



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:39 PM UTC

PDB ID : 4O5P / pdb_00004o5p
Title : Crystal structure of an uncharacterized protein from Pseudomonas aeruginosa
Authors : Hu, H.D.; Gao, Z.Q.; Zhang, H.; Dong, Y.H.
Deposited on : 2013-12-19
Resolution : 2.00 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
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

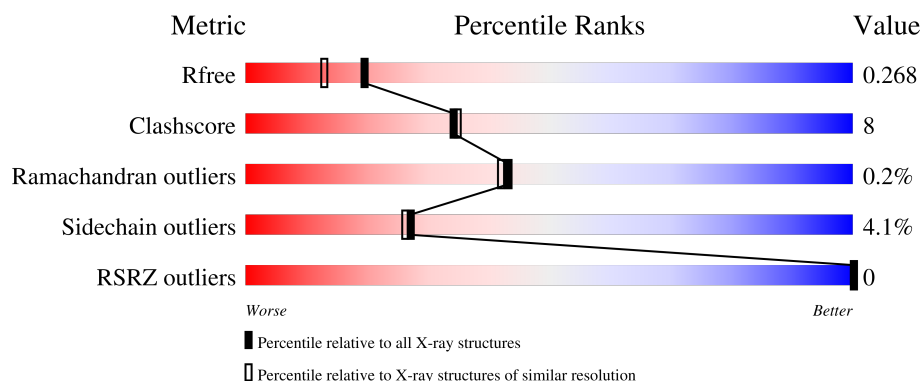
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	884	
1	B	884	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12543 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	Se	0	0	0
			5753	3626	1025	1080	8	14			
1	B	741	Total	C	N	O	S	Se	0	1	0
			5765	3636	1025	1082	8	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9HYV3
A	0	SER	-	expression tag	UNP Q9HYV3
B	-1	GLY	-	expression tag	UNP Q9HYV3
B	0	SER	-	expression tag	UNP Q9HYV3

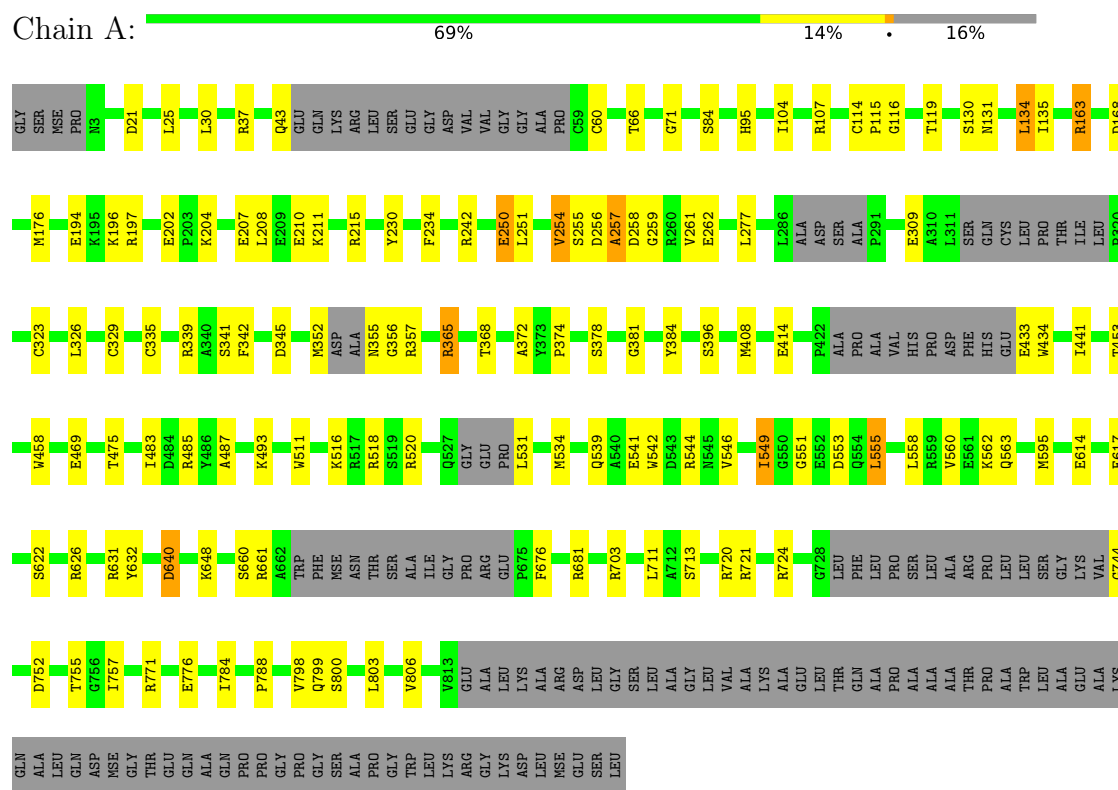
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	520	Total	O	0	0
			520	520		
2	B	505	Total	O	0	0
			505	505		

