



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:14 AM BST

PDB ID : 4OVN  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

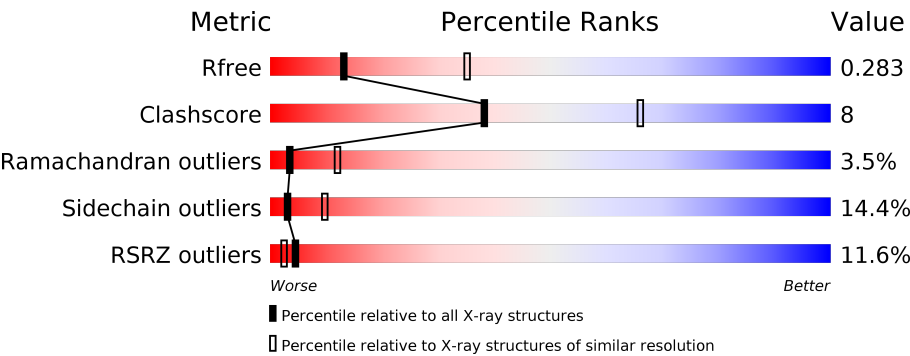
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div>12%</div><div><div></div><div>73%</div><div>23%</div><div>..</div></div></div>
1	B	149	<div><div>18%</div><div><div></div><div>73%</div><div>21%</div><div>..</div></div></div>
1	C	149	<div><div>7%</div><div><div></div><div>77%</div><div>19%</div><div>..</div></div></div>
1	D	149	<div><div>2%</div><div><div></div><div>72%</div><div>21%</div><div>...</div></div></div>
1	E	149	<div><div>20%</div><div><div></div><div>69%</div><div>25%</div><div>..</div></div></div>
2	F	157	<div><div>18%</div><div><div></div><div>68%</div><div>20%</div><div>5% 7%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	157	<div><div></div><div>7%</div><div>64%</div><div>22%</div><div>• • 8%</div></div>
2	H	157	<div><div></div><div>8%</div><div>63%</div><div>26%</div><div>6% • •</div></div>
2	I	157	<div><div></div><div>5%</div><div>61%</div><div>22%</div><div>7% • 9%</div></div>
2	J	157	<div><div></div><div>6%</div><div>69%</div><div>20%</div><div>• • •</div></div>

## 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 (three-letter code: MG) (formula: Mg).

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



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		

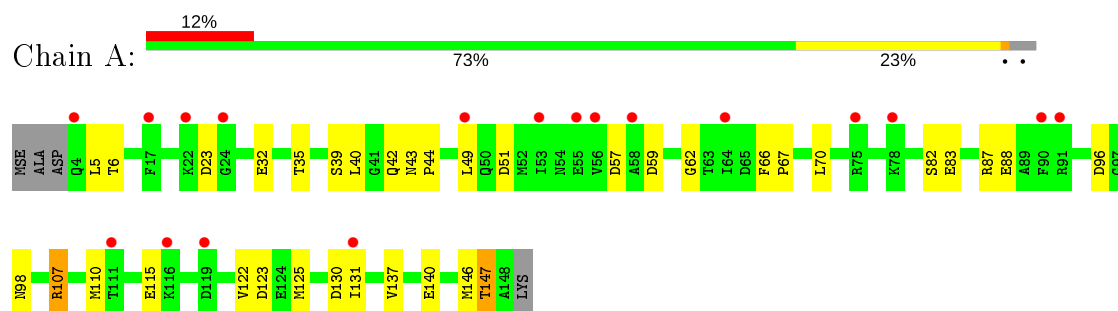
- Molecule 6 is water.

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		

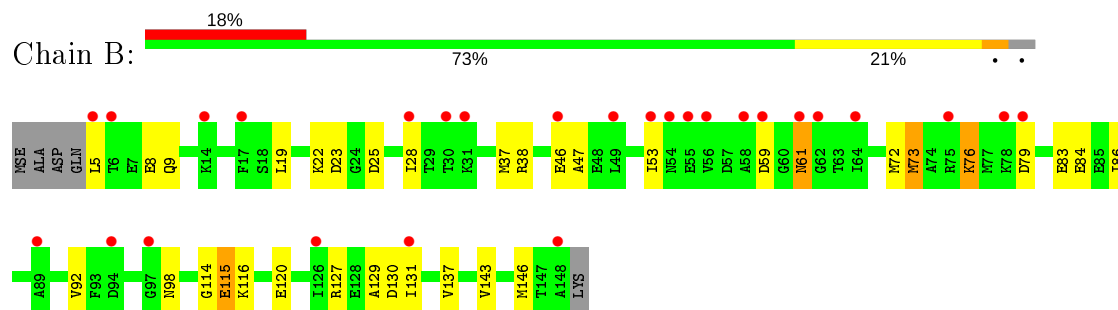
### 3 Residue-property plots [i](#)

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.

