



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:03 PM UTC

PDB ID : 4OVN / pdb_00004ovn
Title : Voltage-gated Sodium Channel 1.5 (Nav1.5) C-terminal domain in complex with Calmodulin poised for activation
Authors : Gabelli, S.B.; Bianchet, M.A.; Boto, A.; Jakoncic, J.; Tomaselli, G.F.; Amzel, L.M.
Deposited on : 2013-12-10
Resolution : 2.80 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:

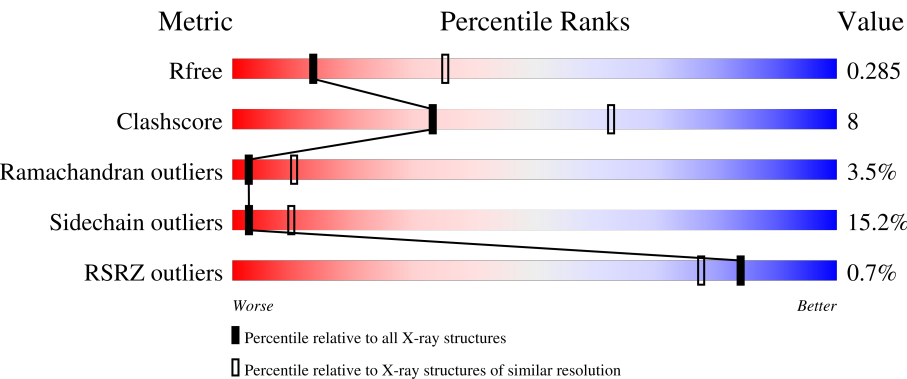
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	149	70%26%..
1	B	149	% 73%19%..
1	C	149	% 77%19%..
1	D	149	71%22%...
1	E	149	% 68%24%..

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Mol	Chain	Length	Quality of chain
2	F	157	% 65%22%5% • 7%
2	G	157	% 62%25%• • 8%
2	H	157	% 64%25%6% • •
2	I	157	62%20%8% • 9%
2	J	157	% 66%22%5% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23011 atoms, of which 11227 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 Calmodulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	H	N	O	Se	0	0	0
			2213	701	1070	184	249	9			
1	B	144	Total	C	H	N	O	Se	0	0	0
			2197	696	1063	182	247	9			
1	C	145	Total	C	H	N	O	Se	0	0	0
			2213	701	1070	184	249	9			
1	D	145	Total	C	H	N	O	Se	0	0	0
			2213	701	1070	184	249	9			
1	E	144	Total	C	H	N	O	Se	0	0	0
			2197	696	1063	182	247	9			

- Molecule 2 is a protein called Sodium channel protein type 5 subunit alpha.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	F	146	Total	C	H	N	O	S	Se	0	0	0
			2361	756	1174	198	224	1	8			
2	G	144	Total	C	H	N	O	S	Se	0	0	0
			2331	747	1158	196	221	1	8			
2	H	151	Total	C	H	N	O	S	Se	0	0	0
			2431	778	1207	203	234	1	8			
2	I	143	Total	C	H	N	O	S	Se	0	0	0
			2317	743	1151	195	219	1	8			
2	J	151	Total	C	H	N	O	S	Se	0	0	0
			2423	775	1201	203	235	1	8			

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

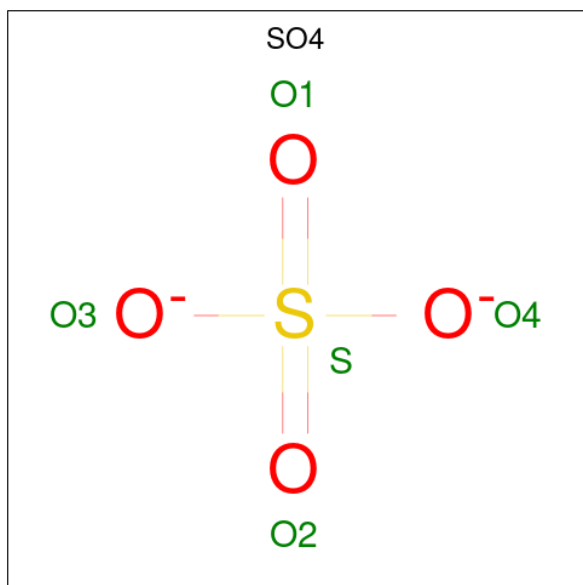
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	3	Total	Mg	0	0
			3	3		

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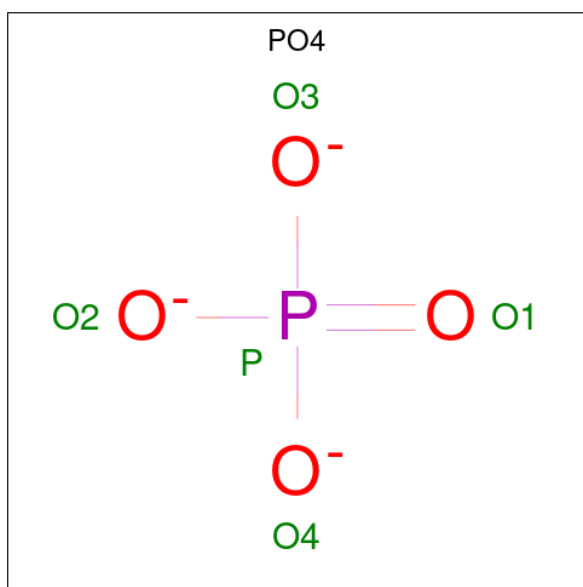
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	5	Total	Mg	0	0
			5	5		
3	D	4	Total	Mg	0	0
			4	4		
3	E	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

