Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2016 – 04:09 PM EDT

PDB ID	:	5L3Q
Title	:	Structure of the GTPase heterodimer of human SRP54 and SRalpha
Authors	:	Wild, K.; Segnitz, B.; Sinning, I.
Deposited on	:	2016-05-24
Resolution	:	3.20 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:

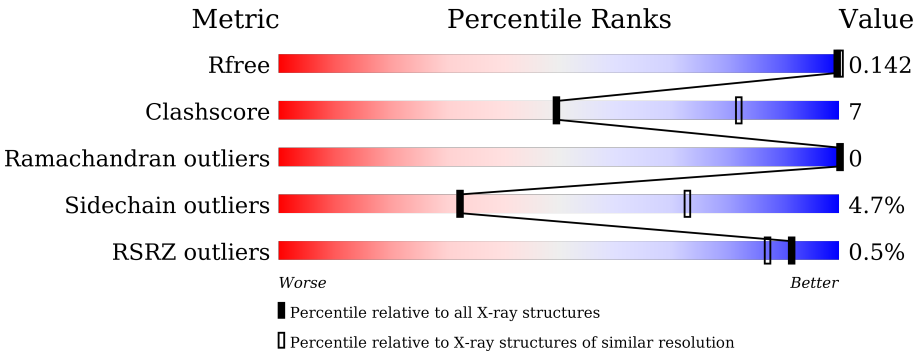
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	442	50% 9% • 40%
1	C	442	% 51% 8% 40%
2	B	638	38% 9% • 52%
2	D	638	39% 8% • 52%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	704	-	-	-	X
6	GOL	B	707	-	-	-	X
6	GOL	D	705	-	-	-	X
7	AMP	A	505	-	-	-	X
7	AMP	C	506	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9156 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 Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2050	1308	345	386	11			
1	C	265	Total	C	N	O	S	0	0	0
			2050	1308	345	386	11			

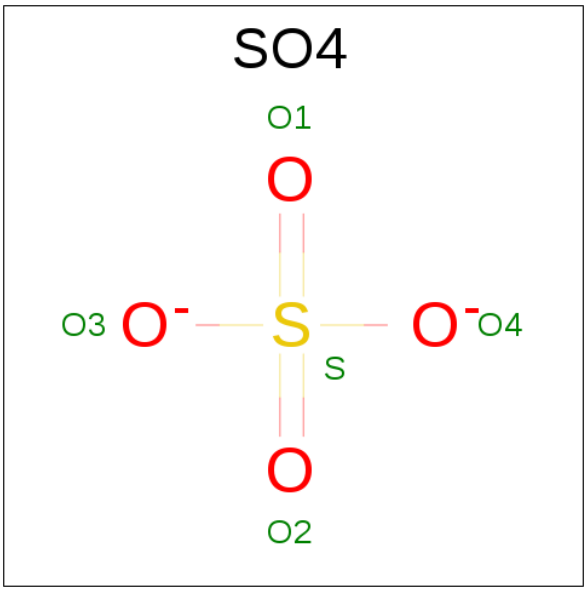
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P61011
A	-4	HIS	-	expression tag	UNP P61011
A	-3	HIS	-	expression tag	UNP P61011
A	-2	HIS	-	expression tag	UNP P61011
A	-1	HIS	-	expression tag	UNP P61011
A	0	HIS	-	expression tag	UNP P61011
C	-5	HIS	-	expression tag	UNP P61011
C	-4	HIS	-	expression tag	UNP P61011
C	-3	HIS	-	expression tag	UNP P61011
C	-2	HIS	-	expression tag	UNP P61011
C	-1	HIS	-	expression tag	UNP P61011
C	0	HIS	-	expression tag	UNP P61011

- Molecule 2 is a protein called Signal recognition particle receptor subunit alpha.

