Full wwPDB X-ray Structure Validation Report

May 13, 2020 – 08:52 pm BST

PDB ID	:	6DCA
Title	:	Fab/epitope complex of mouse monoclonal antibody 6B2 targeting a non-phosphorylated tau epitope.
Authors	:	Chukwu, J.E.; Kong, X.-P.
Deposited on	:	2018-05-04
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 following versions of software and data (see references ①) were used in the production of this report:

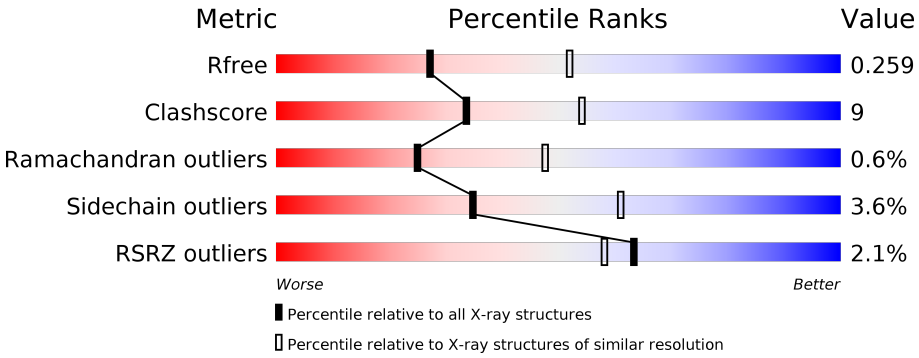
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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 <=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	L	218	77% 20%
1	M	218	75% 23%
1	N	218	83% 15%
1	O	218	78% 19%
2	H	221	4% 74% 19%
2	I	221	2% 79% 16%

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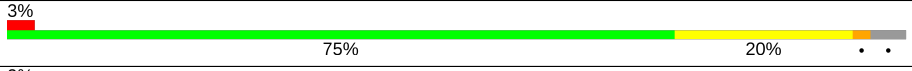
Mol	Chain	Length	Quality of chain
2	J	221	
2	K	221	
3	P	31	
3	Q	31	
3	R	31	
3	S	31	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13662 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1662	1039	281	336	6			
1	M	215	Total	C	N	O	S	0	0	0
			1662	1039	281	336	6			
1	N	215	Total	C	N	O	S	0	0	0
			1662	1039	281	336	6			
1	O	215	Total	C	N	O	S	0	0	0
			1662	1039	281	336	6			

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1623	1030	261	325	7			
2	I	213	Total	C	N	O	S	6	0	0
			1623	1030	261	325	7			
2	J	213	Total	C	N	O	S	0	0	0
			1623	1030	261	325	7			
2	K	213	Total	C	N	O	S	0	0	0
			1623	1030	261	325	7			

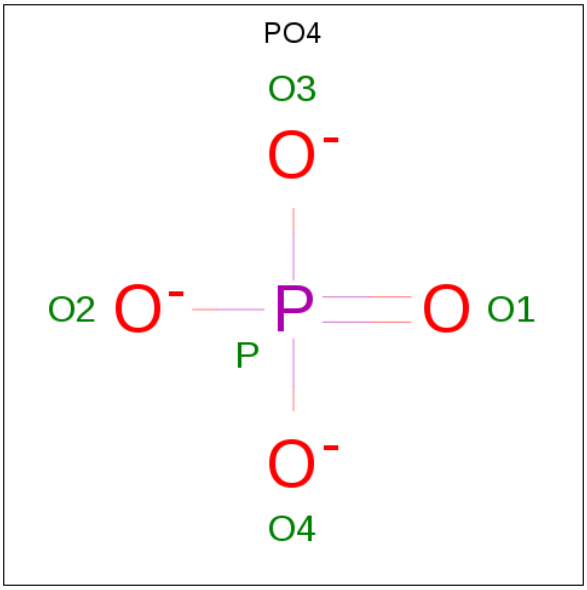
- Molecule 3 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	0	0	1
			50	30	12	8			
3	Q	7	Total	C	N	O	0	0	1
			50	30	12	8			
3	R	7	Total	C	N	O	0	0	1
			50	30	12	8			
3	S	7	Total	C	N	O	0	0	1
			50	30	12	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	409	NH2	-	amidation	UNP P10636
Q	409	NH2	-	amidation	UNP P10636
R	409	NH2	-	amidation	UNP P10636
S	409	NH2	-	amidation	UNP P10636

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	R	1	Total O P 5 4 1	0	0
4	S	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	41	Total O 41 41	0	0
5	H	37	Total O 37 37	0	0
5	P	1	Total O 1 1	0	0

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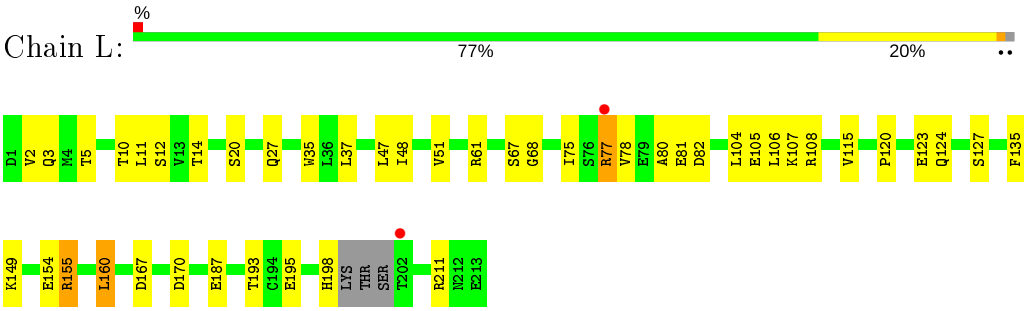
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	42	Total O 42 42	0	0
5	I	35	Total O 35 35	0	0
5	N	38	Total O 38 38	0	0
5	J	38	Total O 38 38	0	0
5	R	2	Total O 2 2	0	0
5	O	38	Total O 38 38	0	0
5	K	28	Total O 28 28	0	0
5	S	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