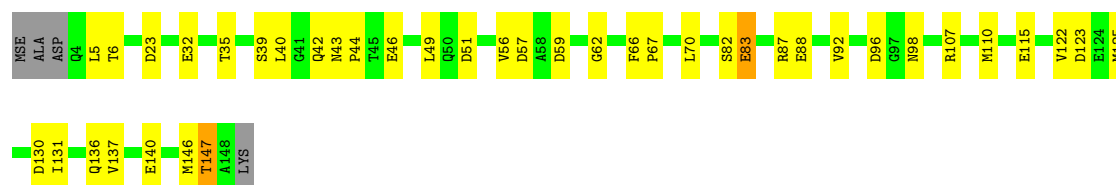
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	F	3	Total	O	0	0
			3	3		
6	B	4	Total	O	0	0
			4	4		
6	G	3	Total	O	0	0
			3	3		
6	C	10	Total	O	0	0
			10	10		
6	H	4	Total	O	0	0
			4	4		
6	D	13	Total	O	0	0
			13	13		
6	I	3	Total	O	0	0
			3	3		
6	E	4	Total	O	0	0
			4	4		
6	J	8	Total	O	0	0
			8	8		

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.

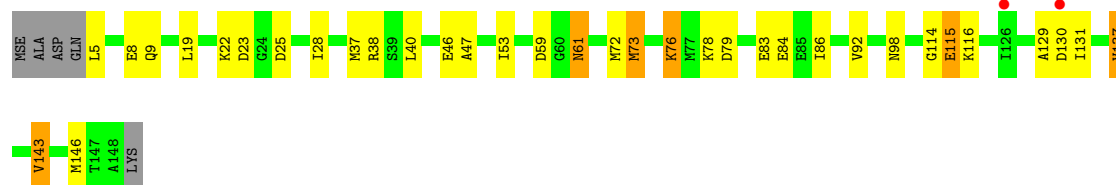
• Molecule 1: Calmodulin

Chain A: 



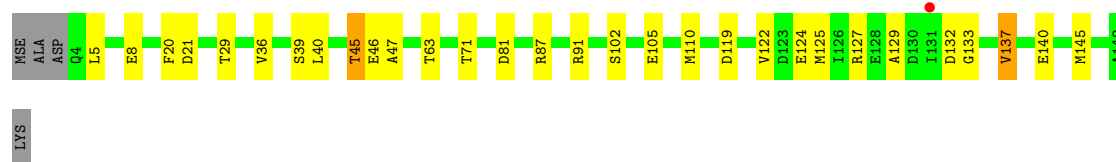
• Molecule 1: Calmodulin

Chain B: 



• Molecule 1: Calmodulin

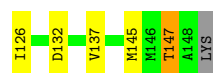
Chain C: 



• Molecule 1: Calmodulin

Chain D: 





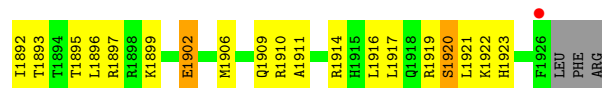
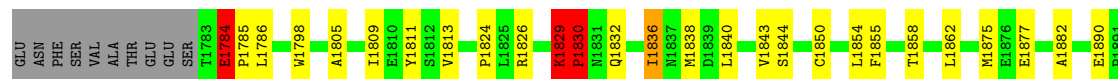
• Molecule 1: Calmodulin



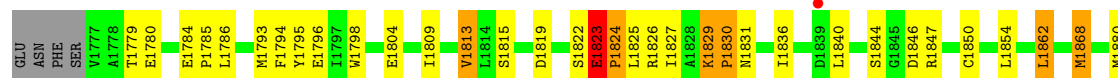
• Molecule 2: Sodium channel protein type 5 subunit alpha



• Molecule 2: Sodium channel protein type 5 subunit alpha



• Molecule 2: Sodium channel protein type 5 subunit alpha



• Molecule 2: Sodium channel protein type 5 subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.13Å 99.01Å 109.28Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	28.70 – 2.80 28.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.2 (28.70-2.80) 90.2 (28.70-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.211 , 0.282 0.218 , 0.285	Depositor DCC
R_{free} test set	2393 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23011	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PO4, 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	0.63	1/1146 (0.1%)	0.89	2/1524 (0.1%)
1	B	0.54	0/1137	0.83	0/1512
1	C	0.61	0/1146	0.99	5/1524 (0.3%)
1	D	0.60	0/1146	0.89	0/1524
1	E	0.50	0/1137	0.84	0/1512
2	F	0.58	0/1204	0.86	0/1608
2	G	0.60	0/1190	0.93	4/1589 (0.3%)
2	H	0.62	0/1241	0.87	0/1659
2	I	0.66	0/1183	0.93	4/1579 (0.3%)
2	J	0.62	0/1239	0.94	4/1656 (0.2%)
All	All	0.60	1/11769 (0.0%)	0.90	19/15687 (0.1%)

