



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:27 PM UTC

PDB ID : 1WXR / pdb_00001wxr
Title : Crystal structure of Heme Binding protein, an autotransporter hemoglobine protease from pathogenic Escherichia coli
Authors : Otto, B.R.; Sijbrandi, R.; Luijck, J.; Oudega, B.; Hedde, J.G.; Mizutani, K.; Park, S.-Y.; Tame, J.R.H.
Deposited on : 2005-01-31
Resolution : 2.20 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

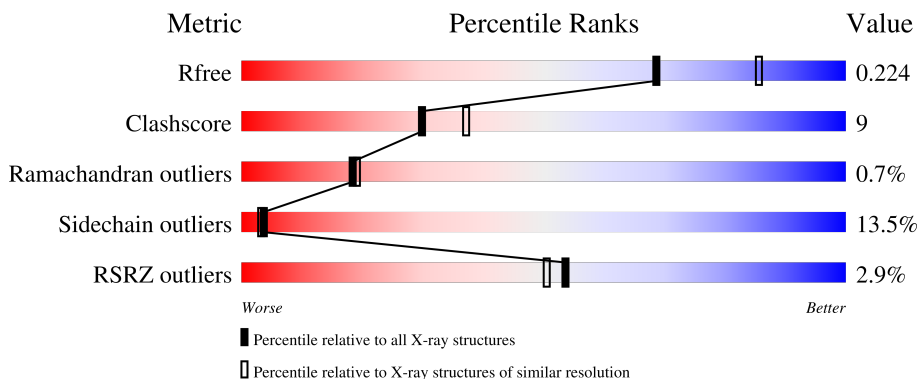
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1048	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8197 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 haemoglobin protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1035	Total	C	N	O	S	0	0	0
			7802	4847	1355	1586	14			

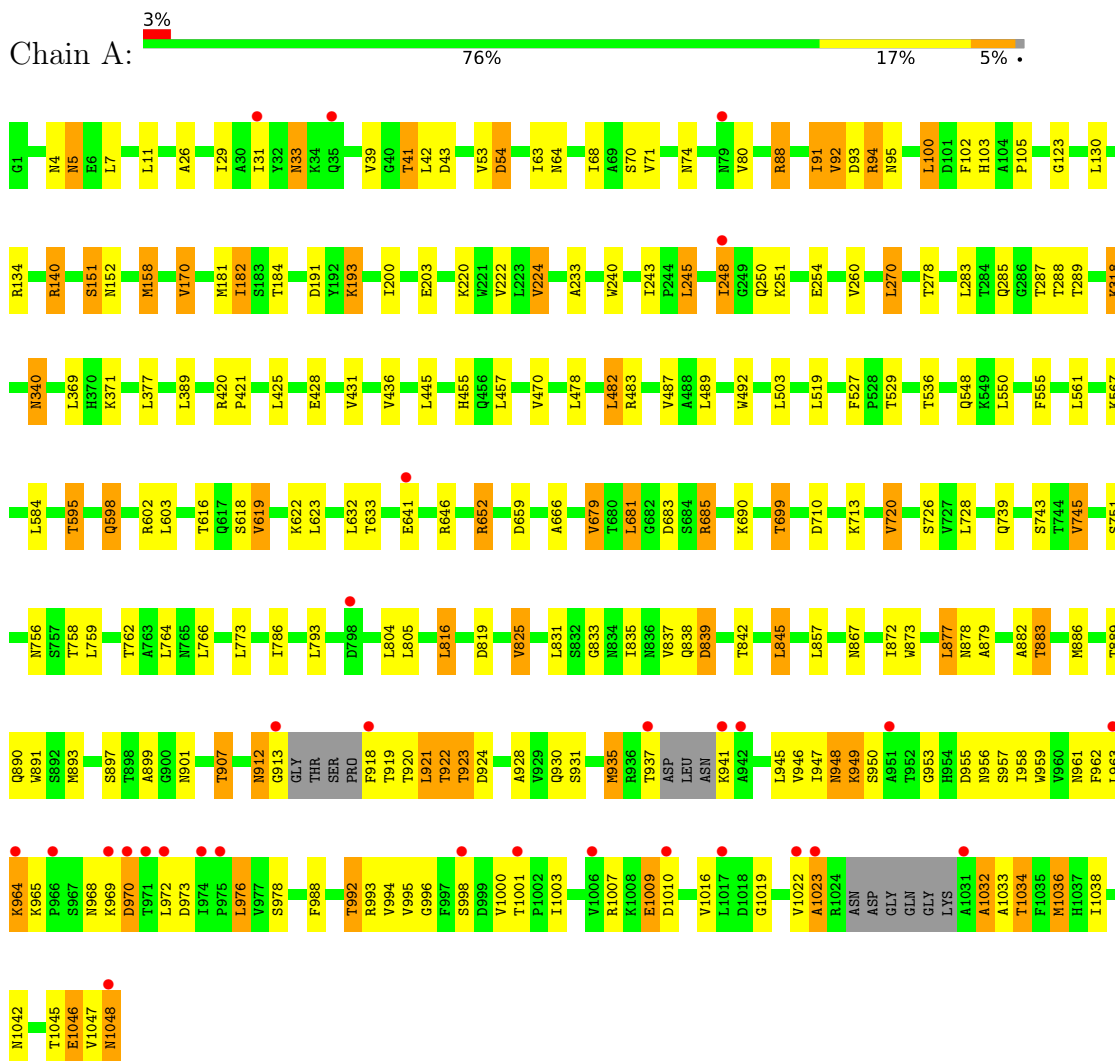
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	395	Total	O	0	0
			395	395		

