W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 02:02 PM EDT

|		
PDB ID	:	4OM9
Title	:	X-Ray Crystal Structure of the passenger domain of Plasmid encoded toxin, an Autrotansporter Enterotoxin from enteroaggregative Escherichia coli (EAEC)
Authors	:	Meza-Aguilar, J.D.; Fromme, P.; Torres-Larios, A.; Mendoza-Hernandez, G.; Hernandez-Chinas, U.; Arreguin-Espinosa de Los Monteros, R.A.; Eslava-Campos, C.A.; Fromme, R.
Deposited on	:	2014-01-27
Resolution	:	2.30 Å(reported)

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 2.30 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.
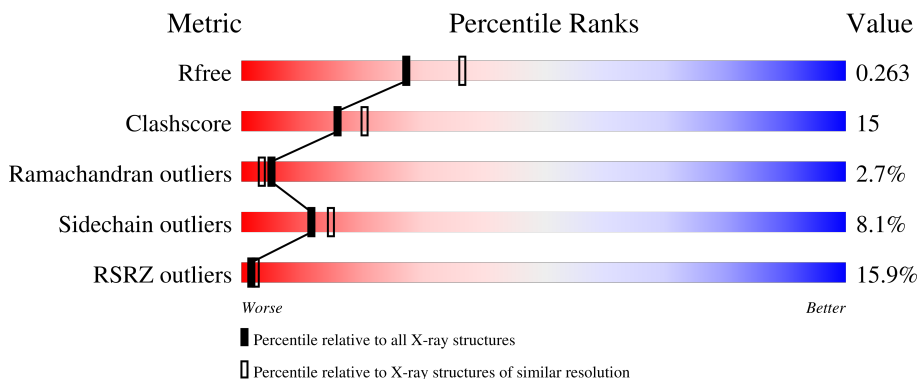
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	966	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7586 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 Serine protease pet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	930	Total	C	N	O	S	0	0	0
			7043	4368	1219	1446	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	543	Total	O	0	0
			543	543		

