



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:59 PM UTC

PDB ID : 2IGN / pdb_00002ign
Title : Crystal structure of recombinant pyranose 2-oxidase H167A mutant
Authors : Divne, C.
Deposited on : 2006-09-22
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

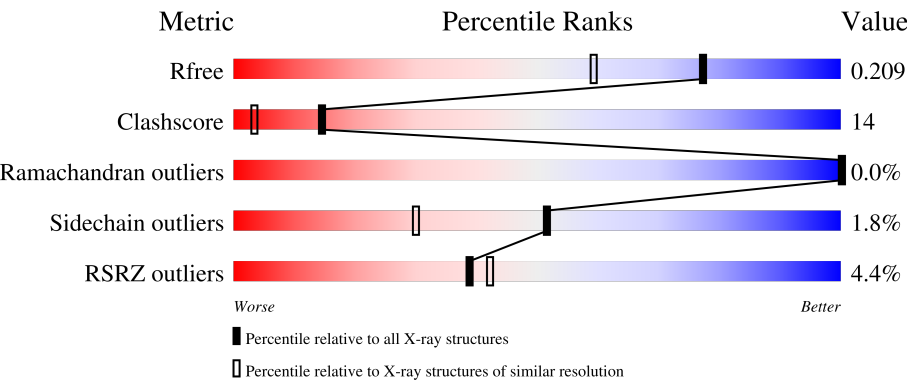
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	5% 80%12%• 7%
1	B	623	4% 78%14%• 7%
1	C	623	5% 79%12%• 7%
1	D	623	4% 79%13%• 7%
1	E	623	5% 78%14%7%

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Mol	Chain	Length	Quality of chain
1	F	623	 3% 81% 11% • 7%
1	G	623	 4% 76% 15% • 7%
1	H	623	 3% 76% 15% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	B	8003	-	-	X	-
3	MES	C	8008	-	-	X	-
3	MES	D	8005	-	-	X	-
3	MES	E	8007	-	-	X	-
3	MES	G	8006	-	-	X	-
3	MES	H	8004	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41758 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	1	0
			4551	2874	777	875	25			
1	B	577	Total	C	N	O	S	0	2	0
			4560	2879	779	877	25			
1	D	577	Total	C	N	O	S	0	2	0
			4560	2879	779	877	25			
1	C	577	Total	C	N	O	S	0	2	0
			4560	2879	779	877	25			
1	E	577	Total	C	N	O	S	0	2	0
			4560	2879	779	877	25			
1	F	577	Total	C	N	O	S	0	1	0
			4551	2874	777	875	25			
1	H	577	Total	C	N	O	S	0	3	0
			4568	2884	780	878	26			
1	G	577	Total	C	N	O	S	0	3	0
			4570	2885	782	878	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
E	167	ALA	HIS	engineered mutation	UNP Q7ZA32
F	167	ALA	HIS	engineered mutation	UNP Q7ZA32
G	167	ALA	HIS	engineered mutation	UNP Q7ZA32
H	167	ALA	HIS	engineered mutation	UNP Q7ZA32

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	H	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	G	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	705	Total	O	0	0
			705	705		
4	B	670	Total	O	0	0
			670	670		
4	D	577	Total	O	0	0
			577	577		
4	C	528	Total	O	0	0
			528	528		

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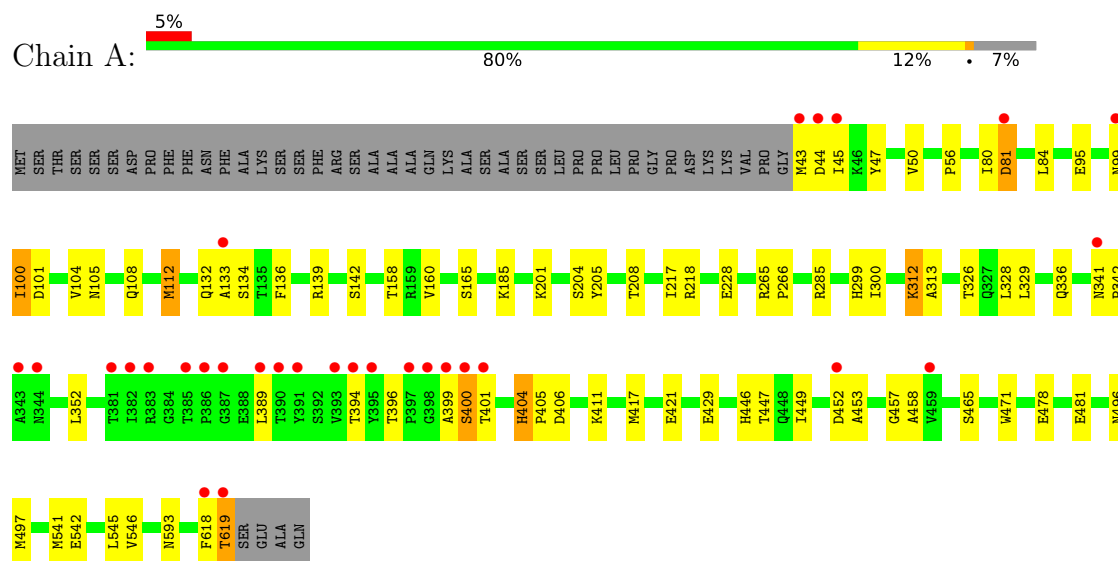
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	565	Total 565	O 565	0	0
4	F	498	Total 498	O 498	0	0
4	H	611	Total 611	O 611	0	0
4	G	604	Total 604	O 604	0	0

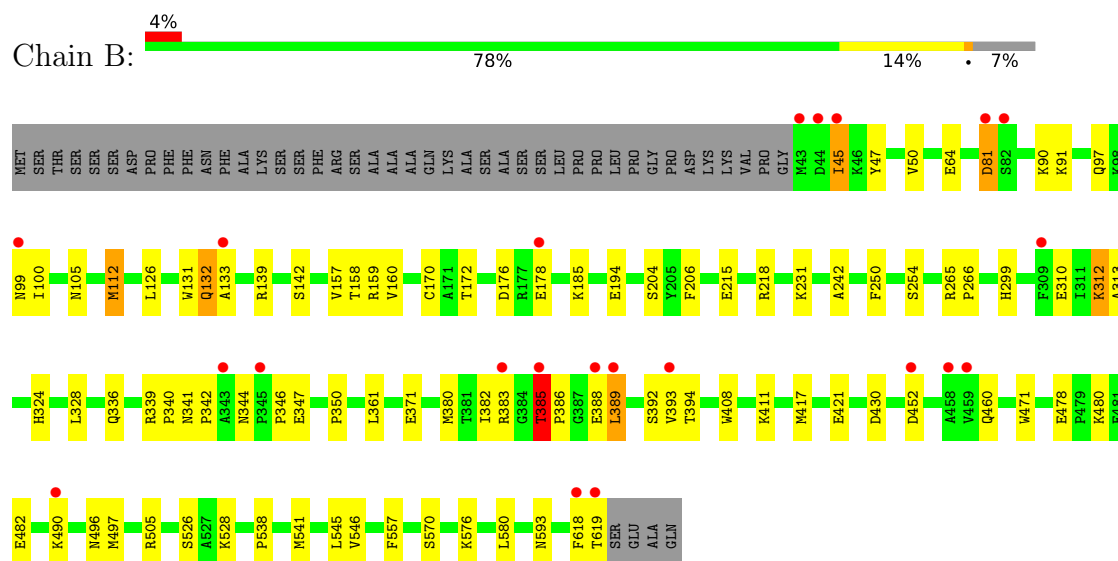
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyranose oxidase

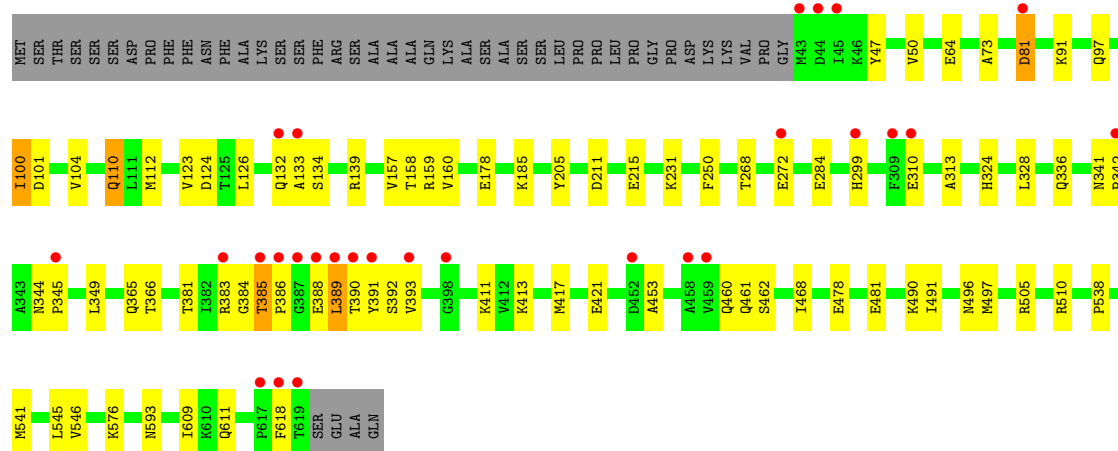


• Molecule 1: Pyranose oxidase



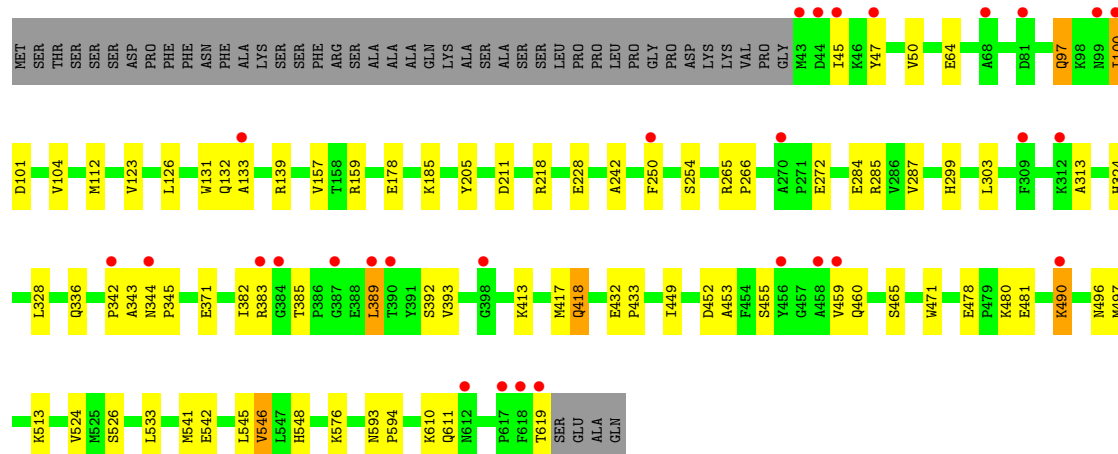
• Molecule 1: Pyranose oxidase

Chain D: 



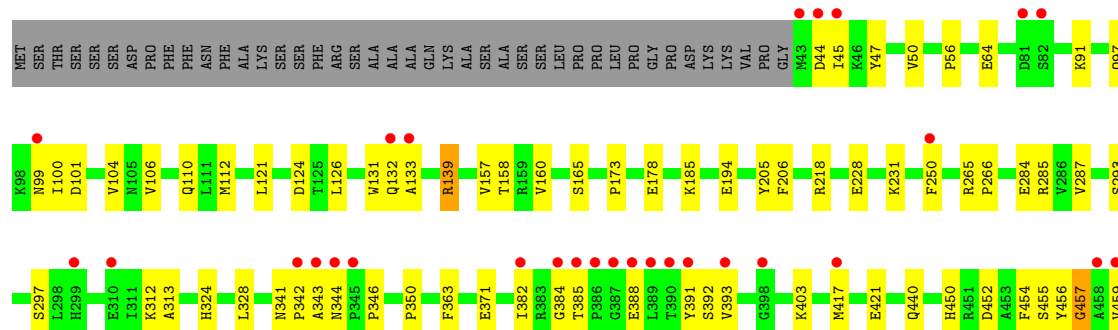
• Molecule 1: Pyranose oxidase

Chain C: 



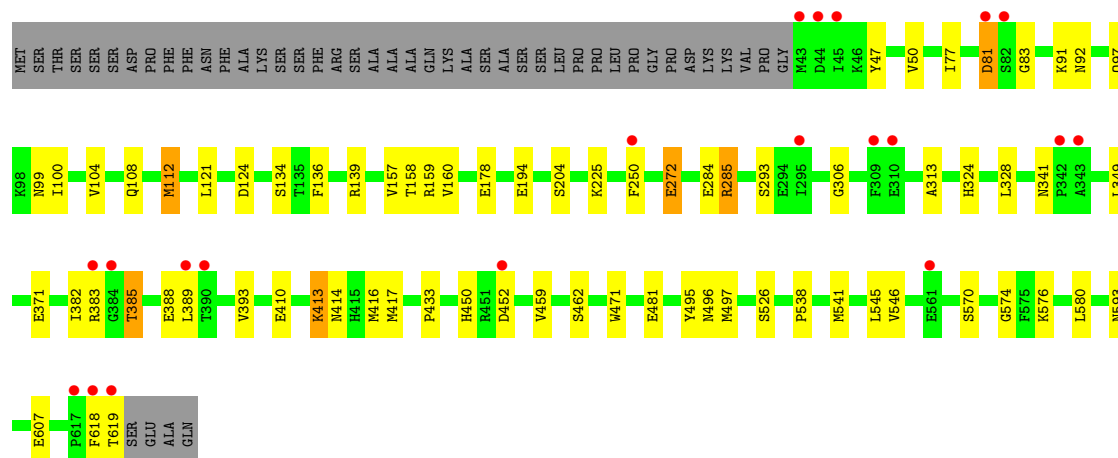
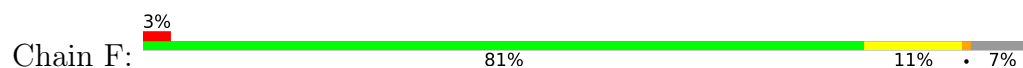
• Molecule 1: Pyranose oxidase

Chain E: 

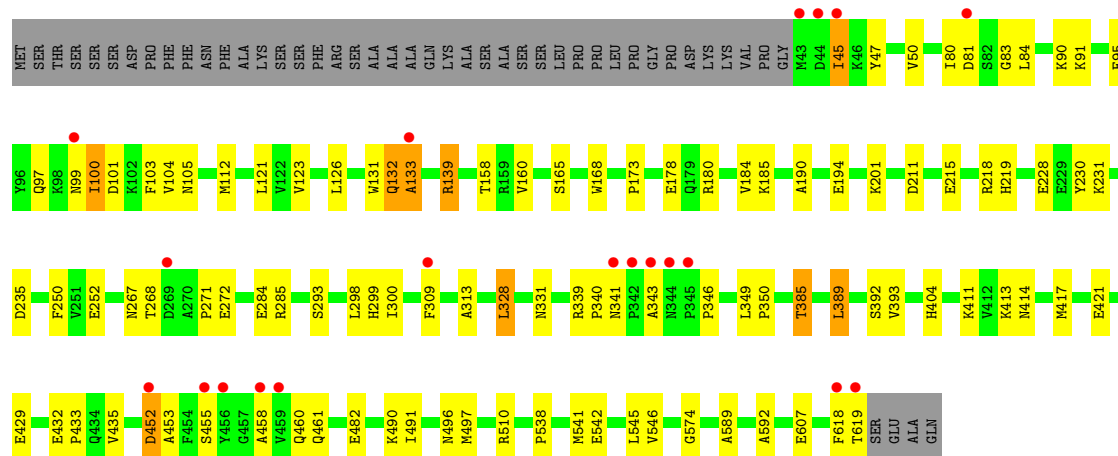
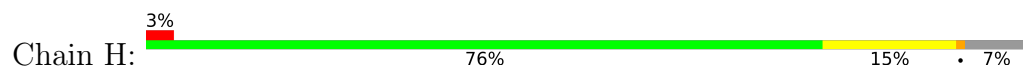




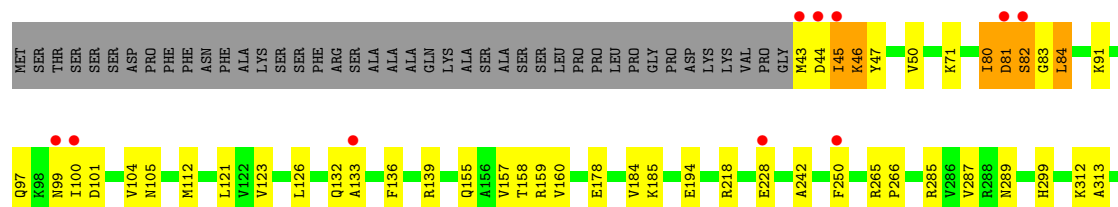
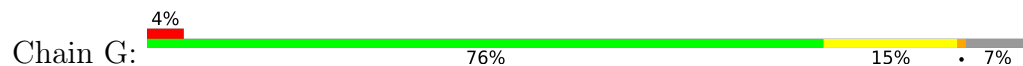
• Molecule 1: Pyranose oxidase

