



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 24, 2025 – 12:05 AM EDT

PDB ID : 2E2V / pdb_00002e2v
Title : Substrate Schiff-base analogue of copper amine oxidase from *Arthrobacter globiformis* formed with benzylhydrazine
Authors : Murakawa, T.; Okajima, T.; Taki, M.; Yamamoto, Y.; Kuroda, S.; Hayashi, H.; Tanizawa, K.
Deposited on : 2006-11-17
Resolution : 1.80 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

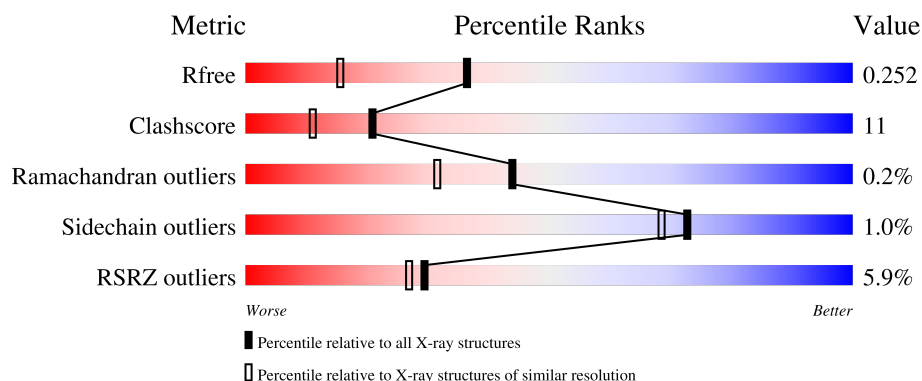
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	628	<div> <div>9%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	B	628	<div> <div>2%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10959 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4876	3081	857	929	9			
1	B	620	Total	C	N	O	S	0	0	0
			4876	3081	857	929	9			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

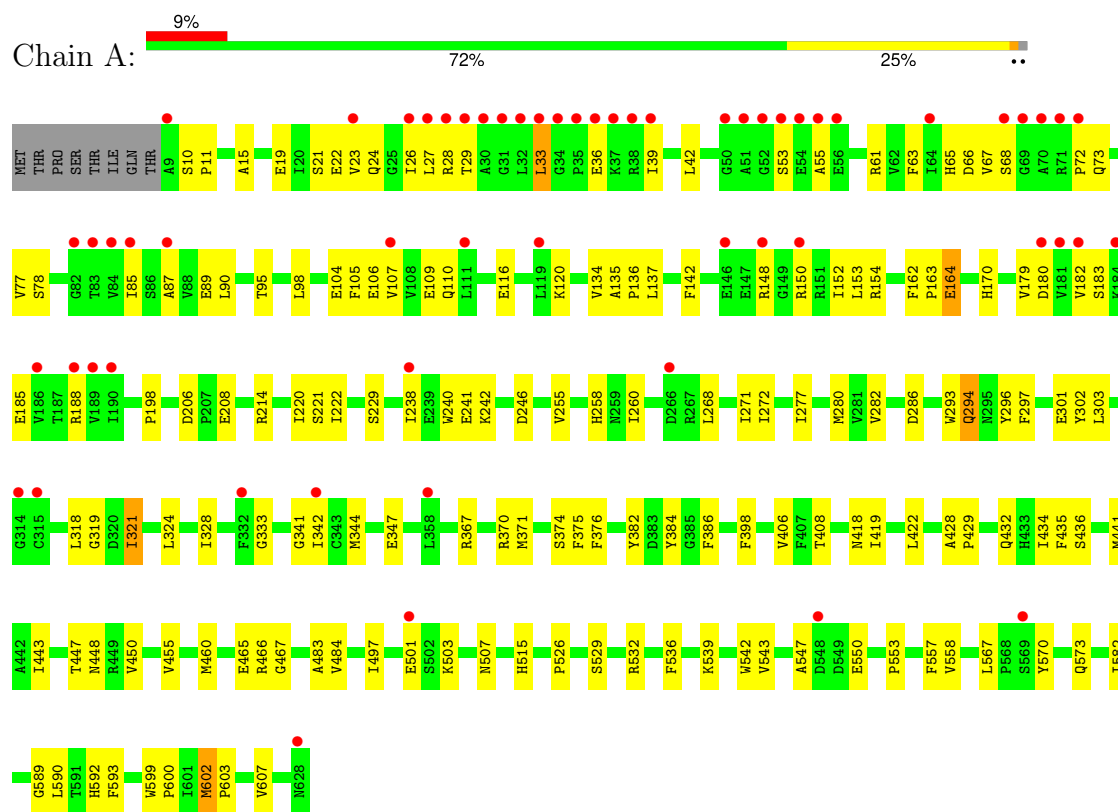
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	550	Total	O	0	0
			550	550		
3	B	655	Total	O	0	0
			655	655		

