Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RH1
Title	:	High resolution crystal structure of human B2-adrenergic G protein-coupled receptor.
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Deposited on	:	2007-10-05
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

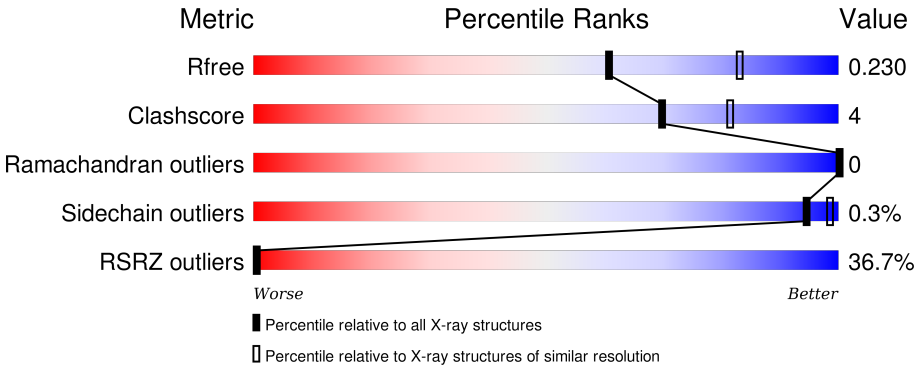
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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	500	32% 80% 8% 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
2	MAL	A	401	X	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3804 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.

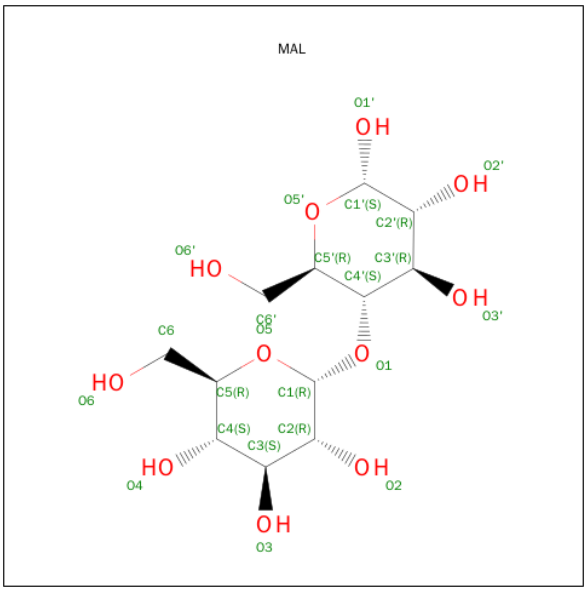
- Molecule 1 is a protein called beta-2-adrenergic receptor/T4-lysozyme chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3543	2315	590	614	24			

There are 10 discrepancies between the modelled and reference sequences:

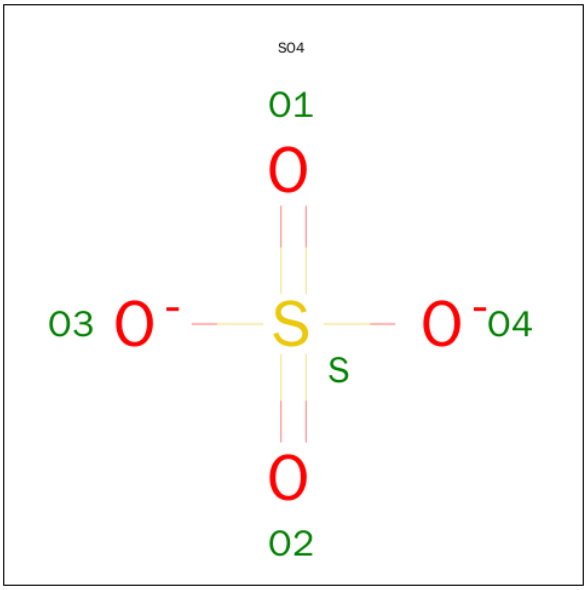
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	EXPRESSION TAG	UNP P07550
A	-5	TYR	-	EXPRESSION TAG	UNP P07550
A	-4	LYS	-	EXPRESSION TAG	UNP P07550
A	-3	ASP	-	EXPRESSION TAG	UNP P07550
A	-2	ASP	-	EXPRESSION TAG	UNP P07550
A	-1	ASP	-	EXPRESSION TAG	UNP P07550
A	0	ALA	-	EXPRESSION TAG	UNP P07550
A	187	GLU	ASN	ENGINEERED	UNP P07550
A	1054	THR	CYS	ENGINEERED	UNP P00720
A	1097	ALA	CYS	ENGINEERED	UNP P00720