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: Serine protease pet
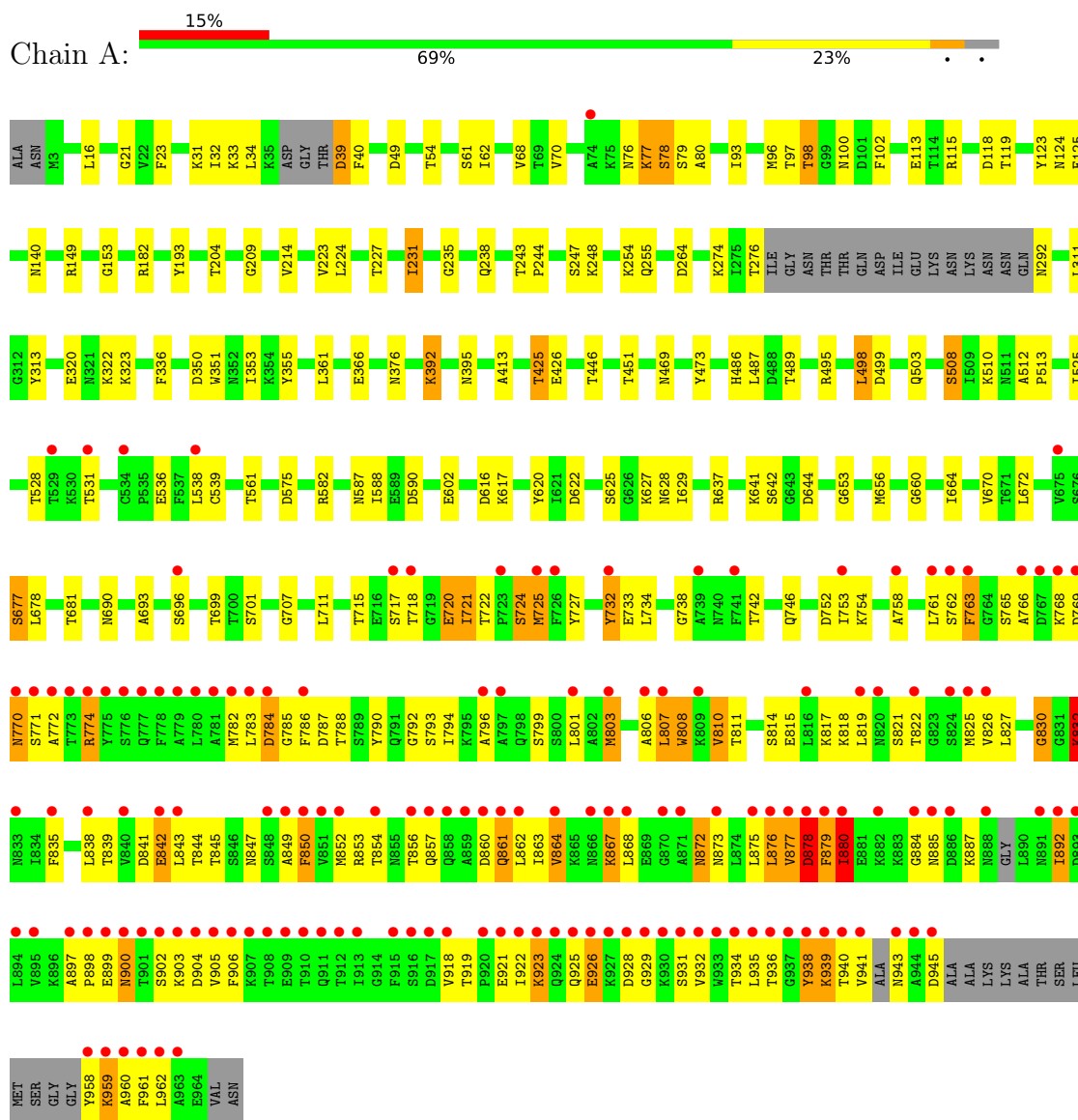
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.76Å 95.93Å 164.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.46 – 2.30 47.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.46-2.30) 99.6 (47.96-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1439)	Depositor
R, R_{free}	0.220 , 0.263 0.223 , 0.263	Depositor DCC
R_{free} test set	2814 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.0	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	0.46	0/7143	0.62	5/9656 (0.1%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	877	VAL	CB-CA-C	-8.13	95.96	111.40
1	A	878	ASP	N-CA-C	6.62	128.87	111.00
1	A	879	PHE	N-CA-C	5.98	127.16	111.00
1	A	877	VAL	N-CA-C	5.76	126.55	111.00
1	A	876	LEU	N-CA-C	5.57	126.05	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	878	ASP	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	7043	0	6844	203	0
2	A	543	0	0	55	2
All	All	7586	0	6844	203	2

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 15.