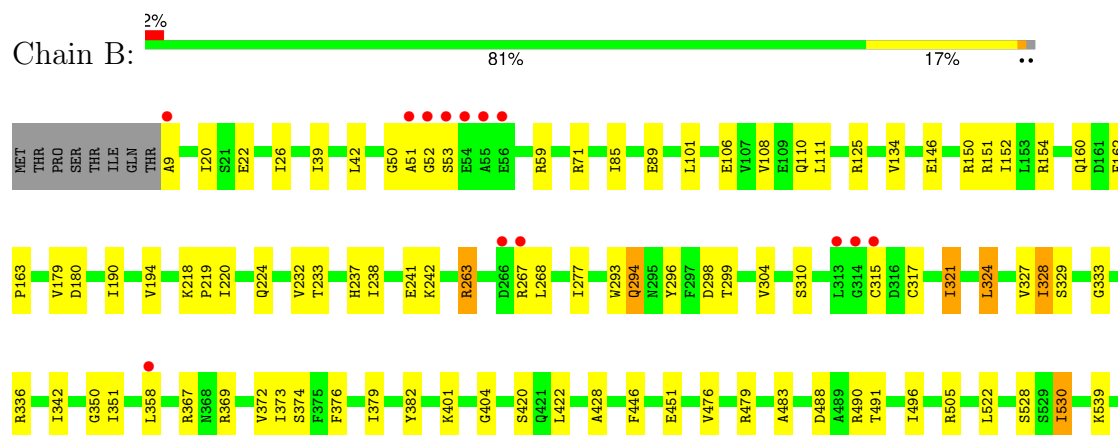
3 Residue-property plots [i](#)

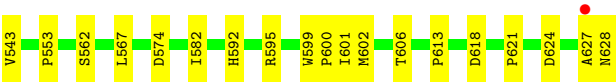
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phenylethylamine oxidase



• Molecule 1: Phenylethylamine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.05Å 62.64Å 183.95Å 90.00° 112.16° 90.00°	Depositor
Resolution (Å)	26.52 – 1.80 26.52 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.52-1.80) 99.1 (26.52-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.252 0.215 , 0.252	Depositor DCC
R_{free} test set	7711 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10959	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 76.66 % 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 9.9438e-07. 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: 3TY, CU

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	0.35	0/4975	0.90	10/6774 (0.1%)
1	B	0.38	0/4975	0.92	12/6774 (0.2%)
All	All	0.36	0/9950	0.91	22/13548 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	MET	N-CA-C	8.39	120.33	109.93
1	A	294	GLN	N-CA-C	6.76	118.88	109.15
1	B	602	MET	N-CA-C	6.64	118.44	110.07
1	B	224	GLN	CA-C-N	6.60	126.84	119.32
1	B	224	GLN	C-N-CA	6.60	126.84	119.32
1	A	582	ILE	N-CA-C	5.96	117.43	108.96
1	A	592	HIS	N-CA-C	5.92	118.16	108.52
1	A	374	SER	N-CA-C	5.89	117.92	109.14
1	A	321	ILE	N-CA-C	5.85	116.36	108.17
1	B	310	SER	N-CA-C	-5.78	99.77	108.96
1	B	294	GLN	N-CA-C	5.60	117.83	109.59
1	B	321	ILE	N-CA-C	5.49	116.89	108.71
1	B	592	HIS	N-CA-C	5.39	117.54	107.99
1	B	374	SER	N-CA-C	5.33	116.90	108.96
1	A	455	VAL	N-CA-C	-5.29	102.76	109.58
1	A	408	THR	N-CA-C	5.27	117.89	110.14
1	A	593	PHE	N-CA-C	-5.27	97.29	108.66
1	A	558	VAL	N-CA-C	5.20	115.97	110.72
1	B	277	ILE	N-CA-C	-5.09	99.15	106.88
1	B	582	ILE	N-CA-C	5.03	116.84	108.99
1	B	446	PHE	N-CA-C	5.03	119.27	113.18
1	B	324	LEU	N-CA-C	-5.00	101.24	109.40