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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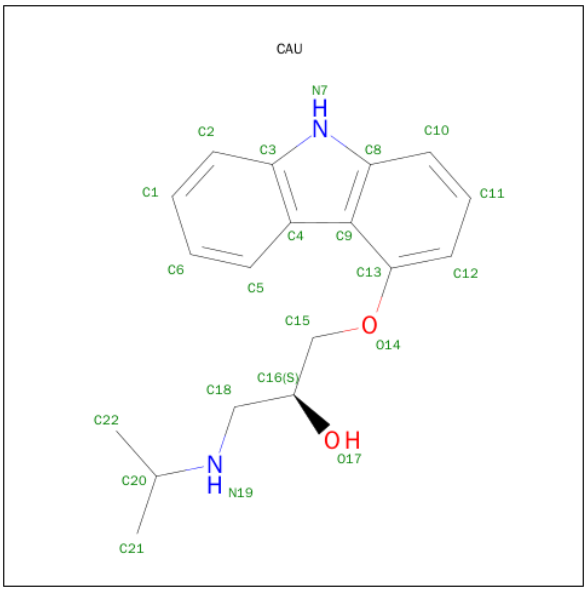
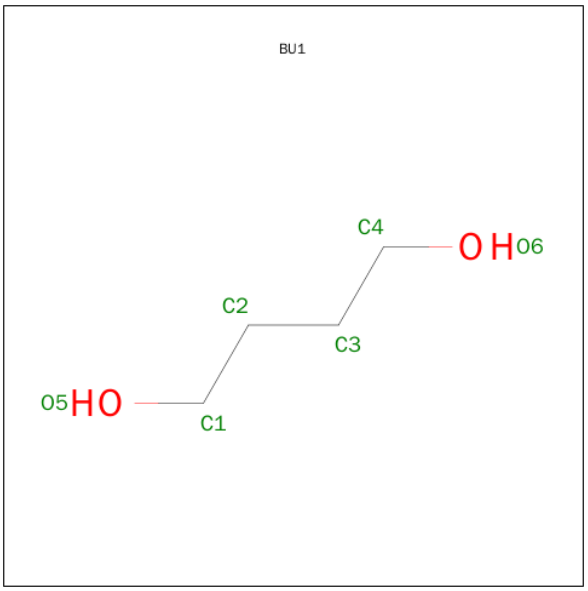
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is (2S)-1-(9H-CARBAZOL-4-YLOXY)-3-(ISOPROPYLAMINO)PROPAN-2-OL (three-letter code: CAU) (formula: $C_{18}H_{22}N_2O_2$).



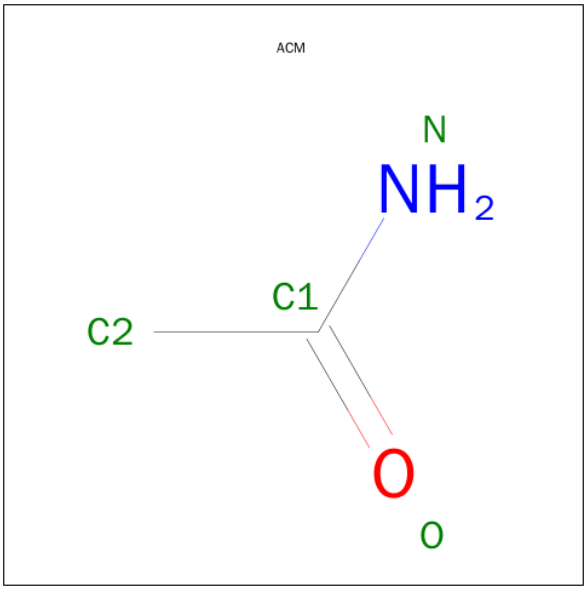
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 18 2 2	0	0

- Molecule 5 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).



