



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:01 AM UTC

PDB ID : 6B8Q / pdb_00006b8q
Title : Crystal Structure of the Mg²⁺/CaM:Kv7.5 (KCNQ5) AB domain complex
Authors : Chang, A.; Abderemane-Ali, F.; Minor, D.L.
Deposited on : 2017-10-09
Resolution : 2.60 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

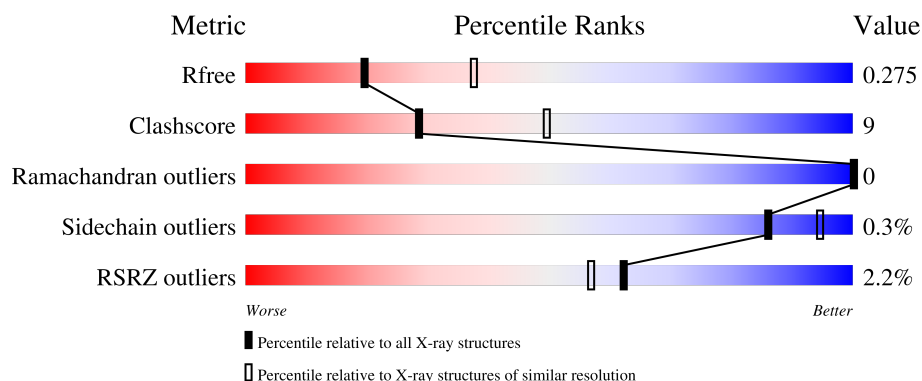
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	75	
1	C	75	
1	E	75	
1	G	75	
2	B	149	

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Mol	Chain	Length	Quality of chain
2	D	149	2% 81% 15%
2	F	149	5% 73% 23%
2	H	149	85% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6648 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 Potassium voltage-gated channel subfamily KQT member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	0	0
			511	330	96	83	2			
1	C	60	Total	C	N	O	S	0	0	0
			494	318	93	81	2			
1	E	60	Total	C	N	O	S	0	0	0
			491	318	90	81	2			
1	G	66	Total	C	N	O	S	0	0	0
			550	356	103	89	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	GLY	-	expression tag	UNP Q9NR82
A	357	HIS	-	expression tag	UNP Q9NR82
A	358	MET	-	expression tag	UNP Q9NR82
A	359	ALA	-	expression tag	UNP Q9NR82
A	360	SER	-	expression tag	UNP Q9NR82
A	395	LYS	-	linker	UNP Q9NR82
A	396	LEU	VAL	linker	UNP Q9NR82
C	356	GLY	-	expression tag	UNP Q9NR82
C	357	HIS	-	expression tag	UNP Q9NR82
C	358	MET	-	expression tag	UNP Q9NR82
C	359	ALA	-	expression tag	UNP Q9NR82
C	360	SER	-	expression tag	UNP Q9NR82
C	395	LYS	-	linker	UNP Q9NR82
C	396	LEU	VAL	linker	UNP Q9NR82
E	356	GLY	-	expression tag	UNP Q9NR82
E	357	HIS	-	expression tag	UNP Q9NR82
E	358	MET	-	expression tag	UNP Q9NR82
E	359	ALA	-	expression tag	UNP Q9NR82
E	360	SER	-	expression tag	UNP Q9NR82
E	395	LYS	-	linker	UNP Q9NR82
E	396	LEU	VAL	linker	UNP Q9NR82

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Chain	Residue	Modelled	Actual	Comment	Reference
G	356	GLY	-	expression tag	UNP Q9NR82
G	357	HIS	-	expression tag	UNP Q9NR82
G	358	MET	-	expression tag	UNP Q9NR82
G	359	ALA	-	expression tag	UNP Q9NR82
G	360	SER	-	expression tag	UNP Q9NR82
G	395	LYS	-	linker	UNP Q9NR82
G	396	LEU	VAL	linker	UNP Q9NR82

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1151	705	185	252	9			
2	D	143	Total	C	N	O	S	0	0	0
			1126	690	181	246	9			
2	F	144	Total	C	N	O	S	0	0	0
			1134	696	182	247	9			
2	H	146	Total	C	N	O	S	0	0	0
			1151	705	185	252	9			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	D	4	Total	Mg	0	0
			4	4		
3	F	4	Total	Mg	0	0
			4	4		
3	H	4	Total	Mg	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	O 3	0	0
4	E	1	Total 1	O 1	0	0
4	F	2	Total 2	O 2	0	0
4	G	4	Total 4	O 4	0	0
4	H	8	Total 8	O 8	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.