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	4876	0	4693	131	0
1	B	4876	0	4693	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	550	0	0	10	0
3	B	655	0	0	10	0
All	All	10959	0	9386	208	0

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 11.

All (208) 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:263:ARG:HB2	1:B:263:ARG:HH11	1.38	0.88
1:A:78:SER:HB2	1:A:85:ILE:HD11	1.55	0.84
1:B:505:ARG:HD3	1:B:618:ASP:HB3	1.63	0.81
1:A:238:ILE:HD11	1:A:344:MET:SD	2.22	0.79
1:A:297:PHE:HB2	1:A:301:GLU:HG3	1.67	0.76
1:A:27:LEU:HB3	1:A:33:LEU:HD13	1.65	0.76
1:A:441:MET:HE3	1:A:443:ILE:HD11	1.67	0.75
1:B:263:ARG:HB2	1:B:263:ARG:NH1	2.01	0.75
1:B:530:ILE:HD13	1:B:530:ILE:O	1.88	0.74
1:B:328:ILE:HD13	1:B:336:ARG:O	1.88	0.74
1:A:104:GLU:O	1:A:107:VAL:HG22	1.87	0.73
1:B:263:ARG:NH1	1:B:268:LEU:HD13	2.04	0.72
1:B:263:ARG:HH12	1:B:268:LEU:HD13	1.54	0.72
1:A:450:VAL:HG22	1:A:497:ILE:CD1	2.22	0.70
1:A:450:VAL:HG22	1:A:497:ILE:HD12	1.75	0.68
1:A:460:MET:HE1	1:B:528:SER:HA	1.76	0.67
1:A:441:MET:CE	1:A:443:ILE:HD11	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:HG2	1:A:164:GLU:OE2	1.95	0.66
1:A:347:GLU:OE1	1:A:370:ARG:HD3	1.96	0.66
1:A:10:SER:HB3	3:A:1608:HOH:O	1.95	0.65
1:A:116:GLU:O	1:A:120:LYS:HG3	1.96	0.65
1:A:137:LEU:HD13	1:A:296:TYR:OH	1.96	0.65
1:A:66:ASP:OD1	1:A:68:SER:HB3	1.97	0.64
1:A:170:HIS:HD2	1:A:198:PRO:O	1.80	0.64
1:A:280:MET:HE1	1:A:384:TYR:CE2	2.33	0.64
1:A:294:GLN:HG3	1:A:296:TYR:CZ	2.33	0.64
1:A:162:PHE:HB2	1:A:163:PRO:HD2	1.80	0.63
1:A:443:ILE:HD12	1:A:443:ILE:N	2.15	0.62
1:B:232:VAL:HG22	1:B:238:ILE:CD1	2.30	0.62
1:B:146:GLU:O	1:B:150:ARG:HD3	1.99	0.61
1:A:148:ARG:C	1:A:148:ARG:HD2	2.26	0.61
1:B:328:ILE:HD13	1:B:328:ILE:H	1.66	0.60
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.84	0.60
1:B:496:ILE:HD12	1:B:496:ILE:N	2.16	0.60
1:A:188:ARG:HH21	1:A:188:ARG:HG2	1.65	0.60
1:B:263:ARG:HH11	1:B:263:ARG:CB	2.11	0.60
1:A:222:ILE:HD12	1:A:222:ILE:N	2.16	0.60
1:B:22:GLU:O	1:B:26:ILE:HG12	2.02	0.59
1:B:26:ILE:HD11	3:B:1355:HOH:O	2.01	0.59
1:A:206:ASP:CG	1:A:208:GLU:HG2	2.26	0.59
1:A:105:PHE:O	1:A:136:PRO:HG3	2.02	0.59
1:A:73:GLN:HG2	1:A:89:GLU:HA	1.84	0.59
1:A:526:PRO:HG3	3:B:1193:HOH:O	2.03	0.59
1:B:9:ALA:HB3	3:B:1249:HOH:O	2.02	0.58
1:B:106:GLU:O	1:B:110:GLN:HG3	2.03	0.58
1:A:419:ILE:HD13	1:A:429:PRO:HA	1.86	0.58