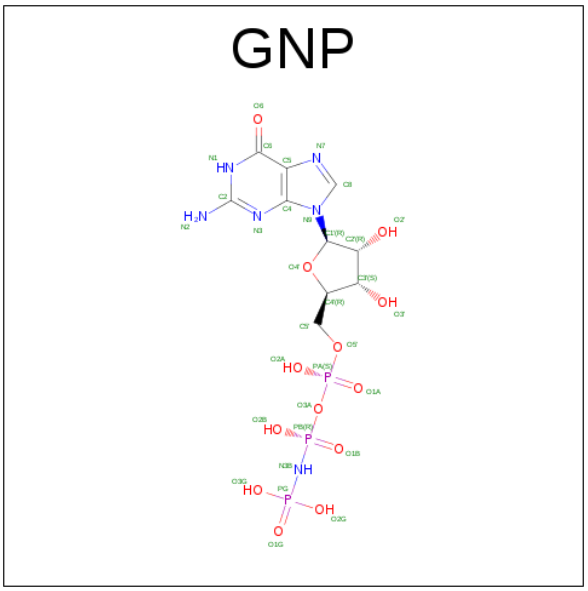
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2340	1471	415	438	16			
2	D	307	Total	C	N	O	S	0	0	0
			2340	1471	415	438	16			

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



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

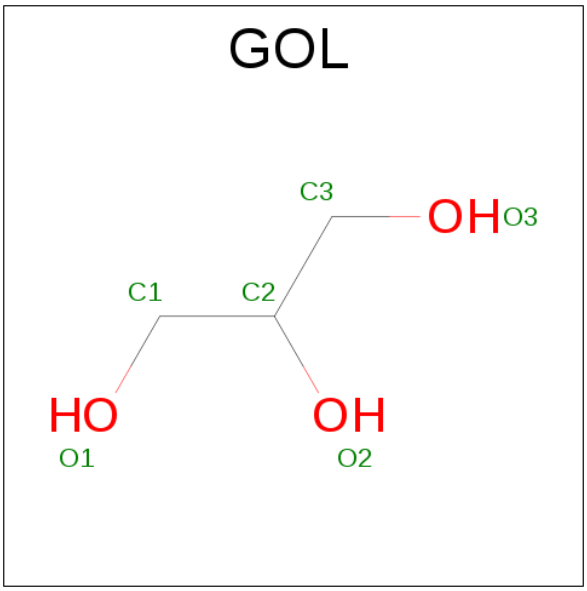


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

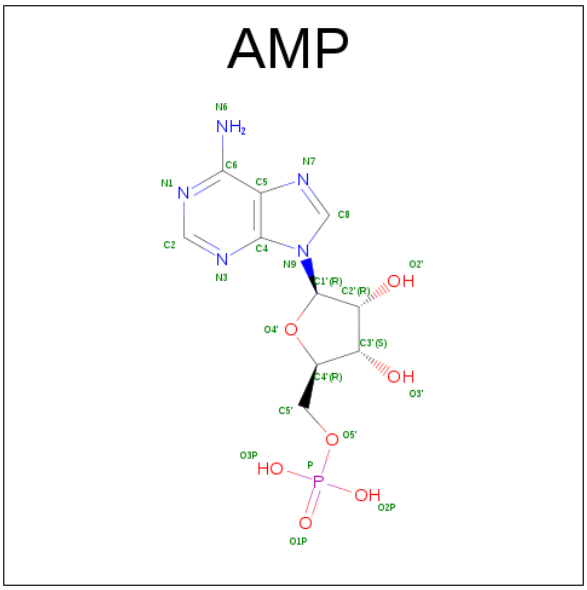
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 8 is water.