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
2	F	0	1
2	G	0	1
2	H	0	2
2	I	0	2
2	J	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	GLN	C-O	-5.28	1.17	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ASP	OD1-CG-OD2	8.56	143.45	122.90
2	G	1890	GLU	CA-C-N	7.54	128.73	119.98
2	G	1890	GLU	C-N-CA	7.54	128.73	119.98
1	A	56	VAL	N-CA-C	-6.13	106.78	111.62
2	J	1823	GLU	CA-C-N	-6.08	112.24	119.84
2	J	1823	GLU	C-N-CA	-6.08	112.24	119.84
2	I	1908	ILE	CB-CA-C	-5.86	104.39	112.24
2	I	1909	GLN	N-CA-C	-5.60	105.25	111.36
1	C	63	THR	N-CA-C	5.56	118.64	110.30
1	A	83	GLU	N-CA-C	-5.49	106.94	113.97
1	C	81	ASP	N-CA-C	5.30	117.37	110.43
2	G	1784	GLU	CA-C-N	-5.27	113.26	119.84
2	G	1784	GLU	C-N-CA	-5.27	113.26	119.84
2	J	1783	THR	N-CA-C	5.07	121.61	110.80
2	I	1890	GLU	CA-C-N	5.07	125.06	119.89
2	I	1890	GLU	C-N-CA	5.07	125.06	119.89
1	C	21	ASP	CB-CG-OD2	-5.05	106.78	118.40
2	J	1866	GLY	N-CA-C	-5.04	106.32	112.77
1	C	63	THR	CB-CA-C	-5.03	103.07	110.06

