



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:58 PM UTC

PDB ID : 1JZD / pdb_00001jzd
Title : DsbC-DsbDalpa complex
Authors : Haebel, P.W.; Goldstone, D.; Katzen, F.; Beckwith, J.; Metcalf, P.
Deposited on : 2001-09-15
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

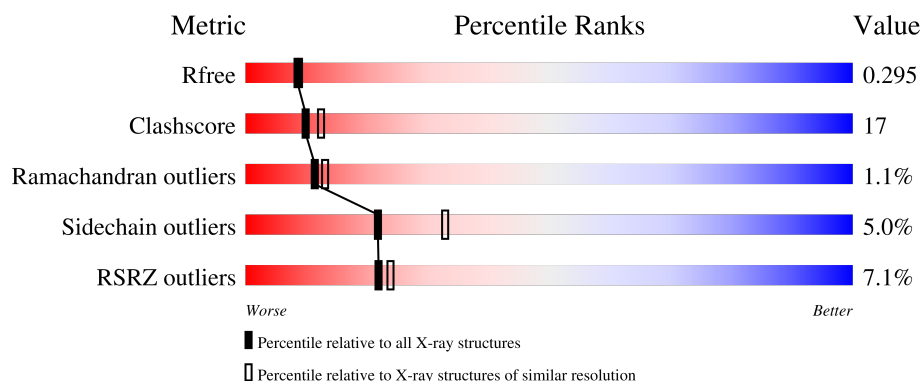
1 Overall quality at a glance

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	220	10% 64% 29% 5%
1	B	220	4% 64% 32% ..
2	C	132	6% 58% 27% .. 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4347 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 thiol:disulfide interchange protein dsbc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1652	1042	275	321	14			
1	B	214	Total	C	N	O	S	0	0	0
			1626	1027	270	316	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P21892
A	-2	ALA	-	expression tag	UNP P21892
A	-1	MET	-	expression tag	UNP P21892
A	0	ALA	-	expression tag	UNP P21892
A	101	SER	CYS	engineered mutation	UNP P21892
B	-3	GLY	-	expression tag	UNP P21892
B	-2	ALA	-	expression tag	UNP P21892
B	-1	MET	-	expression tag	UNP P21892
B	0	ALA	-	expression tag	UNP P21892
B	101	SER	CYS	engineered mutation	UNP P21892

- Molecule 2 is a protein called thiol:disulfide interchange protein dsbd.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	118	Total	C	N	O	S	4	0	0
			945	605	158	181	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	103	ALA	CYS	engineered mutation	UNP P36655

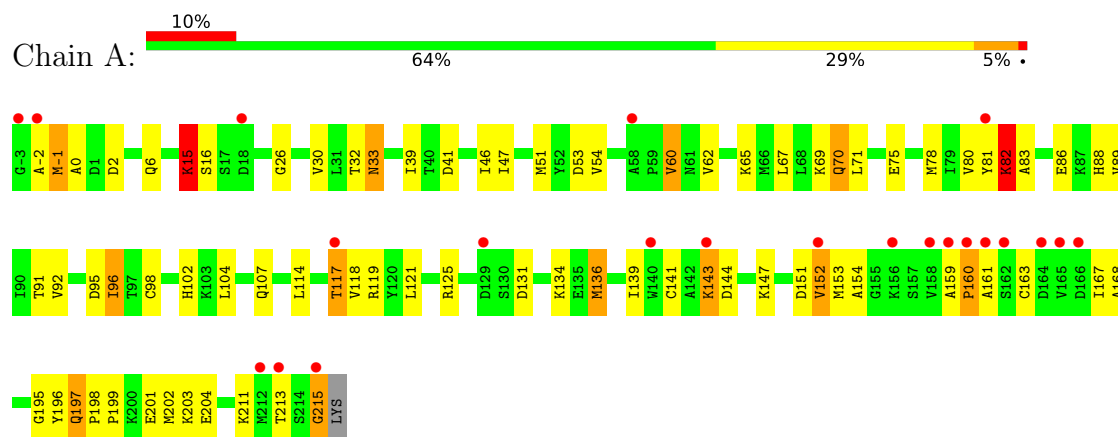
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	46	Total 46	O 46	0	0
3	C	41	Total 41	O 41	0	0

