



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:20 PM UTC

PDB ID : 2OJZ / pdb_00002ojz
Title : Anti-DNA antibody ED10
Authors : Stanfield, R.L.; Sanguineti, S.; Wilson, I.A.; de Prat-Gay, G.
Deposited on : 2007-01-15
Resolution : 2.73 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

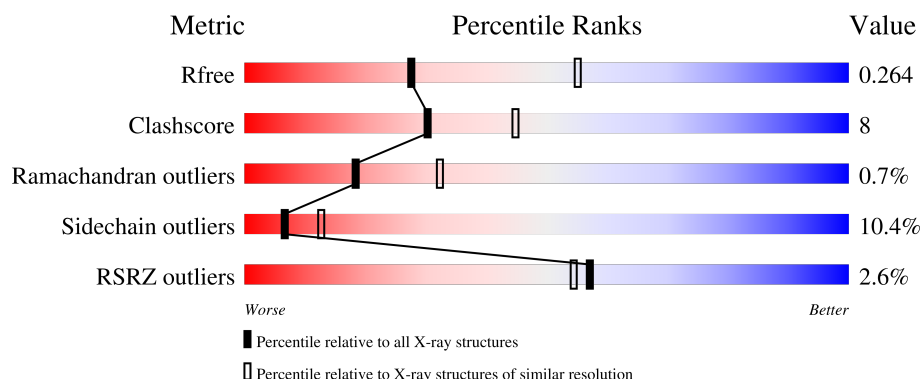
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	L	219	0.2% 78% 16% 5%
1	M	219	2% 77% 20% ..
2	H	216	3% 71% 23% 5% .
2	I	216	5% 73% 21% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6708 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 Fab ED10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	0	0
			1690	1056	285	343	6			
1	M	218	Total	C	N	O	S	0	0	0
			1690	1056	285	343	6			

- Molecule 2 is a protein called Fab ED10 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1654	1058	262	327	7			
2	I	216	Total	C	N	O	S	0	0	0
			1654	1058	262	327	7			

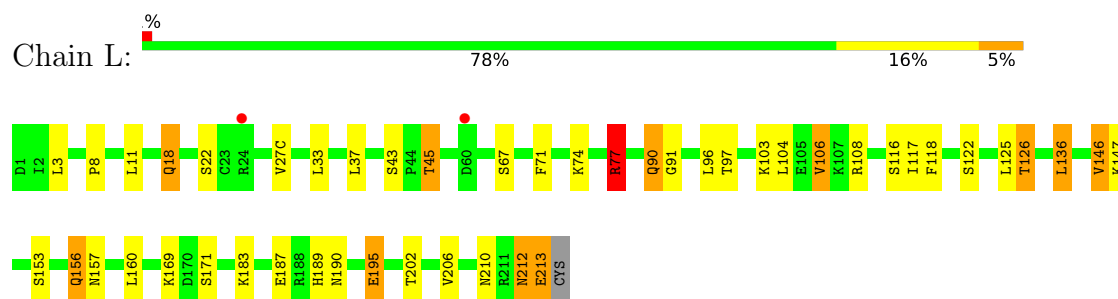
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	6	Total	O	0	0
			6	6		
3	H	4	Total	O	0	0
			4	4		
3	M	4	Total	O	0	0
			4	4		
3	I	6	Total	O	0	0
			6	6		

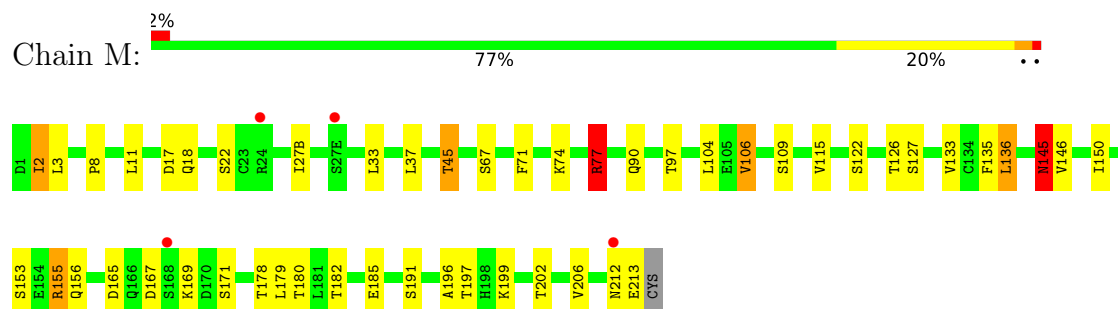
3 Residue-property plots

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.