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	1829	LYS	Peptide
2	G	1829	LYS	Peptide
2	H	1823	GLU	Peptide
2	H	1829	LYS	Peptide
2	I	1823	GLU	Peptide
2	I	1829	LYS	Peptide
2	J	1829	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	1143	1070	1070	17	0
1	B	1134	1063	1063	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1143	1070	1070	8	0
1	D	1143	1070	1070	11	0
1	E	1134	1063	1063	18	0
2	F	1187	1174	1174	20	0
2	G	1173	1158	1158	23	0
2	H	1224	1207	1207	32	0
2	I	1166	1151	1151	27	0
2	J	1222	1201	1201	27	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
3	E	2	0	0	1	0
4	A	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	1	0
4	H	5	0	0	1	0
4	J	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	10	0	0	1	0
6	B	4	0	0	1	0
6	C	10	0	0	0	0
6	D	13	0	0	0	0
6	E	4	0	0	3	0
6	F	3	0	0	0	0
6	G	3	0	0	0	0
6	H	4	0	0	0	0
6	I	3	0	0	0	0
6	J	8	0	0	0	0
All	All	11784	11227	11227	179	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 (179) 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:107:ARG:NH2	1:A:123:ASP:OD1	2.10	0.84
2:F:1927:LEU:O	2:F:1927:LEU:HD23	1.78	0.83
2:H:1925:SER:O	2:H:1926:PHE:HB3	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1854:LEU:O	2:I:1858:THR:OG1	2.03	0.75
2:F:1927:LEU:HD23	2:F:1927:LEU:C	2.15	0.71
2:J:1780:GLU:OE2	2:J:1781:GLU:N	2.25	0.69
2:H:1925:SER:OG	2:H:1926:PHE:N	2.17	0.69
1:D:79:ASP:N	1:D:79:ASP:OD1	2.25	0.69
1:A:43:ASN:ND2	1:A:88:GLU:OE1	2.27	0.68
2:J:1778:ALA:HB1	2:J:1780:GLU:HA	1.78	0.66
1:B:114:GLY:O	1:B:116:LYS:N	2.32	0.63
1:B:76:LYS:O	1:B:76:LYS:NZ	2.29	0.63
1:E:136:GLN:O	3:E:202:MG:MG	1.39	0.62
1:A:82:SER:OG	1:A:83:GLU:N	2.32	0.62
1:E:115:GLU:O	2:J:1909:GLN:NE2	2.34	0.61
2:H:1925:SER:O	2:H:1926:PHE:CB	2.48	0.61
2:F:1792:ASP:OD1	2:G:1922:LYS:NZ	2.31	0.60
1:E:29:THR:OG1	1:E:30:THR:N	2.34	0.60
2:H:1823:GLU:O	2:H:1825:LEU:N	2.34	0.60
1:A:87:ARG:NE	1:A:140:GLU:OE1	2.33	0.58
1:E:130:ASP:HA	6:E:301:HOH:O	2.04	0.58
2:H:1844:SER:O	2:H:1847:ARG:HD3	2.04	0.57
2:I:1798:TRP:CZ2	2:I:1850:CYS:HB3	2.40	0.57
2:J:1778:ALA:HB1	2:J:1779:THR:C	2.29	0.57
1:B:115:GLU:O	2:G:1909:GLN:NE2	2.38	0.57
2:F:1784:GLU:HB3	2:F:1785:PRO:HD2	1.86	0.57
2:H:1926:PHE:CD1	2:H:1927:LEU:N	2.73	0.56
2:I:1823:GLU:O	2:I:1826:ARG:N	2.30	0.56
2:J:1783:THR:O	2:J:1784:GLU:HB2	2.05	0.55
2:F:1795:TYR:CE1	2:F:1799:GLU:HG3	2.41	0.55
2:H:1798:TRP:CZ2	2:H:1850:CYS:HB3	2.42	0.55
1:A:32:GLU:O	1:A:35:THR:N	2.39	0.54
1:A:130:ASP:HA	6:A:305:HOH:O	2.07	0.54
2:H:1926:PHE:CD1	2:H:1926:PHE:C	2.85	0.54
2:J:1783:THR:OG1	2:J:1784:GLU:N	2.39	0.54
1:E:110:MSE:HE3	1:E:117:LEU:HD11	1.89	0.54
2:H:1795:TYR:O	2:H:1798:TRP:N	2.41	0.54
2:G:1784:GLU:CB	2:G:1785:PRO:CD	2.85	0.54
2:H:1846:ASP:OD2	2:H:1898:ARG:NH1	2.30	0.53
1:E:45:THR:O	1:E:47:ALA:N	2.41	0.53
1:B:73:MSE:HE2	1:B:73:MSE:HA	1.90	0.53
1:A:57:ASP:OD2	1:A:62:GLY:N	2.41	0.53
2:H:1925:SER:O	2:H:1926:PHE:CD2	2.62	0.53
2:G:1826:ARG:NH2	4:G:2101:SO4:O4	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1911:ALA:HA	2:G:1914:ARG:HD2	1.91	0.52
2:J:1784:GLU:N	2:J:1785:PRO:HD2	2.25	0.52
2:F:1836:ILE:HA	2:F:1895:THR:HB	1.91	0.52
2:G:1854:LEU:O	2:G:1858:THR:OG1	2.22	0.52
1:D:115:GLU:O	2:I:1913:ARG:NH2	2.43	0.52
2:J:1823:GLU:OE2	2:J:1826:ARG:NH1	2.43	0.52
1:C:124:GLU:OE1	1:C:127:ARG:NH1	2.43	0.51
2:J:1778:ALA:HB1	2:J:1780:GLU:CA	2.40	0.51
1:D:20:PHE:CD2	1:D:36:VAL:HG22	2.45	0.51
2:J:1916:LEU:O	2:J:1920:SER:OG	2.16	0.50
2:J:1836:ILE:HG12	2:J:1896:LEU:HA	1.92	0.50
1:B:130:ASP:HA	6:B:302:HOH:O	2.10	0.50
1:C:87:ARG:NE	1:C:140:GLU:OE2	2.43	0.50
1:D:110:MSE:HE1	2:I:1908:ILE:CG2	2.42	0.50
2:G:1902:GLU:O	2:G:1906:MSE:HG3	2.12	0.50
2:J:1777:VAL:O	2:J:1778:ALA:HB3	2.11	0.50
2:G:1916:LEU:O	2:G:1920:SER:OG	2.30	0.50
1:D:115:GLU:N	2:I:1909:GLN:OE1	2.44	0.50
2:G:1798:TRP:CZ2	2:G:1850:CYS:HB3	2.47	0.49
2:I:1832:GLN:O	2:I:1836:ILE:HG23	2.13	0.49
1:A:107:ARG:HG3	1:A:122:VAL:HG11	1.95	0.49
2:F:1811:TYR:O	2:F:1813:VAL:N	2.42	0.48
2:H:1919:ARG:NH1	4:H:2101:SO4:O1	2.43	0.48
2:H:1784:GLU:N	2:H:1785:PRO:CD	2.76	0.48
2:I:1823:GLU:O	2:I:1825:LEU:N	2.45	0.48
1:A:98:ASN:OD1	1:A:98:ASN:N	2.43	0.48
1:C:129:ALA:HB1	1:C:137:VAL:HG21	1.95	0.48
1:E:87:ARG:NE	1:E:140:GLU:OE2	2.42	0.48
2:J:1798:TRP:CZ2	2:J:1850:CYS:HB3	2.49	0.48
2:J:1892:ILE:HG22	2:J:1893:THR:N	2.29	0.48
2:G:1784:GLU:HB3	2:G:1785:PRO:HD3	1.94	0.48
2:J:1851:MSE:HE1	2:J:1875:MSE:HB3	1.95	0.48
2:F:1829:LYS:HB3	2:F:1830:PRO:HD2	1.95	0.47
2:H:1862:LEU:HD23	2:H:1868:MSE:HE2	1.96	0.47
2:I:1823:GLU:HB3	2:I:1824:PRO:HD3	1.95	0.47
2:G:1798:TRP:CH2	2:G:1809:ILE:HG23	2.49	0.47
2:I:1784:GLU:N	2:I:1785:PRO:CD	2.77	0.47
1:E:6:THR:OG1	1:E:7:GLU:N	2.47	0.47
2:J:1826:ARG:O	2:J:1860:ARG:NH2	2.42	0.47
2:J:1827:ILE:HG12	2:J:1860:ARG:CZ	2.44	0.47