All (203) 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:A:124:ASN:ND2	2:A:1291:HOH:O	1.95	0.96
1:A:292:ASN:N	2:A:1004:HOH:O	2.02	0.92
1:A:446:THR:HG22	1:A:628:ASN:HB2	1.52	0.89
1:A:699:THR:HG22	1:A:701:SER:H	1.35	0.88
1:A:707:GLY:O	2:A:1481:HOH:O	1.91	0.87
1:A:923:LYS:HB2	1:A:934:THR:HG22	1.56	0.87
1:A:806:ALA:HB3	1:A:807:LEU:HD22	1.57	0.86
1:A:940:THR:HG23	2:A:1443:HOH:O	1.73	0.86
1:A:761:LEU:HB3	1:A:762:SER:HB3	1.59	0.84
1:A:561:THR:O	2:A:1025:HOH:O	1.96	0.83
1:A:724:SER:HB2	1:A:746:GLN:HB3	1.62	0.80
1:A:835:PHE:HB3	1:A:860:ASP:HB3	1.63	0.79
1:A:817:LYS:HG3	1:A:818:LYS:HG3	1.64	0.77
1:A:918:VAL:HG13	1:A:938:TYR:HB2	1.66	0.77
1:A:98:THR:O	2:A:1300:HOH:O	2.01	0.77
1:A:677:SER:OG	2:A:1520:HOH:O	2.02	0.76
1:A:782:MET:SD	2:A:1534:HOH:O	2.43	0.74
1:A:718:THR:HB	1:A:721:ILE:HB	1.69	0.74
1:A:486:HIS:NE2	1:A:508:SER:OG	2.16	0.73
1:A:885:ASN:HA	1:A:938:TYR:CE2	2.23	0.73
1:A:806:ALA:HB1	1:A:807:LEU:HA	1.72	0.72
1:A:693:ALA:O	1:A:727:TYR:OH	2.06	0.71
1:A:39:ASP:N	2:A:1370:HOH:O	2.22	0.71
1:A:238:GLN:OE1	2:A:1013:HOH:O	2.09	0.70
1:A:885:ASN:HA	1:A:938:TYR:HE2	1.56	0.69
1:A:786:PHE:N	1:A:787:ASP:HA	2.08	0.69
1:A:681:THR:HA	2:A:1509:HOH:O	1.92	0.69
1:A:366:GLU:OE2	2:A:1244:HOH:O	2.10	0.68
1:A:248:LYS:NZ	2:A:1494:HOH:O	2.21	0.68
1:A:853:ARG:O	2:A:1519:HOH:O	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ASP:OD2	2:A:1197:HOH:O	2.11	0.67
1:A:892:ILE:HG13	1:A:935:LEU:HD13	1.76	0.66
1:A:98:THR:HG23	1:A:100:ASN:H	1.61	0.66
1:A:209:GLY:O	2:A:1033:HOH:O	2.14	0.66
1:A:864:VAL:HG23	2:A:1471:HOH:O	1.96	0.65
1:A:49:ASP:OD2	2:A:1352:HOH:O	2.14	0.64
1:A:149:ARG:NE	2:A:1028:HOH:O	2.24	0.64
1:A:376:ASN:O	2:A:1224:HOH:O	2.14	0.64
1:A:469:ASN:ND2	2:A:1499:HOH:O	2.15	0.64
1:A:808:TRP:H	1:A:808:TRP:HD1	1.45	0.64
1:A:486:HIS:CE1	1:A:510:LYS:HE3	2.32	0.63
1:A:803:MET:HB2	1:A:821:SER:HA	1.81	0.63
1:A:119:THR:OG1	2:A:1474:HOH:O	2.16	0.62
1:A:425:THR:HG23	1:A:629:ILE:HB	1.82	0.62
1:A:900:ASN:ND2	1:A:902:SER:O	2.33	0.62
1:A:715:THR:HA	1:A:722:THR:HG22	1.83	0.61
1:A:98:THR:HG22	1:A:102:PHE:H	1.66	0.61
1:A:720:GLU:HB3	1:A:721:ILE:HD12	1.83	0.60
1:A:876:LEU:O	1:A:877:VAL:HG13	2.01	0.60
1:A:807:LEU:HB2	1:A:825:MET:HA	1.84	0.59
1:A:323:LYS:NZ	1:A:350:ASP:OD2	2.28	0.59