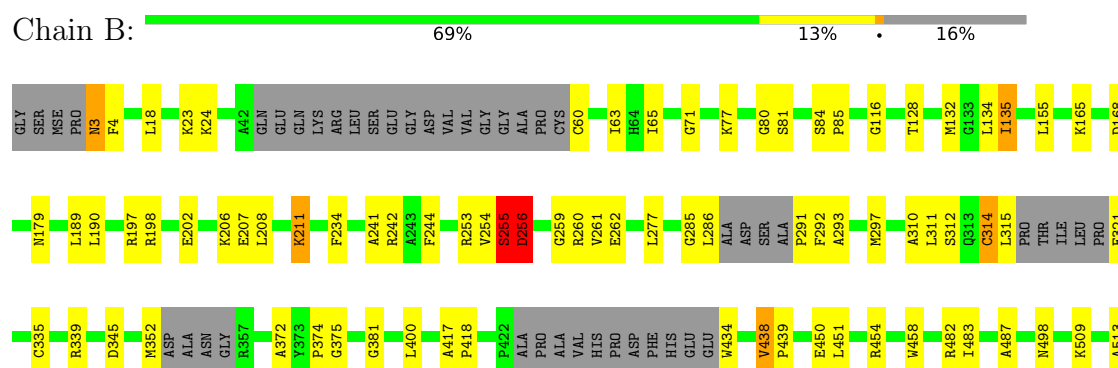
3 Residue-property plots [i](#)

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.60Å 81.08Å 92.14Å 97.83° 89.96° 90.01°	Depositor
Resolution (Å)	28.30 – 2.00 28.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (28.30-2.00) 91.7 (28.30-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.226 , 0.269 0.225 , 0.268	Depositor DCC
R_{free} test set	5464 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.480 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12543	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.53	2/5859 (0.0%)	0.84	6/7902 (0.1%)
1	B	0.55	1/5872 (0.0%)	0.88	7/7921 (0.1%)
All	All	0.54	3/11731 (0.0%)	0.86	13/15823 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	SER	CA-C	-6.59	1.44	1.52
1	A	631	ARG	C-O	-5.90	1.17	1.24
1	A	632	TYR	C-O	-5.56	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	GLY	N-CA-C	-7.85	105.34	114.69
1	B	764	GLY	N-CA-C	7.63	121.00	111.85
1	B	314	CYS	N-CA-C	6.49	118.00	108.14
1	B	626	ARG	N-CA-C	5.72	117.21	110.97
1	B	762	VAL	N-CA-C	-5.37	101.18	108.06
1	A	408	MSE	N-CA-C	-5.30	105.58	111.36
1	B	752	ASP	CA-C-N	-5.25	114.34	119.64
1	B	752	ASP	C-N-CA	-5.25	114.34	119.64
1	A	256	ASP	N-CA-C	-5.19	101.54	108.34
1	A	475	THR	N-CA-C	-5.08	105.82	111.36
1	A	788	PRO	CA-C-N	5.01	125.54	120.38
1	A	788	PRO	C-N-CA	5.01	125.54	120.38
1	B	4	PHE	N-CA-C	5.00	117.50	110.14

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	5753	0	5631	80	0
1	B	5765	0	5639	93	0
2	A	520	0	0	14	0
2	B	505	0	0	16	1
All	All	12543	0	11270	173	1

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 8.