2:G:1836:ILE:HA	2:G:1895:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1826:ARG:CG	2:H:1827:ILE:N	2.77	0.47
2:J:1836:ILE:C	2:J:1836:ILE:HD13	2.40	0.47
2:H:1927:LEU:HD11	2:I:1786:LEU:HD21	1.97	0.47
1:B:46:GLU:HG2	1:B:47:ALA:N	2.30	0.47
2:J:1832:GLN:O	2:J:1836:ILE:HG22	2.14	0.47
1:B:25:ASP:N	1:B:25:ASP:OD1	2.48	0.46
2:H:1898:ARG:HA	2:H:1901:GLU:HG3	1.97	0.46
2:H:1823:GLU:HB3	2:H:1824:PRO:CD	2.45	0.46
2:G:1811:TYR:CE2	2:G:1895:THR:HG22	2.50	0.46
1:D:16:ALA:HA	2:I:1833:ILE:HG21	1.98	0.46
2:I:1827:ILE:HG22	2:I:1831:ASN:ND2	2.31	0.46
1:C:20:PHE:CD2	1:C:36:VAL:HG22	2.51	0.46
1:E:93:PHE:CE2	1:E:109:VAL:HG11	2.51	0.46
1:D:110:MSE:HE1	2:I:1908:ILE:HG21	1.98	0.45
1:A:66:PHE:CE2	1:A:70:LEU:HD11	2.51	0.45
2:H:1815:SER:O	2:H:1831:ASN:ND2	2.50	0.45
2:I:1786:LEU:O	2:I:1786:LEU:HD23	2.16	0.45
1:B:146:MSE:HE3	2:G:1911:ALA:HB1	1.99	0.45
1:B:72:MSE:HE3	1:B:73:MSE:HE3	1.99	0.45
2:I:1823:GLU:O	2:I:1824:PRO:C	2.59	0.45
2:I:1823:GLU:HB3	2:I:1824:PRO:CD	2.47	0.45
1:E:117:LEU:HD12	1:E:122:VAL:HG22	1.98	0.45
2:G:1829:LYS:HB3	2:G:1830:PRO:CD	2.46	0.45
2:H:1862:LEU:HB2	2:H:1868:MSE:HE3	1.99	0.45
2:H:1926:PHE:CG	2:H:1927:LEU:N	2.85	0.44
2:H:1882:ALA:O	2:H:1884:PRO:HD3	2.17	0.44
2:I:1899:LYS:O	2:I:1903:VAL:HG13	2.18	0.44
2:G:1784:GLU:HB3	2:G:1785:PRO:CD	2.48	0.44
2:J:1917:LEU:O	2:J:1920:SER:N	2.49	0.44
2:F:1926:PHE:O	2:F:1926:PHE:CD1	2.70	0.44
1:B:129:ALA:HB1	1:B:137:VAL:HG21	1.98	0.44
1:E:136:GLN:O	6:E:301:HOH:O	2.21	0.44
1:A:146:MSE:O	1:A:147:THR:OG1	2.28	0.44
2:G:1811:TYR:C	2:G:1813:VAL:H	2.26	0.44
2:J:1844:SER:O	2:J:1847:ARG:NH2	2.42	0.44
2:J:1776:SER:C	2:J:1778:ALA:N	2.76	0.44
2:J:1779:THR:O	2:J:1780:GLU:O	2.35	0.44
2:H:1798:TRP:CH2	2:H:1809:ILE:HG23	2.53	0.44
2:I:1871:LEU:HG	2:I:1875:MSE:HE2	2.00	0.44
1:E:137:VAL:HA	6:E:301:HOH:O	2.17	0.44
1:A:115:GLU:O	2:F:1913:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:OD1	1:B:61:ASN:ND2	2.51	0.43
1:A:66:PHE:HB3	1:A:67:PRO:HD3	2.00	0.43
2:F:1836:ILE:HD13	2:F:1837:ASN:N	2.34	0.43
2:J:1778:ALA:HB1	2:J:1780:GLU:N	2.34	0.43
2:J:1795:TYR:CD1	2:J:1795:TYR:C	2.96	0.43
2:H:1822:SER:O	2:H:1826:ARG:HB2	2.17	0.43
2:H:1925:SER:O	2:H:1926:PHE:HD2	2.01	0.43
1:A:110:MSE:CE	2:F:1909:GLN:HG3	2.48	0.43
2:F:1809:ILE:HD11	2:F:1853:ILE:CD1	2.49	0.43
1:E:42:GLN:HB3	1:E:44:PRO:HD3	2.00	0.43
2:G:1855:PHE:HD1	2:G:1875:MSE:HE2	1.84	0.42
1:A:125:MSE:HA	2:F:1912:PHE:CZ	2.54	0.42
2:H:1862:LEU:HD23	2:H:1868:MSE:CE	2.49	0.42
1:E:110:MSE:HE1	2:J:1909:GLN:HA	2.01	0.42
1:C:45:THR:O	1:C:47:ALA:N	2.53	0.42
2:J:1843:VAL:O	2:J:1844:SER:C	2.63	0.42
2:G:1843:VAL:CG1	2:G:1844:SER:N	2.82	0.42
2:H:1794:PHE:CD1	2:H:1854:LEU:HD13	2.54	0.42
2:H:1922:LYS:HE3	2:H:1922:LYS:HA	2.02	0.42
1:D:45:THR:OG1	1:D:48:GLU:OE2	2.37	0.42
1:C:102:SER:O	1:C:105:GLU:N	2.53	0.42
1:D:110:MSE:HG3	1:D:125:MSE:SE	2.69	0.42
1:B:98:ASN:N	1:B:98:ASN:OD1	2.45	0.42
2:F:1798:TRP:CZ2	2:F:1850:CYS:HB3	2.55	0.42
2:F:1902:GLU:O	2:F:1906:MSE:HG3	2.19	0.42
2:G:1882:ALA:HB2	2:I:1923:HIS:CG	2.54	0.42
1:E:17:PHE:HD2	1:E:69:PHE:CD2	2.38	0.41
1:C:45:THR:C	1:C:47:ALA:N	2.77	0.41
1:C:110:MSE:HE2	1:C:125:MSE:HE1	2.03	0.41
2:F:1784:GLU:O	2:F:1786:LEU:N	2.53	0.41
2:H:1819:ASP:OD2	2:H:1826:ARG:NH2	2.51	0.41
1:E:49:LEU:HA	1:E:52:MSE:HE2	2.02	0.41
1:B:86:ILE:HG22	1:B:143:VAL:HG22	2.02	0.41
2:I:1829:LYS:HB3	2:I:1830:PRO:HD2	2.02	0.41
2:H:1793:MSE:HE2	2:H:1822:SER:HB3	2.02	0.41
2:I:1793:MSE:HE3	2:I:1797:ILE:HD11	2.02	0.41
2:I:1808:PHE:HB3	2:I:1847:ARG:HB3	2.02	0.41
1:E:56:VAL:HG13	1:E:64:ILE:HD11	2.02	0.41
1:A:125:MSE:HE3	2:F:1912:PHE:CG	2.56	0.41
2:G:1843:VAL:HG12	2:G:1844:SER:N	2.36	0.41
2:I:1786:LEU:HD11	2:I:1858:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1802:ASP:OD2	2:I:1807:GLN:N	2.53	0.41
1:E:90:PHE:HB3	1:E:139:TYR:CG	2.56	0.41
1:A:110:MSE:HE1	2:F:1908:ILE:HG22	2.03	0.41
2:H:1889:TYR:CD2	2:H:1889:TYR:C	2.99	0.41
2:F:1852:ASP:OD2	2:F:1889:TYR:OH	2.33	0.40
1:B:129:ALA:HB1	1:B:137:VAL:CG2	2.51	0.40
2:H:1793:MSE:HE2	2:H:1822:SER:N	2.36	0.40
1:D:6:THR:O	1:D:7:GLU:HB2	2.22	0.40
2:G:1805:ALA:HA	2:I:1917:LEU:HD12	2.04	0.40
2:G:1836:ILE:HG13	2:G:1899:LYS:HB2	2.03	0.40
1:D:66:PHE:CE2	1:D:70:LEU:HD11	2.56	0.40
2:I:1826:ARG:HG2	2:I:1827:ILE:N	2.36	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	143/149 (96%)	127 (89%)	14 (10%)	2 (1%)	9	30
1	B	142/149 (95%)	122 (86%)	18 (13%)	2 (1%)	9	30
1	C	143/149 (96%)	126 (88%)	15 (10%)	2 (1%)	9	30
1	D	143/149 (96%)	124 (87%)	13 (9%)	6 (4%)	2	7
1	E	142/149 (95%)	120 (84%)	16 (11%)	6 (4%)	2	7
2	F	144/157 (92%)	118 (82%)	19 (13%)	7 (5%)	1	6
2	G	142/157 (90%)	118 (83%)	19 (13%)	5 (4%)	3	10
2	H	149/157 (95%)	125 (84%)	16 (11%)	8 (5%)	1	4
2	I	141/157 (90%)	119 (84%)	17 (12%)	5 (4%)	3	10
2	J	149/157 (95%)	126 (85%)	16 (11%)	7 (5%)	2	6
All	All	1438/1530 (94%)	1225 (85%)	163 (11%)	50 (4%)	3	10