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: haemoglobin protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.03Å 115.03Å 437.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.36 – 2.20 29.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (29.36-2.20) 92.4 (29.36-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.203 , 0.243 (Not available) , 0.224	Depositor DCC
R_{free} test set	4077 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8197	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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	0.95	3/7945 (0.0%)	1.13	17/10799 (0.2%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	652	ARG	NE-CZ	5.53	1.39	1.33
1	A	1047	VAL	CA-C	5.42	1.59	1.52
1	A	1048	ASN	N-CA	5.12	1.55	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CA-C-N	-8.12	112.00	123.20
1	A	94	ARG	C-N-CA	-8.12	112.00	123.20
1	A	94	ARG	N-CA-C	-7.75	98.82	110.28
1	A	64	ASN	N-CA-C	-6.82	99.31	108.11
1	A	151	SER	N-CA-C	-6.50	101.33	110.50
1	A	970	ASP	N-CA-C	6.42	121.36	107.49
1	A	1042	ASN	N-CA-C	-6.25	104.39	111.07
1	A	92	VAL	CB-CA-C	6.18	116.71	110.65
1	A	833	GLY	N-CA-C	6.11	117.76	111.95
1	A	912	ASN	N-CA-C	6.01	118.09	109.14
1	A	720	VAL	CB-CA-C	5.83	119.47	110.96
1	A	1033	ALA	N-CA-C	5.80	118.35	111.33
1	A	968	ASN	N-CA-C	5.75	117.49	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	VAL	N-CA-C	-5.68	107.97	113.53
1	A	455	HIS	N-CA-C	-5.55	106.55	113.38
1	A	699	THR	OG1-CB-CG2	-5.29	98.72	109.30
1	A	340	ASN	CB-CA-C	-5.02	100.94	109.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	970	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	7802	0	7482	130	0
2	A	395	0	0	6	0
All	All	8197	0	7482	130	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 9.