1:A:959:LYS:HE2	1:A:962:LEU:HD13	1.83	0.59
1:A:792:GLY:O	1:A:811:THR:N	2.29	0.59
1:A:867:LYS:HG2	1:A:900:ASN:HA	1.84	0.59
1:A:656:MET:HG2	2:A:1226:HOH:O	2.02	0.58
1:A:68:VAL:HG12	1:A:227:THR:HG21	1.84	0.58
1:A:413:ALA:N	2:A:1489:HOH:O	2.35	0.58
1:A:276:THR:O	2:A:1036:HOH:O	2.17	0.57
1:A:958:TYR:O	1:A:960:ALA:N	2.34	0.57
1:A:76:ASN:O	1:A:78:SER:N	2.38	0.57
1:A:718:THR:HG21	1:A:721:ILE:HD13	1.88	0.56
1:A:699:THR:HG22	1:A:701:SER:N	2.15	0.55
1:A:235:GLY:N	2:A:1141:HOH:O	2.17	0.55
1:A:732:TYR:HB3	1:A:752:ASP:O	2.06	0.55
1:A:842:GLU:N	2:A:1471:HOH:O	2.39	0.54
1:A:617:LYS:HG3	1:A:644:ASP:OD1	2.08	0.54
1:A:841:ASP:O	1:A:842:GLU:HB2	2.08	0.54
1:A:495:ARG:NE	2:A:1116:HOH:O	2.32	0.54
1:A:875:LEU:HB2	1:A:906:PHE:CD1	2.43	0.53
1:A:718:THR:HG22	1:A:720:GLU:H	1.73	0.53
1:A:451:THR:OG1	2:A:1245:HOH:O	2.19	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:GLU:H	1:A:929:GLY:C	2.11	0.53
1:A:140:ASN:N	2:A:1389:HOH:O	2.42	0.53
1:A:690:ASN:ND2	2:A:1447:HOH:O	2.40	0.53
1:A:525:ILE:HD11	1:A:627:LYS:HZ3	1.74	0.53
1:A:254:LYS:NZ	2:A:1180:HOH:O	2.42	0.52
1:A:34:LEU:HD11	1:A:40:PHE:HB2	1.91	0.52
1:A:62:ILE:HD11	1:A:224:LEU:HD22	1.92	0.52
1:A:660:GLY:C	2:A:1509:HOH:O	2.47	0.52
1:A:885:ASN:C	1:A:938:TYR:HD2	2.13	0.52
1:A:711:LEU:HB3	1:A:727:TYR:CE2	2.44	0.51
1:A:446:THR:CG2	1:A:629:ILE:HG12	2.40	0.51
1:A:945:ASP:OD2	1:A:958:TYR:N	2.43	0.51
1:A:724:SER:OG	1:A:725:MET:N	2.42	0.51
1:A:921:GLU:N	1:A:936:THR:OG1	2.40	0.51
1:A:113:GLU:OE1	1:A:113:GLU:N	2.43	0.51
1:A:123:TYR:O	1:A:182:ARG:NH2	2.32	0.51
1:A:392:LYS:HE3	1:A:395:ASN:OD1	2.11	0.51
1:A:734:LEU:HD22	1:A:754:LYS:HE3	1.93	0.51
1:A:838:LEU:HD23	1:A:839:THR:H	1.77	0.50
1:A:860:ASP:OD1	2:A:1519:HOH:O	2.18	0.50
1:A:495:ARG:HG2	1:A:513:PRO:HB2	1.92	0.50
1:A:753:ILE:HG23	1:A:794:ILE:HG12	1.94	0.50
1:A:762:SER:N	2:A:1495:HOH:O	2.20	0.50
1:A:794:ILE:HG13	1:A:808:TRP:CZ3	2.47	0.50
1:A:904:ASP:N	2:A:1160:HOH:O	2.44	0.50
1:A:77:LYS:O	1:A:79:SER:N	2.44	0.49
1:A:590:ASP:OD2	2:A:1292:HOH:O	2.20	0.49
1:A:786:PHE:CE1	1:A:959:LYS:HB2	2.47	0.49
1:A:876:LEU:HD22	1:A:876:LEU:N	2.27	0.49
1:A:877:VAL:O	1:A:878:ASP:HB2	2.13	0.49
1:A:854:THR:O	1:A:879:PHE:HD1	1.95	0.49
1:A:899:GLU:N	1:A:929:GLY:O	2.44	0.49