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1813	VAL
2	F	1830	PRO
1	B	115	GLU
2	G	1784	GLU
2	G	1829	LYS
2	G	1830	PRO
2	H	1823	GLU
2	H	1824	PRO
2	H	1830	PRO
1	D	5	LEU
1	D	7	GLU
2	I	1822	SER
2	I	1823	GLU
2	I	1830	PRO
1	E	46	GLU
2	J	1780	GLU
2	J	1783	THR
2	J	1784	GLU
2	J	1830	PRO
2	F	1785	PRO
2	F	1787	SER
2	H	1813	VAL
2	H	1926	PHE
1	E	61	ASN
1	A	147	THR
2	F	1812	SER
1	B	22	LYS
2	H	1779	THR
1	D	81	ASP
2	I	1785	PRO
2	I	1889	TYR
1	E	21	ASP
1	E	29	THR
1	E	103	ALA
2	J	1829	LYS
1	A	44	PRO
2	H	1796	GLU
1	D	132	ASP
1	D	147	THR
2	J	1888	SER
2	F	1854	LEU
2	G	1910	ARG

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Mol	Chain	Res	Type
1	C	46	GLU
1	E	82	SER
2	J	1781	GLU
1	C	133	GLY
1	D	6	THR
2	F	1824	PRO
2	H	1829	LYS
2	G	1824	PRO