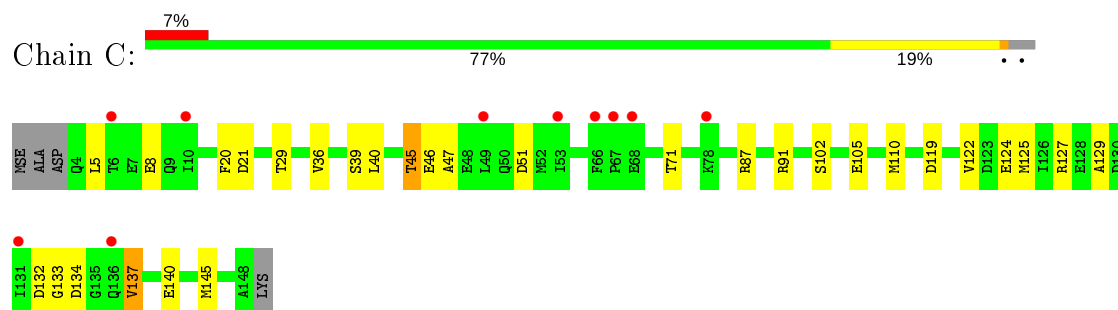
#### • Molecule 1: Calmodulin



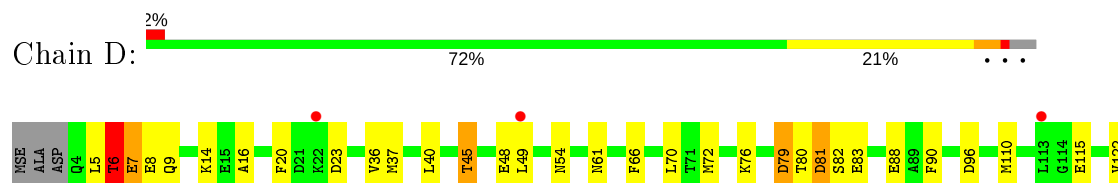
#### • Molecule 1: Calmodulin



#### • Molecule 1: Calmodulin

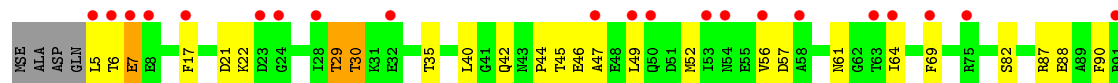


#### • Molecule 1: Calmodulin

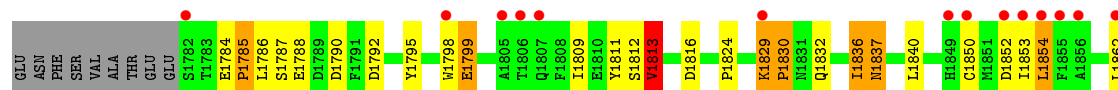




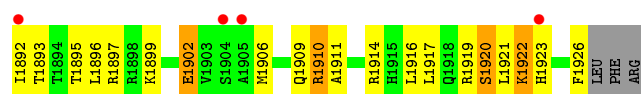
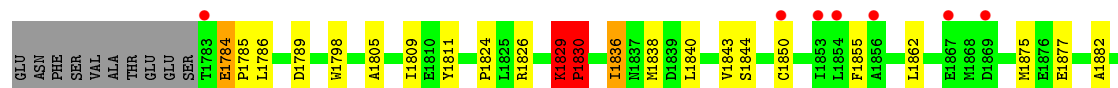
• Molecule 1: Calmodulin



