Full wwPDB X-ray Structure Validation Report (i)

Mar 17, 2022 – 01:04 PM JST

PDB ID	:	7ETR
Title	:	Crystal structure of SO_1444-SO_1445 complex from Shewanella oneidensis
Authors	:	Zhou, J.; Zhang, H.
Deposited on	:	2021-05-13
Resolution	:	3.80 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:

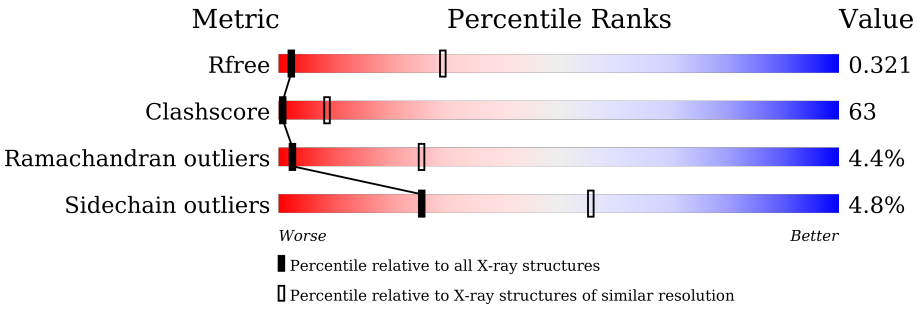
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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%

Mol	Chain	Length	Quality of chain
1	A	102	41% 43% • 14%
1	B	102	42% 25% • 28%
2	C	97	31% 46% 7% 15%
2	D	97	33% 35% 5% • 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2582 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 Transcriptional regulator CopG family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	Se	0	0	0
			721	443	135	141	2			
1	B	73	Total	C	N	O	Se	0	0	0
			608	375	116	115	2			

- Molecule 2 is a protein called Toxin module of toxin-antitoxin system RelE/StbE family.

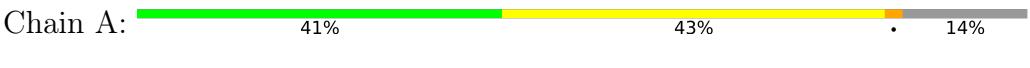
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	82	Total	C	N	O	S	Se	0	0	0
			671	427	123	119	1	1			
2	D	72	Total	C	N	O	S	Se	0	0	0
			582	374	102	104	1	1			

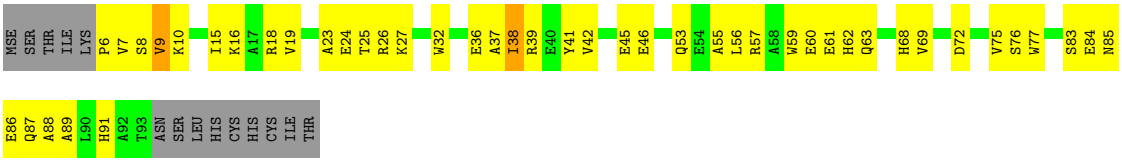
3 Residue-property plots (i)

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. 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. 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: Transcriptional regulator CopG family

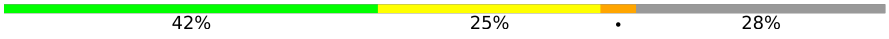
Chain A:

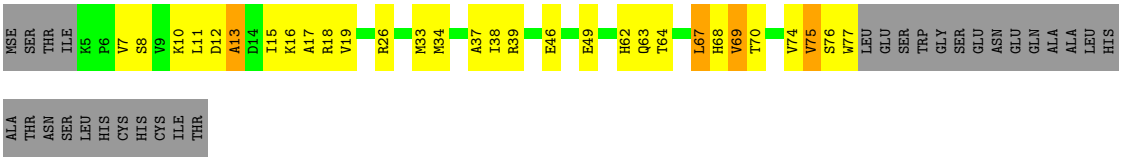




- Molecule 1: Transcriptional regulator CopG family

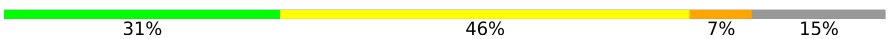
Chain B:

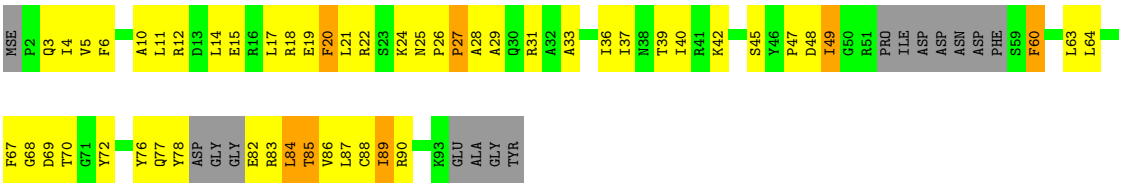




- Molecule 2: Toxin module of toxin-antitoxin system RelE/StbE family

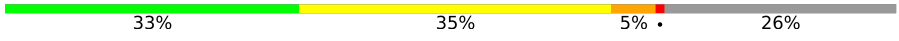
Chain C:

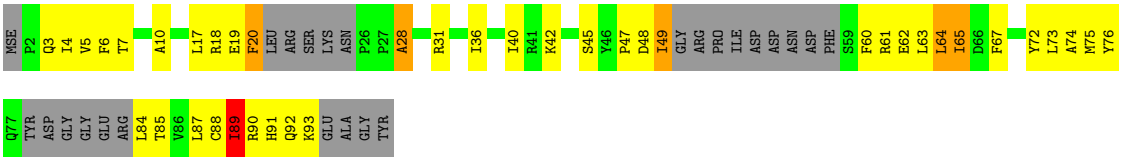




- Molecule 2: Toxin module of toxin-antitoxin system RelE/StbE family

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.40Å 85.40Å 110.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.93 – 3.80 46.51 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.93-3.80) 98.9 (46.51-3.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.41 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.287 , 0.308 0.314 , 0.321	Depositor DCC
R_{free} test set	436 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	133.8	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 109.3	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	0.84	EDS
Total number of atoms	2582	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	0.34	0/733	0.64	0/985
1	B	0.31	0/617	0.67	0/826
2	C	0.41	0/680	0.76	0/911
2	D	0.35	0/589	0.73	0/789
All	All	0.35	0/2619	0.70	0/3511

There are no bond length outliers.

There are no bond angle outliers.

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	721	0	689	73	0
1	B	608	0	595	106	0
2	C	671	0	687	106	0
2	D	582	0	595	120	0
All	All	2582	0	2566	322	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 63.