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	124/117 (106%)	110 (89%)	14 (11%)	5	19
1	B	123/117 (105%)	102 (83%)	21 (17%)	2	7
1	C	124/117 (106%)	111 (90%)	13 (10%)	6	22
1	D	124/117 (106%)	97 (78%)	27 (22%)	1	3
1	E	123/117 (105%)	108 (88%)	15 (12%)	5	16
2	F	132/134 (98%)	111 (84%)	21 (16%)	2	9
2	G	130/134 (97%)	111 (85%)	19 (15%)	3	11
2	H	136/134 (102%)	116 (85%)	20 (15%)	3	10
2	I	129/134 (96%)	107 (83%)	22 (17%)	2	7
2	J	136/134 (102%)	113 (83%)	23 (17%)	2	7
All	All	1281/1255 (102%)	1086 (85%)	195 (15%)	3	10

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	THR
1	A	23	ASP
1	A	39	SER
1	A	40	LEU

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Mol	Chain	Res	Type
1	A	42	GLN
1	A	46	GLU
1	A	49	LEU
1	A	51	ASP
1	A	59	ASP
1	A	92	VAL
1	A	96	ASP
1	A	131	ILE
1	A	137	VAL
2	F	1788	GLU
2	F	1790	ASP
2	F	1799	GLU
2	F	1800	LYS
2	F	1813	VAL
2	F	1816	ASP
2	F	1829	LYS
2	F	1832	GLN
2	F	1836	ILE
2	F	1837	ASN
2	F	1840	LEU
2	F	1854	LEU
2	F	1862	LEU
2	F	1890	GLU
2	F	1893	THR
2	F	1897	ARG
2	F	1902	GLU
2	F	1921	LEU
2	F	1922	LYS
2	F	1925	SER
2	F	1927	LEU
1	B	5	LEU
1	B	8	GLU
1	B	9	GLN
1	B	19	LEU
1	B	23	ASP
1	B	28	ILE
1	B	37	MSE
1	B	38	ARG
1	B	40	LEU
1	B	53	ILE
1	B	61	ASN
1	B	73	MSE

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Mol	Chain	Res	Type
1	B	76	LYS
1	B	78	LYS
1	B	79	ASP
1	B	83	GLU
1	B	84	GLU
1	B	92	VAL
1	B	131	ILE
1	B	137	VAL
1	B	143	VAL
2	G	1786	LEU
2	G	1829	LYS
2	G	1830	PRO
2	G	1832	GLN
2	G	1836	ILE
2	G	1838	MSE
2	G	1840	LEU
2	G	1862	LEU
2	G	1877	GLU
2	G	1892	ILE
2	G	1893	THR
2	G	1896	LEU
2	G	1897	ARG
2	G	1902	GLU
2	G	1917	LEU
2	G	1919	ARG
2	G	1920	SER
2	G	1921	LEU
2	G	1923	HIS
1	C	5	LEU
1	C	8	GLU
1	C	29	THR
1	C	39	SER
1	C	40	LEU
1	C	45	THR
1	C	71	THR
1	C	91	ARG
1	C	119	ASP
1	C	122	VAL
1	C	132	ASP
1	C	137	VAL
1	C	145	MSE
2	H	1780	GLU

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Mol	Chain	Res	Type
2	H	1786	LEU
2	H	1804	GLU
2	H	1813	VAL
2	H	1830	PRO
2	H	1836	ILE
2	H	1840	LEU
2	H	1862	LEU
2	H	1868	MSE
2	H	1880	MSE
2	H	1886	LYS
2	H	1887	ILE
2	H	1888	SER
2	H	1893	THR
2	H	1901	GLU
2	H	1902	GLU
2	H	1903	VAL
2	H	1917	LEU
2	H	1922	LYS
2	H	1927	LEU
1	D	6	THR
1	D	8	GLU
1	D	9	GLN
1	D	14	LYS
1	D	23	ASP
1	D	37	MSE
1	D	40	LEU
1	D	45	THR
1	D	49	LEU
1	D	54	ASN
1	D	61	ASN
1	D	72	MSE
1	D	76	LYS
1	D	79	ASP
1	D	80	THR
1	D	81	ASP
1	D	82	SER
1	D	83	GLU
1	D	88	GLU
1	D	90	PHE
1	D	96	ASP
1	D	109	VAL
1	D	122	VAL

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Mol	Chain	Res	Type
1	D	126	ILE
1	D	137	VAL
1	D	145	MSE
1	D	147	THR
2	I	1786	LEU
2	I	1787	SER
2	I	1789	ASP
2	I	1822	SER
2	I	1823	GLU
2	I	1829	LYS
2	I	1831	ASN
2	I	1833	ILE
2	I	1836	ILE
2	I	1840	LEU
2	I	1862	LEU
2	I	1878	LYS
2	I	1880	MSE
2	I	1887	ILE
2	I	1889	TYR
2	I	1893	THR
2	I	1896	LEU
2	I	1899	LYS
2	I	1903	VAL
2	I	1909	GLN
2	I	1917	LEU
2	I	1922	LYS
1	E	5	LEU
1	E	7	GLU
1	E	22	LYS
1	E	30	THR
1	E	35	THR
1	E	40	LEU
1	E	46	GLU
1	E	64	ILE
1	E	72	MSE
1	E	88	GLU
1	E	120	GLU
1	E	125	MSE
1	E	126	ILE
1	E	137	VAL
1	E	145	MSE
2	J	1777	VAL