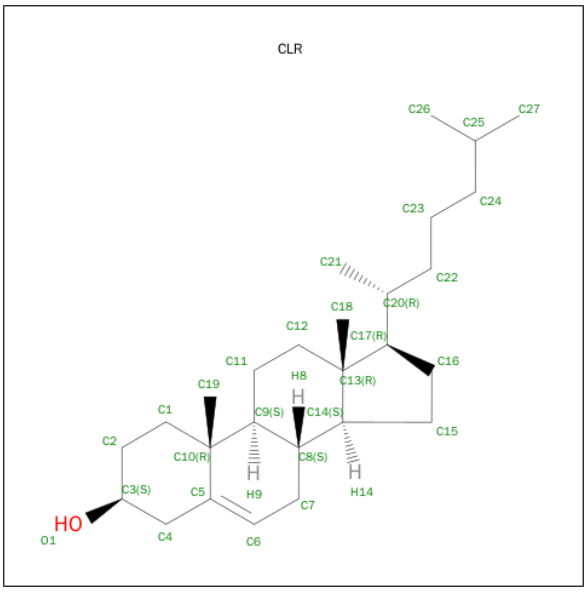
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 4 2	0	0
5	A	1	Total C O 6 4 2	0	0

- Molecule 6 is ACETAMIDE (three-letter code: ACM) (formula: C_2H_5NO).



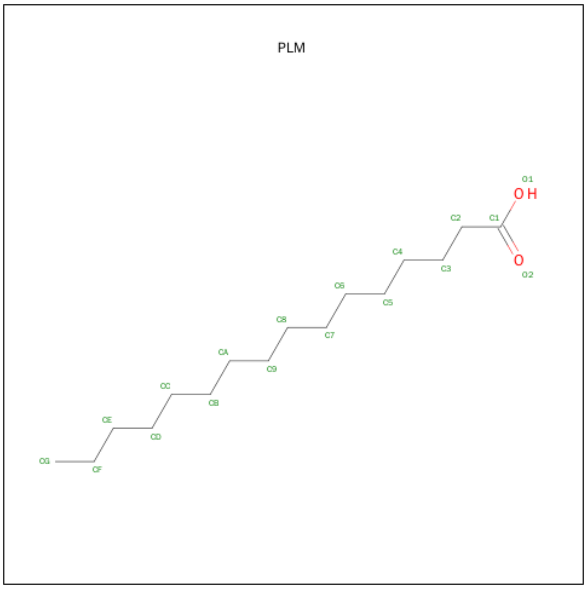
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 4 2 1 1	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



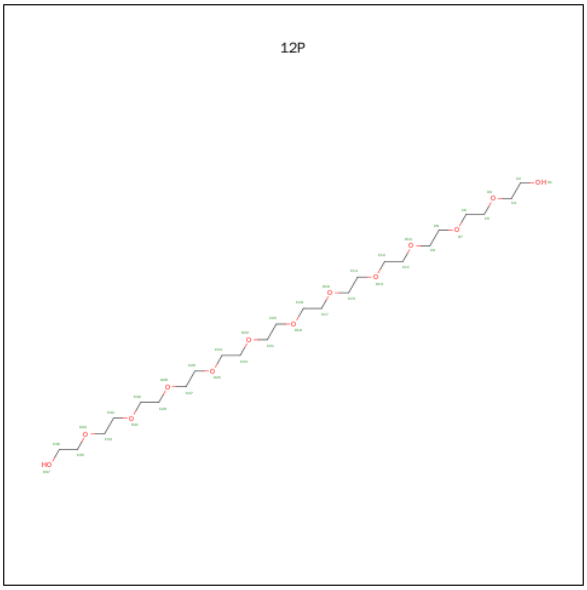
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 28 27 1	0	0
7	A	1	Total C O 28 27 1	0	0
7	A	1	Total C O 28 27 1	0	0