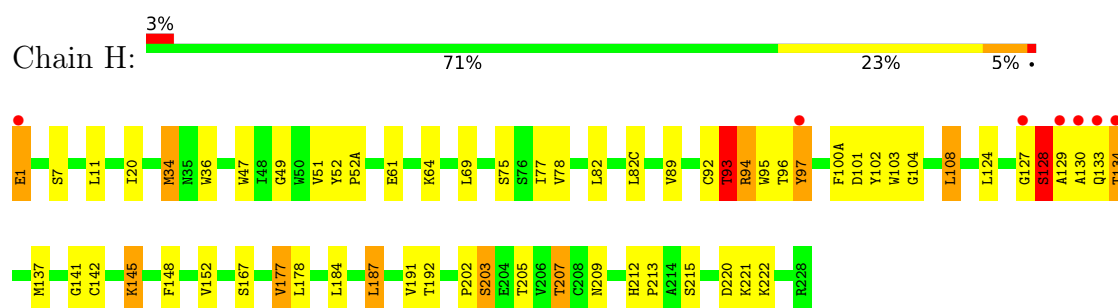
- Molecule 1: Fab ED10 light chain



- Molecule 1: Fab ED10 light chain

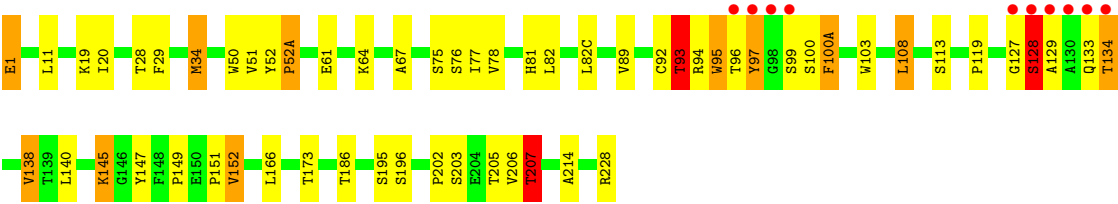


- Molecule 2: Fab ED10 heavy chain



- Molecule 2: Fab ED10 heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.90Å 194.04Å 61.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.24 – 2.73 25.24 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.24-2.73) 96.8 (25.24-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	11.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.32 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.264 0.206 , 0.264	Depositor DCC
R_{free} test set	1349 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6708	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	L	1.21	6/1728 (0.3%)	1.10	5/2346 (0.2%)
1	M	1.16	2/1728 (0.1%)	1.09	4/2346 (0.2%)
2	H	1.32	7/1703 (0.4%)	1.14	7/2332 (0.3%)
2	I	1.38	10/1703 (0.6%)	1.08	7/2332 (0.3%)
All	All	1.27	25/6862 (0.4%)	1.10	23/9356 (0.2%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	134	THR	CA-CB	9.20	1.67	1.53
2	H	134	THR	CA-CB	8.40	1.66	1.53
2	I	128	SER	N-CA	7.18	1.55	1.46
1	L	106	VAL	CA-CB	6.88	1.62	1.54
2	H	20	ILE	CA-C	-6.83	1.44	1.52
2	H	128	SER	N-CA	6.70	1.54	1.46
1	L	189	HIS	CA-C	-6.38	1.44	1.52
2	I	97	TYR	N-CA	6.38	1.54	1.46
1	M	146	VAL	C-O	-6.18	1.17	1.24
2	I	173	THR	C-O	-5.95	1.17	1.24
2	I	152	VAL	C-O	-5.91	1.18	1.24
2	H	213	PRO	C-O	-5.86	1.16	1.24
2	H	130	ALA	CA-C	5.73	1.59	1.52