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Mol	Chain	Res	Type
2	J	1780	GLU
2	J	1781	GLU
2	J	1782	SER
2	J	1783	THR
2	J	1786	LEU
2	J	1829	LYS
2	J	1836	ILE
2	J	1840	LEU
2	J	1842	MSE
2	J	1844	SER
2	J	1862	LEU
2	J	1865	SER
2	J	1871	LEU
2	J	1886	LYS
2	J	1890	GLU
2	J	1892	ILE
2	J	1893	THR
2	J	1896	LEU
2	J	1910	ARG
2	J	1918	GLN
2	J	1922	LYS
2	J	1923	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	GLN
2	G	1923	HIS
2	H	1923	HIS
2	I	1909	GLN
1	E	9	GLN
1	E	112	ASN
2	J	1837	ASN
2	J	1883	ASN

5.3.3 RNA ⓘ

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 25 ligands modelled in this entry, 18 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	B	204	-	4,4,4	0.82	0	6,6,6	0.50	0
4	SO4	A	205	-	4,4,4	0.27	0	6,6,6	0.19	0
4	SO4	J	2101	-	4,4,4	0.27	0	6,6,6	0.11	0
4	SO4	F	2101	-	4,4,4	0.29	0	6,6,6	0.13	0
5	PO4	C	205	-	4,4,4	0.75	0	6,6,6	0.63	0
4	SO4	H	2101	-	4,4,4	0.29	0	6,6,6	0.13	0
4	SO4	G	2101	-	4,4,4	0.28	0	6,6,6	0.20	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2101	SO4	1	0
4	G	2101	SO4	1	0

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	136/149 (91%)	-0.31	0 100 100	67, 92, 126, 150	0
1	B	135/149 (90%)	-0.30	2 (1%) 72 63	71, 108, 151, 191	0
1	C	136/149 (91%)	-0.38	1 (0%) 84 77	68, 90, 113, 126	0
1	D	136/149 (91%)	-0.41	0 100 100	68, 88, 112, 138	0
1	E	135/149 (90%)	-0.03	1 (0%) 84 77	75, 117, 151, 168	0
2	F	138/157 (87%)	-0.36	1 (0%) 84 77	66, 89, 127, 155	0
2	G	136/157 (86%)	-0.36	1 (0%) 84 77	67, 86, 112, 133	0
2	H	143/157 (91%)	-0.29	1 (0%) 84 77	67, 84, 115, 132	0
2	I	135/157 (85%)	-0.44	0 100 100	63, 76, 105, 117	0
2	J	143/157 (91%)	-0.43	2 (1%) 73 64	64, 82, 100, 115	0
All	All	1373/1530 (89%)	-0.33	9 (0%) 84 77	63, 88, 132, 191	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	ILE	2.7
2	G	1926	PHE	2.6
2	H	1839	ASP	2.6
2	J	1926	PHE	2.6
1	C	131	ILE	2.5
2	F	1856	ALA	2.4
1	E	99	GLY	2.4
1	B	130	ASP	2.3
2	J	1828	ALA	2.2

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($\text{\AA}^2$)	Q<0.9
5	PO4	B	204	5/5	0.65	0.14	103,108,111,135	0
4	SO4	G	2101	5/5	0.73	0.14	98,105,111,140	0
4	SO4	A	205	5/5	0.74	0.11	79,103,129,142	0
3	MG	E	202	1/1	0.82	0.17	83,83,83,83	0
3	MG	B	202	1/1	0.82	0.13	66,66,66,66	0
4	SO4	J	2101	5/5	0.85	0.09	97,103,108,125	0
4	SO4	H	2101	5/5	0.85	0.10	83,91,96,133	0
5	PO4	C	205	5/5	0.85	0.11	67,92,112,124	0
3	MG	D	203	1/1	0.87	0.06	96,96,96,96	0
3	MG	B	203	1/1	0.88	0.07	95,95,95,95	0
3	MG	C	206	1/1	0.89	0.20	66,66,66,66	0
3	MG	C	201	1/1	0.90	0.07	94,94,94,94	0
3	MG	B	201	1/1	0.91	0.13	113,113,113,113	0
3	MG	D	204	1/1	0.93	0.06	91,91,91,91	0
3	MG	C	203	1/1	0.93	0.06	80,80,80,80	0
4	SO4	F	2101	5/5	0.94	0.05	66,82,101,114	0
3	MG	A	203	1/1	0.94	0.07	66,66,66,66	0
3	MG	E	201	1/1	0.94	0.08	113,113,113,113	0
3	MG	D	201	1/1	0.96	0.06	89,89,89,89	0
3	MG	A	202	1/1	0.96	0.10	115,115,115,115	0
3	MG	C	204	1/1	0.97	0.07	102,102,102,102	0
3	MG	A	201	1/1	0.97	0.03	89,89,89,89	0
3	MG	C	202	1/1	0.98	0.05	68,68,68,68	0
3	MG	D	202	1/1	0.99	0.03	71,71,71,71	0
3	MG	A	204	1/1	0.99	0.03	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.