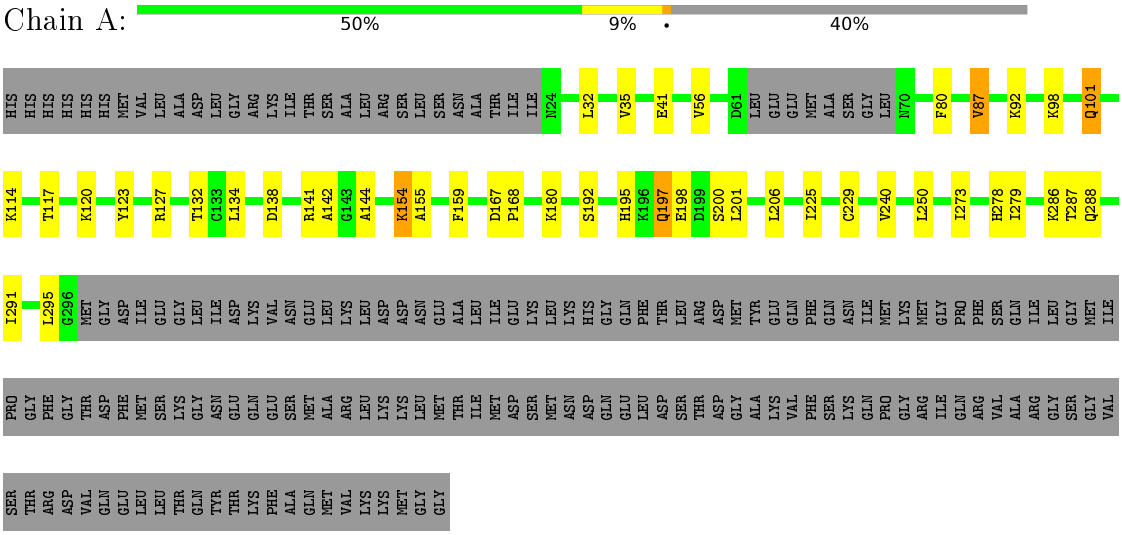
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	31	Total	O	0	0
			31	31		
8	B	42	Total	O	0	0
			42	42		
8	C	20	Total	O	0	0
			20	20		
8	D	36	Total	O	0	0
			36	36		

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.

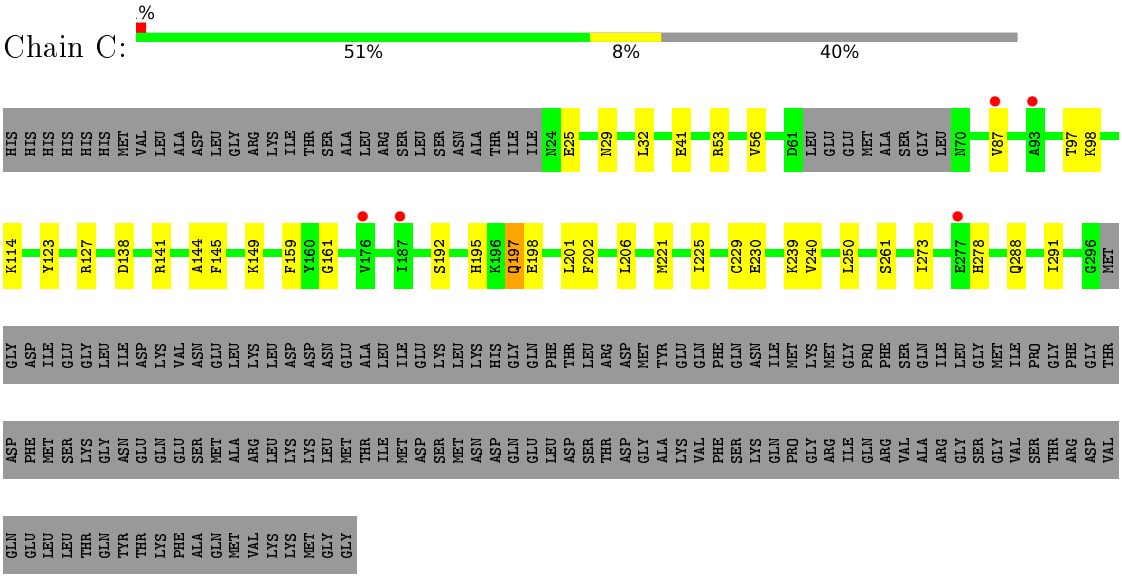
- Molecule 1: Signal recognition particle 54 kDa protein

Chain A:



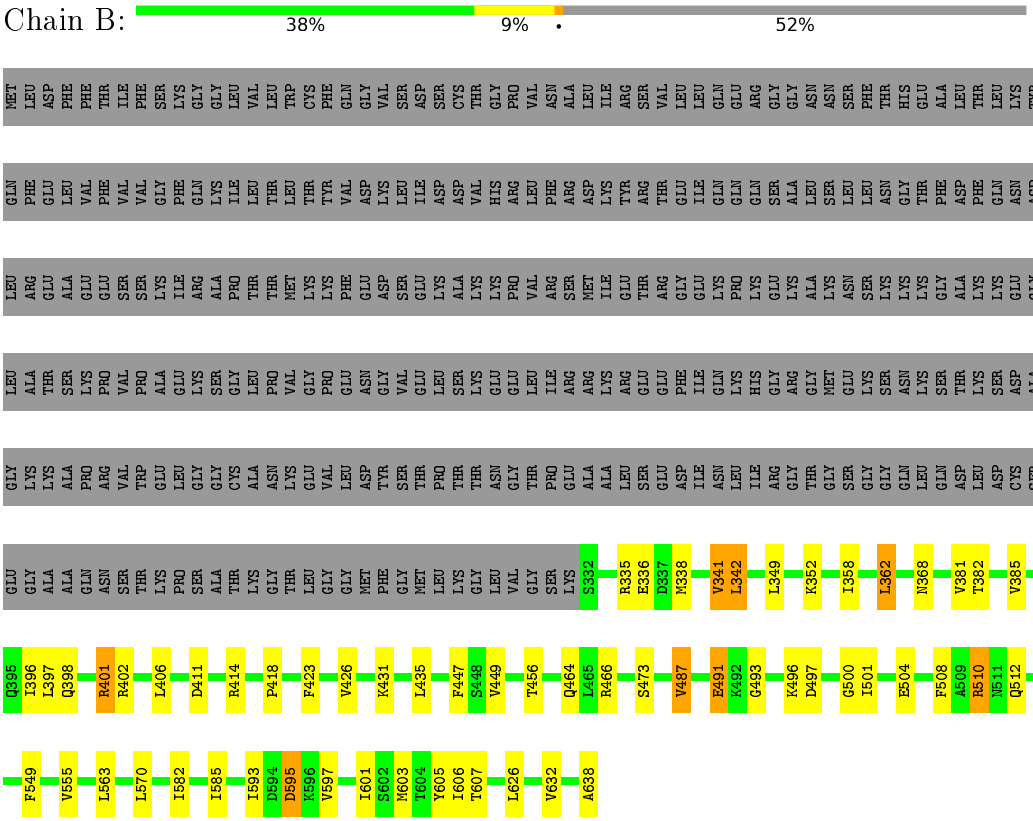
- Molecule 1: Signal recognition particle 54 kDa protein

Chain C:



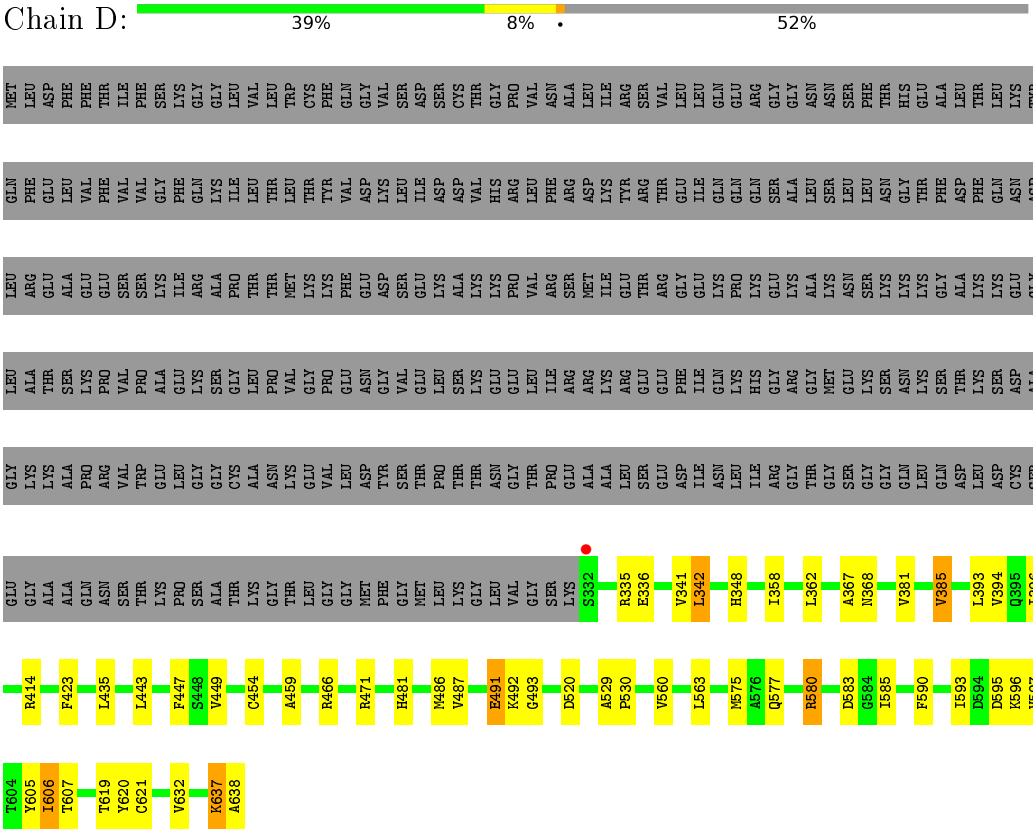
- Molecule 2: Signal recognition particle receptor subunit alpha