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 17 16 1	0	0

- Molecule 9 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	21	14	7	0	0

- Molecule 10 is water.

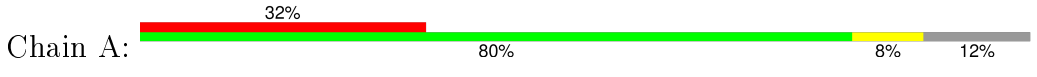
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	48	48	48	0	0

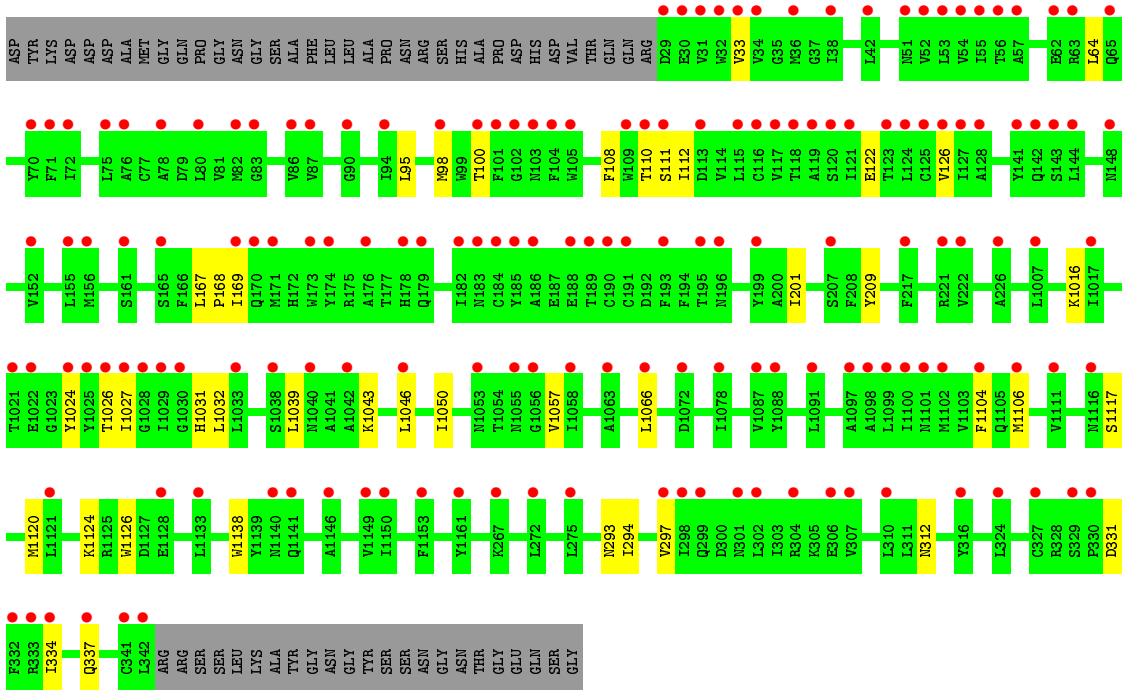
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: beta-2-adrenergic receptor/T4-lysozyme chimera