All (322) 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:68:HIS:CG	1:B:74:VAL:HG23	1.36	1.54
2:D:73:LEU:CD1	2:D:93:LYS:HB2	1.49	1.42
1:B:67:LEU:HD21	2:D:5:VAL:CG1	1.55	1.35
2:D:62:GLU:CB	2:D:75:MSE:HA	1.63	1.28
2:D:62:GLU:HB3	2:D:75:MSE:SE	1.81	1.28
2:D:62:GLU:CB	2:D:75:MSE:SE	2.38	1.22
1:B:68:HIS:CG	1:B:74:VAL:CG2	2.24	1.21
2:D:6:PHE:CZ	2:D:87:LEU:HD23	1.77	1.19
2:D:62:GLU:HB3	2:D:75:MSE:CB	1.70	1.18
1:B:68:HIS:CB	1:B:74:VAL:HG23	1.75	1.15
2:D:64:LEU:HD12	2:D:65:ILE:N	1.63	1.14
1:B:68:HIS:ND1	1:B:74:VAL:HG23	1.64	1.12
1:B:69:VAL:HG11	2:D:5:VAL:HA	1.21	1.12
1:B:69:VAL:HG11	2:D:5:VAL:CA	1.79	1.12
2:D:73:LEU:HD11	2:D:93:LYS:HD2	1.23	1.11
2:D:73:LEU:HD13	2:D:93:LYS:CB	1.80	1.11
2:D:62:GLU:CB	2:D:75:MSE:CA	2.27	1.11
2:C:21:LEU:HD22	2:C:29:ALA:HB2	1.15	1.10
2:D:62:GLU:OE1	2:D:75:MSE:HB2	1.49	1.10
2:D:64:LEU:O	2:D:65:ILE:HG13	1.49	1.10
2:C:45:SER:O	2:C:47:PRO:HD3	1.50	1.09
2:D:62:GLU:CG	2:D:75:MSE:SE	2.51	1.07
1:B:69:VAL:CG1	2:D:5:VAL:HA	1.86	1.05
2:C:21:LEU:CD2	2:C:29:ALA:HB2	1.87	1.03
2:D:64:LEU:O	2:D:65:ILE:CG1	2.06	1.03
1:B:67:LEU:HD21	2:D:5:VAL:HG13	1.05	1.02
2:D:62:GLU:HB3	2:D:75:MSE:CG	1.89	1.02
1:A:91:HIS:HE1	2:C:11:LEU:CD2	1.73	1.01
2:D:73:LEU:CD1	2:D:93:LYS:CB	2.38	1.01
2:D:62:GLU:HB2	2:D:75:MSE:CA	1.88	1.01
2:C:24:LYS:HG2	2:C:25:ASN:H	1.20	1.00
2:C:21:LEU:HA	2:C:24:LYS:HB3	1.43	1.00
2:C:77:GLN:HG2	2:C:78:TYR:CD2	1.98	0.99
2:D:73:LEU:HD11	2:D:93:LYS:CD	1.92	0.98
2:D:48:ASP:OD2	2:D:63:LEU:HD11	1.62	0.98
1:B:67:LEU:CD2	2:D:5:VAL:CG1	2.40	0.97
2:D:62:GLU:HG2	2:D:75:MSE:SE	2.13	0.97
1:A:32:TRP:CH2	1:A:36:GLU:HG3	2.00	0.97
2:D:62:GLU:CB	2:D:75:MSE:CB	2.43	0.97
1:A:91:HIS:HE1	2:C:11:LEU:HD23	1.29	0.96
2:D:62:GLU:HB2	2:D:75:MSE:HA	1.46	0.95
2:C:21:LEU:HD13	2:C:29:ALA:HA	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:HIS:CE1	2:C:11:LEU:CD2	2.50	0.94
2:C:4:ILE:O	2:C:4:ILE:HG13	1.66	0.94
1:B:69:VAL:HG21	2:D:5:VAL:HA	1.50	0.94
1:B:26:ARG:HD2	1:B:33:MSE:HE1	1.53	0.91
2:D:62:GLU:CA	2:D:75:MSE:HA	1.99	0.91
2:C:21:LEU:CD1	2:C:29:ALA:HA	2.02	0.90
2:D:49:ILE:O	2:D:61:ARG:HG3	1.70	0.90
2:C:21:LEU:HD22	2:C:29:ALA:CB	2.01	0.90
2:D:62:GLU:HB3	2:D:75:MSE:CA	1.95	0.89
2:C:25:ASN:HB2	2:C:28:ALA:HB3	1.52	0.89
1:B:69:VAL:HG11	2:D:5:VAL:CB	2.03	0.89
2:D:4:ILE:O	2:D:4:ILE:HG13	1.68	0.88
1:B:69:VAL:CG2	2:D:4:ILE:O	2.22	0.88
1:B:67:LEU:HD21	2:D:5:VAL:HG11	1.54	0.87
2:C:24:LYS:CE	2:C:69:ASP:OD2	2.23	0.86