All (130) 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:958:ILE:HD11	1:A:988:PHE:HB3	1.44	0.98
1:A:1022:VAL:HG12	1:A:1023:ALA:H	1.28	0.95
1:A:886:MET:HE3	1:A:889:THR:HG21	1.48	0.93
1:A:959:TRP:HE3	1:A:995:VAL:HG22	1.38	0.87
1:A:158:MET:CE	1:A:622:LYS:HB3	2.03	0.87
1:A:958:ILE:CD1	1:A:988:PHE:HB3	2.06	0.85
1:A:998:SER:HB3	1:A:1000:VAL:HG22	1.59	0.82
1:A:886:MET:HE1	1:A:891:TRP:HB2	1.62	0.82
1:A:158:MET:HE1	1:A:622:LYS:HB3	1.62	0.81
1:A:959:TRP:CE3	1:A:995:VAL:HG22	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HB	1:A:652:ARG:HB3	1.65	0.78
1:A:683:ASP:OD1	1:A:685:ARG:HD3	1.84	0.78
1:A:948:ASN:O	1:A:949:LYS:HB2	1.83	0.76
1:A:1022:VAL:CG1	1:A:1023:ALA:H	1.99	0.76
1:A:158:MET:HA	1:A:158:MET:HE3	1.70	0.74
1:A:879:ALA:HB1	1:A:882:ALA:HB3	1.71	0.71
1:A:886:MET:HE3	1:A:889:THR:CG2	2.21	0.70
1:A:995:VAL:O	1:A:1032:ALA:O	2.10	0.70
1:A:158:MET:HE2	1:A:622:LYS:HB3	1.73	0.69
1:A:1022:VAL:HG12	1:A:1023:ALA:N	2.03	0.68
1:A:158:MET:CE	1:A:158:MET:HA	2.24	0.68
1:A:250:GLN:HG3	2:A:1428:HOH:O	1.94	0.67
1:A:270:LEU:HD13	1:A:285:GLN:HB2	1.77	0.67
1:A:883:THR:HG22	1:A:901:ASN:HD22	1.59	0.67
1:A:598:GLN:HG3	1:A:603:LEU:HD22	1.77	0.67
1:A:897:SER:HB2	1:A:921:LEU:HD23	1.78	0.64
1:A:972:LEU:HD13	1:A:1019:GLY:HA2	1.79	0.64
1:A:151:SER:O	1:A:152:ASN:HB2	1.96	0.64
1:A:1034:THR:HG22	1:A:1036:MET:H	1.62	0.63
1:A:962:PHE:HB2	1:A:998:SER:OG	1.98	0.62
1:A:616:THR:OG1	1:A:619:VAL:HG13	2.01	0.60
1:A:937:THR:HG23	1:A:941:LYS:O	2.01	0.60
1:A:961:ASN:ND2	1:A:996:GLY:HA3	2.17	0.59
1:A:959:TRP:HB3	1:A:995:VAL:CG2	2.33	0.59
1:A:68:ILE:HG13	1:A:105:PRO:HD2	1.85	0.58
1:A:957:SER:OG	1:A:1046:GLU:OE1	2.17	0.58
1:A:224:VAL:O	1:A:243:ILE:HG12	2.03	0.58
1:A:54:ASP:HB2	1:A:80:VAL:HG22	1.84	0.58
1:A:845:LEU:HG	1:A:886:MET:HG2	1.87	0.57
1:A:726:SER:O	1:A:743:SER:HB3	2.05	0.56
1:A:825:VAL:HG13	1:A:845:LEU:HD22	1.86	0.56
1:A:182:ILE:HG22	1:A:240:TRP:HB2	1.87	0.56
1:A:250:GLN:CG	2:A:1428:HOH:O	2.51	0.56
1:A:838:GLN:O	1:A:839:ASP:HB2	2.05	0.56
