



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 04:31 am BST

PDB ID : 5N8P  
Title : S-layer protein RsaA from *C. crescentus*  
Authors : Bharat, T.A.M.; Kureisaite-Ciziene, D.; Lowe, J.  
Deposited on : 2017-02-24  
Resolution : 2.70 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](mailto: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>.

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

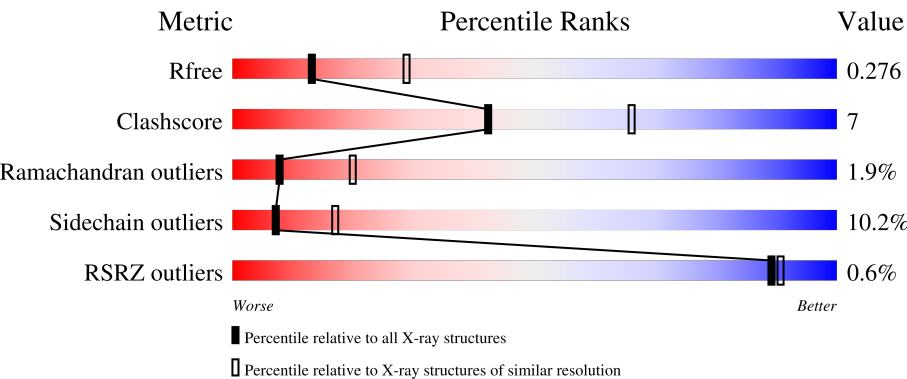
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 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 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	1026	<div><div></div><div>61%13%•24%</div></div>
1	B	1026	<div><div>%</div><div>60%13%•24%</div></div>
1	C	1026	<div><div>%</div><div>61%13%•24%</div></div>
1	D	1026	<div><div></div><div>61%13%•24%</div></div>
1	E	1026	<div><div></div><div>60%13%•24%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	1026	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 61%, a yellow segment representing 13%, and a grey segment representing 24%. A small black dot is located on the yellow segment.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31059 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 S-layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	B	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	C	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	D	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	E	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	F	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	Ca	0	0
			19	19		
2	B	19	Total	Ca	0	0
			19	19		
2	C	19	Total	Ca	0	0
			19	19		
2	D	19	Total	Ca	0	0
			19	19		
2	E	19	Total	Ca	0	0
			19	19		
2	F	19	Total	Ca	0	0
			19	19		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	29	Total 29	O 29	0	0
3	C	24	Total 24	O 24	0	0
3	D	32	Total 32	O 32	0	0
3	E	16	Total 16	O 16	0	0
3	F	27	Total 27	O 27	0	0

