



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:52 PM UTC

PDB ID : 7MK6 / pdb_00007mk6
Title : KcsA open gate E71V mutant with sodium
Authors : Rohaim, A.; Li, J.; Weingarth, M.; Roux, B.
Deposited on : 2021-04-21
Resolution : 3.10 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

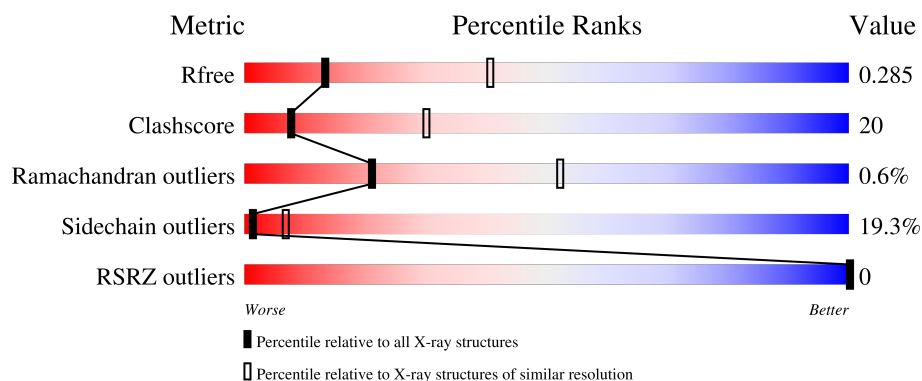
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

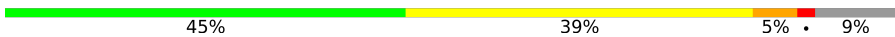
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	229	
2	B	215	
3	C	96	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3805 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1568	994	264	305	5			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1513	948	255	305	5			

- Molecule 3 is a protein called pH-gated potassium channel KcsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			660	437	106	113	4			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	28	CYS	ALA	engineered mutation	UNP P0A334
C	71	VAL	GLU	engineered mutation	UNP P0A334
C	90	CYS	LEU	engineered mutation	UNP P0A334
C	117	GLN	ARG	engineered mutation	UNP P0A334
C	118	CYS	GLU	engineered mutation	UNP P0A334
C	120	GLN	GLU	engineered mutation	UNP P0A334
C	121	GLN	ARG	engineered mutation	UNP P0A334

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		

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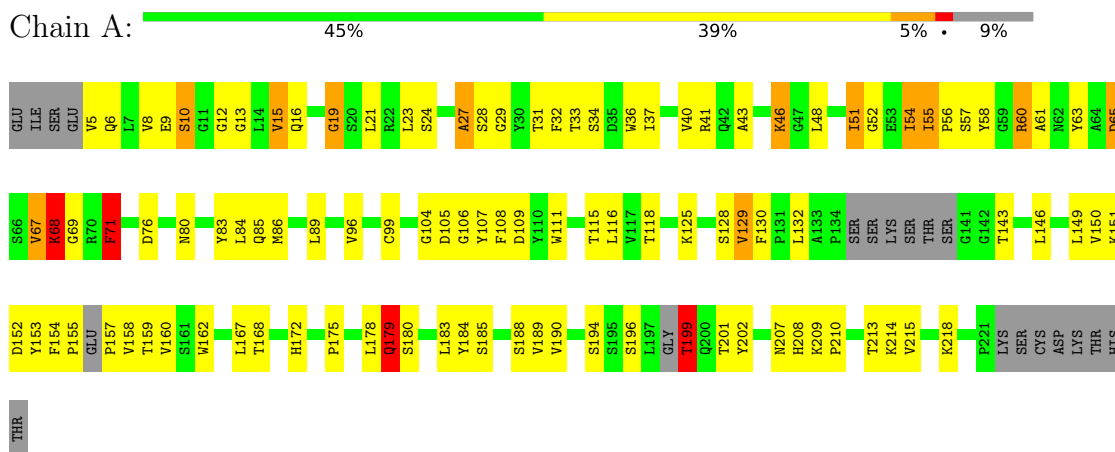
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	21	Total	O	0	0
			21	21		
4	C	10	Total	O	0	0
			10	10		

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.