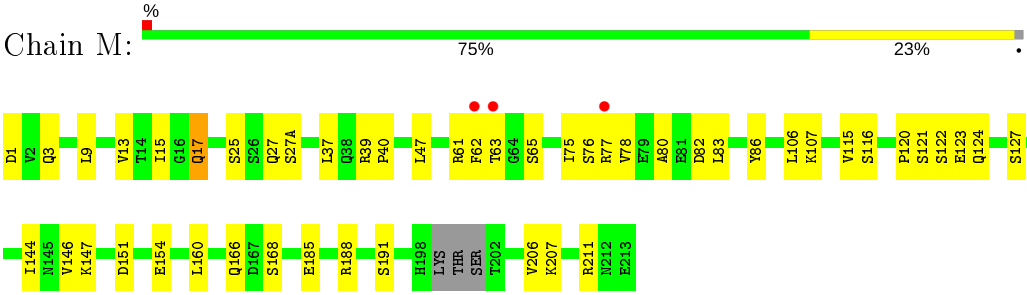
- Molecule 1: Fab light chain

Chain L:



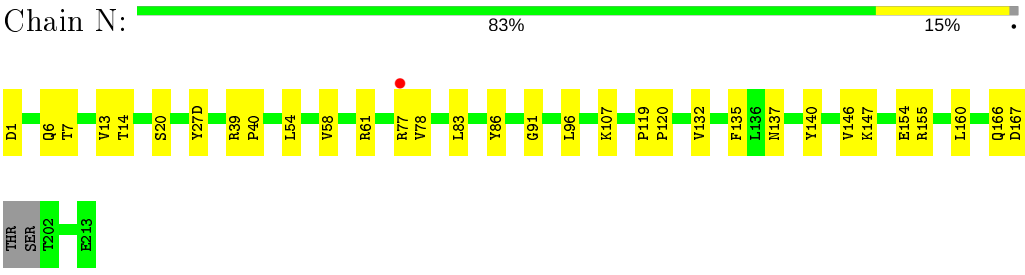
- Molecule 1: Fab light chain

Chain M:



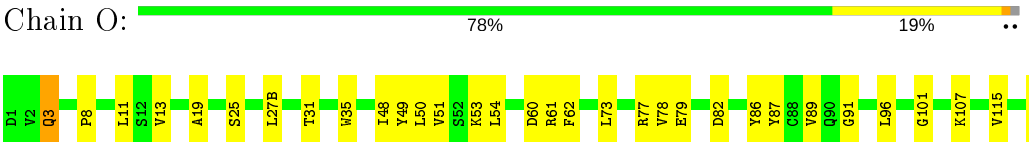
- Molecule 1: Fab light chain

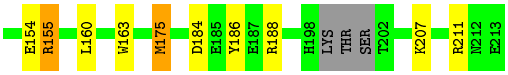
Chain N:



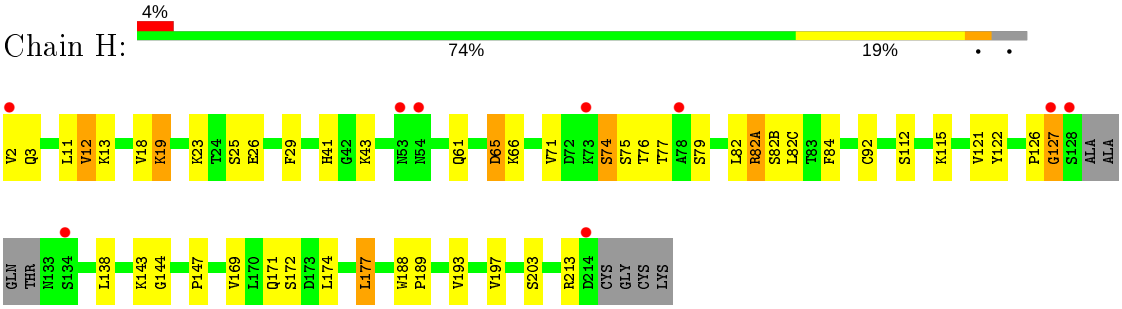
- Molecule 1: Fab light chain

Chain O:

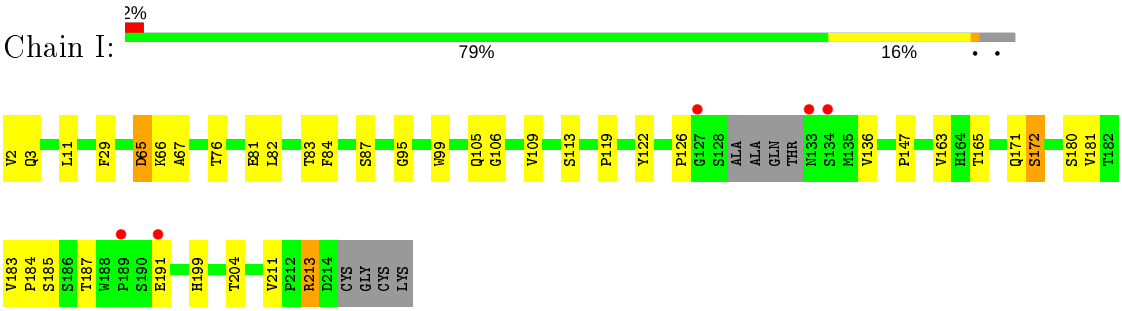




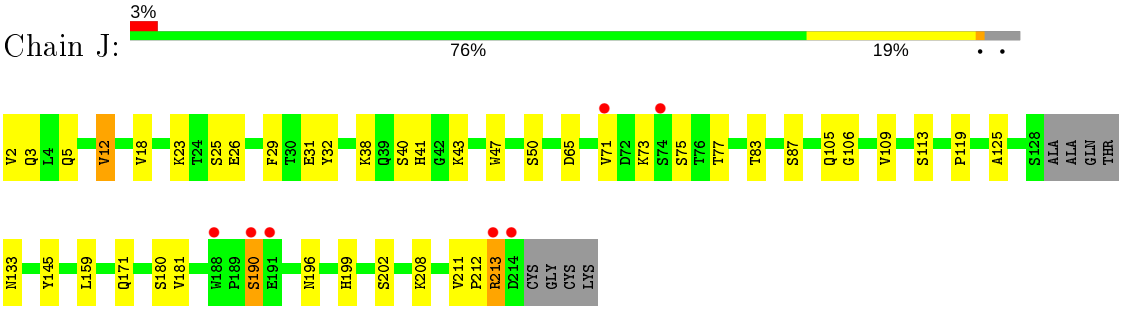
• Molecule 2: Fab heavy chain



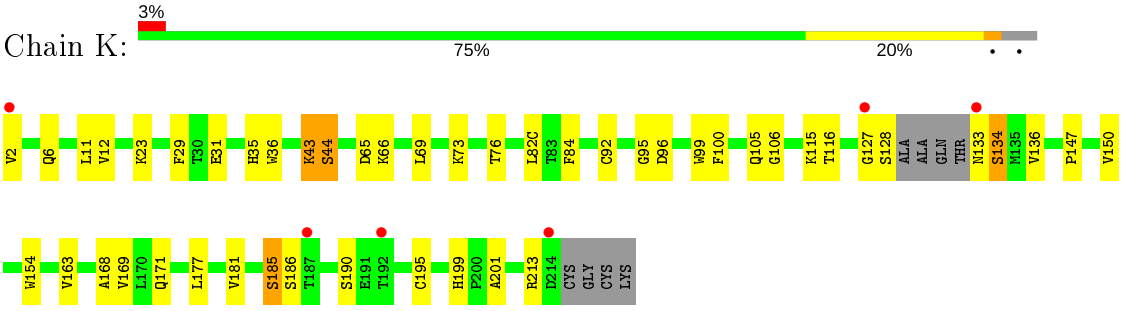
• Molecule 2: Fab heavy chain



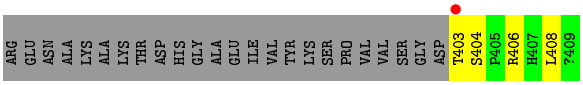
• Molecule 2: Fab heavy chain



• Molecule 2: Fab heavy chain

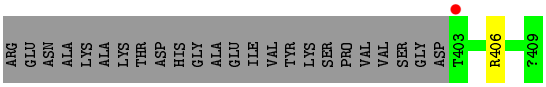


• Molecule 3: Microtubule-associated protein tau



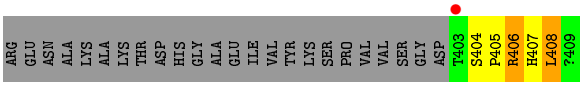
- Molecule 3: Microtubule-associated protein tau

Chain Q:



- Molecule 3: Microtubule-associated protein tau

Chain R:



- Molecule 3: Microtubule-associated protein tau

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.01Å 59.70Å 143.85Å 89.43° 92.69° 97.35°	Depositor
Resolution (Å)	45.60 – 2.60 45.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.60-2.60) 96.5 (45.60-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.189 , 0.259 0.189 , 0.259	Depositor DCC
R_{free} test set	1980 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13662	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, NH2

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	L	0.47	0/1696	0.66	0/2302
1	M	0.46	0/1696	0.64	0/2302
1	N	0.46	0/1696	0.61	0/2302
1	O	0.42	0/1696	0.64	1/2302 (0.0%)
2	H	0.47	0/1667	0.65	1/2280 (0.0%)
2	I	0.45	0/1667	0.65	1/2280 (0.0%)
2	J	0.49	0/1667	0.65	0/2280
2	K	0.47	0/1667	0.63	0/2280
3	P	0.41	0/50	0.55	0/67
3	Q	0.50	0/50	0.56	0/67
3	R	0.61	0/50	0.77	0/67
3	S	0.68	0/50	0.69	0/67
All	All	0.46	0/13652	0.64	3/18596 (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	H	0	1
2	I	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	177	LEU	CA-CB-CG	6.01	129.12	115.30
2	I	165	THR	C-N-CA	-5.73	107.37	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	155	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	65	ASP	Peptide
2	I	65	ASP	Peptide