All (173) 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:255:SER:HB3	1:B:261:VAL:HA	1.18	1.17
1:B:255:SER:CB	1:B:261:VAL:HA	1.81	1.09
1:B:255:SER:HB3	1:B:260:ARG:O	1.71	0.90
1:B:255:SER:HA	1:B:256:ASP:O	1.74	0.88
1:A:755:THR:HG23	1:A:757:ILE:H	1.39	0.84
1:B:255:SER:HB3	1:B:261:VAL:CA	2.07	0.80
1:A:721:ARG:NH2	1:A:744:GLY:O	2.16	0.78
1:B:255:SER:HB2	1:B:261:VAL:HG22	1.66	0.78
1:B:255:SER:CB	1:B:261:VAL:HG22	2.19	0.72
1:B:255:SER:OG	1:B:261:VAL:HG13	1.89	0.71
1:B:771:ARG:NH2	2:B:1208:HOH:O	2.22	0.71
1:B:755:THR:HG23	1:B:757:ILE:H	1.56	0.71
1:B:721:ARG:NH1	2:B:1377:HOH:O	2.25	0.69
1:B:253:ARG:NH1	2:B:1172:HOH:O	2.22	0.69
1:A:255:SER:HB3	1:A:261:VAL:HG22	1.76	0.68
1:B:616:ASP:OD2	1:B:694:ARG:HD3	1.94	0.67
1:A:215:ARG:NH1	2:A:1071:HOH:O	2.27	0.67
1:B:197:ARG:NH2	2:B:1111:HOH:O	2.19	0.67
1:A:703:ARG:NH2	1:A:784:ILE:O	2.28	0.66
1:B:579:GLU:OE2	1:B:661:ARG:NH2	2.30	0.64
1:A:595:MSE:HE2	1:A:721:ARG:O	1.97	0.64
1:A:771:ARG:NH2	2:A:1390:HOH:O	2.30	0.63
1:B:450:GLU:OE2	1:B:454:ARG:NE	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:NH1	2:A:1138:HOH:O	2.30	0.63
1:B:595:MSE:HE2	1:B:721:ARG:O	1.99	0.63
1:A:355:ASN:HB3	1:A:357:ARG:H	1.64	0.63
1:A:131:ASN:O	1:A:131:ASN:ND2	2.33	0.62
1:B:314:CYS:SG	1:B:315:LEU:N	2.73	0.61
1:B:255:SER:OG	1:B:261:VAL:HA	2.01	0.60
1:B:615:GLU:OE2	1:B:721:ARG:NH1	2.35	0.59
1:B:254:VAL:O	1:B:255:SER:OG	2.16	0.59
1:B:80:GLY:HA2	1:B:85:PRO:HB3	1.85	0.58
1:A:309:GLU:OE2	1:A:365:ARG:NH2	2.35	0.58
1:A:617:GLU:OE1	1:A:720:ARG:NH2	2.25	0.58
1:B:255:SER:HA	1:B:256:ASP:C	2.30	0.57
1:B:135:ILE:H	1:B:285:GLY:HA3	1.70	0.57
1:B:375:GLY:HA2	1:B:657:VAL:HG13	1.86	0.57
1:A:752:ASP:OD2	1:A:755:THR:HG22	2.05	0.56
1:B:752:ASP:OD2	1:B:755:THR:HG22	2.05	0.56
1:B:516:LYS:HG2	1:B:517:ARG:N	2.19	0.56
1:A:254:VAL:HG13	1:A:255:SER:H	1.71	0.56
1:B:255:SER:CB	1:B:261:VAL:CA	2.70	0.56
1:B:291:PRO:HB3	1:B:597:VAL:HG11	1.86	0.55
1:B:617:GLU:OE1	1:B:720:ARG:NH2	2.30	0.55
1:B:71:GLY:O	1:B:116:GLY:HA3	2.07	0.55
1:B:242:ARG:HD2	1:B:277:LEU:HD13	1.89	0.55
1:A:511:TRP:CZ2	1:A:549:ILE:HG21	2.41	0.54
1:B:77:LYS:O	1:B:81:SER:HB3	2.07	0.54
1:A:130:SER:O	1:A:563:GLN:HG3	2.08	0.54
1:A:163:ARG:NH1	2:A:1395:HOH:O	2.39	0.54
1:A:250:GLU:HG2	1:A:251:LEU:N	2.24	0.53
1:B:482:ARG:NH2	2:B:940:HOH:O	2.27	0.53
1:B:614:GLU:HG3	1:B:720:ARG:NH1	2.24	0.52
1:A:595:MSE:HE3	1:A:720:ARG:NE	2.25	0.52
1:A:30:LEU:HA	1:A:37:ARG:HH22	1.73	0.52
1:A:257:ALA:C	1:A:259:GLY:H	2.17	0.52
1:A:541:GLU:HG2	1:A:544:ARG:HH21	1.74	0.52