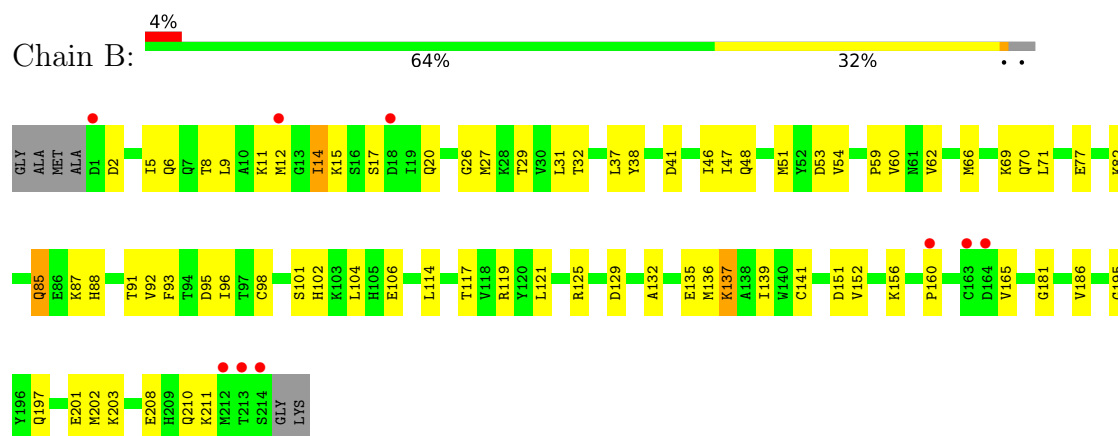
3 Residue-property plots [i](#)

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.

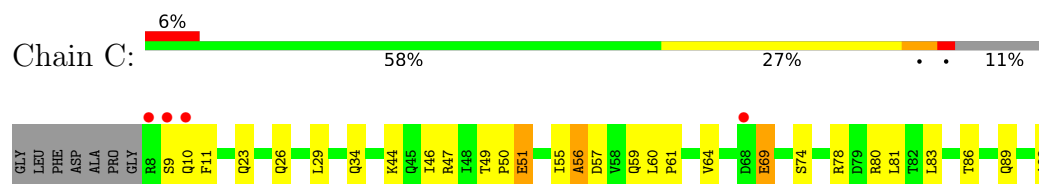
- Molecule 1: thiol:disulfide interchange protein dsbc



- Molecule 1: thiol:disulfide interchange protein dsbc



- Molecule 2: thiol:disulfide interchange protein dsbd



A106	G107	F108	C109	E113	S120	E121	V122	V123	A124	V125	ASN	ALA	ALA	PRO	GLN	PRO	VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.91Å 68.91Å 230.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.30 29.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.77-2.30) 98.3 (29.77-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.293 0.235 , 0.295	Depositor DCC
R_{free} test set	1995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4347	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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