1:B:125:ARG:HG2	1:B:194:VAL:HG23	1.84	0.58
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.86	0.58
1:A:324:LEU:HB2	1:A:342:ILE:HB	1.84	0.58
1:A:222:ILE:HD13	1:A:318:LEU:HD21	1.85	0.58
1:A:271:ILE:HG22	1:A:272:ILE:HG13	1.86	0.58
1:A:277:ILE:HD12	1:A:277:ILE:N	2.19	0.58
1:A:460:MET:HE3	1:A:467:GLY:HA3	1.86	0.57
1:B:267:ARG:HG2	1:B:267:ARG:HH11	1.68	0.57
1:A:24:GLN:O	1:A:28:ARG:HG2	2.05	0.57
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.40	0.57
1:B:530:ILE:HD13	1:B:530:ILE:C	2.30	0.57
1:A:72:PRO:HG2	1:A:90:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:HD12	1:B:327:VAL:HG12	1.87	0.56
1:A:85:ILE:HD12	1:A:85:ILE:N	2.21	0.56
1:B:351:ILE:HD12	1:B:351:ILE:N	2.21	0.56
1:A:53:SER:HB3	3:A:1582:HOH:O	2.06	0.56
1:A:460:MET:HE2	1:A:466:ARG:C	2.30	0.56
1:B:59:ARG:CZ	1:B:85:ILE:HD13	2.35	0.56
1:B:39:ILE:HD12	1:B:333:GLY:HA2	1.88	0.56
1:B:101:LEU:HD13	1:B:151:ARG:HH21	1.71	0.56
1:B:372:VAL:C	1:B:373:ILE:HD12	2.30	0.56
1:A:206:ASP:OD1	1:A:208:GLU:HG2	2.06	0.55
1:A:328:ILE:C	1:A:328:ILE:HD12	2.31	0.55
3:A:1411:HOH:O	1:B:621:PRO:HD2	2.06	0.55
1:A:255:VAL:CG2	1:A:342:ILE:HD12	2.37	0.55
1:A:260:ILE:HD12	1:A:260:ILE:N	2.22	0.55
1:A:443:ILE:HD12	1:A:443:ILE:H	1.72	0.55
1:A:547:ALA:HB3	1:A:550:GLU:HG3	1.87	0.55
1:B:71:ARG:HD3	1:B:89:GLU:HG2	1.89	0.54
1:A:367:ARG:HD3	1:B:315:CYS:O	2.08	0.54
1:B:101:LEU:HD13	1:B:151:ARG:NH2	2.22	0.54
1:A:42:LEU:C	1:A:42:LEU:HD23	2.32	0.54
1:A:27:LEU:HB2	1:A:33:LEU:HD22	1.89	0.53
3:A:1577:HOH:O	1:B:490:ARG:HD3	2.08	0.53
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.43	0.53
1:A:286:ASP:CG	1:A:419:ILE:HD11	2.34	0.53
1:A:78:SER:CB	1:A:85:ILE:HD11	2.33	0.53
1:A:447:THR:HG21	1:A:501:GLU:OE2	2.08	0.53
1:B:451:GLU:HG2	1:B:476:VAL:HG22	1.92	0.52
1:A:106:GLU:O	1:A:110:GLN:HG3	2.10	0.52
1:A:370:ARG:O	1:A:370:ARG:HG2	2.09	0.52
1:A:85:ILE:HD12	1:A:85:ILE:H	1.75	0.52
1:B:373:ILE:HD12	1:B:373:ILE:N	2.25	0.52
1:A:36:GLU:O	1:A:66:ASP:HA	2.10	0.52
1:A:61:ARG:NH1	3:A:1401:HOH:O	2.41	0.52
1:A:39:ILE:HD12	1:A:333:GLY:HA2	1.93	0.51
1:A:434:ILE:HD13	1:A:589:GLY:HA3	1.92	0.51
1:A:280:MET:HG3	1:A:435:PHE:CE2	2.45	0.51
1:B:190:ILE:HD12	1:B:190:ILE:N	2.25	0.51
1:B:298:ASP:HB3	1:B:379:ILE:HD13	1.92	0.51
1:A:483:ALA:HB1	1:A:543:VAL:HB	1.93	0.51
1:A:341:GLY:O	1:A:342:ILE:HD13	2.11	0.51
1:A:375:PHE:CE1	1:A:386:PHE:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG21	1:A:422:LEU:HD11	1.93	0.51