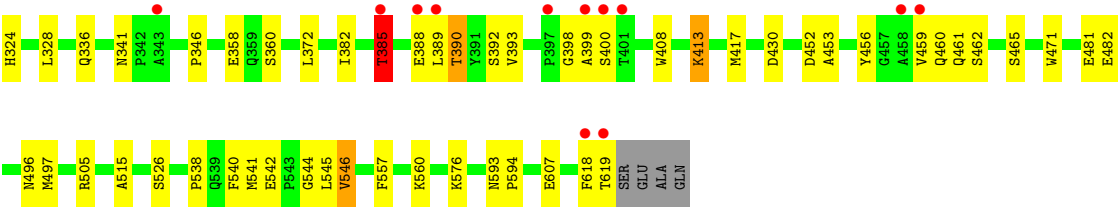


• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.07Å 103.00Å 168.56Å 90.00° 106.43° 90.00°	Depositor
Resolution (Å)	39.00 – 1.65 39.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.00-1.65) 99.9 (39.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.205 0.179 , 0.209	Depositor DCC
R_{free} test set	6563 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	41758	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9631e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	2/4666 (0.0%)	1.04	4/6345 (0.1%)
1	B	1.05	1/4675 (0.0%)	0.99	3/6357 (0.0%)
1	C	1.01	1/4675 (0.0%)	1.00	8/6357 (0.1%)
1	D	1.00	3/4675 (0.1%)	0.95	4/6357 (0.1%)
1	E	0.97	2/4675 (0.0%)	0.96	4/6357 (0.1%)
1	F	0.96	3/4666 (0.1%)	0.95	1/6345 (0.0%)
1	G	1.07	7/4686 (0.1%)	1.01	8/6372 (0.1%)
1	H	1.05	5/4683 (0.1%)	0.99	7/6367 (0.1%)
All	All	1.03	24/37401 (0.1%)	0.99	39/50857 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	ASP	CA-C	14.06	1.70	1.53
1	B	81	ASP	CA-C	8.26	1.63	1.52
1	D	81	ASP	CA-C	8.05	1.63	1.52
1	H	349	LEU	C-O	7.26	1.27	1.23
1	H	349	LEU	N-CA	6.73	1.51	1.46
1	F	81	ASP	CA-C	6.21	1.61	1.52
1	G	82	SER	C-O	6.14	1.32	1.23
1	C	449	ILE	CA-C	-5.96	1.48	1.53
1	G	139	ARG	CD-NE	-5.86	1.38	1.46
1	D	139	ARG	CD-NE	-5.80	1.38	1.46
1	F	139	ARG	CD-NE	-5.79	1.38	1.46
1	A	80	ILE	C-O	-5.71	1.18	1.24
1	A	81	ASP	CA-C	5.69	1.60	1.52
1	E	450	HIS	C-O	-5.68	1.20	1.24
1	E	440	GLN	N-CA	5.60	1.50	1.45
1	H	133	ALA	CA-C	-5.45	1.45	1.52
1	G	82	SER	N-CA	5.43	1.52	1.46
1	G	546	VAL	CA-CB	5.42	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	242	ALA	CA-CB	5.34	1.60	1.52
1	H	589	ALA	CA-CB	-5.28	1.46	1.53
1	H	139	ARG	CD-NE	-5.21	1.39	1.46
1	D	349	LEU	C-O	5.11	1.26	1.23
1	G	82	SER	CA-C	5.04	1.59	1.52
1	F	349	LEU	C-O	5.00	1.26	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	-9.42	110.72	119.20
1	G	139	ARG	NE-CZ-NH2	-8.97	111.12	119.20
1	E	139	ARG	NE-CZ-NH2	-8.49	111.56	119.20
1	G	46	LYS	N-CA-C	8.41	122.22	108.26
1	F	139	ARG	NE-CZ-NH2	-8.27	111.76	119.20
1	B	139	ARG	NE-CZ-NH2	-8.13	111.89	119.20
1	G	139	ARG	NE-CZ-NH1	7.53	129.03	121.50
1	A	139	ARG	NE-CZ-NH2	-7.43	112.52	119.20
1	H	139	ARG	NE-CZ-NH2	-7.40	112.54	119.20
1	C	139	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	H	389	LEU	CA-CB-CG	6.76	139.96	116.30
1	H	389	LEU	N-CA-CB	-6.21	99.99	110.49
1	D	139	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	G	546	VAL	N-CA-C	6.06	117.52	110.62
1	E	139	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	C	139	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	H	452	ASP	CB-CA-C	5.83	121.84	110.30
1	B	139	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	G	372	LEU	N-CA-C	5.75	117.54	111.28
1	A	217	ILE	N-CA-C	5.58	115.78	110.42
1	G	385	THR	CB-CA-C	5.58	116.95	109.42
1	G	81	ASP	N-CA-CB	-5.57	103.01	111.19
1	A	404	HIS	CA-C-N	5.40	125.38	120.03
1	A	404	HIS	C-N-CA	5.40	125.38	120.03
1	D	139	ARG	CD-NE-CZ	5.36	131.91	124.40
1	D	139	ARG	CG-CD-NE	-5.30	100.33	112.00
1	B	385	THR	CB-CA-C	5.30	117.14	109.20
1	G	80	ILE	O-C-N	5.23	128.68	122.83
1	E	484	LYS	N-CA-C	5.18	117.26	109.23
1	C	139	ARG	CD-NE-CZ	5.18	131.65	124.40
1	E	457	GLY	N-CA-C	-5.16	105.93	112.54
1	H	385	THR	CB-CA-C	5.12	116.34	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	VAL	N-CA-C	5.12	115.33	110.42
1	H	180	ARG	CA-C-N	-5.09	114.99	120.03
1	H	180	ARG	C-N-CA	-5.09	114.99	120.03
1	C	97	GLN	N-CA-C	-5.08	105.92	111.82
1	C	546	VAL	N-CA-C	5.07	116.41	110.62
1	C	533	LEU	CA-C-N	-5.03	114.77	119.90
1	C	533	LEU	C-N-CA	-5.03	114.77	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4551	0	4401	128	0
1	B	4560	0	4408	152	0
1	C	4560	0	4408	112	0
1	D	4560	0	4408	94	0
1	E	4560	0	4408	102	0
1	F	4551	0	4401	75	0
1	G	4570	0	4414	174	0
1	H	4568	0	4416	169	1
2	A	53	0	31	0	0
2	B	53	0	30	2	0
2	C	53	0	28	1	0
2	D	53	0	30	1	0
2	E	53	0	29	0	0
2	F	53	0	30	1	0
2	G	53	0	30	1	0
2	H	53	0	29	0	0
3	A	12	0	12	4	0
3	B	12	0	12	9	0
3	C	12	0	12	10	0
3	D	12	0	12	14	0
3	E	12	0	12	11	0
3	F	12	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	12	0	12	9	0
3	H	12	0	12	17	0
4	A	705	0	0	100	2
4	B	670	0	0	110	1
4	C	528	0	0	73	0
4	D	577	0	0	54	0
4	E	565	0	0	65	0
4	F	498	0	0	47	0
4	G	604	0	0	110	3
4	H	611	0	0	122	1
All	All	41758	0	35597	1015	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1015) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LYS:HE3	4:B:8620:HOH:O	1.23	1.38
1:B:452:ASP:HB2	4:B:8464:HOH:O	1.26	1.34
1:G:104[A]:VAL:HG23	4:G:8521:HOH:O	1.28	1.33
1:B:142:SER:HB3	4:B:8632:HOH:O	1.28	1.33
1:A:204:SER:HB2	4:A:8479:HOH:O	1.16	1.31
1:D:546:VAL:HG12	4:D:8527:HOH:O	1.15	1.30
1:C:328:LEU:HG	4:C:8437:HOH:O	1.28	1.29
1:A:208:THR:HG21	4:A:8588:HOH:O	1.16	1.27
1:C:546:VAL:HA	4:C:8472:HOH:O	1.10	1.27
1:D:328:LEU:HG	4:D:8462:HOH:O	1.34	1.27
1:H:413:LYS:HD2	4:H:8507:HOH:O	1.24	1.26
1:A:546:VAL:HA	4:A:8473:HOH:O	1.09	1.25
1:A:133:ALA:HB1	4:A:8381:HOH:O	1.36	1.25
1:G:546:VAL:HA	4:G:8455:HOH:O	1.25	1.25
1:B:328:LEU:HG	4:B:8525:HOH:O	1.37	1.25
1:F:546:VAL:HA	4:F:8436:HOH:O	1.21	1.25
1:B:133:ALA:HA	4:B:8607:HOH:O	1.38	1.23
1:F:204:SER:HB2	4:F:8421:HOH:O	1.28	1.23
1:A:204:SER:CB	4:A:8479:HOH:O	1.70	1.23
1:G:497:MET:HE2	4:G:8374:HOH:O	1.34	1.23
1:F:134:SER:HB2	4:F:8441:HOH:O	1.35	1.23
1:E:371:GLU:HB3	4:E:8522:HOH:O	1.38	1.22
4:H:8528:HOH:O	1:G:121:LEU:HD12	1.33	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:ASP:HB2	4:F:8405:HOH:O	1.32	1.21
1:A:160:VAL:HB	4:A:8654:HOH:O	1.04	1.20
1:C:104[A]:VAL:HG23	4:C:8397:HOH:O	1.41	1.19
1:C:452:ASP:HB2	4:C:8432:HOH:O	1.39	1.18
1:G:328:LEU:HG	4:G:8550:HOH:O	1.38	1.18
1:B:497:MET:HE2	4:B:8369:HOH:O	1.43	1.18
1:A:108:GLN:HG2	4:A:8376:HOH:O	1.43	1.18
1:A:142:SER:HB3	4:A:8535:HOH:O	1.42	1.17
1:G:465:SER:HB2	4:G:8570:HOH:O	1.01	1.17
1:B:204:SER:HB2	4:B:8547:HOH:O	0.99	1.16
1:B:478:GLU:HB2	4:B:8610:HOH:O	1.45	1.15
1:B:45:ILE:HD12	4:B:8338:HOH:O	1.47	1.15
1:H:133:ALA:HA	4:H:8544:HOH:O	1.45	1.14
1:E:459:VAL:HG22	4:E:8545:HOH:O	1.48	1.13
1:D:133:ALA:HB3	3:D:8005:MES:C7	1.77	1.13
1:D:609:ILE:HG22	4:D:8536:HOH:O	1.49	1.13
1:H:331:ASN:HB3	4:H:8576:HOH:O	1.48	1.13
1:H:546:VAL:HA	4:H:8375:HOH:O	0.94	1.12
1:D:546:VAL:HA	4:D:8470:HOH:O	0.98	1.12
1:E:454:PHE:HE2	4:E:8500:HOH:O	1.32	1.12
1:A:134:SER:HB2	4:A:8630:HOH:O	1.46	1.12
1:A:465:SER:HB2	4:A:8522:HOH:O	0.96	1.10
1:E:497:MET:CE	4:E:8276:HOH:O	1.99	1.08
1:C:497:MET:HE2	4:C:8350:HOH:O	1.53	1.08
1:A:399:ALA:HB1	4:A:8622:HOH:O	1.53	1.08
1:A:545:LEU:HD13	4:A:8649:HOH:O	1.53	1.07
1:B:371:GLU:HB3	4:B:8526:HOH:O	1.52	1.07
1:A:497:MET:HE2	4:A:8380:HOH:O	1.52	1.06
1:C:465:SER:HB2	4:C:8393:HOH:O	0.89	1.06
1:F:112:MET:CG	4:F:8442:HOH:O	2.02	1.06
1:H:104[A]:VAL:HG23	4:H:8555:HOH:O	1.55	1.06
1:H:435:VAL:HG23	4:H:8587:HOH:O	1.56	1.05
1:H:452:ASP:HB2	4:H:8499:HOH:O	1.54	1.05
1:D:468:ILE:HG23	4:D:8526:HOH:O	1.56	1.05
1:G:155:GLN:HG2	4:G:8530:HOH:O	1.53	1.04
1:D:497:MET:HE2	4:D:8282:HOH:O	1.57	1.04
1:A:44:ASP:HB3	4:A:8394:HOH:O	1.57	1.04
1:E:497:MET:HE2	4:E:8276:HOH:O	1.54	1.04
1:F:417:MET:HE3	4:F:8415:HOH:O	1.55	1.03
1:G:452:ASP:HB2	4:G:8460:HOH:O	1.56	1.03
1:B:340:PRO:HD2	4:B:8553:HOH:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:LEU:HD13	4:C:8502:HOH:O	1.56	1.03
1:F:459:VAL:HG13	4:F:8302:HOH:O	1.57	1.02
1:G:453:ALA:HB1	4:G:8521:HOH:O	1.60	1.02
1:A:405:PRO:C	4:A:8625:HOH:O	2.02	1.01
1:A:542:GLU:HB3	4:A:8649:HOH:O	1.59	1.01
1:F:393:VAL:H	1:F:417:MET:HE1	1.27	1.00
1:B:133:ALA:HB3	3:B:8003:MES:C7	1.91	1.00
1:G:312:LYS:HB2	4:G:8555:HOH:O	1.62	0.99
3:D:8005:MES:H72	4:D:8310:HOH:O	1.62	0.99
1:C:453:ALA:HB1	4:C:8397:HOH:O	1.60	0.99
1:A:312:LYS:HB3	4:A:8623:HOH:O	1.61	0.99
1:D:133:ALA:HB3	3:D:8005:MES:H72	1.42	0.99
1:G:594:PRO:HG3	4:G:8572:HOH:O	1.62	0.99
1:D:133:ALA:HB3	3:D:8005:MES:H71	1.42	0.98
4:B:8469:HOH:O	1:C:542:GLU:HB2	1.62	0.98
1:F:92:ASN:C	4:F:8419:HOH:O	2.05	0.98
1:H:97:GLN:HB2	4:H:8480:HOH:O	1.63	0.98
1:H:298:LEU:HB3	4:H:8578:HOH:O	1.63	0.98
1:C:541:MET:HE3	4:C:8146:HOH:O	1.63	0.98
1:A:112:MET:HB2	4:B:8609:HOH:O	1.62	0.98
1:B:172:THR:HG23	4:B:8594:HOH:O	1.61	0.98
1:H:298:LEU:CD1	4:H:8520:HOH:O	2.10	0.97
1:E:459:VAL:HG13	4:E:8503:HOH:O	1.64	0.97
1:H:104[B]:VAL:HG13	4:H:8555:HOH:O	1.64	0.97
1:H:497:MET:HE2	4:H:8307:HOH:O	1.63	0.97
1:B:204:SER:CB	4:B:8547:HOH:O	1.68	0.97
1:B:133:ALA:CA	4:B:8607:HOH:O	2.03	0.97
1:E:454:PHE:CE2	4:E:8500:HOH:O	2.10	0.97
4:H:8615:HOH:O	1:G:84:LEU:HG	1.64	0.97
1:D:133:ALA:CB	3:D:8005:MES:C7	2.42	0.96
1:A:352:LEU:HD21	4:A:8656:HOH:O	1.63	0.96
1:H:453:ALA:HB1	4:H:8555:HOH:O	1.66	0.96
1:C:541:MET:CE	4:C:8146:HOH:O	2.12	0.96
1:G:465:SER:CB	4:G:8570:HOH:O	1.67	0.95
1:H:230:TYR:C	4:H:8510:HOH:O	2.08	0.95
1:B:393:VAL:H	1:B:417:MET:HE1	1.32	0.95
1:D:541:MET:HE3	4:D:8191:HOH:O	1.65	0.95
1:E:541:MET:SD	4:E:8502:HOH:O	2.24	0.95
1:H:211:ASP:HB3	4:H:8421:HOH:O	1.66	0.95
1:C:542:GLU:HB3	4:C:8502:HOH:O	1.66	0.95
1:D:272:GLU:HG2	4:D:8433:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:VAL:H	1:D:417:MET:HE1	1.31	0.94
1:H:84:LEU:HD21	4:G:8586:HOH:O	1.65	0.94
1:H:458:ALA:C	4:H:8528:HOH:O	2.10	0.94
1:D:100:ILE:HG12	4:D:8425:HOH:O	1.68	0.93
1:H:300:ILE:HG13	4:H:8590:HOH:O	1.69	0.92
1:D:133:ALA:CB	3:D:8005:MES:H71	1.98	0.92
3:B:8003:MES:H72	4:B:8503:HOH:O	1.70	0.92
1:H:81:ASP:HB2	4:H:8304:HOH:O	1.69	0.92
1:G:389:LEU:HD13	4:G:8577:HOH:O	1.68	0.92
1:C:619:THR:HG22	4:C:8291:HOH:O	1.68	0.92
1:C:393:VAL:H	1:C:417:MET:HE1	1.34	0.91
1:A:542:GLU:HG3	4:D:8339:HOH:O	1.69	0.91
1:E:133:ALA:HB2	3:E:8007:MES:O1S	1.70	0.91
1:D:133:ALA:HB2	3:D:8005:MES:O3S	1.71	0.91
1:E:126:LEU:CD1	1:E:132[B]:GLN:HG3	2.00	0.91
1:A:43:MET:HE1	4:A:8342:HOH:O	1.69	0.91
1:A:112:MET:CB	4:B:8609:HOH:O	2.18	0.90
1:B:112:MET:CE	4:B:8592:HOH:O	2.18	0.90
1:D:126:LEU:HD12	1:D:132[B]:GLN:HG3	1.51	0.90
1:H:541:MET:HG3	4:H:8603:HOH:O	1.70	0.90
1:H:458:ALA:O	4:H:8528:HOH:O	1.90	0.90
1:B:178:GLU:HG3	4:B:8262:HOH:O	1.72	0.90
1:G:101:ASP:O	4:G:8521:HOH:O	1.89	0.90
1:C:285:ARG:HD3	4:C:8385:HOH:O	1.70	0.90
1:B:178:GLU:HB2	4:B:8626:HOH:O	1.70	0.89
1:B:385:THR:HG23	1:B:388:GLU:OE1	1.72	0.89
1:C:611:GLN:HG2	4:C:8423:HOH:O	1.73	0.89
1:C:126:LEU:HD12	1:C:132[B]:GLN:HG3	1.51	0.89
1:B:299:HIS:CD2	4:B:8612:HOH:O	2.25	0.89
1:G:393:VAL:H	1:G:417:MET:HE1	1.38	0.89
1:H:393:VAL:H	1:H:417[B]:MET:HE1	1.37	0.88
1:G:360:SER:HB3	4:G:8588:HOH:O	1.74	0.88
1:B:250:PHE:HD2	4:B:8670:HOH:O	1.55	0.88
1:B:133:ALA:HB3	3:B:8003:MES:H71	1.54	0.88
1:B:133:ALA:HB3	3:B:8003:MES:H72	1.56	0.88
1:E:121:LEU:HB3	4:F:8302:HOH:O	1.74	0.88
1:H:298:LEU:HD11	4:H:8520:HOH:O	1.68	0.88
1:F:497:MET:HE2	4:F:8284:HOH:O	1.73	0.87
3:H:8004:MES:H72	1:G:462:SER:O	1.73	0.87
1:D:126:LEU:CD1	1:D:132[B]:GLN:HG3	2.03	0.87
1:F:112:MET:SD	4:F:8442:HOH:O	2.31	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LEU:CD1	1:D:132[B]:GLN:CG	2.54	0.85
3:C:8008:MES:H72	4:C:8251:HOH:O	1.76	0.84
1:A:545:LEU:HB2	4:A:8649:HOH:O	1.77	0.84
1:C:594:PRO:HG3	4:C:8370:HOH:O	1.76	0.84
1:A:112:MET:SD	4:B:8609:HOH:O	2.35	0.84
1:C:303:LEU:HD21	4:C:8361:HOH:O	1.77	0.83
1:A:312:LYS:HE2	4:A:8623:HOH:O	1.78	0.83
1:A:618:PHE:HB3	4:A:8553:HOH:O	1.79	0.83
1:A:112:MET:CG	4:B:8609:HOH:O	2.26	0.83
1:A:447:THR:HG22	4:A:8655:HOH:O	1.77	0.83
1:G:312:LYS:HD2	4:G:8555:HOH:O	1.79	0.83
1:C:126:LEU:CD1	1:C:132[B]:GLN:HG3	2.08	0.83
1:C:287:VAL:CG2	4:C:8497:HOH:O	2.26	0.83
1:B:133:ALA:HB2	3:B:8003:MES:O2S	1.79	0.82
1:F:112:MET:HG2	4:F:8442:HOH:O	1.71	0.82
1:A:404:HIS:O	4:A:8625:HOH:O	1.97	0.82
1:H:132[B]:GLN:OE1	3:H:8004:MES:H52	1.80	0.82
1:B:393:VAL:H	1:B:417:MET:CE	1.93	0.82
1:B:126:LEU:CD1	1:B:132[B]:GLN:HG3	2.09	0.82
1:E:459:VAL:CG2	4:E:8545:HOH:O	2.14	0.82
1:H:618:PHE:HB3	4:H:8344:HOH:O	1.79	0.82
1:H:133:ALA:CB	3:H:8004:MES:H81	2.09	0.81
1:G:312:LYS:CB	4:G:8555:HOH:O	2.24	0.81
1:H:228:GLU:OE1	4:H:8446:HOH:O	1.96	0.81
1:G:126:LEU:CD1	1:G:132[B]:GLN:HG3	2.10	0.81
1:A:541:MET:SD	4:A:8689:HOH:O	2.38	0.81
4:H:8279:HOH:O	1:G:81:ASP:HA	1.79	0.81
3:A:8002:MES:H72	4:A:8414:HOH:O	1.80	0.81
1:G:133:ALA:HB3	3:G:8006:MES:C7	2.11	0.81
1:H:100:ILE:HG12	4:H:8387:HOH:O	1.80	0.80
1:G:299[A]:HIS:CE1	4:G:8370:HOH:O	2.34	0.80
1:B:126:LEU:HD12	1:B:132[B]:GLN:HG3	1.63	0.80
1:B:250:PHE:CD2	4:B:8670:HOH:O	2.31	0.80
1:H:133:ALA:CA	4:H:8544:HOH:O	2.15	0.80
1:B:172:THR:CG2	4:B:8594:HOH:O	2.25	0.80
1:H:417[B]:MET:HE3	4:H:8345:HOH:O	1.81	0.80
1:A:133:ALA:CB	4:A:8381:HOH:O	2.07	0.79
1:B:112:MET:SD	4:B:8592:HOH:O	2.39	0.79
3:G:8006:MES:H72	4:G:8371:HOH:O	1.82	0.79
1:B:170:CYS:O	4:B:8594:HOH:O	1.99	0.79
1:A:389:LEU:HA	4:A:8611:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:PHE:CD2	4:H:8480:HOH:O	2.34	0.79
1:B:482:GLU:HG3	4:B:8564:HOH:O	1.82	0.79
1:B:328:LEU:CD1	4:B:8525:HOH:O	2.30	0.78
1:C:610:LYS:O	4:C:8494:HOH:O	2.01	0.78
4:E:8545:HOH:O	1:F:121:LEU:HD22	1.82	0.78
1:G:184:VAL:HG12	4:G:8589:HOH:O	1.83	0.78
1:D:478:GLU:HB2	4:D:8535:HOH:O	1.83	0.78
1:A:545:LEU:HD22	4:A:8649:HOH:O	1.82	0.78
1:A:619:THR:HG22	4:A:8659:HOH:O	1.83	0.78
1:F:204:SER:CB	4:F:8421:HOH:O	2.00	0.78
1:A:228:GLU:HG3	4:A:8362:HOH:O	1.83	0.77
1:G:456:TYR:HB3	4:G:8463:HOH:O	1.85	0.77
1:H:123:VAL:H	3:H:8004:MES:H22	1.49	0.77
1:A:133:ALA:N	4:A:8633:HOH:O	2.18	0.77
1:A:452:ASP:CB	4:A:8367:HOH:O	2.33	0.77
1:D:341:ASN:ND2	4:D:8533:HOH:O	2.15	0.77
1:E:228:GLU:OE1	4:E:8412:HOH:O	2.02	0.77
1:F:341:ASN:ND2	4:F:8423:HOH:O	2.16	0.77
1:A:133:ALA:O	4:A:8679:HOH:O	2.04	0.76
1:A:452:ASP:HB2	4:A:8367:HOH:O	1.84	0.76
1:G:413:LYS:HD2	4:G:8496:HOH:O	1.85	0.76
1:E:619:THR:HG23	4:E:8531:HOH:O	1.86	0.76
1:G:460:GLN:C	4:G:8463:HOH:O	2.27	0.76
1:C:133:ALA:HB3	3:C:8008:MES:H72	1.67	0.76
1:G:619:THR:HG21	4:G:8569:HOH:O	1.84	0.76
1:F:393:VAL:H	1:F:417:MET:CE	1.98	0.76
1:C:45:ILE:HG23	4:C:8400:HOH:O	1.86	0.75
1:C:133:ALA:HB3	3:C:8008:MES:C7	2.15	0.75
1:H:133:ALA:HB3	3:H:8004:MES:H51	1.68	0.75
1:G:81:ASP:CA	4:G:8299:HOH:O	2.32	0.75
1:G:133:ALA:HB3	3:G:8006:MES:H71	1.67	0.75
1:C:465:SER:CB	4:C:8393:HOH:O	1.68	0.75
1:B:131:TRP:CZ3	4:B:8607:HOH:O	2.38	0.75
1:D:384:GLY:HA3	4:D:8483:HOH:O	1.87	0.75
1:D:391:TYR:HB3	4:D:8401:HOH:O	1.86	0.75
1:D:611:GLN:HG2	4:D:8393:HOH:O	1.87	0.75
1:G:132[A]:GLN:HG2	4:G:8290:HOH:O	1.86	0.74
1:G:285:ARG:HD3	4:G:8414:HOH:O	1.85	0.74
1:B:385:THR:HG23	1:B:388:GLU:CD	2.11	0.74
1:C:104[B]:VAL:HG13	4:C:8397:HOH:O	1.87	0.74
1:E:126:LEU:HD13	1:E:132[B]:GLN:CG	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:541:MET:HE3	1:F:545:LEU:HD23	1.69	0.74
1:A:299:HIS:NE2	4:A:8599:HOH:O	2.20	0.74
1:D:541:MET:CE	4:D:8191:HOH:O	2.29	0.74
1:C:132[A]:GLN:HG2	4:C:8244:HOH:O	1.86	0.74
1:C:101:ASP:HA	4:C:8397:HOH:O	1.87	0.74
1:H:393:VAL:H	1:H:417[B]:MET:CE	2.00	0.74
1:B:176:ASP:OD1	4:B:8626:HOH:O	2.05	0.74
1:E:126:LEU:CD1	1:E:132[B]:GLN:CG	2.65	0.73
1:G:360:SER:CB	4:G:8588:HOH:O	2.34	0.73
1:B:100:ILE:HD13	4:B:8444:HOH:O	1.87	0.73
1:B:528:LYS:NZ	4:B:8620:HOH:O	2.14	0.73
1:D:133:ALA:CB	3:D:8005:MES:H72	2.11	0.73
3:D:8005:MES:C7	4:D:8310:HOH:O	2.23	0.73
1:G:126:LEU:HD13	1:G:132[B]:GLN:CG	2.19	0.73
1:E:460:GLN:NE2	4:E:8500:HOH:O	2.21	0.73
1:A:100:ILE:HG12	4:A:8662:HOH:O	1.88	0.73
1:B:133:ALA:CB	3:B:8003:MES:C7	2.67	0.73
3:B:8003:MES:C7	4:B:8503:HOH:O	2.29	0.73
1:F:92:ASN:O	4:F:8419:HOH:O	2.03	0.73
1:F:124:ASP:OD1	4:F:8449:HOH:O	2.07	0.73
1:G:133:ALA:HB2	3:G:8006:MES:O3S	1.87	0.73
1:A:399:ALA:CB	4:A:8622:HOH:O	2.20	0.72
1:D:178:GLU:OE1	4:D:8307:HOH:O	2.05	0.72
1:B:341:ASN:HB3	4:B:8604:HOH:O	1.88	0.72
1:E:133:ALA:HA	4:E:8271:HOH:O	1.88	0.72
1:F:410:GLU:HB3	4:F:8476:HOH:O	1.89	0.72
1:G:541:MET:SD	4:G:8540:HOH:O	2.46	0.72
1:B:421:GLU:OE2	4:B:8672:HOH:O	2.07	0.72
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.70	0.72
1:B:361:LEU:HB2	4:B:8629:HOH:O	1.90	0.72
1:G:393:VAL:H	1:G:417:MET:CE	2.02	0.72
1:B:45:ILE:HD12	1:B:45:ILE:H	1.55	0.72
1:H:133:ALA:HB2	3:H:8004:MES:H81	1.72	0.72
1:B:385:THR:HB	4:B:8392:HOH:O	1.89	0.72
1:E:126:LEU:HD12	1:E:132[B]:GLN:HG3	1.71	0.72
1:C:126:LEU:CD1	1:C:132[B]:GLN:CG	2.67	0.72
1:E:297:SER:HB2	4:E:8536:HOH:O	1.87	0.72
1:G:81:ASP:HB2	4:G:8299:HOH:O	1.90	0.72
1:A:112:MET:HE2	4:B:8609:HOH:O	1.90	0.72
1:A:329:LEU:HB2	4:A:8656:HOH:O	1.89	0.72
1:A:545:LEU:CG	4:A:8649:HOH:O	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:460:GLN:O	4:H:8562:HOH:O	2.06	0.72
1:A:133:ALA:O	4:A:8633:HOH:O	2.08	0.71
1:B:126:LEU:CD1	1:B:132[B]:GLN:CG	2.66	0.71
1:B:133:ALA:CB	3:B:8003:MES:H71	2.19	0.71
1:E:178:GLU:OE1	4:E:8277:HOH:O	2.07	0.71
1:F:413:LYS:HE2	4:F:8470:HOH:O	1.89	0.71
1:A:394:THR:HG23	4:A:8486:HOH:O	1.90	0.71
1:G:100:ILE:HG13	4:G:8331:HOH:O	1.89	0.71
1:D:211:ASP:HB3	4:D:8348:HOH:O	1.89	0.70
1:E:421:GLU:OE2	4:E:8571:HOH:O	2.08	0.70
1:A:300:ILE:O	4:A:8599:HOH:O	2.10	0.70
1:D:299:HIS:HB2	1:D:310:GLU:OE1	1.91	0.70
1:D:393:VAL:H	1:D:417:MET:CE	2.04	0.70