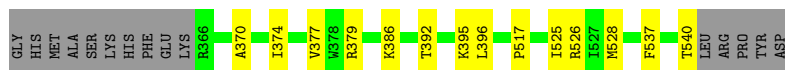
- Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

Chain A: 



- Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

Chain C: 



- Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

Chain E: 



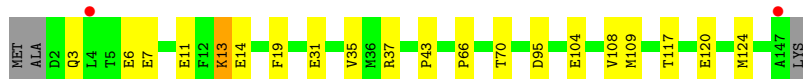
- Molecule 1: Potassium voltage-gated channel subfamily KQT member 5

Chain G: 

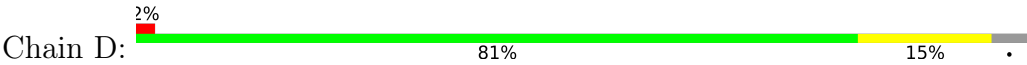


- Molecule 2: Calmodulin-1

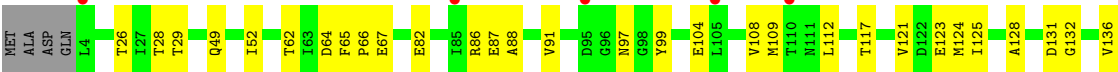
Chain B: 



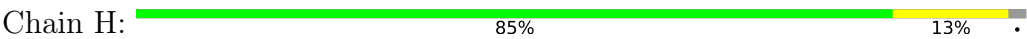
- Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.82Å 116.84Å 119.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.74 – 2.60 45.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.74-2.60) 100.0 (45.74-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.222 , 0.270 0.228 , 0.275	Depositor DCC
R_{free} test set	1556 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.15	0/521	0.43	0/700
1	C	0.12	0/504	0.30	0/678
1	E	0.15	0/501	0.33	0/675
1	G	0.14	0/562	0.34	0/754
2	B	0.40	2/1163 (0.2%)	0.30	0/1562
2	D	0.14	0/1138	0.34	0/1528
2	F	0.17	0/1146	0.38	0/1539
2	H	0.13	0/1163	0.28	0/1562
All	All	0.21	2/6698 (0.0%)	0.34	0/8998

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	GLU	C-O	-6.76	1.16	1.24
2	B	13	LYS	C-O	-5.54	1.17	1.24

There are no bond angle outliers.

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	A	511	0	553	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	494	0	529	13	0
1	E	491	0	527	12	0
1	G	550	0	588	10	0
2	B	1151	0	1075	14	0
2	D	1126	0	1052	20	0
2	F	1134	0	1063	37	0
2	H	1151	0	1075	15	0
3	B	3	0	0	0	0
3	D	4	0	0	0	0
3	F	4	0	0	0	0
3	H	4	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	1	0
4	G	4	0	0	0	0
4	H	8	0	0	0	0
All	All	6648	0	6462	115	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 9.