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	0.56	2/1682 (0.1%)	0.99	14/2277 (0.6%)
1	B	0.41	0/1656	0.93	6/2243 (0.3%)
2	C	0.79	5/971 (0.5%)	1.40	14/1326 (1.1%)
All	All	0.57	7/4309 (0.2%)	1.08	34/5846 (0.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	123	VAL	CA-C	11.95	1.67	1.53
2	C	125	ASN	N-CA	6.22	1.58	1.46
1	A	82	LYS	N-CA	6.09	1.54	1.46
1	A	82	LYS	CB-CG	5.98	1.70	1.52
2	C	122	VAL	CA-C	5.94	1.60	1.52
2	C	124	ALA	CA-CB	-5.36	1.45	1.54
2	C	123	VAL	N-CA	5.26	1.55	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	123	VAL	N-CA-C	24.10	137.44	110.21
2	C	124	ALA	N-CA-C	19.56	144.38	114.64
1	B	2	ASP	N-CA-C	-11.34	100.16	114.56
2	C	125	ASN	N-CA-C	8.73	135.44	111.00
2	C	124	ALA	CA-C-O	-8.32	108.03	118.43
2	C	122	VAL	CA-C-N	6.93	131.28	120.34
2	C	122	VAL	C-N-CA	6.93	131.28	120.34
2	C	125	ASN	CB-CA-C	-6.87	97.05	110.10
2	C	26	GLN	CB-CA-C	-6.76	108.04	117.23
2	C	124	ALA	CB-CA-C	-6.62	99.29	109.29
1	A	82	LYS	CB-CG-CD	6.12	125.37	111.30
1	B	195	GLY	N-CA-C	6.01	119.02	112.29
1	A	121	LEU	N-CA-C	-6.00	100.02	109.50
1	A	131	ASP	N-CA-C	-5.96	105.50	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ALA	N-CA-C	-5.92	101.04	109.62
1	A	195	GLY	N-CA-C	5.86	123.13	112.58
2	C	49	THR	CA-C-N	5.80	125.71	119.85
2	C	49	THR	C-N-CA	5.80	125.71	119.85
1	B	15	LYS	N-CA-C	5.75	118.50	111.82
1	B	101	SER	N-CA-C	-5.75	105.09	111.36
2	C	34	GLN	N-CA-C	-5.71	99.43	108.73
1	A	15	LYS	N-CA-C	5.65	118.20	111.71
1	B	137	LYS	N-CA-C	-5.65	105.03	111.07
1	A	82	LYS	N-CA-C	5.63	122.80	110.80
1	A	134	LYS	N-CA-C	5.60	117.19	111.14
1	A	92	VAL	N-CA-C	5.59	115.91	107.75
1	A	118	VAL	N-CA-C	5.55	115.93	108.17
1	A	215	GLY	N-CA-C	5.41	128.99	113.30
1	B	92	VAL	N-CA-C	5.30	115.49	107.75
1	A	136	MET	N-CA-C	-5.27	105.59	112.23
2	C	56	ALA	N-CA-C	-5.25	105.46	111.07
2	C	64	VAL	N-CA-C	5.05	116.42	109.46
1	A	197	GLN	CA-C-N	5.04	123.34	119.66
1	A	197	GLN	C-N-CA	5.04	123.34	119.66

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	1652	0	1658	58	6
1	B	1626	0	1633	54	0
2	C	945	0	896	44	6
3	A	37	0	0	0	0
3	B	46	0	0	0	0
3	C	41	0	0	2	0
All	All	4347	0	4187	147	6

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 17.