1:H:126:LEU:CD1	1:H:132[B]:GLN:HG3	2.21	0.70
1:B:312:LYS:HE2	4:B:8573:HOH:O	1.91	0.70
1:B:45:ILE:HB	4:B:8568:HOH:O	1.92	0.70
1:B:194:GLU:CD	4:B:8505:HOH:O	2.34	0.70
1:F:541:MET:HE1	4:F:8480:HOH:O	1.91	0.69
4:E:8545:HOH:O	1:F:121:LEU:HD13	1.92	0.69
1:A:396:THR:HG22	4:A:8593:HOH:O	1.91	0.69
1:D:126:LEU:HD13	1:D:132[B]:GLN:HG2	1.73	0.69
1:D:546:VAL:CG1	4:D:8527:HOH:O	1.92	0.69
1:G:390:THR:CB	4:G:8559:HOH:O	2.39	0.69
1:B:328:LEU:HD13	4:B:8639:HOH:O	1.93	0.69
1:B:528:LYS:CE	4:B:8620:HOH:O	1.94	0.69
1:F:462:SER:OG	4:F:8327:HOH:O	2.05	0.69
1:H:126:LEU:HD13	1:H:132[B]:GLN:CG	2.23	0.69
1:C:133:ALA:HB2	3:C:8008:MES:O1S	1.93	0.69
1:A:396:THR:HB	4:A:8640:HOH:O	1.91	0.68
1:H:298:LEU:HD12	4:H:8520:HOH:O	1.86	0.68
1:G:126:LEU:CD1	1:G:132[B]:GLN:CG	2.71	0.68
1:D:366:THR:O	4:D:8526:HOH:O	2.11	0.68
1:E:91:LYS:CE	4:E:8307:HOH:O	2.42	0.68
1:A:411:LYS:NZ	4:A:8518:HOH:O	2.14	0.68
1:G:453:ALA:HB3	4:G:8552:HOH:O	1.92	0.68
1:A:101:ASP:O	1:A:104[A]:VAL:HG23	1.94	0.68
1:C:178:GLU:OE1	4:C:8276:HOH:O	2.12	0.68
1:A:465:SER:CB	4:A:8522:HOH:O	1.74	0.67
1:A:112:MET:HE1	4:A:8372:HOH:O	1.95	0.67
1:D:421:GLU:HG3	4:D:8542:HOH:O	1.93	0.67
1:E:393:VAL:H	1:E:417:MET:HE1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:GLN:CB	4:H:8480:HOH:O	2.25	0.67
1:C:545:LEU:CG	4:C:8502:HOH:O	2.42	0.67
1:H:194:GLU:HG2	4:H:8356:HOH:O	1.92	0.67
1:H:131:TRP:CH2	4:H:8544:HOH:O	2.47	0.67
1:G:44:ASP:HB3	4:G:8492:HOH:O	1.95	0.67
1:B:64:GLU:OE1	4:B:8366:HOH:O	2.12	0.67
1:F:413:LYS:NZ	1:F:414:ASN:OD1	2.27	0.67
1:H:267:ASN:O	4:H:8596:HOH:O	2.12	0.67
1:G:178:GLU:OE1	4:G:8332:HOH:O	2.12	0.67
1:G:461:GLN:N	4:G:8463:HOH:O	2.26	0.67
1:E:194:GLU:HG2	4:E:8441:HOH:O	1.94	0.67
4:F:8449:HOH:O	1:G:542:GLU:HG3	1.93	0.67
1:G:289:ASN:N	4:G:8562:HOH:O	2.28	0.67
1:G:389:LEU:HD12	4:G:8491:HOH:O	1.93	0.67
1:D:124:ASP:OD1	4:D:8339:HOH:O	2.12	0.67
1:D:462:SER:OG	4:D:8439:HOH:O	2.13	0.67
1:C:371:GLU:HB3	4:C:8492:HOH:O	1.94	0.67
1:F:272:GLU:HG2	4:F:8328:HOH:O	1.93	0.67
1:G:44:ASP:CB	4:G:8492:HOH:O	2.43	0.67
1:A:458:ALA:HA	4:A:8638:HOH:O	1.93	0.66
1:C:576:LYS:HD3	4:C:8260:HOH:O	1.94	0.66
1:B:131:TRP:CH2	4:B:8607:HOH:O	2.47	0.66
1:B:112:MET:HE1	4:B:8328:HOH:O	1.96	0.66
4:H:8279:HOH:O	1:G:81:ASP:CA	2.41	0.66
1:A:446:HIS:O	4:A:8655:HOH:O	2.12	0.66
1:H:461:GLN:HA	4:H:8562:HOH:O	1.94	0.66
1:G:44:ASP:HB3	4:G:8305:HOH:O	1.94	0.66
1:A:100:ILE:HD13	1:A:100:ILE:O	1.95	0.66
1:E:133:ALA:HB2	3:E:8007:MES:H81	1.78	0.66
1:H:331:ASN:CB	4:H:8576:HOH:O	2.22	0.66
4:H:8528:HOH:O	1:G:121:LEU:CD1	2.12	0.66
1:C:393:VAL:H	1:C:417:MET:CE	2.07	0.66
1:B:194:GLU:CG	4:B:8505:HOH:O	2.43	0.66
1:E:297:SER:CB	4:E:8536:HOH:O	2.43	0.66
1:C:545:LEU:CD1	4:C:8502:HOH:O	2.27	0.65
1:H:132[B]:GLN:C	4:H:8544:HOH:O	2.38	0.65
1:C:481:GLU:HG2	4:C:8336:HOH:O	1.96	0.65
1:G:80:ILE:HD13	4:G:8586:HOH:O	1.95	0.65
1:C:460:GLN:O	4:C:8263:HOH:O	2.14	0.65
1:H:131:TRP:CZ3	4:H:8544:HOH:O	2.49	0.65
1:A:285:ARG:HA	1:A:328:LEU:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:LEU:HD22	1:C:389:LEU:H	1.61	0.65
1:A:100:ILE:HD12	4:A:8505:HOH:O	1.96	0.65
1:A:132:GLN:HB3	4:A:8633:HOH:O	1.97	0.65
1:F:481:GLU:HG2	4:F:8289:HOH:O	1.97	0.65
1:C:460:GLN:C	4:C:8263:HOH:O	2.40	0.65
1:E:539:GLN:HG3	4:E:8502:HOH:O	1.94	0.65
1:F:306:GLY:O	4:F:8466:HOH:O	2.14	0.65
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.79	0.65
1:H:126:LEU:CD1	1:H:132[B]:GLN:CG	2.75	0.65
1:G:312:LYS:HE3	4:G:8468:HOH:O	1.96	0.65
1:E:538:PRO:HG2	1:G:538:PRO:HG2	1.78	0.65
1:H:178:GLU:OE1	4:H:8329:HOH:O	2.14	0.64
1:G:83:GLY:N	4:G:8288:HOH:O	2.16	0.64
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.32	0.64
3:A:8002:MES:C7	4:A:8414:HOH:O	2.41	0.64
1:G:81:ASP:CB	4:G:8299:HOH:O	2.45	0.64
1:A:545:LEU:CD1	4:A:8649:HOH:O	2.24	0.64
1:E:133:ALA:CB	4:E:8271:HOH:O	2.45	0.64
1:G:104[B]:VAL:HG13	4:G:8521:HOH:O	1.98	0.64
1:G:385:THR:HG22	1:G:388:GLU:OE2	1.96	0.64
1:D:100:ILE:HD13	1:D:453:ALA:HA	1.80	0.64
1:E:393:VAL:H	1:E:417:MET:CE	2.09	0.64
1:A:43:MET:HG2	4:A:8636:HOH:O	1.97	0.64
1:H:133:ALA:HB2	3:H:8004:MES:O3S	1.98	0.64
1:E:126:LEU:HD13	1:E:132[B]:GLN:HG3	1.76	0.64
1:H:126:LEU:HD12	1:H:132[B]:GLN:HG3	1.80	0.64
1:G:540:PHE:CE1	4:G:8588:HOH:O	2.50	0.64
1:C:132[A]:GLN:CD	4:C:8462:HOH:O	2.40	0.64
1:C:545:LEU:HD22	4:C:8502:HOH:O	1.98	0.64
4:E:8371:HOH:O	1:H:542:GLU:HG3	1.98	0.64
1:B:194:GLU:HG2	4:B:8505:HOH:O	1.98	0.63
1:G:126:LEU:HD12	1:G:132[B]:GLN:HG3	1.80	0.63
1:H:101:ASP:O	4:H:8555:HOH:O	2.15	0.63
1:F:121:LEU:CD2	1:G:121:LEU:HD21	2.28	0.63
1:F:607:GLU:HG3	4:F:8394:HOH:O	1.96	0.63
1:G:81:ASP:OD1	1:G:81:ASP:C	2.37	0.63
1:F:225:LYS:NZ	4:F:8427:HOH:O	2.30	0.63
1:H:252:GLU:CD	4:H:8565:HOH:O	2.42	0.63
1:C:541:MET:HE3	1:C:541:MET:HA	1.80	0.63
1:G:400:SER:HA	4:G:8493:HOH:O	1.99	0.63
1:G:497:MET:CE	4:G:8374:HOH:O	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:HG3	4:B:8553:HOH:O	1.98	0.62
1:C:287:VAL:HG23	4:C:8497:HOH:O	1.93	0.62
1:H:343:ALA:CB	4:H:8537:HOH:O	2.47	0.62
1:H:97:GLN:HG2	4:H:8488:HOH:O	1.98	0.62
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.64	0.62
1:C:382:ILE:HD13	4:C:8388:HOH:O	2.00	0.62
1:F:121:LEU:HD21	1:G:121:LEU:CD2	2.29	0.62
1:H:104[B]:VAL:HG21	1:H:455:SER:OG	2.00	0.62
1:G:388:GLU:CG	4:G:8559:HOH:O	2.47	0.62
1:A:112:MET:CE	4:B:8609:HOH:O	2.45	0.62
1:D:385:THR:OG1	1:D:388:GLU:OE1	2.09	0.62
1:A:545:LEU:CD2	4:A:8649:HOH:O	2.44	0.62
1:H:133:ALA:HB3	3:H:8004:MES:H81	1.80	0.62
1:H:271:PRO:CD	4:H:8596:HOH:O	2.47	0.62
1:B:178:GLU:CB	4:B:8626:HOH:O	2.37	0.62
1:G:328:LEU:CG	4:G:8550:HOH:O	2.17	0.61
1:D:541:MET:HE2	1:D:545:LEU:HD23	1.81	0.61
1:H:250:PHE:HD2	4:H:8480:HOH:O	1.77	0.61
1:B:99:ASN:HB3	4:B:8326:HOH:O	2.00	0.61
1:C:545:LEU:HB2	4:C:8502:HOH:O	2.00	0.61
1:F:121:LEU:CD2	1:G:121:LEU:CD2	2.78	0.61
1:H:343:ALA:HB3	4:H:8537:HOH:O	2.01	0.61
1:A:478:GLU:HB2	4:A:8519:HOH:O	2.00	0.61
4:H:8279:HOH:O	1:G:81:ASP:C	2.44	0.61
1:G:560:LYS:HE2	4:G:8549:HOH:O	1.99	0.61
1:D:126:LEU:CD1	1:D:132[B]:GLN:HG2	2.30	0.61
1:E:132[A]:GLN:CG	4:E:8344:HOH:O	2.48	0.61
1:H:392:SER:HA	1:H:417[B]:MET:HE1	1.82	0.61
1:H:339:ARG:HG2	4:H:8511:HOH:O	2.00	0.61
1:B:312:LYS:CE	4:B:8573:HOH:O	2.48	0.60
1:C:389:LEU:CD2	4:C:8365:HOH:O	2.49	0.60
1:E:312:LYS:HB2	4:E:8565:HOH:O	2.00	0.60
1:E:456:TYR:CD1	4:E:8500:HOH:O	2.51	0.60
1:H:228:GLU:HB2	4:H:8560:HOH:O	2.00	0.60
1:A:411:LYS:HE3	4:A:8590:HOH:O	2.01	0.60
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.84	0.60
1:G:328:LEU:CD1	4:G:8550:HOH:O	2.45	0.60
1:C:345:PRO:CB	4:C:8443:HOH:O	2.49	0.60
1:A:545:LEU:CB	4:A:8649:HOH:O	2.41	0.60
1:E:133:ALA:CB	3:E:8007:MES:H81	2.31	0.60
4:A:8679:HOH:O	1:D:505:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:MET:CB	4:F:8442:HOH:O	2.40	0.60
1:C:211:ASP:HB3	4:C:8440:HOH:O	2.02	0.60
1:G:133:ALA:HB3	3:G:8006:MES:H72	1.81	0.60
1:A:396:THR:O	4:A:8640:HOH:O	2.17	0.60
1:B:393:VAL:N	1:B:417:MET:HE1	2.12	0.60
1:H:132[A]:GLN:C	4:H:8544:HOH:O	2.43	0.60
1:H:219:HIS:HA	4:H:8587:HOH:O	2.00	0.59
1:G:194:GLU:HG2	4:G:8360:HOH:O	2.02	0.59
1:H:393:VAL:N	1:H:417[B]:MET:HE1	2.13	0.59
1:D:393:VAL:N	1:D:417:MET:HE1	2.11	0.59
1:E:384:GLY:HA3	4:E:8490:HOH:O	2.02	0.59
1:B:339:ARG:CG	4:B:8553:HOH:O	2.50	0.59
1:E:363:PHE:HB3	4:E:8502:HOH:O	2.01	0.59
1:G:541:MET:HE3	1:G:545:LEU:HD23	1.84	0.59
1:A:326:THR:O	4:A:8656:HOH:O	2.17	0.59
1:D:133:ALA:HB2	3:D:8005:MES:C7	2.32	0.59
1:E:619:THR:HG22	4:E:8169:HOH:O	2.01	0.59
1:H:97:GLN:CG	4:H:8480:HOH:O	2.49	0.59
1:G:358:GLU:OE2	4:G:8530:HOH:O	2.16	0.59
1:C:490:LYS:HB2	4:C:8450:HOH:O	2.02	0.59
1:H:271:PRO:HD3	4:H:8596:HOH:O	2.02	0.59
1:G:540:PHE:HE1	4:G:8588:HOH:O	1.83	0.59
1:A:285:ARG:HA	1:A:328:LEU:HD11	1.84	0.59
1:F:393:VAL:N	1:F:417:MET:HE1	2.09	0.58
4:H:8279:HOH:O	1:G:82:SER:N	2.36	0.58
1:A:481:GLU:HG2	4:A:8352:HOH:O	2.03	0.58
1:B:126:LEU:HD13	1:B:132[B]:GLN:CG	2.32	0.58
1:A:447:THR:CG2	4:A:8655:HOH:O	2.42	0.58
1:A:452:ASP:HB3	4:A:8367:HOH:O	2.01	0.58
3:C:8008:MES:C7	4:C:8251:HOH:O	2.42	0.58
1:H:429:GLU:HG2	4:H:8571:HOH:O	2.03	0.58
1:A:44:ASP:O	4:A:8572:HOH:O	2.17	0.58
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.39	0.58
1:E:460:GLN:C	4:E:8533:HOH:O	2.47	0.58
1:F:538:PRO:HG2	1:H:538:PRO:CG	2.34	0.58
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.38	0.58
1:D:481:GLU:HG2	4:D:8251:HOH:O	2.04	0.58
1:H:404:HIS:CE1	4:H:8295:HOH:O	2.57	0.58
1:B:81:ASP:OD1	1:B:81:ASP:C	2.45	0.57
1:C:133:ALA:HB3	3:C:8008:MES:H71	1.86	0.57
1:H:101:ASP:HA	4:H:8555:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:MET:CE	4:G:8302:HOH:O	2.51	0.57
1:F:47:TYR:O	1:F:313:ALA:HA	2.04	0.57
1:H:432:GLU:OE2	4:H:8512:HOH:O	2.17	0.57
1:B:385:THR:HG23	1:B:388:GLU:OE2	2.05	0.57
1:C:389:LEU:HD22	4:C:8365:HOH:O	2.04	0.57
1:H:201:LYS:NZ	4:H:8552:HOH:O	2.36	0.57
1:H:228:GLU:HG3	4:H:8297:HOH:O	2.03	0.57
1:A:341:ASN:HD22	1:A:342:PRO:HD2	1.69	0.57
1:D:496:ASN:CB	4:D:8575:HOH:O	2.53	0.57
1:E:421:GLU:CB	4:E:8513:HOH:O	2.52	0.57
1:E:452:ASP:HB3	4:E:8303:HOH:O	2.05	0.57
1:G:413:LYS:CD	4:G:8496:HOH:O	2.48	0.57
1:B:133:ALA:N	4:B:8607:HOH:O	2.31	0.57
1:D:510:ARG:NH2	4:D:8535:HOH:O	2.37	0.57
1:E:194:GLU:CD	4:E:8441:HOH:O	2.47	0.57
1:H:80:ILE:HG21	1:G:84:LEU:HD21	1.87	0.57
1:A:99:ASN:HB3	4:A:8357:HOH:O	2.05	0.57
1:B:100:ILE:HD11	4:B:8252:HOH:O	2.04	0.57
1:B:347:GLU:HG3	4:B:8551:HOH:O	2.05	0.57
1:E:392:SER:HA	1:E:417:MET:HE1	1.86	0.57
1:G:101:ASP:C	4:G:8521:HOH:O	2.42	0.57
1:A:421:GLU:HG3	4:B:8486:HOH:O	2.05	0.57
1:A:429:GLU:HG2	4:A:8644:HOH:O	2.04	0.57
1:H:298:LEU:CB	4:H:8578:HOH:O	2.35	0.57
1:B:310:GLU:CB	4:B:8535:HOH:O	2.52	0.56
1:B:380:MET:HA	4:B:8496:HOH:O	2.06	0.56
1:B:541:MET:HE3	1:B:545:LEU:HD23	1.86	0.56
1:D:478:GLU:CB	4:D:8535:HOH:O	2.49	0.56
1:E:133:ALA:CA	4:E:8271:HOH:O	2.50	0.56
1:E:497:MET:HE1	4:E:8276:HOH:O	1.83	0.56
3:H:8004:MES:C7	4:H:8306:HOH:O	2.53	0.56
1:G:155:GLN:NE2	4:G:8530:HOH:O	2.12	0.56
1:B:557:PHE:HA	4:B:8477:HOH:O	2.04	0.56
1:C:343:ALA:HB3	4:C:8445:HOH:O	2.06	0.56
1:F:619:THR:HG23	1:F:619:THR:O	2.06	0.56
1:B:81:ASP:HB3	4:B:8572:HOH:O	2.06	0.56
1:E:228:GLU:HG3	4:E:8554:HOH:O	2.06	0.56
1:H:389:LEU:HB3	4:H:8517:HOH:O	2.06	0.56
1:A:394:THR:CG2	4:A:8486:HOH:O	2.52	0.56
1:B:242:ALA:N	4:B:8594:HOH:O	2.38	0.56
1:E:284:GLU:C	1:E:328:LEU:CD1	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:435:VAL:CG2	4:H:8587:HOH:O	2.31	0.56
1:C:611:GLN:CG	4:C:8423:HOH:O	2.39	0.56
1:F:91:LYS:NZ	4:F:8319:HOH:O	2.38	0.56
3:F:8001:MES:C8	4:F:8407:HOH:O	2.54	0.56
1:A:100:ILE:HG21	4:A:8505:HOH:O	2.06	0.56
1:H:230:TYR:CA	4:H:8510:HOH:O	2.52	0.56
4:E:8250:HOH:O	1:F:81:ASP:HA	2.06	0.55
1:H:299:HIS:CD2	4:H:8526:HOH:O	2.59	0.55
1:D:496:ASN:HB2	4:D:8575:HOH:O	2.06	0.55
1:H:219:HIS:ND1	4:H:8587:HOH:O	2.33	0.55
1:H:619:THR:O	1:H:619:THR:HG23	2.05	0.55
1:G:312:LYS:CD	4:G:8555:HOH:O	2.46	0.55
1:B:385:THR:OG1	1:B:388:GLU:OE2	2.19	0.55
4:E:8503:HOH:O	1:F:121:LEU:HB3	2.06	0.55
1:H:45:ILE:C	1:H:45:ILE:HD12	2.32	0.55
1:G:126:LEU:HD13	1:G:132[B]:GLN:HG3	1.83	0.55
1:F:459:VAL:HG22	4:F:8302:HOH:O	2.05	0.55
1:G:459:VAL:HG12	4:G:8563:HOH:O	2.06	0.55
1:G:482:GLU:HG3	4:G:8580:HOH:O	2.05	0.55
1:E:126:LEU:HD13	1:E:132[B]:GLN:HG2	1.89	0.55
1:B:619:THR:HA	4:B:8373:HOH:O	2.05	0.55
1:B:126:LEU:HD13	1:B:132[B]:GLN:HG2	1.89	0.55
1:B:328:LEU:HB2	4:B:8639:HOH:O	2.06	0.55
3:F:8001:MES:C7	4:F:8407:HOH:O	2.55	0.55
1:H:389:LEU:CB	4:H:8514:HOH:O	2.54	0.55
1:A:405:PRO:CA	4:A:8625:HOH:O	2.45	0.54
1:A:541:MET:HE3	1:A:545:LEU:HD23	1.89	0.54
1:E:132[B]:GLN:NE2	3:E:8007:MES:O3S	2.35	0.54
1:E:194:GLU:OE2	4:E:8441:HOH:O	2.18	0.54
4:A:8705:HOH:O	1:B:421:GLU:HG3	2.06	0.54
1:E:610:LYS:HE3	4:E:8482:HOH:O	2.06	0.54
1:G:83:GLY:CA	4:G:8288:HOH:O	2.54	0.54
1:B:132[A]:GLN:HG2	4:B:8347:HOH:O	2.07	0.54
1:F:99:ASN:HB3	4:F:8219:HOH:O	2.06	0.54
1:H:80:ILE:HG21	1:G:84:LEU:CD2	2.37	0.54
1:H:340:PRO:HD2	4:H:8511:HOH:O	2.06	0.54
1:G:47:TYR:O	1:G:313:ALA:HA	2.07	0.54
1:C:185:LYS:HD3	4:C:8530:HOH:O	2.07	0.54
1:H:194:GLU:CG	4:H:8356:HOH:O	2.53	0.54
1:G:390:THR:OG1	4:G:8559:HOH:O	1.87	0.54
1:D:461:GLN:HA	4:D:8453:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:HB3	4:A:8483:HOH:O	2.07	0.54
1:A:542:GLU:CB	4:D:8339:HOH:O	2.55	0.54
1:A:136:PHE:HA	4:A:8414:HOH:O	2.08	0.54
1:D:299:HIS:CB	1:D:310:GLU:OE1	2.55	0.54
1:C:131:TRP:O	1:C:132[B]:GLN:HG2	2.08	0.54
1:G:126:LEU:HD13	1:G:132[B]:GLN:HG2	1.90	0.54
1:A:100:ILE:CG2	4:A:8505:HOH:O	2.57	0.53
3:A:8002:MES:C8	4:A:8414:HOH:O	2.56	0.53
1:B:392:SER:HA	1:B:417:MET:HE1	1.90	0.53
1:H:411:LYS:HE3	4:H:8436:HOH:O	2.06	0.53
1:G:45:ILE:N	4:G:8305:HOH:O	2.41	0.53
1:E:421:GLU:HB3	4:E:8513:HOH:O	2.09	0.53
1:A:201:LYS:HE2	1:A:205:TYR:OH	2.08	0.53
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.91	0.53
1:E:112:MET:CE	4:E:8332:HOH:O	2.55	0.53
3:E:8007:MES:H51	4:F:8327:HOH:O	2.08	0.53
1:H:230:TYR:HA	4:H:8510:HOH:O	2.08	0.53
1:C:611:GLN:HA	4:C:8423:HOH:O	2.09	0.53
3:G:8006:MES:C7	4:G:8371:HOH:O	2.49	0.53
1:A:336:GLN:HG3	4:A:8568:HOH:O	2.08	0.53
1:H:458:ALA:HB1	4:H:8528:HOH:O	2.07	0.53
1:H:490:LYS:HD3	1:H:491:ILE:HD13	1.91	0.53
1:A:133:ALA:CA	4:A:8381:HOH:O	2.47	0.53
1:C:343:ALA:CB	4:C:8445:HOH:O	2.57	0.53
1:D:101:ASP:O	1:D:104[B]:VAL:HG22	2.08	0.52
3:H:8004:MES:C8	4:H:8306:HOH:O	2.55	0.52
1:G:184:VAL:C	4:G:8589:HOH:O	2.52	0.52
1:D:112:MET:CE	4:D:8311:HOH:O	2.57	0.52
1:G:398:GLY:O	1:G:399:ALA:C	2.52	0.52
1:A:336:GLN:HA	4:A:8568:HOH:O	2.10	0.52
1:D:460:GLN:C	4:D:8453:HOH:O	2.52	0.52
1:A:100:ILE:HD13	1:A:100:ILE:C	2.35	0.52
1:D:365:GLN:HB3	4:D:8526:HOH:O	2.09	0.52
1:C:344:ASN:ND2	4:C:8445:HOH:O	2.42	0.52
3:H:8004:MES:H71	4:H:8306:HOH:O	2.10	0.52
1:B:389:LEU:N	1:B:389:LEU:HD22	2.24	0.52
1:E:541:MET:HE3	1:E:545:LEU:HD23	1.92	0.52
1:H:218:ARG:HD2	4:H:8090:HOH:O	2.10	0.52
1:B:100:ILE:HG13	4:B:8336:HOH:O	2.09	0.52
1:G:81:ASP:C	4:G:8299:HOH:O	2.52	0.52
1:A:45:ILE:C	1:A:45:ILE:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ARG:HD3	3:E:8007:MES:H82	1.92	0.52
1:B:394:THR:OG1	4:B:8653:HOH:O	2.19	0.52
1:B:157:VAL:HG21	1:B:324:HIS:CE1	2.45	0.51
1:E:158:THR:HG22	1:E:160:VAL:HG22	1.93	0.51
1:H:404:HIS:HE1	4:H:8295:HOH:O	1.91	0.51
1:B:328:LEU:HD22	4:B:8639:HOH:O	2.09	0.51
1:E:101:ASP:O	1:E:104[B]:VAL:HG22	2.09	0.51
1:D:47:TYR:O	1:D:313:ALA:HA	2.09	0.51
1:C:336:GLN:NE2	1:C:344:ASN:O	2.43	0.51
1:E:173:PRO:HG2	1:E:592:ALA:HB1	1.91	0.51
1:H:158:THR:HG22	1:H:160:VAL:HG22	1.91	0.51
3:F:8001:MES:H72	4:F:8407:HOH:O	2.10	0.51
1:H:133:ALA:HB2	3:H:8004:MES:C8	2.40	0.51
1:B:541:MET:HE3	1:B:545:LEU:CD2	2.40	0.51
1:G:515:ALA:HB1	4:G:8588:HOH:O	2.10	0.51
1:A:95:GLU:HG3	1:B:112:MET:HE3	1.93	0.51
1:E:385:THR:O	4:E:8379:HOH:O	2.18	0.51
1:D:284:GLU:C	1:D:328:LEU:CD1	2.83	0.51
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.92	0.51
1:E:91:LYS:NZ	4:E:8307:HOH:O	2.42	0.51
3:A:8002:MES:H71	4:A:8633:HOH:O	2.11	0.51
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.93	0.51
1:D:576:LYS:CD	4:D:8297:HOH:O	2.58	0.51
1:C:133:ALA:CB	3:C:8008:MES:C7	2.87	0.51
1:C:285:ARG:HD2	4:C:8522:HOH:O	2.10	0.51
1:C:342:PRO:C	4:C:8466:HOH:O	2.53	0.51
1:B:132[B]:GLN:C	4:B:8607:HOH:O	2.52	0.51
1:C:47:TYR:O	1:C:313:ALA:HA	2.10	0.51
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.93	0.51
1:G:389:LEU:HA	4:G:8491:HOH:O	2.11	0.51
1:A:132:GLN:C	4:A:8633:HOH:O	2.52	0.51
1:A:457:GLY:HA3	4:A:8341:HOH:O	2.11	0.51
1:H:607:GLU:HG3	4:H:8367:HOH:O	2.10	0.51
1:G:576:LYS:HG3	4:G:8579:HOH:O	2.11	0.51
1:B:478:GLU:CG	4:B:8615:HOH:O	2.59	0.50
1:A:95:GLU:OE2	4:A:8460:HOH:O	2.18	0.50
1:F:541:MET:CE	1:F:545:LEU:HD23	2.41	0.50
1:B:576:LYS:HG3	4:B:8622:HOH:O	2.10	0.50
1:G:619:THR:HG23	1:G:619:THR:O	2.11	0.50
4:A:8705:HOH:O	1:B:421:GLU:CG	2.59	0.50
1:E:385:THR:O	1:E:388:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:GLN:HB2	1:G:346:PRO:HG3	1.92	0.50
1:A:619:THR:HG22	4:A:8645:HOH:O	2.10	0.50
1:B:178:GLU:CG	4:B:8626:HOH:O	2.59	0.50
1:D:268:THR:HG22	4:D:8553:HOH:O	2.12	0.50
1:E:478:GLU:HG2	4:E:8399:HOH:O	2.12	0.50
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.47	0.50
1:G:100:ILE:CG1	4:G:8331:HOH:O	2.55	0.50
1:G:133:ALA:CB	3:G:8006:MES:H71	2.40	0.50
1:G:218:ARG:HD2	4:G:8031:HOH:O	2.12	0.50
1:B:342:PRO:HB3	4:B:8576:HOH:O	2.12	0.49
1:C:383:ARG:HB3	1:C:392:SER:HB3	1.93	0.49
1:C:513:LYS:HD3	4:C:8335:HOH:O	2.12	0.49
1:H:194:GLU:CD	4:H:8356:HOH:O	2.55	0.49
1:G:84:LEU:CD2	1:G:84:LEU:N	2.74	0.49
1:G:393:VAL:N	1:G:417:MET:HE1	2.18	0.49
1:G:541:MET:HE2	4:G:8540:HOH:O	2.12	0.49
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.46	0.49
1:E:47:TYR:O	1:E:313:ALA:HA	2.11	0.49
1:E:132[B]:GLN:OE1	3:E:8007:MES:H31	2.12	0.49
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.49
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.94	0.49
1:H:339:ARG:CG	4:H:8511:HOH:O	2.59	0.49
1:H:482:GLU:HG3	4:H:8472:HOH:O	2.11	0.49
1:B:505:ARG:HD2	4:C:8462:HOH:O	2.12	0.49