All (115) 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:F:86:ARG:NH2	2:F:139:GLU:HG2	1.78	0.97
2:F:86:ARG:CZ	2:F:139:GLU:HG2	2.00	0.90
1:E:392:THR:HG23	1:E:526:ARG:HH12	1.40	0.84
1:E:535:ARG:HG3	1:E:538:LYS:HE3	1.63	0.81
2:D:14:GLU:N	2:D:14:GLU:OE1	2.14	0.80
2:F:108:VAL:HA	2:F:112:LEU:HD23	1.65	0.79
2:F:121:VAL:HG22	2:F:125:ILE:HD11	1.69	0.74
2:F:138:TYR:CZ	2:F:139:GLU:HG3	2.24	0.73
2:F:86:ARG:HB3	2:F:138:TYR:HE1	1.56	0.69
2:H:83:GLU:OE2	2:H:86:ARG:NH1	2.26	0.68
2:F:125:ILE:HD12	2:F:125:ILE:H	1.59	0.68
1:A:394:LYS:NZ	2:B:117:THR:OG1	2.28	0.66
2:F:49:GLN:NE2	4:F:301:HOH:O	2.30	0.65
1:C:517:PRO:HG3	2:D:14:GLU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PRO:HG2	1:A:540:THR:HG21	1.80	0.64
2:F:121:VAL:O	2:F:125:ILE:HD12	1.98	0.64
2:F:29:THR:HG22	2:F:52:ILE:HG13	1.79	0.64
1:G:527:ILE:HD11	2:H:71:MET:HG2	1.80	0.63
2:F:86:ARG:NH2	2:F:139:GLU:CG	2.58	0.62
2:F:109:MET:HE3	2:F:124:MET:HE1	1.82	0.62
2:F:121:VAL:O	2:F:125:ILE:CD1	2.48	0.61
1:E:374:ILE:HD11	2:F:88:ALA:HB1	1.83	0.61
1:C:525:ILE:HA	1:C:528:MET:HE3	1.83	0.60
2:B:6:GLU:N	2:B:6:GLU:OE1	2.36	0.59
1:E:535:ARG:HA	1:E:538:LYS:HG3	1.84	0.59
2:H:4:LEU:HD11	2:H:73:ALA:HB2	1.84	0.59
1:A:385:GLU:H	1:A:385:GLU:CD	2.11	0.58
2:F:121:VAL:HG22	2:F:125:ILE:CD1	2.32	0.58
2:F:140:GLU:OE1	2:F:140:GLU:N	2.31	0.57
2:F:86:ARG:HH21	2:F:139:GLU:HG2	1.68	0.57
1:A:391:ALA:O	1:A:394:LYS:HG3	2.05	0.57
2:F:137:ASN:OD1	2:F:138:TYR:N	2.37	0.57
1:A:394:LYS:HZ3	2:B:120:GLU:HG3	1.68	0.57
2:D:27:ILE:HB	2:D:63:ILE:HB	1.85	0.57
1:C:386:LYS:NZ	2:D:147:ALA:O	2.38	0.56
1:G:527:ILE:HG21	2:H:75:LYS:HE3	1.88	0.56
2:F:137:ASN:HB3	2:F:140:GLU:OE2	2.05	0.56
2:F:86:ARG:HB3	2:F:138:TYR:CE1	2.41	0.55
2:H:31:GLU:O	2:H:35:VAL:HG23	2.07	0.55
1:C:525:ILE:HD13	2:D:36:MET:HG2	1.90	0.54
2:F:125:ILE:HD12	2:F:125:ILE:N	2.23	0.54
2:B:7:GLU:O	2:B:11:GLU:HG3	2.08	0.53
1:G:523:ARG:O	1:G:527:ILE:HG23	2.10	0.52
1:E:374:ILE:HB	2:F:109:MET:HE1	1.92	0.52
2:F:86:ARG:NE	2:F:139:GLU:HG2	2.22	0.52
2:D:10:ALA:O	2:D:14:GLU:OE1	2.27	0.52
2:B:95:ASP:OD1	2:B:95:ASP:N	2.39	0.52
1:A:365:LYS:HG3	1:A:367:ARG:HG2	1.92	0.51
2:D:86:ARG:HE	2:D:139:GLU:HG3	1.76	0.51
1:A:394:LYS:NZ	2:B:120:GLU:HG3	2.26	0.51
2:F:97:ASN:HB2	2:F:99:TYR:H	1.75	0.50
2:H:86:ARG:HD3	2:H:139:GLU:OE1	2.11	0.50
2:B:66:PRO:O	2:B:70:THR:HG23	2.12	0.50
1:A:533:ALA:HA	1:A:536:LYS:HE2	1.94	0.50
1:C:537:PHE:O	1:C:540:THR:OG1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:O	2:B:13:LYS:HG3	2.13	0.48
2:F:131:ASP:OD2	2:F:132:GLY:N	2.47	0.48
2:F:82:GLU:O	2:F:86:ARG:HG3	2.13	0.48
1:E:513:ASP:CG	1:E:515:THR:HG1	2.21	0.48
2:H:106:ARG:NH1	2:H:122:ASP:OD2	2.47	0.47
1:C:377:VAL:HG21	2:D:85:ILE:HG12	1.95	0.47
2:F:128:ALA:HB1	2:F:136:VAL:HG21	1.96	0.47
2:H:138:TYR:HA	2:H:141:PHE:HB3	1.96	0.47
1:G:396:LEU:HD23	1:G:514:LEU:HD21	1.97	0.47
2:H:71:MET:HE2	2:H:71:MET:HB3	1.76	0.46
1:E:374:ILE:H	1:E:374:ILE:HD12	1.80	0.46
2:F:117:THR:O	2:F:121:VAL:HG12	2.15	0.46
