



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 AM UTC

PDB ID : 4OM9 / pdb_00004om9
Title : X-Ray Crystal Structure of the passenger domain of Plasmid encoded toxin, an Autotransporter 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)

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
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

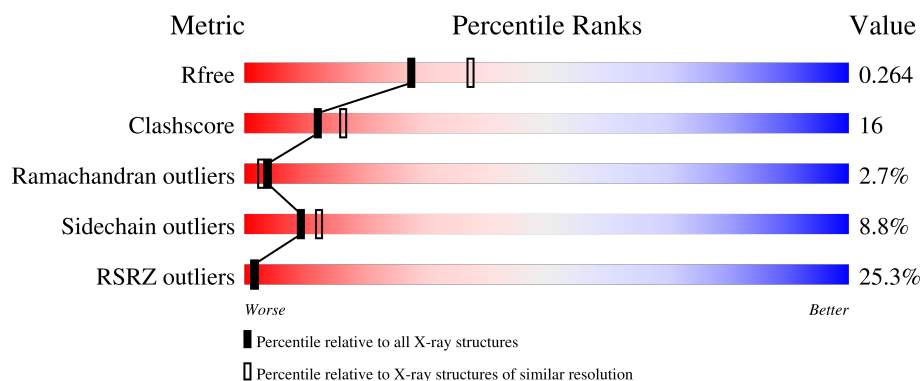
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	966	24% 68% 23% 5% .

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			

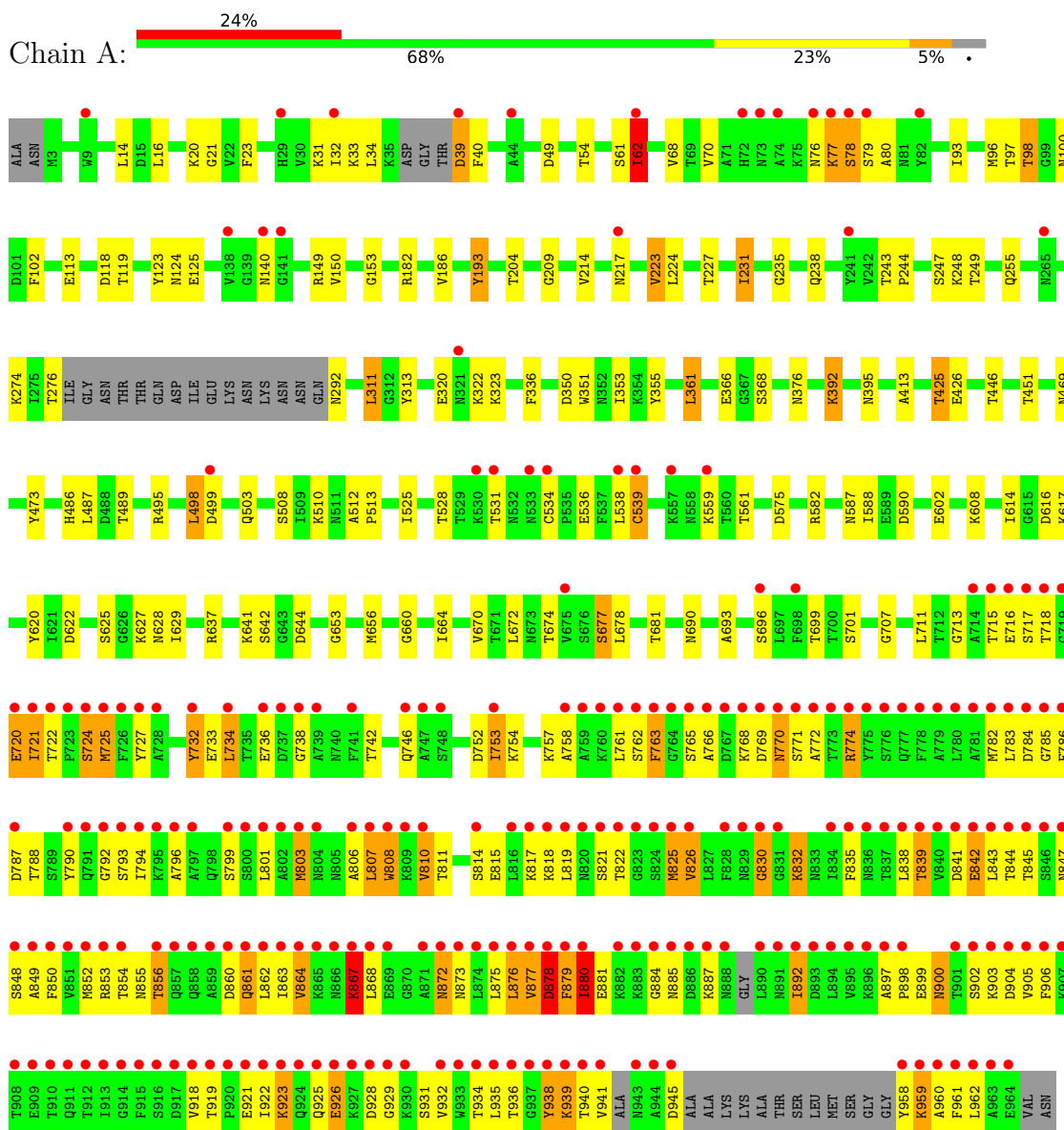
- Molecule 2 is water.