1:F:382:ILE:HD11	1:F:416:MET:HE1	1.93	0.49
1:C:218:ARG:HD2	4:C:8029:HOH:O	2.11	0.49
1:G:385:THR:CG2	1:G:388:GLU:OE2	2.59	0.49
1:G:576:LYS:HG2	4:G:8295:HOH:O	2.12	0.49
1:F:371:GLU:HB3	4:F:8435:HOH:O	2.12	0.49
1:B:178:GLU:CD	4:B:8626:HOH:O	2.56	0.49
1:E:124:ASP:OD1	4:E:8371:HOH:O	2.19	0.49
1:E:619:THR:CG2	4:E:8531:HOH:O	2.54	0.49
1:G:81:ASP:HA	4:G:8299:HOH:O	2.02	0.49
1:G:184:VAL:CG1	4:G:8589:HOH:O	2.53	0.49
1:B:380:MET:CA	4:B:8496:HOH:O	2.61	0.49
1:E:99:ASN:CG	4:E:8537:HOH:O	2.55	0.49
1:E:619:THR:HG23	4:E:8372:HOH:O	2.11	0.49
1:H:413:LYS:HE3	1:H:414:ASN:OD1	2.13	0.49
1:G:45:ILE:HD12	4:G:8305:HOH:O	2.12	0.49
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.94	0.49
1:B:478:GLU:HG2	4:B:8615:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:PHE:HA	4:F:8407:HOH:O	2.12	0.49
1:B:242:ALA:HB1	1:B:254:SER:HB2	1.95	0.49
1:B:478:GLU:CD	1:B:480:LYS:HE2	2.38	0.49
1:G:43:MET:CE	4:G:8501:HOH:O	2.60	0.49
1:G:155:GLN:CG	4:G:8530:HOH:O	2.29	0.49
1:G:618:PHE:CD1	1:G:618:PHE:C	2.89	0.49
1:B:546:VAL:HG11	4:B:8629:HOH:O	2.13	0.48
1:D:345:PRO:CA	4:D:8484:HOH:O	2.61	0.48
3:D:8005:MES:C8	4:D:8310:HOH:O	2.59	0.48
1:C:299:HIS:HB2	4:C:8497:HOH:O	2.13	0.48
1:H:541:MET:HE2	4:H:8603:HOH:O	2.11	0.48
1:C:619:THR:O	1:C:619:THR:HG23	2.13	0.48
1:E:218:ARG:HD2	4:E:8073:HOH:O	2.13	0.48
3:E:8007:MES:H71	1:F:462:SER:O	2.12	0.48
3:F:8001:MES:H32	3:F:8001:MES:O3S	2.13	0.48
1:G:481:GLU:HG2	4:G:8293:HOH:O	2.13	0.48
1:C:284:GLU:C	1:C:328:LEU:CD1	2.87	0.48
4:E:8371:HOH:O	1:H:542:GLU:CG	2.61	0.48
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.77	0.48
1:H:112:MET:CE	4:H:8331:HOH:O	2.61	0.48
1:G:99:ASN:CG	4:G:8551:HOH:O	2.56	0.48
1:A:81:ASP:C	1:A:81:ASP:OD1	2.54	0.48
1:D:490:LYS:HD3	1:D:491:ILE:HD13	1.95	0.48
1:C:126:LEU:HD13	1:C:132[B]:GLN:CG	2.42	0.48
1:C:389:LEU:CD1	4:C:8365:HOH:O	2.61	0.48
1:C:545:LEU:CD2	4:C:8502:HOH:O	2.56	0.48
1:G:91:LYS:NZ	4:G:8508:HOH:O	2.29	0.48
1:B:389:LEU:HD22	1:B:389:LEU:H	1.76	0.48
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.14	0.48
1:B:336:GLN:NE2	1:B:344:ASN:O	2.46	0.48
1:D:576:LYS:HD3	4:D:8297:HOH:O	2.13	0.48
1:G:400:SER:CA	4:G:8493:HOH:O	2.57	0.48
1:B:158:THR:HG22	1:B:160:VAL:HG22	1.94	0.48
1:A:312:LYS:CD	4:A:8546:HOH:O	2.61	0.48
1:B:231:LYS:HE2	4:B:8482:HOH:O	2.14	0.48
1:D:134:SER:HB2	4:D:8459:HOH:O	2.13	0.48
1:D:81:ASP:C	1:D:81:ASP:OD1	2.54	0.48
1:F:121:LEU:HD23	1:G:121:LEU:HD21	1.95	0.48
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.96	0.48
1:H:452:ASP:CB	4:H:8499:HOH:O	2.35	0.48
1:A:299:HIS:CE1	4:A:8599:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:GLU:CG	4:F:8336:HOH:O	2.62	0.47
1:G:158:THR:CG2	1:G:160:VAL:HG22	2.44	0.47
1:A:341:ASN:HB3	4:A:8641:HOH:O	2.13	0.47
1:B:382:ILE:HD13	4:B:8420:HOH:O	2.14	0.47
1:H:99:ASN:HB3	4:H:8312:HOH:O	2.13	0.47
1:H:228:GLU:CD	4:H:8465:HOH:O	2.57	0.47
1:A:541:MET:CE	1:A:545:LEU:HD23	2.44	0.47
1:C:490:LYS:HG3	4:C:8450:HOH:O	2.14	0.47
1:E:284:GLU:O	1:E:328:LEU:HD12	2.14	0.47
1:H:268:THR:C	4:H:8596:HOH:O	2.57	0.47
1:G:133:ALA:CB	3:G:8006:MES:O3S	2.60	0.47
1:C:185:LYS:CE	4:C:8507:HOH:O	2.63	0.47
1:G:100:ILE:HD11	4:G:8311:HOH:O	2.14	0.47
1:G:389:LEU:HG	4:G:8599:HOH:O	2.14	0.47
1:A:497:MET:CE	4:A:8380:HOH:O	2.33	0.47
1:D:336:GLN:NE2	1:D:344:ASN:O	2.48	0.47
1:C:101:ASP:O	4:C:8397:HOH:O	2.20	0.47
1:C:159:ARG:HA	2:C:7004:FAD:O2B	2.15	0.47
1:E:158:THR:CG2	1:E:160:VAL:HG22	2.44	0.47
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.97	0.47
4:E:8371:HOH:O	1:H:542:GLU:CB	2.62	0.47
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.79	0.47
1:C:548:HIS:C	4:C:8370:HOH:O	2.57	0.47
1:H:100:ILE:HD13	1:H:100:ILE:O	2.14	0.47
1:G:336:GLN:NE2	4:G:8482:HOH:O	2.47	0.47
1:G:388:GLU:HG3	4:G:8559:HOH:O	2.13	0.47
1:G:541:MET:CE	4:G:8540:HOH:O	2.63	0.47
1:D:496:ASN:CG	4:D:8575:HOH:O	2.57	0.47
4:D:8439:HOH:O	3:C:8008:MES:H52	2.15	0.47
1:H:184:VAL:HG11	1:H:190:ALA:HB3	1.97	0.47
1:H:331:ASN:C	4:H:8576:HOH:O	2.56	0.47
1:F:459:VAL:HA	4:F:8302:HOH:O	2.13	0.47
1:G:83:GLY:HA2	4:G:8288:HOH:O	2.13	0.47
1:D:345:PRO:HA	4:D:8484:HOH:O	2.14	0.47
4:F:8449:HOH:O	1:G:542:GLU:CB	2.63	0.47
1:A:84:LEU:HD23	4:B:8332:HOH:O	2.14	0.46
1:A:541:MET:HE3	1:A:545:LEU:CD2	2.45	0.46
1:D:132[B]:GLN:OE1	3:D:8005:MES:H71	2.15	0.46
1:G:218:ARG:HG3	1:G:430:ASP:OD2	2.15	0.46
1:G:388:GLU:CD	4:G:8559:HOH:O	2.58	0.46
1:B:91:LYS:CE	4:B:8327:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:541:MET:CE	1:H:545:LEU:HD23	2.46	0.46
4:H:8615:HOH:O	1:G:84:LEU:CG	2.42	0.46
1:G:471:TRP:CH2	1:G:526:SER:HA	2.51	0.46
1:A:47:TYR:O	1:A:313:ALA:HA	2.16	0.46
1:A:312:LYS:HD3	4:A:8546:HOH:O	2.15	0.46
1:B:158:THR:CG2	1:B:160:VAL:HG22	2.46	0.46
1:D:110:GLN:NE2	4:D:8488:HOH:O	2.22	0.46
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.51	0.46
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.98	0.46
1:F:83:GLY:HA2	4:F:8157:HOH:O	2.15	0.46
1:G:388:GLU:CB	4:G:8598:HOH:O	2.63	0.46
1:F:83:GLY:N	4:F:8157:HOH:O	2.42	0.46
1:H:45:ILE:C	1:H:45:ILE:CD1	2.89	0.46
1:H:104[A]:VAL:CG2	4:H:8555:HOH:O	2.34	0.46
1:H:139:ARG:HD3	3:H:8004:MES:H82	1.97	0.46
1:B:47:TYR:O	1:B:313:ALA:HA	2.15	0.46
1:F:293:SER:HA	1:F:574:GLY:O	2.15	0.46
3:H:8004:MES:H51	4:H:8306:HOH:O	2.16	0.46
1:G:544:GLY:CA	4:G:8530:HOH:O	2.64	0.46
1:B:385:THR:CG2	1:B:388:GLU:OE2	2.63	0.46
1:D:389:LEU:HB2	4:D:8465:HOH:O	2.16	0.46
1:C:272:GLU:HG2	4:C:8442:HOH:O	2.16	0.46
1:C:345:PRO:HB3	4:C:8443:HOH:O	2.12	0.46
1:G:285:ARG:NH2	1:G:287:VAL:HG22	2.31	0.46
1:G:619:THR:HA	4:G:8582:HOH:O	2.16	0.46
1:A:265:ARG:HA	1:A:266:PRO:C	2.40	0.46
1:B:460:GLN:HB3	4:B:8558:HOH:O	2.15	0.46
1:H:91:LYS:CG	4:H:8488:HOH:O	2.64	0.46
1:G:46:LYS:N	4:G:8305:HOH:O	2.25	0.46
1:B:45:ILE:HD13	4:B:8488:HOH:O	2.15	0.45
1:B:90:LYS:HD3	4:B:8528:HOH:O	2.15	0.45
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.80	0.45
1:A:100:ILE:CD1	1:A:453:ALA:HB2	2.45	0.45
1:F:459:VAL:CG1	4:F:8302:HOH:O	2.37	0.45
3:H:8004:MES:H31	1:G:462:SER:OG	2.15	0.45
1:A:43:MET:HG3	4:A:8572:HOH:O	2.15	0.45
1:B:100:ILE:HA	4:B:8336:HOH:O	2.14	0.45
1:C:123:VAL:HB	3:C:8008:MES:H62	1.99	0.45
1:C:418:GLN:HE21	1:C:418:GLN:HB3	1.51	0.45
1:F:194:GLU:HG2	4:F:8264:HOH:O	2.17	0.45
1:G:123:VAL:HB	3:G:8006:MES:H22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASP:N	4:A:8625:HOH:O	2.34	0.45
1:D:576:LYS:HG3	4:D:8297:HOH:O	2.16	0.45
1:H:284:GLU:C	1:H:328:LEU:CD1	2.90	0.45
1:E:341:ASN:C	1:E:341:ASN:HD22	2.24	0.45
1:G:43:MET:HE2	4:G:8501:HOH:O	2.16	0.45
1:C:432:GLU:HB2	1:C:433:PRO:HD2	1.99	0.45
1:H:126:LEU:HD13	1:H:132[B]:GLN:HG2	1.98	0.45
1:H:133:ALA:N	4:H:8544:HOH:O	2.35	0.45
1:H:389:LEU:HB2	4:H:8514:HOH:O	2.16	0.45
1:H:429:GLU:CG	4:H:8571:HOH:O	2.61	0.45
1:G:112:MET:HE1	4:G:8302:HOH:O	2.15	0.45
1:A:285:ARG:HA	1:A:328:LEU:HD12	1.98	0.45
1:B:132[A]:GLN:C	4:B:8607:HOH:O	2.57	0.45
1:B:218:ARG:HD2	4:B:8041:HOH:O	2.17	0.45
1:B:310:GLU:HB2	4:B:8535:HOH:O	2.16	0.45
1:E:64:GLU:OE2	1:E:205:TYR:OH	2.32	0.45
1:A:285:ARG:CA	1:A:328:LEU:HD11	2.47	0.45
1:A:299:HIS:CD2	4:A:8599:HOH:O	2.66	0.45
1:B:265:ARG:HA	1:B:266:PRO:C	2.42	0.45
1:D:618:PHE:CD1	1:D:618:PHE:C	2.94	0.45
1:D:133:ALA:HB2	3:D:8005:MES:H71	1.88	0.44
1:B:112:MET:CE	4:B:8328:HOH:O	2.60	0.44
1:B:328:LEU:CG	4:B:8525:HOH:O	2.12	0.44
1:B:546:VAL:HB	4:B:8629:HOH:O	2.17	0.44
1:C:541:MET:HE2	1:C:545:LEU:HD23	1.99	0.44
1:C:576:LYS:CD	4:C:8260:HOH:O	2.57	0.44
1:E:312:LYS:HD3	4:E:8565:HOH:O	2.16	0.44
1:H:231:LYS:CE	4:H:8297:HOH:O	2.66	0.44
1:G:158:THR:HG22	1:G:160:VAL:HG22	1.99	0.44
1:C:133:ALA:CB	3:C:8008:MES:H71	2.47	0.44
1:H:105:ASN:HB3	1:G:105:ASN:O	2.17	0.44
1:H:389:LEU:CA	4:H:8514:HOH:O	2.64	0.44
1:C:185:LYS:CD	4:C:8530:HOH:O	2.64	0.44
1:G:413:LYS:CE	4:G:8496:HOH:O	2.65	0.44
1:A:50:VAL:HG13	1:A:313:ALA:HB2	2.00	0.44
1:B:242:ALA:HB2	4:B:8594:HOH:O	2.17	0.44
1:E:132[A]:GLN:HG2	4:E:8344:HOH:O	2.12	0.44
1:G:84:LEU:N	1:G:84:LEU:HD23	2.32	0.44
3:D:8005:MES:H32	3:D:8005:MES:O2S	2.18	0.44
1:C:460:GLN:HB3	4:C:8263:HOH:O	2.18	0.44
1:G:299[A]:HIS:CG	4:G:8370:HOH:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LYS:NZ	4:D:8250:HOH:O	2.49	0.44
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.83	0.44
1:D:159:ARG:HA	2:D:7003:FAD:O2B	2.18	0.44
1:H:123:VAL:HG22	1:G:459:VAL:CG1	2.48	0.44
1:C:478:GLU:OE2	1:C:480:LYS:HE2	2.18	0.44
1:H:101:ASP:C	4:H:8555:HOH:O	2.59	0.44
1:G:157:VAL:HG21	1:G:324:HIS:HE1	1.82	0.44
1:G:385:THR:CB	1:G:388:GLU:OE2	2.66	0.44
1:G:385:THR:HB	1:G:388:GLU:OE2	2.18	0.44
1:B:383:ARG:HG3	4:B:8514:HOH:O	2.18	0.43
1:B:385:THR:CB	1:B:388:GLU:OE2	2.66	0.43
1:H:211:ASP:CB	4:H:8421:HOH:O	2.44	0.43
1:G:159:ARG:HA	2:G:7008:FAD:O2B	2.18	0.43
1:A:400:SER:CB	4:A:8523:HOH:O	2.66	0.43
1:A:421:GLU:OE2	4:A:8681:HOH:O	2.21	0.43
1:D:123:VAL:HG22	1:C:459:VAL:HG12	1.98	0.43
1:C:100:ILE:HD13	1:C:100:ILE:O	2.17	0.43
1:C:478:GLU:CD	1:C:480:LYS:HE2	2.43	0.43
1:F:158:THR:HG22	1:F:160:VAL:HG22	2.00	0.43
1:G:544:GLY:HA2	4:G:8530:HOH:O	2.18	0.43
1:D:215:GLU:O	1:D:411:LYS:NZ	2.51	0.43
1:E:45:ILE:HG13	4:E:8442:HOH:O	2.16	0.43
1:H:101:ASP:O	1:H:104[B]:VAL:HG22	2.19	0.43
1:C:471:TRP:CH2	1:C:526:SER:HA	2.54	0.43
1:E:44:ASP:HB3	4:E:8443:HOH:O	2.18	0.43
1:E:91:LYS:HE2	4:E:8307:HOH:O	2.13	0.43
1:F:159:ARG:HA	2:F:7006:FAD:O2B	2.19	0.43
1:H:309:PHE:HD2	4:H:8590:HOH:O	2.01	0.43
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.53	0.43
1:D:158:THR:CG2	1:D:160:VAL:HG22	2.48	0.43
1:C:100:ILE:HD13	1:C:453:ALA:HB2	2.00	0.43
1:E:265:ARG:HA	1:E:266:PRO:C	2.43	0.43
3:E:8007:MES:C8	4:E:8255:HOH:O	2.66	0.43
1:H:293:SER:HA	1:H:574:GLY:O	2.18	0.43
1:H:343:ALA:HB1	4:H:8537:HOH:O	2.15	0.43
1:D:299:HIS:CA	1:D:310:GLU:OE1	2.67	0.43
1:D:342:PRO:HD2	4:D:8533:HOH:O	2.18	0.43
1:E:459:VAL:HA	4:E:8503:HOH:O	2.18	0.43
1:H:105:ASN:O	1:G:105:ASN:HB3	2.19	0.43
1:G:505:ARG:NH1	4:G:8363:HOH:O	2.51	0.43
1:A:417:MET:HE3	1:A:417:MET:HB3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:PRO:HG2	1:D:538:PRO:HG2	2.00	0.43
1:C:242:ALA:HB1	1:C:254:SER:HB2	2.01	0.43
1:C:413:LYS:NZ	4:C:8269:HOH:O	2.51	0.43
1:H:231:LYS:HD3	4:H:8416:HOH:O	2.19	0.43
1:A:56:PRO:HD3	1:A:165:SER:HB3	2.01	0.43
1:B:97:GLN:HB2	4:B:8633:HOH:O	2.19	0.43
1:E:194:GLU:CG	4:E:8441:HOH:O	2.58	0.43
1:A:312:LYS:CE	4:A:8623:HOH:O	2.52	0.43
1:A:542:GLU:CG	4:D:8339:HOH:O	2.43	0.43
1:E:56:PRO:HD3	1:E:165:SER:HB3	2.01	0.43
1:E:133:ALA:HB1	4:E:8271:HOH:O	2.17	0.43
1:G:265:ARG:HA	1:G:266:PRO:C	2.44	0.43
1:B:45:ILE:CD1	4:B:8488:HOH:O	2.67	0.42
1:B:100:ILE:CD1	4:B:8252:HOH:O	2.64	0.42
1:B:328:LEU:CB	4:B:8639:HOH:O	2.66	0.42
1:B:478:GLU:CD	4:B:8671:HOH:O	2.61	0.42
1:A:399:ALA:N	4:A:8593:HOH:O	2.51	0.42
1:D:47:TYR:CD2	1:D:73:ALA:HB2	2.54	0.42
1:D:385:THR:HA	1:D:386:PRO:HD3	1.93	0.42
1:H:91:LYS:HG3	4:H:8488:HOH:O	2.19	0.42
1:H:95:GLU:HG3	1:G:112:MET:HE3	2.01	0.42
1:C:112:MET:CE	4:C:8372:HOH:O	2.68	0.42
1:H:47:TYR:O	1:H:313:ALA:HA	2.20	0.42
1:H:271:PRO:N	4:H:8596:HOH:O	2.51	0.42
1:H:285:ARG:HG2	4:H:8576:HOH:O	2.19	0.42
1:H:341:ASN:C	1:H:341:ASN:HD22	2.26	0.42
1:B:385:THR:HA	1:B:386:PRO:HD3	1.91	0.42
1:D:541:MET:HE2	1:D:545:LEU:CD2	2.48	0.42
1:C:64:GLU:OE2	1:C:205:TYR:OH	2.35	0.42
3:E:8007:MES:H81	4:E:8255:HOH:O	2.19	0.42
1:F:459:VAL:CB	4:F:8302:HOH:O	2.65	0.42
1:G:312:LYS:CG	4:G:8555:HOH:O	2.58	0.42
1:E:293:SER:HA	1:E:574:GLY:O	2.19	0.42
1:E:452:ASP:OD1	1:E:452:ASP:N	2.52	0.42
1:B:204:SER:OG	4:B:8547:HOH:O	2.05	0.42
1:G:136:PHE:HA	4:G:8371:HOH:O	2.20	0.42
1:G:185:LYS:HD2	4:G:8567:HOH:O	2.19	0.42
1:A:104[A]:VAL:HG13	4:A:8551:HOH:O	2.20	0.42
1:B:619:THR:HB	4:B:8625:HOH:O	2.20	0.42
1:E:382:ILE:CG2	1:E:391:TYR:CE1	3.03	0.42
1:E:541:MET:CE	1:E:545:LEU:HD23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:GLY:CA	4:F:8157:HOH:O	2.67	0.42
1:B:50:VAL:HG13	1:B:313:ALA:HB2	2.02	0.42
1:D:392:SER:HA	1:D:417:MET:HE1	2.02	0.42
1:F:77:ILE:HD11	1:F:495:TYR:CD2	2.55	0.42
1:F:385:THR:OG1	1:F:388:GLU:OE1	2.21	0.42
1:H:103:PHE:HB2	4:H:8387:HOH:O	2.20	0.42
1:H:231:LYS:N	4:H:8510:HOH:O	2.39	0.42
1:B:341:ASN:HD22	1:B:342:PRO:HD2	1.85	0.42
1:E:541:MET:HE3	1:E:545:LEU:CD2	2.50	0.42
1:D:383:ARG:HB3	1:D:392:SER:HB3	2.02	0.41
1:H:81:ASP:O	1:H:90:LYS:HE2	2.19	0.41
1:H:458:ALA:CB	4:H:8528:HOH:O	2.66	0.41
1:G:46:LYS:CE	4:G:8576:HOH:O	2.67	0.41
1:D:413:LYS:HE3	4:D:8443:HOH:O	2.20	0.41
1:E:285:ARG:HH21	1:E:287:VAL:HG22	1.86	0.41
1:F:91:LYS:HG2	4:F:8296:HOH:O	2.21	0.41
1:H:389:LEU:HA	4:H:8514:HOH:O	2.20	0.41
1:G:101:ASP:O	1:G:104[B]:VAL:HG22	2.19	0.41
1:G:392:SER:HA	1:G:417:MET:HE1	2.02	0.41
1:G:408:TRP:CD1	1:G:408:TRP:C	2.98	0.41
2:B:7002:FAD:H8A	4:B:8158:HOH:O	2.20	0.41
1:C:101:ASP:C	4:C:8397:HOH:O	2.60	0.41
1:C:389:LEU:HD13	4:C:8365:HOH:O	2.18	0.41
1:E:505:ARG:NH2	4:E:8354:HOH:O	2.53	0.41
1:H:231:LYS:HE2	4:H:8297:HOH:O	2.20	0.41
1:B:618:PHE:HD1	4:B:8417:HOH:O	2.03	0.41
1:H:83:GLY:N	4:H:8279:HOH:O	2.36	0.41
1:H:101:ASP:O	1:H:104[A]:VAL:HG23	2.20	0.41
1:H:510:ARG:NH2	4:H:8504:HOH:O	2.53	0.41
1:A:218:ARG:HD2	4:A:8189:HOH:O	2.20	0.41
1:E:106:VAL:O	1:E:110:GLN:HG2	2.21	0.41
1:G:557:PHE:HA	4:G:8584:HOH:O	2.20	0.41
1:C:541:MET:HE2	1:C:545:LEU:CD2	2.51	0.41
1:F:481:GLU:CG	4:F:8289:HOH:O	2.64	0.41
1:H:331:ASN:ND2	4:H:8576:HOH:O	2.52	0.41
1:H:460:GLN:C	4:H:8562:HOH:O	2.60	0.41
1:H:541:MET:HE3	4:H:8149:HOH:O	2.20	0.41
1:D:344:ASN:C	4:D:8398:HOH:O	2.63	0.41
1:C:157:VAL:HG21	1:C:324:HIS:CE1	2.54	0.41
1:C:265:ARG:HA	1:C:266:PRO:C	2.45	0.41
1:C:619:THR:CG2	4:C:8291:HOH:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:TRP:CH2	1:E:526:SER:HA	2.56	0.41
1:H:123:VAL:N	3:H:8004:MES:H22	2.26	0.41
1:G:607:GLU:HG3	4:G:8317:HOH:O	2.21	0.41
1:A:105:ASN:HB3	1:B:105:ASN:O	2.20	0.41
1:B:388:GLU:HB3	1:B:389:LEU:HD22	2.02	0.41
1:C:228:GLU:HG3	4:C:8249:HOH:O	2.20	0.41
1:E:576:LYS:HD2	4:E:8386:HOH:O	2.20	0.41
1:F:570:SER:HB3	1:F:580:LEU:O	2.20	0.41
1:H:215:GLU:O	1:H:411:LYS:NZ	2.54	0.41
1:H:421:GLU:H	1:H:421:GLU:CD	2.28	0.41
1:A:312:LYS:HD2	4:A:8456:HOH:O	2.21	0.41
1:B:408:TRP:CD1	1:B:408:TRP:C	2.99	0.41
1:C:545:LEU:CB	4:C:8502:HOH:O	2.58	0.41
1:E:457:GLY:H	1:E:460:GLN:HE21	1.67	0.41
1:F:433:PRO:O	1:F:450:HIS:HA	2.21	0.41
1:H:126:LEU:CD1	1:H:132[B]:GLN:CD	2.94	0.41
1:H:541:MET:HE3	1:H:545:LEU:HD23	2.02	0.41
3:H:8004:MES:C7	1:G:462:SER:O	2.56	0.41
1:G:382:ILE:HD13	4:G:8401:HOH:O	2.20	0.41
1:B:159:ARG:HA	2:B:7002:FAD:O2B	2.21	0.41
1:B:383:ARG:HD2	4:B:8485:HOH:O	2.20	0.41
1:D:576:LYS:CG	4:D:8297:HOH:O	2.68	0.41
1:F:104[A]:VAL:HG12	1:F:108:GLN:NE2	2.36	0.41
1:H:81:ASP:CB	4:H:8304:HOH:O	2.48	0.41
1:B:133:ALA:CB	3:B:8003:MES:O2S	2.62	0.40
1:B:389:LEU:H	1:B:389:LEU:HD13	1.86	0.40
1:B:471:TRP:CH2	1:B:526:SER:HA	2.56	0.40
1:C:101:ASP:O	1:C:104[B]:VAL:HG22	2.20	0.40
1:G:619:THR:O	1:G:619:THR:CG2	2.68	0.40
1:B:570:SER:HB3	1:B:580:LEU:O	2.21	0.40
4:B:8469:HOH:O	1:C:542:GLU:CB	2.42	0.40
1:D:211:ASP:CB	4:D:8348:HOH:O	2.59	0.40
1:E:131:TRP:O	1:E:132[B]:GLN:HG2	2.22	0.40
1:F:618:PHE:C	1:F:618:PHE:CD1	3.00	0.40
1:H:173:PRO:HG2	1:H:592:ALA:HB1	2.02	0.40
1:H:343:ALA:CA	4:H:8588:HOH:O	2.69	0.40
1:B:242:ALA:CB	4:B:8594:HOH:O	2.70	0.40
1:B:497:MET:CE	4:B:8369:HOH:O	2.26	0.40
1:D:64:GLU:OE2	1:D:205:TYR:OH	2.36	0.40
3:E:8007:MES:H51	1:F:462:SER:OG	2.21	0.40
1:F:284:GLU:C	1:F:285:ARG:HG2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:471:TRP:CH2	1:F:526:SER:HA	2.56	0.40
1:H:165:SER:HA	1:H:168:TRP:CD1	2.57	0.40
1:G:71:LYS:NZ	4:G:8492:HOH:O	2.54	0.40
1:B:215:GLU:O	1:B:411:LYS:NZ	2.55	0.40
1:E:121:LEU:CD2	1:H:121:LEU:CD2	3.00	0.40
1:H:81:ASP:HA	4:G:8288:HOH:O	2.21	0.40
1:H:421:GLU:OE2	4:H:8273:HOH:O	2.22	0.40
1:H:432:GLU:HB2	1:H:433:PRO:HD2	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:8534:HOH:O	4:G:8089:HOH:O[2_646]	1.69	0.51
4:A:8707:HOH:O	4:G:8089:HOH:O[2_646]	1.73	0.47
4:H:8261:HOH:O	4:G:8557:HOH:O[2_655]	1.81	0.39
1:H:235:ASP:OD2	4:B:8535:HOH:O[2_666]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/623 (92%)	563 (98%)	13 (2%)	0	100	100
1	B	577/623 (93%)	564 (98%)	13 (2%)	0	100	100
1	C	577/623 (93%)	558 (97%)	19 (3%)	0	100	100
1	D	577/623 (93%)	564 (98%)	13 (2%)	0	100	100
1	E	577/623 (93%)	561 (97%)	15 (3%)	1 (0%)	43	27
1	F	576/623 (92%)	563 (98%)	13 (2%)	0	100	100
1	G	578/623 (93%)	562 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	578/623 (93%)	562 (97%)	16 (3%)	0	100	100
All	All	4616/4984 (93%)	4497 (97%)	118 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	343	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/541 (93%)	496 (98%)	9 (2%)	51	30
1	B	506/541 (94%)	494 (98%)	12 (2%)	43	20
1	C	506/541 (94%)	498 (98%)	8 (2%)	55	34
1	D	506/541 (94%)	497 (98%)	9 (2%)	51	30
1	E	506/541 (94%)	499 (99%)	7 (1%)	59	39
1	F	505/541 (93%)	492 (97%)	13 (3%)	40	17
1	G	507/541 (94%)	498 (98%)	9 (2%)	51	30
1	H	507/541 (94%)	498 (98%)	9 (2%)	51	30
All	All	4048/4328 (94%)	3972 (98%)	76 (2%)	51	28