• Molecule 2: Sodium channel protein type 5 subunit alpha



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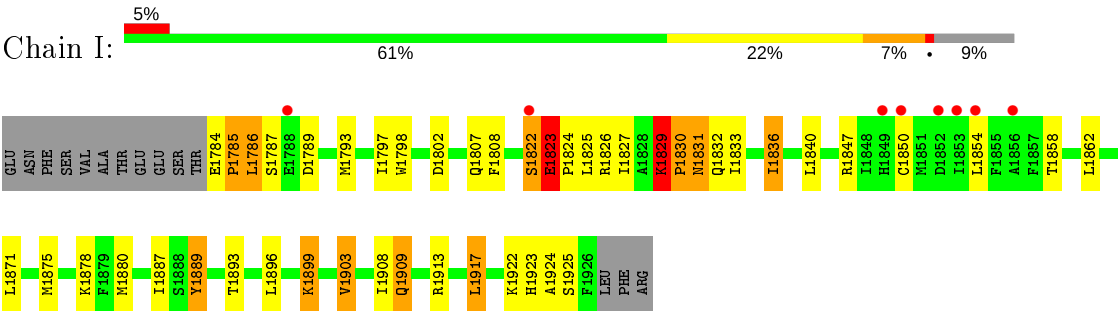


• Molecule 2: Sodium channel protein type 5 subunit alpha

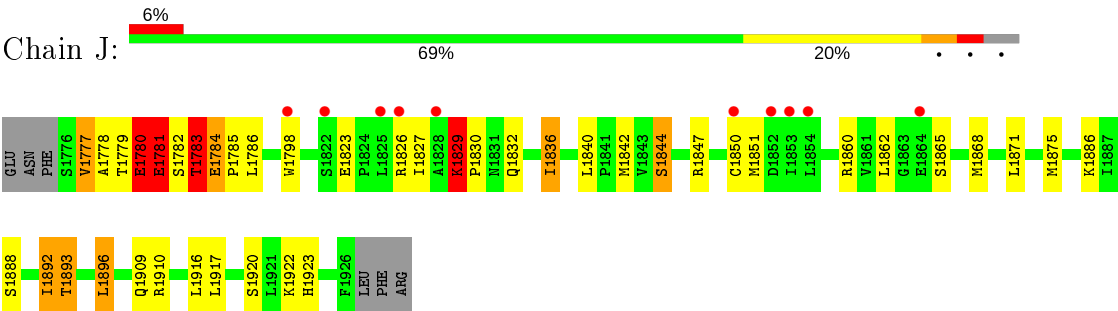


• Molecule 2: Sodium channel protein type 5 subunit alpha





• 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, $\alpha$ , $\beta$ , $\gamma$	106.13 Å 99.01 Å 109.28 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.211 , 0.282 0.214 , 0.283	Depositor DCC
$R_{free}$ test set	2393 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, PO4, SO4

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	0.50	0/1146	0.66	0/1524
1	B	0.44	0/1137	0.58	0/1512
1	C	0.48	0/1146	0.82	3/1524 (0.2%)
1	D	0.49	0/1146	0.68	0/1524
1	E	0.42	0/1137	0.58	0/1512
2	F	0.44	0/1204	0.60	0/1608
2	G	0.45	0/1190	0.61	0/1589
2	H	0.49	0/1241	0.65	2/1659 (0.1%)
2	I	0.50	0/1183	0.67	1/1579 (0.1%)
2	J	0.51	0/1239	0.68	0/1656
All	All	0.47	0/11769	0.66	6/15687 (0.0%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ASP	CB-CG-OD2	-12.80	106.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ASP	OD1-CG-OD2	10.61	143.45	123.30
1	C	21	ASP	CB-CG-OD1	-9.63	109.64	118.30
2	H	1829	LYS	C-N-CD	-6.77	105.70	120.60
2	I	1829	LYS	C-N-CD	-6.19	106.97	120.60
2	H	1786	LEU	CA-CB-CG	5.38	127.66	115.30