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 41.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.46-2.30) 99.6 (41.46-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1439)	Depositor
R, R_{free}	0.220 , 0.263 0.224 , 0.264	Depositor DCC
R_{free} test set	2814 reflections (5.06%)	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)	0.31 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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 i

5.1 Standard geometry i

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	0.59	6/7143 (0.1%)	0.90	13/9656 (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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	878	ASP	CA-C	8.07	1.62	1.52
1	A	876	LEU	CA-C	8.03	1.63	1.52
1	A	877	VAL	N-CA	6.81	1.54	1.46
1	A	876	LEU	N-CA	6.30	1.54	1.46
1	A	878	ASP	N-CA	6.23	1.54	1.46
1	A	877	VAL	CA-C	6.16	1.60	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	878	ASP	N-CA-C	13.13	128.87	107.73
1	A	877	VAL	CB-CA-C	-9.35	95.96	111.29
1	A	877	VAL	N-CA-C	8.27	126.55	109.34
1	A	879	PHE	N-CA-C	7.68	127.16	110.80
1	A	876	LEU	N-CA-C	7.16	126.05	110.80
1	A	825	MET	N-CA-C	6.95	117.15	108.19
1	A	839	THR	N-CA-C	6.53	118.09	107.32
1	A	62	ILE	N-CA-C	-6.08	106.83	112.43
1	A	826	VAL	N-CA-C	5.60	117.25	109.80
1	A	848	SER	N-CA-C	5.37	117.26	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	867	LYS	CB-CA-C	-5.28	108.92	115.89
1	A	368	SER	N-CA-C	5.09	117.26	109.07
1	A	217	ASN	N-CA-C	5.06	116.79	111.28

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	217	0
2	A	543	0	0	55	2
All	All	7586	0	6844	217	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 16.

All (217) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:713:GLY:HA2	1:A:725:MET:HE2	1.70	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
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:96:MET:HE2	1:A:249:THR:HG23	1.82	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:808:TRP:H	1:A:808:TRP:CD1	2.18	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:899:GLU:H	1:A:929:GLY:C	2.11	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:660:GLY:C	2:A:1509:HOH:O	2.47	0.56
1:A:885:ASN:C	1:A:938:TYR:HD2	2.13	0.56
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:725:MET:O	1:A:725:MET:HE3	2.07	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
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:323:LYS:NZ	1:A:350:ASP:OD2	2.28	0.52
1:A:525:ILE:HD11	1:A:627:LYS:HZ3	1.74	0.52
1:A:20:LYS:NZ	2:A:1082: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:THR:OG1	2:A:1474:HOH:O	2.16	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:78:SER:C	1:A:80:ALA:H	2.19	0.49
1:A:876:LEU:HD22	1:A:876:LEU:N	2.27	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
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:877:VAL:O	1:A:878:ASP:HB2	2.13	0.48
1:A:817:LYS:HE2	1:A:818:LYS:HE3	1.95	0.48
1:A:534:CYS:HG	1:A:539:CYS:HG	1.59	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:725:MET:HE1	1:A:727:TYR:CE2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:ASN:O	1:A:856:THR:OG1	2.33	0.47
1:A:879:PHE:C	1:A:880:ILE:HG12	2.41	0.46
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: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:847:ASN:C	1:A:873:ASN:HA	2.41	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:725:MET:HE3	1:A:725:MET:C	2.43	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
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:885:ASN:C	1:A:938:TYR:CD2	2.95	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:736:GLU:C	1:A:757:LYS:HG3	2.43	0.43
1:A:786:PHE:HE1	1:A:959:LYS:HB2	1.84	0.43
1:A:903:LYS:C	1:A:905:VAL:H	2.27	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:559:LYS:C	2:A:1385:HOH:O	2.63	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:884:GLY:C	1:A:938:TYR:CE2	2.98	0.41
1:A:934:THR:C	1:A:935:LEU:HD12	2.45	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:61:SER:C	1:A:62:ILE:HD12	2.47	0.40
1:A:425:THR:HG23	1:A:629:ILE:CB	2.50	0.40
1:A:193:TYR:C	1:A:193:TYR:CD1	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	918/966 (95%)	795 (87%)	98 (11%)	25 (3%)	4 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
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