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.32Å 169.24Å 40.15Å 90.00° 105.62° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.95-2.40) 99.8 (19.95-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.232 0.198 , 0.230	Depositor DCC
R_{free} test set	1310 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 85.3	EDS
Estimated twinning fraction	0.012 for 1/2*h+1/2*k+l,3/2*h-1/2*k+l,-l 0.015 for 1/2*h-1/2*k+l,-3/2*h-1/2*k-l,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 26558 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3804	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BU1, CAU, 12P, ACM, PLM, MAL, CLR, 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	0.64	0/3624	0.67	0/4920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3543	0	3610	25	0
2	A	23	0	22	1	0
3	A	30	0	0	0	0
4	A	22	0	22	0	0
5	A	12	0	20	0	0
6	A	4	0	3	0	0
7	A	84	0	138	9	0
8	A	17	0	31	0	0
9	A	21	0	24	0	0
10	A	48	0	0	0	0
All	All	3804	0	3870	34	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 4.

All (34) 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:1124:LYS:HD3	1:A:1126:TRP:CZ2	2.22	0.74
1:A:334:ILE:HA	1:A:337:GLN:HE21	1.65	0.62
7:A:412:CLR:H272	7:A:414:CLR:H262	1.84	0.60
7:A:412:CLR:H272	7:A:414:CLR:C26	2.32	0.59
7:A:413:CLR:H212	7:A:413:CLR:H183	1.86	0.57
1:A:201:ILE:HD11	1:A:297:VAL:HG11	1.87	0.57
1:A:110:THR:HG22	1:A:169:ILE:HD13	1.86	0.56
1:A:209:TYR:CE1	1:A:294:ILE:HD11	2.42	0.55
7:A:414:CLR:H212	7:A:414:CLR:H121	1.90	0.54
1:A:98:MET:SD	1:A:100:THR:HG22	2.48	0.53
1:A:1124:LYS:HD3	1:A:1126:TRP:CH2	2.45	0.52
1:A:108:PHE:HE2	1:A:112:ILE:HD11	1.76	0.51
1:A:108:PHE:CE2	1:A:112:ILE:HD11	2.46	0.51
1:A:1104:PHE:O	2:A:401:MAL:H4'	2.13	0.48
1:A:1026:THR:HG23	1:A:1031:HIS:O	2.14	0.47
1:A:1024:TYR:HB3	1:A:1032:LEU:HD11	1.97	0.47
1:A:122:GLU:O	1:A:126:VAL:HG23	2.15	0.46
1:A:1016:LYS:HG2	1:A:1057:VAL:HG22	1.97	0.46
1:A:1117:SER:HA	1:A:1120:MET:HE2	1.98	0.46
1:A:64:LEU:HD21	1:A:331:ASP:HB3	1.98	0.45
1:A:1106:MET:HE1	1:A:1138:TRP:CD2	2.52	0.45
7:A:414:CLR:C22	7:A:414:CLR:H263	2.47	0.45
1:A:33:VAL:HG13	1:A:95:LEU:HD22	1.99	0.44
7:A:412:CLR:H193	7:A:414:CLR:C6	2.46	0.44
7:A:412:CLR:H182	7:A:414:CLR:H71	2.00	0.44
7:A:412:CLR:C19	7:A:414:CLR:C6	2.96	0.43
1:A:201:ILE:CD1	1:A:297:VAL:HG11	2.48	0.43
1:A:1039:LEU:HD21	1:A:1043:LYS:HZ3	1.84	0.43
1:A:1050:ILE:HD11	1:A:1066:LEU:HD11	2.02	0.42
1:A:293:ASN:O	1:A:297:VAL:HG23	2.20	0.42
1:A:1027:ILE:HG21	1:A:1046:LEU:HD13	2.02	0.42
1:A:111:SER:HA	1:A:169:ILE:HD12	2.02	0.41
1:A:167:LEU:HB2	1:A:168:PRO:HD3	2.02	0.41
7:A:414:CLR:H222	7:A:414:CLR:H263	2.03	0.41

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	440/500 (88%)	431 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	382/428 (89%)	381 (100%)	1 (0%)	94 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	229	GLN
1	A	1053	ASN
1	A	296	HIS
1	A	337	GLN