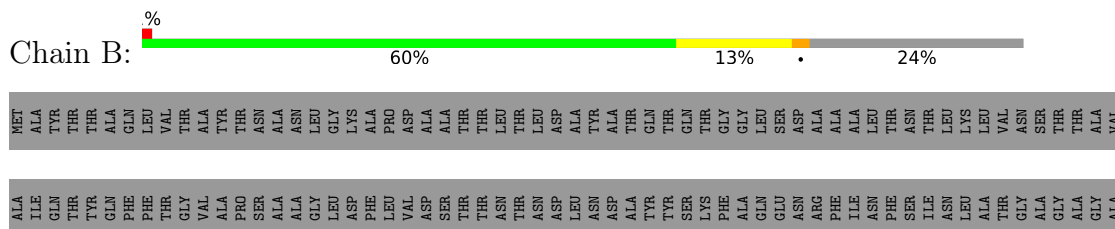
### 3 Residue-property plots

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: S-layer protein



#### • Molecule 1: S-layer protein

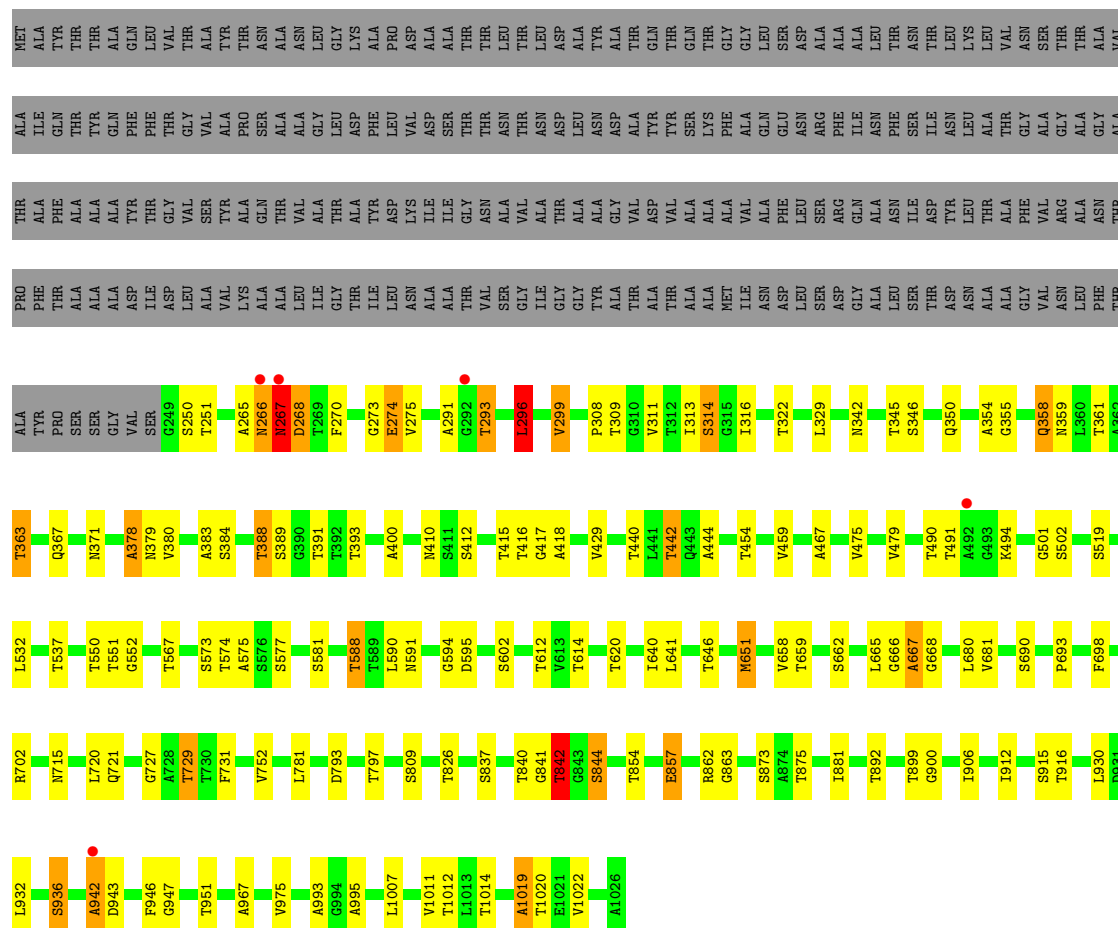






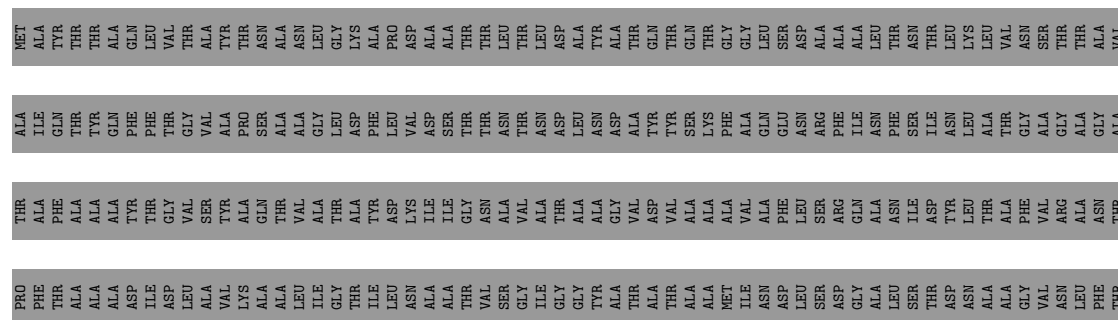
• Molecule 1: S-layer protein

Chain D: 61% 13% 24%

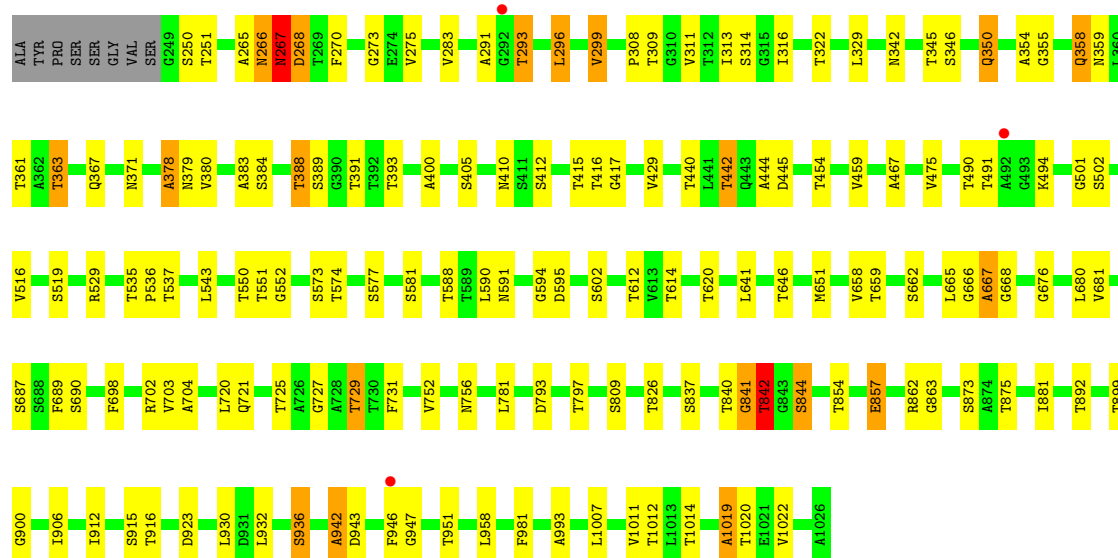


• Molecule 1: S-layer protein

Chain E: 60% 13% 24%

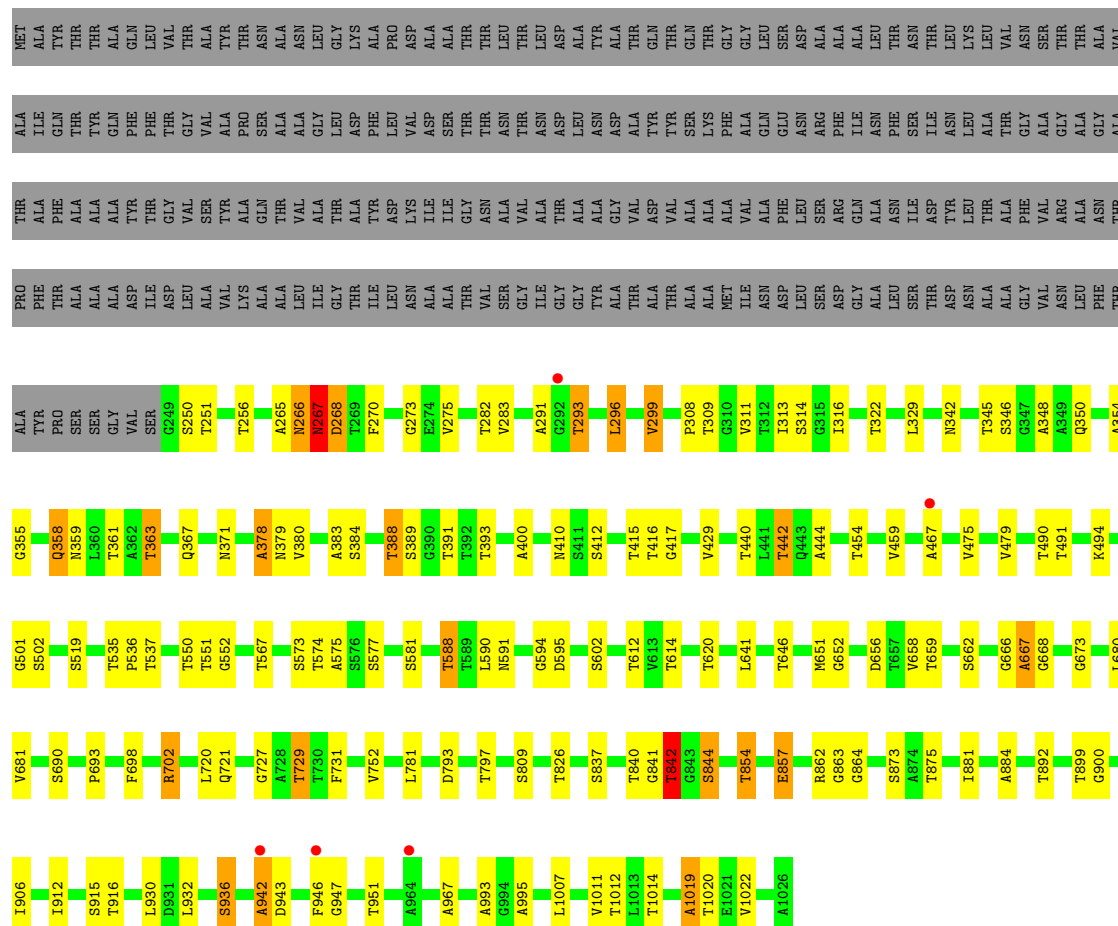






### • Molecule 1: S-layer protein

Chain F: 61% 13% 24%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.88Å 74.96Å 221.66Å 90.00° 118.99° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	69.6 (50.00-2.70) 69.7 (48.95-2.70)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.258 , 0.276 0.258 , 0.276	Depositor DCC
$R_{free}$ test set	6102 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 9.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h-l,k,h 0.028 for l,k,-h-l 0.028 for h,-k,-h-l 0.026 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	31059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 22.57 % 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 5.5499e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA

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	0.70	1/5166 (0.0%)	0.87	3/7112 (0.0%)
1	B	0.68	1/5166 (0.0%)	0.86	2/7112 (0.0%)
1	C	0.70	1/5166 (0.0%)	0.88	3/7112 (0.0%)
1	D	0.70	1/5166 (0.0%)	0.88	5/7112 (0.1%)
1	E	0.69	2/5166 (0.0%)	0.87	5/7112 (0.1%)
1	F	0.69	1/5166 (0.0%)	0.87	3/7112 (0.0%)
All	All	0.69	7/30996 (0.0%)	0.87	21/42672 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	842	THR	CA-CB	6.12	1.69	1.53
1	B	842	THR	CA-CB	5.77	1.68	1.53
1	A	842	THR	CA-CB	5.64	1.68	1.53
1	E	842	THR	CA-CB	5.52	1.67	1.53
1	C	842	THR	CA-CB	5.35	1.67	1.53
1	D	842	THR	CA-CB	5.30	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	841	GLY	N-CA	5.07	1.53	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	840	THR	N-CA-C	6.92	129.68	111.00
1	E	840	THR	N-CA-C	6.87	129.54	111.00
1	C	840	THR	N-CA-C	6.73	129.18	111.00
1	D	840	THR	N-CA-C	6.68	129.05	111.00
1	F	840	THR	N-CA-C	6.68	129.04	111.00
1	A	840	THR	N-CA-C	6.65	128.95	111.00
1	D	274	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	F	900	GLY	N-CA-C	-5.35	99.72	113.10
1	A	900	GLY	N-CA-C	-5.32	99.79	113.10
1	C	900	GLY	N-CA-C	-5.32	99.80	113.10
1	D	296	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	793	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	793	ASP	CB-CG-OD1	5.24	123.02	118.30
1	E	900	GLY	N-CA-C	-5.21	100.08	113.10
1	D	793	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	793	ASP	CB-CG-OD1	5.14	122.93	118.30
1	F	793	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	445	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	E	793	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	900	GLY	N-CA-C	-5.01	100.56	113.10
1	E	923	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	594	GLY	Peptide
1	B	594	GLY	Peptide
1	C	594	GLY	Peptide
1	D	594	GLY	Peptide
1	E	594	GLY	Peptide
1	F	594	GLY	Peptide

## 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	5133	0	5071	64	0
1	B	5133	0	5071	73	0
1	C	5133	0	5071	69	8
1	D	5133	0	5071	73	7
1	E	5133	0	5071	73	0
1	F	5133	0	5072	71	1
2	A	19	0	0	0	0
2	B	19	0	0	1	0
2	C	19	0	0	1	0
2	D	19	0	0	0	0
2	E	19	0	0	0	0
2	F	19	0	0	4	0
3	A	19	0	0	1	0
3	B	29	0	0	3	0
3	C	24	0	0	3	0
3	D	32	0	0	5	0
3	E	16	0	0	8	0
3	F	27	0	0	10	0
All	All	31059	0	30427	422	8

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 7.