1:A:582:ARG:HD3	1:A:602:GLU:HB3	1.94	0.49
1:A:852:MET:SD	1:A:861:GLN:HG3	2.52	0.49
1:A:118:ASP:OD1	1:A:223:VAL:HG22	2.13	0.49
1:A:884:GLY:O	1:A:938:TYR:HE2	1.94	0.49
1:A:696:SER:OG	1:A:725:MET:HB2	2.13	0.49
1:A:16:LEU:HD13	1:A:23:PHE:CD1	2.48	0.48
1:A:801:LEU:HG	1:A:803:MET:SD	2.52	0.48
1:A:753:ILE:HG22	1:A:790:TYR:OH	2.12	0.48
1:A:884:GLY:O	1:A:938:TYR:CE2	2.66	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:MET:SD	1:A:807:LEU:HD21	2.53	0.48
1:A:366:GLU:HB3	2:A:1244:HOH:O	2.13	0.48
1:A:808:TRP:CD1	1:A:808:TRP:N	2.82	0.48
1:A:817:LYS:HE2	1:A:818:LYS:HE3	1.95	0.48
1:A:664:ILE:HD13	1:A:670:VAL:HG21	1.96	0.48
1:A:732:TYR:CG	1:A:752:ASP:HB2	2.49	0.48
1:A:887:LYS:HD3	1:A:887:LYS:HA	1.69	0.48
1:A:93:ILE:HG21	1:A:313:TYR:CE1	2.49	0.48
1:A:786:PHE:N	1:A:787:ASP:CA	2.77	0.47
1:A:255:GLN:HG2	2:A:1175:HOH:O	2.14	0.47
1:A:873:ASN:ND2	1:A:905:VAL:O	2.46	0.47
1:A:742:THR:HA	1:A:762:SER:OG	2.15	0.47
1:A:762:SER:OG	1:A:763:PHE:N	2.46	0.47
1:A:616:ASP:OD1	1:A:617:LYS:N	2.48	0.47
1:A:752:ASP:OD1	1:A:793:SER:HB3	2.14	0.47
1:A:149:ARG:NH2	2:A:1028:HOH:O	2.47	0.46
1:A:446:THR:HG21	2:A:1020:HOH:O	2.15	0.46
1:A:425:THR:HB	1:A:426:GLU:H	1.53	0.46
1:A:738:GLY:HA2	1:A:758:ALA:O	2.15	0.46
1:A:940:THR:O	2:A:1444:HOH:O	2.20	0.46
1:A:96:MET:HE3	2:A:1124:HOH:O	2.15	0.46
1:A:681:THR:HG23	2:A:1509:HOH:O	2.16	0.45
1:A:926:GLU:HB2	1:A:932:VAL:HG22	1.98	0.45
1:A:934:THR:OG1	1:A:935:LEU:N	2.48	0.45
1:A:660:GLY:O	2:A:1509:HOH:O	2.21	0.45
1:A:806:ALA:CB	1:A:807:LEU:HA	2.42	0.45
1:A:153:GLY:HA3	1:A:204:THR:OG1	2.16	0.45
1:A:78:SER:C	1:A:80:ALA:H	2.19	0.45
1:A:852:MET:O	1:A:877:VAL:HA	2.17	0.45
1:A:938:TYR:CE1	1:A:939:LYS:O	2.70	0.44
1:A:311:LEU:HG	1:A:336:PHE:HE1	1.82	0.44
1:A:125:GLU:HA	2:A:1450:HOH:O	2.16	0.44
1:A:799:SER:O	1:A:817:LYS:HB3	2.18	0.44
1:A:622:ASP:HB3	1:A:625:SER:HB2	1.99	0.44
1:A:885:ASN:CA	1:A:938:TYR:CE2	2.97	0.44
1:A:898:PRO:O	1:A:900:ASN:N	2.42	0.44
1:A:941:VAL:HA	2:A:1444:HOH:O	2.18	0.44
1:A:473:TYR:HB3	1:A:498:LEU:HD12	2.00	0.44
1:A:503:GLN:OE1	2:A:1281:HOH:O	2.21	0.44
1:A:718:THR:HA	2:A:1118:HOH:O	2.18	0.44
1:A:742:THR:HA	1:A:762:SER:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:GLU:O	1:A:935:LEU:HA	2.17	0.44
1:A:78:SER:O	1:A:80:ALA:N	2.45	0.44