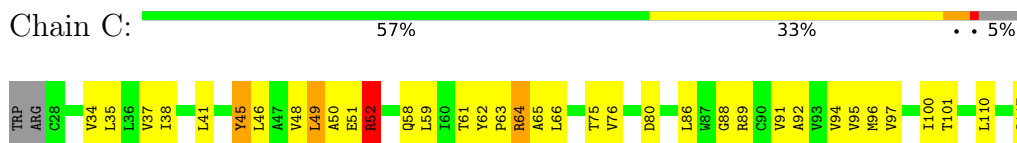
• Molecule 1: Fab heavy chain



• Molecule 2: Fab light chain



• Molecule 3: pH-gated potassium channel KcsA



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.14Å 140.14Å 69.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.10) 99.5 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.253 0.231 , 0.285	Depositor DCC
R_{free} test set	647 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	125.5	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3805	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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	1.35	8/1606 (0.5%)	1.65	22/2187 (1.0%)
2	B	1.26	5/1544 (0.3%)	1.56	10/2092 (0.5%)
3	C	1.18	1/676 (0.1%)	1.74	8/933 (0.9%)
All	All	1.28	14/3826 (0.4%)	1.63	40/5212 (0.8%)

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	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	GLY	C-O	8.76	1.33	1.23
2	B	39	GLN	C-O	7.95	1.32	1.23
2	B	20	VAL	C-O	7.51	1.32	1.24
1	A	99	CYS	C-O	7.13	1.33	1.23
1	A	19	GLY	C-O	6.61	1.32	1.23
1	A	54	ILE	C-O	6.26	1.31	1.24
3	C	52	ARG	C-O	6.24	1.31	1.23
2	B	75	THR	C-O	6.10	1.31	1.24
2	B	172	SER	C-O	5.79	1.30	1.23
1	A	51	ILE	CA-C	5.76	1.60	1.52
1	A	71	PHE	C-O	5.52	1.30	1.23
1	A	106	GLY	C-O	-5.32	1.16	1.23
2	B	61	SER	C-O	5.24	1.30	1.24
1	A	52	GLY	CA-C	-5.15	1.45	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LYS	N-CA-C	11.74	126.15	108.31
1	A	28	SER	N-CA-C	9.87	125.01	111.39
1	A	199	THR	CA-C-N	9.04	135.20	122.72
1	A	199	THR	C-N-CA	9.04	135.20	122.72
2	B	92	SER	CB-CA-C	8.73	120.42	109.16
2	B	181	THR	CB-CA-C	7.29	121.76	109.80
3	C	64	ARG	N-CA-C	-7.24	102.39	112.45
1	A	69	GLY	N-CA-C	-7.24	96.03	113.18
1	A	199	THR	CB-CA-C	7.13	124.79	109.10
1	A	76	ASP	N-CA-C	7.07	120.82	111.28
1	A	180	SER	CA-C-N	6.80	129.28	120.44
1	A	180	SER	C-N-CA	6.80	129.28	120.44
3	C	97	VAL	N-CA-C	6.70	117.20	110.23
2	B	60	PRO	CB-CA-C	-6.68	102.83	111.39
3	C	76	VAL	N-CA-C	6.61	117.23	110.82
2	B	32	THR	CA-CB-OG1	-6.56	99.76	109.60
3	C	64	ARG	CB-CA-C	6.42	122.24	110.11
3	C	76	VAL	CB-CA-C	-6.14	104.00	112.04
2	B	90	GLN	CA-C-N	6.01	129.66	120.82
2	B	90	GLN	C-N-CA	6.01	129.66	120.82
2	B	60	PRO	N-CA-C	6.00	120.65	111.11
1	A	27	ALA	N-CA-C	5.95	117.64	111.03
1	A	106	GLY	O-C-N	5.91	130.38	122.70
1	A	109	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	179	GLN	CA-C-O	-5.83	114.77	121.19
1	A	37	ILE	N-CA-CB	5.80	117.04	110.72
1	A	109	ASP	CB-CA-C	5.79	120.05	110.90
3	C	97	VAL	CB-CA-C	-5.74	104.36	111.70
1	A	151	LYS	N-CA-CB	5.62	119.33	110.56
1	A	57	SER	N-CA-C	5.61	117.86	111.02
1	A	58	TYR	N-CA-C	-5.52	106.54	113.72
1	A	151	LYS	CA-C-N	5.46	130.16	122.46
1	A	151	LYS	C-N-CA	5.46	130.16	122.46
1	A	152	ASP	N-CA-C	5.40	118.64	111.30
2	B	70	THR	N-CA-C	-5.29	107.37	113.88
3	C	94	VAL	O-C-N	5.21	127.15	121.94
3	C	58	GLN	N-CA-C	-5.17	106.12	112.90
2	B	29	SER	N-CA-C	-5.12	102.27	109.96
2	B	111	VAL	CB-CA-C	5.12	119.68	111.29
1	A	32	PHE	CA-CB-CG	5.09	118.89	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	THR	Peptide
1	A	60	ARG	Peptide
2	B	191	LYS	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	1568	0	1521	77	0
2	B	1513	0	1472	64	0
3	C	660	0	679	23	0
4	A	33	0	0	5	0
4	B	21	0	0	1	0
4	C	10	0	0	0	0
All	All	3805	0	3672	148	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 20.

