Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2017 – 09:40 AM EDT

PDB ID	:	4PJJ
Title	:	MYOSIN VI (MD-INSERT2-CAM, DELTA-INSERT1) post-rigor state - long soaking with PO4
Authors	:	Isabet, T.; Benisty, H.; Llinas, P.; Sweeney, H.L.; Houdusse, A.
Deposited on	:	unknown
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 2.40 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.
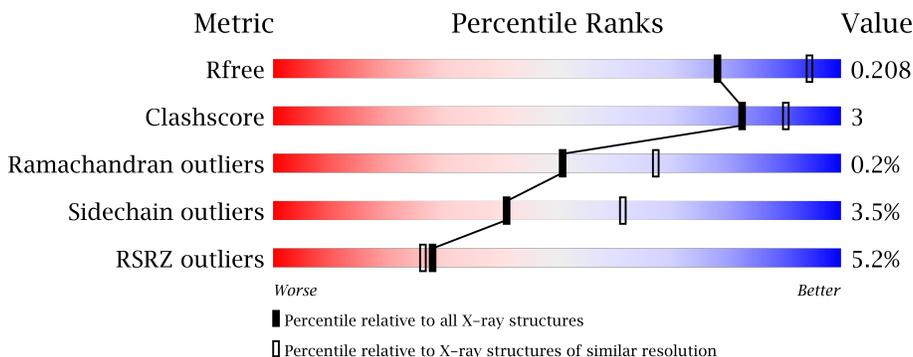
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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	A	788	5% · 86% · 8% · 6%
2	B	149	2% · 83% · 12% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	903	-	-	-	X
6	GOL	A	906	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7479 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 Unconventional myosin-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	743	5948	3793	1032	1095	28	0	2	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	MET	ARG	conflict	UNP F1RQI7
A	?	-	CYS	deletion	UNP F1RQI7
A	?	-	THR	deletion	UNP F1RQI7
A	?	-	ARG	deletion	UNP F1RQI7
A	?	-	TYR	deletion	UNP F1RQI7
A	?	-	PHE	deletion	UNP F1RQI7
A	?	-	ALA	deletion	UNP F1RQI7
A	?	-	ASN	deletion	UNP F1RQI7
A	?	-	LYS	deletion	UNP F1RQI7
A	?	-	GLU	deletion	UNP F1RQI7
A	?	-	THR	deletion	UNP F1RQI7
A	?	-	ASP	deletion	UNP F1RQI7
A	?	-	LYS	deletion	UNP F1RQI7
A	?	-	GLN	deletion	UNP F1RQI7
A	?	-	ILE	deletion	UNP F1RQI7
A	?	-	LEU	deletion	UNP F1RQI7
A	?	-	GLN	deletion	UNP F1RQI7
A	?	-	ASN	deletion	UNP F1RQI7
A	?	-	ARG	deletion	UNP F1RQI7
A	?	-	LYS	deletion	UNP F1RQI7
A	?	-	SER	deletion	UNP F1RQI7
A	?	-	PRO	deletion	UNP F1RQI7
A	?	-	GLU	deletion	UNP F1RQI7
A	?	-	TYR	deletion	UNP F1RQI7
A	?	-	LEU	deletion	UNP F1RQI7
A	?	-	LYS	deletion	UNP F1RQI7
A	?	-	ALA	deletion	UNP F1RQI7

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total 1125	C 689	N 181	O 246	S 9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	128	SER	ALA	conflict	UNP P62152

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ —— P ═══ O O1

P

O⁻

O4
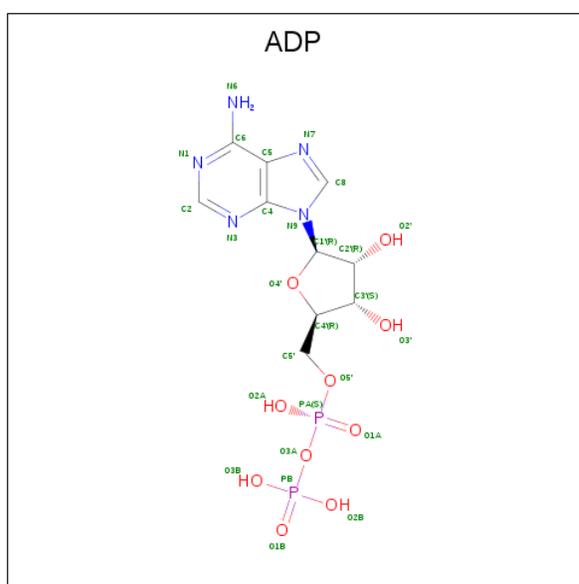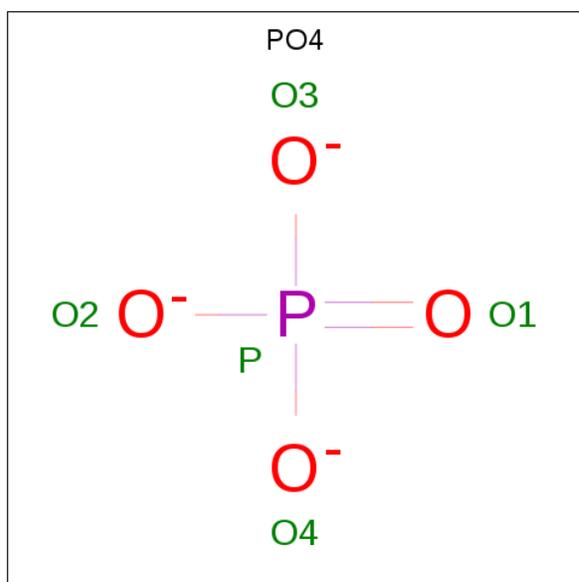
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	A	1	Total 5	O 4	P 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1 C2