1:A:653:GLY:O	1:A:672:LEU:HA	2.18	0.43
1:A:575:ASP:OD1	1:A:575:ASP:N	2.49	0.43
1:A:721:ILE:HG13	1:A:774:ARG:HD2	1.99	0.43
1:A:746:GLN:N	1:A:787:ASP:O	2.51	0.43
1:A:746:GLN:H	1:A:787:ASP:HB2	1.83	0.43
1:A:830:GLY:HA2	1:A:853:ARG:CZ	2.47	0.43
1:A:587:ASN:OD1	2:A:1034:HOH:O	2.21	0.43
1:A:32:ILE:HD12	1:A:33:LYS:H	1.84	0.43
1:A:803:MET:SD	1:A:807:LEU:HD11	2.58	0.43
1:A:487:LEU:HD12	1:A:512:ALA:HB2	1.99	0.43
1:A:785:GLY:HA3	1:A:786:PHE:CD1	2.54	0.43
1:A:790:TYR:HD2	1:A:808:TRP:HB3	1.84	0.43
1:A:838:LEU:HD23	1:A:839:THR:N	2.33	0.43
1:A:786:PHE:HE1	1:A:959:LYS:HB2	1.84	0.43
1:A:641:LYS:HA	1:A:641:LYS:HD3	1.81	0.42
1:A:718:THR:HB	1:A:720:GLU:O	2.19	0.42
1:A:796:ALA:HB1	1:A:799:SER:OG	2.19	0.42
1:A:839:THR:O	1:A:839:THR:HG22	2.18	0.42
1:A:231:ILE:H	1:A:231:ILE:HD13	1.84	0.42
1:A:351:TRP:CH2	1:A:353:ILE:HD11	2.54	0.42
1:A:355:TYR:CG	1:A:361:LEU:HB2	2.53	0.42
1:A:897:ALA:HA	1:A:898:PRO:HD2	1.87	0.42
1:A:54:THR:HB	2:A:1045:HOH:O	2.20	0.42
1:A:885:ASN:HA	1:A:938:TYR:CD2	2.54	0.42
1:A:879:PHE:C	1:A:880:ILE:HG12	2.41	0.41
1:A:919:THR:OG1	1:A:939:LYS:HB2	2.20	0.41
1:A:838:LEU:O	1:A:861:GLN:NE2	2.53	0.41
1:A:149:ARG:CZ	2:A:1028:HOH:O	2.67	0.41
1:A:877:VAL:O	1:A:877:VAL:HG23	2.21	0.41
1:A:61:SER:O	1:A:62:ILE:HD12	2.19	0.41
1:A:320:GLU:O	1:A:322:LYS:HG2	2.21	0.41
1:A:770:ASN:HB3	1:A:771:SER:H	1.61	0.41
1:A:765:SER:HB3	1:A:768:LYS:HB2	2.02	0.41
1:A:21:GLY:HA3	2:A:1031:HOH:O	2.21	0.41
1:A:832:LYS:HD3	1:A:832:LYS:HA	1.88	0.40
1:A:867:LYS:HE2	1:A:898:PRO:HG2	2.03	0.40
1:A:815:GLU:N	2:A:1351:HOH:O	2.55	0.40
1:A:425:THR:HG23	1:A:629:ILE:CB	2.50	0.40
1:A:847:ASN:C	1:A:873:ASN:HA	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:ASN:C	1:A:938:TYR:CD2	2.95	0.40
1:A:243:THR:HA	1:A:244:PRO:HD3	1.95	0.40
1:A:808:TRP:CD2	1:A:810:VAL:HG22	2.56	0.40
1:A:819:LEU:HD13	1:A:843:LEU:HD13	2.02	0.40
1:A:903:LYS:NZ	1:A:925:GLN:HB2	2.36	0.40
1:A:918:VAL:CG1	1:A:938:TYR:HB2	2.45	0.40
1:A:119:THR:HA	2:A:1165:HOH:O	2.21	0.40
1:A:620:TYR:CD2	1:A:642:SER:HB3	2.56	0.40
1:A:786:PHE:H	1:A:788:THR:H	1.68	0.40

All (2) 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:A:1273:HOH:O	2:A:1295:HOH:O[4_554]	2.02	0.18
2:A:1049:HOH:O	2:A:1364:HOH:O[4_454]	2.04	0.16