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	112	MET
1	A	185	LYS
1	A	312	LYS
1	A	400	SER
1	A	401	THR
1	A	496	ASN

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Mol	Chain	Res	Type
1	A	593	ASN
1	A	619	THR
1	B	45	ILE
1	B	112	MET
1	B	132[A]	GLN
1	B	132[B]	GLN
1	B	185	LYS
1	B	206	PHE
1	B	312	LYS
1	B	385	THR
1	B	389	LEU
1	B	490	LYS
1	B	496	ASN
1	B	593	ASN
1	D	100	ILE
1	D	110	GLN
1	D	185	LYS
1	D	231	LYS
1	D	381	THR
1	D	385	THR
1	D	389	LEU
1	D	390	THR
1	D	593	ASN
1	C	100	ILE
1	C	385	THR
1	C	389	LEU
1	C	418	GLN
1	C	455	SER
1	C	490	LYS
1	C	496	ASN
1	C	593	ASN
1	E	100	ILE
1	E	185	LYS
1	E	206	PHE
1	E	231	LYS
1	E	403	LYS
1	E	455	SER
1	E	496	ASN
1	F	100	ILE
1	F	112	MET
1	F	178	GLU
1	F	272	GLU

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Mol	Chain	Res	Type
1	F	285	ARG
1	F	328	LEU
1	F	383	ARG
1	F	385	THR
1	F	389	LEU
1	F	413	LYS
1	F	496	ASN
1	F	576	LYS
1	F	593	ASN
1	H	45	ILE
1	H	100	ILE
1	H	132[A]	GLN
1	H	132[B]	GLN
1	H	185	LYS
1	H	272	GLU
1	H	328	LEU
1	H	385	THR
1	H	496	ASN
1	G	45	ILE
1	G	84	LEU
1	G	228	GLU
1	G	341	ASN
1	G	385	THR
1	G	390	THR
1	G	413	LYS
1	G	496	ASN
1	G	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	108	GLN
1	A	257	ASN
1	A	263	GLN
1	A	299	HIS
1	A	341	ASN
1	A	409	ASN
1	A	419	HIS
1	A	461	GLN
1	B	105	ASN
1	B	257	ASN

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	276	ASN
1	B	341	ASN
1	B	344	ASN
1	B	440	GLN
1	B	460	GLN
1	B	461	GLN
1	D	105	ASN
1	D	257	ASN
1	D	299	HIS
1	D	341	ASN
1	D	419	HIS
1	D	460	GLN
1	C	105	ASN
1	C	224	ASN
1	C	237	GLN
1	C	257	ASN
1	C	263	GLN
1	C	276	ASN
1	C	341	ASN
1	C	344	ASN
1	C	418	GLN
1	C	461	GLN
1	E	99	ASN
1	E	105	ASN
1	E	233	GLN
1	E	263	GLN
1	E	276	ASN
1	E	336	GLN
1	E	341	ASN
1	E	418	GLN
1	E	460	GLN
1	E	499	GLN
1	F	105	ASN
1	F	108	GLN
1	F	132	GLN
1	F	257	ASN
1	F	263	GLN
1	F	341	ASN
1	F	419	HIS
1	H	105	ASN
1	H	257	ASN

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Mol	Chain	Res	Type
1	H	276	ASN
1	H	341	ASN
1	H	418	GLN
1	H	419	HIS
1	H	460	GLN
1	G	105	ASN
1	G	108	GLN
1	G	257	ASN
1	G	263	GLN
1	G	276	ASN
1	G	418	GLN
1	G	419	HIS
1	G	460	GLN
1	G	461	GLN
1	G	499	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MES	B	8003	-	12,12,12	2.03	1 (8%)	15,16,16	4.01	6 (40%)
3	MES	E	8007	-	12,12,12	1.94	1 (8%)	15,16,16	5.58	11 (73%)
2	FAD	E	7005	-	58,58,58	1.48	8 (13%)	85,89,89	2.03	25 (29%)
3	MES	H	8004	-	12,12,12	2.28	1 (8%)	15,16,16	3.22	7 (46%)
3	MES	C	8008	-	12,12,12	1.72	1 (8%)	15,16,16	4.65	8 (53%)
2	FAD	D	7003	-	58,58,58	1.40	9 (15%)	85,89,89	2.26	27 (31%)
3	MES	D	8005	-	12,12,12	1.74	1 (8%)	15,16,16	5.47	7 (46%)
3	MES	G	8006	-	12,12,12	1.89	1 (8%)	15,16,16	4.81	8 (53%)
2	FAD	H	7007	-	58,58,58	1.30	9 (15%)	85,89,89	2.10	22 (25%)
2	FAD	F	7006	-	58,58,58	1.31	9 (15%)	85,89,89	2.12	24 (28%)
2	FAD	G	7008	-	58,58,58	1.35	10 (17%)	85,89,89	2.19	30 (35%)
2	FAD	C	7004	-	58,58,58	1.53	11 (18%)	85,89,89	2.10	30 (35%)
3	MES	F	8001	-	12,12,12	1.68	1 (8%)	15,16,16	3.53	8 (53%)
2	FAD	B	7002	-	58,58,58	1.43	7 (12%)	85,89,89	2.22	25 (29%)
2	FAD	A	7001	-	58,58,58	1.40	5 (8%)	85,89,89	1.87	20 (23%)
3	MES	A	8002	-	12,12,12	1.71	1 (8%)	15,16,16	3.64	7 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '–' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	B	8003	-	-	2/6/14/14	0/1/1/1
3	MES	E	8007	-	-	5/6/14/14	0/1/1/1
2	FAD	E	7005	-	-	3/34/50/50	0/6/6/6
3	MES	H	8004	-	-	5/6/14/14	0/1/1/1
3	MES	C	8008	-	-	2/6/14/14	0/1/1/1
2	FAD	D	7003	-	-	2/34/50/50	0/6/6/6
3	MES	D	8005	-	-	2/6/14/14	0/1/1/1
3	MES	G	8006	-	-	2/6/14/14	0/1/1/1
2	FAD	H	7007	-	-	2/34/50/50	0/6/6/6
2	FAD	F	7006	-	-	3/34/50/50	0/6/6/6
2	FAD	G	7008	-	-	1/34/50/50	0/6/6/6
2	FAD	C	7004	-	-	3/34/50/50	0/6/6/6
3	MES	F	8001	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	7002	-	-	1/34/50/50	0/6/6/6
2	FAD	A	7001	-	-	1/34/50/50	0/6/6/6
3	MES	A	8002	-	-	2/6/14/14	0/1/1/1

