



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:05 AM UTC

PDB ID : 3GL3 / pdb_00003gl3
Title : Crystal structure of a putative Thiol:disulfide interchange protein DsbE from *Chlorobium tepidum*
Authors : Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-03-11
Resolution : 2.09 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

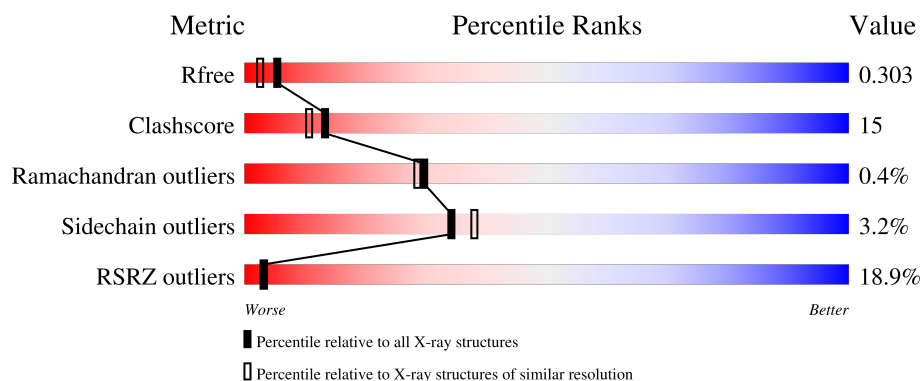
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	152	6% 76% 16% • 7%
1	B	152	7% 71% 20% • 7%
1	C	152	13% 63% 25% • 9%
1	D	152	41% 55% 32% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4488 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 Putative Thiol:disulfide interchange protein DsbE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	Se	0	0	0
			1084	701	184	193	2	4			
1	B	141	Total	C	N	O	S	Se	0	0	0
			1083	700	184	193	2	4			
1	C	138	Total	C	N	O	S	Se	0	0	0
			1067	690	181	190	2	4			
1	D	137	Total	C	N	O	S	Se	0	0	0
			1053	683	177	187	2	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	-	expression tag	UNP Q8KDH8
A	28	SER	-	expression tag	UNP Q8KDH8
A	29	LEU	-	expression tag	UNP Q8KDH8
A	171	GLU	-	expression tag	UNP Q8KDH8
A	172	GLY	-	expression tag	UNP Q8KDH8
A	173	HIS	-	expression tag	UNP Q8KDH8
A	174	HIS	-	expression tag	UNP Q8KDH8
A	175	HIS	-	expression tag	UNP Q8KDH8
A	176	HIS	-	expression tag	UNP Q8KDH8
A	177	HIS	-	expression tag	UNP Q8KDH8
A	178	HIS	-	expression tag	UNP Q8KDH8
B	27	MSE	-	expression tag	UNP Q8KDH8
B	28	SER	-	expression tag	UNP Q8KDH8
B	29	LEU	-	expression tag	UNP Q8KDH8
B	171	GLU	-	expression tag	UNP Q8KDH8
B	172	GLY	-	expression tag	UNP Q8KDH8
B	173	HIS	-	expression tag	UNP Q8KDH8
B	174	HIS	-	expression tag	UNP Q8KDH8
B	175	HIS	-	expression tag	UNP Q8KDH8
B	176	HIS	-	expression tag	UNP Q8KDH8
B	177	HIS	-	expression tag	UNP Q8KDH8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	178	HIS	-	expression tag	UNP Q8KDH8
C	27	MSE	-	expression tag	UNP Q8KDH8
C	28	SER	-	expression tag	UNP Q8KDH8
C	29	LEU	-	expression tag	UNP Q8KDH8
C	171	GLU	-	expression tag	UNP Q8KDH8
C	172	GLY	-	expression tag	UNP Q8KDH8
C	173	HIS	-	expression tag	UNP Q8KDH8
C	174	HIS	-	expression tag	UNP Q8KDH8
C	175	HIS	-	expression tag	UNP Q8KDH8
C	176	HIS	-	expression tag	UNP Q8KDH8
C	177	HIS	-	expression tag	UNP Q8KDH8
C	178	HIS	-	expression tag	UNP Q8KDH8
D	27	MSE	-	expression tag	UNP Q8KDH8
D	28	SER	-	expression tag	UNP Q8KDH8
D	29	LEU	-	expression tag	UNP Q8KDH8
D	171	GLU	-	expression tag	UNP Q8KDH8
D	172	GLY	-	expression tag	UNP Q8KDH8
D	173	HIS	-	expression tag	UNP Q8KDH8
D	174	HIS	-	expression tag	UNP Q8KDH8
D	175	HIS	-	expression tag	UNP Q8KDH8
D	176	HIS	-	expression tag	UNP Q8KDH8
D	177	HIS	-	expression tag	UNP Q8KDH8
D	178	HIS	-	expression tag	UNP Q8KDH8