1:A:152:ILE:HG22	1:A:153:LEU:N	2.25	0.51
1:B:111:LEU:HD12	1:B:179:VAL:HG11	1.93	0.51
1:A:28:ARG:HG3	1:A:29:THR:N	2.26	0.51
1:A:63:PHE:HB3	1:A:98:LEU:HD22	1.93	0.51
1:A:29:THR:HG21	3:A:1250:HOH:O	2.10	0.51
1:A:443:ILE:H	1:A:448:ASN:HD21	1.58	0.50
1:B:553:PRO:HA	1:B:567:LEU:HG	1.93	0.50
1:A:246:ASP:HB2	1:A:258:HIS:HB2	1.94	0.50
1:B:150:ARG:HD2	3:B:1450:HOH:O	2.11	0.50
1:A:36:GLU:HA	1:A:67:VAL:HG22	1.94	0.49
1:B:595:ARG:HG3	3:B:1256:HOH:O	2.12	0.49
1:A:22:GLU:O	1:A:26:ILE:HG12	2.13	0.49
1:A:220:ILE:HG22	1:A:222:ILE:HD11	1.94	0.49
1:B:479:ARG:HB3	1:B:574:ASP:OD1	2.14	0.48
1:B:220:ILE:HD12	1:B:220:ILE:N	2.28	0.48
1:B:324:LEU:HB2	1:B:342:ILE:HB	1.95	0.48
1:B:488:ASP:HB3	1:B:491:THR:HG22	1.96	0.48
1:A:183:SER:OG	1:A:185:GLU:HG2	2.14	0.47
1:A:277:ILE:HD11	1:A:398:PHE:CE1	2.49	0.47
1:A:318:LEU:HD12	1:A:319:GLY:H	1.79	0.47
1:A:241:GLU:O	1:A:242:LYS:HB2	2.14	0.47
1:B:613:PRO:HD2	3:B:1261:HOH:O	2.14	0.47
1:A:603:PRO:HG2	3:A:1411:HOH:O	2.14	0.47
1:B:294:GLN:HG2	1:B:296:TYR:OH	2.14	0.47
1:A:28:ARG:HA	1:A:33:LEU:HB2	1.97	0.47
1:A:515:HIS:HE1	3:A:1112:HOH:O	1.98	0.47
1:A:321:ILE:N	1:A:321:ILE:HD12	2.29	0.47
1:B:321:ILE:HD12	1:B:321:ILE:N	2.30	0.47
1:A:260:ILE:HD12	1:A:260:ILE:H	1.79	0.47
1:A:23:VAL:HG13	1:A:77:VAL:HG21	1.97	0.46
1:A:319:GLY:C	1:A:321:ILE:HD12	2.41	0.46
1:B:522:LEU:HD11	1:B:530:ILE:HD12	1.97	0.46
1:A:182:VAL:HG23	1:A:183:SER:N	2.31	0.46
1:A:443:ILE:H	1:A:443:ILE:CD1	2.29	0.46
1:A:150:ARG:NE	1:A:180:ASP:OD2	2.48	0.46
1:B:350:GLY:HA2	1:B:367:ARG:NH2	2.31	0.46
1:A:180:ASP:OD1	1:A:182:VAL:HG22	2.16	0.46
1:B:317:CYS:HB3	1:B:321:ILE:HG12	1.97	0.46
1:A:105:PHE:HA	1:A:136:PRO:CG	2.47	0.45
1:A:441:MET:HE3	1:A:443:ILE:CD1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:TYR:HA	1:A:573:GLN:HE21	1.81	0.45
1:A:65:HIS:CG	1:A:66:ASP:N	2.84	0.45
1:A:154:ARG:HD2	1:A:293:TRP:CE3	2.51	0.45
1:B:39:ILE:HD12	1:B:333:GLY:CA	2.47	0.45
1:A:148:ARG:C	1:A:148:ARG:CD	2.88	0.45
1:B:328:ILE:HD13	1:B:328:ILE:N	2.31	0.45
1:A:460:MET:CE	1:A:467:GLY:HA3	2.46	0.45
1:B:51:ALA:C	1:B:53:SER:H	2.25	0.45
1:B:232:VAL:HG22	1:B:238:ILE:HD13	1.97	0.45
1:B:267:ARG:HG2	1:B:267:ARG:NH1	2.32	0.45
1:A:590:LEU:HD21	1:A:607:VAL:HB	1.99	0.45
1:B:401:LYS:HG2	1:B:606:THR:HG22	1.99	0.45
1:B:539:LYS:HD3	1:B:539:LYS:HA	1.80	0.44