All (148) 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:A:189:VAL:HG11	2:B:136:LEU:HD11	1.55	0.88
1:A:36:TRP:CE2	1:A:55:ILE:HG12	2.17	0.80
1:A:9:GLU:HA	1:A:24:SER:O	1.83	0.79
1:A:67:VAL:O	1:A:67:VAL:HG13	1.85	0.76
1:A:167:LEU:HD21	1:A:190:VAL:HG11	1.68	0.75
1:A:128:SER:HB3	1:A:130:PHE:CE2	2.29	0.68
1:A:43:ALA:HB3	1:A:46:LYS:HG3	1.76	0.67
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.77	0.66
3:C:62:TYR:N	3:C:63:PRO:HD2	2.10	0.65
2:B:38:GLN:O	2:B:46:LYS:N	2.27	0.65
2:B:167:GLN:HG2	2:B:172:SER:HA	1.79	0.64
1:A:189:VAL:CG1	2:B:136:LEU:HD11	2.26	0.64
1:A:160:VAL:HG11	1:A:188:SER:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:HIS:CD2	2:B:175:SER:OG	2.52	0.62
3:C:88:GLY:O	3:C:91:VAL:HB	2.00	0.62
1:A:21:LEU:O	1:A:86:MET:HB2	2.00	0.62
1:A:54:ILE:HD12	1:A:61:ALA:HB2	1.82	0.61
1:A:179:GLN:HB2	1:A:183:LEU:O	2.00	0.61
1:A:160:VAL:HG11	1:A:188:SER:CB	2.31	0.60
1:A:86:MET:HB3	1:A:89:LEU:HD21	1.83	0.60
1:A:153:TYR:CZ	1:A:208:HIS:ND1	2.70	0.60
3:C:91:VAL:O	3:C:95:VAL:HG23	2.00	0.60
2:B:81:PRO:HA	2:B:107:ILE:HD13	1.85	0.59
1:A:130:PHE:CD2	2:B:125:GLN:HG3	2.38	0.59
1:A:29:GLY:O	1:A:31:THR:HG23	2.03	0.59
3:C:37:VAL:O	3:C:41:LEU:HD12	2.02	0.59
1:A:43:ALA:HB3	1:A:46:LYS:CG	2.32	0.59
3:C:48:VAL:HG23	3:C:65:ALA:HB2	1.84	0.59
1:A:155:PRO:O	1:A:157:PRO:HD2	2.04	0.58
2:B:34:ILE:CG2	2:B:72:PHE:CE2	2.85	0.58
2:B:88:TYR:CE1	2:B:102:GLY:HA3	2.39	0.58
1:A:27:ALA:HB2	1:A:80:ASN:O	2.05	0.56
1:A:107:TYR:HA	2:B:90:GLN:HE22	1.69	0.56
2:B:34:ILE:HA	2:B:90:GLN:O	2.05	0.56
2:B:91:GLN:OE1	2:B:94:ARG:O	2.23	0.56
2:B:34:ILE:HD12	2:B:89:CYS:SG	2.47	0.55
1:A:67:VAL:O	1:A:67:VAL:CG1	2.55	0.55
1:A:61:ALA:O	1:A:63:TYR:CE1	2.60	0.54
2:B:15:SER:HB2	4:B:313:HOH:O	2.08	0.54
1:A:12:GLY:HA2	1:A:21:LEU:HD21	1.90	0.53
1:A:36:TRP:NE1	1:A:55:ILE:HG12	2.21	0.53
2:B:137:LEU:O	2:B:175:SER:HA	2.09	0.53
1:A:36:TRP:CZ2	1:A:55:ILE:HD11	2.43	0.53
2:B:131:ALA:N	2:B:182:LEU:O	2.42	0.53
2:B:167:GLN:HG3	2:B:174:TYR:CE1	2.44	0.53
1:A:5:VAL:HA	1:A:29:GLY:HA3	1.90	0.52
1:A:107:TYR:HB3	2:B:35:HIS:CG	2.44	0.52
2:B:149:TRP:HB2	2:B:156:GLN:HB2	1.90	0.52
3:C:89:ARG:O	3:C:92:ALA:HB3	2.09	0.52
1:A:107:TYR:HB3	2:B:35:HIS:CD2	2.45	0.52
2:B:62:ARG:NH2	2:B:83:ASP:OD1	2.43	0.52
1:A:15:VAL:HG12	1:A:19:GLY:HA3	1.92	0.51