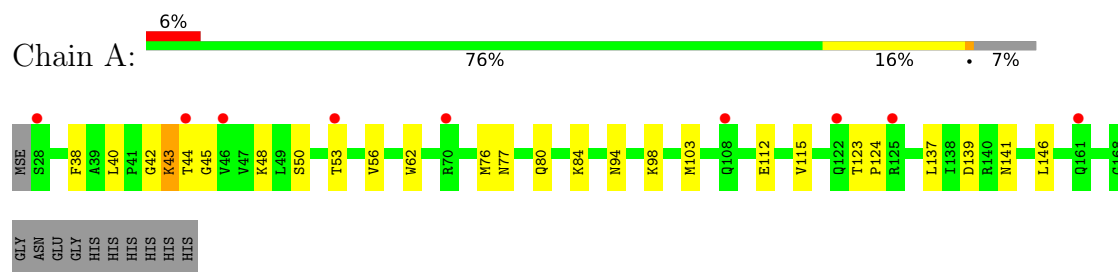
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	45	Total O 45 45	0	0
2	C	55	Total O 55 55	0	0
2	D	35	Total O 35 35	0	0

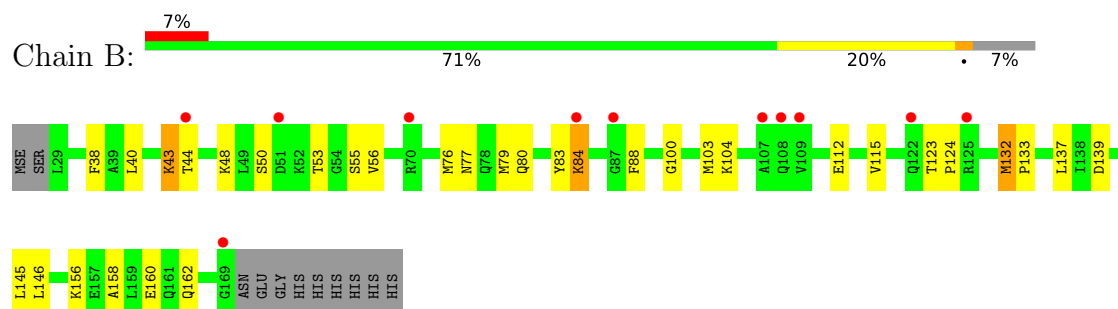
3 Residue-property plots [i](#)

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.

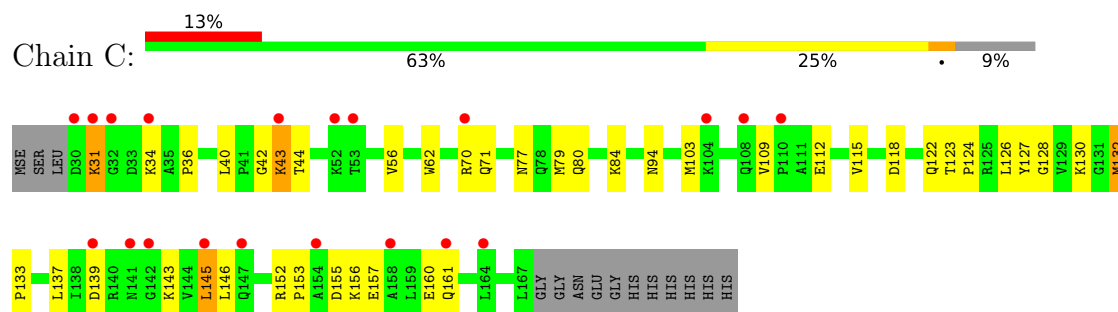
- Molecule 1: Putative Thiol:disulfide interchange protein DsbE