All (422) 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)
2:C:9002:CA:CA	3:C:9103:HOH:O	1.22	1.11
2:F:9007:CA:CA	3:F:9103:HOH:O	1.30	1.07
1:D:265:ALA:HA	1:D:291:ALA:H	1.22	1.04
1:F:265:ALA:HA	1:F:291:ALA:H	1.22	1.02
1:E:265:ALA:HA	1:E:291:ALA:H	1.22	1.01
1:F:864:GLY:O	3:F:9102:HOH:O	1.78	1.00
1:A:265:ALA:HA	1:A:291:ALA:H	1.22	0.99
1:B:265:ALA:HA	1:B:291:ALA:H	1.21	0.98
1:C:265:ALA:HA	1:C:291:ALA:H	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:GLU:O	3:D:9101:HOH:O	1.82	0.98
2:F:9003:CA:CA	3:F:9101:HOH:O	1.41	0.95
1:F:282:THR:OG1	3:F:9101:HOH:O	1.67	0.90
2:F:9011:CA:CA	3:F:9102:HOH:O	1.51	0.87
1:F:656:ASP:OD2	3:F:9103:HOH:O	1.93	0.86
1:D:442:THR:HB	1:D:475:VAL:HB	1.60	0.83
1:C:442:THR:HB	1:C:475:VAL:HB	1.60	0.83
1:F:442:THR:HB	1:F:475:VAL:HB	1.60	0.82
1:B:442:THR:HB	1:B:475:VAL:HB	1.59	0.82
1:E:442:THR:HB	1:E:475:VAL:HB	1.60	0.81
1:A:442:THR:HB	1:A:475:VAL:HB	1.61	0.80
2:B:9002:CA:CA	3:B:9103:HOH:O	1.62	0.76
1:B:255:THR:O	3:B:9101:HOH:O	2.04	0.75
1:F:652:GLY:O	3:F:9103:HOH:O	2.06	0.73
1:B:342:ASN:HD22	1:B:361:THR:HB	1.54	0.72
1:D:342:ASN:HD22	1:D:361:THR:HB	1.55	0.71
1:F:342:ASN:HD22	1:F:361:THR:HB	1.55	0.71
1:F:884:ALA:O	3:F:9102:HOH:O	2.08	0.71
1:E:342:ASN:HD22	1:E:361:THR:HB	1.56	0.70
1:A:342:ASN:HD22	1:A:361:THR:HB	1.55	0.70
1:A:265:ALA:HA	1:A:291:ALA:N	2.04	0.70
1:E:725:THR:CG2	3:E:9101:HOH:O	2.38	0.70
1:B:265:ALA:HA	1:B:291:ALA:N	2.04	0.69
1:C:342:ASN:HD22	1:C:361:THR:HB	1.56	0.69
1:D:314:SER:HB3	3:D:9110:HOH:O	1.92	0.69
1:E:265:ALA:HA	1:E:291:ALA:N	2.04	0.68
1:D:947:GLY:O	1:D:1014:THR:HA	1.94	0.68
1:F:702:ARG:HB2	1:F:721:GLN:HB2	1.76	0.68
1:F:947:GLY:O	1:F:1014:THR:HA	1.94	0.67
1:A:947:GLY:O	1:A:1014:THR:HA	1.94	0.67
1:C:947:GLY:O	1:C:1014:THR:HA	1.94	0.67
1:C:265:ALA:HA	1:C:291:ALA:N	2.04	0.67
1:F:265:ALA:HA	1:F:291:ALA:N	2.04	0.67
1:E:947:GLY:O	1:E:1014:THR:HA	1.94	0.67
1:B:947:GLY:O	1:B:1014:THR:HA	1.94	0.67
1:A:702:ARG:HB2	1:A:721:GLN:HB2	1.75	0.66
1:E:702:ARG:HB2	1:E:721:GLN:HB2	1.77	0.66
1:B:702:ARG:HB2	1:B:721:GLN:HB2	1.77	0.66
1:D:702:ARG:HB2	1:D:721:GLN:HB2	1.77	0.66
1:D:265:ALA:HA	1:D:291:ALA:N	2.04	0.65
1:B:841:GLY:H	1:B:844:SER:HG	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ARG:HB2	1:C:721:GLN:HB2	1.77	0.65
1:C:586:ASP:OD2	3:C:9101:HOH:O	2.15	0.64
1:E:725:THR:HG23	3:E:9101:HOH:O	1.95	0.64
1:C:841:GLY:H	1:C:844:SER:HG	1.45	0.63
1:E:841:GLY:H	1:E:844:SER:HG	1.46	0.63
1:E:703:VAL:O	3:E:9101:HOH:O	2.16	0.62
1:D:842:THR:HG21	3:D:9102:HOH:O	1.99	0.62
1:D:842:THR:CG2	3:D:9102:HOH:O	2.47	0.61
1:E:704:ALA:HA	3:E:9101:HOH:O	2.00	0.61
1:D:265:ALA:CA	1:D:291:ALA:H	2.08	0.60
1:D:532:LEU:HD13	3:D:9105:HOH:O	2.01	0.60
1:A:841:GLY:N	1:A:844:SER:OG	2.33	0.60
1:B:841:GLY:N	1:B:844:SER:OG	2.33	0.59
1:D:841:GLY:N	1:D:844:SER:OG	2.33	0.59
1:E:265:ALA:CA	1:E:291:ALA:H	2.08	0.58
1:C:265:ALA:CA	1:C:291:ALA:H	2.08	0.58
2:F:9019:CA:CA	3:F:9107:HOH:O	1.78	0.58
1:D:416:THR:O	1:D:416:THR:HG22	2.04	0.58
1:E:410:ASN:OD1	1:E:412:SER:HB3	2.04	0.58
1:A:359:ASN:ND2	1:A:379:ASN:H	2.02	0.58
1:B:440:THR:OG1	1:B:467:ALA:HB2	2.04	0.57
1:F:501:GLY:HA2	1:F:519:SER:HB3	1.86	0.57
1:F:912:ILE:HD12	1:F:912:ILE:H	1.69	0.57
1:B:501:GLY:HA2	1:B:519:SER:HB3	1.86	0.57
1:C:410:ASN:OD1	1:C:412:SER:HB3	2.04	0.57
1:D:410:ASN:OD1	1:D:412:SER:HB3	2.05	0.57
1:A:265:ALA:CA	1:A:291:ALA:H	2.08	0.57
1:A:440:THR:OG1	1:A:467:ALA:HB2	2.04	0.57
1:A:416:THR:O	1:A:416:THR:HG22	2.05	0.57
1:B:416:THR:HG22	1:B:416:THR:O	2.04	0.57
1:E:416:THR:HG22	1:E:416:THR:O	2.05	0.57
1:C:841:GLY:N	1:C:844:SER:OG	2.33	0.57
1:A:410:ASN:OD1	1:A:412:SER:HB3	2.05	0.57
1:A:1019:ALA:HB3	1:A:1022:VAL:HB	1.87	0.57
1:B:410:ASN:OD1	1:B:412:SER:HB3	2.04	0.57
1:C:501:GLY:HA2	1:C:519:SER:HB3	1.87	0.57
1:E:359:ASN:ND2	1:E:379:ASN:H	2.02	0.57
1:F:410:ASN:OD1	1:F:412:SER:HB3	2.04	0.57
1:C:440:THR:OG1	1:C:467:ALA:HB2	2.05	0.57
1:C:799:HIS:HB3	3:C:9123:HOH:O	2.04	0.57
1:F:359:ASN:ND2	1:F:379:ASN:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:THR:OG1	1:F:467:ALA:HB2	2.05	0.57
1:D:313:ILE:HG23	1:D:316:ILE:HD12	1.86	0.56
1:D:359:ASN:ND2	1:D:379:ASN:H	2.03	0.56
1:C:359:ASN:ND2	1:C:379:ASN:H	2.03	0.56
1:D:912:ILE:HD12	1:D:912:ILE:H	1.70	0.56
1:E:1019:ALA:HB3	1:E:1022:VAL:HB	1.88	0.56
1:A:359:ASN:HD22	1:A:379:ASN:H	1.54	0.56
1:C:313:ILE:HG23	1:C:316:ILE:HD12	1.88	0.56
1:C:416:THR:HG22	1:C:416:THR:O	2.05	0.56
1:D:501:GLY:HA2	1:D:519:SER:HB3	1.88	0.56
1:A:501:GLY:HA2	1:A:519:SER:HB3	1.87	0.56
1:E:440:THR:OG1	1:E:467:ALA:HB2	2.05	0.56
1:F:1019:ALA:HB3	1:F:1022:VAL:HB	1.87	0.56
1:B:313:ILE:HG23	1:B:316:ILE:HD12	1.88	0.56
1:C:912:ILE:H	1:C:912:ILE:HD12	1.70	0.55
1:D:440:THR:OG1	1:D:467:ALA:HB2	2.06	0.55
1:B:359:ASN:ND2	1:B:379:ASN:H	2.03	0.55
1:C:1019:ALA:HB3	1:C:1022:VAL:HB	1.87	0.55
1:A:841:GLY:H	1:A:844:SER:HG	1.53	0.55
1:F:416:THR:O	1:F:416:THR:HG22	2.05	0.55
1:E:501:GLY:HA2	1:E:519:SER:HB3	1.87	0.55
1:A:313:ILE:HG23	1:A:316:ILE:HD12	1.89	0.55
1:E:359:ASN:HD22	1:E:379:ASN:H	1.54	0.55
1:E:841:GLY:N	1:E:844:SER:OG	2.33	0.55
1:C:359:ASN:HD22	1:C:379:ASN:H	1.55	0.54
1:D:1019:ALA:HB3	1:D:1022:VAL:HB	1.89	0.54
1:B:265:ALA:CA	1:B:291:ALA:H	2.08	0.54
1:F:313:ILE:HG23	1:F:316:ILE:HD12	1.90	0.54
1:C:715:ASN:ND2	1:D:693:PRO:HB3	2.23	0.54
1:B:1019:ALA:HB3	1:B:1022:VAL:HB	1.88	0.54
1:E:912:ILE:H	1:E:912:ILE:HD12	1.71	0.53
1:C:693:PRO:HB3	1:D:715:ASN:ND2	2.23	0.53
1:E:354:ALA:HB1	1:E:358:GLN:HE21	1.74	0.53
1:E:313:ILE:HG23	1:E:316:ILE:HD12	1.89	0.53
1:A:354:ALA:HB1	1:A:358:GLN:HE21	1.74	0.53
1:D:354:ALA:HB1	1:D:358:GLN:HE21	1.74	0.53
1:E:405:SER:HB3	3:E:9108:HOH:O	2.08	0.53
1:A:912:ILE:HD12	1:A:912:ILE:H	1.73	0.52
1:D:273:GLY:HA2	1:D:299:VAL:HG23	1.91	0.52
1:A:754:LEU:HD23	3:A:9115:HOH:O	2.09	0.52
1:B:359:ASN:HD22	1:B:379:ASN:H	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:SER:HA	1:B:863:GLY:O	2.10	0.52
1:C:273:GLY:HA2	1:C:299:VAL:HG23	1.92	0.52
1:C:354:ALA:HB1	1:C:358:GLN:HE21	1.74	0.52
1:D:359:ASN:HD22	1:D:379:ASN:H	1.56	0.52
1:F:354:ALA:HB1	1:F:358:GLN:HE21	1.75	0.52
1:F:841:GLY:N	1:F:844:SER:OG	2.33	0.52
1:B:354:ALA:HB1	1:B:358:GLN:HE21	1.75	0.51
1:F:273:GLY:HA2	1:F:299:VAL:HG23	1.90	0.51
1:C:367:GLN:NE2	1:C:384:SER:HB3	2.25	0.51
1:F:359:ASN:HD22	1:F:379:ASN:H	1.56	0.51
1:B:367:GLN:NE2	1:B:384:SER:HB3	2.26	0.51
1:C:416:THR:HB	1:C:444:ALA:HB2	1.92	0.51
1:F:930:LEU:HG	1:F:932:LEU:HD21	1.93	0.51
1:B:912:ILE:HD12	1:B:912:ILE:H	1.75	0.51
1:D:837:SER:HA	1:D:863:GLY:O	2.11	0.51
1:B:273:GLY:HA2	1:B:299:VAL:HG23	1.91	0.51
1:A:416:THR:HB	1:A:444:ALA:HB2	1.93	0.51
1:A:837:SER:HA	1:A:863:GLY:O	2.11	0.51
1:E:720:LEU:HD13	1:E:731:PHE:CD1	2.46	0.51
1:E:837:SER:HA	1:E:863:GLY:O	2.11	0.51
1:A:273:GLY:HA2	1:A:299:VAL:HG23	1.91	0.51
1:A:930:LEU:HG	1:A:932:LEU:HD21	1.93	0.51
1:C:363:THR:HG23	1:C:383:ALA:HB3	1.92	0.51
1:C:837:SER:HA	1:C:863:GLY:O	2.11	0.51
1:A:367:GLN:NE2	1:A:384:SER:HB3	2.25	0.51
1:B:930:LEU:HG	1:B:932:LEU:HD21	1.91	0.50
1:E:930:LEU:HG	1:E:932:LEU:HD21	1.93	0.50
1:D:355:GLY:H	1:D:358:GLN:NE2	2.09	0.50
1:E:273:GLY:HA2	1:E:299:VAL:HG23	1.93	0.50
1:E:367:GLN:NE2	1:E:384:SER:HB3	2.26	0.50
1:B:435:ASN:O	3:B:9102:HOH:O	2.19	0.50
1:F:416:THR:HB	1:F:444:ALA:HB2	1.94	0.50
1:D:367:GLN:NE2	1:D:384:SER:HB3	2.27	0.50
1:F:942:ALA:O	1:F:943:ASP:CB	2.60	0.50
1:E:550:THR:HG22	1:E:552:GLY:H	1.77	0.50
1:B:720:LEU:HD13	1:B:731:PHE:CD1	2.47	0.50
1:F:837:SER:HA	1:F:863:GLY:O	2.11	0.50
1:A:415:THR:HB	1:A:442:THR:O	2.12	0.49
1:C:930:LEU:HG	1:C:932:LEU:HD21	1.94	0.49
1:F:673:GLY:O	3:F:9103:HOH:O	2.20	0.49
1:B:388:THR:OG1	1:B:389:SER:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:THR:OG1	1:E:389:SER:N	2.46	0.49
1:F:388:THR:OG1	1:F:389:SER:N	2.45	0.49
1:B:363:THR:HG23	1:B:383:ALA:HB3	1.94	0.49
1:D:308:PRO:HD2	1:D:311:VAL:HG21	1.95	0.49
1:D:942:ALA:O	1:D:943:ASP:CB	2.59	0.49
1:E:942:ALA:O	1:E:943:ASP:CB	2.60	0.49
1:F:355:GLY:H	1:F:358:GLN:NE2	2.10	0.49
1:A:550:THR:HG22	1:A:552:GLY:H	1.77	0.49
1:B:416:THR:HB	1:B:444:ALA:HB2	1.94	0.49
1:E:371:ASN:ND2	1:E:391:THR:H	2.10	0.49
1:D:371:ASN:ND2	1:D:391:THR:H	2.10	0.49
1:D:720:LEU:HD13	1:D:731:PHE:CD1	2.47	0.49
1:A:942:ALA:O	1:A:943:ASP:CB	2.60	0.49
1:F:265:ALA:CA	1:F:291:ALA:H	2.08	0.49
1:F:363:THR:HG23	1:F:383:ALA:HB3	1.94	0.49
1:F:367:GLN:NE2	1:F:384:SER:HB3	2.26	0.49
1:C:942:ALA:O	1:C:943:ASP:CB	2.60	0.49
1:D:930:LEU:HG	1:D:932:LEU:HD21	1.93	0.49
1:A:371:ASN:ND2	1:A:391:THR:H	2.11	0.49
1:B:942:ALA:O	1:B:943:ASP:CB	2.60	0.49
1:D:416:THR:HB	1:D:444:ALA:HB2	1.94	0.49
1:D:641:LEU:HG	1:D:659:THR:HB	1.95	0.49
1:F:720:LEU:HD13	1:F:731:PHE:CD1	2.48	0.49
1:B:415:THR:HB	1:B:442:THR:O	2.13	0.48
1:B:550:THR:HG22	1:B:552:GLY:H	1.78	0.48
1:B:936:SER:O	1:B:936:SER:OG	2.30	0.48
1:E:416:THR:HB	1:E:444:ALA:HB2	1.93	0.48
1:F:415:THR:HB	1:F:442:THR:O	2.13	0.48
1:B:355:GLY:H	1:B:358:GLN:NE2	2.10	0.48
1:B:752:VAL:HB	1:B:781:LEU:HD23	1.95	0.48
1:C:715:ASN:HD21	1:D:693:PRO:HB3	1.78	0.48
1:C:720:LEU:HD13	1:C:731:PHE:CD1	2.48	0.48
1:A:363:THR:HG23	1:A:383:ALA:HB3	1.94	0.48
1:A:388:THR:OG1	1:A:389:SER:N	2.46	0.48
1:A:720:LEU:HD13	1:A:731:PHE:CD1	2.48	0.48
1:D:388:THR:OG1	1:D:389:SER:N	2.46	0.48
1:C:388:THR:OG1	1:C:389:SER:N	2.46	0.48
1:D:550:THR:HG22	1:D:552:GLY:H	1.78	0.48