1:A:798:VAL:HG23	1:A:799:GLN:HG3	1.91	0.51
1:B:255:SER:CB	1:B:260:ARG:O	2.52	0.51
1:A:242:ARG:HD2	1:A:277:LEU:HD13	1.93	0.50
1:B:168:ASP:HA	2:B:1392:HOH:O	2.11	0.50
1:B:80:GLY:HA2	1:B:85:PRO:CB	2.40	0.50
1:B:155:LEU:HB3	1:B:208:LEU:HD13	1.94	0.50
1:A:30:LEU:HD22	1:A:37:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:TRP:CE2	1:A:549:ILE:HD12	2.47	0.49
1:B:23:LYS:HB3	1:B:24:LYS:HZ2	1.76	0.49
1:A:384:TYR:O	2:A:1020:HOH:O	2.20	0.49
1:B:255:SER:HB3	1:B:260:ARG:C	2.35	0.49
1:B:198:ARG:NH2	2:B:1213:HOH:O	2.37	0.49
1:A:676:PHE:O	1:A:681:ARG:NH2	2.45	0.49
1:A:204:LYS:O	1:A:208:LEU:HG	2.13	0.49
1:B:579:GLU:CD	1:B:661:ARG:HH22	2.20	0.49
1:A:434:TRP:H	1:A:434:TRP:CD1	2.30	0.49
1:A:43:GLN:O	2:A:1172:HOH:O	2.20	0.48
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.60	0.48
1:B:63:ILE:HG22	1:B:65:ILE:HD11	1.95	0.48
1:B:614:GLU:HG2	1:B:721:ARG:O	2.13	0.48
1:B:483:ILE:O	1:B:487:ALA:HB3	2.14	0.48
1:B:509:LYS:HG3	2:B:1217:HOH:O	2.14	0.48
1:A:196:LYS:NZ	2:A:1133:HOH:O	2.40	0.48
1:B:513:ALA:HA	1:B:516:LYS:HD3	1.95	0.48
1:A:493:LYS:NZ	1:A:640:ASP:OD1	2.43	0.48
1:A:378:SER:HB2	1:A:384:TYR:CE2	2.49	0.48
1:B:595:MSE:HE3	1:B:720:ARG:NE	2.29	0.48
1:B:3:ASN:HD22	1:B:3:ASN:N	2.11	0.47
1:A:339:ARG:NH1	2:A:1128:HOH:O	2.46	0.47
1:B:662:ALA:O	1:B:663:TRP:HE3	1.96	0.47
1:A:469:GLU:HG3	2:A:1008:HOH:O	2.14	0.47
1:B:134:LEU:HA	1:B:134:LEU:HD12	1.51	0.47
1:B:253:ARG:HH22	1:B:310:ALA:HB2	1.80	0.47
1:B:629:SER:O	1:B:632:TYR:HB3	2.15	0.47
1:A:71:GLY:O	1:A:116:GLY:HA3	2.15	0.47
1:B:165:LYS:HE3	1:B:165:LYS:HB2	1.74	0.46
1:B:211:LYS:HD2	2:B:1102:HOH:O	2.14	0.46
1:B:567:PRO:O	1:B:568:LEU:HD23	2.15	0.46
1:B:543:ASP:O	2:B:1402:HOH:O	2.20	0.46
1:B:234:PHE:CE1	1:B:381:GLY:HA3	2.50	0.46
1:B:255:SER:OG	1:B:261:VAL:HG22	2.16	0.46
1:A:483:ILE:O	1:A:487:ALA:HB3	2.16	0.45
1:A:66:THR:HA	1:A:230:TYR:O	2.16	0.45
1:A:255:SER:OG	1:A:261:VAL:HG13	2.15	0.45
1:A:30:LEU:CA	1:A:37:ARG:HH22	2.29	0.45
1:B:763:GLY:H	1:B:767:LEU:HD22	1.82	0.45
1:A:595:MSE:HE3	1:A:720:ARG:HE	1.80	0.45
1:A:614:GLU:HG2	1:A:721:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:ALA:O	1:B:527:GLN:NE2	2.50	0.45
1:B:374:PRO:HD3	1:B:458:TRP:CZ3	2.52	0.45
1:B:674:GLU:N	2:B:1371:HOH:O	2.50	0.44
1:A:323:CYS:SG	2:A:1400:HOH:O	2.61	0.44
1:B:259:GLY:O	1:B:312:SER:HB2	2.18	0.44
1:B:674:GLU:HG2	1:B:676:PHE:O	2.17	0.44
1:B:293:ALA:HB3	1:B:610:PHE:HB2	1.99	0.44
1:A:534:MSE:HE3	1:A:539:GLN:OE1	2.17	0.44
1:A:30:LEU:HD22	1:A:37:ARG:HH21	1.80	0.44
1:A:640:ASP:OD2	2:A:1138:HOH:O	2.20	0.44