HO OH

O1 O2
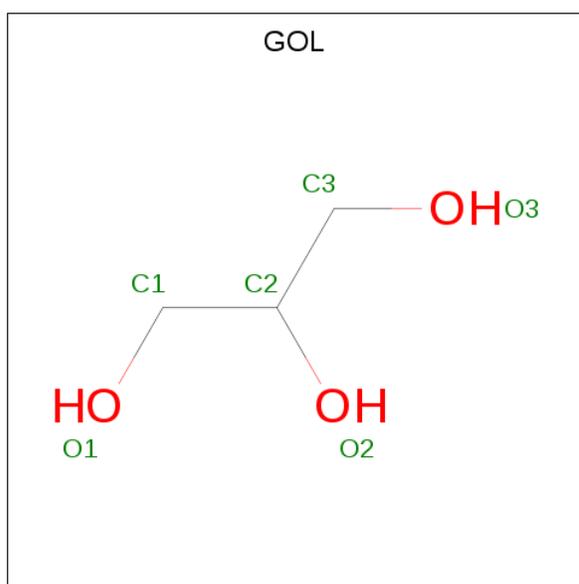
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	Ca 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	310	Total 310	O 310	0	0
8	B	44	Total 44	O 44	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: Unconventional myosin-VI
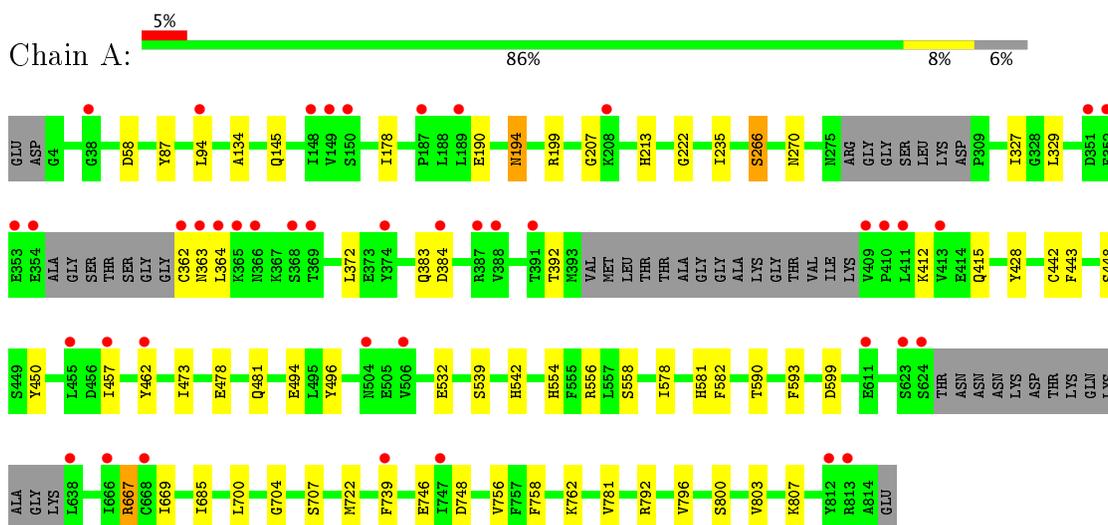
- Molecule 2: Calmodulin
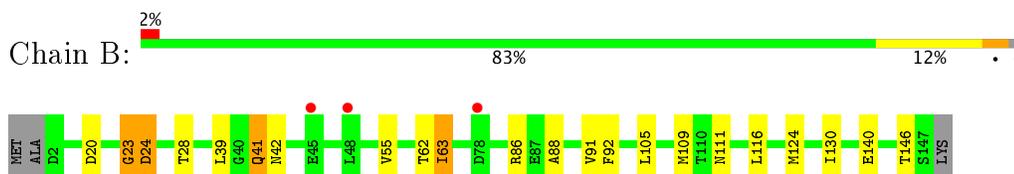
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.01Å 109.24Å 180.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.74 – 2.40 43.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.74-2.40) 99.8 (43.74-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.172 , 0.207 0.178 , 0.208	Depositor DCC
R_{free} test set	2855 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.1	EDS
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7479	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CA, PO4, ADP

