Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 09:35 pm BST

PDB ID	:	4O5P
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

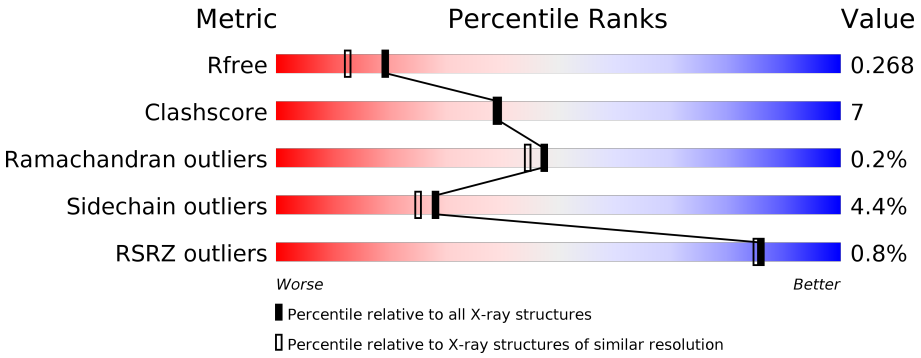
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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 <=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	% 70% 13% • 16%
1	B	884	% 70% 13% • 16%

2 Entry composition (i)

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.

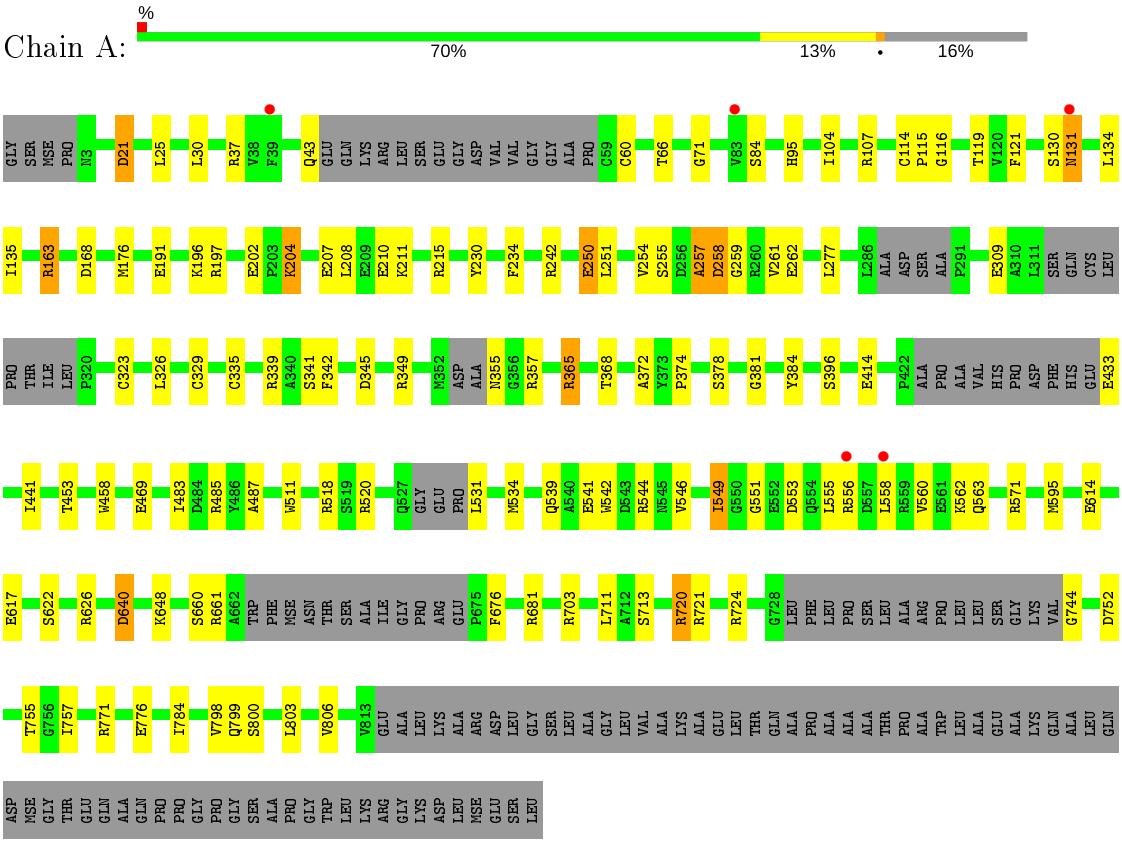
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	520	Total	O	0	0
			520	520		
2	B	505	Total	O	0	0
			505	505		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