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Mol	Chain	Res	Type
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%)	696 (91%)	67 (9%)	9 12

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	31	LYS
1	A	39	ASP
1	A	62	ILE
1	A	70	VAL
1	A	97	THR
1	A	98	THR
1	A	150	VAL
1	A	186	VAL
1	A	193	TYR
1	A	214	VAL
1	A	223	VAL
1	A	231	ILE
1	A	247	SER
1	A	274	LYS

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Mol	Chain	Res	Type
1	A	311	LEU
1	A	361	LEU
1	A	392	LYS
1	A	425	THR
1	A	489	THR
1	A	498	LEU
1	A	499	ASP
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	608	LYS
1	A	614	ILE
1	A	637	ARG
1	A	674	THR
1	A	677	SER
1	A	678	LEU
1	A	716	GLU
1	A	720	GLU
1	A	724	SER
1	A	725	MET
1	A	732	TYR
1	A	733	GLU
1	A	734	LEU
1	A	753	ILE
1	A	769	ASP
1	A	774	ARG
1	A	783	LEU
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	844	THR
1	A	845	THR
1	A	861	GLN
1	A	862	LEU
1	A	864	VAL
1	A	867	LYS

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Mol	Chain	Res	Type
1	A	872	ASN
1	A	878	ASP
1	A	880	ILE
1	A	881	GLU
1	A	892	ILE
1	A	923	LYS
1	A	931	SER
1	A	938	TYR
1	A	939	LYS
1	A	961	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	321	ASN
1	A	409	ASN
1	A	745	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 oligosaccharides 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, 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	930/966 (96%)	1.37	235 (25%) 1 2	23, 43, 148, 220	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	775	TYR	9.1
1	A	961	PHE	8.7
1	A	877	VAL	8.5
1	A	935	LEU	7.4
1	A	774	ARG	7.4
1	A	778	PHE	7.2
1	A	941	VAL	6.9
1	A	857	GLN	6.9
1	A	780	LEU	6.7
1	A	876	LEU	6.7
1	A	962	LEU	6.5
1	A	875	LEU	6.4
1	A	783	LEU	6.3
1	A	912	THR	6.2
1	A	772	ALA	6.1
1	A	725	MET	6.0
1	A	769	ASP	5.9
1	A	807	LEU	5.8
1	A	913	ILE	5.8
1	A	848	SER	5.8
1	A	933	TRP	5.7
1	A	782	MET	5.7
1	A	963	ALA	5.6
1	A	849	ALA	5.6
1	A	826	VAL	5.6
1	A	761	LEU	5.5
1	A	776	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	915	PHE	5.5
1	A	862	LEU	5.4
1	A	868	LEU	5.4
1	A	922	ILE	5.4
1	A	738	GLY	5.4
1	A	864	VAL	5.4
1	A	958	TYR	5.3
1	A	851	VAL	5.3
1	A	850	PHE	5.3
1	A	901	THR	5.2
1	A	785	GLY	5.1
1	A	884	GLY	5.1
1	A	934	THR	5.0
1	A	910	THR	5.0
1	A	771	SER	5.0
1	A	840	VAL	5.0
1	A	773	THR	5.0
1	A	719	GLY	4.9
1	A	895	VAL	4.9
1	A	960	ALA	4.9
1	A	717	SER	4.9
1	A	890	LEU	4.8
1	A	781	ALA	4.8
1	A	538	LEU	4.8
1	A	860	ASP	4.7
1	A	768	LYS	4.6
1	A	886	ASP	4.6
1	A	841	ASP	4.6
1	A	837	THR	4.6
1	A	786	PHE	4.5
1	A	766	ALA	4.4
1	A	905	VAL	4.4
1	A	777	GLN	4.4
1	A	726	PHE	4.4
1	A	762	SER	4.3
1	A	920	PRO	4.3
1	A	894	LEU	4.3
1	A	906	PHE	4.3
1	A	944	ALA	4.3
1	A	732	TYR	4.3
1	A	794	ILE	4.3
1	A	779	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	852	MET	4.2
1	A	908	THR	4.2
1	A	936	THR	4.2
1	A	892	ILE	4.2
1	A	943	ASN	4.2
1	A	959	LYS	4.2
1	A	856	THR	4.2