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	L	1662	0	1624	35	0
1	M	1662	0	1624	42	0
1	N	1662	0	1624	17	0
1	O	1662	0	1624	25	0
2	H	1623	0	1573	29	0
2	I	1623	0	1573	30	0
2	J	1623	0	1573	25	0
2	K	1623	0	1573	35	0
3	P	50	0	49	3	0
3	Q	50	0	49	0	0
3	R	50	0	49	4	0
3	S	50	0	49	5	0
4	L	5	0	0	0	0
4	M	5	0	0	0	0
4	R	5	0	0	1	0
4	S	5	0	0	0	0
5	H	37	0	0	0	0
5	I	35	0	0	0	0
5	J	38	0	0	1	0
5	K	28	0	0	1	0
5	L	41	0	0	5	0
5	M	42	0	0	6	0
5	N	38	0	0	2	0
5	O	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1	0	0	1	0
5	R	2	0	0	0	0
5	S	2	0	0	0	0
All	All	13662	0	12984	225	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 (225) 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:M:17:GLN:OE1	5:M:401:HOH:O	1.90	0.89
1:M:17:GLN:O	5:M:402:HOH:O	1.97	0.81
1:M:185:GLU:OE1	1:M:188:ARG:NH2	2.15	0.80
1:M:120:PRO:HD3	1:M:132:VAL:HG12	1.66	0.77
2:H:115:LYS:HE2	1:M:211:ARG:HH12	1.52	0.73
1:L:81:GLU:OE2	1:L:81:GLU:N	2.18	0.73
1:M:147:LYS:HE3	1:M:154:GLU:HB2	1.70	0.72
2:H:82:LEU:HB3	2:H:82(C):LEU:HD21	1.72	0.72
2:K:128:SER:O	5:K:301:HOH:O	2.08	0.72
2:H:121:VAL:HG21	2:H:197:VAL:HG11	1.73	0.71
1:L:3:GLN:NE2	1:L:5:THR:OG1	2.25	0.69
2:K:136:VAL:HG23	2:K:185:SER:HA	1.73	0.69
1:M:25:SER:OG	1:M:27:GLN:O	2.12	0.67
2:K:96:ASP:H	3:S:409:NH2:N	1.94	0.66
1:L:120:PRO:O	2:H:213:ARG:NH2	2.29	0.66
2:H:23:LYS:HD3	2:H:77:THR:OG1	1.96	0.65
3:P:403:THR:HG22	3:P:404:SER:H	1.60	0.65
2:I:163:VAL:HG22	2:I:181:VAL:HG23	1.78	0.64
1:L:108:ARG:O	5:L:401:HOH:O	2.14	0.64
1:N:61:ARG:HD2	1:N:77:ARG:HG3	1.80	0.64
1:M:206:VAL:O	1:M:207:LYS:HD2	1.99	0.63
2:H:127:GLY:HA3	2:H:213:ARG:HD3	1.81	0.63
2:H:84:PHE:CD2	2:J:65:ASP:HB2	2.34	0.62
2:K:12:VAL:HG11	2:K:82(C):LEU:HD12	1.82	0.62
2:H:11:LEU:HD13	2:H:147:PRO:HG3	1.81	0.62
2:I:119:PRO:HD2	2:I:204:THR:HG21	1.81	0.62
2:I:84:PHE:CD1	2:K:65:ASP:HB2	2.35	0.62
2:I:199:HIS:HB3	2:I:204:THR:CG2	2.30	0.61
1:M:107:LYS:NZ	5:M:401:HOH:O	2.34	0.61
2:J:133:ASN:N	5:J:302:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:VAL:HG22	2:K:181:VAL:HG23	1.82	0.61
1:L:127:SER:OG	1:M:127:SER:O	2.16	0.60
2:I:2:VAL:HG21	2:I:29:PHE:CD2	2.37	0.59
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.84	0.59
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.35	0.58
1:L:155:ARG:HE	1:L:155:ARG:HA	1.67	0.58
2:I:95:GLY:HA2	2:I:99:TRP:HA	1.85	0.58
1:N:96:LEU:O	5:N:301:HOH:O	2.17	0.58
2:K:133:ASN:O	2:K:134:SER:OG	2.19	0.58
1:O:155:ARG:NH2	5:O:302:HOH:O	2.29	0.57
1:M:61:ARG:HD2	1:M:77:ARG:O	2.04	0.57
2:K:186:SER:O	2:K:190:SER:OG	2.18	0.57
3:R:404:SER:OG	4:R:501:PO4:O4	2.22	0.57
2:J:105:GLN:HG2	2:J:106:GLY:N	2.19	0.57
2:I:184:PRO:O	2:I:187:THR:HG22	2.05	0.56
2:I:199:HIS:HB3	2:I:204:THR:HG22	1.86	0.56
2:J:12:VAL:HG11	2:J:18:VAL:HB	1.87	0.56
1:N:107:LYS:HA	1:N:140:TYR:OH	2.06	0.56
2:H:74:SER:HB2	2:H:76:THR:HG23	1.88	0.56
1:M:13:VAL:HG12	1:M:78:VAL:HG21	1.88	0.56
1:M:82:ASP:O	1:M:86:TYR:OH	2.18	0.56
2:H:41:HIS:O	2:H:43:LYS:HG3	2.05	0.55
2:I:2:VAL:HG21	2:I:29:PHE:HD2	1.71	0.55
1:L:195:GLU:OE2	5:L:402:HOH:O	2.18	0.55
1:M:61:ARG:HH21	1:M:82:ASP:CG	2.10	0.55
1:M:61:ARG:HB2	1:M:76:SER:HB3	1.88	0.54
2:H:2:VAL:HG11	2:H:29:PHE:CD2	2.41	0.54
1:O:107:LYS:HA	1:O:140:TYR:OH	2.08	0.54
1:O:13:VAL:HG21	1:O:19:ALA:HB2	1.89	0.54
2:K:43:LYS:HE3	2:K:44:SER:O	2.07	0.54
1:M:37:LEU:HB2	1:M:47:LEU:HD11	1.88	0.54
2:K:36:TRP:CD1	2:K:69:LEU:HD22	2.42	0.54
1:M:80:ALA:HA	1:M:106:LEU:HD13	1.90	0.53
1:M:83:LEU:HD12	1:M:166:GLN:HB3	1.91	0.53
2:J:31:GLU:HG2	2:J:32:TYR:CD2	2.43	0.53
2:K:73:LYS:HE2	2:K:73:LYS:H	1.74	0.53
1:L:106:LEU:O	5:L:403:HOH:O	2.19	0.53
1:M:135:PHE:CE1	2:I:180:SER:HB3	2.44	0.53
2:H:2:VAL:HG12	2:H:26:GLU:CD	2.30	0.53