1:B:69:VAL:HG21	2:D:5:VAL:CA	2.06	0.86
1:B:68:HIS:CB	1:B:74:VAL:CG2	2.51	0.86
2:D:73:LEU:HD13	2:D:93:LYS:HB2	0.87	0.85
1:B:68:HIS:HB2	1:B:75:VAL:H	1.39	0.85
1:B:69:VAL:CG2	2:D:5:VAL:HA	2.07	0.84
2:C:12:ARG:HD3	2:C:15:GLU:OE1	1.76	0.84
1:B:67:LEU:CD2	2:D:5:VAL:HG11	2.07	0.84
2:D:62:GLU:HA	2:D:75:MSE:HA	1.58	0.83
2:C:21:LEU:HA	2:C:24:LYS:CB	2.07	0.83
2:D:62:GLU:N	2:D:75:MSE:SE	2.62	0.82
1:A:55:ALA:HA	2:C:89:ILE:HG13	1.60	0.82
2:D:73:LEU:HD11	2:D:93:LYS:HB2	1.58	0.81
1:B:69:VAL:HG21	2:D:4:ILE:O	1.79	0.81
2:D:62:GLU:H	2:D:75:MSE:SE	2.12	0.81
1:B:68:HIS:HB2	1:B:74:VAL:HG23	1.62	0.81
2:D:6:PHE:CZ	2:D:87:LEU:CD2	2.63	0.80
2:C:77:GLN:HG2	2:C:78:TYR:HD2	1.47	0.79
2:C:60:PHE:CD2	2:C:77:GLN:HG3	2.20	0.77
1:B:68:HIS:ND1	1:B:74:VAL:CG2	2.40	0.77
2:D:62:GLU:HB3	2:D:75:MSE:HB2	1.66	0.77
1:A:26:ARG:HG2	1:B:49:GLU:CD	2.06	0.76
2:C:21:LEU:HD11	2:C:28:ALA:C	2.05	0.76
1:A:7:VAL:HG11	1:B:10:LYS:HE2	1.68	0.75
2:C:49:ILE:HG21	2:C:63:LEU:HD13	1.68	0.75
2:D:73:LEU:O	2:D:90:ARG:HA	1.87	0.74
1:A:26:ARG:CG	1:B:49:GLU:OE1	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:24:LYS:HE3	2:C:69:ASP:OD2	1.86	0.74
2:D:6:PHE:CE2	2:D:87:LEU:HD23	2.23	0.74
2:D:62:GLU:CB	2:D:75:MSE:HB2	2.16	0.74
2:D:64:LEU:HD12	2:D:65:ILE:CA	2.17	0.74
2:D:49:ILE:O	2:D:61:ARG:CG	2.36	0.74
1:B:15:ILE:O	1:B:18:ARG:N	2.21	0.73
1:A:15:ILE:CD1	1:B:39:ARG:HH12	2.01	0.73
2:C:18:ARG:HD2	2:C:18:ARG:O	1.89	0.73
2:C:60:PHE:HD2	2:C:77:GLN:HG3	1.51	0.72
1:A:45:GLU:OE1	1:B:26:ARG:NH2	2.20	0.72
1:B:69:VAL:HB	2:D:6:PHE:H	1.55	0.72
2:C:77:GLN:NE2	2:C:78:TYR:HE2	1.88	0.71
2:D:72:TYR:C	2:D:73:LEU:HD12	2.10	0.71
2:C:25:ASN:CB	2:C:28:ALA:HB3	2.20	0.71
2:D:20:PHE:H	2:D:20:PHE:HD2	1.37	0.71
2:C:24:LYS:HE2	2:C:69:ASP:OD2	1.89	0.71
2:D:64:LEU:CD1	2:D:65:ILE:N	2.50	0.70
1:A:7:VAL:HG12	1:B:10:LYS:CD	2.22	0.70
2:C:77:GLN:NE2	2:C:78:TYR:CE2	2.59	0.70
2:C:24:LYS:HG2	2:C:25:ASN:N	2.02	0.70
2:C:12:ARG:CD	2:C:15:GLU:OE1	2.40	0.70
2:D:73:LEU:HD11	2:D:93:LYS:CB	2.19	0.69
1:A:7:VAL:CG1	1:B:10:LYS:HE2	2.22	0.69
1:A:15:ILE:HD13	1:B:39:ARG:HH12	1.56	0.69
2:D:62:GLU:HB2	2:D:75:MSE:N	2.07	0.69
1:A:15:ILE:CD1	1:B:39:ARG:NH1	2.56	0.69
2:C:21:LEU:HD11	2:C:29:ALA:N	2.08	0.69
2:D:4:ILE:O	2:D:4:ILE:CG1	2.40	0.69
1:A:7:VAL:HG12	1:B:10:LYS:HG2	1.74	0.68
1:B:69:VAL:CB	2:D:5:VAL:HA	2.23	0.68
2:D:17:LEU:HD13	2:D:72:TYR:CE2	2.28	0.68
2:D:45:SER:O	2:D:47:PRO:HD3	1.93	0.67