1:A:108:PHE:HB2	1:A:111:TRP:CZ2	2.46	0.51
3:C:35:LEU:O	3:C:38:ILE:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:VAL:HG23	3:C:65:ALA:CB	2.40	0.51
1:A:15:VAL:CG1	1:A:19:GLY:HA3	2.40	0.51
2:B:38:GLN:N	2:B:46:LYS:O	2.43	0.51
1:A:23:LEU:HB2	1:A:84:LEU:HB3	1.92	0.50
1:A:146:LEU:C	1:A:146:LEU:HD12	2.37	0.50
1:A:175:PRO:HD2	2:B:163:SER:OG	2.10	0.50
3:C:34:VAL:O	3:C:38:ILE:HG13	2.12	0.50
1:A:36:TRP:CZ2	1:A:55:ILE:CD1	2.95	0.49
1:A:65:ASP:O	1:A:68:LYS:HG3	2.13	0.49
1:A:209:LYS:N	1:A:210:PRO:CD	2.75	0.49
2:B:87:TYR:HE1	2:B:105:VAL:CG2	2.26	0.48
2:B:110:THR:O	2:B:111:VAL:C	2.55	0.48
2:B:9:PRO:O	2:B:103:THR:HG23	2.13	0.48
1:A:132:LEU:HB3	2:B:119:PHE:CD1	2.48	0.48
2:B:120:PRO:HG3	2:B:193:TYR:HE2	1.79	0.48
1:A:154:PHE:CD1	1:A:155:PRO:HA	2.49	0.47
1:A:162:TRP:CE2	1:A:190:VAL:CG2	2.97	0.47
2:B:3:ILE:HD11	2:B:28:GLN:OE1	2.14	0.47
3:C:46:LEU:O	3:C:49:LEU:HB3	2.13	0.47
1:A:155:PRO:C	1:A:157:PRO:HD2	2.39	0.47
2:B:62:ARG:HB3	2:B:77:SER:O	2.14	0.46
2:B:34:ILE:HG23	2:B:72:PHE:CE2	2.50	0.46
1:A:23:LEU:O	1:A:83:TYR:HA	2.15	0.46
2:B:141:TYR:CD1	2:B:142:PRO:HA	2.50	0.46
1:A:71:PHE:N	1:A:71:PHE:CD1	2.83	0.46
2:B:89:CYS:O	2:B:99:PHE:HA	2.16	0.46
3:C:37:VAL:O	3:C:41:LEU:CD1	2.64	0.46
1:A:71:PHE:N	1:A:71:PHE:HD1	2.14	0.46
3:C:59:LEU:HD11	3:C:65:ALA:HA	1.97	0.46
2:B:95:TRP:CG	2:B:96:PRO:HA	2.51	0.45
3:C:46:LEU:O	3:C:50:ALA:N	2.39	0.45
1:A:155:PRO:O	1:A:157:PRO:CD	2.64	0.45
3:C:86:LEU:O	3:C:89:ARG:N	2.48	0.45
2:B:135:CYS:HB2	2:B:149:TRP:CH2	2.52	0.45
3:C:75:THR:HG22	3:C:100:ILE:HG12	1.98	0.45
1:A:41:ARG:HA	1:A:96:VAL:O	2.17	0.45
1:A:96:VAL:HA	1:A:115:THR:O	2.17	0.45
2:B:7:GLN:OE1	2:B:89:CYS:CB	2.64	0.44
2:B:66:SER:OG	2:B:67:ARG:N	2.46	0.44
3:C:51:GLU:O	3:C:52:ARG:C	2.60	0.44
1:A:27:ALA:CB	1:A:80:ASN:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HB1	1:A:31:THR:HG21	1.98	0.44
1:A:105:ASP:OD2	1:A:107:TYR:CZ	2.71	0.44
2:B:164:VAL:CG2	2:B:176:LEU:HD12	2.48	0.44
1:A:33:THR:HG22	1:A:34:SER:OG	2.18	0.43
2:B:34:ILE:HG21	2:B:72:PHE:CE2	2.53	0.43
2:B:3:ILE:HD11	2:B:94:ARG:CG	2.48	0.43
2:B:37:TYR:HA	2:B:46:LYS:O	2.19	0.43
2:B:40:LYS:O	2:B:41:PRO:C	2.61	0.43
2:B:88:TYR:CE1	2:B:102:GLY:CA	3.02	0.43
2:B:93:ASN:O	3:C:64:ARG:NH1	2.51	0.43
1:A:55:ILE:HD12	3:C:49:LEU:CD1	2.48	0.43
2:B:131:ALA:HB3	2:B:182:LEU:HB2	2.00	0.43