1:E:355:GLY:H	1:E:358:GLN:NE2	2.10	0.48
1:A:355:GLY:H	1:A:358:GLN:NE2	2.11	0.48
1:C:415:THR:HB	1:C:442:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:THR:HG22	1:C:552:GLY:H	1.77	0.48
1:B:371:ASN:ND2	1:B:391:THR:H	2.11	0.48
1:E:363:THR:HG23	1:E:383:ALA:HB3	1.95	0.48
1:F:371:ASN:ND2	1:F:391:THR:H	2.11	0.48
1:C:265:ALA:C	1:C:291:ALA:HB3	2.34	0.48
1:C:355:GLY:H	1:C:358:GLN:NE2	2.11	0.48
1:C:371:ASN:ND2	1:C:391:THR:H	2.11	0.48
1:D:415:THR:HB	1:D:442:THR:O	2.13	0.48
1:E:752:VAL:HB	1:E:781:LEU:HD23	1.95	0.48
1:C:752:VAL:HB	1:C:781:LEU:HD23	1.96	0.47
1:F:936:SER:O	1:F:936:SER:OG	2.30	0.47
1:E:415:THR:HB	1:E:442:THR:O	2.14	0.47
1:E:756:ASN:HB2	1:F:693:PRO:HD2	1.96	0.47
1:A:936:SER:O	1:A:936:SER:OG	2.31	0.47
1:D:752:VAL:HB	1:D:781:LEU:HD23	1.96	0.47
1:F:641:LEU:HG	1:F:659:THR:HB	1.96	0.47
1:C:693:PRO:HB3	1:D:715:ASN:HD21	1.78	0.47
1:F:265:ALA:C	1:F:291:ALA:HB3	2.35	0.47
1:F:345:THR:HG22	1:F:346:SER:N	2.30	0.47
1:F:550:THR:HG22	1:F:552:GLY:H	1.78	0.47
1:A:265:ALA:C	1:A:291:ALA:HB3	2.35	0.47
1:A:345:THR:HG22	1:A:346:SER:N	2.30	0.47
1:A:752:VAL:HB	1:A:781:LEU:HD23	1.96	0.47
1:C:345:THR:HG22	1:C:346:SER:N	2.30	0.46
1:C:641:LEU:HG	1:C:659:THR:HB	1.97	0.46
1:D:265:ALA:C	1:D:291:ALA:HB3	2.35	0.46
1:E:936:SER:O	1:E:936:SER:OG	2.30	0.46
1:E:265:ALA:C	1:E:291:ALA:HB3	2.35	0.46
1:E:345:THR:HG22	1:E:346:SER:N	2.31	0.46
1:F:752:VAL:HB	1:F:781:LEU:HD23	1.96	0.46
1:B:265:ALA:C	1:B:291:ALA:HB3	2.36	0.46
1:F:367:GLN:HE21	1:F:384:SER:HB3	1.79	0.46
1:B:345:THR:HG22	1:B:346:SER:N	2.31	0.46
1:D:345:THR:HG22	1:D:346:SER:N	2.30	0.46
1:B:641:LEU:HG	1:B:659:THR:HB	1.97	0.46
1:E:854:THR:HB	1:E:857:GLU:CG	2.46	0.46
1:B:350:GLN:HE21	1:B:350:GLN:HB2	1.57	0.46
1:B:573:SER:HA	1:B:595:ASP:HB3	1.98	0.46
1:C:308:PRO:HD2	1:C:311:VAL:HG21	1.98	0.46
1:C:535:THR:HA	1:C:536:PRO:HD3	1.82	0.46
1:D:854:THR:HB	1:D:857:GLU:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASN:HA	1:C:293:THR:OG1	2.16	0.45
1:D:250:SER:H	1:D:268:ASP:HB3	1.82	0.45
1:D:936:SER:O	1:D:936:SER:OG	2.30	0.45
1:A:573:SER:HA	1:A:595:ASP:HB3	1.98	0.45
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.56	0.45
1:C:854:THR:HB	1:C:857:GLU:CG	2.46	0.45
1:E:267:ASN:HA	1:E:293:THR:OG1	2.16	0.45
1:F:854:THR:HB	1:F:857:GLU:CG	2.47	0.45
1:D:363:THR:HG23	1:D:383:ALA:HB3	1.99	0.45
1:A:267:ASN:HA	1:A:293:THR:OG1	2.16	0.45
1:C:573:SER:HA	1:C:595:ASP:HB3	1.99	0.45
1:B:267:ASN:HA	1:B:293:THR:OG1	2.16	0.45
1:E:641:LEU:HG	1:E:659:THR:HB	1.99	0.45
1:F:267:ASN:HA	1:F:293:THR:OG1	2.16	0.45
1:A:854:THR:HB	1:A:857:GLU:CG	2.46	0.45
1:E:573:SER:HA	1:E:595:ASP:HB3	1.99	0.45
1:A:308:PRO:HD2	1:A:311:VAL:HG21	1.99	0.44
1:C:250:SER:H	1:C:268:ASP:HB3	1.82	0.44
1:E:378:ALA:O	1:E:400:ALA:HB1	2.18	0.44
1:E:725:THR:HG22	3:E:9101:HOH:O	2.09	0.44
1:D:267:ASN:HA	1:D:293:THR:OG1	2.17	0.44
1:E:429:VAL:HG22	1:E:459:VAL:HG13	1.99	0.44
1:B:854:THR:HB	1:B:857:GLU:CG	2.46	0.44
1:E:529:ARG:NH2	3:E:9103:HOH:O	2.51	0.44
1:B:367:GLN:HE21	1:B:384:SER:HB3	1.82	0.44
1:F:573:SER:HA	1:F:595:ASP:HB3	1.99	0.44
1:C:666:GLY:O	1:C:667:ALA:C	2.56	0.44
1:E:308:PRO:HD2	1:E:311:VAL:HG21	2.00	0.44
1:F:666:GLY:O	1:F:667:ALA:C	2.56	0.44
1:A:378:ALA:O	1:A:400:ALA:HB1	2.18	0.44
1:C:367:GLN:HE21	1:C:384:SER:HB3	1.83	0.44
1:F:308:PRO:HD2	1:F:311:VAL:HG21	2.00	0.44
1:C:378:ALA:O	1:C:400:ALA:HB1	2.18	0.44
1:C:429:VAL:HG22	1:C:459:VAL:HG13	1.99	0.43
1:C:581:SER:HA	1:C:602:SER:O	2.19	0.43
1:D:378:ALA:O	1:D:400:ALA:HB1	2.17	0.43
1:F:342:ASN:ND2	1:F:361:THR:HB	2.29	0.43
1:A:573:SER:O	1:A:575:ALA:N	2.46	0.43
1:A:641:LEU:HG	1:A:659:THR:HB	2.00	0.43
1:B:250:SER:H	1:B:268:ASP:HB3	1.83	0.43
1:B:378:ALA:O	1:B:400:ALA:HB1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:SER:HA	1:E:602:SER:O	2.18	0.43
1:D:270:PHE:HB3	1:D:296:LEU:HD23	2.00	0.43
1:D:573:SER:HA	1:D:595:ASP:HB3	1.99	0.43
1:F:429:VAL:HG22	1:F:459:VAL:HG13	2.01	0.43
1:F:535:THR:HA	1:F:536:PRO:HD3	1.82	0.43
1:A:581:SER:HA	1:A:602:SER:O	2.18	0.43
1:C:727:GLY:O	1:C:729:THR:HG22	2.18	0.43
1:F:581:SER:HA	1:F:602:SER:O	2.19	0.43
1:A:666:GLY:O	1:A:667:ALA:C	2.56	0.43
1:B:342:ASN:ND2	1:B:361:THR:HB	2.29	0.43
1:E:666:GLY:O	1:E:667:ALA:C	2.56	0.43
1:F:250:SER:H	1:F:268:ASP:HB3	1.84	0.43
1:F:378:ALA:O	1:F:400:ALA:HB1	2.17	0.43
1:A:359:ASN:ND2	1:A:378:ALA:HB3	2.34	0.43
1:A:429:VAL:HG22	1:A:459:VAL:HG13	2.00	0.43
1:C:936:SER:OG	1:C:936:SER:O	2.30	0.43
1:E:250:SER:H	1:E:268:ASP:HB3	1.82	0.43
1:E:350:GLN:HE21	1:E:350:GLN:HB2	1.57	0.43
1:A:756:ASN:HB2	1:B:693:PRO:HD2	1.99	0.43
1:B:573:SER:O	1:B:575:ALA:N	2.46	0.43
1:D:666:GLY:O	1:D:667:ALA:C	2.56	0.43
1:E:727:GLY:O	1:E:729:THR:HG22	2.18	0.43
1:E:1007:LEU:HD23	1:E:1011:VAL:HG11	2.01	0.43
1:B:429:VAL:HG22	1:B:459:VAL:HG13	2.00	0.43
1:B:270:PHE:HB3	1:B:296:LEU:HD23	2.01	0.43
1:F:1007:LEU:HD23	1:F:1011:VAL:HG11	2.00	0.43
1:A:727:GLY:O	1:A:729:THR:HG22	2.18	0.42
1:F:680:LEU:HB2	1:F:698:PHE:CD1	2.54	0.42
1:B:581:SER:HA	1:B:602:SER:O	2.19	0.42
1:D:429:VAL:HG22	1:D:459:VAL:HG13	2.00	0.42
1:D:581:SER:HA	1:D:602:SER:O	2.19	0.42
1:A:693:PRO:HD2	1:B:756:ASN:HB2	2.01	0.42
1:B:308:PRO:HD2	1:B:311:VAL:HG21	2.01	0.42
1:B:727:GLY:O	1:B:729:THR:HG22	2.19	0.42
1:C:350:GLN:HE21	1:C:350:GLN:HB2	1.57	0.42
1:D:727:GLY:O	1:D:729:THR:HG22	2.19	0.42
1:B:666:GLY:O	1:B:667:ALA:C	2.56	0.42
1:C:680:LEU:HB2	1:C:698:PHE:CD1	2.54	0.42
1:E:367:GLN:HE21	1:E:384:SER:HB3	1.84	0.42
1:E:947:GLY:HA3	1:E:1014:THR:O	2.20	0.42
1:A:687:SER:HB2	1:A:689:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HB2	1:A:698:PHE:CD1	2.54	0.42
1:B:345:THR:HG21	1:B:348:ALA:O	2.20	0.42
1:C:947:GLY:HA3	1:C:1014:THR:O	2.19	0.42
1:A:1007:LEU:HD23	1:A:1011:VAL:HG11	2.02	0.42
1:D:640:ILE:HG12	1:D:651:MET:HE2	2.02	0.42
1:E:359:ASN:ND2	1:E:378:ALA:HB3	2.35	0.42
1:F:591:ASN:HD22	1:F:612:THR:HB	1.84	0.42
1:A:947:GLY:HA3	1:A:1014:THR:O	2.19	0.42
1:B:947:GLY:HA3	1:B:1014:THR:O	2.19	0.42
1:E:676:GLY:HA2	3:E:9113:HOH:O	2.19	0.42
1:E:680:LEU:HB2	1:E:698:PHE:CD1	2.55	0.42
1:B:680:LEU:HB2	1:B:698:PHE:CD1	2.55	0.42
1:C:516:VAL:HB	1:C:543:LEU:HD12	2.02	0.42
1:F:947:GLY:HA3	1:F:1014:THR:O	2.20	0.42
1:B:567:THR:HG22	1:B:588:THR:HG22	2.02	0.41
1:D:947:GLY:HA3	1:D:1014:THR:O	2.20	0.41
1:E:881:ILE:HA	1:E:899:THR:O	2.20	0.41
1:F:270:PHE:HB3	1:F:296:LEU:HD23	2.00	0.41
1:F:359:ASN:ND2	1:F:378:ALA:HB3	2.35	0.41
1:F:573:SER:O	1:F:575:ALA:N	2.46	0.41
1:D:266:ASN:HD22	1:D:267:ASN:H	1.68	0.41
1:D:1007:LEU:HD23	1:D:1011:VAL:HG11	2.02	0.41
1:E:535:THR:HA	1:E:536:PRO:HD3	1.82	0.41
1:F:727:GLY:O	1:F:729:THR:HG22	2.19	0.41
1:A:270:PHE:HB3	1:A:296:LEU:HD23	2.03	0.41
1:B:967:ALA:HA	1:B:995:ALA:HA	2.02	0.41
1:B:591:ASN:HD22	1:B:612:THR:HB	1.85	0.41
1:D:342:ASN:ND2	1:D:361:THR:HB	2.29	0.41
1:D:680:LEU:HB2	1:D:698:PHE:CD1	2.55	0.41
1:E:342:ASN:ND2	1:E:361:THR:HB	2.29	0.41
1:F:345:THR:HG21	1:F:348:ALA:O	2.20	0.41
1:F:967:ALA:HA	1:F:995:ALA:HA	2.03	0.41
1:B:359:ASN:ND2	1:B:378:ALA:HB3	2.35	0.41
1:C:567:THR:HG22	1:C:588:THR:HG22	2.03	0.41
1:C:958:LEU:HB2	1:C:981:PHE:CE1	2.56	0.41
1:F:266:ASN:HD22	1:F:267:ASN:H	1.69	0.41
1:A:591:ASN:HD22	1:A:612:THR:HB	1.85	0.41
1:A:958:LEU:HB2	1:A:981:PHE:CE1	2.55	0.41
1:B:355:GLY:O	1:B:358:GLN:HG3	2.21	0.41
1:C:359:ASN:ND2	1:C:378:ALA:HB3	2.35	0.41
1:E:687:SER:HB2	1:E:689:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ILE:HA	1:A:899:THR:O	2.21	0.41
1:B:266:ASN:HD22	1:B:267:ASN:H	1.69	0.41
1:C:881:ILE:HA	1:C:899:THR:O	2.21	0.41
1:D:359:ASN:ND2	1:D:378:ALA:HB3	2.35	0.41
1:D:573:SER:O	1:D:575:ALA:N	2.46	0.41
1:D:881:ILE:HA	1:D:899:THR:O	2.21	0.41
1:E:266:ASN:HD22	1:E:267:ASN:H	1.68	0.41
1:E:270:PHE:HB3	1:E:296:LEU:HD23	2.02	0.41
1:C:681:VAL:HG13	1:C:702:ARG:HG2	2.03	0.41
1:C:967:ALA:HA	1:C:995:ALA:HA	2.03	0.41
1:D:967:ALA:HA	1:D:995:ALA:HA	2.03	0.41
1:A:250:SER:H	1:A:268:ASP:HB3	1.84	0.41
1:A:967:ALA:HA	1:A:995:ALA:HA	2.02	0.41
1:B:535:THR:HA	1:B:536:PRO:HD3	1.82	0.41
1:D:250:SER:O	1:D:268:ASP:CB	2.69	0.41
1:D:591:ASN:HD22	1:D:612:THR:HB	1.85	0.41
1:D:681:VAL:HG13	1:D:702:ARG:HG2	2.03	0.41
1:E:591:ASN:HD22	1:E:612:THR:HB	1.86	0.41
1:E:681:VAL:HG13	1:E:702:ARG:HG2	2.03	0.41
1:F:881:ILE:HA	1:F:899:THR:O	2.20	0.41
1:A:367:GLN:HE21	1:A:384:SER:HB3	1.85	0.41
1:D:567:THR:HG22	1:D:588:THR:HG22	2.03	0.41
1:F:355:GLY:O	1:F:358:GLN:HG3	2.22	0.41
1:F:567:THR:HG22	1:F:588:THR:HG22	2.02	0.41
1:B:597:ARG:HH22	1:B:637:ALA:HB3	1.87	0.40
1:B:1007:LEU:HD23	1:B:1011:VAL:HG11	2.01	0.40
1:D:367:GLN:HE21	1:D:384:SER:HB3	1.85	0.40
1:E:958:LEU:HB2	1:E:981:PHE:CE1	2.56	0.40
1:F:250:SER:O	1:F:268:ASP:CB	2.69	0.40
1:A:681:VAL:HG13	1:A:702:ARG:HG2	2.04	0.40
1:B:687:SER:HB2	1:B:689:PHE:CE1	2.56	0.40
1:C:355:GLY:O	1:C:358:GLN:HG3	2.21	0.40
1:C:951:THR:O	1:C:952:LEU:HD23	2.22	0.40
1:E:516:VAL:HB	1:E:543:LEU:HD12	2.03	0.40
1:B:250:SER:O	1:B:268:ASP:CB	2.69	0.40
1:B:274:GLU:OE1	1:B:277:GLY:HA2	2.22	0.40
1:B:958:LEU:HB2	1:B:981:PHE:CE1	2.57	0.40
1:C:591:ASN:HD22	1:C:612:THR:HB	1.87	0.40
1:E:250:SER:O	1:E:268:ASP:CB	2.70	0.40
1:B:854:THR:HB	1:B:857:GLU:HG3	2.04	0.40
1:C:1007:LEU:HD23	1:C:1011:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:GLY:O	1:D:358:GLN:HG3	2.22	0.40
1:D:841:GLY:O	1:D:842:THR:C	2.60	0.40
1:F:681:VAL:HG13	1:F:702:ARG:HG2	2.03	0.40