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	0/6072	0.64	0/8186
2	B	0.49	0/1137	0.69	1/1531 (0.1%)
All	All	0.50	0/7209	0.65	1/9717 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	23	GLY	C-N-CA	7.00	139.21	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5948	0	5849	34	0
2	B	1125	0	1027	11	0
3	A	27	0	12	0	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
6	A	12	0	16	1	0
7	B	2	0	0	0	0
8	A	310	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	44	0	0	0	0
All	All	7479	0	6904	41	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 3.

All (41) 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:496:TYR:OH	1:A:704:GLY:HA3	1.75	0.86
1:A:554:HIS:HD2	1:A:556:ARG:H	1.28	0.78
1:A:532:GLU:OE2	1:A:542:HIS:HD2	1.75	0.70
1:A:554:HIS:CD2	1:A:556:ARG:H	2.13	0.64
1:A:739:PHE:HZ	1:A:756:VAL:HG11	1.66	0.60
1:A:667:ARG:NH2	8:A:1001:HOH:O	2.33	0.60
1:A:473:ILE:HD11	6:A:906:GOL:H32	1.86	0.57
1:A:190:GLU:O	1:A:194:ASN:HB2	2.06	0.56
1:A:178:ILE:HD11	1:A:222:GLY:HA2	1.87	0.55
1:A:372:LEU:HD23	1:A:383:GLN:HE21	1.73	0.54
2:B:55:VAL:HG23	2:B:63:ILE:HG21	1.90	0.53
1:A:412:LYS:H	1:A:415:GLN:HE21	1.57	0.53
1:A:213:HIS:HD2	1:A:448:SER:OG	1.92	0.52
1:A:748:ASP:HB3	1:A:762:LYS:HG3	1.93	0.51
1:A:739:PHE:CZ	1:A:756:VAL:HG11	2.48	0.48
2:B:130:ILE:HD12	2:B:140:GLU:HG2	1.96	0.48
1:A:478:GLU:OE1	1:A:581:HIS:HD2	1.98	0.47
1:A:481:GLN:HG2	1:A:582:PHE:CD1	2.50	0.47
1:A:722:MET:CE	1:A:781:VAL:HG21	2.45	0.47
1:A:554:HIS:HE1	8:A:1279:HOH:O	1.98	0.46
1:A:266:SER:HB2	1:A:270:ASN:HD22	1.81	0.46
2:B:28:THR:HG22	2:B:62:THR:HG22	1.99	0.45
1:A:134:ALA:O	1:A:145:GLN:HG3	2.16	0.45
2:B:116:LEU:HD11	2:B:124:MET:HE1	1.99	0.44
1:A:554:HIS:HD2	1:A:556:ARG:N	2.06	0.43
1:A:807:LYS:HB2	2:B:41:GLN:HG2	2.01	0.42
1:A:590:THR:HA	1:A:593:PHE:CD1	2.54	0.42
1:A:87:TYR:HB3	1:A:94:LEU:HD11	2.02	0.42
1:A:803:VAL:HG21	2:B:39:LEU:HD12	2.00	0.42
1:A:207:GLY:HA3	1:A:457:ILE:HD12	2.02	0.42
1:A:707:SER:HB2	1:A:758:PHE:HB2	2.02	0.42
2:B:105:LEU:O	2:B:109:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HD13	1:A:428:TYR:HB3	2.01	0.41
1:A:558:SER:HB3	1:A:578:ILE:HB	2.01	0.41
1:A:669:ILE:HG21	1:A:685:ILE:HG23	2.03	0.41
1:A:800:SER:HA	2:B:39:LEU:HD13	2.03	0.41
2:B:88:ALA:O	2:B:91:VAL:HB	2.21	0.41
1:A:796:VAL:HG23	2:B:92:PHE:HZ	1.86	0.40
1:A:762:LYS:HA	1:A:762:LYS:HD3	1.91	0.40
2:B:20:ASP:OD1	2:B:24:ASP:HB3	2.22	0.40
1:A:462:TYR:HA	8:A:1195:HOH:O	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	A	735/788 (93%)	721 (98%)	14 (2%)	0	100	100
2	B	144/149 (97%)	140 (97%)	2 (1%)	2 (1%)	13	18
All	All	879/937 (94%)	861 (98%)	16 (2%)	2 (0%)	51	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	24	ASP
2	B	23	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	A	647/697 (93%)	626 (97%)	21 (3%)	44	65
2	B	120/129 (93%)	114 (95%)	6 (5%)	28	45
All	All	767/826 (93%)	740 (96%)	27 (4%)	41	61