All (147) 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)
2:C:124:ALA:C	2:C:125:ASN:ND2	1.72	1.47
1:A:141:CYS:SG	1:A:163:CYS:SG	2.31	1.28
2:C:124:ALA:O	2:C:125:ASN:ND2	1.85	1.10
1:A:53:ASP:HB3	1:A:60:VAL:HG13	1.50	0.92
2:C:124:ALA:CA	2:C:125:ASN:ND2	2.36	0.88
1:B:29:THR:HG21	1:B:66:MET:HE2	1.58	0.84
1:A:15:LYS:HD2	1:A:16:SER:H	1.40	0.83
2:C:124:ALA:HA	2:C:125:ASN:ND2	1.92	0.82
1:A:51:MET:HE2	1:B:47:ILE:HD11	1.58	0.82
1:A:15:LYS:HD2	1:A:16:SER:N	1.95	0.81
1:B:14:ILE:HD11	1:B:32:THR:HG21	1.64	0.80
2:C:92:ALA:HB2	2:C:121:GLU:OE2	1.82	0.79
1:A:198:PRO:HB2	1:A:201:GLU:OE1	1.83	0.78
2:C:50:PRO:HG3	2:C:55:ILE:HD11	1.64	0.77
1:A:211:LYS:O	1:A:215:GLY:HA2	1.86	0.76
1:A:71:LEU:HD11	1:A:91:THR:HG21	1.69	0.75
1:A:102:HIS:HA	1:A:153:MET:HE3	1.69	0.74
1:A:102:HIS:HA	1:A:153:MET:CE	2.19	0.72
1:B:98:CYS:SG	2:C:109:CYS:SG	2.88	0.71
1:B:87:LYS:HA	1:B:87:LYS:HE2	1.71	0.71
2:C:123:VAL:HG12	2:C:124:ALA:N	2.07	0.70
2:C:125:ASN:ND2	2:C:125:ASN:N	2.40	0.69
1:A:197:GLN:HB3	1:A:202:MET:HE2	1.75	0.69
1:B:14:ILE:HG12	1:B:17:SER:OG	1.93	0.68
1:B:8:THR:HG22	1:B:12:MET:HE2	1.74	0.67
1:B:14:ILE:HG12	1:B:14:ILE:O	1.94	0.67
2:C:78:ARG:HD3	3:C:158:HOH:O	1.95	0.66
1:B:27:MET:HE2	1:B:38:TYR:HB3	1.78	0.66
2:C:69:GLU:H	2:C:69:GLU:CD	2.05	0.65
1:B:125:ARG:HH11	1:B:125:ARG:HG2	1.61	0.65
2:C:50:PRO:HG3	2:C:55:ILE:CD1	2.26	0.64
1:A:95:ASP:OD2	1:A:125:ARG:HG2	1.99	0.63
1:A:69:LYS:HB3	1:A:70:GLN:NE2	2.14	0.62
2:C:124:ALA:C	2:C:125:ASN:CG	2.57	0.62
1:B:14:ILE:HD11	1:B:32:THR:CG2	2.29	0.62
2:C:69:GLU:CD	2:C:69:GLU:N	2.58	0.62
2:C:124:ALA:O	2:C:125:ASN:CG	2.42	0.61
1:B:151:ASP:HA	1:B:156:LYS:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASP:O	1:A:6:GLN:HG3	2.00	0.60
2:C:46:ILE:O	2:C:47:ARG:HD2	2.02	0.60
2:C:78:ARG:HH11	2:C:78:ARG:HG3	1.66	0.60
1:A:96:ILE:HD12	1:A:136:MET:CG	2.31	0.59
2:C:120:SER:O	2:C:122:VAL:HG23	2.02	0.59
1:B:54:VAL:HG12	1:B:59:PRO:HB3	1.82	0.59
1:A:96:ILE:HD12	1:A:136:MET:HG3	1.83	0.58
1:A:211:LYS:O	1:A:215:GLY:CA	2.51	0.58
1:B:211:LYS:NZ	1:B:211:LYS:HB3	2.18	0.58
1:B:53:ASP:HB3	1:B:60:VAL:HG12	1.84	0.58