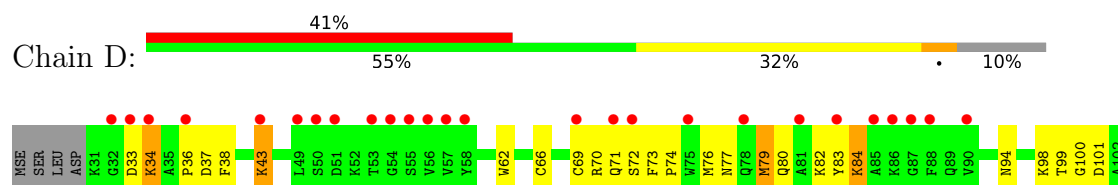
- Molecule 1: Putative Thiol:disulfide interchange protein DsbE

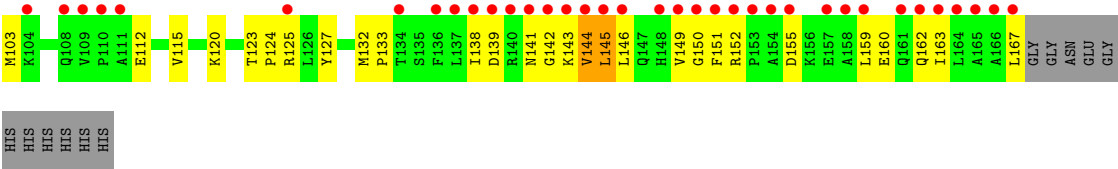


- Molecule 1: Putative Thiol:disulfide interchange protein DsbE



- Molecule 1: Putative Thiol:disulfide interchange protein DsbE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.20Å 42.07Å 82.52Å 90.00° 108.77° 90.00°	Depositor
Resolution (Å)	39.07 – 2.09 39.07 – 2.09	Depositor EDS
% Data completeness (in resolution range)	90.8 (39.07-2.09) 95.6 (39.07-2.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.296 0.279 , 0.303	Depositor DCC
R_{free} test set	1557 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9020e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.61	2/1107 (0.2%)	0.87	1/1490 (0.1%)
1	B	0.59	3/1106 (0.3%)	0.88	2/1488 (0.1%)
1	C	0.55	2/1090 (0.2%)	0.86	3/1467 (0.2%)
1	D	0.62	5/1076 (0.5%)	0.91	2/1449 (0.1%)
All	All	0.59	12/4379 (0.3%)	0.88	8/5894 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MSE	SE-CE	-8.35	1.70	1.95
1	D	132	MSE	SE-CE	-7.68	1.72	1.95
1	B	76	MSE	SE-CE	-7.12	1.74	1.95
1	B	103	MSE	SE-CE	-6.43	1.76	1.95
1	D	76	MSE	SE-CE	-6.26	1.76	1.95
1	A	103	MSE	SE-CE	-6.25	1.76	1.95
1	D	79	MSE	SE-CE	-6.14	1.77	1.95
1	C	132	MSE	SE-CE	-6.02	1.77	1.95
1	B	132	MSE	SE-CE	-5.64	1.78	1.95
1	D	103	MSE	SE-CE	-5.60	1.78	1.95
1	C	103	MSE	SE-CE	-5.44	1.79	1.95
1	D	103	MSE	CG-SE	-5.38	1.79	1.95

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	LYS	N-CA-C	7.17	119.10	111.28
1	B	56	VAL	N-CA-C	-6.60	101.05	109.30
1	B	156	LYS	N-CA-C	6.53	118.94	111.11
1	D	145	LEU	N-CA-C	-6.16	106.37	114.31
1	A	56	VAL	N-CA-C	-6.01	100.96	108.89
1	C	42	GLY	N-CA-C	-5.82	104.78	112.81
1	C	145	LEU	N-CA-C	-5.77	106.78	113.88
1	C	56	VAL	N-CA-C	-5.68	101.49	109.21

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	1084	0	1091	21	0
1	B	1083	0	1092	21	0
1	C	1067	0	1075	32	0
1	D	1053	0	1060	54	0
2	A	66	0	0	3	0
2	B	45	0	0	0	0
2	C	55	0	0	3	0
2	D	35	0	0	1	0
All	All	4488	0	4318	127	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 15.