1:B:369:ARG:HG3	3:B:1114:HOH:O	2.18	0.44
1:A:280:MET:HG3	1:A:435:PHE:CD2	2.52	0.44
1:A:553:PRO:HA	1:A:567:LEU:HG	2.00	0.44
1:B:194:VAL:CG2	3:B:1182:HOH:O	2.65	0.44
1:B:483:ALA:HB1	1:B:543:VAL:HB	1.99	0.43
1:B:233:THR:O	1:B:237:HIS:HB3	2.18	0.43
1:B:160:GLN:HG2	1:B:162:PHE:O	2.18	0.43
1:A:135:ALA:HA	1:A:136:PRO:HD3	1.76	0.43
1:A:153:LEU:O	1:A:179:VAL:HG22	2.18	0.43
1:B:51:ALA:C	1:B:53:SER:N	2.77	0.43
1:B:162:PHE:HB2	1:B:163:PRO:HD2	2.01	0.43
1:A:28:ARG:HG3	1:A:29:THR:H	1.83	0.43
1:A:15:ALA:HA	1:A:19:GLU:OE1	2.19	0.43
1:A:154:ARG:HD2	1:A:293:TRP:CD2	2.53	0.43
1:A:443:ILE:N	1:A:443:ILE:CD1	2.81	0.43
1:B:299:THR:HA	1:B:304:VAL:HG13	2.01	0.42
1:B:50:GLY:C	1:B:52:GLY:H	2.27	0.42
1:A:418:ASN:O	1:A:419:ILE:HD13	2.19	0.42
1:A:503:LYS:HD3	1:A:507:ASN:ND2	2.34	0.42
1:A:152:ILE:CG2	1:A:153:LEU:N	2.82	0.42
1:A:465:GLU:H	1:A:465:GLU:CD	2.28	0.42
1:B:152:ILE:HD13	1:B:180:ASP:HA	2.00	0.42
1:A:441:MET:HE2	1:A:497:ILE:HG13	2.01	0.42
1:A:450:VAL:HG22	1:A:497:ILE:HD13	2.00	0.42
1:A:590:LEU:CD2	1:A:607:VAL:HB	2.49	0.42
1:B:628:ASN:N	1:B:628:ASN:HD22	2.17	0.42
1:A:21:SER:HB3	3:A:1598:HOH:O	2.19	0.42
1:A:214:ARG:HG3	1:B:624:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:TRP:CE3	1:A:371:MET:HB2	2.55	0.42
1:B:42:LEU:HD13	1:B:329:SER:HB2	2.02	0.42
1:B:404:GLY:O	1:B:601:ILE:HD12	2.20	0.42
1:B:562:SER:HB2	3:B:1115:HOH:O	2.19	0.42
1:A:87:ALA:HB1	3:A:1307:HOH:O	2.19	0.41
1:B:42:LEU:C	1:B:42:LEU:HD23	2.45	0.41
1:B:241:GLU:O	1:B:242:LYS:HB2	2.20	0.41
1:A:10:SER:HA	1:A:11:PRO:HD3	1.87	0.41
1:A:536:PHE:HA	1:A:542:TRP:CZ2	2.56	0.41
1:A:529:SER:HA	1:A:532:ARG:NH1	2.35	0.41
1:A:302:TYR:O	1:A:303:LEU:HB2	2.20	0.41
1:A:282:VAL:HA	1:A:432:GLN:O	2.21	0.41
1:B:219:PRO:C	1:B:220:ILE:HD12	2.46	0.41
1:A:436:SER:HB2	1:A:536:PHE:CE2	2.56	0.41
1:B:71:ARG:NH1	3:B:1210:HOH:O	2.52	0.41
1:B:108:VAL:HG12	1:B:134:VAL:HG11	2.03	0.41
1:A:240:TRP:O	1:A:241:GLU:C	2.64	0.40
1:A:95:THR:O	1:A:557:PHE:HB2	2.21	0.40
1:A:221:SER:C	1:A:222:ILE:HD12	2.46	0.40
1:A:484:VAL:HG12	1:A:539:LYS:HG3	2.03	0.40
1:B:59:ARG:NE	1:B:85:ILE:HD13	2.36	0.40
1:A:602:MET:HA	1:A:603:PRO:HD3	1.85	0.40
1:B:154:ARG:HD2	1:B:293:TRP:CE3	2.56	0.40
1:A:106:GLU:N	1:A:106:GLU:CD	2.80	0.40
1:A:109:GLU:HB2	1:A:134:VAL:HB	2.02	0.40
1:A:142:PHE:CZ	1:A:293:TRP:HA	2.56	0.40
1:A:229:SER:HA	1:B:218:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