1:A:151:SER:O	1:A:152:ASN:CB	2.54	0.55
1:A:786:ILE:O	1:A:816:LEU:HA	2.06	0.55
1:A:924:ASP:HB3	1:A:949:LYS:HD3	1.89	0.55
1:A:786:ILE:HD12	1:A:816:LEU:HD22	1.88	0.55
1:A:743:SER:C	1:A:762:THR:HG23	2.33	0.53
1:A:428:GLU:HB2	2:A:1331:HOH:O	2.08	0.53
1:A:937:THR:C	1:A:963:LEU:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:N	1:A:421:PRO:CD	2.72	0.53
1:A:102:PHE:CZ	1:A:248:ILE:HD11	2.44	0.52
1:A:745:VAL:HG22	1:A:764:LEU:HD13	1.91	0.52
1:A:893:MET:O	1:A:893:MET:HG2	2.10	0.52
1:A:371:LYS:HD3	1:A:371:LYS:C	2.34	0.52
1:A:922:THR:HB	1:A:946:VAL:HB	1.91	0.51
1:A:482:LEU:HB2	1:A:555:PHE:CD1	2.46	0.51
1:A:1034:THR:HG22	1:A:1036:MET:N	2.26	0.51
1:A:886:MET:HE1	1:A:891:TRP:CB	2.39	0.50
1:A:877:LEU:O	1:A:897:SER:HA	2.11	0.50
1:A:1045:THR:O	1:A:1048:ASN:HA	2.12	0.49
1:A:886:MET:CE	1:A:891:TRP:HB2	2.40	0.49
1:A:91:ILE:HG13	1:A:105:PRO:HB3	1.95	0.49
1:A:102:PHE:HZ	1:A:248:ILE:HD11	1.78	0.48
1:A:492:TRP:HB2	1:A:527:PHE:CE2	2.48	0.48
1:A:959:TRP:HB3	1:A:995:VAL:HG21	1.95	0.48
1:A:487:VAL:HB	1:A:548:GLN:HG2	1.95	0.48
1:A:93:ASP:O	1:A:105:PRO:HA	2.15	0.47
1:A:912:ASN:CG	1:A:913:GLY:H	2.22	0.47
1:A:91:ILE:CD1	1:A:91:ILE:N	2.78	0.47
1:A:100:LEU:HD11	2:A:1249:HOH:O	2.13	0.47
1:A:825:VAL:CG1	1:A:845:LEU:HD22	2.44	0.47
1:A:947:ILE:HG21	1:A:950:SER:O	2.15	0.47
1:A:646:ARG:O	1:A:666:ALA:HA	2.15	0.47
1:A:937:THR:O	1:A:964:LYS:HE3	2.15	0.47
1:A:602:ARG:HG2	1:A:659:ASP:HB3	1.97	0.47
1:A:931:SER:O	1:A:956:ASN:HA	2.15	0.47
1:A:816:LEU:HG	1:A:837:VAL:HG22	1.96	0.47
1:A:959:TRP:CZ2	1:A:1046:GLU:HG2	2.49	0.46
1:A:4:ASN:OD1	1:A:4:ASN:C	2.59	0.46
1:A:243:ILE:HG22	1:A:248:ILE:HD13	1.97	0.46
1:A:992:THR:HB	1:A:1046:GLU:OE2	2.16	0.46
1:A:74:ASN:O	1:A:94:ARG:NH1	2.47	0.45
1:A:95:ASN:HB3	1:A:251:LYS:HD2	1.98	0.45
1:A:26:ALA:CB	1:A:29:ILE:HD11	2.47	0.45
1:A:123:GLY:HA3	2:A:1227:HOH:O	2.15	0.45
1:A:170:VAL:HG13	1:A:184:THR:HG21	1.98	0.45
1:A:140:ARG:HE	1:A:200:ILE:HG23	1.82	0.45
1:A:191:ASP:OD1	1:A:193:LYS:HG3	2.17	0.45
1:A:318:LYS:O	1:A:340:ASN:ND2	2.51	0.44