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8004	MES	C8-S	-7.80	1.66	1.77
3	B	8003	MES	C8-S	-6.66	1.68	1.77
3	G	8006	MES	C8-S	-6.19	1.68	1.77
3	E	8007	MES	C8-S	-6.18	1.68	1.77
3	C	8008	MES	C8-S	-5.57	1.69	1.77
3	A	8002	MES	C8-S	-5.55	1.69	1.77
2	E	7005	FAD	P-O3P	5.52	1.65	1.59
2	B	7002	FAD	PA-O3P	5.50	1.65	1.59
3	D	8005	MES	C8-S	-5.42	1.70	1.77
3	F	8001	MES	C8-S	-5.23	1.70	1.77
2	D	7003	FAD	PA-O3P	3.93	1.63	1.59
2	C	7004	FAD	PA-O3P	3.88	1.63	1.59
2	D	7003	FAD	O4B-C4B	-3.75	1.36	1.45
2	C	7004	FAD	O4B-C4B	-3.42	1.37	1.45
2	F	7006	FAD	PA-O3P	3.32	1.63	1.59
2	B	7002	FAD	C8A-N9A	-3.21	1.32	1.37
2	G	7008	FAD	PA-O3P	3.17	1.62	1.59
2	A	7001	FAD	C10-N1	3.12	1.39	1.33
2	A	7001	FAD	C2B-C3B	-3.08	1.45	1.53
2	F	7006	FAD	C2-N3	-3.07	1.32	1.39
2	E	7005	FAD	C8A-N9A	-3.03	1.32	1.37
2	F	7006	FAD	C4X-N5	3.03	1.37	1.30
2	G	7008	FAD	C8A-N9A	-2.95	1.32	1.37
2	D	7003	FAD	P-O3P	2.95	1.62	1.59
2	E	7005	FAD	O4B-C4B	-2.90	1.38	1.45
2	A	7001	FAD	C4X-N5	2.89	1.37	1.30
2	E	7005	FAD	O3B-C3B	-2.89	1.35	1.43
2	F	7006	FAD	O4B-C4B	-2.85	1.38	1.45
2	C	7004	FAD	O3B-C3B	-2.83	1.35	1.43
2	E	7005	FAD	C5X-N5	-2.83	1.34	1.39
2	C	7004	FAD	C4X-N5	2.81	1.36	1.30
2	C	7004	FAD	C10-N1	2.76	1.38	1.33
2	C	7004	FAD	C2B-C3B	-2.71	1.46	1.53
2	H	7007	FAD	C5A-N7A	-2.66	1.34	1.39
2	H	7007	FAD	O3B-C3B	-2.65	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7002	FAD	C8A-N7A	2.65	1.36	1.31
2	G	7008	FAD	C5'-C4'	2.57	1.55	1.51
2	C	7004	FAD	C5X-N5	-2.57	1.34	1.39
2	D	7003	FAD	C10-N1	2.54	1.38	1.33
2	E	7005	FAD	C2B-C3B	-2.50	1.46	1.53
2	H	7007	FAD	C10-N1	2.44	1.38	1.33
2	H	7007	FAD	C5X-N5	-2.42	1.35	1.39
2	A	7001	FAD	P-O3P	2.41	1.62	1.59
2	H	7007	FAD	C8A-N9A	-2.40	1.33	1.37
2	F	7006	FAD	C10-N1	2.40	1.38	1.33
2	C	7004	FAD	C2A-N1A	2.37	1.38	1.33
2	F	7006	FAD	C8A-N9A	-2.36	1.33	1.37
2	C	7004	FAD	C6-C5X	2.34	1.43	1.40
2	C	7004	FAD	C8A-N9A	-2.33	1.33	1.37
2	F	7006	FAD	C2B-C3B	-2.32	1.47	1.53
2	F	7006	FAD	O3B-C3B	-2.31	1.37	1.43
2	D	7003	FAD	C2B-C3B	-2.29	1.47	1.53
2	G	7008	FAD	C8A-N7A	2.27	1.36	1.31
2	C	7004	FAD	C2-N3	-2.26	1.34	1.39
2	D	7003	FAD	C9-C8	2.25	1.42	1.39
2	G	7008	FAD	P-O1P	-2.25	1.43	1.50
2	B	7002	FAD	C5A-N7A	-2.24	1.35	1.39
2	G	7008	FAD	C4X-N5	2.24	1.35	1.30
2	E	7005	FAD	C6-C5X	2.22	1.43	1.40
2	G	7008	FAD	C2'-C3'	2.18	1.57	1.53
2	H	7007	FAD	O4-C4	2.17	1.27	1.23
2	F	7006	FAD	C5X-N5	-2.16	1.35	1.39
2	D	7003	FAD	C4X-C10	-2.14	1.37	1.44
2	G	7008	FAD	P-O3P	2.14	1.61	1.59
2	D	7003	FAD	O3B-C3B	-2.13	1.37	1.43
2	G	7008	FAD	O4B-C4B	-2.13	1.40	1.45
2	H	7007	FAD	C2B-C3B	-2.11	1.47	1.53
2	H	7007	FAD	C9-C8	2.10	1.42	1.39
2	B	7002	FAD	C5X-N5	-2.09	1.35	1.39
2	A	7001	FAD	C5'-C4'	2.07	1.54	1.51
2	B	7002	FAD	C4-N3	-2.07	1.35	1.38
2	D	7003	FAD	C2-N3	-2.05	1.34	1.39
2	B	7002	FAD	C2A-N1A	2.04	1.37	1.33
2	H	7007	FAD	C2A-N1A	2.04	1.37	1.33
2	E	7005	FAD	C10-N1	2.01	1.37	1.33
2	G	7008	FAD	C2A-N1A	2.01	1.37	1.33

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8005	MES	O2S-S-C8	-17.48	80.31	106.73
3	G	8006	MES	O2S-S-C8	-14.59	84.68	106.73
3	C	8008	MES	O3S-S-C8	-11.36	83.79	106.00
3	B	8003	MES	O1S-S-C8	-10.44	90.95	106.73
3	E	8007	MES	C6-C5-N4	-10.22	94.59	110.12
3	E	8007	MES	O1S-S-C8	-10.15	91.40	106.73
3	E	8007	MES	O3S-S-C8	-9.70	87.02	106.00
3	A	8002	MES	O1S-S-C8	-9.44	92.47	106.73
3	E	8007	MES	C7-N4-C3	7.93	132.38	111.24
2	G	7008	FAD	C4A-N9A-C8A	7.88	114.01	105.74
2	H	7007	FAD	N3A-C2A-N1A	-7.86	116.69	128.58
3	F	8001	MES	O3S-S-C8	-7.56	91.22	106.00
2	D	7003	FAD	C4A-N9A-C8A	7.47	113.58	105.74
2	B	7002	FAD	C4A-N9A-C8A	7.39	113.50	105.74
3	H	8004	MES	O2S-S-C8	-7.31	95.68	106.73
3	C	8008	MES	C5-N4-C3	7.17	124.28	108.84
3	C	8008	MES	O1S-S-C8	-7.10	96.00	106.73
2	F	7006	FAD	C4A-N9A-C8A	7.04	113.12	105.74
2	A	7001	FAD	N3A-C2A-N1A	-7.02	117.95	128.58
3	G	8006	MES	C5-N4-C3	6.84	123.57	108.84
2	G	7008	FAD	N9A-C8A-N7A	-6.80	104.29	113.94
2	E	7005	FAD	C4A-N9A-C8A	6.68	112.75	105.74
2	G	7008	FAD	N3A-C2A-N1A	-6.46	118.80	128.58
3	D	8005	MES	C5-N4-C3	6.35	122.52	108.84
2	B	7002	FAD	C4-C4X-N5	6.32	126.93	118.21
3	B	8003	MES	C5-N4-C3	6.27	122.34	108.84
3	B	8003	MES	O2S-S-C8	-6.24	97.30	106.73
3	F	8001	MES	O1S-S-C8	-6.15	97.44	106.73
3	A	8002	MES	C5-N4-C3	6.08	121.94	108.84
2	E	7005	FAD	N3A-C2A-N1A	-6.08	119.38	128.58
3	H	8004	MES	C5-N4-C3	6.06	121.89	108.84
2	C	7004	FAD	C4A-N9A-C8A	6.00	112.04	105.74
2	D	7003	FAD	N9A-C8A-N7A	-5.95	105.50	113.94
2	B	7002	FAD	N9A-C8A-N7A	-5.91	105.56	113.94
2	B	7002	FAD	N3A-C2A-N1A	-5.70	119.95	128.58
3	F	8001	MES	C5-N4-C3	5.70	121.11	108.84
2	D	7003	FAD	O4B-C1B-N9A	5.69	119.02	108.09
2	A	7001	FAD	N9A-C8A-N7A	-5.55	106.06	113.94
2	C	7004	FAD	O4B-C1B-N9A	5.45	118.56	108.09
2	F	7006	FAD	N9A-C8A-N7A	-5.30	106.42	113.94
3	D	8005	MES	O3S-S-O2S	5.19	124.37	111.40
2	F	7006	FAD	O4B-C1B-N9A	5.08	117.84	108.09
3	E	8007	MES	O1-C6-C5	-5.07	100.85	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7005	FAD	N9A-C8A-N7A	-5.07	106.74	113.94
2	H	7007	FAD	C2A-N1A-C6A	5.00	126.95	118.73
3	C	8008	MES	O1-C2-C3	-4.92	101.18	111.77
3	F	8001	MES	C7-N4-C3	4.88	124.24	111.24
3	D	8005	MES	O3S-S-C8	-4.80	96.61	106.00
3	H	8004	MES	O1S-S-C8	-4.76	99.53	106.73
2	G	7008	FAD	O3B-C3B-C4B	4.76	124.75	111.08
3	G	8006	MES	O3S-S-C8	-4.71	96.78	106.00
2	H	7007	FAD	C4A-N9A-C8A	4.66	110.63	105.74
2	D	7003	FAD	O3B-C3B-C4B	4.62	124.36	111.08
2	C	7004	FAD	C2B-C1B-N9A	4.53	124.56	113.30
2	A	7001	FAD	C5A-N7A-C8A	4.51	110.54	103.45
3	G	8006	MES	O3S-S-O2S	4.51	122.68	111.40
3	A	8002	MES	C7-N4-C5	4.48	123.17	111.24
2	E	7005	FAD	C2B-C1B-N9A	4.48	124.42	113.30
2	H	7007	FAD	N9A-C8A-N7A	-4.44	107.64	113.94
3	E	8007	MES	O3S-S-O1S	4.42	122.46	111.40
2	F	7006	FAD	C2B-C1B-N9A	4.39	124.22	113.30
3	D	8005	MES	C7-N4-C3	4.39	122.94	111.24
3	B	8003	MES	C7-N4-C3	4.39	122.93	111.24
2	B	7002	FAD	C2A-N1A-C6A	4.34	125.87	118.73
2	A	7001	FAD	C4A-N9A-C8A	4.30	110.25	105.74
3	E	8007	MES	C2-C3-N4	-4.25	103.66	110.12
3	A	8002	MES	O2S-S-C8	-4.23	100.34	106.73
2	D	7003	FAD	O4-C4-C4X	-4.20	115.45	126.53
2	H	7007	FAD	O2B-C2B-C3B	4.19	125.25	111.82
2	H	7007	FAD	C2B-C1B-N9A	4.17	123.67	113.30
2	D	7003	FAD	N3A-C2A-N1A	-4.15	122.30	128.58
2	C	7004	FAD	N9A-C8A-N7A	-4.12	108.09	113.94
2	F	7006	FAD	O2B-C2B-C1B	4.10	124.22	110.10
2	D	7003	FAD	N3A-C4A-N9A	4.08	134.10	127.17
3	C	8008	MES	O2S-S-C8	-4.04	100.63	106.73
2	G	7008	FAD	C5A-N7A-C8A	4.01	109.75	103.45
3	G	8006	MES	C7-N4-C3	3.98	121.85	111.24
2	A	7001	FAD	C2A-N1A-C6A	3.98	125.27	118.73
2	B	7002	FAD	O3B-C3B-C4B	3.96	122.46	111.08
3	E	8007	MES	O2S-S-C8	-3.96	100.75	106.73
2	C	7004	FAD	O2B-C2B-C3B	3.95	124.47	111.82
3	C	8008	MES	C7-N4-C5	3.92	121.69	111.24
3	C	8008	MES	O3S-S-O1S	3.88	121.09	111.40
2	D	7003	FAD	C5A-N7A-C8A	3.87	109.53	103.45
2	D	7003	FAD	O2B-C2B-C1B	3.86	123.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7003	FAD	C4-N3-C2	-3.85	118.80	125.64
2	E	7005	FAD	O4B-C1B-N9A	3.83	115.45	108.09
2	F	7006	FAD	N3A-C2A-N1A	-3.83	122.78	128.58
3	B	8003	MES	O1-C6-C5	-3.83	103.52	111.77
2	D	7003	FAD	C4-C4X-N5	3.79	123.45	118.21
2	B	7002	FAD	C5A-N7A-C8A	3.77	109.38	103.45
2	F	7006	FAD	C5A-N7A-C8A	3.74	109.33	103.45
2	F	7006	FAD	O2A-PA-O3P	3.74	117.39	107.27
2	C	7004	FAD	O2B-C2B-C1B	3.74	122.98	110.10
2	E	7005	FAD	C2A-N1A-C6A	3.68	124.77	118.73
3	D	8005	MES	O1-C6-C5	-3.67	103.86	111.77
2	G	7008	FAD	O4'-C4'-C3'	3.65	117.79	109.25
2	C	7004	FAD	N3A-C4A-N9A	3.65	133.37	127.17
2	F	7006	FAD	O3B-C3B-C4B	3.61	121.45	111.08
2	C	7004	FAD	N3A-C2A-N1A	-3.60	123.13	128.58
2	H	7007	FAD	O3B-C3B-C4B	3.60	121.41	111.08
3	H	8004	MES	O3S-S-O1S	3.60	120.39	111.40
2	B	7002	FAD	O4-C4-C4X	-3.55	117.16	126.53
2	B	7002	FAD	C2B-C1B-N9A	3.53	122.07	113.30
2	C	7004	FAD	O2A-PA-O1A	3.52	128.81	112.44
3	B	8003	MES	O3S-S-O2S	3.49	120.12	111.40
2	E	7005	FAD	O4B-C4B-C5B	3.43	120.31	109.33
2	G	7008	FAD	C2A-N1A-C6A	3.43	124.36	118.73
3	C	8008	MES	O3S-S-O2S	3.42	119.95	111.40
2	D	7003	FAD	O2B-C2B-C3B	3.42	122.77	111.82
2	G	7008	FAD	C5'-C4'-C3'	-3.39	105.82	112.22
2	D	7003	FAD	C2B-C1B-N9A	3.37	121.68	113.30
3	D	8005	MES	O1S-S-C8	-3.32	101.71	106.73
2	D	7003	FAD	O2-C2-N1	-3.32	116.29	121.80
2	A	7001	FAD	C2B-C1B-N9A	3.32	121.55	113.30
2	G	7008	FAD	N3A-C4A-N9A	3.32	132.81	127.17
2	F	7006	FAD	O2B-C2B-C3B	3.29	122.37	111.82
2	E	7005	FAD	O3B-C3B-C4B	3.29	120.53	111.08
2	B	7002	FAD	O2B-C2B-C1B	3.27	121.36	110.10
2	E	7005	FAD	C5A-N7A-C8A	3.26	108.57	103.45
2	E	7005	FAD	O2B-C2B-C3B	3.25	122.24	111.82
2	A	7001	FAD	O3B-C3B-C4B	3.25	120.42	111.08
2	A	7001	FAD	O2B-C2B-C3B	3.25	122.23	111.82
2	C	7004	FAD	C4-C4X-N5	3.24	122.68	118.21
2	B	7002	FAD	C10-C4X-N5	-3.23	118.21	124.81
2	F	7006	FAD	C1B-N9A-C8A	-3.22	119.95	127.09
3	H	8004	MES	C7-N4-C5	3.21	119.80	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7007	FAD	C1B-N9A-C8A	-3.21	119.97	127.09
2	G	7008	FAD	C1B-N9A-C8A	-3.20	119.99	127.09
2	A	7001	FAD	C4A-C5A-N7A	-3.19	106.93	110.58
2	H	7007	FAD	O4B-C1B-N9A	3.18	114.19	108.09
3	G	8006	MES	O1-C6-C5	-3.17	104.94	111.77
2	D	7003	FAD	O4B-C4B-C3B	3.17	111.44	105.15
2	H	7007	FAD	O2'-C2'-C3'	3.14	116.59	109.25
3	A	8002	MES	O3S-S-O2S	3.12	119.22	111.40
3	A	8002	MES	O3S-S-C8	-3.12	99.90	106.00
2	G	7008	FAD	O2B-C2B-C3B	3.10	121.76	111.82
2	H	7007	FAD	C5B-C4B-C3B	3.08	126.31	115.21
2	A	7001	FAD	C2A-N3A-C4A	3.06	119.31	111.83
2	C	7004	FAD	O4-C4-N3	-3.06	114.36	120.11
2	F	7006	FAD	O4-C4-N3	3.02	125.80	120.11
2	G	7008	FAD	C2B-C1B-N9A	3.02	120.81	113.30
2	H	7007	FAD	C9A-C5X-N5	-3.01	119.26	122.45
2	C	7004	FAD	C1B-N9A-C8A	-2.99	120.45	127.09
2	C	7004	FAD	C5A-C4A-N3A	-2.99	122.60	126.72
2	H	7007	FAD	O2B-C2B-C1B	2.99	120.39	110.10
2	H	7007	FAD	C4-N3-C2	-2.98	120.34	125.64
3	F	8001	MES	O3S-S-O2S	2.98	118.86	111.40
2	H	7007	FAD	C5A-N7A-C8A	2.98	108.13	103.45
2	H	7007	FAD	O2-C2-N1	-2.98	116.85	121.80
3	F	8001	MES	O3S-S-O1S	2.96	118.80	111.40
2	E	7005	FAD	N3A-C4A-N9A	2.96	132.20	127.17
2	H	7007	FAD	N6A-C6A-N1A	2.95	124.95	118.38
2	D	7003	FAD	O2A-PA-O3P	2.95	115.24	107.27
2	B	7002	FAD	N3A-C4A-N9A	2.95	132.18	127.17
2	B	7002	FAD	O4B-C4B-C3B	2.94	110.98	105.15
2	C	7004	FAD	O5'-P-O1P	-2.93	97.32	108.94
2	F	7006	FAD	O3P-PA-O1A	-2.93	101.89	110.70
3	F	8001	MES	C2-C3-N4	2.92	114.56	110.12
2	C	7004	FAD	O3P-PA-O1A	-2.92	101.92	110.70
2	F	7006	FAD	C2A-N1A-C6A	2.91	123.52	118.73
2	D	7003	FAD	C4X-C4-N3	2.90	120.63	113.25
2	C	7004	FAD	C10-C4X-N5	-2.90	118.90	124.81
2	F	7006	FAD	C5A-C4A-N9A	-2.87	102.68	105.81
2	F	7006	FAD	O3B-C3B-C2B	2.87	121.01	111.82
2	D	7003	FAD	O4B-C1B-C2B	2.86	112.73	106.62
2	B	7002	FAD	C5A-C4A-N9A	-2.85	102.70	105.81
2	B	7002	FAD	O2B-C2B-C3B	2.85	120.94	111.82
2	D	7003	FAD	C5A-C4A-N9A	-2.84	102.72	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7008	FAD	C4-C4X-N5	2.83	122.12	118.21
2	E	7005	FAD	O2-C2-N1	-2.82	117.11	121.80
2	C	7004	FAD	O3B-C3B-C4B	2.81	119.15	111.08
2	F	7006	FAD	C4'-C3'-C2'	-2.79	108.93	113.57
2	E	7005	FAD	C5A-C4A-N9A	-2.78	102.78	105.81
2	G	7008	FAD	O4-C4-C4X	-2.77	119.21	126.53
2	G	7008	FAD	O4B-C1B-N9A	2.77	113.42	108.09
2	F	7006	FAD	C4X-C10-N10	2.73	120.39	116.48
2	H	7007	FAD	O4B-C1B-C2B	2.71	112.42	106.62
2	C	7004	FAD	O4B-C4B-C5B	2.71	118.02	109.33
3	A	8002	MES	O3S-S-O1S	2.70	118.17	111.40
2	F	7006	FAD	O2A-PA-O1A	2.70	125.00	112.44
2	B	7002	FAD	C10-N1-C2	2.70	122.69	116.85
2	B	7002	FAD	O4B-C1B-N9A	2.70	113.27	108.09
2	C	7004	FAD	C6A-C5A-C4A	2.69	120.85	117.18
2	B	7002	FAD	C5'-C4'-C3'	-2.68	107.17	112.22
2	G	7008	FAD	C2A-N3A-C4A	2.67	118.35	111.83
2	D	7003	FAD	C5A-C4A-N3A	-2.66	123.06	126.72
3	H	8004	MES	C7-N4-C3	2.64	118.28	111.24
2	B	7002	FAD	C5X-N5-C4X	2.64	122.36	118.09
2	G	7008	FAD	C5B-C4B-C3B	2.63	124.67	115.21
2	F	7006	FAD	C5B-C4B-C3B	2.61	124.59	115.21
3	E	8007	MES	O2S-S-O1S	2.59	122.26	113.82
2	E	7005	FAD	O2B-C2B-C1B	2.58	118.99	110.10
2	B	7002	FAD	C1'-N10-C9A	2.58	125.64	120.63
2	C	7004	FAD	C7M-C7-C6	-2.58	115.03	119.57
2	B	7002	FAD	O4B-C4B-C5B	2.58	117.58	109.33
2	H	7007	FAD	N3A-C4A-N9A	2.57	131.53	127.17
2	H	7007	FAD	C5A-C4A-N9A	-2.56	103.03	105.81
2	A	7001	FAD	C1B-N9A-C8A	-2.55	121.44	127.09
2	H	7007	FAD	C2A-N3A-C4A	2.54	118.04	111.83
2	G	7008	FAD	O2P-P-O1P	2.54	124.25	112.44
2	H	7007	FAD	O4B-C4B-C3B	2.53	110.18	105.15
2	D	7003	FAD	O4B-C4B-C5B	2.50	117.34	109.33
2	E	7005	FAD	O4B-C4B-C3B	2.50	110.11	105.15
2	D	7003	FAD	C1B-N9A-C8A	-2.49	121.57	127.09
2	E	7005	FAD	C4'-C3'-C2'	-2.47	109.46	113.57
3	H	8004	MES	O2S-S-O1S	2.47	121.84	113.82
2	F	7006	FAD	O2'-C2'-C3'	2.46	115.00	109.25
2	G	7008	FAD	C10-N1-C2	2.46	122.17	116.85
2	D	7003	FAD	O5'-P-O1P	-2.45	99.22	108.94
2	B	7002	FAD	C9A-C5X-N5	-2.44	119.86	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7004	FAD	O4-C4-C4X	-2.43	120.13	126.53
2	C	7004	FAD	O4B-C1B-C2B	2.42	111.80	106.62
3	G	8006	MES	O1S-S-C8	-2.42	103.08	106.73
2	F	7006	FAD	O4B-C1B-C2B	2.42	111.79	106.62
2	F	7006	FAD	N3A-C4A-N9A	2.42	131.28	127.17
2	G	7008	FAD	O4-C4-N3	2.41	124.64	120.11
2	A	7001	FAD	O4B-C4B-C3B	2.39	109.89	105.15
3	E	8007	MES	C5-N4-C3	2.39	113.98	108.84
2	E	7005	FAD	C5B-C4B-C3B	2.37	123.74	115.21
2	G	7008	FAD	O2B-C2B-C1B	2.36	118.24	110.10
2	F	7006	FAD	C10-C4X-N5	-2.36	119.99	124.81
2	D	7003	FAD	O2A-PA-O1A	2.34	123.34	112.44
2	G	7008	FAD	O3P-PA-O1A	-2.34	103.67	110.70
3	G	8006	MES	O3S-S-O1S	2.33	117.24	111.40
2	E	7005	FAD	O4B-C1B-C2B	2.33	111.61	106.62
2	D	7003	FAD	C5B-C4B-C3B	2.32	123.55	115.21
3	E	8007	MES	C6-O1-C2	2.31	117.36	109.88
2	E	7005	FAD	C1B-N9A-C8A	-2.29	122.01	127.09
2	A	7001	FAD	O4'-C4'-C3'	2.28	114.58	109.25
2	C	7004	FAD	C2B-C3B-C4B	2.27	106.99	102.61
2	G	7008	FAD	C5A-C4A-N3A	-2.27	123.59	126.72
2	C	7004	FAD	C5A-N7A-C8A	2.25	106.99	103.45
2	G	7008	FAD	O2P-P-O3P	-2.25	101.18	107.27
2	A	7001	FAD	O2A-PA-O3P	2.23	113.31	107.27
2	D	7003	FAD	O3P-PA-O1A	-2.21	104.04	110.70
2	E	7005	FAD	O2A-PA-O1A	2.20	122.67	112.44
2	E	7005	FAD	C10-N1-C2	2.19	121.59	116.85
2	A	7001	FAD	C5'-C4'-C3'	-2.18	108.10	112.22
2	A	7001	FAD	O4B-C1B-N9A	2.17	112.25	108.09
2	E	7005	FAD	C5'-C4'-C3'	-2.16	108.14	112.22
2	G	7008	FAD	C4X-C10-N10	2.15	119.56	116.48
2	B	7002	FAD	N6A-C6A-N1A	2.15	123.16	118.38
2	C	7004	FAD	C5B-C4B-C3B	2.13	122.87	115.21
2	C	7004	FAD	O2-C2-N3	2.12	122.65	118.58
2	E	7005	FAD	O2P-P-O1P	2.11	122.28	112.44
2	E	7005	FAD	C2A-N3A-C4A	2.11	116.99	111.83
2	G	7008	FAD	C4A-C5A-N7A	-2.11	108.17	110.58
2	C	7004	FAD	C4X-C10-N10	2.10	119.49	116.48
2	B	7002	FAD	C2A-N3A-C4A	2.10	116.96	111.83
2	G	7008	FAD	C4'-C3'-C2'	-2.09	110.10	113.57
2	A	7001	FAD	O2P-P-O3P	-2.09	101.63	107.27
2	G	7008	FAD	O4B-C4B-C5B	2.08	116.00	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7003	FAD	C4X-C10-N10	2.08	119.46	116.48
2	C	7004	FAD	C10-N1-C2	2.07	121.33	116.85
2	C	7004	FAD	O2P-P-O1P	2.07	122.06	112.44
2	A	7001	FAD	C3B-C2B-C1B	2.06	105.37	101.46
3	F	8001	MES	O1-C2-C3	-2.05	107.35	111.77
2	G	7008	FAD	C5A-C4A-N9A	-2.05	103.58	105.81
2	G	7008	FAD	O3'-C3'-C4'	2.04	113.56	108.93
2	C	7004	FAD	O2P-P-O3P	-2.03	101.78	107.27
2	A	7001	FAD	O2'-C2'-C3'	2.03	114.00	109.25
2	B	7002	FAD	O2P-P-O1P	2.03	121.89	112.44
2	A	7001	FAD	C4X-C10-N10	2.02	119.38	116.48
2	E	7005	FAD	O2P-P-O3P	-2.02	101.82	107.27

