



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:41 PM GMT

PDB ID : 1BZ7
Title : FAB FRAGMENT FROM MURINE ASCITES
Authors : Kaminski, M.J.; Mackenzie, C.R.; Mooibroek, M.J.; Dahms, T.E.S.; Hirama, T.; Houghton, A.N.; Chapman, P.B.; Evans, S.V.
Deposited on : 1998-11-06
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

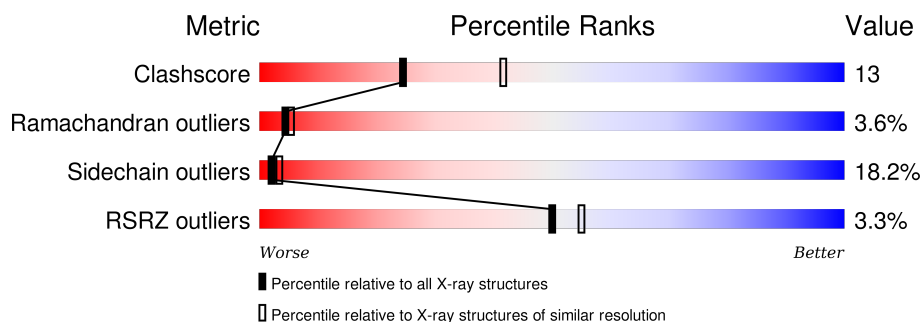
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	206	
2	B	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3232 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 PROTEIN (ANTIBODY R24 (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1598	1004	264	325	5			

- Molecule 2 is a protein called PROTEIN (ANTIBODY R24 (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1621	1023	273	319	6			

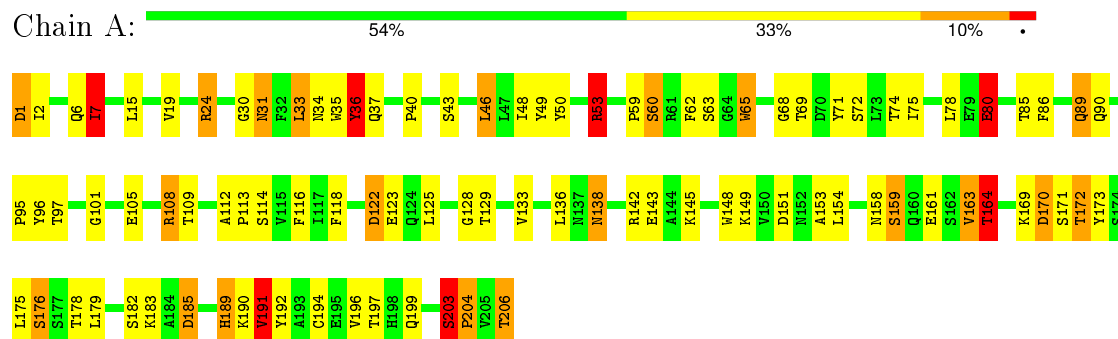
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	6	Total	O	0	0
			6	6		

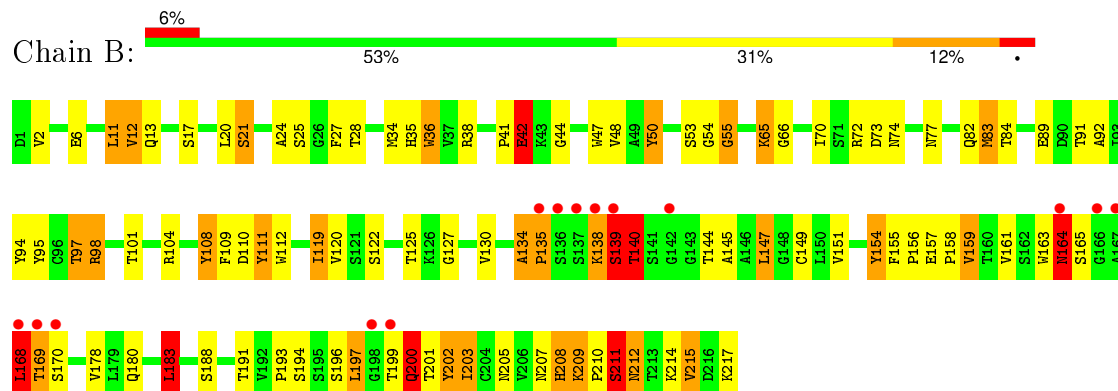
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN (ANTIBODY R24 (LIGHT CHAIN))



• Molecule 2: PROTEIN (ANTIBODY R24 (HEAVY CHAIN))