1	A	874	LEU	4.1
1	A	932	VAL	4.1
1	A	822	THR	4.0
1	A	499	ASP	4.0
1	A	930	LYS	4.0
1	A	878	ASP	4.0
1	A	859	ALA	4.0
1	A	32	ILE	3.9
1	A	964	GLU	3.9
1	A	828	PHE	3.9
1	A	918	VAL	3.9
1	A	891	ASN	3.9
1	A	77	LYS	3.8
1	A	897	ALA	3.8
1	A	880	ILE	3.8
1	A	838	LEU	3.8
1	A	819	LEU	3.8
1	A	843	LEU	3.8
1	A	739	ALA	3.7
1	A	835	PHE	3.7
1	A	767	ASP	3.7
1	A	721	ILE	3.7
1	A	914	GLY	3.7
1	A	718	THR	3.7
1	A	879	PHE	3.6
1	A	898	PRO	3.6
1	A	865	LYS	3.6
1	A	829	ASN	3.6
1	A	758	ALA	3.6
1	A	806	ALA	3.6
1	A	825	MET	3.6
1	A	882	LYS	3.6
1	A	816	LEU	3.6
1	A	809	LYS	3.6
1	A	907	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	824	SER	3.5
1	A	928	ASP	3.5
1	A	921	GLU	3.5
1	A	896	LYS	3.5
1	A	746	GLN	3.5
1	A	44	ALA	3.5
1	A	534	CYS	3.5
1	A	924	GLN	3.5
1	A	861	GLN	3.4
1	A	803	MET	3.4
1	A	867	LYS	3.3
1	A	885	ASN	3.3
1	A	808	TRP	3.3
1	A	74	ALA	3.2
1	A	802	ALA	3.2
1	A	863	ILE	3.2
1	A	810	VAL	3.2
1	A	945	ASP	3.2
1	A	887	LYS	3.2
1	A	927	LYS	3.2
1	A	715	THR	3.2
1	A	727	TYR	3.2
1	A	866	ASN	3.2
1	A	872	ASN	3.2
1	A	904	ASP	3.2
1	A	801	LEU	3.2
1	A	883	LYS	3.2
1	A	73	ASN	3.1
1	A	723	PRO	3.1
1	A	814	SER	3.1
1	A	873	ASN	3.1
1	A	888	ASN	3.1
1	A	929	GLY	3.1
1	A	747	ALA	3.1
1	A	760	LYS	3.1
1	A	763	PHE	3.1
1	A	533	ASN	3.1
1	A	893	ASP	3.1
1	A	916	SER	3.0
1	A	858	GLN	3.0
1	A	926	GLU	3.0
1	A	903	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	748	SER	3.0
1	A	217	ASN	3.0
1	A	138	VAL	2.9
1	A	78	SER	2.9
1	A	842	GLU	2.9
1	A	817	LYS	2.9
1	A	797	ALA	2.9
1	A	753	ILE	2.9
1	A	39	ASP	2.9
1	A	140	ASN	2.9
1	A	902	SER	2.9
1	A	940	THR	2.9
1	A	741	PHE	2.8
1	A	939	LYS	2.8
1	A	834	ILE	2.8
1	A	72	HIS	2.8
1	A	787	ASP	2.8
1	A	818	LYS	2.8
1	A	770	ASN	2.7
1	A	795	LYS	2.7
1	A	804	ASN	2.7
1	A	839	THR	2.7
1	A	530	LYS	2.7
1	A	675	VAL	2.7
1	A	869	GLU	2.7
1	A	853	ARG	2.7
1	A	728	ALA	2.6
1	A	871	ALA	2.6
1	A	696	SER	2.6
1	A	9	TRP	2.6
1	A	796	ALA	2.6
1	A	722	THR	2.6
1	A	854	THR	2.6
1	A	791	GLN	2.6
1	A	925	GLN	2.6
1	A	76	ASN	2.6
1	A	830	GLY	2.5
1	A	79	SER	2.5
1	A	539	CYS	2.5
1	A	911	GLN	2.5
1	A	937	GLY	2.5
1	A	800	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	917	ASP	2.4
1	A	919	THR	2.4
1	A	799	SER	2.4
1	A	724	SER	2.4
1	A	736	GLU	2.4
1	A	784	ASP	2.4
1	A	909	GLU	2.4
1	A	764	GLY	2.4
1	A	792	GLY	2.4
1	A	831	GLY	2.3
1	A	845	THR	2.3
1	A	759	ALA	2.3
1	A	62	ILE	2.3
1	A	559	LYS	2.3
1	A	820	ASN	2.3
1	A	844	THR	2.3
1	A	821	SER	2.3
1	A	716	GLU	2.3
1	A	720	GLU	2.3
1	A	923	LYS	2.3
1	A	141	GLY	2.2
1	A	531	THR	2.2
1	A	737	ASP	2.2
1	A	793	SER	2.2
1	A	790	TYR	2.1
1	A	938	TYR	2.1
1	A	836	ASN	2.1
1	A	698	PHE	2.1
1	A	823	GLY	2.1
1	A	765	SER	2.1
1	A	714	ALA	2.1
1	A	847	ASN	2.1
1	A	29	HIS	2.0
1	A	265	ASN	2.0
1	A	321	ASN	2.0
1	A	734	LEU	2.0
1	A	82	TYR	2.0
1	A	241	TYR	2.0
1	A	846	SER	2.0
1	A	557	LYS	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 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.