2	H	134	THR	N-CA	5.64	1.53	1.46
2	I	97	TYR	CA-C	5.50	1.60	1.52
2	I	128	SER	CA-C	5.46	1.60	1.52
2	H	129	ALA	CA-C	5.42	1.60	1.52
1	L	146	VAL	CA-CB	-5.37	1.47	1.54
2	I	129	ALA	CA-C	5.36	1.59	1.52
1	M	145	ASN	CB-CG	-5.36	1.38	1.52
2	I	28	THR	CA-CB	5.30	1.59	1.53
1	L	103	LYS	CE-NZ	5.25	1.65	1.49
1	L	118	PHE	CA-C	-5.14	1.48	1.52
2	I	207	THR	CA-CB	5.11	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	117	ILE	C-O	-5.04	1.19	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	145	LYS	N-CA-C	8.78	122.49	109.24
2	I	145	LYS	N-CA-C	7.71	121.47	109.52
2	H	34	MET	CB-CG-SD	-7.54	90.07	112.70
1	L	202	THR	N-CA-C	-6.42	103.57	111.40
1	M	106	VAL	N-CA-CB	6.12	117.20	110.53
1	M	202	THR	N-CA-C	-6.08	103.98	111.40
1	L	27(C)	VAL	N-CA-C	-5.99	100.98	108.89
2	I	128	SER	N-CA-C	5.92	123.42	110.80
2	H	95	TRP	N-CA-C	5.87	118.03	108.76
1	M	182	THR	N-CA-C	-5.87	102.63	110.55
2	I	52(A)	PRO	CA-C-N	-5.86	116.47	123.44
2	I	52(A)	PRO	C-N-CA	-5.86	116.47	123.44
1	L	106	VAL	N-CA-CB	5.71	117.33	110.31
1	L	146	VAL	CB-CA-C	-5.59	102.31	110.81
2	H	222	LYS	CB-CA-C	5.50	118.61	109.53
2	H	93	THR	CB-CA-C	-5.42	98.69	109.79
1	L	77	ARG	CG-CD-NE	5.35	123.77	112.00
2	H	128	SER	N-CA-C	5.28	122.04	110.80
2	H	221	LYS	CB-CA-C	-5.11	101.96	110.14
2	I	93	THR	CB-CA-C	-5.09	100.22	110.30
2	I	95	TRP	N-CA-C	5.09	116.57	108.79
2	I	34	MET	CB-CG-SD	-5.07	97.50	112.70
1	M	77	ARG	CG-CD-NE	5.06	123.14	112.00

There are no chirality outliers.

There are no planarity outliers.