1:A:935:MET:HE1	1:A:976:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:CG2	1:A:248:ILE:HD13	2.47	0.44
1:A:710:ASP:HA	1:A:713:LYS:HD2	1.99	0.44
1:A:41:THR:OG1	1:A:43:ASP:HB3	2.18	0.44
1:A:54:ASP:HB2	1:A:80:VAL:CG2	2.47	0.44
1:A:958:ILE:HD11	1:A:988:PHE:CB	2.31	0.44
1:A:681:LEU:HD22	1:A:728:LEU:HD11	1.99	0.44
1:A:948:ASN:O	1:A:949:LYS:CB	2.56	0.44
1:A:203:GLU:OE1	1:A:233:ALA:HA	2.17	0.44
1:A:616:THR:OG1	1:A:619:VAL:CG1	2.66	0.44
1:A:961:ASN:HD21	1:A:996:GLY:HA3	1.83	0.43
1:A:883:THR:HA	1:A:901:ASN:O	2.19	0.43
1:A:819:ASP:OD1	1:A:839:ASP:HB3	2.18	0.43
1:A:1022:VAL:CG1	1:A:1023:ALA:N	2.69	0.43
1:A:181:MET:HE3	1:A:181:MET:HB3	1.95	0.43
1:A:679:VAL:HG22	1:A:728:LEU:HD12	2.00	0.43
1:A:995:VAL:HG13	1:A:1038:ILE:HD11	2.01	0.43
1:A:921:LEU:HD12	1:A:945:LEU:HD13	2.00	0.43
1:A:928:ALA:O	1:A:953:GLY:HA3	2.20	0.42
1:A:70:SER:HB3	1:A:103:HIS:CD2	2.55	0.42
1:A:959:TRP:HE3	1:A:995:VAL:CG2	2.20	0.42
1:A:920:THR:HG22	1:A:922:THR:HG22	2.01	0.42
1:A:889:THR:HB	1:A:907:THR:HB	2.02	0.42
1:A:53:VAL:O	1:A:54:ASP:C	2.61	0.41
1:A:930:GLN:HA	1:A:955:ASP:O	2.21	0.41
1:A:123:GLY:CA	1:A:245:LEU:HD22	2.50	0.41
1:A:758:THR:C	1:A:759:LEU:HD12	2.46	0.41
1:A:835:ILE:HG13	1:A:873:TRP:CZ2	2.56	0.41
1:A:5:ASN:H	1:A:5:ASN:HD22	1.69	0.41
1:A:872:ILE:HD13	1:A:890:GLN:HB3	2.02	0.41
1:A:899:ALA:O	1:A:923:THR:HA	2.21	0.41
1:A:1045:THR:O	1:A:1048:ASN:N	2.54	0.41
1:A:26:ALA:HB1	1:A:29:ILE:HD11	2.02	0.40
1:A:70:SER:HB3	1:A:103:HIS:NE2	2.36	0.40
1:A:88:ARG:NH1	2:A:1394:HOH:O	2.54	0.40
1:A:420:ARG:N	1:A:421:PRO:HD3	2.36	0.40
1:A:816:LEU:N	1:A:816:LEU:HD23	2.37	0.40
1:A:679:VAL:HG22	1:A:728:LEU:CD1	2.51	0.40
1:A:973:ASP:OD2	1:A:1007:ARG:NH1	2.53	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	1027/1048 (98%)	974 (95%)	46 (4%)	7 (1%)	18	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	949	LYS
1	A	1010	ASP
1	A	1032	ALA
1	A	1023	ALA
1	A	33	ASN
1	A	1009	GLU
1	A	839	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	838/848 (99%)	725 (86%)	113 (14%)	4	3