2:D:97:ASN:ND2	2:D:99:TYR:HB2	2.31	0.46
1:G:369:PRO:HG2	1:G:540:THR:HG21	1.97	0.46
1:G:515:THR:HG22	1:G:517:PRO:HG2	1.98	0.45
1:E:368:ASN:N	1:E:369:PRO:HD2	2.31	0.45
2:D:6:GLU:O	2:D:7:GLU:HB2	2.15	0.45
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.74	0.45
2:D:138:TYR:O	2:D:142:VAL:HG13	2.17	0.45
2:F:104:GLU:O	2:F:108:VAL:HG13	2.16	0.45
2:B:31:GLU:O	2:B:35:VAL:HG23	2.16	0.44
2:B:109:MET:HE2	2:B:124:MET:SD	2.58	0.44
2:B:37:ARG:HG2	2:B:43:PRO:HD2	1.99	0.44
1:G:527:ILE:CD1	2:H:71:MET:HG2	2.46	0.44
2:D:28:THR:HG22	2:D:62:THR:HG22	1.99	0.44
1:E:385:GLU:OE1	1:E:523:ARG:NH2	2.50	0.44
2:F:26:THR:HG23	2:F:62:THR:HB	2.00	0.44
2:F:125:ILE:H	2:F:125:ILE:CD1	2.29	0.44
2:H:82:GLU:O	2:H:86:ARG:HG3	2.17	0.44
2:B:104:GLU:O	2:B:108:VAL:HG12	2.18	0.44
1:C:370:ALA:O	1:C:374:ILE:HG12	2.17	0.44
1:C:517:PRO:HG3	2:D:14:GLU:CB	2.45	0.44
2:D:6:GLU:O	2:D:6:GLU:CD	2.61	0.44
2:D:26:THR:HB	2:D:62:THR:HB	2.00	0.44
1:C:392:THR:HB	1:C:526:ARG:HH12	1.84	0.43
2:F:64:ASP:OD2	2:F:67:GLU:HB2	2.19	0.43
1:C:379:ARG:NH1	2:D:114:GLU:HG2	2.33	0.43
1:C:374:ILE:HB	2:D:109:MET:HE1	2.01	0.43
2:F:28:THR:HG22	2:F:62:THR:HG22	2.00	0.42
1:G:368:ASN:HB3	1:G:369:PRO:HD3	2.02	0.42
2:F:65:PHE:HB3	2:F:66:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLU:HG3	1:A:523:ARG:CZ	2.50	0.42
1:C:525:ILE:HG23	2:D:51:MET:HE1	2.01	0.41
1:A:535:ARG:HE	1:A:535:ARG:HB3	1.74	0.41
2:B:3:GLN:HG3	2:H:24:ASP:O	2.20	0.41
1:C:395:LYS:C	1:C:396:LEU:HD23	2.45	0.41
1:E:383:ALA:O	1:E:523:ARG:NH1	2.47	0.41
2:H:119:GLU:OE1	2:H:119:GLU:N	2.44	0.41
2:D:86:ARG:NE	2:D:139:GLU:HG3	2.35	0.41
1:E:513:ASP:OD2	1:E:515:THR:OG1	2.36	0.41
1:G:538:LYS:HB2	2:H:84:GLU:OE1	2.21	0.41
1:A:512:GLU:N	1:A:512:GLU:OE1	2.54	0.41
1:A:515:THR:HB	1:A:518:LEU:HD12	2.03	0.41
2:F:87:GLU:O	2:F:91:VAL:HG23	2.21	0.41
2:H:87:GLU:O	2:H:91:VAL:HG23	2.21	0.41
1:G:537:PHE:O	1:G:540:THR:OG1	2.34	0.40
1:E:389:SER:OG	2:F:123:GLU:OE1	2.38	0.40
2:D:51:MET:O	2:D:55:VAL:HG12	2.22	0.40
2:F:86:ARG:HG2	2:F:142:VAL:HG21	2.04	0.40
1:A:521:VAL:HG13	2:B:19:PHE:CZ	2.57	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	60/75 (80%)	58 (97%)	2 (3%)	0	100	100
1	C	58/75 (77%)	55 (95%)	3 (5%)	0	100	100
1	E	58/75 (77%)	51 (88%)	7 (12%)	0	100	100
1	G	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
2	B	144/149 (97%)	141 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
2	F	142/149 (95%)	137 (96%)	5 (4%)	0	100	100
2	H	144/149 (97%)	140 (97%)	4 (3%)	0	100	100
All	All	811/896 (90%)	775 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	55/66 (83%)	55 (100%)	0	100	100
1	C	53/66 (80%)	53 (100%)	0	100	100
1	E	53/66 (80%)	53 (100%)	0	100	100
1	G	59/66 (89%)	58 (98%)	1 (2%)	53	78
2	B	125/127 (98%)	125 (100%)	0	100	100
2	D	122/127 (96%)	121 (99%)	1 (1%)	73	88
2	F	123/127 (97%)	123 (100%)	0	100	100
2	H	125/127 (98%)	125 (100%)	0	100	100
All	All	715/772 (93%)	713 (100%)	2 (0%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	18	LEU
1	G	396	LEU