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	L	1690	0	1631	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1690	0	1631	23	0
2	H	1654	0	1605	34	0
2	I	1654	0	1605	30	0
3	H	4	0	0	0	0
3	I	6	0	0	1	0
3	L	6	0	0	0	0
3	M	4	0	0	0	0
All	All	6708	0	6472	110	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 (110) 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:H:34:MET:HE2	2:H:78:VAL:HG21	1.44	0.98
2:I:34:MET:HE1	2:I:92:CYS:HB2	1.60	0.83
2:H:34:MET:HE1	2:H:92:CYS:HB2	1.61	0.82
1:M:133:VAL:HG22	1:M:178:THR:HG23	1.63	0.78
2:I:19:LYS:HE3	3:I:230:HOH:O	1.83	0.78
1:L:77:ARG:HB2	1:L:77:ARG:HH11	1.52	0.74
2:I:93:THR:HG21	2:I:100(A):PHE:HB3	1.69	0.74
1:L:122:SER:O	1:L:126:THR:HG23	1.91	0.71
1:M:127:SER:OG	1:M:127:SER:O	2.09	0.70
1:M:77:ARG:HH11	1:M:77:ARG:HB2	1.57	0.69
2:H:93:THR:HG21	2:H:100(A):PHE:HB3	1.75	0.69
2:I:34:MET:HE2	2:I:78:VAL:HG21	1.74	0.69
1:M:150:ILE:HD11	1:M:179:LEU:HD21	1.76	0.68
1:L:77:ARG:HH11	1:L:77:ARG:CB	2.07	0.68
2:H:124:LEU:HD12	2:H:141:GLY:HA3	1.77	0.67
2:I:89:VAL:HG22	2:I:108:LEU:HD22	1.76	0.66
2:H:89:VAL:HG22	2:H:108:LEU:HD22	1.79	0.64
1:M:122:SER:O	1:M:126:THR:HG23	1.98	0.63
2:H:202:PRO:O	2:H:203:SER:C	2.43	0.61
2:I:93:THR:HG23	2:I:103:TRP:CD2	2.34	0.61
2:I:1:GLU:OE1	2:I:1:GLU:N	2.32	0.61
1:L:37:LEU:O	1:L:45:THR:HG22	2.01	0.60
2:H:137:MET:HE3	2:H:192:THR:HG22	1.83	0.60
2:H:93:THR:HG23	2:H:103:TRP:CD2	2.38	0.58
1:M:77:ARG:HH11	1:M:77:ARG:CB	2.16	0.58
2:I:127:GLY:O	2:I:128:SER:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:ILE:N	1:M:2:ILE:HD13	2.20	0.57
2:H:1:GLU:OE1	2:H:1:GLU:N	2.34	0.57
2:I:89:VAL:HG22	2:I:108:LEU:CD2	2.36	0.56
2:H:89:VAL:HG22	2:H:108:LEU:CD2	2.34	0.56
1:M:37:LEU:O	1:M:45:THR:HG22	2.05	0.56
2:H:61:GLU:OE2	2:H:64:LYS:NZ	2.25	0.55
2:H:127:GLY:O	2:H:128:SER:HB2	2.06	0.54
2:I:205:THR:HG22	2:I:207:THR:HG22	1.89	0.54
1:L:77:ARG:CB	1:L:77:ARG:NH1	2.70	0.54
1:L:91:GLY:HA2	1:L:96:LEU:HD22	1.90	0.54
1:L:160:LEU:HD13	2:H:177:VAL:CG2	2.38	0.54
1:M:145:ASN:O	1:M:196:ALA:HA	2.09	0.52
1:L:212:ASN:O	1:L:213:GLU:HG3	2.10	0.52
2:H:209:ASN:ND2	2:H:220:ASP:OD1	2.31	0.52
2:H:34:MET:HE2	2:H:78:VAL:CG2	2.29	0.52
1:M:33:LEU:HD13	1:M:71:PHE:CD2	2.45	0.52
1:L:37:LEU:O	1:L:45:THR:CG2	2.58	0.51
2:H:52:TYR:CD1	2:H:52(A):PRO:HD2	2.46	0.50
1:M:8:PRO:HG3	1:M:11:LEU:HD13	1.92	0.50
2:I:149:PRO:HD2	2:I:214:ALA:CB	2.41	0.50
2:I:82:LEU:HB3	2:I:82(C):LEU:HD21	1.93	0.50
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.47	0.49
1:M:77:ARG:CB	1:M:77:ARG:NH1	2.75	0.49
2:I:138:VAL:HG12	2:I:195:SER:HB3	1.94	0.49
1:M:133:VAL:CG2	1:M:178:THR:HG23	2.40	0.48
2:H:137:MET:HE3	2:H:192:THR:CG2	2.42	0.48
1:M:77:ARG:HB2	1:M:77:ARG:NH1	2.26	0.48
2:I:140:LEU:HD12	2:I:206:VAL:HG11	1.94	0.48
1:M:155:ARG:NH2	1:M:185:GLU:OE1	2.47	0.47
1:L:8:PRO:HG3	1:L:11:LEU:HD13	1.97	0.47