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	918/966 (95%)	795 (87%)	98 (11%)	25 (3%)	5	3

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	763	PHE
1	A	842	GLU
1	A	863	ILE
1	A	880	ILE
1	A	959	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	78	SER
1	A	721	ILE
1	A	810	VAL
1	A	856	THR
1	A	717	SER
1	A	766	ALA
1	A	770	ASN
1	A	784	ASP
1	A	832	LYS
1	A	850	PHE
1	A	868	LEU
1	A	872	ASN
1	A	928	ASP
1	A	772	ALA
1	A	900	ASN
1	A	926	GLU
1	A	849	ALA
1	A	922	ILE
1	A	830	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	763/797 (96%)	701 (92%)	62 (8%)	11	15

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	39	ASP
1	A	70	VAL
1	A	97	THR
1	A	98	THR
1	A	115	ARG
1	A	193	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	VAL
1	A	231	ILE
1	A	247	SER
1	A	264	ASP
1	A	274	LYS
1	A	392	LYS
1	A	425	THR
1	A	489	THR
1	A	498	LEU
1	A	499	ASP
1	A	508	SER
1	A	528	THR
1	A	531	THR
1	A	536	GLU
1	A	538	LEU
1	A	539	CYS
1	A	588	ILE
1	A	637	ARG
1	A	677	SER
1	A	678	LEU
1	A	720	GLU
1	A	724	SER
1	A	725	MET
1	A	732	TYR
1	A	733	GLU
1	A	769	ASP
1	A	774	ARG
1	A	783	LEU
1	A	784	ASP
1	A	803	MET
1	A	807	LEU
1	A	808	TRP
1	A	814	SER
1	A	822	THR
1	A	826	VAL
1	A	827	LEU
1	A	832	LYS
1	A	844	THR
1	A	845	THR
1	A	850	PHE
1	A	857	GLN
1	A	861	GLN

Continued from previous page...

Mol	Chain	Res	Type
1	A	862	LEU
1	A	864	VAL
1	A	867	LYS
1	A	872	ASN
1	A	878	ASP
1	A	880	ILE
1	A	892	ILE
1	A	923	LYS
1	A	931	SER
1	A	938	TYR
1	A	939	LYS
1	A	943	ASN
1	A	961	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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 (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(Å²)	Q<0.9
1	A	930/966 (96%)	0.85	148 (15%)	1	2	23, 43, 148, 220	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	775	TYR	15.8
1	A	774	ARG	11.0
1	A	901	THR	11.0
1	A	868	LEU	10.4
1	A	962	LEU	10.3
1	A	778	PHE	9.7
1	A	961	PHE	8.9
1	A	943	ASN	8.4
1	A	908	THR	7.8
1	A	941	VAL	7.6
1	A	922	ILE	7.5
1	A	912	THR	6.9
1	A	779	ALA	6.7
1	A	717	SER	6.7
1	A	769	ASP	6.7
1	A	773	THR	6.5
1	A	780	LEU	6.5
1	A	877	VAL	6.4
1	A	905	VAL	6.3
1	A	933	TRP	6.2
1	A	920	PRO	6.2
1	A	909	GLU	6.1
1	A	935	LEU	6.0
1	A	898	PRO	6.0
1	A	777	GLN	5.9
1	A	884	GLY	5.8