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	617/628 (98%)	589 (96%)	27 (4%)	1 (0%)	44	31
1	B	617/628 (98%)	588 (95%)	28 (4%)	1 (0%)	44	31
All	All	1234/1256 (98%)	1177 (95%)	55 (4%)	2 (0%)	44	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	627	ALA
1	A	55	ALA

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	513/521 (98%)	509 (99%)	4 (1%)	79	76
1	B	513/521 (98%)	507 (99%)	6 (1%)	67	62
All	All	1026/1042 (98%)	1016 (99%)	10 (1%)	73	68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	164	GLU
1	A	268	LEU
1	A	376	PHE
1	B	263	ARG
1	B	328	ILE
1	B	358	LEU
1	B	376	PHE
1	B	420	SER
1	B	530	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	170	HIS
1	A	294	GLN
1	A	309	ASN
1	A	458	GLN
1	A	507	ASN
1	A	515	HIS
1	A	519	GLN
1	A	573	GLN
1	A	628	ASN
1	B	126	ASN
1	B	224	GLN
1	B	306	GLN
1	B	340	ASN
1	B	345	HIS
1	B	418	ASN
1	B	507	ASN
1	B	519	GLN
1	B	628	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	3TY	A	382	1	22,23,24	2.53	11 (50%)	19,30,32	1.78	3 (15%)
1	3TY	B	382	1	22,23,24	2.35	11 (50%)	19,30,32	1.81	2 (10%)