1:A:10:SER:C	4:A:309:HOH:O	2.60	0.43
1:A:10:SER:CA	4:A:309:HOH:O	2.66	0.43
1:A:48:LEU:HB2	2:B:99:PHE:CD2	2.54	0.43
1:A:150:VAL:O	1:A:185:SER:HA	2.18	0.43
1:A:54:ILE:O	1:A:56:PRO:HD3	2.19	0.42
1:A:10:SER:HA	4:A:309:HOH:O	2.18	0.42
1:A:153:TYR:CG	1:A:154:PHE:N	2.87	0.42
1:A:172:HIS:HD2	2:B:175:SER:OG	2.01	0.42
2:B:10:SER:O	2:B:104:LYS:N	2.47	0.42
2:B:52:ALA:O	2:B:65:GLY:O	2.37	0.42
2:B:159:ASN:O	2:B:180:LEU:HA	2.20	0.42
1:A:108:PHE:H	2:B:37:TYR:HH	1.67	0.42
3:C:62:TYR:N	3:C:63:PRO:CD	2.81	0.42
1:A:129:VAL:HA	1:A:149:LEU:O	2.20	0.42
1:A:15:VAL:CG2	1:A:21:LEU:HD22	2.50	0.42
2:B:123:ASP:O	2:B:126:LEU:N	2.53	0.42
2:B:80:GLN:HB3	2:B:82:GLU:OE2	2.19	0.41
1:A:178:LEU:HD13	1:A:184:TYR:CE1	2.54	0.41
2:B:15:SER:O	2:B:18:ASP:HB2	2.21	0.41
2:B:50:LYS:C	2:B:52:ALA:H	2.27	0.41
1:A:146:LEU:HD21	1:A:202:TYR:CD2	2.55	0.41
3:C:48:VAL:HG22	3:C:61:THR:N	2.35	0.41
1:A:178:LEU:HD13	1:A:184:TYR:HE1	1.85	0.41
2:B:87:TYR:HE1	2:B:105:VAL:HG22	1.84	0.41
2:B:167:GLN:HG2	2:B:172:SER:CA	2.47	0.41
2:B:37:TYR:CE1	2:B:47:LEU:HB2	2.55	0.41
1:A:184:TYR:HB2	4:A:302:HOH:O	2.20	0.41
2:B:3:ILE:HD11	2:B:94:ARG:HG3	2.03	0.41
1:A:167:LEU:HD21	1:A:190:VAL:CG1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:TYR:C	3:C:45:TYR:CD1	2.99	0.41
1:A:104:GLY:O	3:C:61:THR:HB	2.20	0.41
1:A:132:LEU:HB3	2:B:119:PHE:CG	2.56	0.41
1:A:158:VAL:HG13	1:A:208:HIS:CE1	2.56	0.41
2:B:39:GLN:HB2	2:B:45:PRO:HA	2.03	0.41
3:C:62:TYR:HB2	3:C:63:PRO:CD	2.50	0.41
1:A:40:VAL:HG12	1:A:41:ARG:N	2.35	0.40
1:A:213:THR:HG23	1:A:215:VAL:HG23	2.03	0.40
1:A:60:ARG:HB3	4:A:318:HOH:O	2.21	0.40
1:A:85:GLN:OE1	1:A:85:GLN:HA	2.20	0.40
2:B:15:SER:O	2:B:18:ASP:CG	2.64	0.40
2:B:86:THR:CG2	2:B:88:TYR:CE2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	201/229 (88%)	163 (81%)	36 (18%)	2 (1%)	12	41
2	B	189/215 (88%)	159 (84%)	29 (15%)	1 (0%)	24	57
3	C	89/96 (93%)	69 (78%)	20 (22%)	0	100	100
All	All	479/540 (89%)	391 (82%)	85 (18%)	3 (1%)	21	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLY
2	B	67	ARG
1	A	129	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	171/190 (90%)	145 (85%)	26 (15%)	3	13
2	B	174/191 (91%)	130 (75%)	44 (25%)	0	2
3	C	65/71 (92%)	56 (86%)	9 (14%)	3	15
All	All	410/452 (91%)	331 (81%)	79 (19%)	1	7