All (127) 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:D:43:LYS:HD2	1:D:43:LYS:H	1.18	1.06
1:A:77:ASN:HD21	1:A:112:GLU:H	1.16	0.93
1:D:43:LYS:HD2	1:D:43:LYS:N	1.85	0.89
1:D:139:ASP:HB3	1:D:145:LEU:HD21	1.59	0.84
1:B:77:ASN:HD21	1:B:112:GLU:H	1.24	0.84
1:A:50:SER:O	1:A:53:THR:HG23	1.77	0.83
1:B:43:LYS:HD3	1:B:43:LYS:H	1.41	0.83
1:C:43:LYS:HD2	1:C:43:LYS:H	1.45	0.81
1:A:77:ASN:ND2	1:A:112:GLU:H	1.80	0.79
1:D:34:LYS:HA	1:D:143:LYS:HA	1.66	0.76
1:A:43:LYS:HD3	1:A:43:LYS:H	1.52	0.75
1:C:70:ARG:HH11	1:C:109:VAL:HG22	1.52	0.74
1:B:77:ASN:ND2	1:B:112:GLU:H	1.87	0.72
1:D:43:LYS:H	1:D:43:LYS:CD	1.83	0.72
1:D:80:GLN:HE21	1:D:84:LYS:HB2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:MSE:SE	1:C:160:GLU:HG3	2.41	0.71
1:A:43:LYS:HE3	1:A:115:VAL:HB	1.73	0.71
1:D:143:LYS:O	1:D:144:VAL:HB	1.90	0.70
1:C:77:ASN:HD21	1:C:112:GLU:H	1.37	0.70
1:C:157:GLU:O	1:C:161:GLN:HG2	1.92	0.70
1:D:77:ASN:HD21	1:D:112:GLU:H	1.38	0.70
1:D:70:ARG:NH1	1:D:70:ARG:HB3	2.07	0.69
1:D:77:ASN:ND2	1:D:112:GLU:H	1.91	0.68
1:D:139:ASP:CB	1:D:145:LEU:HD21	2.23	0.68
1:D:143:LYS:O	1:D:144:VAL:CB	2.42	0.66
1:D:79:MSE:SE	1:D:160:GLU:HG3	2.46	0.66
1:D:80:GLN:NE2	1:D:84:LYS:HB2	2.11	0.66
1:D:71:GLN:O	1:D:74:PRO:HD2	1.95	0.65
1:D:138:ILE:CG2	1:D:142:GLY:HA2	2.27	0.65
1:B:43:LYS:HE3	1:B:115:VAL:H	1.60	0.65
1:C:77:ASN:ND2	1:C:112:GLU:H	1.95	0.65
1:C:43:LYS:HE3	1:C:115:VAL:H	1.62	0.64
1:D:43:LYS:HE2	1:D:115:VAL:H	1.62	0.63
1:D:70:ARG:HB3	1:D:70:ARG:HH11	1.63	0.63
1:C:31:LYS:HE2	1:C:145:LEU:O	1.98	0.62
1:B:139:ASP:HB3	1:B:145:LEU:HD11	1.80	0.61
1:C:130:LYS:HE2	2:C:228:HOH:O	1.98	0.61
1:A:139:ASP:OD1	1:A:141:ASN:N	2.35	0.60
1:C:152:ARG:HG2	1:C:155:ASP:OD2	2.03	0.59
1:A:146:LEU:C	1:A:146:LEU:HD12	2.28	0.59
1:B:43:LYS:HD3	1:B:43:LYS:N	2.15	0.59
1:A:43:LYS:HE3	1:A:115:VAL:H	1.68	0.58
1:D:33:ASP:O	1:D:34:LYS:CB	2.52	0.57
1:D:33:ASP:O	1:D:34:LYS:HB3	2.05	0.57