1:L:136:LEU:N	1:L:136:LEU:CD2	2.77	0.47
2:H:148:PHE:HB2	2:H:184:LEU:HD23	1.96	0.47
2:H:205:THR:HG22	2:H:207:THR:HG22	1.96	0.47
1:L:18:GLN:O	1:L:18:GLN:HG3	2.14	0.47
2:H:93:THR:HG22	2:H:102:TYR:O	2.14	0.47
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.96	0.47
1:L:183:LYS:O	1:L:187:GLU:HG3	2.15	0.46
1:M:37:LEU:O	1:M:45:THR:CG2	2.63	0.46
2:H:34:MET:HG3	2:H:78:VAL:HG11	1.96	0.46
2:I:202:PRO:O	2:I:203:SER:C	2.59	0.46
1:L:125:LEU:HA	1:L:125:LEU:HD23	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:145:LYS:HB3	2:I:186:THR:HG23	1.98	0.46
1:L:136:LEU:N	1:L:136:LEU:HD22	2.31	0.46
2:I:29:PHE:CD1	2:I:76:SER:HB2	2.51	0.45
1:L:43:SER:OG	2:H:104:GLY:O	2.33	0.45
2:H:82:LEU:HB3	2:H:82(C):LEU:HD21	1.97	0.45
2:I:95:TRP:CG	2:I:96:THR:N	2.84	0.45
1:L:156:GLN:HE21	1:L:156:GLN:HB2	1.66	0.45
2:H:96:THR:O	2:H:97:TYR:C	2.59	0.45
1:L:77:ARG:HB2	1:L:77:ARG:NH1	2.24	0.44
2:I:50:TRP:C	2:I:50:TRP:CD1	2.95	0.44
2:I:119:PRO:HB3	2:I:147:TYR:HB3	1.98	0.44
1:L:90:GLN:NE2	1:L:97:THR:OG1	2.50	0.44
1:M:90:GLN:NE2	1:M:97:THR:OG1	2.51	0.44
2:I:61:GLU:OE2	2:I:64:LYS:NZ	2.34	0.44
1:L:33:LEU:HD13	1:L:71:PHE:CD2	2.53	0.44
2:I:29:PHE:CG	2:I:76:SER:HB2	2.52	0.44
2:H:205:THR:CG2	2:H:207:THR:HG22	2.48	0.44
2:I:34:MET:HB3	2:I:34:MET:HE3	1.33	0.43
1:M:115:VAL:HA	1:M:135:PHE:O	2.18	0.43
2:I:67:ALA:HA	2:I:81:HIS:O	2.17	0.43
2:I:93:THR:CG2	2:I:103:TRP:CE2	3.02	0.43
1:M:212:ASN:O	1:M:213:GLU:HG3	2.19	0.42
2:I:51:VAL:HG11	2:I:78:VAL:HB	2.00	0.42
1:L:146:VAL:HG12	1:L:147:LYS:N	2.33	0.42
2:H:187:LEU:C	2:H:187:LEU:HD23	2.44	0.42
1:M:169:LYS:N	1:M:169:LYS:CD	2.83	0.42
2:H:191:VAL:O	2:H:191:VAL:HG13	2.20	0.42
1:M:27(B):ILE:HD13	1:M:27(B):ILE:HG21	1.75	0.42
2:I:145:LYS:CB	2:I:186:THR:HG23	2.49	0.42
1:L:212:ASN:O	1:L:213:GLU:CG	2.68	0.42
2:H:36:TRP:CD1	2:H:69:LEU:HD22	2.55	0.42
2:H:94:ARG:NH1	2:H:101:ASP:OD2	2.53	0.42
2:H:127:GLY:O	2:H:128:SER:CB	2.68	0.42
2:I:149:PRO:HD2	2:I:214:ALA:HB3	2.02	0.41
2:H:34:MET:HB3	2:H:34:MET:HE3	1.21	0.41
2:H:212:HIS:ND1	2:H:215:SER:OG	2.52	0.41
2:I:20:ILE:HD13	2:I:20:ILE:HG21	1.87	0.41
1:M:136:LEU:N	1:M:136:LEU:CD2	2.83	0.41
1:L:108:ARG:HD2	1:L:171:SER:HB2	2.02	0.40
2:H:51:VAL:HG11	2:H:78:VAL:HB	2.03	0.40
2:I:52:TYR:CD1	2:I:52(A):PRO:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:ASN:O	1:L:210:ASN:HA	2.21	0.40
1:M:167:ASP:O	1:M:171:SER:HA	2.20	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	L	216/219 (99%)	205 (95%)	11 (5%)	0	100	100
1	M	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
2	H	214/216 (99%)	204 (95%)	7 (3%)	3 (1%)	9	15
2	I	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	9	15
All	All	860/870 (99%)	816 (95%)	38 (4%)	6 (1%)	18	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	128	SER
2	H	128	SER
2	H	133	GLN
2	I	133	GLN
2	I	97	TYR
2	H	97	TYR