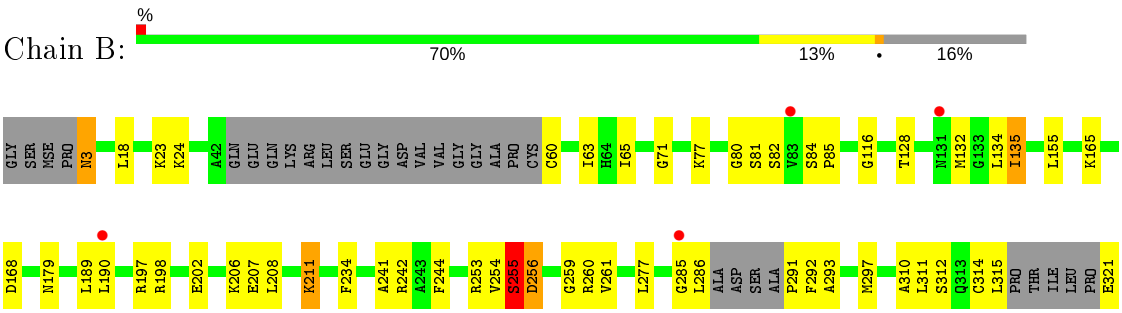
- Molecule 1: Uncharacterized protein

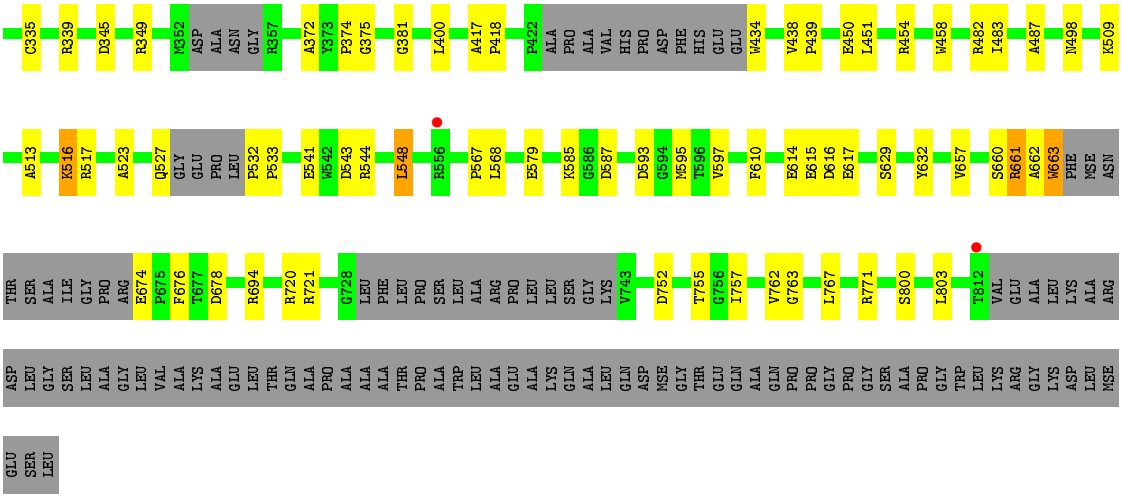
Chain A:



- Molecule 1: Uncharacterized protein

Chain B:




C335 R339 D345 R349 M352 ASP ALA ASN GLY R357 A372 Y373 P374 G375 G381 L400 A417 P418 P422 ALA PRO ALA VAL HIS PRO ASP PHE HIS GLU GLU W434 V438 P439 E450 L451 R454 W458 R482 I483 A487 N498 K509
A513 K516 R517 A523 Q527 GLY GLU PRO LEU P532 P533 E541 W542 D543 R544 L548 R556 P567 L568 E579 K585 G586 D587 D593 G594 M595 T596 V597 F610 E614 E615 D616 E617 S629 Y632 V657 S660 R661 A662 W663 PHE MSE ASN
THR SER ALA ILE GLY PRO ARG E674 P675 F676 T677 D678 R694 R720 R721 G728 LEU PHE LEU PRO SER LEU ALA ARG PRO LEU LEU SER GLY LYS V743 D752 T755 G756 I757 V762 G763 L767 R771 S800 L803 T812 VAL GLU ALA LEU LYS ARG
ASP LEU GLY SER LEU ALA GLY LEU VAL ALA LYS ALA GLU LEU THR GLN ALA PRO ALA ALA ALA THR PRO ALA TRP LEU ALA GLU ALA LYS GLN ALA LEU GLN ASP MSE GLY THR GLU GLN ALA GLN PRO PRO GLY PRO GLY SER ALA PRO GLY TRP LEU LYS ARG GLY LYS ASP LEU MSE
GLU SER LEU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	5443 reflections (4.98%)	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)	0.30 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.480 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	1/5859 (0.0%)	0.60	1/7902 (0.0%)
1	B	0.45	0/5872	0.62	0/7921
All	All	0.44	1/11731 (0.0%)	0.61	1/15823 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	ASP	CB-CG	-5.12	1.41	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	720	ARG	NE-CZ-NH1	5.15	122.88	120.30

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	77	0
1	B	5765	0	5639	92	0
2	A	520	0	0	13	0
2	B	505	0	0	16	1
All	All	12543	0	11270	169	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 7.