1:B:62:HIS:HD2	1:B:67:LEU:HD13	1.60	0.67
2:C:48:ASP:O	2:C:49:ILE:HB	1.93	0.67
1:B:67:LEU:CD2	2:D:5:VAL:HG13	2.01	0.67
1:B:69:VAL:HG22	2:D:4:ILE:O	1.93	0.67
2:D:64:LEU:O	2:D:65:ILE:HG12	1.96	0.66
2:D:73:LEU:HD11	2:D:93:LYS:CG	2.24	0.66
1:A:59:TRP:CZ3	2:C:86:VAL:HG11	2.31	0.65
1:B:69:VAL:HG21	2:D:5:VAL:C	2.16	0.65
2:D:17:LEU:HD13	2:D:72:TYR:CZ	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:TYR:HB3	2:D:87:LEU:HD13	1.77	0.65
1:A:7:VAL:HG12	1:B:10:LYS:CG	2.26	0.65
1:A:91:HIS:CE1	2:C:11:LEU:HD23	2.21	0.65
1:A:32:TRP:CZ3	1:A:36:GLU:HG3	2.31	0.65
1:B:68:HIS:O	1:B:69:VAL:HB	1.96	0.65
1:B:12:ASP:OD1	1:B:12:ASP:O	2.15	0.65
2:D:6:PHE:CE1	2:D:87:LEU:HD23	2.32	0.65
1:B:62:HIS:CD2	1:B:67:LEU:HD13	2.31	0.65
1:A:26:ARG:HG2	1:B:49:GLU:OE1	1.97	0.65
2:C:17:LEU:HD13	2:C:72:TYR:CE2	2.32	0.64
1:B:69:VAL:HG11	2:D:5:VAL:CG1	2.27	0.64
1:B:69:VAL:CG1	2:D:5:VAL:HG13	2.27	0.64
2:C:21:LEU:HD21	2:C:29:ALA:N	2.11	0.64
1:B:68:HIS:HB2	1:B:74:VAL:CG2	2.22	0.64
2:D:64:LEU:C	2:D:65:ILE:HG13	2.16	0.64
2:C:4:ILE:O	2:C:4:ILE:CG1	2.39	0.64
2:D:72:TYR:O	2:D:73:LEU:HD12	1.98	0.64
1:B:74:VAL:HG22	1:B:75:VAL:N	2.13	0.63
2:C:21:LEU:CD2	2:C:29:ALA:CB	2.70	0.63
2:C:67:PHE:O	2:C:67:PHE:CD1	2.51	0.63
1:A:91:HIS:CE1	2:C:11:LEU:HD21	2.34	0.62
2:D:28:ALA:HA	2:D:31:ARG:HB3	1.81	0.62
2:D:62:GLU:CA	2:D:75:MSE:SE	2.97	0.62
1:B:69:VAL:HG11	2:D:5:VAL:CG2	2.29	0.62
2:C:21:LEU:CD1	2:C:29:ALA:CA	2.76	0.62
1:B:69:VAL:CG1	2:D:5:VAL:HG22	2.29	0.62
2:C:48:ASP:O	2:C:49:ILE:CB	2.47	0.61
1:A:89:ALA:CB	2:C:11:LEU:HD11	2.29	0.61
1:A:36:GLU:OE2	1:A:39:ARG:NH1	2.34	0.61
1:B:15:ILE:HG22	1:B:16:LYS:N	2.14	0.61
2:C:3:GLN:OE1	2:C:84:LEU:HD23	2.00	0.61
2:C:17:LEU:O	2:C:20:PHE:HB3	2.00	0.61
1:B:69:VAL:HG11	2:D:5:VAL:HG22	1.83	0.60
2:D:3:GLN:O	2:D:4:ILE:CG2	2.49	0.60
1:B:69:VAL:HG11	2:D:5:VAL:HG13	1.80	0.60
2:C:21:LEU:CA	2:C:24:LYS:HB3	2.26	0.60
2:D:48:ASP:OD2	2:D:63:LEU:CD1	2.45	0.60
1:B:67:LEU:HD12	2:D:7:THR:HA	1.84	0.60
1:B:74:VAL:HG21	1:B:77:TRP:CD1	2.36	0.59
1:A:10:LYS:HD3	1:B:34:MSE:SE	2.53	0.59
2:C:24:LYS:CG	2:C:25:ASN:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:VAL:HG21	2:D:84:LEU:HD23	1.83	0.59
2:C:5:VAL:O	2:C:87:LEU:N	2.28	0.59
1:B:15:ILE:O	1:B:16:LYS:C	2.37	0.59
2:C:4:ILE:HG12	2:C:40:ILE:HG23	1.85	0.58
1:A:32:TRP:CH2	1:A:36:GLU:CG	2.81	0.58
2:C:82:GLU:O	2:C:82:GLU:HG2	2.04	0.58
1:B:74:VAL:CG2	1:B:77:TRP:CD1	2.86	0.58
2:C:20:PHE:C	2:C:20:PHE:CD1	2.72	0.58