1:A:82:LYS:NZ	1:A:86:GLU:OE1	2.35	0.58
2:C:56:ALA:HB3	2:C:86:THR:HB	1.85	0.57
1:B:98:CYS:HG	2:C:109:CYS:HG	1.41	0.57
1:B:12:MET:HE1	1:B:46:ILE:HD11	1.88	0.56
1:A:211:LYS:O	1:A:215:GLY:N	2.38	0.56
2:C:123:VAL:CG1	2:C:124:ALA:N	2.69	0.55
1:B:71:LEU:HD11	1:B:91:THR:HG21	1.89	0.55
1:A:54:VAL:HG11	1:B:12:MET:SD	2.47	0.54
1:A:104:LEU:HD23	1:A:104:LEU:C	2.32	0.54
1:A:39:ILE:HG12	1:A:46:ILE:HG12	1.89	0.53
1:A:47:ILE:HD11	1:B:51:MET:HE2	1.91	0.53
1:A:67:LEU:O	1:A:70:GLN:HG2	2.08	0.52
1:B:77:GLU:HG2	1:B:165:VAL:HG22	1.92	0.52
1:B:82:LYS:HA	1:B:117:THR:HG23	1.92	0.51
1:B:37:LEU:CD2	1:B:48:GLN:HG2	2.40	0.51
1:A:213:THR:O	1:A:213:THR:HG22	2.10	0.50
1:B:53:ASP:HB3	1:B:60:VAL:CG1	2.40	0.50
1:B:12:MET:HE1	1:B:46:ILE:CD1	2.42	0.50
1:B:137:LYS:HE2	1:B:141:CYS:SG	2.51	0.50
1:A:51:MET:O	1:A:62:VAL:HG22	2.11	0.49
1:B:201:GLU:N	1:B:201:GLU:OE1	2.45	0.49
1:B:104:LEU:C	1:B:104:LEU:HD23	2.38	0.49
2:C:44:LYS:NZ	2:C:74:SER:HB3	2.28	0.49
1:B:125:ARG:HG2	1:B:125:ARG:NH1	2.27	0.49
2:C:44:LYS:HG3	3:C:142:HOH:O	2.11	0.49
2:C:89:GLN:HA	2:C:122:VAL:O	2.12	0.49
1:A:143:LYS:HD2	1:A:143:LYS:N	2.28	0.49
1:B:88:HIS:HE1	1:B:210:GLN:CG	2.26	0.48
1:A:89:VAL:HG13	1:A:117:THR:HG22	1.95	0.48
1:A:-2:ALA:HB1	1:A:2:ASP:OD2	2.13	0.48
1:B:14:ILE:CD1	1:B:32:THR:HG21	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:GLN:O	2:C:29:LEU:HD12	2.14	0.48
1:A:30:VAL:HG21	1:A:39:ILE:HD12	1.96	0.48
1:A:15:LYS:CD	1:A:16:SER:N	2.74	0.47
1:B:93:PHE:HE1	1:B:186:VAL:HG21	1.78	0.47
1:B:20:GLN:HE22	1:B:69:LYS:HD3	1.79	0.47
2:C:69:GLU:N	2:C:69:GLU:OE1	2.49	0.46
1:A:139:ILE:HD11	1:A:152:VAL:HG21	1.98	0.46
2:C:78:ARG:NH2	2:C:105:ASP:OD2	2.45	0.46
1:A:167:ILE:HD12	1:A:167:ILE:N	2.31	0.46
2:C:56:ALA:O	2:C:57:ASP:HB3	2.16	0.46
1:A:53:ASP:HB3	1:A:60:VAL:CG1	2.34	0.45
1:A:98:CYS:O	1:A:102:HIS:HD2	1.99	0.45
1:A:144:ASP:HB3	1:A:147:LYS:HB3	1.98	0.45
2:C:11:PHE:CE2	2:C:106:ALA:HB3	2.51	0.45
1:A:26:GLY:HA2	1:A:41:ASP:OD2	2.16	0.45
1:A:96:ILE:HG23	1:A:136:MET:HG2	1.98	0.45
2:C:60:LEU:HD23	2:C:83:LEU:HD11	1.99	0.45
2:C:92:ALA:N	2:C:121:GLU:HG2	2.31	0.45
2:C:51:GLU:HA	2:C:51:GLU:OE1	2.17	0.45