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	L	196/197 (100%)	176 (90%)	20 (10%)	7	13
1	M	196/197 (100%)	173 (88%)	23 (12%)	5	9
2	H	189/189 (100%)	171 (90%)	18 (10%)	8	15
2	I	189/189 (100%)	170 (90%)	19 (10%)	7	14
All	All	770/772 (100%)	690 (90%)	80 (10%)	7	13

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	LEU
1	L	18	GLN
1	L	22	SER
1	L	45	THR
1	L	67	SER
1	L	74	LYS
1	L	77	ARG
1	L	90	GLN
1	L	104	LEU
1	L	106	VAL
1	L	116	SER
1	L	126	THR
1	L	136	LEU
1	L	153	SER
1	L	156	GLN
1	L	157	ASN
1	L	169	LYS
1	L	195	GLU
1	L	212	ASN
1	L	213	GLU
2	H	1	GLU
2	H	7	SER
2	H	11	LEU
2	H	75	SER
2	H	77	ILE
2	H	93	THR
2	H	94	ARG
2	H	108	LEU
2	H	134	THR
2	H	142	CYS

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Mol	Chain	Res	Type
2	H	145	LYS
2	H	152	VAL
2	H	167	SER
2	H	177	VAL
2	H	178	LEU
2	H	187	LEU
2	H	203	SER
2	H	207	THR
1	M	2	ILE
1	M	3	LEU
1	M	17	ASP
1	M	18	GLN
1	M	22	SER
1	M	45	THR
1	M	67	SER
1	M	74	LYS
1	M	77	ARG
1	M	104	LEU
1	M	106	VAL
1	M	109	SER
1	M	136	LEU
1	M	145	ASN
1	M	153	SER
1	M	155	ARG
1	M	156	GLN
1	M	165	ASP
1	M	180	THR
1	M	191	SER
1	M	197	THR
1	M	199	LYS
1	M	206	VAL
2	I	1	GLU
2	I	11	LEU
2	I	75	SER
2	I	77	ILE
2	I	93	THR
2	I	94	ARG
2	I	99	SER
2	I	100	SER
2	I	100(A)	PHE
2	I	108	LEU
2	I	113	SER

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Mol	Chain	Res	Type
2	I	134	THR
2	I	138	VAL
2	I	151	PRO
2	I	152	VAL
2	I	166	LEU
2	I	196	SER
2	I	207	THR
2	I	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	137	ASN
1	L	156	GLN
1	M	124	GLN
1	M	156	GLN
2	I	133	GLN

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 ⓘ

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	L	218/219 (99%)	-0.02	2 (0%) 81 81	18, 30, 37, 50	0
1	M	218/219 (99%)	-0.02	4 (1%) 67 64	18, 30, 37, 51	0
2	H	216/216 (100%)	-0.01	7 (3%) 50 48	14, 28, 39, 52	0
2	I	216/216 (100%)	0.06	10 (4%) 37 36	14, 28, 38, 53	0
All	All	868/870 (99%)	0.00	23 (2%) 57 54	14, 29, 38, 53	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	129	ALA	6.6
2	I	134	THR	5.8
2	H	130	ALA	5.2
2	H	129	ALA	5.2
2	I	130	ALA	4.9
2	H	134	THR	4.8
2	H	97	TYR	3.8
2	I	97	TYR	3.6
2	I	96	THR	3.0
2	H	1	GLU	2.9
2	H	133	GLN	2.9
2	I	99	SER	2.9
1	M	168	SER	2.8
1	M	27(E)	SER	2.7
1	M	24	ARG	2.7
2	I	133	GLN	2.5
2	I	127	GLY	2.5
2	I	128	SER	2.3
2	H	127	GLY	2.2
1	M	212	ASN	2.1
1	L	24	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	60	ASP	2.0
2	I	98	GLY	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.