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
1	C	1143	1070	1070	8	0
1	D	1143	1070	1070	12	0
1	E	1134	1063	1063	18	0
2	F	1187	1174	1174	20	0
2	G	1173	1158	1158	21	0
2	H	1224	1207	1207	31	0
2	I	1166	1151	1151	28	0
2	J	1222	1201	1201	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	175	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 (175) 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:HD23	2:F:1927:LEU:O	1.78	0.83
2:H:1925:SER:OG	2:H:1926:PHE:N	2.17	0.78
2:H:1925:SER:O	2:H:1926:PHE:HB3	1.84	0.76
2:I:1854:LEU:O	2:I:1858:THR:OG1	2.03	0.75
2:J:1780:GLU:OE2	2:J:1781:GLU:N	2.25	0.69
1:D:79:ASP:OD1	1:D:79:ASP:N	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
2:F:1927:LEU:HD23	2:F:1927:LEU:C	2.15	0.65
1:B:114:GLY:O	1:B:116:LYS:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:130:ASP:HA	6:A:305:HOH:O	2.07	0.54
1:A:32:GLU:O	1:A:35:THR:N	2.39	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:J:1778:ALA:HB1	2:J:1779:THR:C	2.29	0.52
1:B:76:LYS:NZ	1:B:76:LYS:O	2.29	0.52
2:G:1826:ARG:NH2	4:G:2101:SO4:O4	2.42	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:1926:PHE:C	2:H:1926:PHE:CD1	2.85	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
2:H:1826:ARG:CG	2:H:1827:ILE:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1815:SER:O	2:H:1831:ASN:ND2	2.50	0.45
2:I:1786:LEU:HD23	2:I:1786:LEU:O	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
1:E:117:LEU:HD12	1:E:122:VAL:HG22	1.98	0.45
2:I:1823:GLU:HB3	2:I:1824:PRO:CD	2.47	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
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
2:F:1926:PHE:CD1	2:F:1926:PHE:O	2.70	0.44
1:A:146:MSE:O	1:A:147:THR:OG1	2.28	0.44
2:J:1844:SER:O	2:J:1847:ARG:NH2	2.42	0.44
2:J:1779:THR:O	2:J:1780:GLU:O	2.35	0.44
1:E:137:VAL:HA	6:E:301:HOH:O	2.17	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:A:115:GLU:O	2:F:1913:ARG:NH2	2.50	0.43
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: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
1:E:42:GLN:HB3	1:E:44:PRO:HD3	2.00	0.43
2:F:1809:ILE:HD11	2:F:1853:ILE:CD1	2.49	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
1:D:45:THR:OG1	1:D:48:GLU:OE2	2.37	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:HA	2:H:1922:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1836:ILE:HD13	2:J:1836:ILE:C	2.40	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
2:I:1924:ALA:O	2:I:1925:SER:OG	2.34	0.42
1:B:98:ASN:N	1:B:98:ASN:OD1	2.45	0.42
1:C:134:ASP:N	1:C:134:ASP:OD1	2.53	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:110:MSE:HE2	1:C:125:MSE:HE1	2.03	0.41
1:D:134:ASP:OD1	1:D:134:ASP:N	2.54	0.41
2:F:1784:GLU:O	2:F:1786:LEU:N	2.53	0.41
1:E:49:LEU:HA	1:E:52:MSE:HE2	2.02	0.41
2:H:1819:ASP:OD2	2:H:1826:ARG:NH2	2.51	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
1:E:56:VAL:HG13	1:E:64:ILE:HD11	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:A:125:MSE:HE3	2:F:1912:PHE:CG	2.56	0.41
1:E:90:PHE:HB3	1:E:139:TYR: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
2:I:1802:ASP:OD2	2:I:1807:GLN:N	2.53	0.41
1:A:110:MSE:HE1	2:F:1908:ILE:HG22	2.03	0.41
1:B:129:ALA:HB1	1:B:137:VAL:CG2	2.51	0.40
2:F:1852:ASP:OD2	2:F:1889:TYR:OH	2.33	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
1:D:66:PHE:CE2	1:D:70:LEU:HD11	2.56	0.40
2:G:1836:ILE:HG13	2:G:1899:LYS:HB2	2.03	0.40
2:I:1823:GLU:O	2:I:1824:PRO:C	2.59	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

### 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	143/149 (96%)	127 (89%)	14 (10%)	2 (1%)	11	34
1	B	142/149 (95%)	122 (86%)	18 (13%)	2 (1%)	11	34
1	C	143/149 (96%)	126 (88%)	15 (10%)	2 (1%)	11	34
1	D	143/149 (96%)	124 (87%)	13 (9%)	6 (4%)	3	9
1	E	142/149 (95%)	120 (84%)	16 (11%)	6 (4%)	3	9
2	F	144/157 (92%)	118 (82%)	19 (13%)	7 (5%)	2	7
2	G	142/157 (90%)	118 (83%)	19 (13%)	5 (4%)	3	12
2	H	149/157 (95%)	125 (84%)	16 (11%)	8 (5%)	2	5
2	I	141/157 (90%)	119 (84%)	17 (12%)	5 (4%)	3	12
2	J	149/157 (95%)	126 (85%)	16 (11%)	7 (5%)	2	7
All	All	1438/1530 (94%)	1225 (85%)	163 (11%)	50 (4%)	3	12