1:B:335:CYS:SG	1:B:372:ALA:HB1	2.58	0.44
1:A:433:GLU:N	2:A:1309:HOH:O	2.50	0.43
1:B:603:LEU:HD22	1:B:702:GLY:C	2.43	0.43
1:B:3:ASN:N	1:B:3:ASN:ND2	2.66	0.43
1:A:339:ARG:CZ	1:A:660:SER:HB2	2.48	0.43
1:A:622:SER:O	1:A:626:ARG:HG3	2.19	0.43
1:B:339:ARG:NE	1:B:660:SER:HB3	2.33	0.43
1:B:532:PRO:HA	1:B:533:PRO:HD2	1.78	0.43
1:A:104:ILE:HD13	1:A:107:ARG:HH12	1.84	0.43
1:A:549:ILE:O	1:A:551:GLY:N	2.44	0.42
1:A:234:PHE:CE1	1:A:381:GLY:HA3	2.53	0.42
1:A:374:PRO:HD3	1:A:458:TRP:CZ3	2.54	0.42
1:A:21:ASP:O	1:A:25:LEU:HG	2.18	0.42
1:B:179:ASN:O	1:B:189:LEU:HD23	2.19	0.42
1:A:84:SER:O	1:A:84:SER:OG	2.26	0.42
1:A:335:CYS:SG	1:A:372:ALA:HB1	2.59	0.42
1:B:207:GLU:O	1:B:211:LYS:HG2	2.19	0.42
1:B:291:PRO:HA	1:B:292:PHE:HA	1.84	0.42
1:A:207:GLU:O	1:A:211:LYS:HG2	2.20	0.42
1:A:541:GLU:HG2	1:A:544:ARG:NH2	2.33	0.42
1:A:711:LEU:HD12	2:A:1164:HOH:O	2.19	0.42
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.83	0.42
1:B:241:ALA:O	1:B:244:PHE:HB3	2.20	0.42
1:A:95:HIS:HB3	1:A:441:ILE:HD12	2.01	0.42
1:A:204:LYS:HD3	1:A:204:LYS:HA	1.83	0.42
1:A:595:MSE:HE3	1:A:720:ARG:HG3	2.02	0.42
1:A:194:GLU:HG3	1:A:250:GLU:CD	2.45	0.41
1:A:755:THR:HG21	1:A:806:VAL:HG22	2.02	0.41
1:B:544:ARG:O	1:B:548:LEU:HD22	2.20	0.41
1:B:755:THR:HG21	1:B:757:ILE:HD12	2.02	0.41
1:A:800:SER:HB2	1:A:803:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:THR:HG21	1:A:648:LYS:HE3	2.01	0.41
1:B:498:ASN:HA	2:B:1240:HOH:O	2.18	0.41
1:A:176:MSE:HG2	1:A:197:ARG:HA	2.01	0.41
1:B:297:MSE:SE	2:B:1160:HOH:O	2.87	0.41
1:B:417:ALA:HA	1:B:418:PRO:HD3	1.90	0.41
1:B:434:TRP:N	2:B:1254:HOH:O	2.52	0.41
1:B:438:VAL:HG13	1:B:439:PRO:HD2	2.03	0.41
1:A:562:LYS:NZ	2:A:1271:HOH:O	2.53	0.41
1:B:206:LYS:HD3	1:B:206:LYS:HA	1.60	0.41
1:B:800:SER:HB3	1:B:803:LEU:HB2	2.02	0.41
1:A:341:SER:HG	1:A:342:PHE:HD1	1.65	0.41
1:A:520:ARG:CB	1:A:531:LEU:HD11	2.51	0.41
1:B:374:PRO:HB3	1:B:458:TRP:CE2	2.56	0.41
1:B:254:VAL:O	1:B:255:SER:CB	2.68	0.40
1:B:661:ARG:HD3	1:B:678:ASP:HB2	2.03	0.40
1:A:114:CYS:HA	1:A:115:PRO:HD2	1.97	0.40
1:A:326:LEU:HB3	1:A:365:ARG:NH2	2.36	0.40
1:A:542:TRP:O	1:A:546:VAL:HG23	2.21	0.40
1:A:555:LEU:O	1:A:558:LEU:HB2	2.20	0.40
1:A:614:GLU:HG3	1:A:720:ARG:NH1	2.37	0.40
1:B:541:GLU:HG2	2:B:1123:HOH:O	2.20	0.40
1:A:119:THR:HG22	1:A:562:LYS:HG2	2.03	0.40
1:B:60:CYS:N	2:B:990:HOH:O	2.54	0.40
1:B:400:LEU:HA	1:B:451:LEU:HD11	2.04	0.40
1:A:329:CYS:HB3	1:A:368:THR:HG22	2.04	0.40
1:A:614:GLU:OE2	1:A:720:ARG:HB2	2.22	0.40
1:B:595:MSE:HE3	1:B:720:ARG:HE	1.85	0.40