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	LEU
1	A	11	LEU
1	A	31	ILE

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Mol	Chain	Res	Type
1	A	33	ASN
1	A	39	VAL
1	A	41	THR
1	A	42	LEU
1	A	54	ASP
1	A	63	ILE
1	A	71	VAL
1	A	88	ARG
1	A	91	ILE
1	A	92	VAL
1	A	100	LEU
1	A	130	LEU
1	A	134	ARG
1	A	140	ARG
1	A	158	MET
1	A	170	VAL
1	A	182	ILE
1	A	193	LYS
1	A	220	LYS
1	A	222	VAL
1	A	224	VAL
1	A	245	LEU
1	A	248	ILE
1	A	254	GLU
1	A	260	VAL
1	A	270	LEU
1	A	278	THR
1	A	283	LEU
1	A	287	THR
1	A	288	THR
1	A	289	THR
1	A	318	LYS
1	A	369	LEU
1	A	377	LEU
1	A	389	LEU
1	A	425	LEU
1	A	431	VAL
1	A	436	VAL
1	A	445	LEU
1	A	457	LEU
1	A	470	VAL
1	A	478	LEU

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Mol	Chain	Res	Type
1	A	482	LEU
1	A	483	ARG
1	A	489	LEU
1	A	503	LEU
1	A	519	LEU
1	A	529	THR
1	A	536	THR
1	A	550	LEU
1	A	561	LEU
1	A	567	LYS
1	A	584	LEU
1	A	595	THR
1	A	598	GLN
1	A	618	SER
1	A	619	VAL
1	A	623	LEU
1	A	632	LEU
1	A	633	THR
1	A	641	GLU
1	A	679	VAL
1	A	681	LEU
1	A	685	ARG
1	A	690	LYS
1	A	699	THR
1	A	720	VAL
1	A	739	GLN
1	A	745	VAL
1	A	751	SER
1	A	756	ASN
1	A	766	LEU
1	A	773	LEU
1	A	793	LEU
1	A	804	LEU
1	A	805	LEU
1	A	816	LEU
1	A	825	VAL
1	A	831	LEU
1	A	842	THR
1	A	845	LEU
1	A	857	LEU
1	A	867	ASN
1	A	877	LEU

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Mol	Chain	Res	Type
1	A	878	ASN
1	A	883	THR
1	A	907	THR
1	A	918	PHE
1	A	919	THR
1	A	921	LEU
1	A	922	THR
1	A	923	THR
1	A	935	MET
1	A	948	ASN
1	A	964	LYS
1	A	965	LYS
1	A	969	LYS
1	A	976	LEU
1	A	978	SER
1	A	992	THR
1	A	993	ARG
1	A	994	VAL
1	A	1001	THR
1	A	1003	ILE
1	A	1009	GLU
1	A	1016	VAL
1	A	1034	THR
1	A	1036	MET
1	A	1046	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	90	ASN
1	A	219	ASN
1	A	312	ASN
1	A	380	GLN
1	A	399	ASN
1	A	407	GLN
1	A	502	ASN
1	A	512	ASN
1	A	521	GLN
1	A	600	ASN
1	A	676	ASN
1	A	717	ASN

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Mol	Chain	Res	Type
1	A	746	ASN
1	A	756	ASN
1	A	815	ASN
1	A	824	ASN
1	A	836	ASN
1	A	838	GLN
1	A	867	ASN
1	A	905	ASN
1	A	948	ASN
1	A	961	ASN
1	A	1037	HIS
1	A	1041	ASN

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 ⓘ

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	1035/1048 (98%)	-0.04	30 (2%) 53 50	18, 33, 56, 86	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	964	LYS	5.0
1	A	918	PHE	4.9
1	A	972	LEU	4.3
1	A	798	ASP	4.3
1	A	913	GLY	4.2
1	A	971	THR	4.1
1	A	1031	ALA	4.0
1	A	970	ASP	3.8
1	A	969	LYS	3.4
1	A	1023	ALA	3.2
1	A	941	LYS	3.2
1	A	974	ILE	3.1
1	A	1048	ASN	2.9
1	A	1022	VAL	2.9
1	A	1010	ASP	2.7
1	A	963	LEU	2.6
1	A	35	GLN	2.5
1	A	1001	THR	2.4
1	A	937	THR	2.4
1	A	975	PRO	2.4
1	A	998	SER	2.3
1	A	966	PRO	2.3
1	A	79	ASN	2.2
1	A	31	ILE	2.2
1	A	1006	VAL	2.2
1	A	942	ALA	2.2
1	A	248	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	641	GLU	2.1
1	A	951	ALA	2.0
1	A	1017	LEU	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.