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

16 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	$\#\|Z\| > 2$
2	MAL	A	401	-	24,24,24	1.12	2 (8%)	35,35,35	2.40	9 (25%)
3	SO4	A	402	-	4,4,4	0.18	0	6,6,6	0.34	0
3	SO4	A	403	-	4,4,4	0.47	0	6,6,6	0.65	0
3	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.40	0
3	SO4	A	405	-	4,4,4	0.29	0	6,6,6	0.18	0
3	SO4	A	406	-	4,4,4	0.10	0	6,6,6	0.17	0
3	SO4	A	407	-	4,4,4	0.08	0	6,6,6	0.08	0
4	CAU	A	408	-	22,24,24	1.10	2 (9%)	30,33,33	1.18	1 (3%)
5	BU1	A	409	-	5,5,5	0.19	0	4,4,4	0.41	0
5	BU1	A	410	-	5,5,5	0.44	0	4,4,4	0.23	0
6	ACM	A	411	1	3,3,3	0.83	0	3,3,3	0.74	0
7	CLR	A	412	-	31,31,31	0.80	1 (3%)	48,48,48	1.20	5 (10%)
7	CLR	A	413	-	31,31,31	0.62	0	48,48,48	1.04	3 (6%)
7	CLR	A	414	-	31,31,31	0.55	0	48,48,48	0.93	1 (2%)
8	PLM	A	415	1	16,16,17	0.45	0	14,15,17	0.49	0
9	12P	A	416	-	20,20,36	0.62	0	19,19,35	0.53	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
2	MAL	A	401	-	1/1/10/10	0/8/48/48	0/2/2/2
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	SO4	A	403	-	-	0/0/0/0	0/0/0/0
3	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	SO4	A	405	-	-	0/0/0/0	0/0/0/0
3	SO4	A	406	-	-	0/0/0/0	0/0/0/0
3	SO4	A	407	-	-	0/0/0/0	0/0/0/0
4	CAU	A	408	-	-	0/10/10/10	0/3/3/3
5	BU1	A	409	-	-	0/3/3/3	0/0/0/0
5	BU1	A	410	-	-	0/3/3/3	0/0/0/0
6	ACM	A	411	1	-	0/0/0/0	0/0/0/0
7	CLR	A	412	-	-	0/10/68/68	0/4/4/4
7	CLR	A	413	-	-	0/10/68/68	0/4/4/4
7	CLR	A	414	-	-	0/10/68/68	0/4/4/4
8	PLM	A	415	1	-	0/13/14/15	0/0/0/0
9	12P	A	416	-	-	0/18/18/34	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	CAU	C10-C8	-2.76	1.36	1.41
7	A	412	CLR	C19-C10	-2.44	1.50	1.54
4	A	408	CAU	C2-C3	-2.12	1.38	1.41
2	A	401	MAL	O1-C1	2.04	1.47	1.41
2	A	401	MAL	O2-C2	3.31	1.50	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	MAL	C4-C3-C2	-6.51	98.64	110.79
2	A	401	MAL	O5-C1-C2	-5.78	98.41	110.28
7	A	412	CLR	C19-C10-C5	-4.23	101.81	108.36
2	A	401	MAL	O3'-C3'-C2'	-3.73	101.93	110.34
4	A	408	CAU	C12-C13-C9	-3.60	117.51	121.28
7	A	413	CLR	C3-C4-C5	-3.09	105.45	111.82
7	A	414	CLR	C19-C10-C5	-2.42	104.61	108.36
7	A	413	CLR	C19-C10-C5	-2.20	104.96	108.36
2	A	401	MAL	C1-O5-C5	2.10	117.83	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	412	CLR	C1-C10-C9	2.33	111.64	108.64