1:D:145:LEU:HD22	1:D:145:LEU:N	2.20	0.57
1:C:70:ARG:NH1	1:C:109:VAL:HG22	2.18	0.57
1:B:80:GLN:O	1:B:84:LYS:HB3	2.05	0.57
1:C:34:LYS:HD2	2:C:224:HOH:O	2.05	0.56
1:B:40:LEU:HD11	1:B:123:THR:HG21	1.86	0.56
1:B:79:MSE:SE	1:B:160:GLU:HG3	2.57	0.55
1:D:43:LYS:HE2	1:D:115:VAL:O	2.07	0.55
1:D:143:LYS:O	1:D:144:VAL:HG23	2.06	0.55
1:D:43:LYS:N	1:D:43:LYS:CD	2.54	0.53
1:B:137:LEU:HB3	1:B:146:LEU:HG	1.90	0.52
1:D:138:ILE:HG21	1:D:142:GLY:HA2	1.92	0.52
1:B:43:LYS:HE3	1:B:115:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:NE2	1:C:161:GLN:HA	2.25	0.51
1:D:144:VAL:C	1:D:145:LEU:HD22	2.34	0.51
1:A:80:GLN:HE21	1:A:84:LYS:HB3	1.74	0.51
1:D:143:LYS:O	1:D:144:VAL:CG2	2.58	0.51
1:C:139:ASP:OD2	1:C:143:LYS:HB2	2.11	0.51
2:A:220:HOH:O	1:D:125:ARG:HD2	2.09	0.50
1:C:123:THR:N	1:C:124:PRO:HD2	2.26	0.50
1:D:123:THR:N	1:D:124:PRO:HD2	2.26	0.50
1:B:100:GLY:O	1:B:104:LYS:HG3	2.11	0.50
1:B:50:SER:O	1:B:53:THR:HG23	2.12	0.49
1:B:123:THR:N	1:B:124:PRO:HD2	2.27	0.49
1:C:43:LYS:CE	1:C:115:VAL:H	2.26	0.49
1:C:40:LEU:HD13	1:C:118:ASP:HB2	1.94	0.49
1:C:137:LEU:HB3	1:C:146:LEU:HG	1.95	0.48
1:C:43:LYS:H	1:C:43:LYS:CD	2.11	0.48
1:D:139:ASP:O	1:D:142:GLY:N	2.46	0.48
1:A:43:LYS:HD3	1:A:43:LYS:N	2.23	0.48
1:D:62:TRP:CZ2	1:D:94:ASN:HB2	2.48	0.48
1:D:133:PRO:HD2	1:D:150:GLY:HA2	1.96	0.47
1:D:71:GLN:HG3	2:D:181:HOH:O	2.15	0.47
1:B:146:LEU:C	1:B:146:LEU:HD12	2.39	0.47
1:C:44:THR:O	1:D:120:LYS:NZ	2.46	0.47
1:D:34:LYS:HB3	1:D:34:LYS:HE3	1.77	0.47
1:D:145:LEU:N	1:D:145:LEU:CD2	2.77	0.46
1:B:132:MSE:HA	1:B:133:PRO:HA	1.78	0.46
1:D:159:LEU:O	1:D:163:ILE:HG13	2.16	0.46
1:C:161:GLN:HA	1:C:161:GLN:HE21	1.80	0.46
1:A:43:LYS:HE3	1:A:115:VAL:N	2.32	0.45
1:C:153:PRO:HA	1:C:156:LYS:HE2	1.98	0.45
1:A:38:PHE:O	1:A:48:LYS:HA	2.16	0.45
1:A:43:LYS:H	1:A:43:LYS:CD	2.20	0.45
1:D:34:LYS:O	1:D:34:LYS:HD2	2.17	0.45
1:D:43:LYS:CE	1:D:115:VAL:H	2.26	0.45