All (8) 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)
1:C:267:ASN:ND2	1:D:418:ALA:CB[2_455]	1.49	0.71
1:C:267:ASN:OD1	1:D:418:ALA:CB[2_455]	1.56	0.64
1:C:249:GLY:CA	1:D:391:THR:CG2[2_455]	1.57	0.63
1:C:249:GLY:N	1:D:391:THR:CG2[2_455]	1.60	0.60
1:C:267:ASN:CG	1:D:418:ALA:CB[2_455]	1.60	0.60
1:C:267:ASN:OD1	1:D:418:ALA:N[2_455]	1.77	0.43
1:C:267:ASN:OD1	1:D:418:ALA:CA[2_455]	1.84	0.36
1:C:275:VAL:O	1:F:256:THR:O[2_455]	1.88	0.32

## 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	776/1026 (76%)	709 (91%)	52 (7%)	15 (2%)	8	20
1	B	776/1026 (76%)	710 (92%)	52 (7%)	14 (2%)	8	21
1	C	776/1026 (76%)	711 (92%)	51 (7%)	14 (2%)	8	21
1	D	776/1026 (76%)	710 (92%)	51 (7%)	15 (2%)	8	20
1	E	776/1026 (76%)	712 (92%)	49 (6%)	15 (2%)	8	20
1	F	776/1026 (76%)	712 (92%)	50 (6%)	14 (2%)	8	21
All	All	4656/6156 (76%)	4264 (92%)	305 (7%)	87 (2%)	8	20