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	VAL
1	A	10	SER
1	A	15	VAL
1	A	16	GLN
1	A	46	LYS
1	A	51	ILE
1	A	55	ILE
1	A	65	ASP
1	A	67	VAL
1	A	68	LYS
1	A	71	PHE
1	A	116	LEU
1	A	118	THR
1	A	125	LYS
1	A	143	THR
1	A	159	THR
1	A	168	THR
1	A	179	GLN
1	A	194	SER
1	A	196	SER
1	A	199	THR
1	A	201	THR
1	A	207	ASN
1	A	214	LYS
1	A	218	LYS

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Mol	Chain	Res	Type
2	B	3	ILE
2	B	13	SER
2	B	16	VAL
2	B	20	VAL
2	B	21	THR
2	B	23	THR
2	B	24	CYS
2	B	25	ARG
2	B	28	GLN
2	B	29	SER
2	B	34	ILE
2	B	55	SER
2	B	66	SER
2	B	67	ARG
2	B	68	SER
2	B	75	THR
2	B	78	SER
2	B	82	GLU
2	B	86	THR
2	B	90	GLN
2	B	91	GLN
2	B	92	SER
2	B	96	PRO
2	B	110	THR
2	B	115	SER
2	B	122	SER
2	B	124	SER
2	B	127	LYS
2	B	130	THR
2	B	136	LEU
2	B	137	LEU
2	B	143	ARG
2	B	147	VAL
2	B	148	GLN
2	B	150	LYS
2	B	151	VAL
2	B	160	SER
2	B	161	GLN
2	B	170	LYS
2	B	171	ASP
2	B	184	LYS
2	B	186	ASP

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Mol	Chain	Res	Type
2	B	190	HIS
2	B	192	VAL
3	C	45	TYR
3	C	49	LEU
3	C	52	ARG
3	C	66	LEU
3	C	80	ASP
3	C	96	MET
3	C	101	THR
3	C	110	LEU
3	C	117	GLN

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	42	GLN
1	A	172	HIS
2	B	39	GLN
2	B	90	GLN
2	B	148	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	209/229 (91%)	-0.48	0 100 100	101, 162, 215, 232	0
2	B	195/215 (90%)	-0.61	0 100 100	85, 149, 194, 219	0
3	C	91/96 (94%)	-0.40	0 100 100	93, 139, 194, 224	0
All	All	495/540 (91%)	-0.52	0 100 100	85, 154, 208, 232	0

There are no RSRZ outliers to report.

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.