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.80 Å 56.00 Å 80.00 Å 90.00° 119.20° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 28.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.0 (6.00-2.50) 87.5 (28.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.51 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.162 , (Not available) 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18143 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3232	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.02	3/1630 (0.2%)	1.89	44/2210 (2.0%)
2	B	1.02	1/1661 (0.1%)	2.03	61/2259 (2.7%)
All	All	1.02	4/3291 (0.1%)	1.96	105/4469 (2.3%)

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	2
2	B	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	GLU	CG-CD	6.03	1.60	1.51
2	B	47	TRP	CG-CD2	-5.46	1.34	1.43
1	A	72	SER	CA-CB	-5.22	1.45	1.52
1	A	80	GLU	CB-CG	5.01	1.61	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	TYR	CB-CG-CD2	-10.86	114.48	121.00
2	B	163	TRP	CD1-CG-CD2	10.46	114.67	106.30
2	B	211	SER	CA-C-N	-9.99	95.23	117.20
2	B	83	MET	CG-SD-CE	-9.77	84.56	100.20
1	A	142	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	148	TRP	CE2-CD2-CG	-8.24	100.71	107.30
2	B	47	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	A	24	ARG	NE-CZ-NH1	8.11	124.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	TYR	CB-CG-CD1	-8.05	116.17	121.00
1	A	1	ASP	CA-C-N	-8.01	99.58	117.20
1	A	148	TRP	CD1-CG-CD2	7.94	112.66	106.30
2	B	50	TYR	CB-CG-CD1	-7.79	116.32	121.00
2	B	98	ARG	CB-CG-CD	-7.63	91.75	111.60
1	A	35	TRP	CD1-CG-CD2	7.61	112.39	106.30
2	B	42	GLU	N-CA-C	-7.57	90.55	111.00
2	B	138	LYS	CA-C-N	-7.49	100.72	117.20
2	B	211	SER	O-C-N	7.48	134.67	122.70
2	B	47	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	B	217	LYS	N-CA-CB	7.36	123.85	110.60
2	B	163	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	35	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	B	36	TRP	CD1-CG-CD2	7.19	112.05	106.30
2	B	211	SER	N-CA-C	7.14	130.27	111.00
1	A	2	ILE	N-CA-C	-7.12	91.77	111.00
2	B	34	MET	CG-SD-CE	-7.09	88.85	100.20
2	B	119	ILE	CG1-CB-CG2	-7.09	95.81	111.40
2	B	50	TYR	CB-CG-CD2	6.98	125.19	121.00
2	B	95	TYR	CB-CG-CD1	-6.94	116.84	121.00
2	B	98	ARG	NE-CZ-NH2	-6.89	116.86	120.30
2	B	183	LEU	CA-CB-CG	6.88	131.13	115.30
2	B	36	TRP	CE2-CD2-CG	-6.87	101.80	107.30
2	B	168	LEU	CA-C-N	-6.82	102.20	117.20
1	A	136	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	2	ILE	N-CA-CB	-6.62	95.57	110.80
1	A	192	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	A	65	TRP	CE2-CD2-CG	-6.51	102.09	107.30
2	B	163	TRP	CG-CD1-NE1	-6.49	103.61	110.10
1	A	191	VAL	CA-CB-CG2	-6.45	101.22	110.90
1	A	136	LEU	CB-CG-CD1	-6.44	100.05	111.00
1	A	36	TYR	CB-CG-CD1	-6.44	117.14	121.00
2	B	169	THR	CA-CB-CG2	-6.37	103.48	112.40
1	A	123	GLU	CA-CB-CG	6.36	127.39	113.40
1	A	46	LEU	CA-CB-CG	6.35	129.91	115.30
1	A	1	ASP	CA-C-O	6.34	133.41	120.10
2	B	108	TYR	CB-CG-CD2	-6.29	117.22	121.00
2	B	112	TRP	CD1-CG-CD2	6.27	111.31	106.30
1	A	163	VAL	CG1-CB-CG2	-6.26	100.88	110.90
2	B	134	ALA	N-CA-CB	-6.19	101.44	110.10
1	A	65	TRP	CD1-CG-CD2	6.19	111.25	106.30
2	B	44	GLY	CA-C-N	-6.15	103.67	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	CYS	CA-CB-SG	-6.09	103.03	114.00
2	B	164	ASN	CA-CB-CG	6.05	126.72	113.40
2	B	163	TRP	CA-C-N	-6.04	103.91	117.20
2	B	215	VAL	CG1-CB-CG2	-6.01	101.28	110.90
2	B	138	LYS	O-C-N	6.00	132.31	122.70
2	B	112	TRP	CE2-CD2-CG	-5.99	102.50	107.30
2	B	202	TYR	CA-C-N	5.98	130.36	117.20
2	B	97	THR	CA-CB-CG2	5.96	120.74	112.40
1	A	179	LEU	N-CA-C	-5.89	95.09	111.00
1	A	6	GLN	N-CA-C	-5.82	95.29	111.00
2	B	217	LYS	CB-CA-C	-5.78	98.83	110.40
2	B	147	LEU	CA-CB-CG	5.78	128.58	115.30
2	B	38	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	B	139	SER	CA-C-N	-5.66	104.74	117.20
2	B	73	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	2	ILE	CB-CA-C	5.63	122.85	111.60
2	B	98	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	B	101	THR	CA-CB-CG2	5.60	120.25	112.40
2	B	201	THR	N-CA-CB	-5.60	99.66	110.30
1	A	53	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	11	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	A	142	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	208	HIS	CA-CB-CG	5.53	123.01	113.60
1	A	189	HIS	CB-CG-ND1	5.52	137.00	123.20
1	A	148	TRP	CG-CD2-CE3	5.51	138.85	133.90
1	A	69	THR	N-CA-CB	5.47	120.70	110.30
1	A	172	THR	N-CA-CB	-5.47	99.91	110.30
2	B	12	VAL	CG1-CB-CG2	-5.43	102.22	110.90
2	B	211	SER	C-N-CA	5.38	135.15	121.70
2	B	36	TRP	CG-CD2-CE3	5.37	138.73	133.90
2	B	97	THR	N-CA-CB	-5.36	100.11	110.30
1	A	53	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	B	209	LYS	N-CA-C	5.33	125.40	111.00
1	A	33	LEU	CB-CG-CD2	-5.33	101.94	111.00
2	B	135	PRO	N-CA-C	5.32	125.94	112.10
1	A	206	THR	N-CA-CB	-5.32	100.19	110.30
2	B	163	TRP	CA-CB-CG	5.31	123.79	113.70
1	A	35	TRP	CG-CD2-CE3	5.30	138.68	133.90
2	B	159	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	96	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	170	ASP	CA-C-N	5.25	128.74	117.20
1	A	24	ARG	NE-CZ-NH2	-5.23	117.68	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	GLY	CA-C-N	5.23	128.71	117.20
1	A	7	ILE	CB-CG1-CD1	5.19	128.43	113.90
1	A	164	THR	N-CA-CB	-5.19	100.44	110.30
1	A	65	TRP	CG-CD2-CE3	5.17	138.56	133.90
2	B	111	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	35	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	A	191	VAL	CA-CB-CG1	5.11	118.56	110.90
1	A	203	SER	N-CA-C	-5.08	97.27	111.00
2	B	200	GLN	CA-CB-CG	5.08	124.58	113.40
2	B	165	SER	N-CA-C	-5.06	97.33	111.00
2	B	154	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	1	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	90	GLN	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	SER	Peptide
1	A	36	TYR	Sidechain
2	B	111	TYR	Sidechain
2	B	210	PRO	Peptide