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	7003	FAD	PA-O3P-P-O5'
2	F	7006	FAD	PA-O3P-P-O5'
3	A	8002	MES	C8-C7-N4-C5
3	A	8002	MES	N4-C7-C8-S
3	B	8003	MES	C8-C7-N4-C3
3	B	8003	MES	N4-C7-C8-S
3	D	8005	MES	C8-C7-N4-C3
3	D	8005	MES	N4-C7-C8-S
3	C	8008	MES	C8-C7-N4-C5
3	C	8008	MES	N4-C7-C8-S
3	E	8007	MES	C8-C7-N4-C5
3	E	8007	MES	C7-C8-S-O1S
3	E	8007	MES	C7-C8-S-O2S
3	E	8007	MES	C7-C8-S-O3S
3	F	8001	MES	C8-C7-N4-C3
3	F	8001	MES	N4-C7-C8-S
3	H	8004	MES	C8-C7-N4-C5
3	H	8004	MES	C7-C8-S-O1S
3	H	8004	MES	C7-C8-S-O2S
3	H	8004	MES	C7-C8-S-O3S
3	G	8006	MES	C8-C7-N4-C3
3	G	8006	MES	N4-C7-C8-S
2	A	7001	FAD	PA-O3P-P-O5'
2	C	7004	FAD	PA-O3P-P-O5'
2	E	7005	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
2	G	7008	FAD	PA-O3P-P-O5'
3	E	8007	MES	N4-C7-C8-S
3	H	8004	MES	N4-C7-C8-S
2	C	7004	FAD	O4B-C4B-C5B-O5B
2	F	7006	FAD	O4B-C4B-C5B-O5B
2	C	7004	FAD	P-O3P-PA-O2A
2	E	7005	FAD	P-O3P-PA-O2A
2	F	7006	FAD	P-O3P-PA-O2A
2	H	7007	FAD	PA-O3P-P-O5'
2	E	7005	FAD	O4B-C4B-C5B-O5B
2	D	7003	FAD	P-O3P-PA-O2A
2	B	7002	FAD	O4B-C4B-C5B-O5B
2	H	7007	FAD	O4B-C4B-C5B-O5B

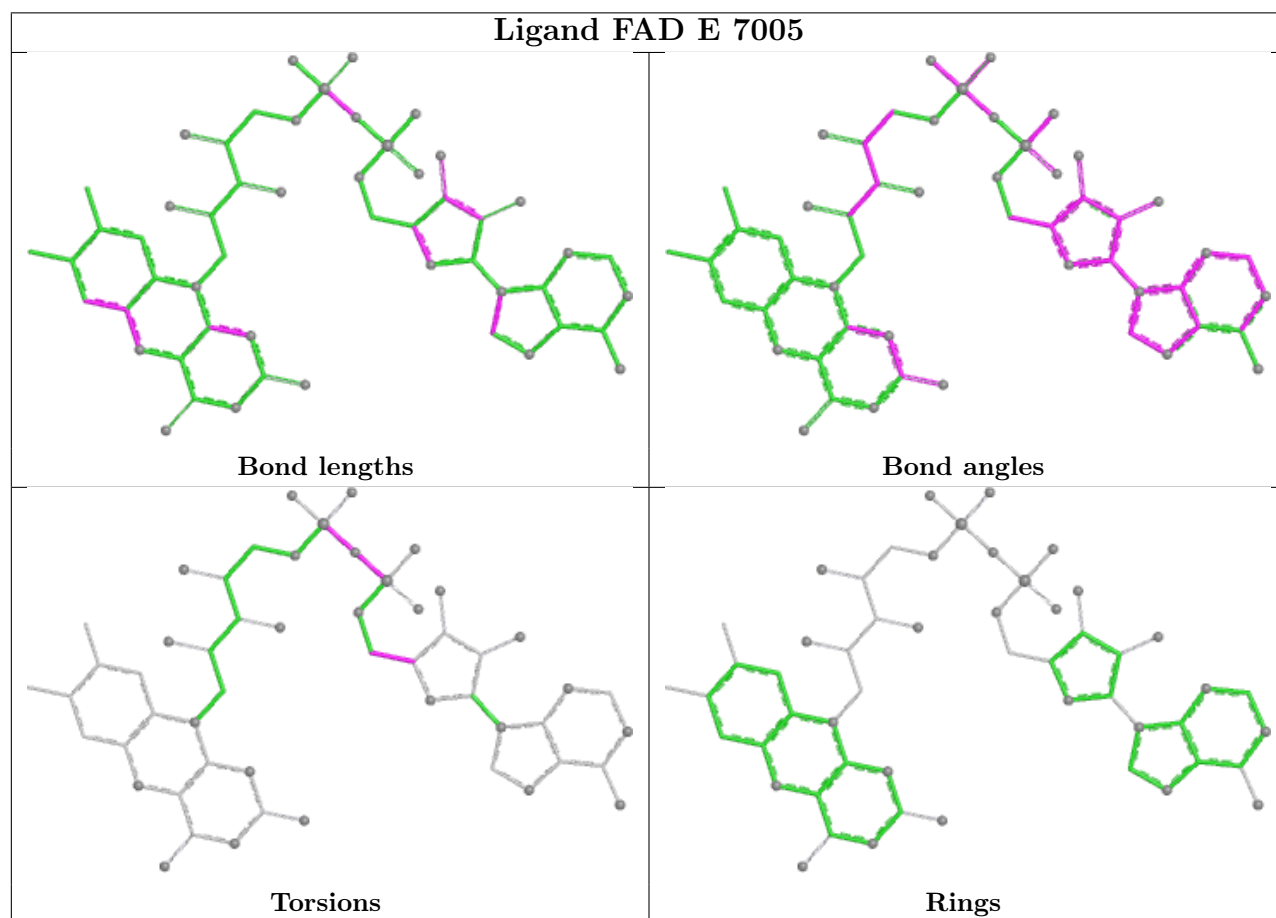
There are no ring outliers.

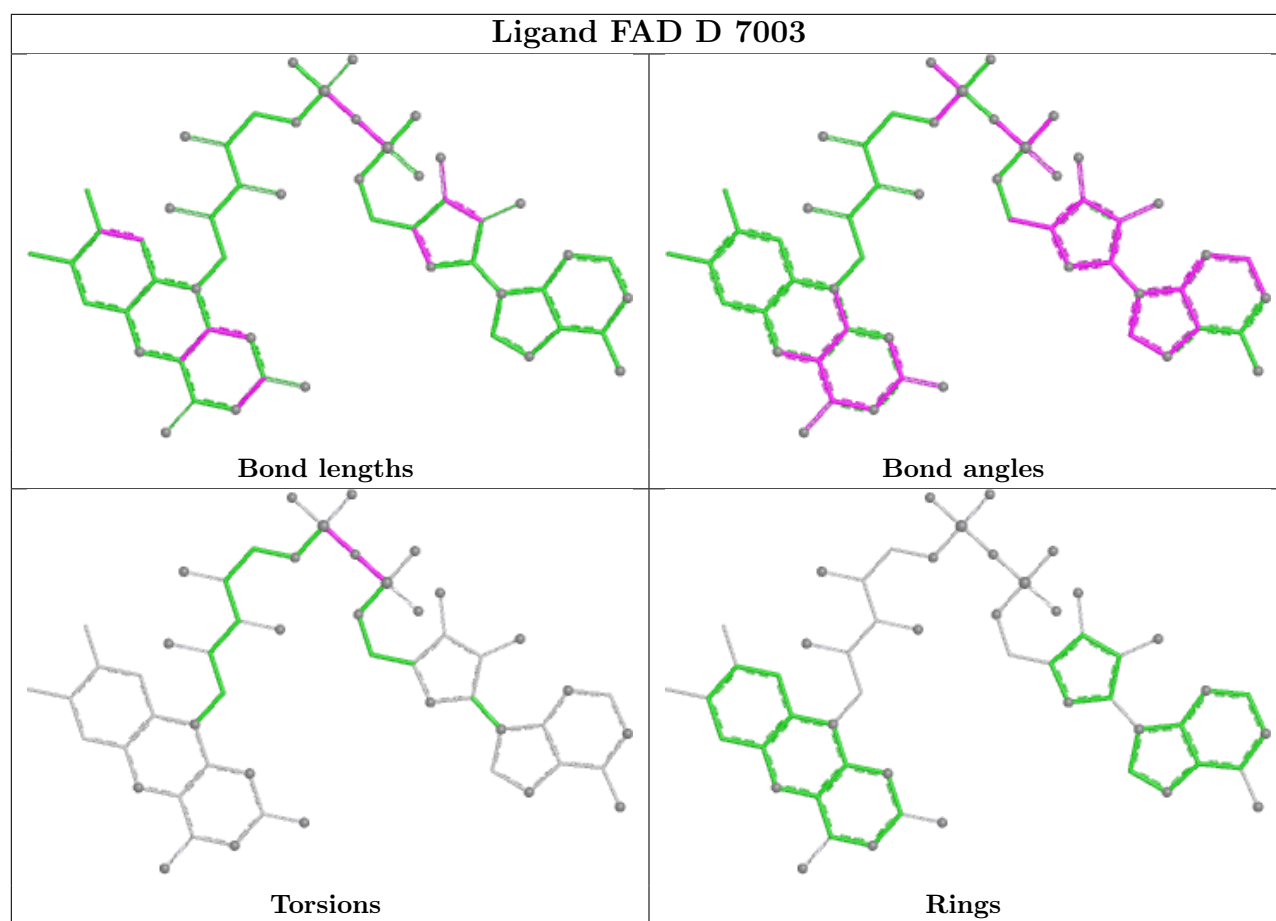
13 monomers are involved in 84 short contacts:

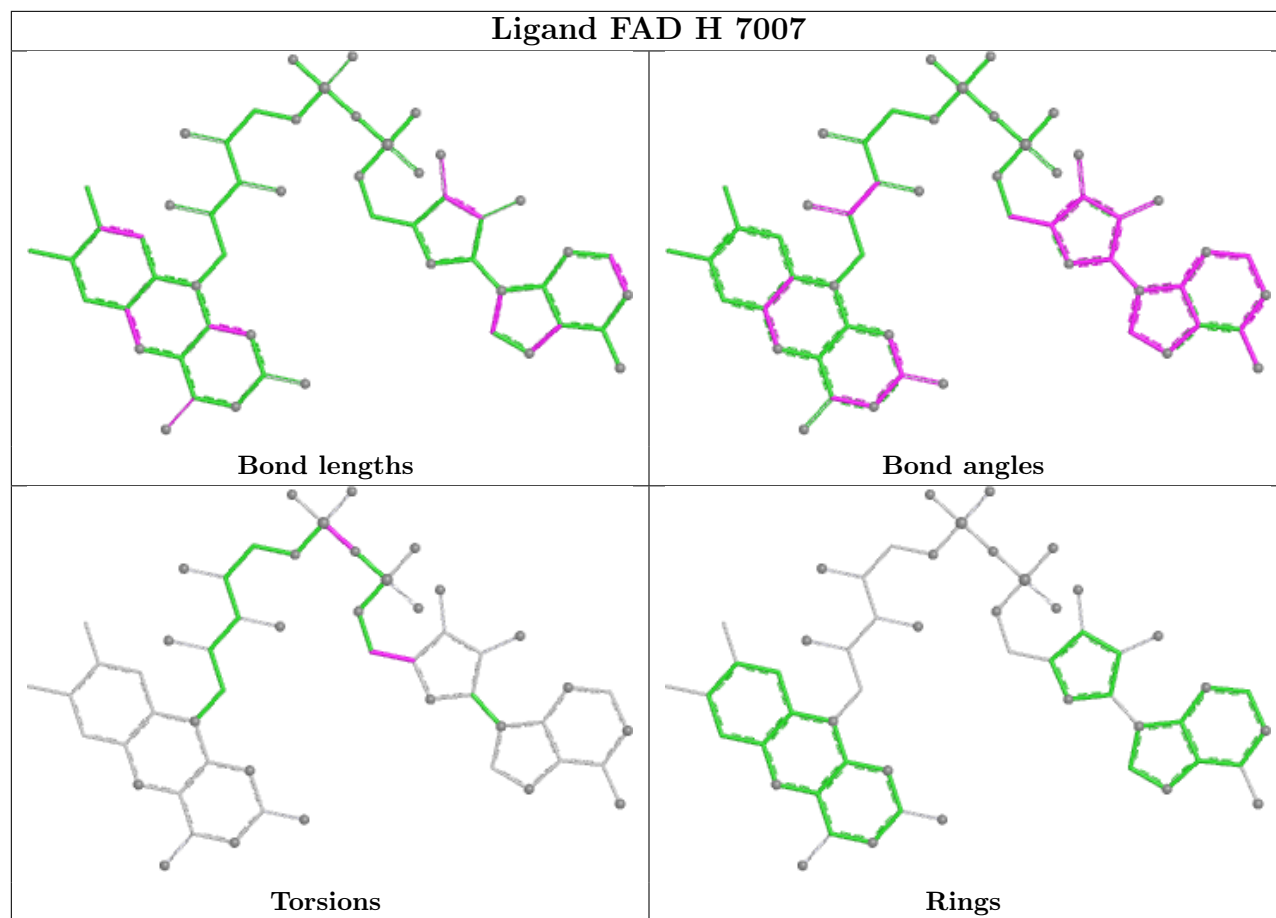
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	8003	MES	9	0
3	E	8007	MES	11	0
3	H	8004	MES	17	0
3	C	8008	MES	10	0
2	D	7003	FAD	1	0
3	D	8005	MES	14	0
3	G	8006	MES	9	0
2	F	7006	FAD	1	0
2	G	7008	FAD	1	0
2	C	7004	FAD	1	0
3	F	8001	MES	4	0
2	B	7002	FAD	2	0
3	A	8002	MES	4	0

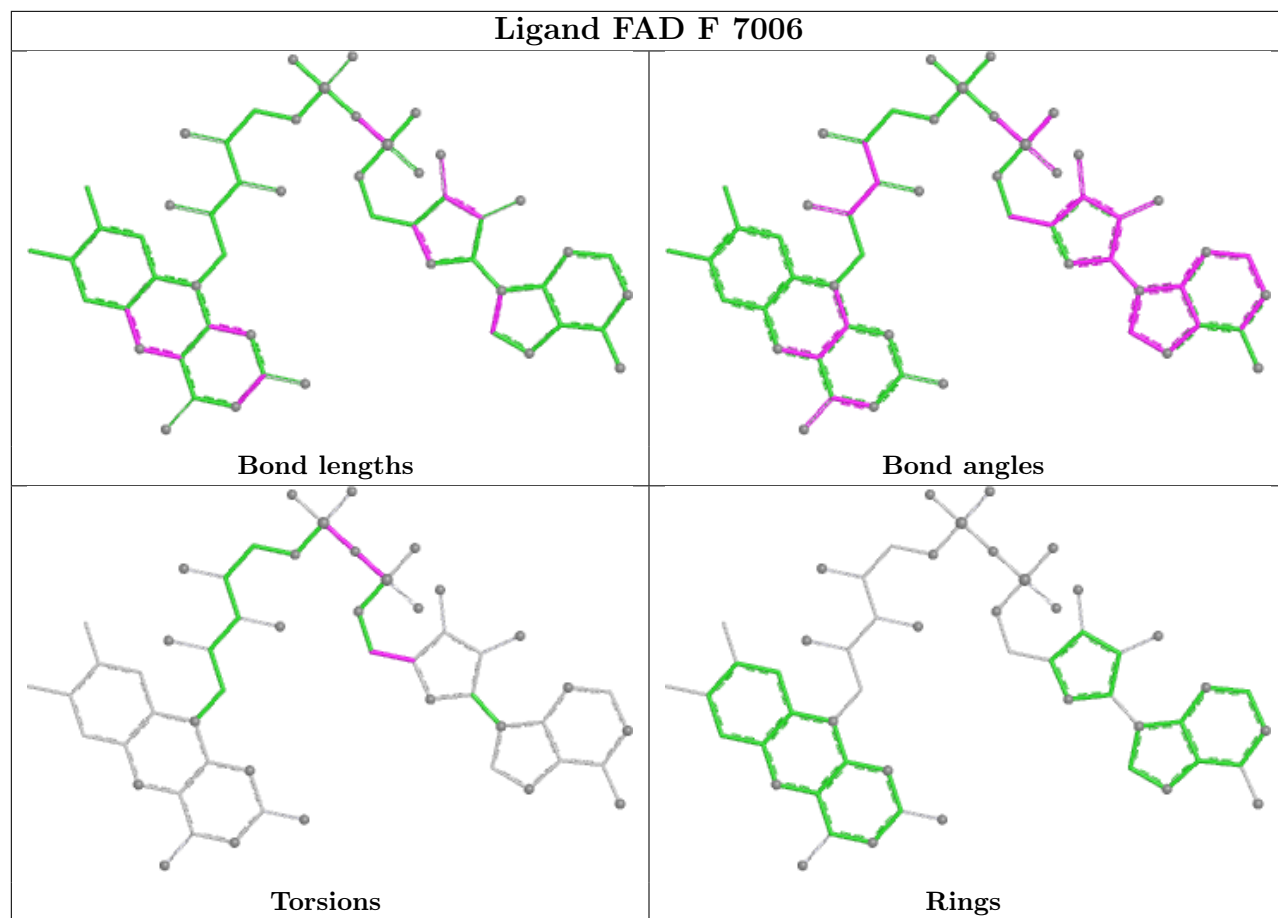
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