All (1) 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)
2:B:1264:HOH:O	2:B:1387:HOH:O[1_455]	2.17	0.03

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	724/884 (82%)	697 (96%)	26 (4%)	1 (0%)	48	46
1	B	724/884 (82%)	702 (97%)	20 (3%)	2 (0%)	36	35
All	All	1448/1768 (82%)	1399 (97%)	46 (3%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ALA
1	B	255	SER
1	B	256	ASP

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	596/687 (87%)	569 (96%)	27 (4%)	24	23
1	B	598/687 (87%)	576 (96%)	22 (4%)	30	30
All	All	1194/1374 (87%)	1145 (96%)	49 (4%)	27	26

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	CYS
1	A	134	LEU
1	A	135	ILE
1	A	163	ARG
1	A	168	ASP
1	A	202	GLU
1	A	210	GLU
1	A	250	GLU
1	A	254	VAL

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Mol	Chain	Res	Type
1	A	258	ASP
1	A	262	GLU
1	A	345	ASP
1	A	352	MSE
1	A	365	ARG
1	A	396	SER
1	A	414	GLU
1	A	516	LYS
1	A	518	ARG
1	A	549	ILE
1	A	553	ASP
1	A	555	LEU
1	A	560	VAL
1	A	640	ASP
1	A	661	ARG
1	A	713	SER
1	A	724	ARG
1	A	776	GLU
1	B	3	ASN
1	B	18	LEU
1	B	84	SER
1	B	128	THR
1	B	132	MSE
1	B	135	ILE
1	B	202	GLU
1	B	211	LYS
1	B	255	SER
1	B	256	ASP
1	B	262	GLU
1	B	286	LEU
1	B	311	LEU
1	B	321	GLU
1	B	345	ASP
1	B	352	MSE
1	B	438	VAL
1	B	516	LYS
1	B	548	LEU
1	B	585	LYS
1	B	590	VAL
1	B	762	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	179	ASN
1	A	223	HIS
1	B	105	ASN
1	B	131	ASN
1	B	179	ASN
1	B	507	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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	728/884 (82%)	-1.28	0 100 100	11, 24, 42, 65	2 (0%)
1	B	727/884 (82%)	-1.30	0 100 100	9, 24, 41, 56	1 (0%)
All	All	1455/1768 (82%)	-1.29	0 100 100	9, 24, 42, 65	3 (0%)

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.