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

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Mol	Chain	Res	Type
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
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%)	111 (90%)	13 (10%)	7	20
1	B	123/117 (105%)	104 (85%)	19 (15%)	2	8
1	C	124/117 (106%)	110 (89%)	14 (11%)	6	18
1	D	124/117 (106%)	99 (80%)	25 (20%)	1	4
1	E	123/117 (105%)	111 (90%)	12 (10%)	8	24
2	F	132/134 (98%)	117 (89%)	15 (11%)	5	18
2	G	130/134 (97%)	108 (83%)	22 (17%)	2	6
2	H	136/134 (102%)	114 (84%)	22 (16%)	2	7
2	I	129/134 (96%)	108 (84%)	21 (16%)	2	7
2	J	136/134 (102%)	114 (84%)	22 (16%)	2	7
All	All	1281/1255 (102%)	1096 (86%)	185 (14%)	3	10

All (185) 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
1	A	42	GLN
1	A	49	LEU
1	A	51	ASP
1	A	59	ASP
1	A	96	ASP
1	A	107	ARG
1	A	131	ILE
1	A	137	VAL
2	F	1788	GLU
2	F	1790	ASP
2	F	1799	GLU
2	F	1813	VAL
2	F	1816	ASP
2	F	1832	GLN
2	F	1836	ILE
2	F	1837	ASN
2	F	1840	LEU

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Mol	Chain	Res	Type
2	F	1854	LEU
2	F	1862	LEU
2	F	1893	THR
2	F	1897	ARG
2	F	1921	LEU
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	53	ILE
1	B	61	ASN
1	B	73	MSE
1	B	76	LYS
1	B	79	ASP
1	B	83	GLU
1	B	84	GLU
1	B	92	VAL
1	B	120	GLU
1	B	127	ARG
1	B	131	ILE
2	G	1786	LEU
2	G	1789	ASP
2	G	1829	LYS
2	G	1830	PRO
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	1910	ARG
2	G	1917	LEU
2	G	1919	ARG

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Mol	Chain	Res	Type
2	G	1920	SER
2	G	1921	LEU
2	G	1922	LYS
2	G	1923	HIS
2	G	1926	PHE
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	51	ASP
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
2	H	1786	LEU
2	H	1800	LYS
2	H	1804	GLU
2	H	1813	VAL
2	H	1816	ASP
2	H	1829	LYS
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	1887	ILE
2	H	1888	SER
2	H	1889	TYR
2	H	1893	THR
2	H	1902	GLU
2	H	1903	VAL
2	H	1917	LEU
2	H	1922	LYS
2	H	1927	LEU
1	D	6	THR

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Mol	Chain	Res	Type
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	122	VAL
1	D	126	ILE
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	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