All (87) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	574	THR
1	A	936	SER
1	A	942	ALA
1	A	1019	ALA
1	B	574	THR
1	B	936	SER
1	B	942	ALA
1	B	1019	ALA
1	C	574	THR
1	C	936	SER
1	C	942	ALA
1	C	1019	ALA
1	D	574	THR
1	D	936	SER
1	D	942	ALA
1	D	1019	ALA
1	E	574	THR
1	E	936	SER
1	E	942	ALA
1	E	1019	ALA
1	F	574	THR
1	F	936	SER
1	F	942	ALA
1	F	1019	ALA
1	A	267	ASN
1	A	667	ALA
1	A	946	PHE
1	A	993	ALA
1	B	267	ASN
1	B	417	GLY
1	B	667	ALA
1	B	946	PHE
1	B	993	ALA
1	C	267	ASN
1	C	667	ALA
1	C	946	PHE
1	C	993	ALA
1	D	267	ASN
1	D	417	GLY
1	D	667	ALA
1	D	946	PHE
1	D	993	ALA
1	E	267	ASN

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Mol	Chain	Res	Type
1	E	667	ALA
1	E	946	PHE
1	E	993	ALA
1	F	267	ASN
1	F	667	ALA
1	F	946	PHE
1	F	993	ALA
1	A	417	GLY
1	A	502	SER
1	C	417	GLY
1	E	417	GLY
1	F	417	GLY
1	A	378	ALA
1	B	378	ALA
1	B	502	SER
1	B	842	THR
1	C	378	ALA
1	C	502	SER
1	C	842	THR
1	D	378	ALA
1	D	502	SER
1	D	842	THR
1	E	378	ALA
1	E	502	SER
1	E	842	THR
1	F	378	ALA
1	F	502	SER
1	F	842	THR
1	A	665	LEU
1	A	842	THR
1	B	665	LEU
1	D	665	LEU
1	D	1020	THR
1	A	1020	THR
1	C	665	LEU
1	E	665	LEU
1	E	1020	THR
1	F	1020	THR
1	A	668	GLY
1	B	668	GLY
1	C	668	GLY
1	D	668	GLY

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Mol	Chain	Res	Type
1	E	668	GLY
1	F	668	GLY

### 5.3.2 Protein sidechains ⓘ

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	526/699 (75%)	473 (90%)	53 (10%)	7	17
1	B	526/699 (75%)	471 (90%)	55 (10%)	7	16
1	C	526/699 (75%)	472 (90%)	54 (10%)	7	16
1	D	526/699 (75%)	473 (90%)	53 (10%)	7	17
1	E	526/699 (75%)	474 (90%)	52 (10%)	8	18
1	F	526/699 (75%)	471 (90%)	55 (10%)	7	16
All	All	3156/4194 (75%)	2834 (90%)	322 (10%)	7	17

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	THR
1	A	266	ASN
1	A	267	ASN
1	A	268	ASP
1	A	275	VAL
1	A	293	THR
1	A	296	LEU
1	A	299	VAL
1	A	309	THR
1	A	314	SER
1	A	322	THR
1	A	329	LEU
1	A	350	GLN
1	A	358	GLN
1	A	363	THR
1	A	380	VAL