1:A:139:ASP:OD1	1:A:139:ASP:C	2.60	0.45
1:D:152:ARG:N	1:D:155:ASP:OD2	2.40	0.45
1:A:123:THR:N	1:A:124:PRO:HD2	2.32	0.45
1:D:34:LYS:N	1:D:143:LYS:O	2.50	0.44
1:D:36:PRO:HD2	1:D:127:TYR:CZ	2.52	0.44
1:D:99:THR:O	1:D:100:GLY:C	2.60	0.44
1:D:138:ILE:HG22	1:D:142:GLY:HA2	2.00	0.44
1:A:40:LEU:HD11	1:A:123:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ALA:O	1:B:162:GLN:HG2	2.18	0.44
1:A:42:GLY:N	1:A:45:GLY:O	2.47	0.43
1:D:72:SER:HA	1:D:151:PHE:CE2	2.53	0.43
1:D:36:PRO:O	1:D:127:TYR:OH	2.30	0.43
1:B:43:LYS:HE3	1:B:115:VAL:N	2.29	0.43
1:B:43:LYS:H	1:B:43:LYS:CD	2.15	0.43
1:A:98:LYS:HD2	2:A:204:HOH:O	2.18	0.43
1:C:122:GLN:O	1:C:126:LEU:HG	2.19	0.43
1:B:38:PHE:O	1:B:48:LYS:HA	2.19	0.43
1:D:66:CYS:HB3	1:D:69:CYS:SG	2.59	0.43
1:D:37:ASP:CG	1:D:38:PHE:H	2.27	0.43
1:D:139:ASP:OD1	1:D:141:ASN:N	2.51	0.43
1:C:36:PRO:HD2	1:C:127:TYR:CZ	2.54	0.42
1:B:83:TYR:O	1:B:88:PHE:HB3	2.20	0.42
1:D:80:GLN:O	1:D:84:LYS:HB3	2.19	0.42
1:C:80:GLN:O	1:C:84:LYS:HB2	2.20	0.42
1:C:40:LEU:HD11	1:C:123:THR:HG21	2.02	0.41
1:A:137:LEU:HD12	1:A:137:LEU:HA	1.85	0.41
1:C:77:ASN:HD22	1:C:77:ASN:HA	1.70	0.41
1:C:79:MSE:HA	1:C:79:MSE:HE2	2.01	0.41
1:C:132:MSE:HA	1:C:133:PRO:C	2.45	0.41
1:D:83:TYR:HB3	1:D:167:LEU:CD1	2.51	0.41
1:C:62:TRP:CZ2	1:C:94:ASN:HB2	2.56	0.41
1:D:98:LYS:O	1:D:101:ASP:HB2	2.21	0.40
1:D:73:PHE:O	1:D:74:PRO:C	2.63	0.40
1:A:62:TRP:CZ2	1:A:94:ASN:HB2	2.57	0.40
1:A:141:ASN:HB2	2:A:192:HOH:O	2.21	0.40
1:D:141:ASN:O	1:D:143:LYS:HG3	2.21	0.40
1:C:43:LYS:HD2	2:C:18:HOH:O	2.21	0.40
1:C:128:GLY:O	1:C:130:LYS:HG3	2.22	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	139/152 (91%)	136 (98%)	3 (2%)	0	100	100
1	B	139/152 (91%)	134 (96%)	5 (4%)	0	100	100
1	C	136/152 (90%)	133 (98%)	3 (2%)	0	100	100
1	D	135/152 (89%)	126 (93%)	7 (5%)	2 (2%)	8	4
All	All	549/608 (90%)	529 (96%)	18 (3%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	34	LYS
1	D	144	VAL