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	1598	0	1559	38	0
2	B	1621	0	1580	47	0
3	A	7	0	0	0	0
3	B	6	0	0	0	0
All	All	3232	0	3139	82	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 13.

All (82) 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:B:11:LEU:HD11	2:B:155:PHE:HE1	1.52	0.73
2:B:196:SER:HB3	2:B:200:GLN:HE22	1.52	0.72
1:A:159:SER:HA	1:A:178:THR:O	1.94	0.68
2:B:164:ASN:HD21	2:B:170:SER:HA	1.60	0.67
1:A:163:VAL:HG12	1:A:164:THR:O	1.95	0.66
2:B:65:LYS:HE3	2:B:66:GLY:N	2.12	0.64
2:B:138:LYS:HA	2:B:194:SER:HB3	1.80	0.64
2:B:12:VAL:O	2:B:120:VAL:HA	1.99	0.62
1:A:145:LYS:HB3	1:A:197:THR:HB	1.81	0.62
2:B:20:LEU:HD13	2:B:83:MET:CE	2.29	0.61
1:A:86:PHE:O	1:A:101:GLY:HA2	2.00	0.61
1:A:118:PHE:HB2	1:A:133:VAL:HG22	1.82	0.60
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.36	0.60
2:B:11:LEU:HD11	2:B:155:PHE:CE1	2.37	0.60
2:B:161:VAL:HG11	2:B:188:SER:CB	2.33	0.58
2:B:72:ARG:NE	2:B:74:ASN:HD21	2.01	0.58
2:B:97:THR:OG1	2:B:109:PHE:HB3	2.03	0.58
1:A:116:PHE:CD1	2:B:140:THR:HB	2.39	0.57
2:B:91:THR:HG23	2:B:119:ILE:HA	1.87	0.56
2:B:98:ARG:HD3	2:B:110:ASP:OD1	2.06	0.55
1:A:31:ASN:HB3	1:A:50:TYR:CE1	2.43	0.53
2:B:20:LEU:HD13	2:B:83:MET:HE1	1.91	0.52
1:A:116:PHE:HD1	2:B:140:THR:HB	1.73	0.52
1:A:185:ASP:O	1:A:189:HIS:CD2	2.64	0.51
2:B:72:ARG:HE	2:B:74:ASN:ND2	2.09	0.51
1:A:53:ARG:HA	1:A:53:ARG:NE	2.26	0.51
1:A:1:ASP:HB2	1:A:95:PRO:HD2	1.93	0.51
2:B:41:PRO:O	2:B:42:GLU:HB2	2.11	0.51
1:A:19:VAL:HG21	1:A:78:LEU:HD13	1.93	0.51
1:A:149:LYS:HA	1:A:153:ALA:O	2.12	0.49
1:A:34:ASN:ND2	2:B:108:TYR:HB3	2.28	0.49
1:A:151:ASP:HA	1:A:191:VAL:HG12	1.93	0.49
2:B:145:ALA:CB	2:B:197:LEU:HD21	2.43	0.49
1:A:128:GLY:HA2	1:A:183:LYS:HB2	1.94	0.49
2:B:196:SER:HB3	2:B:202:TYR:OH	2.13	0.49
1:A:33:LEU:HD22	1:A:71:TYR:CD2	2.48	0.49
1:A:182:SER:OG	1:A:185:ASP:HB2	2.12	0.49
2:B:35:HIS:CE1	2:B:50:TYR:CD1	3.01	0.48
2:B:92:ALA:HB3	2:B:94:TYR:CE1	2.49	0.48
2:B:205:ASN:HB3	2:B:215:VAL:HG12	1.95	0.48
1:A:161:GLU:HA	1:A:176:SER:O	2.14	0.48
2:B:139:SER:HB2	2:B:145:ALA:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:CYS:O	1:A:206:THR:HA	2.14	0.47