1:M:115:VAL:HA	1:M:135:PHE:O	2.09	0.53
1:N:137:ASN:ND2	5:N:307:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:GLN:HG3	2:H:122:TYR:CZ	2.44	0.52
1:O:87:TYR:HE2	2:K:44:SER:HB2	1.75	0.52
1:L:3:GLN:HE22	1:L:5:THR:HG1	1.52	0.52
2:H:71:VAL:HG22	2:H:75:SER:HA	1.91	0.52
1:M:115:VAL:HB	1:M:207:LYS:HD3	1.90	0.52
1:L:14:THR:HG23	1:L:107:LYS:HE2	1.92	0.51
1:L:187:GLU:HA	1:L:211:ARG:HE	1.75	0.51
2:I:67:ALA:HA	2:I:81:GLU:O	2.10	0.51
2:J:3:GLN:HB2	2:J:25:SER:HB2	1.92	0.51
2:J:41:HIS:O	2:J:43:LYS:HG3	2.10	0.51
2:I:172:SER:O	2:I:172:SER:OG	2.29	0.51
2:J:199:HIS:ND1	2:J:202:SER:OG	2.37	0.51
1:M:160:LEU:HD13	2:I:171:GLN:HG3	1.91	0.51
1:N:6:GLN:NE2	1:N:86:TYR:O	2.35	0.51
2:I:2:VAL:HG22	2:I:3:GLN:H	1.76	0.51
1:O:160:LEU:HD13	2:K:171:GLN:HG3	1.93	0.51
1:M:121:SER:OG	1:M:123:GLU:HG2	2.10	0.51
1:M:13:VAL:HG13	1:M:17:GLN:HG2	1.93	0.51
2:I:105:GLN:HG2	2:I:106:GLY:N	2.26	0.50
2:I:65:ASP:HB2	2:K:84:PHE:CD1	2.47	0.50
2:J:38:LYS:HE2	2:J:40:SER:OG	2.12	0.50
1:L:80:ALA:HA	1:L:106:LEU:HD13	1.92	0.50
1:M:124:GLN:HG3	2:I:122:TYR:CZ	2.45	0.50
2:K:6:GLN:H	2:K:105:GLN:HE22	1.59	0.50
2:K:95:GLY:HA2	2:K:99:TRP:HA	1.94	0.50
1:O:35:TRP:HD1	1:O:48:ILE:HB	1.76	0.50
2:K:154:TRP:CZ3	2:K:195:CYS:HB3	2.47	0.50
1:M:77:ARG:NH2	5:M:407:HOH:O	2.44	0.50
1:N:83:LEU:HD12	1:N:166:GLN:HB3	1.94	0.50
2:K:115:LYS:HD2	2:K:116:THR:H	1.77	0.49
1:L:155:ARG:HD3	5:L:404:HOH:O	2.11	0.49
1:M:3:GLN:NE2	5:M:404:HOH:O	2.26	0.49
1:N:54:LEU:HD22	1:N:58:VAL:HB	1.94	0.49
1:O:186:TYR:CZ	1:O:211:ARG:HG3	2.47	0.49
1:L:61:ARG:HD2	1:L:77:ARG:O	2.12	0.49
2:H:19:LYS:NZ	2:H:79:SER:OG	2.41	0.49
1:L:27:GLN:HG3	5:L:418:HOH:O	2.12	0.49
1:L:61:ARG:HH12	1:L:82:ASP:CG	2.17	0.48
2:I:11:LEU:HD13	2:I:147:PRO:HG3	1.94	0.48
1:M:75:ILE:HG21	1:M:78:VAL:HG12	1.95	0.48
1:O:8:PRO:HG3	1:O:11:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:127:GLY:O	2:K:213:ARG:HD2	2.13	0.48
1:M:15:ILE:HA	1:M:78:VAL:HG23	1.94	0.48
2:J:71:VAL:CG1	2:J:75:SER:HA	2.44	0.48
2:J:2:VAL:HG11	2:J:29:PHE:CE2	2.48	0.48
2:K:154:TRP:CH2	2:K:195:CYS:HB3	2.49	0.48
1:N:160:LEU:HD13	2:J:171:GLN:HG3	1.95	0.47
2:K:2:VAL:HG21	2:K:29:PHE:CD2	2.49	0.47
2:H:144:GLY:HA2	2:H:174:LEU:HB3	1.96	0.47
1:L:115:VAL:HA	1:L:135:PHE:O	2.14	0.47
1:M:39:ARG:HB3	1:M:40:PRO:HD2	1.96	0.47
1:O:3:GLN:O	1:O:25:SER:HA	2.15	0.47
1:O:120:PRO:HD3	1:O:132:VAL:HG22	1.97	0.47
1:L:10:THR:HG22	1:L:11:LEU:N	2.30	0.47
1:L:160:LEU:HD21	2:H:169:VAL:HB	1.96	0.46
2:J:23:LYS:HG3	2:J:77:THR:OG1	2.15	0.46
2:K:11:LEU:HD22	2:K:147:PRO:HG3	1.97	0.46
1:N:91:GLY:O	3:R:407:HIS:NE2	2.47	0.46
2:I:183:VAL:HB	2:I:187:THR:HG21	1.98	0.46
3:P:403:THR:N	5:P:501:HOH:O	2.47	0.46
1:M:13:VAL:HG13	1:M:17:GLN:CG	2.46	0.45
1:M:77:ARG:HA	5:M:402:HOH:O	2.16	0.45
2:I:187:THR:O	2:I:191:GLU:N	2.48	0.45
2:I:213:ARG:H	2:I:213:ARG:HG2	1.64	0.45
3:S:406:ARG:HD2	3:S:406:ARG:H	1.81	0.45
1:N:135:PHE:CE1	2:J:180:SER:HB3	2.52	0.45
1:N:147:LYS:HG2	1:N:154:GLU:HG3	1.99	0.45
1:O:61:ARG:NH1	1:O:82:ASP:OD2	2.42	0.45
2:I:84:PHE:CE1	2:K:65:ASP:HB2	2.53	0.44
2:J:159:LEU:HD13	2:J:181:VAL:HG21	1.98	0.44
2:K:43:LYS:HB3	2:K:43:LYS:HE2	1.72	0.44
1:M:39:ARG:NH2	1:M:168:SER:HB2	2.31	0.44
1:M:61:ARG:NH2	1:M:82:ASP:OD1	2.46	0.44
1:O:49:TYR:CE2	1:O:53:LYS:HD3	2.52	0.44
2:H:2:VAL:HG11	2:H:29:PHE:CE2	2.51	0.44
3:S:408:LEU:HA	3:S:408:LEU:HD23	1.81	0.44
2:H:138:LEU:HD12	2:H:193:VAL:HG11	1.99	0.44
2:H:121:VAL:CG2	2:H:197:VAL:HG11	2.44	0.44
1:N:119:PRO:HD2	2:J:213:ARG:NH2	2.33	0.44
1:M:136:LEU:HD23	1:M:144:ILE:HD13	1.98	0.44
1:M:151:ASP:HA	1:M:191:SER:OG	2.17	0.44
1:N:167:ASP:O	1:N:171:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:GLY:HA2	1:O:96:LEU:HG	1.98	0.43