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	194	ASN
1	A	199	ARG
1	A	266	SER
1	A	327	ILE
1	A	329	LEU
1	A	362	CYS
1	A	363	ASN
1	A	364	LEU
1	A	384	ASP
1	A	392	THR
1	A	442	CYS
1	A	443	PHE
1	A	450	TYR
1	A	494	GLU
1	A	539	SER
1	A	599	ASP
1	A	667	ARG
1	A	700	LEU
1	A	746	GLU
1	A	792	ARG
2	B	41	GLN
2	B	42	ASN
2	B	63	ILE
2	B	86	ARG
2	B	111	ASN
2	B	146	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN

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Mol	Chain	Res	Type
1	A	194	ASN
1	A	213	HIS
1	A	246	HIS
1	A	270	ASN
1	A	383	GLN
1	A	415	GLN
1	A	466	ASN
1	A	481	GLN
1	A	485	ASN
1	A	493	GLN
1	A	542	HIS
1	A	554	HIS
1	A	581	HIS
1	A	678	HIS
2	B	107	HIS
2	B	111	ASN
2	B	135	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\#\|Z\|>2$
3	ADP	A	901	4	25,29,29	0.63	0	24,45,45	0.71	0
5	PO4	A	903	-	4,4,4	2.63	1 (25%)	6,6,6	0.46	0
5	PO4	A	904	-	4,4,4	2.64	1 (25%)	6,6,6	0.39	0
6	GOL	A	905	-	5,5,5	0.17	0	5,5,5	0.18	0
6	GOL	A	906	-	5,5,5	0.12	0	5,5,5	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	901	4	-	0/12/32/32	0/3/3/3
5	PO4	A	903	-	-	0/0/0/0	0/0/0/0
5	PO4	A	904	-	-	0/0/0/0	0/0/0/0
6	GOL	A	905	-	-	0/4/4/4	0/0/0/0
6	GOL	A	906	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	PO4	P-O1	4.67	1.60	1.50
5	A	903	PO4	P-O1	4.68	1.60	1.50

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
6	A	906	GOL	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	743/788 (94%)	0.09	43 (5%)	24 22	31, 54, 96, 117	0
2	B	146/149 (97%)	-0.07	3 (2%)	64 61	46, 67, 100, 121	0
All	All	889/937 (94%)	0.06	46 (5%)	28 26	31, 56, 97, 121	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	VAL	6.1
1	A	352	PHE	5.8
1	A	812	TYR	5.4
1	A	362	CYS	5.2
1	A	364	LEU	4.4
1	A	411	LEU	4.1
1	A	623	SER	3.7
1	A	363	ASN	3.6
1	A	354	GLU	3.4
1	A	353	GLU	3.3
1	A	366	ASN	3.3
1	A	506	VAL	3.3
1	A	624	SER	3.3
1	A	611	GLU	3.2
2	B	78	ASP	3.2
1	A	368	SER	3.1
1	A	391	THR	3.1
1	A	149	VAL	3.0
1	A	409	VAL	3.0
1	A	638	LEU	2.9
1	A	666	ILE	2.9
1	A	387	ARG	2.7
1	A	455	LEU	2.6
1	A	410	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	38	GLY	2.6
1	A	369	THR	2.5
1	A	94	LEU	2.5
1	A	384	ASP	2.5
1	A	747	ILE	2.5
2	B	48	LEU	2.4
1	A	504	ASN	2.4
1	A	739	PHE	2.4
1	A	351	ASP	2.4
1	A	374	TYR	2.3
1	A	150	SER	2.3
1	A	388	VAL	2.2
1	A	668	CYS	2.2
1	A	365	LYS	2.2
1	A	813	ARG	2.1
1	A	148	ILE	2.1
1	A	189	LEU	2.1
1	A	208	LYS	2.1
2	B	45	GLU	2.1
1	A	462	TYR	2.0
1	A	457	ILE	2.0
1	A	187	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
6	GOL	A	906	6/6	0.89	0.40	5.26	76,78,80,82	0
5	PO4	A	903	5/5	0.91	0.28	2.80	50,56,57,58	5
6	GOL	A	905	6/6	0.83	0.31	1.52	81,85,86,88	0
4	MG	A	902	1/1	0.99	0.21	-0.52	43,43,43,43	0
3	ADP	A	901	27/27	0.99	0.15	-0.83	37,43,47,55	0
7	CA	B	201	1/1	0.99	0.07	-1.40	52,52,52,52	0
7	CA	B	202	1/1	0.99	0.05	-2.06	54,54,54,54	0
5	PO4	A	904	5/5	0.84	0.17	-	102,104,105,108	0

6.5 Other polymers (i)

There are no such residues in this entry.