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Mol	Chain	Res	Type
1	A	388	THR
1	A	393	THR
1	A	442	THR
1	A	454	THR
1	A	479	VAL
1	A	490	THR
1	A	491	THR
1	A	494	LYS
1	A	537	THR
1	A	551	THR
1	A	577	SER
1	A	588	THR
1	A	590	LEU
1	A	614	THR
1	A	620	THR
1	A	646	THR
1	A	651	MET
1	A	658	VAL
1	A	662	SER
1	A	690	SER
1	A	729	THR
1	A	797	THR
1	A	809	SER
1	A	826	THR
1	A	842	THR
1	A	844	SER
1	A	857	GLU
1	A	862	ARG
1	A	873	SER
1	A	875	THR
1	A	892	THR
1	A	906	ILE
1	A	915	SER
1	A	916	THR
1	A	951	THR
1	A	973	THR
1	A	1012	THR
1	B	251	THR
1	B	266	ASN
1	B	267	ASN
1	B	268	ASP
1	B	275	VAL

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Mol	Chain	Res	Type
1	B	283	VAL
1	B	293	THR
1	B	296	LEU
1	B	299	VAL
1	B	309	THR
1	B	314	SER
1	B	322	THR
1	B	329	LEU
1	B	350	GLN
1	B	358	GLN
1	B	363	THR
1	B	380	VAL
1	B	388	THR
1	B	393	THR
1	B	442	THR
1	B	454	THR
1	B	479	VAL
1	B	490	THR
1	B	491	THR
1	B	494	LYS
1	B	537	THR
1	B	551	THR
1	B	577	SER
1	B	588	THR
1	B	590	LEU
1	B	614	THR
1	B	620	THR
1	B	646	THR
1	B	651	MET
1	B	658	VAL
1	B	662	SER
1	B	690	SER
1	B	729	THR
1	B	797	THR
1	B	809	SER
1	B	826	THR
1	B	842	THR
1	B	844	SER
1	B	857	GLU
1	B	862	ARG
1	B	873	SER
1	B	875	THR

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Mol	Chain	Res	Type
1	B	892	THR
1	B	906	ILE
1	B	915	SER
1	B	916	THR
1	B	951	THR
1	B	973	THR
1	B	975	VAL
1	B	1012	THR
1	C	251	THR
1	C	266	ASN
1	C	267	ASN
1	C	268	ASP
1	C	275	VAL
1	C	283	VAL
1	C	293	THR
1	C	296	LEU
1	C	299	VAL
1	C	309	THR
1	C	314	SER
1	C	322	THR
1	C	329	LEU
1	C	350	GLN
1	C	358	GLN
1	C	363	THR
1	C	380	VAL
1	C	388	THR
1	C	393	THR
1	C	442	THR
1	C	454	THR
1	C	479	VAL
1	C	490	THR
1	C	491	THR
1	C	494	LYS
1	C	537	THR
1	C	551	THR
1	C	577	SER
1	C	588	THR
1	C	590	LEU
1	C	614	THR
1	C	620	THR
1	C	646	THR
1	C	651	MET

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Mol	Chain	Res	Type
1	C	662	SER
1	C	690	SER
1	C	729	THR
1	C	797	THR
1	C	809	SER
1	C	826	THR
1	C	842	THR
1	C	844	SER
1	C	857	GLU
1	C	862	ARG
1	C	873	SER
1	C	875	THR
1	C	892	THR
1	C	906	ILE
1	C	915	SER
1	C	916	THR
1	C	951	THR
1	C	973	THR
1	C	975	VAL
1	C	1012	THR
1	D	251	THR
1	D	266	ASN
1	D	267	ASN
1	D	268	ASP
1	D	275	VAL
1	D	293	THR
1	D	296	LEU
1	D	299	VAL
1	D	309	THR
1	D	314	SER
1	D	322	THR
1	D	329	LEU
1	D	350	GLN
1	D	358	GLN
1	D	363	THR
1	D	380	VAL
1	D	388	THR
1	D	393	THR
1	D	442	THR
1	D	454	THR
1	D	479	VAL
1	D	490	THR

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Mol	Chain	Res	Type
1	D	491	THR
1	D	494	LYS
1	D	537	THR
1	D	551	THR
1	D	577	SER
1	D	588	THR
1	D	590	LEU
1	D	614	THR
1	D	620	THR
1	D	646	THR
1	D	651	MET
1	D	658	VAL
1	D	662	SER
1	D	690	SER
1	D	729	THR
1	D	797	THR
1	D	809	SER
1	D	826	THR
1	D	842	THR
1	D	844	SER
1	D	857	GLU
1	D	862	ARG
1	D	873	SER
1	D	875	THR
1	D	892	THR
1	D	906	ILE
1	D	915	SER
1	D	916	THR
1	D	951	THR
1	D	975	VAL
1	D	1012	THR
1	E	251	THR
1	E	266	ASN
1	E	267	ASN
1	E	268	ASP
1	E	275	VAL
1	E	283	VAL
1	E	293	THR
1	E	296	LEU
1	E	299	VAL
1	E	309	THR
1	E	314	SER

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Mol	Chain	Res	Type
1	E	322	THR
1	E	329	LEU
1	E	350	GLN
1	E	358	GLN
1	E	363	THR
1	E	380	VAL
1	E	388	THR
1	E	393	THR
1	E	442	THR
1	E	454	THR
1	E	490	THR
1	E	491	THR
1	E	494	LYS
1	E	537	THR
1	E	551	THR
1	E	577	SER
1	E	588	THR
1	E	590	LEU
1	E	614	THR
1	E	620	THR
1	E	646	THR
1	E	651	MET
1	E	658	VAL
1	E	662	SER
1	E	690	SER
1	E	729	THR
1	E	797	THR
1	E	809	SER
1	E	826	THR
1	E	842	THR
1	E	844	SER
1	E	857	GLU
1	E	862	ARG
1	E	873	SER
1	E	875	THR
1	E	892	THR
1	E	906	ILE
1	E	915	SER
1	E	916	THR
1	E	951	THR
1	E	1012	THR
1	F	251	THR

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Mol	Chain	Res	Type
1	F	266	ASN
1	F	267	ASN
1	F	268	ASP
1	F	275	VAL
1	F	283	VAL
1	F	293	THR
1	F	296	LEU
1	F	299	VAL
1	F	309	THR
1	F	314	SER
1	F	322	THR
1	F	329	LEU
1	F	350	GLN
1	F	358	GLN
1	F	363	THR
1	F	380	VAL
1	F	388	THR
1	F	393	THR
1	F	442	THR
1	F	454	THR
1	F	479	VAL
1	F	490	THR
1	F	491	THR
1	F	494	LYS
1	F	537	THR
1	F	551	THR
1	F	577	SER
1	F	588	THR
1	F	590	LEU
1	F	614	THR
1	F	620	THR
1	F	646	THR
1	F	651	MET
1	F	658	VAL
1	F	662	SER
1	F	690	SER
1	F	702	ARG
1	F	729	THR
1	F	797	THR
1	F	809	SER
1	F	826	THR
1	F	842	THR

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Mol	Chain	Res	Type
1	F	844	SER
1	F	854	THR
1	F	857	GLU
1	F	862	ARG
1	F	873	SER
1	F	875	THR
1	F	892	THR
1	F	906	ILE
1	F	915	SER
1	F	916	THR
1	F	951	THR
1	F	1012	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	267	ASN
1	A	342	ASN
1	A	350	GLN
1	A	358	GLN
1	A	359	ASN
1	A	367	GLN
1	A	371	ASN
1	A	685	ASN
1	A	709	GLN
1	B	266	ASN
1	B	267	ASN
1	B	342	ASN
1	B	350	GLN
1	B	358	GLN
1	B	359	ASN
1	B	367	GLN
1	B	371	ASN
1	B	685	ASN
1	B	709	GLN
1	C	266	ASN
1	C	267	ASN
1	C	342	ASN
1	C	350	GLN
1	C	358	GLN
1	C	359	ASN