1:L:2:VAL:HG22	1:L:27:GLN:HB2	2.00	0.43
1:M:75:ILE:HD13	1:M:75:ILE:HA	1.77	0.43
1:O:163:TRP:NE1	1:O:175:MET:HG3	2.33	0.43
1:L:37:LEU:HB2	1:L:47:LEU:HD11	1.99	0.43
1:L:61:ARG:H	1:L:61:ARG:HG2	1.62	0.43
2:J:73:LYS:HE2	2:J:73:LYS:HB2	1.83	0.43
2:J:211:VAL:HG12	2:J:212:PRO:O	2.18	0.43
1:O:89:VAL:HG21	2:K:100:PHE:HE1	1.83	0.43
1:L:78:VAL:HG11	1:L:104:LEU:HD21	2.01	0.43
2:J:105:GLN:CG	2:J:106:GLY:N	2.81	0.43
1:M:61:ARG:CB	1:M:76:SER:HB3	2.49	0.43
1:O:54:LEU:HD11	1:O:62:PHE:O	2.18	0.43
2:J:87:SER:HA	2:J:109:VAL:O	2.19	0.43
1:L:167:ASP:HB3	1:L:170:ASP:OD1	2.18	0.43
1:O:160:LEU:HD21	2:K:169:VAL:HB	1.99	0.43
2:H:3:GLN:HB3	2:H:25:SER:OG	2.19	0.43
2:I:83:THR:HG22	2:I:84:PHE:H	1.84	0.43
1:L:149:LYS:HB2	1:L:193:THR:HB	2.01	0.43
2:I:136:VAL:HG23	2:I:185:SER:HA	2.01	0.42
2:K:116:THR:HG22	2:K:147:PRO:HD3	2.00	0.42
1:M:39:ARG:HH22	1:M:168:SER:HB2	1.84	0.42
3:S:406:ARG:CD	3:S:406:ARG:H	2.31	0.42
2:I:65:ASP:HB2	2:K:84:PHE:HD1	1.84	0.42
2:I:66:LYS:O	2:I:82:LEU:HA	2.19	0.42
2:K:35:HIS:HE2	3:S:409:NH2:N	2.17	0.42
1:M:62:PHE:CD2	1:M:75:ILE:HD11	2.55	0.42
2:H:12:VAL:HG11	2:H:18:VAL:HB	2.00	0.42
1:L:123:GLU:OE1	1:L:123:GLU:N	2.40	0.42
1:L:35:TRP:HB2	1:L:48:ILE:HB	2.02	0.42
1:N:120:PRO:HD3	1:N:132:VAL:HG22	2.02	0.42
3:R:408:LEU:HD12	3:R:408:LEU:HA	1.78	0.42
2:J:47:TRP:HZ2	2:J:50:SER:HB3	1.85	0.42
2:I:105:GLN:CG	2:I:106:GLY:N	2.83	0.42
1:L:12:SER:HA	1:L:105:GLU:O	2.20	0.42
1:M:9:LEU:HD23	1:M:9:LEU:HA	1.85	0.41
2:I:183:VAL:HB	2:I:187:THR:CG2	2.49	0.41
2:K:168:ALA:HB2	2:K:177:LEU:HD23	2.01	0.41
2:K:2:VAL:HG11	2:K:29:PHE:CE2	2.55	0.41
1:O:184:ASP:O	1:O:188:ARG:HG3	2.20	0.41
2:K:23:LYS:HG2	2:K:76:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:LYS:HG3	1:L:154:GLU:OE2	2.20	0.41
2:H:188:TRP:CG	2:H:189:PRO:HA	2.56	0.41
2:I:87:SER:HA	2:I:109:VAL:O	2.21	0.41
2:J:125:ALA:O	2:J:213:ARG:NH2	2.53	0.41
1:L:61:ARG:O	1:L:75:ILE:HA	2.20	0.41
1:O:50:LEU:O	1:O:51:VAL:HB	2.20	0.41
2:K:150:VAL:HG23	2:K:199:HIS:HD2	1.85	0.41
2:H:66:LYS:HE2	2:H:82(A):ARG:O	2.20	0.41
2:I:2:VAL:HG22	2:I:3:GLN:N	2.35	0.41
2:K:105:GLN:HG2	2:K:106:GLY:N	2.36	0.41
1:L:187:GLU:C	1:L:211:ARG:HH11	2.21	0.41
2:K:147:PRO:HD2	2:K:201:ALA:HB3	2.03	0.41
1:M:62:PHE:CE2	1:M:75:ILE:HD11	2.56	0.41
1:N:13:VAL:HG21	1:N:78:VAL:HG21	2.02	0.41
1:O:27(B):LEU:O	1:O:31:THR:HG23	2.21	0.41
1:O:78:VAL:O	1:O:79:GLU:HG3	2.21	0.41
2:H:13:LYS:HA	2:H:112:SER:O	2.21	0.41
1:L:143:ASP:O	1:L:198:HIS:HD2	2.04	0.41
1:O:86:TYR:O	1:O:101:GLY:HA2	2.19	0.41
1:N:39:ARG:HB3	1:N:40:PRO:HD2	2.03	0.41
1:O:35:TRP:CE2	1:O:73:LEU:HB2	2.56	0.41
3:P:408:LEU:HA	3:P:408:LEU:HD12	1.91	0.41
2:H:19:LYS:HE3	2:H:19:LYS:HB3	1.94	0.40
2:H:84:PHE:CE2	2:J:65:ASP:HB2	2.57	0.40
1:N:27(D):TYR:CZ	3:R:405:PRO:HB3	2.56	0.40
1:L:187:GLU:O	1:L:211:ARG:NH1	2.45	0.40
2:H:82:LEU:CB	2:H:82(C):LEU:HD21	2.47	0.40
2:J:2:VAL:HG12	2:J:26:GLU:CD	2.41	0.40
2:H:171:GLN:O	2:H:172:SER:OG	2.38	0.40
1:O:154:GLU:HG2	1:O:155:ARG:N	2.36	0.40
1:O:115:VAL:O	1:O:207:LYS:HE3	2.21	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	L	211/218 (97%)	204 (97%)	5 (2%)	2 (1%)	17 35
1	M	211/218 (97%)	202 (96%)	9 (4%)	0	100 100
1	N	211/218 (97%)	198 (94%)	13 (6%)	0	100 100
1	O	211/218 (97%)	204 (97%)	7 (3%)	0	100 100
2	H	209/221 (95%)	190 (91%)	15 (7%)	4 (2%)	8 15
2	I	209/221 (95%)	197 (94%)	11 (5%)	1 (0%)	29 52
2	J	209/221 (95%)	196 (94%)	12 (6%)	1 (0%)	29 52
2	K	209/221 (95%)	196 (94%)	11 (5%)	2 (1%)	15 32
3	P	5/31 (16%)	5 (100%)	0	0	100 100
3	Q	5/31 (16%)	5 (100%)	0	0	100 100
3	R	5/31 (16%)	4 (80%)	0	1 (20%)	0 0
3	S	5/31 (16%)	4 (80%)	1 (20%)	0	100 100
All	All	1700/1880 (90%)	1605 (94%)	84 (5%)	11 (1%)	25 47