2:C:83:ARG:HG3	2:C:83:ARG:O	2.03	0.58
2:C:85:THR:O	2:C:85:THR:HG23	2.03	0.58
2:D:64:LEU:HD12	2:D:64:LEU:C	2.23	0.58
1:A:59:TRP:O	1:A:62:HIS:N	2.37	0.57
2:D:74:ALA:HB1	2:D:87:LEU:HD11	1.85	0.57
1:A:86:GLU:OE1	2:C:18:ARG:NH2	2.37	0.57
1:B:68:HIS:HA	1:B:75:VAL:HG13	1.86	0.57
2:D:47:PRO:O	2:D:76:TYR:OH	2.23	0.57
1:B:69:VAL:HB	2:D:6:PHE:N	2.20	0.56
2:C:21:LEU:HD21	2:C:29:ALA:H	1.69	0.56
1:A:32:TRP:CZ2	1:A:36:GLU:HG3	2.41	0.56
1:A:45:GLU:HB3	1:B:26:ARG:NH2	2.21	0.56
1:B:68:HIS:O	1:B:69:VAL:CB	2.55	0.55
2:D:7:THR:HG21	2:D:88:CYS:HB3	1.87	0.55
2:C:18:ARG:HD2	2:C:18:ARG:C	2.27	0.55
2:C:12:ARG:NE	2:C:15:GLU:OE1	2.39	0.55
2:D:20:PHE:N	2:D:20:PHE:CD2	2.73	0.55
1:A:26:ARG:HG2	1:B:49:GLU:OE2	2.07	0.55
2:C:36:ILE:O	2:C:40:ILE:N	2.39	0.54
1:A:89:ALA:HB1	2:C:11:LEU:HD11	1.89	0.54
2:D:62:GLU:HB3	2:D:75:MSE:HA	1.55	0.54
2:C:3:GLN:H	2:C:84:LEU:HA	1.72	0.54
1:A:32:TRP:CZ2	1:A:36:GLU:CG	2.90	0.54
2:C:33:ALA:HA	2:C:36:ILE:HD12	1.89	0.54
2:D:3:GLN:C	2:D:4:ILE:HG22	2.28	0.54
1:B:15:ILE:O	1:B:17:ALA:N	2.41	0.54
2:D:7:THR:OG1	2:D:88:CYS:HA	2.09	0.53
1:A:26:ARG:CD	1:B:49:GLU:OE1	2.57	0.53
2:C:21:LEU:HD11	2:C:28:ALA:O	2.09	0.53
2:D:62:GLU:CD	2:D:75:MSE:SE	2.98	0.53
1:B:69:VAL:HG23	2:D:6:PHE:HD1	1.75	0.52
1:B:68:HIS:ND1	1:B:74:VAL:CB	2.71	0.52
2:C:76:TYR:HB3	2:C:87:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:PHE:CD2	2:C:77:GLN:CG	2.92	0.52
2:D:3:GLN:O	2:D:4:ILE:HG23	2.09	0.52
1:B:74:VAL:HG22	1:B:77:TRP:HD1	1.74	0.52
2:C:21:LEU:HD11	2:C:29:ALA:CA	2.39	0.52
2:C:28:ALA:HA	2:C:31:ARG:HB2	1.91	0.51
2:D:10:ALA:HB2	2:D:89:ILE:H	1.76	0.51
1:B:74:VAL:HG22	1:B:75:VAL:H	1.75	0.51
2:D:62:GLU:CD	2:D:75:MSE:HB2	2.26	0.51
1:A:83:SER:O	1:A:85:ASN:N	2.43	0.51
2:D:6:PHE:CE2	2:D:87:LEU:CD2	2.89	0.51
1:B:69:VAL:O	1:B:70:THR:C	2.49	0.51
2:C:18:ARG:C	2:C:20:PHE:H	2.13	0.51
1:A:7:VAL:CG1	1:B:10:LYS:CE	2.89	0.50
2:D:5:VAL:HG12	2:D:6:PHE:N	2.25	0.50
2:D:60:PHE:CE1	2:D:75:MSE:HE3	2.46	0.50
1:A:15:ILE:HD13	1:B:39:ARG:NH1	2.21	0.50
2:C:25:ASN:CB	2:C:28:ALA:CB	2.89	0.50
2:C:45:SER:O	2:C:47:PRO:CD	2.41	0.50
2:C:88:CYS:O	2:C:89:ILE:HB	2.12	0.50
1:A:26:ARG:HD2	1:B:49:GLU:OE1	2.12	0.50
1:A:68:HIS:HB2	2:C:5:VAL:HG13	1.93	0.50
2:C:26:PRO:HG2	2:C:27:PRO:HD3	1.93	0.50
2:D:36:ILE:O	2:D:40:ILE:N	2.38	0.49
1:B:74:VAL:CG2	1:B:75:VAL:N	2.75	0.49
2:D:5:VAL:CG1	2:D:6:PHE:N	2.75	0.49
1:B:49:GLU:HG2	1:B:49:GLU:O	2.13	0.49