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
1	3TY	A	382	1	-	1/10/28/30	0/2/2/2
1	3TY	B	382	1	-	1/10/28/30	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	3TY	C5-N5	7.06	1.43	1.31
1	B	382	3TY	C5-N5	6.87	1.42	1.31
1	A	382	3TY	C1-C2	4.25	1.54	1.49
1	B	382	3TY	C1-C2	3.69	1.54	1.49
1	A	382	3TY	C3-C2	3.12	1.53	1.44
1	B	382	3TY	C3-C2	2.78	1.52	1.44
1	A	382	3TY	CT3-NB1	2.65	1.49	1.45
1	B	382	3TY	C3-C4	2.53	1.40	1.36
1	A	382	3TY	C3-C4	2.45	1.40	1.36
1	B	382	3TY	C4-C5	-2.36	1.42	1.46
1	A	382	3TY	CT6-CT5	2.34	1.42	1.38
1	B	382	3TY	CT3-NB1	2.32	1.48	1.45
1	A	382	3TY	CT9-CT4	2.31	1.43	1.38
1	A	382	3TY	CT5-CT4	2.28	1.43	1.38
1	A	382	3TY	C6-C1	2.26	1.40	1.34
1	B	382	3TY	CT9-CT4	2.22	1.43	1.38
1	B	382	3TY	CT5-CT4	2.18	1.43	1.38
1	B	382	3TY	CT6-CT5	2.13	1.42	1.38
1	A	382	3TY	CT8-CT9	2.12	1.42	1.38
1	A	382	3TY	CB-C1	2.08	1.54	1.50
1	B	382	3TY	C6-C1	2.05	1.39	1.34
1	B	382	3TY	CT8-CT9	2.03	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	3TY	C5-N5-NB1	6.16	130.29	118.05
1	A	382	3TY	C5-N5-NB1	5.99	129.94	118.05
1	A	382	3TY	C6-C5-C4	3.07	120.91	117.44
1	B	382	3TY	C6-C5-C4	3.04	120.88	117.44
1	A	382	3TY	CT4-CT3-NB1	2.08	114.92	111.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382	3TY	N-CA-CB-C1
1	B	382	3TY	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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, 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	619/628 (98%)	0.54	59 (9%) 15 13	17, 32, 52, 77	0
1	B	619/628 (98%)	0.01	14 (2%) 61 59	16, 26, 38, 74	0
All	All	1238/1256 (98%)	0.28	73 (5%) 29 27	16, 28, 49, 77	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	5.8
1	B	627	ALA	5.7
1	B	54	GLU	5.4
1	A	53	SER	5.0
1	A	148	ARG	4.9
1	B	52	GLY	4.8
1	A	52	GLY	4.7
1	A	26	ILE	4.4
1	B	51	ALA	4.4
1	B	53	SER	4.3
1	A	266	ASP	4.1
1	A	628	ASN	3.9
1	A	30	ALA	3.6
1	A	51	ALA	3.6
1	A	27	LEU	3.5
1	A	182	VAL	3.5
1	B	55	ALA	3.4
1	B	9	ALA	3.3
1	A	33	LEU	3.2
1	A	358	LEU	3.2
1	A	32	LEU	3.1
1	A	186	VAL	3.1
1	B	314	GLY	3.0
1	A	29	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	315	CYS	3.0
1	A	82	GLY	2.9
1	A	84	VAL	2.9
1	A	31	GLY	2.9
1	A	83	THR	2.8
1	A	39	ILE	2.8
1	A	314	GLY	2.8
1	B	358	LEU	2.7
1	A	332	PHE	2.7
1	A	64	ILE	2.7
1	A	111	LEU	2.7
1	A	56	GLU	2.6
1	A	70	ALA	2.6
1	A	238	ILE	2.6
1	A	501	GLU	2.5
1	A	34	GLY	2.5
1	A	184	LYS	2.5
1	A	71	ARG	2.5
1	A	55	ALA	2.5
1	A	68	SER	2.4
1	A	69	GLY	2.4
1	A	23	VAL	2.4
1	A	342	ILE	2.4
1	A	38	ARG	2.4
1	A	548	ASP	2.4
1	A	107	VAL	2.4
1	A	85	ILE	2.3
1	A	35	PRO	2.3
1	B	56	GLU	2.3
1	A	54	GLU	2.3
1	B	266	ASP	2.3
1	A	72	PRO	2.2
1	A	569	SER	2.2
1	A	87	ALA	2.2
1	A	180	ASP	2.2
1	B	267	ARG	2.2
1	A	189	VAL	2.2
1	B	315	CYS	2.1
1	A	150	ARG	2.1
1	A	37	LYS	2.1
1	A	36	GLU	2.1
1	A	28	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	ARG	2.1
1	A	119	LEU	2.0
1	A	146	GLU	2.0
1	A	190	ILE	2.0
1	A	50	GLY	2.0
1	A	181	VAL	2.0
1	B	313	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	3TY	A	382	22/23	0.90	0.12	24,38,47,48	0
1	3TY	B	382	22/23	0.96	0.08	19,29,34,34	0

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(Å ²)	Q<0.9
2	CU	B	701	1/1	0.99	0.03	22,22,22,22	0
2	CU	A	701	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.