1:B:132:ALA:O	1:B:136:MET:HG3	2.17	0.44
1:B:211:LYS:HB3	1:B:211:LYS:HZ2	1.81	0.44
1:B:197:GLN:HB2	1:B:202:MET:HE2	1.99	0.44
1:B:51:MET:O	1:B:62:VAL:HG22	2.17	0.44
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.80	0.44
1:B:114:LEU:HB3	1:B:203:LYS:HD3	2.00	0.43
1:A:151:ASP:O	1:A:154:ALA:HB3	2.18	0.43
1:A:144:ASP:O	1:A:147:LYS:HB3	2.17	0.43
1:A:88:HIS:O	1:A:117:THR:HB	2.19	0.43
1:A:114:LEU:O	1:A:203:LYS:HE3	2.18	0.43
1:B:5:ILE:O	1:B:9:LEU:HG	2.19	0.43
1:B:181:GLY:HA3	2:C:108:PHE:CZ	2.54	0.43
1:A:151:ASP:O	1:A:152:VAL:C	2.61	0.43
1:A:75:GLU:HA	1:A:78:MET:HG3	2.01	0.43
1:B:95:ASP:OD2	1:B:125:ARG:HG2	2.19	0.43
1:A:-2:ALA:O	1:A:-1:MET:C	2.61	0.42
1:B:14:ILE:HG12	1:B:17:SER:HG	1.84	0.42
1:B:91:THR:OG1	1:B:119:ARG:NH2	2.49	0.42
1:A:96:ILE:O	1:A:102:HIS:NE2	2.48	0.42
1:A:104:LEU:HD23	1:A:104:LEU:O	2.19	0.42
1:A:107:GLN:NE2	1:A:196:TYR:OH	2.48	0.42
2:C:124:ALA:O	2:C:125:ASN:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:ARG:HG3	2:C:78:ARG:NH1	2.32	0.42
1:B:102:HIS:HB2	2:C:69:GLU:HB2	2.02	0.42
1:B:96:ILE:HD11	1:B:135:GLU:HB2	2.01	0.41
2:C:57:ASP:OD2	2:C:59:GLN:NE2	2.52	0.41
2:C:46:ILE:C	2:C:47:ARG:HD2	2.45	0.41
1:B:69:LYS:HG3	1:B:70:GLN:N	2.34	0.41
2:C:80:ARG:HG2	2:C:81:LEU:N	2.35	0.41
1:B:152:VAL:HA	1:B:156:LYS:O	2.20	0.41
1:A:-2:ALA:O	1:A:0:ALA:N	2.54	0.41
1:A:32:THR:HG22	1:A:33:ASN:N	2.35	0.41
2:C:121:GLU:C	2:C:122:VAL:CG2	2.93	0.41
2:C:124:ALA:HA	2:C:125:ASN:HD21	1.76	0.41
1:A:51:MET:HE2	1:B:47:ILE:CD1	2.40	0.41
1:A:159:ALA:O	1:A:160:PRO:O	2.39	0.41
1:B:31:LEU:HD12	1:B:31:LEU:N	2.36	0.41
1:A:96:ILE:HD12	1:A:136:MET:HG2	2.03	0.41
2:C:60:LEU:HA	2:C:61:PRO:HD3	1.96	0.41
1:A:198:PRO:HA	1:A:199:PRO:HD3	1.95	0.40
1:A:197:GLN:HA	1:A:198:PRO:HD3	1.95	0.40
1:A:54:VAL:HG21	1:B:46:ILE:HD11	2.03	0.40
1:A:80:VAL:HG13	1:A:119:ARG:HG2	2.04	0.40
1:B:26:GLY:HA2	1:B:41:ASP:OD2	2.22	0.40
1:B:85:GLN:HE21	1:B:85:GLN:HB3	1.58	0.40
1:A:104:LEU:C	1:A:104:LEU:CD2	2.95	0.40
1:B:139:ILE:HD11	1:B:152:VAL:HG21	2.03	0.40
2:C:100:TYR:CE1	2:C:113:GLU:HB2	2.56	0.40
2:C:105:ASP:C	2:C:107:GLY:H	2.30	0.40