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	65	ASP
2	I	126	PRO
3	R	406	ARG
1	L	68	GLY
2	H	82(B)	SER
2	H	126	PRO
2	J	190	SER
2	K	44	SER
2	K	134	SER
1	L	51	VAL
2	H	127	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	192/195 (98%)	187 (97%)	5 (3%)	46 72
1	M	192/195 (98%)	184 (96%)	8 (4%)	30 55
1	N	192/195 (98%)	186 (97%)	6 (3%)	40 66
1	O	192/195 (98%)	188 (98%)	4 (2%)	53 77
2	H	188/193 (97%)	179 (95%)	9 (5%)	25 49
2	I	188/193 (97%)	183 (97%)	5 (3%)	44 71
2	J	188/193 (97%)	180 (96%)	8 (4%)	29 54
2	K	188/193 (97%)	183 (97%)	5 (3%)	44 71
3	P	6/25 (24%)	5 (83%)	1 (17%)	2 3
3	Q	6/25 (24%)	5 (83%)	1 (17%)	2 3
3	R	6/25 (24%)	4 (67%)	2 (33%)	0 0
3	S	6/25 (24%)	4 (67%)	2 (33%)	0 0
All	All	1544/1652 (94%)	1488 (96%)	56 (4%)	35 61

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	SER
1	L	67	SER
1	L	77	ARG
1	L	155	ARG
1	L	160	LEU
2	H	12	VAL
2	H	19	LYS
2	H	61	GLN
2	H	74	SER
2	H	82(A)	ARG
2	H	92	CYS
2	H	143	LYS
2	H	177	LEU
2	H	203	SER
3	P	406	ARG
1	M	1	ASP
1	M	17	GLN
1	M	27(A)	SER
1	M	63	THR
1	M	65	SER