2:C:48:ASP:CG	2:C:49:ILE:N	2.65	0.49
2:C:12:ARG:HD3	2:C:15:GLU:CD	2.33	0.49
1:A:7:VAL:HG12	1:B:10:LYS:HD3	1.94	0.49
2:C:21:LEU:HD11	2:C:29:ALA:HA	1.91	0.49
1:A:45:GLU:HB3	1:B:26:ARG:HH22	1.78	0.48
1:A:75:VAL:HG22	2:C:37:ILE:HG23	1.93	0.48
2:C:18:ARG:NH1	2:C:29:ALA:CB	2.76	0.48
2:D:89:ILE:HG23	2:D:91:HIS:ND1	2.28	0.48
2:C:84:LEU:O	2:C:86:VAL:N	2.46	0.48
1:B:67:LEU:C	1:B:76:SER:O	2.51	0.48
1:A:19:VAL:O	1:A:23:ALA:N	2.39	0.48
2:C:69:ASP:OD1	2:C:70:THR:N	2.45	0.47
2:D:3:GLN:C	2:D:4:ILE:CG2	2.82	0.47
1:A:7:VAL:HG11	1:B:10:LYS:CE	2.41	0.47
1:A:59:TRP:O	1:A:60:GLU:C	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:CD1	2:D:6:PHE:O	2.62	0.47
2:C:18:ARG:HH12	2:C:29:ALA:HB2	1.79	0.47
1:B:74:VAL:CG2	1:B:75:VAL:H	2.27	0.47
2:D:42:LYS:HE3	2:D:63:LEU:HD21	1.97	0.47
1:A:59:TRP:CZ2	1:A:63:GLN:OE1	2.68	0.47
1:A:69:VAL:HG23	2:C:6:PHE:HB2	1.97	0.47
1:B:67:LEU:HD22	2:D:5:VAL:HG11	1.91	0.47
2:C:39:THR:HA	2:C:42:LYS:HE2	1.96	0.47
2:C:3:GLN:HB3	2:C:84:LEU:HB3	1.96	0.46
1:A:77:TRP:CG	1:A:88:ALA:O	2.68	0.46
2:D:88:CYS:O	2:D:89:ILE:HB	2.16	0.46
1:B:74:VAL:CG2	1:B:77:TRP:HD1	2.29	0.46
1:A:46:GLU:OE1	1:B:18:ARG:NH2	2.35	0.46
1:B:62:HIS:C	1:B:64:THR:H	2.19	0.46
2:C:21:LEU:HA	2:C:24:LYS:HB2	1.96	0.45
1:B:67:LEU:HD11	2:D:6:PHE:O	2.16	0.45
1:A:37:ALA:HB1	1:B:37:ALA:O	2.17	0.45
2:D:31:ARG:HE	2:D:67:PHE:HD1	1.64	0.45
1:A:7:VAL:CG1	1:B:10:LYS:CD	2.93	0.45
1:B:67:LEU:HD11	2:D:5:VAL:HG12	1.99	0.45
1:A:6:PRO:HB2	1:B:11:LEU:H	1.82	0.45
1:B:15:ILE:C	1:B:17:ALA:N	2.70	0.45
2:C:21:LEU:O	2:C:22:ARG:C	2.55	0.45
1:A:42:VAL:HG21	1:B:19:VAL:HG22	1.98	0.45
2:C:21:LEU:CD2	2:C:29:ALA:CA	2.95	0.45
2:C:21:LEU:C	2:C:24:LYS:H	2.19	0.45
1:A:25:THR:HB	1:B:49:GLU:OE2	2.16	0.45
1:A:15:ILE:HG12	1:B:39:ARG:NH1	2.32	0.45
2:C:18:ARG:C	2:C:20:PHE:N	2.69	0.44
1:A:16:LYS:HE3	1:B:7:VAL:HG21	2.00	0.44
1:A:41:TYR:CE2	1:A:45:GLU:HG3	2.53	0.44
1:A:77:TRP:HD1	1:A:87:GLN:HB2	1.81	0.44
2:C:68:GLY:O	2:C:69:ASP:C	2.56	0.44
2:C:48:ASP:O	2:C:49:ILE:HG22	2.17	0.44
2:C:14:LEU:O	2:C:17:LEU:HB3	2.18	0.44
1:A:6:PRO:HB2	1:A:7:VAL:H	1.59	0.43
1:A:25:THR:C	1:A:27:LYS:H	2.21	0.43
2:C:6:PHE:CZ	2:C:87:LEU:HD23	2.53	0.43
1:A:53:GLN:O	1:A:57:ARG:N	2.32	0.43
2:D:64:LEU:CD1	2:D:64:LEU:C	2.85	0.43
2:D:74:ALA:HB2	2:D:90:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ALA:HB2	2:C:89:ILE:H	1.83	0.43
2:C:18:ARG:NH1	2:C:29:ALA:HB2	2.33	0.43
2:D:4:ILE:HA	2:D:85:THR:OG1	2.17	0.43