7	A	413	CLR	O1-C3-C2	2.36	116.74	110.05
7	A	412	CLR	C4-C5-C10	2.39	119.91	116.43
2	A	401	MAL	O2-C2-C1	2.40	115.27	110.02
7	A	412	CLR	C17-C13-C14	2.48	103.01	100.09
7	A	412	CLR	C2-C3-C4	2.63	115.00	110.32
2	A	401	MAL	C1'-C2'-C3'	2.79	114.58	110.43
2	A	401	MAL	O1-C4'-C3'	2.93	114.72	107.17
2	A	401	MAL	O5-C5-C4	3.34	115.95	109.68
2	A	401	MAL	O1-C1-C2	6.79	124.63	108.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	MAL	C1'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	MAL	1	0
7	A	412	CLR	5	0
7	A	413	CLR	1	0
7	A	414	CLR	8	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^{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	A	442/500 (88%)	1.80	162 (36%)	0	0	63, 75, 86, 99	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	VAL	6.8
1	A	117	VAL	6.5
1	A	183	ASN	6.0
1	A	193	PHE	5.8
1	A	72	ILE	5.7
1	A	1027	ILE	5.7
1	A	176	ALA	5.7
1	A	306	GLU	5.6
1	A	1099	LEU	5.5
1	A	1053	ASN	5.4
1	A	1098	ALA	5.3
1	A	1091	LEU	5.3
1	A	337	GLN	5.3
1	A	32	TRP	5.2
1	A	1153	PHE	5.2
1	A	116	CYS	5.1
1	A	1087	VAL	4.6
1	A	57	ALA	4.5
1	A	76	ALA	4.5
1	A	127	ILE	4.4
1	A	62	GLU	4.4
1	A	1140	ASN	4.4
1	A	1038	SER	4.3
1	A	173	TRP	4.3
1	A	1022	GLU	4.2
1	A	1102	MET	4.2
1	A	55	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	SER	4.2
1	A	90	GLY	4.2
1	A	75	LEU	4.2
1	A	42	LEU	4.1
1	A	31	VAL	4.1
1	A	1100	ILE	4.1
1	A	143	SER	3.9
1	A	184	CYS	3.9
1	A	34	VAL	3.9
1	A	1046	LEU	3.9
1	A	30	GLU	3.9
1	A	100	THR	3.9
1	A	199	TYR	3.8
1	A	1133	LEU	3.8
1	A	342	LEU	3.8
1	A	1150	ILE	3.8
1	A	195	THR	3.8
1	A	78	ALA	3.8
1	A	63	ARG	3.7
1	A	1024	TYR	3.7
1	A	1128	GLU	3.7
1	A	29	ASP	3.7
1	A	65	GLN	3.7
1	A	1028	GLY	3.7
1	A	152	VAL	3.6
1	A	1141	GLN	3.6
1	A	105	TRP	3.6
1	A	56	THR	3.6
1	A	54	VAL	3.5
1	A	126	VAL	3.5
1	A	1066	LEU	3.4
1	A	1021	THR	3.4
1	A	1121	LEU	3.4
1	A	121	ILE	3.4
1	A	124	LEU	3.4
1	A	123	THR	3.4
1	A	196	ASN	3.4
1	A	171	MET	3.4
1	A	1033	LEU	3.3
1	A	310	LEU	3.3
1	A	307	VAL	3.2
1	A	1097	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	TYR	3.2
1	A	302	LEU	3.2
1	A	304	ARG	3.2
1	A	333	ARG	3.2
1	A	1116	ASN	3.2
1	A	341	CYS	3.2
1	A	182	ILE	3.1
1	A	1072	ASP	3.1
1	A	170	GLN	3.1
1	A	217	PHE	3.1
1	A	272	LEU	3.1
1	A	1017	ILE	3.0
1	A	33	VAL	3.0
1	A	297	VAL	3.0
1	A	1078	ILE	3.0
1	A	51	ASN	3.0
1	A	144	LEU	3.0