1:A:108:ARG:HG2	1:A:171:SER:CB	2.44	0.47
1:A:49:TYR:O	1:A:53:ARG:HB2	2.14	0.46
2:B:161:VAL:HG11	2:B:188:SER:HB2	1.96	0.46
1:A:59:PRO:HG2	1:A:62:PHE:CE1	2.50	0.46
1:A:196:VAL:O	1:A:204:PRO:HA	2.15	0.46
1:A:7:ILE:HD12	1:A:7:ILE:H	1.80	0.46
2:B:65:LYS:HD2	2:B:65:LYS:HA	1.56	0.45
2:B:145:ALA:HB1	2:B:197:LEU:HD21	1.98	0.45
1:A:33:LEU:HD22	1:A:71:TYR:CG	2.52	0.45
1:A:138:ASN:HA	1:A:173:TYR:O	2.16	0.45
1:A:59:PRO:HG2	1:A:62:PHE:CD1	2.52	0.45
1:A:37:GLN:HG3	1:A:86:PHE:CE1	2.51	0.45
2:B:130:VAL:HG21	2:B:214:LYS:HG2	1.99	0.44
2:B:20:LEU:HD13	2:B:83:MET:HE3	2.00	0.44
2:B:211:SER:OG	2:B:212:ASN:N	2.50	0.44
1:A:19:VAL:O	1:A:74:THR:HA	2.18	0.44
2:B:24:ALA:HB1	2:B:27:PHE:CZ	2.53	0.44
2:B:36:TRP:O	2:B:48:VAL:HB	2.17	0.44
1:A:36:TYR:HE2	1:A:89:GLN:HG2	1.83	0.43
1:A:48:ILE:HA	1:A:53:ARG:O	2.19	0.43
2:B:209:LYS:HB3	2:B:209:LYS:HE2	1.73	0.43
1:A:75:ILE:HG21	1:A:78:LEU:HD12	2.00	0.43
2:B:203:ILE:HG22	2:B:205:ASN:ND2	2.33	0.43
1:A:108:ARG:HG2	1:A:171:SER:HB2	2.01	0.43
2:B:154:TYR:O	2:B:183:LEU:HB3	2.19	0.43
1:A:36:TYR:O	1:A:86:PHE:HA	2.19	0.42
2:B:72:ARG:NE	2:B:74:ASN:ND2	2.67	0.42
2:B:127:GLY:HA2	2:B:208:HIS:CD2	2.55	0.42
2:B:17:SER:HB3	2:B:82:GLN:HE22	1.85	0.42
2:B:144:THR:HA	2:B:193:PRO:HA	2.00	0.42
1:A:163:VAL:CG2	1:A:175:LEU:HD12	2.49	0.42
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.81	0.41
2:B:139:SER:OG	2:B:197:LEU:HD11	2.21	0.41
2:B:70:ILE:HG21	2:B:70:ILE:HD13	1.87	0.41
2:B:125:THR:HA	2:B:155:PHE:O	2.21	0.41
2:B:134:ALA:HA	2:B:135:PRO:HD3	1.90	0.41
2:B:196:SER:O	2:B:199:THR:HB	2.22	0.40
2:B:6:GLU:HA	2:B:21:SER:O	2.21	0.40
1:A:80:GLU:CD	1:A:80:GLU:H	2.24	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	204/206 (99%)	187 (92%)	10 (5%)	7 (3%)	5	6
2	B	215/217 (99%)	186 (86%)	21 (10%)	8 (4%)	4	5
All	All	419/423 (99%)	373 (89%)	31 (7%)	15 (4%)	4	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
2	B	42	GLU
2	B	139	SER
2	B	140	THR
2	B	168	LEU
2	B	211	SER
2	B	212	ASN
1	A	30	GLY
1	A	60	SER
1	A	68	GLY
1	A	138	ASN
2	B	55	GLY
1	A	199	GLN
2	B	54	GLY
1	A	203	SER