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Mol	Chain	Res	Type
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	57	ASP
1	E	88	GLU
1	E	120	GLU
1	E	125	MSE
1	E	137	VAL
1	E	145	MSE
2	J	1777	VAL
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	1868	MSE
2	J	1871	LEU
2	J	1886	LYS
2	J	1892	ILE
2	J	1893	THR
2	J	1896	LEU
2	J	1910	ARG
2	J	1922	LYS
2	J	1923	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
4	SO4	A	205	-	4,4,4	0.16	0	6,6,6	0.21	0
4	SO4	F	2101	-	4,4,4	0.18	0	6,6,6	0.11	0
4	SO4	H	2101	-	4,4,4	0.18	0	6,6,6	0.11	0
4	SO4	G	2101	-	4,4,4	0.17	0	6,6,6	0.17	0
5	PO4	C	205	-	4,4,4	0.70	0	6,6,6	0.60	0
5	PO4	B	204	-	4,4,4	0.77	0	6,6,6	0.47	0
4	SO4	J	2101	-	4,4,4	0.16	0	6,6,6	0.09	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	136/149 (91%)	0.66	18 (13%) <b>3</b> <b>2</b>	55, 89, 132, 165	0
1	B	135/149 (90%)	1.15	27 (20%) <b>1</b> <b>0</b>	65, 109, 181, 219	0
1	C	136/149 (91%)	0.39	10 (7%) <b>14</b> <b>8</b>	59, 87, 118, 138	0
1	D	136/149 (91%)	0.27	3 (2%) 62 52	57, 84, 119, 148	0
1	E	135/149 (90%)	1.10	30 (22%) <b>0</b> <b>0</b>	67, 122, 165, 200	0
2	F	138/157 (87%)	0.96	29 (21%) <b>1</b> <b>0</b>	55, 84, 138, 185	0
2	G	136/157 (86%)	0.67	11 (8%) <b>12</b> <b>6</b>	56, 80, 119, 153	0
2	H	143/157 (91%)	0.59	13 (9%) <b>9</b> <b>5</b>	54, 77, 119, 149	0
2	I	135/157 (85%)	0.42	8 (5%) <b>22</b> <b>14</b>	52, 67, 102, 115	0
2	J	143/157 (91%)	0.54	10 (6%) <b>16</b> <b>9</b>	53, 74, 100, 122	0
All	All	1373/1530 (89%)	0.67	159 (11%) <b>4</b> <b>2</b>	52, 84, 142, 219	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	53	ILE	10.1
1	E	54	ASN	9.1
1	B	62	GLY	8.0
1	B	54	ASN	7.9
1	B	56	VAL	6.7
1	B	30	THR	6.4
1	B	55	GLU	6.2
2	F	1867	GLU	5.8
2	H	1779	THR	5.8
1	E	100	TYR	5.7
1	E	63	THR	5.2
1	E	6	THR	5.2
2	F	1865	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	131	ILE	5.0
1	E	58	ALA	4.9
2	F	1850	CYS	4.9
1	B	5	LEU	4.8
1	B	17	PHE	4.8
1	E	99	GLY	4.6
1	B	58	ALA	4.4
1	E	5	LEU	4.4
2	H	1777	VAL	4.4
2	G	1850	CYS	4.4
1	B	79	ASP	4.4
1	B	78	LYS	4.4
2	I	1850	CYS	4.3
1	B	148	ALA	4.3
2	F	1864	GLU	4.3
2	G	1783	THR	4.2
1	B	131	ILE	4.1
2	J	1850	CYS	4.1
1	A	64	ILE	4.1
1	B	59	ASP	4.0
1	B	75	ARG	4.0
1	A	22	LYS	3.9
2	H	1852	ASP	3.9
2	H	1790	ASP	3.9
2	F	1849	HIS	3.7
2	F	1874	GLN	3.7
2	F	1878	LYS	3.6
1	A	111	THR	3.6
1	E	17	PHE	3.5
1	B	64	ILE	3.5
1	E	56	VAL	3.5
1	E	50	GLN	3.4
1	E	69	PHE	3.4
1	E	7	GLU	3.3
1	E	139	TYR	3.3
1	A	75	ARG	3.2
1	A	4	GLN	3.2
2	H	1780	GLU	3.2
1	A	17	PHE	3.2
1	A	56	VAL	3.2
2	H	1782	SER	3.2
2	H	1850	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	1873	ILE	3.1
1	B	6	THR	3.1
2	I	1852	ASP	3.1
1	B	97	GLY	3.0
2	F	1869	ASP	3.0
2	G	1853	ILE	3.0
2	F	1807	GLN	2.9
2	J	1825	LEU	2.9
2	G	1867	GLU	2.9
2	F	1806	THR	2.9
2	H	1927	LEU	2.9
1	E	24	GLY	2.9
1	A	58	ALA	2.9
1	B	49	LEU	2.9
2	J	1822	SER	2.8
1	E	28	ILE	2.8
1	C	78	LYS	2.8