1	A	275	LEU	3.0
1	A	267	LYS	3.0
1	A	53	LEU	3.0
1	A	83	GLY	3.0
1	A	86	VAL	2.9
1	A	156	MET	2.9
1	A	174	TYR	2.9
1	A	185	TYR	2.9
1	A	98	MET	2.9
1	A	222	VAL	2.8
1	A	1101	ASN	2.8
1	A	330	PRO	2.8
1	A	82	MET	2.8
1	A	104	PHE	2.8
1	A	148	ASN	2.7
1	A	110	THR	2.7
1	A	142	GLN	2.7
1	A	70	TYR	2.7
1	A	169	ILE	2.7
1	A	301	ASN	2.7
1	A	178	HIS	2.7
1	A	1104	PHE	2.7
1	A	1055	ASN	2.6
1	A	190	CYS	2.6
1	A	1042	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	109	TRP	2.6
1	A	1007	LEU	2.6
1	A	1063	ALA	2.6
1	A	115	LEU	2.6
1	A	103	ASN	2.5
1	A	119	ALA	2.5
1	A	71	PHE	2.5
1	A	1029	ILE	2.5
1	A	1056	GLY	2.5
1	A	125	CYS	2.4
1	A	221	ARG	2.4
1	A	36	MET	2.4
1	A	118	THR	2.4
1	A	80	LEU	2.4
1	A	165	SER	2.4
1	A	1058	ILE	2.3
1	A	298	ILE	2.3
1	A	186	ALA	2.3
1	A	161	SER	2.3
1	A	1026	THR	2.3
1	A	316	TYR	2.3
1	A	128	ALA	2.3
1	A	332	PHE	2.3
1	A	329	SER	2.3
1	A	191	CYS	2.3
1	A	101	PHE	2.3
1	A	324	LEU	2.3
1	A	1161	TYR	2.2
1	A	188	GLU	2.2
1	A	87	VAL	2.2
1	A	1146	ALA	2.2
1	A	299	GLN	2.2
1	A	113	ASP	2.2
1	A	1025	TYR	2.2
1	A	327	CYS	2.2
1	A	111	SER	2.2
1	A	207	SER	2.2
1	A	1111	VAL	2.2
1	A	226	ALA	2.1
1	A	102	GLY	2.1
1	A	52	VAL	2.1
1	A	1106	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	155	LEU	2.1
1	A	1030	GLY	2.1
1	A	179	GLN	2.1
1	A	38	ILE	2.1
1	A	189	THR	2.1
1	A	334	ILE	2.0
1	A	94	ILE	2.0
1	A	1088	TYR	2.0
1	A	1040	ASN	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	MAL	A	401	23/23	0.68	0.45	3.37	101,116,118,120	0
3	SO4	A	404	5/5	0.94	0.37	1.44	76,78,81,85	0
5	BU1	A	410	6/6	0.69	0.24	1.31	70,72,80,82	0
7	CLR	A	414	28/28	0.74	0.33	1.11	111,114,116,117	0
9	12P	A	416	21/37	0.68	0.36	1.10	77,91,108,110	0
5	BU1	A	409	6/6	0.91	0.25	0.79	46,52,60,65	0
7	CLR	A	412	28/28	0.80	0.25	0.30	96,100,106,107	0
3	SO4	A	402	5/5	0.95	0.29	0.15	79,79,88,91	0
6	ACM	A	411	4/4	0.90	0.21	-0.27	69,71,72,74	0
8	PLM	A	415	17/18	0.66	0.24	-0.65	86,92,101,101	0
7	CLR	A	413	28/28	0.86	0.22	-0.95	81,89,93,94	0
4	CAU	A	408	22/22	0.93	0.16	-1.60	45,54,59,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	407	5/5	0.93	0.58	-	100,103,106,107	0
3	SO4	A	403	5/5	0.94	0.39	-	84,84,93,95	0
3	SO4	A	405	5/5	0.96	0.31	-	62,74,76,77	0
3	SO4	A	406	5/5	0.76	0.43	-	129,131,133,137	0

6.5 Other polymers (i)

There are no such residues in this entry.