All (169) 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
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:ND2	1:A:131:ASN:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:SER:HA	1:B:256:ASP:C	2.30	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: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:155:LEU:HB3	1:B:208:LEU:HD13	1.94	0.50
1:B:80:GLY:HA2	1:B:85:PRO:CB	2.40	0.50
1:A:30:LEU:HD22	1:A:37:ARG:NH2	2.27	0.49
1:A:511:TRP:CE2	1:A:549:ILE:HD12	2.47	0.49
1:A:384:TYR:O	2:A:1020:HOH:O	2.20	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:A:134:LEU:HD12	1:A:134:LEU:HA	1.60	0.48
1:A:43:GLN:O	2:A:1172:HOH:O	2.20	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:23:LYS:HB3	1:B:24:LYS:HZ2	1.78	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:B:513:ALA:HA	1:B:516:LYS:HD3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ALA:C	1:A:259:GLY:H	2.17	0.47
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:A:341:SER:HG	1:A:342:PHE:HD1	1.59	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:255:SER:OG	1:B:261:VAL:HG22	2.16	0.46
1:B:234:PHE:CE1	1:B:381:GLY:HA3	2.50	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
1:B:523:ALA:O	1:B:527:GLN:NE2	2.50	0.45
1:B:255:SER:HB3	1:B:260:ARG:C	2.35	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:B:579:GLU:CD	1:B:661:ARG:HH22	2.20	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:3:ASN:ND2	1:B:3:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:GLU:OE1	1:A:196:LYS:NZ	2.50	0.42
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:335:CYS:SG	1:A:372:ALA:HB1	2.59	0.42
1:A:84:SER:O	1:A:84:SER:OG	2.26	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: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:95:HIS:HB3	1:A:441:ILE:HD12	2.01	0.42
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
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:B:206:LYS:HA	1:B:206:LYS:HD3	1.60	0.41
1:A:562:LYS:NZ	2:A:1271:HOH:O	2.53	0.41
1:B:800:SER:HB3	1:B:803:LEU:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:400:LEU:HA	1:B:451:LEU:HD11	2.04	0.40
1:B:60:CYS:N	2:B:990:HOH:O	2.54	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 (i)

5.3.1 Protein backbone (i)

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%)	51 49
1	B	724/884 (82%)	702 (97%)	20 (3%)	2 (0%)	41 37
All	All	1448/1768 (82%)	1399 (97%)	46 (3%)	3 (0%)	47 44

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	596/687 (87%)	567 (95%)	29 (5%)	25	21
1	B	598/687 (87%)	575 (96%)	23 (4%)	33	31
All	All	1194/1374 (87%)	1142 (96%)	52 (4%)	28	25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	60	CYS
1	A	121	PHE
1	A	131	ASN
1	A	135	ILE
1	A	163	ARG
1	A	168	ASP
1	A	202	GLU
1	A	204	LYS
1	A	210	GLU
1	A	250	GLU
1	A	258	ASP
1	A	262	GLU
1	A	345	ASP
1	A	349	ARG
1	A	365	ARG
1	A	396	SER
1	A	414	GLU
1	A	518	ARG
1	A	549	ILE
1	A	553	ASP
1	A	556	ARG
1	A	560	VAL
1	A	571	ARG
1	A	640	ASP
1	A	661	ARG
1	A	713	SER

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Mol	Chain	Res	Type
1	A	724	ARG
1	A	776	GLU
1	B	3	ASN
1	B	18	LEU
1	B	82	SER
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	286	LEU
1	B	311	LEU
1	B	321	GLU
1	B	345	ASP
1	B	349	ARG
1	B	516	LYS
1	B	548	LEU
1	B	585	LYS
1	B	587	ASP
1	B	593	ASP
1	B	661	ARG
1	B	663	TRP
1	B	762	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	646	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	-0.26	5 (0%)	87	87	11, 24, 42, 65	2 (0%)
1	B	727/884 (82%)	-0.25	6 (0%)	86	85	11, 24, 41, 56	0
All	All	1455/1768 (82%)	-0.26	11 (0%)	86	85	11, 24, 42, 65	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	VAL	4.7
1	B	83	VAL	3.3
1	A	39	PHE	2.5
1	B	190	LEU	2.3
1	B	556	ARG	2.3
1	B	131	ASN	2.2
1	A	556	ARG	2.1
1	B	285	GLY	2.1
1	B	812	THR	2.1
1	A	131	ASN	2.1
1	A	558	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.