1	A	900	ASN	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	929	GLY	5.5
1	A	906	PHE	5.4
1	A	782	MET	5.4
1	A	732	TYR	5.3
1	A	825	MET	5.1
1	A	807	LEU	5.0
1	A	766	ALA	4.9
1	A	934	THR	4.9
1	A	875	LEU	4.9
1	A	851	VAL	4.9
1	A	894	LEU	4.8
1	A	862	LEU	4.6
1	A	885	ASN	4.6
1	A	963	ALA	4.5
1	A	913	ILE	4.5
1	A	725	MET	4.5
1	A	857	GLN	4.4
1	A	783	LEU	4.4
1	A	939	LYS	4.4
1	A	926	GLU	4.3
1	A	892	ILE	4.2
1	A	876	LEU	4.2
1	A	850	PHE	4.1
1	A	907	LYS	4.1
1	A	776	SER	4.0
1	A	843	LEU	3.9
1	A	849	ALA	3.9
1	A	937	GLY	3.9
1	A	848	SER	3.8
1	A	910	THR	3.8
1	A	878	ASP	3.8
1	A	915	PHE	3.7
1	A	886	ASP	3.7
1	A	936	THR	3.7
1	A	880	ILE	3.7
1	A	840	VAL	3.6
1	A	803	MET	3.6
1	A	893	ASP	3.6
1	A	867	LYS	3.6
1	A	902	SER	3.6
1	A	917	ASP	3.5
1	A	960	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	786	PHE	3.4
1	A	538	LEU	3.4
1	A	767	ASP	3.4
1	A	897	ALA	3.4
1	A	854	THR	3.3
1	A	899	GLU	3.3
1	A	895	VAL	3.3
1	A	852	MET	3.3
1	A	761	LEU	3.3
1	A	816	LEU	3.3
1	A	882	LYS	3.2
1	A	864	VAL	3.2
1	A	797	ALA	3.2
1	A	944	ALA	3.2
1	A	921	GLU	3.2
1	A	871	ALA	3.2
1	A	762	SER	3.1
1	A	945	ASP	3.1
1	A	835	PHE	3.1
1	A	870	GLY	3.0
1	A	927	LYS	3.0
1	A	781	ALA	3.0
1	A	873	ASN	3.0
1	A	928	ASP	3.0
1	A	838	LEU	2.9
1	A	534	CYS	2.9
1	A	932	VAL	2.8
1	A	859	ALA	2.8
1	A	860	ASP	2.8
1	A	858	GLN	2.8
1	A	771	SER	2.8
1	A	931	SER	2.8
1	A	856	THR	2.8
1	A	809	LYS	2.8
1	A	801	LEU	2.7
1	A	904	ASP	2.7
1	A	806	ALA	2.7
1	A	866	ASN	2.7
1	A	958	TYR	2.7
1	A	891	ASN	2.7
1	A	826	VAL	2.7
1	A	819	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	940	THR	2.7
1	A	824	SER	2.6
1	A	796	ALA	2.6
1	A	529	THR	2.6
1	A	753	ILE	2.6
1	A	770	ASN	2.5
1	A	772	ALA	2.5
1	A	938	TYR	2.5
1	A	768	LYS	2.5
1	A	822	THR	2.5
1	A	842	GLU	2.4
1	A	903	LYS	2.4
1	A	833	ASN	2.4
1	A	923	LYS	2.3
1	A	916	SER	2.3
1	A	918	VAL	2.3
1	A	723	PRO	2.3
1	A	675	VAL	2.3
1	A	888	ASN	2.2
1	A	696	SER	2.2
1	A	531	THR	2.2
1	A	911	GLN	2.2
1	A	739	ALA	2.2
1	A	758	ALA	2.2
1	A	820	ASN	2.2
1	A	861	GLN	2.2
1	A	718	THR	2.2
1	A	763	PHE	2.1
1	A	741	PHE	2.1
1	A	924	GLN	2.1
1	A	879	PHE	2.1
1	A	959	LYS	2.1
1	A	925	GLN	2.0
1	A	726	PHE	2.0
1	A	930	LYS	2.0
1	A	74	ALA	2.0
1	A	784	ASP	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 monosaccharides 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.