1:A:10:LYS:HZ2	1:B:38:ILE:HD11	1.83	0.43
2:C:77:GLN:O	2:C:85:THR:HA	2.19	0.43
1:A:56:LEU:O	1:A:59:TRP:HB3	2.18	0.43
2:D:3:GLN:O	2:D:4:ILE:HG22	2.19	0.43
1:B:13:ALA:O	1:B:16:LYS:HB3	2.19	0.43
1:B:69:VAL:CB	2:D:6:PHE:H	2.28	0.43
1:A:38:ILE:HG23	1:B:34:MSE:HG2	2.00	0.42
2:D:92:GLN:CD	2:D:92:GLN:H	2.22	0.42
2:C:26:PRO:CB	2:C:27:PRO:HD3	2.50	0.42
2:C:3:GLN:HB3	2:C:84:LEU:CB	2.50	0.42
2:D:19:GLU:O	2:D:20:PHE:C	2.55	0.42
1:A:18:ARG:HD2	1:B:46:GLU:OE2	2.19	0.42
1:A:59:TRP:O	1:A:61:GLU:N	2.53	0.42
2:C:24:LYS:NZ	2:C:67:PHE:HE1	2.18	0.42
2:C:26:PRO:HB2	2:C:27:PRO:HD3	2.01	0.42
2:C:18:ARG:HH12	2:C:29:ALA:CB	2.32	0.41
1:A:57:ARG:O	1:A:61:GLU:HG3	2.20	0.41
1:A:72:ASP:O	1:A:76:SER:N	2.41	0.41
2:C:48:ASP:O	2:C:49:ILE:CG2	2.68	0.41
1:A:9:VAL:HG12	1:B:8:SER:OG	2.21	0.41
1:B:67:LEU:O	1:B:76:SER:O	2.39	0.41
2:C:36:ILE:HG12	2:C:90:ARG:NH1	2.34	0.41
1:A:7:VAL:HG23	1:A:7:VAL:O	2.21	0.41
2:D:76:TYR:CB	2:D:87:LEU:HA	2.51	0.41
1:A:7:VAL:HG12	1:B:10:LYS:CE	2.51	0.40
1:A:7:VAL:CG1	1:B:10:LYS:HD3	2.52	0.40
1:A:9:VAL:HB	1:B:8:SER:HA	2.04	0.40
1:A:32:TRP:CZ2	1:A:36:GLU:CD	2.95	0.40
2:C:36:ILE:CD1	2:C:90:ARG:HH22	2.35	0.40
2:C:26:PRO:CG	2:C:27:PRO:HD3	2.52	0.40
2:C:63:LEU:HD12	2:C:64:LEU:N	2.36	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	86/102 (84%)	73 (85%)	11 (13%)	2 (2%)	6 38
1	B	71/102 (70%)	59 (83%)	9 (13%)	3 (4%)	3 26
2	C	76/97 (78%)	57 (75%)	14 (18%)	5 (7%)	1 19
2	D	64/97 (66%)	56 (88%)	5 (8%)	3 (5%)	2 24
All	All	297/398 (75%)	245 (82%)	39 (13%)	13 (4%)	2 25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	84	GLU
1	B	69	VAL
2	C	49	ILE
2	C	85	THR
1	B	13	ALA
1	B	63	GLN
2	C	19	GLU
2	C	27	PRO
2	C	89	ILE
2	D	65	ILE
2	D	89	ILE
2	D	28	ALA

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	75/86 (87%)	72 (96%)	3 (4%)	31	59
1	B	64/86 (74%)	62 (97%)	2 (3%)	40	65
2	C	71/80 (89%)	68 (96%)	3 (4%)	30	58
2	D	62/80 (78%)	57 (92%)	5 (8%)	11	41
All	All	272/332 (82%)	259 (95%)	13 (5%)	25	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	VAL
1	A	38	ILE
1	B	67	LEU
1	B	75	VAL
2	C	20	PHE
2	C	60	PHE
2	C	84	LEU
2	D	18	ARG
2	D	20	PHE
2	D	49	ILE
2	D	64	LEU
2	D	89	ILE

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

Mol	Chain	Res	Type
1	A	91	HIS
1	B	62	HIS

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 (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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.