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	183/183 (100%)	148 (81%)	35 (19%)	2	3
2	B	180/180 (100%)	149 (83%)	31 (17%)	2	4
All	All	363/363 (100%)	297 (82%)	66 (18%)	2	3

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	15	LEU
1	A	24	ARG
1	A	31	ASN
1	A	40	PRO
1	A	43	SER
1	A	46	LEU
1	A	53	ARG
1	A	60	SER
1	A	63	SER
1	A	65	TRP
1	A	80	GLU
1	A	85	THR
1	A	89	GLN
1	A	97	THR
1	A	105	GLU
1	A	108	ARG
1	A	109	THR
1	A	114	SER
1	A	122	ASP
1	A	125	LEU
1	A	129	THR
1	A	143	GLU
1	A	154	LEU
1	A	158	ASN
1	A	159	SER
1	A	164	THR
1	A	169	LYS
1	A	170	ASP
1	A	172	THR
1	A	176	SER
1	A	185	ASP
1	A	190	LYS
1	A	191	VAL
1	A	204	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	13	GLN
2	B	21	SER
2	B	25	SER
2	B	28	THR
2	B	42	GLU
2	B	53	SER
2	B	65	LYS
2	B	77	ASN
2	B	84	THR
2	B	89	GLU
2	B	104	ARG
2	B	122	SER
2	B	140	THR
2	B	147	LEU
2	B	151	VAL
2	B	156	PRO
2	B	157	GLU
2	B	158	PRO
2	B	159	VAL
2	B	164	ASN
2	B	168	LEU
2	B	169	THR
2	B	178	VAL
2	B	180	GLN
2	B	183	LEU
2	B	191	THR
2	B	197	LEU
2	B	200	GLN
2	B	203	ILE
2	B	207	ASN
2	B	211	SER

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	152	ASN
1	A	158	ASN
1	A	189	HIS
2	B	74	ASN
2	B	82	GLN
2	B	164	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	173	HIS
2	B	180	GLN
2	B	200	GLN
2	B	205	ASN
2	B	208	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 carbohydrates 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	206/206 (100%)	-0.51	0 100 100	5, 25, 52, 73	0
2	B	217/217 (100%)	-0.14	14 (6%) 22 25	3, 23, 80, 111	0
All	All	423/423 (100%)	-0.32	14 (3%) 50 55	3, 24, 64, 111	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	169	THR	9.8
2	B	168	LEU	7.2
2	B	166	GLY	4.9
2	B	167	ALA	3.9
2	B	139	SER	3.3
2	B	164	ASN	3.1
2	B	198	GLY	3.0
2	B	170	SER	2.7
2	B	138	LYS	2.7
2	B	135	PRO	2.5
2	B	142	GLY	2.5
2	B	136	SER	2.4
2	B	199	THR	2.2
2	B	137	SER	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.