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Mol	Chain	Res	Type
1	C	367	GLN
1	C	371	ASN
1	C	685	ASN
1	C	709	GLN
1	C	715	ASN
1	D	266	ASN
1	D	267	ASN
1	D	342	ASN
1	D	350	GLN
1	D	358	GLN
1	D	359	ASN
1	D	367	GLN
1	D	371	ASN
1	D	685	ASN
1	D	709	GLN
1	D	715	ASN
1	E	266	ASN
1	E	267	ASN
1	E	342	ASN
1	E	350	GLN
1	E	358	GLN
1	E	359	ASN
1	E	367	GLN
1	E	371	ASN
1	E	685	ASN
1	E	709	GLN
1	F	266	ASN
1	F	267	ASN
1	F	342	ASN
1	F	350	GLN
1	F	358	GLN
1	F	359	ASN
1	F	367	GLN
1	F	371	ASN
1	F	685	ASN
1	F	709	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 114 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	778/1026 (75%)	-0.25	3 (0%) 92 93	7, 16, 52, 102	0
1	B	778/1026 (75%)	-0.20	6 (0%) 86 87	9, 21, 46, 97	0
1	C	778/1026 (75%)	-0.10	6 (0%) 86 87	11, 22, 46, 140	0
1	D	778/1026 (75%)	-0.19	5 (0%) 89 91	9, 20, 40, 92	0
1	E	778/1026 (75%)	-0.18	3 (0%) 92 93	9, 22, 45, 85	0
1	F	778/1026 (75%)	-0.20	5 (0%) 89 91	9, 18, 48, 94	0
All	All	4668/6156 (75%)	-0.19	28 (0%) 89 91	7, 20, 46, 140	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	GLY	7.0
1	C	267	ASN	6.1
1	D	292	GLY	4.9
1	F	946	PHE	4.5
1	A	971	SER	4.2
1	F	292	GLY	4.0
1	C	250	SER	3.9
1	B	946	PHE	3.4
1	A	292	GLY	3.4
1	A	946	PHE	3.3
1	D	267	ASN	3.2
1	B	1015	THR	3.1
1	B	971	SER	2.7
1	E	292	GLY	2.6
1	F	942	ALA	2.6
1	F	964	ALA	2.4
1	B	972	GLY	2.4
1	F	467	ALA	2.4
1	E	946	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	266	ASN	2.4
1	D	942	ALA	2.2
1	C	292	GLY	2.2
1	B	995	ALA	2.2
1	B	796	THR	2.2
1	D	492	ALA	2.1
1	C	471	VAL	2.1
1	E	492	ALA	2.0
1	C	436	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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	CA	A	9017	1/1	0.60	0.19	80,80,80,80	0
2	CA	F	9017	1/1	0.70	0.26	90,90,90,90	0
2	CA	B	9018	1/1	0.77	0.31	95,95,95,95	0
2	CA	E	9004	1/1	0.80	0.09	49,49,49,49	0
2	CA	B	9017	1/1	0.81	0.12	59,59,59,59	0
2	CA	C	9017	1/1	0.84	0.35	78,78,78,78	0
2	CA	B	9019	1/1	0.85	0.10	51,51,51,51	0
2	CA	E	9017	1/1	0.85	0.11	33,33,33,33	0
2	CA	A	9010	1/1	0.85	0.07	30,30,30,30	0
2	CA	A	9018	1/1	0.87	0.27	98,98,98,98	0
2	CA	C	9010	1/1	0.88	0.06	39,39,39,39	0
2	CA	E	9016	1/1	0.89	0.08	34,34,34,34	0
2	CA	E	9018	1/1	0.90	0.41	105,105,105,105	0
2	CA	A	9014	1/1	0.90	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	E	9010	1/1	0.91	0.06	44,44,44,44	0
2	CA	E	9013	1/1	0.91	0.06	30,30,30,30	0
2	CA	D	9004	1/1	0.91	0.05	42,42,42,42	0
2	CA	E	9001	1/1	0.92	0.09	42,42,42,42	0
2	CA	F	9001	1/1	0.92	0.11	27,27,27,27	0
2	CA	D	9005	1/1	0.92	0.09	23,23,23,23	0
2	CA	A	9008	1/1	0.93	0.06	11,11,11,11	0
2	CA	D	9002	1/1	0.93	0.10	30,30,30,30	0
2	CA	D	9013	1/1	0.93	0.08	33,33,33,33	0
2	CA	B	9002	1/1	0.94	0.07	43,43,43,43	0
2	CA	D	9001	1/1	0.94	0.07	31,31,31,31	0
2	CA	E	9015	1/1	0.94	0.10	46,46,46,46	0
2	CA	D	9015	1/1	0.94	0.08	31,31,31,31	0
2	CA	B	9016	1/1	0.94	0.05	31,31,31,31	0
2	CA	E	9002	1/1	0.94	0.06	43,43,43,43	0
2	CA	A	9001	1/1	0.94	0.05	15,15,15,15	0
2	CA	F	9016	1/1	0.94	0.09	22,22,22,22	0
2	CA	E	9009	1/1	0.94	0.05	12,12,12,12	0
2	CA	F	9018	1/1	0.94	0.41	109,109,109,109	0
2	CA	B	9001	1/1	0.95	0.08	25,25,25,25	0
2	CA	D	9008	1/1	0.95	0.07	36,36,36,36	0
2	CA	E	9006	1/1	0.95	0.08	26,26,26,26	0
2	CA	A	9006	1/1	0.95	0.10	20,20,20,20	0
2	CA	B	9004	1/1	0.95	0.05	25,25,25,25	0
2	CA	D	9017	1/1	0.95	0.06	37,37,37,37	0
2	CA	A	9019	1/1	0.95	0.04	39,39,39,39	0
2	CA	B	9013	1/1	0.96	0.05	19,19,19,19	0
2	CA	C	9018	1/1	0.96	0.39	82,82,82,82	0
2	CA	B	9005	1/1	0.96	0.06	35,35,35,35	0
2	CA	C	9004	1/1	0.96	0.06	32,32,32,32	0
2	CA	C	9006	1/1	0.96	0.08	26,26,26,26	0
2	CA	C	9009	1/1	0.96	0.05	28,28,28,28	0
2	CA	E	9011	1/1	0.96	0.07	29,29,29,29	0
2	CA	D	9006	1/1	0.96	0.07	22,22,22,22	0
2	CA	B	9008	1/1	0.96	0.07	22,22,22,22	0
2	CA	D	9010	1/1	0.96	0.07	44,44,44,44	0
2	CA	D	9012	1/1	0.96	0.11	21,21,21,21	0
2	CA	C	9012	1/1	0.96	0.07	26,26,26,26	0
2	CA	E	9019	1/1	0.96	0.07	67,67,67,67	0
2	CA	D	9014	1/1	0.96	0.08	26,26,26,26	0
2	CA	F	9005	1/1	0.96	0.07	29,29,29,29	0
2	CA	F	9009	1/1	0.96	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	C	9014	1/1	0.96	0.06	20,20,20,20	0
2	CA	C	9016	1/1	0.96	0.05	18,18,18,18	0
2	CA	D	9018	1/1	0.96	0.23	81,81,81,81	0
2	CA	A	9013	1/1	0.97	0.04	20,20,20,20	0
2	CA	C	9013	1/1	0.97	0.06	35,35,35,35	0
2	CA	B	9006	1/1	0.97	0.09	17,17,17,17	0
2	CA	C	9015	1/1	0.97	0.06	39,39,39,39	0
2	CA	E	9014	1/1	0.97	0.07	22,22,22,22	0
2	CA	A	9007	1/1	0.97	0.06	17,17,17,17	0
2	CA	C	9002	1/1	0.97	0.11	29,29,29,29	0
2	CA	D	9016	1/1	0.97	0.07	23,23,23,23	0
2	CA	B	9012	1/1	0.97	0.07	26,26,26,26	0
2	CA	A	9004	1/1	0.97	0.04	19,19,19,19	0
2	CA	D	9019	1/1	0.97	0.06	27,27,27,27	0
2	CA	F	9002	1/1	0.97	0.12	17,17,17,17	0
2	CA	C	9007	1/1	0.97	0.05	21,21,21,21	0
2	CA	F	9008	1/1	0.97	0.07	11,11,11,11	0
2	CA	B	9014	1/1	0.97	0.12	31,31,31,31	0
2	CA	F	9010	1/1	0.97	0.05	30,30,30,30	0
2	CA	F	9012	1/1	0.97	0.06	19,19,19,19	0
2	CA	F	9014	1/1	0.97	0.09	12,12,12,12	0
2	CA	F	9015	1/1	0.97	0.09	48,48,48,48	0
2	CA	A	9002	1/1	0.97	0.10	18,18,18,18	0
2	CA	E	9005	1/1	0.97	0.06	26,26,26,26	0
2	CA	C	9011	1/1	0.97	0.04	21,21,21,21	0
2	CA	F	9019	1/1	0.97	0.18	61,61,61,61	0
2	CA	E	9008	1/1	0.98	0.07	18,18,18,18	0
2	CA	F	9003	1/1	0.98	0.09	37,37,37,37	0
2	CA	F	9004	1/1	0.98	0.05	36,36,36,36	0
2	CA	D	9003	1/1	0.98	0.10	9,9,9,9	0
2	CA	C	9005	1/1	0.98	0.04	29,29,29,29	0
2	CA	B	9010	1/1	0.98	0.07	27,27,27,27	0
2	CA	A	9011	1/1	0.98	0.06	17,17,17,17	0
2	CA	C	9008	1/1	0.98	0.04	29,29,29,29	0
2	CA	F	9013	1/1	0.98	0.06	16,16,16,16	0
2	CA	D	9009	1/1	0.98	0.04	15,15,15,15	0
2	CA	A	9009	1/1	0.98	0.09	11,11,11,11	0
2	CA	B	9007	1/1	0.98	0.06	16,16,16,16	0
2	CA	C	9003	1/1	0.98	0.08	15,15,15,15	0
2	CA	A	9005	1/1	0.98	0.04	14,14,14,14	0
2	CA	E	9007	1/1	0.98	0.07	23,23,23,23	0
2	CA	A	9015	1/1	0.99	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	9016	1/1	0.99	0.06	13,13,13,13	0
2	CA	A	9003	1/1	0.99	0.10	10,10,10,10	0
2	CA	F	9006	1/1	0.99	0.06	9,9,9,9	0
2	CA	F	9007	1/1	0.99	0.04	27,27,27,27	0
2	CA	B	9015	1/1	0.99	0.08	47,47,47,47	0
2	CA	E	9012	1/1	0.99	0.08	20,20,20,20	0
2	CA	B	9003	1/1	0.99	0.08	17,17,17,17	0
2	CA	F	9011	1/1	0.99	0.04	44,44,44,44	0
2	CA	D	9007	1/1	0.99	0.06	14,14,14,14	0
2	CA	B	9009	1/1	0.99	0.06	9,9,9,9	0
2	CA	A	9012	1/1	0.99	0.06	19,19,19,19	0
2	CA	E	9003	1/1	0.99	0.05	13,13,13,13	0
2	CA	B	9011	1/1	0.99	0.06	18,18,18,18	0
2	CA	D	9011	1/1	0.99	0.09	23,23,23,23	0
2	CA	C	9019	1/1	0.99	0.09	97,97,97,97	0
2	CA	C	9001	1/1	0.99	0.09	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.