Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:52 AM EDT

PDB ID	:	1WXR
Title	:	Crystal structure of Heme Binding protein, an autotransporter hemoglobine protease from pathogenic Escherichia coli
Authors	:	Otto, B.R.; Sijbrandi, R.; Luirink, J.; Oudega, B.; Heddle, 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 (i) 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 (1)) were used in the production of this report:

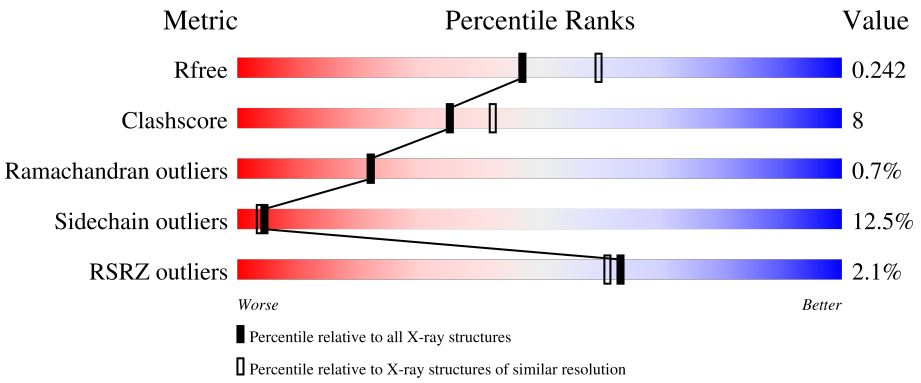
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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% 75% 18% 5% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1035	7802	4847	1355	1586	14	0	0	0

- Molecule 2 is water.

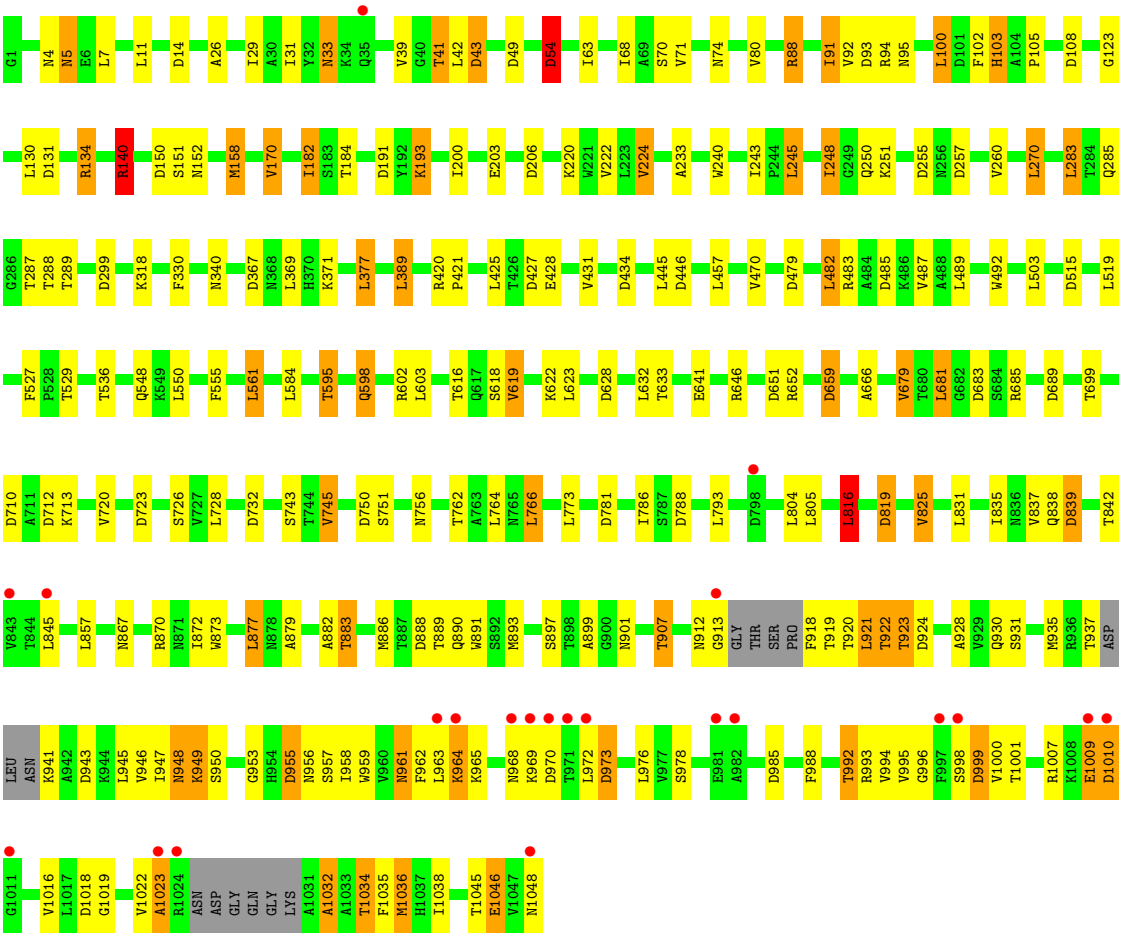
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	395	395	395	0	0

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: haemoglobin protease

Chain A:



4 Data and refinement statistics (i)

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 29.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (29.36-2.20) 92.4 (29.79-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.203 , 0.243 0.206 , 0.242	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 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[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 (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	0.79	1/7945 (0.0%)	1.00	48/10799 (0.4%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	PHE	CE2-CZ	5.10	1.47	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASP	CB-CG-OD2	8.27	125.75	118.30
1	A	43	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	150	ASP	CB-CG-OD2	8.10	125.59	118.30
1	A	49	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	781	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	870	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	A	712	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	973	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	485	ASP	CB-CG-OD2	7.15	124.74	118.30
1	A	131	ASP	CB-CG-OD2	7.07	124.67	118.30
1	A	257	ASP	CB-CG-OD2	6.81	124.42	118.30
1	A	54	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	515	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	689	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	283	LEU	CA-CB-CG	6.56	130.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	479	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	788	ASP	CB-CG-OD2	6.33	123.99	118.30
1	A	732	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	651	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	628	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	993	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	723	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	750	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	1010	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	1018	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	255	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	870	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	659	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	14	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	140	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	206	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	816	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	888	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	561	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	389	LEU	CB-CG-CD2	5.36	120.12	111.00
1	A	134	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	367	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	446	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	999	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	955	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	434	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	766	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	427	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	377	LEU	CB-CG-CD2	5.09	119.66	111.00
1	A	943	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	819	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	985	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	299	ASP	CB-CG-OD1	5.00	122.80	118.30

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 (i)

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	125	0
2	A	395	0	0	6	0
All	All	8197	0	7482	125	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 8.

All (125) 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: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:158:MET:HE1	1:A:622:LYS:HB3	1.59	0.83
1:A:998:SER:HB3	1:A:1000:VAL:HG22	1.59	0.82
1:A:959:TRP:CE3	1:A:995:VAL:HG22	2.15	0.80
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:1022:VAL:HG12	1:A:1023:ALA:N	2.03	0.72
1:A:879:ALA:HB1	1:A:882:ALA:HB3	1.71	0.71
1:A:158:MET:HA	1:A:158:MET:HE3	1.73	0.71
1:A:995:VAL:O	1:A:1032:ALA:O	2.10	0.70
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:158:MET:HE2	1:A:622:LYS:HB3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:886:MET:HE3	1:A:891:TRP:HB2	1.86	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:428:GLU:HB2	2:A:1331:HOH:O	2.08	0.53
1:A:886:MET:HE3	1:A:889:THR:HG21	1.89	0.53
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:886:MET:CE	1:A:891:TRP:HB2	2.40	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:886:MET:CE	1:A:889:THR:HG21	2.40	0.51
1:A:1034:THR:HG22	1:A:1036:MET:N	2.26	0.51
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:743:SER:C	1:A:762:THR:HG23	2.33	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:937:THR:C	1:A:963:LEU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:O	1:A:105:PRO:HA	2.15	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:371:LYS:HD3	1:A:371:LYS:C	2.34	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: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: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: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:912:ASN:CG	1:A:913:GLY:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:ASN:OD1	1:A:4:ASN:C	2.59	0.42
1:A:889:THR:HB	1:A:907:THR:HB	2.02	0.42
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: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 (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	1027/1048 (98%)	974 (95%)	46 (4%)	7 (1%)	22 22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	949	LYS
1	A	1010	ASP
1	A	1032	ALA

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Mol	Chain	Res	Type
1	A	1023	ALA
1	A	33	ASN
1	A	1009	GLU
1	A	839	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	838/848 (99%)	733 (88%)	105 (12%)	4 4

All (105) 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
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	103	HIS
1	A	130	LEU
1	A	134	ARG
1	A	140	ARG
1	A	158	MET
1	A	170	VAL
1	A	182	ILE

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Mol	Chain	Res	Type
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	260	VAL
1	A	270	LEU
1	A	283	LEU
1	A	287	THR
1	A	288	THR
1	A	289	THR
1	A	369	LEU
1	A	377	LEU
1	A	389	LEU
1	A	425	LEU
1	A	431	VAL
1	A	445	LEU
1	A	457	LEU
1	A	470	VAL
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	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	699	THR
1	A	720	VAL

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Mol	Chain	Res	Type
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	857	LEU
1	A	867	ASN
1	A	877	LEU
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	961	ASN
1	A	964	LYS
1	A	965	LYS
1	A	968	ASN
1	A	969	LYS
1	A	976	LEU
1	A	978	SER
1	A	992	THR
1	A	994	VAL
1	A	999	ASP
1	A	1001	THR
1	A	1009	GLU
1	A	1016	VAL
1	A	1034	THR
1	A	1035	PHE
1	A	1036	MET
1	A	1046	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	219	ASN
1	A	380	GLN
1	A	399	ASN
1	A	407	GLN
1	A	521	GLN
1	A	735	ASN
1	A	741	ASN
1	A	756	ASN
1	A	867	ASN
1	A	905	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 monosaccharides 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	1035/1048 (98%)	-0.25	22 (2%) 63 61	18, 33, 56, 86	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	971	THR	5.1
1	A	969	LYS	5.1
1	A	970	ASP	5.0
1	A	1010	ASP	5.0
1	A	798	ASP	3.8
1	A	1023	ALA	3.3
1	A	1024	ARG	3.3
1	A	968	ASN	3.2
1	A	35	GLN	2.9
1	A	845	LEU	2.8
1	A	998	SER	2.8
1	A	913	GLY	2.7
1	A	982	ALA	2.6
1	A	997	PHE	2.6
1	A	963	LEU	2.6
1	A	1009	GLU	2.5
1	A	972	LEU	2.4
1	A	1011	GLY	2.3
1	A	964	LYS	2.2
1	A	843	VAL	2.1
1	A	1048	ASN	2.1
1	A	981	GLU	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 monosaccharides 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.