2	H	1789	ASP	2.8
1	C	136	GLN	2.8
2	F	1782	SER	2.8
1	A	78	LYS	2.8
2	F	1829	LYS	2.8
2	F	1863	GLY	2.8
1	C	53	ILE	2.8
2	F	1866	GLY	2.7
2	F	1872	LYS	2.7
1	E	32	GLU	2.7
2	F	1798	TRP	2.7
1	D	49	LEU	2.6
1	B	46	GLU	2.6
1	E	144	GLN	2.6
1	B	31	LYS	2.6
1	B	61	ASN	2.6
1	B	126	ILE	2.6
2	F	1852	ASP	2.6
2	F	1856	ALA	2.6
2	F	1853	ILE	2.6
2	J	1853	ILE	2.6
2	I	1856	ALA	2.6
1	D	22	LYS	2.6
1	A	49	LEU	2.6
1	E	49	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	1854	LEU	2.6
1	C	68	GLU	2.5
2	H	1788	GLU	2.5
1	E	75	ARG	2.5
1	E	148	ALA	2.5
2	F	1886	LYS	2.5
2	G	1923	HIS	2.5
1	E	91	ARG	2.4
1	A	53	ILE	2.4
2	I	1822	SER	2.4
1	E	47	ALA	2.4
1	B	53	ILE	2.4
2	F	1862	LEU	2.4
2	H	1910	ARG	2.4
2	J	1854	LEU	2.4
1	A	119	ASP	2.4
1	A	116	LYS	2.4
2	F	1882	ALA	2.4
2	I	1853	ILE	2.4
2	I	1849	HIS	2.3
1	C	6	THR	2.3
1	B	14	LYS	2.3
2	J	1852	ASP	2.3
2	G	1856	ALA	2.3
1	A	55	GLU	2.3
2	H	1784	GLU	2.3
1	A	24	GLY	2.3
1	C	49	LEU	2.3
2	G	1904	SER	2.3
1	B	94	ASP	2.3
2	F	1923	HIS	2.3
2	I	1854	LEU	2.3
2	J	1864	GLU	2.3
2	F	1854	LEU	2.2
2	J	1828	ALA	2.2
2	I	1788	GLU	2.2
1	B	28	ILE	2.2
1	E	101	ILE	2.2
2	G	1892	ILE	2.2
1	B	89	ALA	2.2
2	G	1869	ASP	2.1
2	F	1870	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	66	PHE	2.1
1	E	119	ASP	2.1
1	E	126	ILE	2.1
1	A	131	ILE	2.1
2	F	1855	PHE	2.1
2	H	1854	LEU	2.1
1	E	23	ASP	2.1
1	E	136	GLN	2.1
2	F	1805	ALA	2.1
2	G	1905	ALA	2.1
2	F	1914	ARG	2.1
1	C	10	ILE	2.0
1	E	64	ILE	2.0
1	D	113	LEU	2.0
1	A	91	ARG	2.0
1	E	8	GLU	2.0
2	J	1798	TRP	2.0
1	A	90	PHE	2.0
2	J	1826	ARG	2.0
1	C	67	PRO	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 monosaccharides 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, 95<sup>th</sup> 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
3	MG	A	202	1/1	0.62	0.14	115,115,115,115	0
3	MG	E	202	1/1	0.67	0.11	83,83,83,83	0
3	MG	B	203	1/1	0.72	0.08	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	G	2101	5/5	0.72	0.35	98,105,111,140	0
3	MG	C	201	1/1	0.73	0.07	94,94,94,94	0
5	PO4	C	205	5/5	0.73	0.21	67,92,112,124	0
5	PO4	B	204	5/5	0.75	0.34	103,108,111,135	0
3	MG	D	203	1/1	0.80	0.07	96,96,96,96	0
4	SO4	A	205	5/5	0.81	0.27	79,103,129,142	0
3	MG	D	204	1/1	0.82	0.11	91,91,91,91	0
3	MG	A	203	1/1	0.85	0.33	66,66,66,66	0
4	SO4	J	2101	5/5	0.86	0.21	97,103,108,125	0
3	MG	D	201	1/1	0.88	0.08	89,89,89,89	0
3	MG	B	202	1/1	0.88	0.39	66,66,66,66	0
3	MG	B	201	1/1	0.90	0.19	113,113,113,113	0
4	SO4	F	2101	5/5	0.90	0.12	66,82,101,114	0
3	MG	A	201	1/1	0.92	0.06	89,89,89,89	0
3	MG	C	206	1/1	0.93	1.04	66,66,66,66	0
4	SO4	H	2101	5/5	0.93	0.15	83,91,96,133	0
3	MG	C	204	1/1	0.94	0.10	102,102,102,102	0
3	MG	E	201	1/1	0.94	0.10	113,113,113,113	0
3	MG	C	203	1/1	0.95	0.10	80,80,80,80	0
3	MG	C	202	1/1	0.96	0.10	68,68,68,68	0
3	MG	D	202	1/1	0.97	0.16	71,71,71,71	0
3	MG	A	204	1/1	0.98	0.15	70,70,70,70	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.