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	112/117 (96%)	110 (98%)	2 (2%)	51	60
1	B	112/117 (96%)	108 (96%)	4 (4%)	31	34
1	C	111/117 (95%)	108 (97%)	3 (3%)	39	45
1	D	109/117 (93%)	104 (95%)	5 (5%)	24	25
All	All	444/468 (95%)	430 (97%)	14 (3%)	34	38

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	44	THR
1	B	43	LYS
1	B	44	THR
1	B	55	SER
1	B	84	LYS

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Mol	Chain	Res	Type
1	C	31	LYS
1	C	43	LYS
1	C	71	GLN
1	D	43	LYS
1	D	84	LYS
1	D	146	LEU
1	D	149	VAL
1	D	162	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	77	ASN
1	A	89	GLN
1	B	71	GLN
1	B	77	ASN
1	C	77	ASN
1	C	148	HIS
1	C	161	GLN
1	D	71	GLN
1	D	77	ASN
1	D	89	GLN
1	D	122	GLN

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

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	137/152 (90%)	0.53	9 (6%) 24 26	13, 24, 39, 46	0
1	B	137/152 (90%)	0.80	11 (8%) 18 19	17, 29, 45, 50	0
1	C	134/152 (88%)	1.10	20 (14%) 5 5	18, 33, 44, 49	0
1	D	133/152 (87%)	1.94	62 (46%) 0 0	21, 41, 53, 55	0
All	All	541/608 (88%)	1.09	102 (18%) 3 3	13, 31, 49, 55	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	GLY	6.2
1	D	159	LEU	4.5
1	D	144	VAL	4.3
1	D	88	PHE	4.2
1	D	139	ASP	4.0
1	D	138	ILE	4.0
1	D	141	ASN	3.9
1	D	57	VAL	3.8
1	D	145	LEU	3.7
1	C	31	LYS	3.7
1	D	164	LEU	3.7
1	D	87	GLY	3.7
1	D	137	LEU	3.7
1	D	158	ALA	3.6
1	D	85	ALA	3.5
1	D	143	LYS	3.5
1	D	167	LEU	3.4
1	D	55	SER	3.4
1	B	109	VAL	3.3
1	D	154	ALA	3.3
1	D	165	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	83	TYR	3.2
1	D	136	PHE	3.2
1	D	142	GLY	3.2
1	D	149	VAL	3.1
1	C	147	GLN	3.1
1	D	161	GLN	3.1
1	A	108	GLN	3.1
1	D	162	GLN	3.0
1	D	53	THR	3.0
1	D	109	VAL	3.0
1	D	140	ARG	2.9
1	A	28	SER	2.9
1	D	54	GLY	2.9
1	C	104	LYS	2.9
1	D	163	ILE	2.8
1	C	145	LEU	2.8
1	A	44	THR	2.8
1	C	52	LYS	2.8
1	C	139	ASP	2.8
1	B	44	THR	2.7
1	D	90	VAL	2.7
1	C	142	GLY	2.7
1	D	108	GLN	2.7
1	D	72	SER	2.7
1	D	32	GLY	2.7
1	C	158	ALA	2.6
1	A	70	ARG	2.6
1	B	70	ARG	2.6
1	D	166	ALA	2.6
1	C	108	GLN	2.6
1	D	75	TRP	2.6
1	D	150	GLY	2.5
1	D	86	LYS	2.5
1	D	104	LYS	2.5
1	D	81	ALA	2.5
1	A	125	ARG	2.5
1	D	34	LYS	2.5
1	D	152	ARG	2.5
1	D	71	GLN	2.4
1	B	108	GLN	2.4
1	D	56	VAL	2.4
1	D	134	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	36	PRO	2.4
1	D	110	PRO	2.4
1	A	122	GLN	2.4
1	B	122	GLN	2.4
1	D	33	ASP	2.4
1	D	51	ASP	2.4
1	D	50	SER	2.4
1	D	148	HIS	2.4
1	C	154	ALA	2.3
1	D	146	LEU	2.3
1	C	43	LYS	2.3
1	C	141	ASN	2.3
1	D	125	ARG	2.3
1	B	107	ALA	2.3
1	D	49	LEU	2.3
1	D	151	PHE	2.3
1	D	153	PRO	2.3
1	D	58	TYR	2.3
1	D	78	GLN	2.2
1	B	84	LYS	2.2
1	D	69	CYS	2.2
1	D	157	GLU	2.2
1	A	46	VAL	2.2
1	B	51	ASP	2.2
1	C	32	GLY	2.2
1	C	161	GLN	2.2
1	A	53	THR	2.2
1	C	53	THR	2.1
1	B	87	GLY	2.1
1	B	125	ARG	2.1
1	D	111	ALA	2.1
1	D	43	LYS	2.1
1	C	30	ASP	2.1
1	D	155	ASP	2.1
1	C	110	PRO	2.1
1	A	161	GLN	2.1
1	C	70	ARG	2.0
1	C	34	LYS	2.0
1	C	164	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.