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

Mol	Chain	Res	Type
2	B	42	ASN

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Mol	Chain	Res	Type
2	D	111	ASN
2	D	137	ASN
1	E	368	ASN
2	H	49	GLN
2	H	107	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](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	62/75 (82%)	0.18	0	100	100	41, 59, 94, 112	0
1	C	60/75 (80%)	0.09	0	100	100	48, 63, 92, 96	0
1	E	60/75 (80%)	0.40	3 (5%)	34	28	53, 68, 106, 113	0
1	G	66/75 (88%)	0.07	3 (4%)	38	32	37, 55, 92, 105	0
2	B	146/149 (97%)	0.03	2 (1%)	73	69	43, 61, 78, 92	0
2	D	143/149 (95%)	0.29	3 (2%)	63	58	46, 72, 92, 122	0
2	F	144/149 (96%)	0.63	7 (4%)	35	29	49, 86, 112, 122	0
2	H	146/149 (97%)	0.00	0	100	100	41, 61, 87, 100	0
All	All	827/896 (92%)	0.22	18 (2%)	62	57	37, 67, 102, 122	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	4	LEU	3.6
2	F	95	ASP	3.1
1	G	363	PHE	2.7
2	D	5	THR	2.7
2	F	138	TYR	2.5
1	E	537	PHE	2.5
2	F	147	ALA	2.4
1	G	362	HIS	2.3
2	D	130	ILE	2.3
2	F	110	THR	2.3
1	G	361	LYS	2.2
1	E	367	ARG	2.2
2	B	4	LEU	2.2
2	B	147	ALA	2.1
2	F	105	LEU	2.1
2	F	85	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	371	ALA	2.1
2	D	15	ALA	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	H	203	1/1	0.76	0.25	76,76,76,76	0
3	MG	F	203	1/1	0.83	0.11	97,97,97,97	0
3	MG	B	203	1/1	0.90	0.12	56,56,56,56	0
3	MG	F	204	1/1	0.94	0.09	55,55,55,55	0
3	MG	B	201	1/1	0.94	0.04	48,48,48,48	0
3	MG	F	202	1/1	0.96	0.09	56,56,56,56	0
3	MG	D	203	1/1	0.96	0.08	75,75,75,75	0
3	MG	H	204	1/1	0.96	0.09	61,61,61,61	0
3	MG	B	202	1/1	0.98	0.11	41,41,41,41	0
3	MG	D	202	1/1	0.98	0.07	43,43,43,43	0
3	MG	F	201	1/1	0.99	0.03	44,44,44,44	0
3	MG	H	201	1/1	0.99	0.03	42,42,42,42	0
3	MG	H	202	1/1	0.99	0.10	31,31,31,31	0
3	MG	D	201	1/1	0.99	0.02	44,44,44,44	0
3	MG	D	204	1/1	0.99	0.04	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.