All (6) 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)
1:A:81:TYR:O	2:C:125:ASN:O[5_655]	1.65	0.55
1:A:81:TYR:C	2:C:125:ASN:O[5_655]	1.65	0.55
1:A:82:LYS:CB	2:C:124:ALA:O[5_655]	1.82	0.38
1:A:82:LYS:NZ	2:C:125:ASN:OD1[5_655]	2.00	0.20
1:A:82:LYS:N	2:C:125:ASN:O[5_655]	2.04	0.16
1:A:80:VAL:CG1	2:C:125:ASN:N[5_655]	2.05	0.15

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	217/220 (99%)	193 (89%)	19 (9%)	5 (2%)	5	4
1	B	212/220 (96%)	202 (95%)	9 (4%)	1 (0%)	24	31
2	C	116/132 (88%)	105 (90%)	11 (10%)	0	100	100
All	All	545/572 (95%)	500 (92%)	39 (7%)	6 (1%)	11	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	160	PRO
1	A	161	ALA
1	A	168	ALA
1	A	152	VAL
1	B	160	PRO

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	179/180 (99%)	169 (94%)	10 (6%)	19	28
1	B	178/180 (99%)	171 (96%)	7 (4%)	28	43
2	C	99/109 (91%)	93 (94%)	6 (6%)	17	24
All	All	456/469 (97%)	433 (95%)	23 (5%)	22	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	33	ASN
1	A	60	VAL
1	A	65	LYS
1	A	70	GLN
1	A	82	LYS
1	A	96	ILE
1	A	117	THR
1	A	143	LYS
1	A	204	GLU
1	B	6	GLN
1	B	11	LYS
1	B	14	ILE
1	B	85	GLN
1	B	106	GLU
1	B	129	ASP
1	B	208	GLU
2	C	9	SER
2	C	10	GLN
2	C	51	GLU
2	C	69	GLU
2	C	122	VAL
2	C	125	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	20	GLN
1	A	45	HIS
1	A	70	GLN
1	A	105	HIS
1	A	107	GLN
1	A	112	ASN
1	A	210	GLN
1	B	20	GLN
1	B	45	HIS
1	B	72	ASN
1	B	85	GLN
1	B	88	HIS
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	197	GLN
1	B	209	HIS
2	C	16	GLN
2	C	23	GLN
2	C	25	ASN
2	C	30	ASN
2	C	66	HIS

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	219/220 (99%)	0.68	22 (10%) 12 14	26, 44, 79, 86	0
1	B	214/220 (97%)	0.35	9 (4%) 40 42	24, 41, 64, 90	0
2	C	118/132 (89%)	0.52	8 (6%) 23 25	19, 34, 63, 101	1 (0%)
All	All	551/572 (96%)	0.52	39 (7%) 22 24	19, 41, 71, 101	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	124	ALA	13.6
2	C	125	ASN	9.3
2	C	123	VAL	6.6
1	A	-3	GLY	3.8
1	A	158	VAL	3.7
1	A	215	GLY	3.5
1	A	213	THR	3.4
1	A	129	ASP	3.2
1	A	161	ALA	3.1
1	B	212	MET	3.1
1	B	214	SER	3.0
2	C	9	SER	3.0
1	B	160	PRO	2.8
1	A	160	PRO	2.7
1	A	152	VAL	2.7
2	C	122	VAL	2.7
2	C	8	ARG	2.7
1	A	165	VAL	2.4
1	A	159	ALA	2.4
1	A	156	LYS	2.4
2	C	10	GLN	2.4
1	B	12	MET	2.4
1	A	140	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	18	ASP	2.3
1	B	1	ASP	2.2
1	B	164	ASP	2.2
1	A	143	LYS	2.2
1	B	213	THR	2.2
1	A	164	ASP	2.2
1	B	163	CYS	2.2
1	A	117	THR	2.2
1	A	212	MET	2.2
1	A	58	ALA	2.2
2	C	68	ASP	2.1
1	A	162	SER	2.1
1	A	81	TYR	2.1
1	A	-2	ALA	2.0
1	A	18	ASP	2.0
1	A	166	ASP	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.