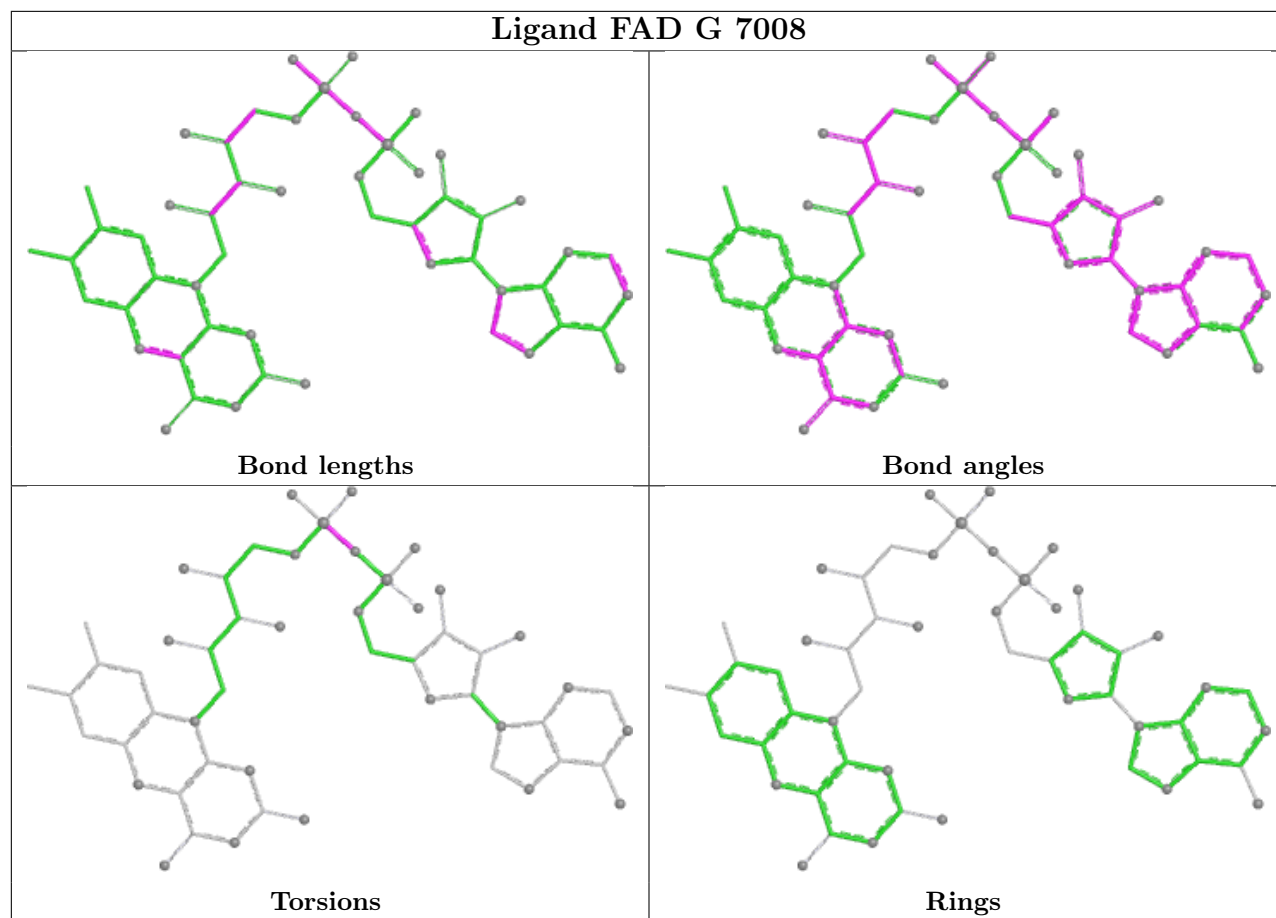
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

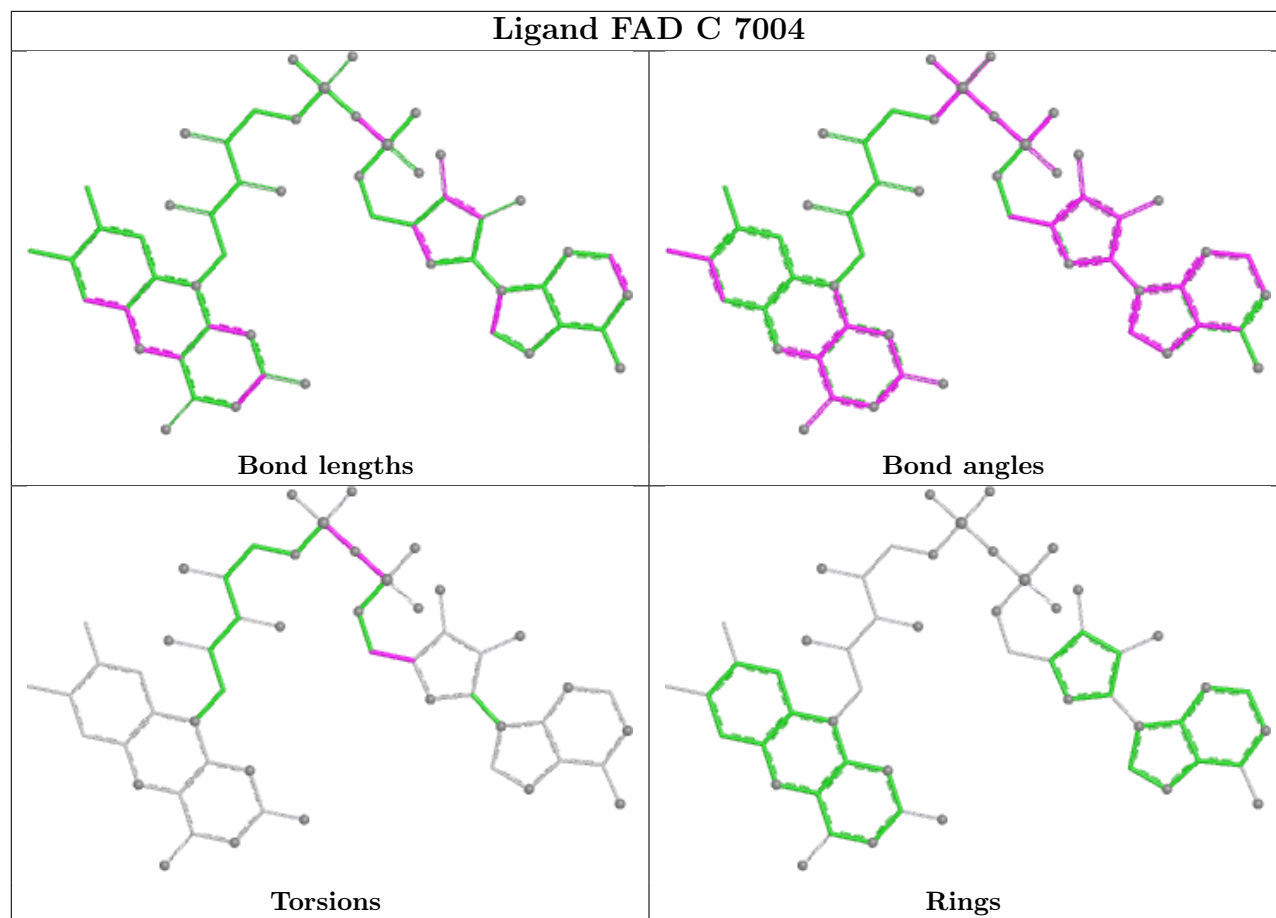


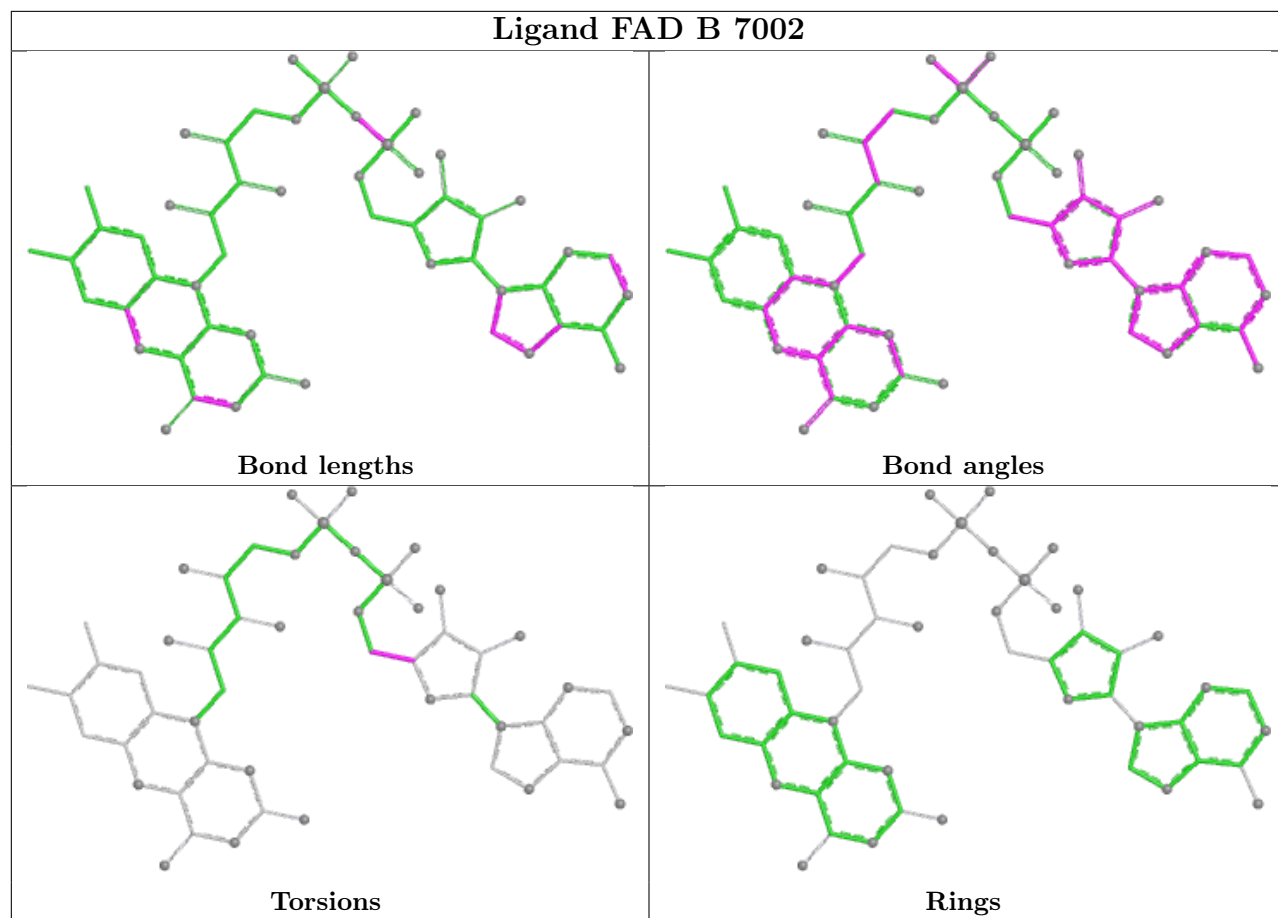


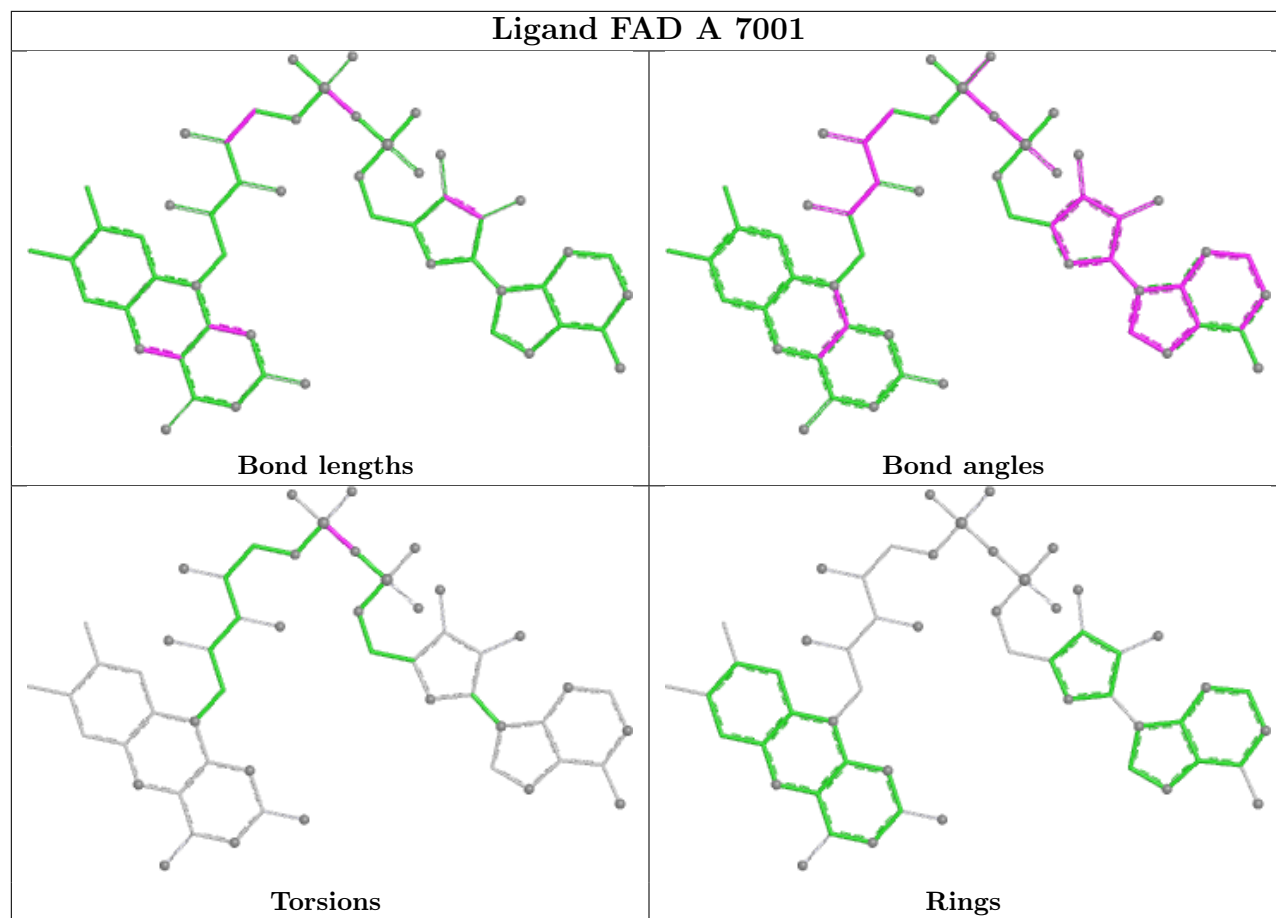












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	577/623 (92%)	-0.10	30 (5%)	33	36	8, 16, 37, 60	1 (0%)
1	B	577/623 (92%)	-0.11	22 (3%)	44	48	8, 17, 36, 54	2 (0%)
1	C	577/623 (92%)	0.35	29 (5%)	34	38	10, 23, 43, 64	2 (0%)
1	D	577/623 (92%)	0.10	28 (4%)	35	39	9, 21, 40, 59	2 (0%)
1	E	577/623 (92%)	0.17	33 (5%)	29	33	9, 21, 41, 58	2 (0%)
1	F	577/623 (92%)	0.22	20 (3%)	47	51	9, 23, 41, 61	1 (0%)
1	G	577/623 (92%)	0.00	22 (3%)	44	48	8, 18, 38, 57	3 (0%)
1	H	577/623 (92%)	-0.08	20 (3%)	47	51	8, 18, 35, 55	3 (0%)
All	All	4616/4984 (92%)	0.07	204 (4%)	39	42	8, 20, 40, 64	16 (0%)

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	619	THR	7.5
1	G	45	ILE	7.4
1	F	44	ASP	6.9
1	C	619	THR	6.1
1	C	45	ILE	6.1
1	E	619	THR	5.8
1	C	44	ASP	5.7
1	G	44	ASP	5.7
1	A	390	THR	5.4
1	F	619	THR	5.1
1	A	389	LEU	4.9
1	E	45	ILE	4.9
1	F	45	ILE	4.9
1	A	619	THR	4.8
1	B	44	ASP	4.6
1	B	618	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	619	THR	4.5
1	H	45	ILE	4.5
1	H	44	ASP	4.5
1	D	44	ASP	4.4
1	B	43	MET	4.4
1	E	618	PHE	4.4
1	H	459	VAL	4.4
1	H	43	MET	4.4
1	F	343	ALA	4.4
1	H	619	THR	4.3
1	B	45	ILE	4.2
1	E	387	GLY	4.1
1	B	619	THR	4.1
1	E	385	THR	4.1
1	B	389	LEU	4.1
1	C	618	PHE	4.1
1	B	133	ALA	4.1
1	D	618	PHE	3.9
1	F	43	MET	3.8
1	D	389	LEU	3.8
1	G	82	SER	3.8
1	D	390	THR	3.7
1	E	44	ASP	3.7
1	G	43	MET	3.6
1	F	389	LEU	3.6
1	A	459	VAL	3.5
1	E	43	MET	3.5
1	H	133	ALA	3.5
1	C	389	LEU	3.5
1	G	618	PHE	3.4
1	G	399	ALA	3.4
1	A	43	MET	3.3
1	B	343	ALA	3.3
1	H	81	ASP	3.3
1	D	45	ILE	3.3
1	C	43	MET	3.3
1	E	386	PRO	3.2
1	E	389	LEU	3.2
1	H	618	PHE	3.2
1	A	399	ALA	3.2
1	H	343	ALA	3.2
1	A	400	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	44	ASP	3.1
1	B	309	PHE	3.1
1	D	385	THR	3.1
1	G	389	LEU	3.0
1	D	388	GLU	3.0
1	C	390	THR	3.0
1	A	393	VAL	3.0
1	G	458	ALA	3.0
1	A	401	THR	3.0
1	B	385	THR	3.0
1	E	390	THR	3.0
1	C	384	GLY	3.0
1	C	617	PRO	3.0
1	G	81	ASP	2.9
1	E	99	ASN	2.9
1	A	618	PHE	2.9
1	C	309	PHE	2.9
1	F	309	PHE	2.9
1	G	385	THR	2.9
1	E	382	ILE	2.9
1	A	386	PRO	2.9
1	E	384	GLY	2.9
1	E	398	GLY	2.9
1	F	618	PHE	2.8
1	E	393	VAL	2.8
1	E	459	VAL	2.8
1	A	397	PRO	2.8
1	B	99	ASN	2.8
1	H	99	ASN	2.8
1	G	397	PRO	2.8
1	A	45	ILE	2.8
1	C	342	PRO	2.8
1	C	383	ARG	2.8
1	A	343	ALA	2.7
1	C	99	ASN	2.7
1	A	382	ILE	2.7
1	A	99	ASN	2.7
1	C	133	ALA	2.7
1	A	391	TYR	2.7
1	D	43	MET	2.7
1	G	99	ASN	2.7
1	B	81	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	388	GLU	2.6
1	E	388	GLU	2.6
1	A	381	THR	2.6
1	A	81	ASP	2.6
1	E	490	LYS	2.6
1	A	387	GLY	2.6
1	A	394	THR	2.6
1	A	452	ASP	2.6
1	E	82	SER	2.6
1	H	342	PRO	2.6
1	D	81	ASP	2.5
1	C	490	LYS	2.5
1	E	391	TYR	2.5
1	D	272	GLU	2.5
1	H	458	ALA	2.5
1	C	81	ASP	2.5
1	F	384	GLY	2.5
1	E	299	HIS	2.5
1	G	388	GLU	2.5
1	E	345	PRO	2.5
1	G	459	VAL	2.5
1	H	455	SER	2.5
1	H	341	ASN	2.5
1	D	132[A]	GLN	2.5
1	G	250	PHE	2.5
1	F	342	PRO	2.5
1	A	398	GLY	2.5
1	E	81	ASP	2.4
1	E	250	PHE	2.4
1	E	343	ALA	2.4
1	A	344	ASN	2.4
1	D	387	GLY	2.4
1	C	387	GLY	2.4
1	B	82	SER	2.4
1	G	133	ALA	2.4
1	G	343	ALA	2.4
1	F	81	ASP	2.4
1	G	100	ILE	2.4
1	G	400	SER	2.3
1	E	342	PRO	2.3
1	E	458	ALA	2.3
1	F	390	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	250	PHE	2.3
1	C	47	TYR	2.3
1	G	401	THR	2.3
1	A	395	TYR	2.3
1	F	295	ILE	2.3
1	F	82	SER	2.3
1	D	393	VAL	2.3
1	C	459	VAL	2.3
1	F	383	ARG	2.3
1	D	452	ASP	2.3
1	F	310	GLU	2.3
1	A	341	ASN	2.3
1	C	312	LYS	2.3
1	D	345	PRO	2.2
1	D	617	PRO	2.2
1	A	385	THR	2.2
1	D	310	GLU	2.2
1	B	458	ALA	2.2
1	A	383	ARG	2.2
1	C	398	GLY	2.2
1	H	456	TYR	2.2
1	C	100	ILE	2.2
1	D	299	HIS	2.2
1	B	393	VAL	2.2
1	B	345	PRO	2.2
1	B	383	ARG	2.2
1	E	344	ASN	2.2
1	B	490	LYS	2.2
1	H	269	ASP	2.2
1	F	561	GLU	2.2
1	C	250	PHE	2.2
1	H	345	PRO	2.2
1	B	452	ASP	2.2
1	C	68	ALA	2.2
1	F	452	ASP	2.2
1	E	132[A]	GLN	2.2
1	B	178	GLU	2.2
1	D	398	GLY	2.2
1	C	344	ASN	2.2
1	D	309	PHE	2.1
1	D	342	PRO	2.1
1	E	617	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	617	PRO	2.1
1	G	228	GLU	2.1
1	D	458	ALA	2.1
1	C	612	ASN	2.1
1	H	452	ASP	2.1
1	H	309	PHE	2.1
1	D	133	ALA	2.1
1	C	458	ALA	2.1
1	B	459	VAL	2.1
1	H	344	ASN	2.1
1	D	391	TYR	2.1
1	A	133	ALA	2.0
1	E	133	ALA	2.0
1	E	417	MET	2.0
1	D	383	ARG	2.0
1	D	459	VAL	2.0
1	D	386	PRO	2.0
1	E	310	GLU	2.0
1	C	456	TYR	2.0
1	C	270	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	E	8007	12/12	0.86	0.14	29,33,38,39	0
3	MES	C	8008	12/12	0.87	0.12	27,32,38,39	0
3	MES	B	8003	12/12	0.88	0.13	28,32,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	D	8005	12/12	0.88	0.13	30,32,34,36	0
3	MES	G	8006	12/12	0.88	0.13	24,30,33,33	0
3	MES	H	8004	12/12	0.90	0.12	27,33,34,35	0
3	MES	A	8002	12/12	0.94	0.10	22,26,28,28	0
3	MES	F	8001	12/12	0.95	0.08	20,22,24,25	0
2	FAD	D	7003	53/53	0.98	0.05	14,17,19,22	0
2	FAD	C	7004	53/53	0.98	0.05	15,18,22,22	0
2	FAD	E	7005	53/53	0.98	0.05	15,17,20,21	0
2	FAD	F	7006	53/53	0.98	0.05	14,17,20,22	0
2	FAD	H	7007	53/53	0.98	0.04	10,14,17,19	0
2	FAD	G	7008	53/53	0.98	0.04	11,14,15,17	0
2	FAD	B	7002	53/53	0.98	0.04	10,13,16,20	0
2	FAD	A	7001	53/53	0.99	0.04	10,12,14,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.