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Mol	Chain	Res	Type
1	M	116	SER
1	M	122	SER
1	M	146	VAL
2	I	76	THR
2	I	113	SER
2	I	172	SER
2	I	211	VAL
2	I	213	ARG
3	Q	406	ARG
1	N	1	ASP
1	N	7	THR
1	N	14	THR
1	N	20	SER
1	N	146	VAL
1	N	155	ARG
2	J	5	GLN
2	J	12	VAL
2	J	83	THR
2	J	113	SER
2	J	190	SER
2	J	196	ASN
2	J	208	LYS
2	J	213	ARG
3	R	406	ARG
3	R	408	LEU
1	O	3	GLN
1	O	60	ASP
1	O	77	ARG
1	O	175	MET
2	K	31	GLU
2	K	43	LYS
2	K	66	LYS
2	K	92	CYS
2	K	185	SER
3	S	406	ARG
3	S	408	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	137	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	PO4	R	501	-	4,4,4	0.60	0	6,6,6	0.78	0
4	PO4	S	501	-	4,4,4	0.65	0	6,6,6	0.69	0
4	PO4	L	301	-	4,4,4	0.80	0	6,6,6	0.87	0
4	PO4	M	301	-	4,4,4	0.68	0	6,6,6	0.78	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	501	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	L	215/218 (98%)	0.02	2 (0%) 84 82	25, 34, 48, 57	0
1	M	215/218 (98%)	-0.03	3 (1%) 75 71	23, 33, 48, 56	0
1	N	215/218 (98%)	-0.06	1 (0%) 91 89	22, 33, 45, 51	0
1	O	215/218 (98%)	0.03	0 100 100	25, 35, 47, 54	0
2	H	213/221 (96%)	0.22	9 (4%) 36 29	20, 37, 51, 73	0
2	I	212/221 (95%)	0.12	5 (2%) 59 53	25, 34, 51, 71	0
2	J	213/221 (96%)	0.17	7 (3%) 46 39	25, 36, 55, 77	0
2	K	213/221 (96%)	0.25	6 (2%) 53 46	26, 38, 57, 86	0
3	P	6/31 (19%)	0.39	1 (16%) 1 1	34, 41, 55, 59	0
3	Q	6/31 (19%)	0.82	1 (16%) 1 1	36, 47, 58, 64	0
3	R	6/31 (19%)	0.65	1 (16%) 1 1	31, 37, 44, 53	0
3	S	6/31 (19%)	0.13	0 100 100	38, 44, 50, 53	0
All	All	1735/1880 (92%)	0.10	36 (2%) 63 58	20, 35, 51, 86	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	127	GLY	5.0
3	Q	403	THR	4.5
2	I	127	GLY	4.0
1	M	62	PHE	3.6
2	H	2	VAL	3.5
2	K	187	THR	3.1
2	H	134	SER	3.1
2	K	214	ASP	3.1
2	I	133	ASN	2.8
2	J	190	SER	2.8
2	H	214	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	P	403	THR	2.5
2	J	213	ARG	2.5
2	I	189	PRO	2.5
2	J	74	SER	2.4
2	J	214	ASP	2.4
2	H	78	ALA	2.3
2	K	133	ASN	2.3
1	M	77	ARG	2.3
2	H	127	GLY	2.3
2	J	191	GLU	2.3
2	J	71	VAL	2.3
1	M	63	THR	2.3
2	H	54	ASN	2.2
2	I	134	SER	2.2
1	N	77	ARG	2.2
3	R	403	THR	2.2
2	J	188	TRP	2.2
2	H	73	LYS	2.2
2	K	192	THR	2.2
2	H	128	SER	2.1
1	L	77	ARG	2.1
2	H	53	ASN	2.1
1	L	202	THR	2.1
2	I	191	GLU	2.0
2	K	2	VAL	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 carbohydrates 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^{th} 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
4	PO4	S	501	5/5	0.86	0.20	50,54,61,73	0
4	PO4	L	301	5/5	0.90	0.26	50,58,71,73	0
4	PO4	R	501	5/5	0.93	0.26	49,51,74,75	0
4	PO4	M	301	5/5	0.93	0.25	55,63,68,78	0

6.5 Other polymers (i)

There are no such residues in this entry.