Chain B:



- Molecule 2: Signal recognition particle receptor subunit alpha

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	241.39Å 241.39Å 241.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.33 – 3.20 98.55 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (76.33-3.20) 95.9 (98.55-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.145 , 0.191 0.147 , 0.142	Depositor DCC
R_{free} test set	1833 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9156	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: GOL, MG, AMP, GNP, 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	0.46	0/2083	0.58	0/2806
1	C	0.40	0/2083	0.56	0/2806
2	B	0.51	0/2370	0.64	0/3202
2	D	0.49	0/2370	0.65	0/3202
All	All	0.47	0/8906	0.61	0/12016

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	2050	0	2090	30	0
1	C	2050	0	2090	21	0
2	B	2340	0	2406	42	0
2	D	2340	0	2406	37	0
3	A	5	0	0	1	0
3	B	20	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	32	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	13	0	0
4	C	32	0	13	1	0
4	D	32	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	8	2	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	2	0
7	A	23	0	12	2	0
7	C	23	0	12	2	0
8	A	31	0	0	0	0
8	B	42	0	0	3	0
8	C	20	0	0	1	0
8	D	36	0	0	3	0
All	All	9156	0	9100	128	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 7.

All (128) 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)
2:B:491:GLU:HG2	2:B:493:GLY:H	1.43	0.83
1:C:198:GLU:HG2	1:C:201:LEU:HG	1.67	0.76
1:A:278:HIS:CE1	7:A:505:AMP:H2'	2.28	0.69
2:D:459:ALA:H	6:D:705:GOL:H12	1.59	0.68
2:D:491:GLU:HG2	2:D:493:GLY:H	1.60	0.67
2:B:473:SER:HB3	2:B:487:VAL:HG23	1.77	0.67
2:B:411:ASP:OD1	2:B:414:ARG:NH1	2.29	0.65
1:A:287:THR:H	6:A:504:GOL:H32	1.63	0.63
1:A:278:HIS:NE2	7:A:505:AMP:H2'	2.12	0.63
1:C:29:ASN:OD1	1:C:53:ARG:NH2	2.32	0.62
1:A:155:ALA:HB2	1:A:279:ILE:HD13	1.82	0.62
1:C:195:HIS:HD2	1:C:197:GLN:HG2	1.62	0.62
1:C:195:HIS:CD2	1:C:197:GLN:HG2	2.35	0.61
2:D:580:ARG:NH2	2:D:583:ASP:OD2	2.33	0.61
2:D:560:VAL:HG13	2:D:606:ILE:HD12	1.83	0.59
2:B:397:LEU:HD22	2:B:626:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:VAL:HG21	1:C:291:ILE:HD11	1.86	0.57
2:B:549:PHE:HB2	2:B:582:ILE:HD13	1.87	0.57
2:B:497:ASP:N	3:B:702:SO4:O1	2.26	0.57
1:A:225:ILE:HG12	1:A:229:CYS:HB2	1.86	0.56
1:A:195:HIS:CD2	1:A:197:GLN:HG2	2.41	0.56
1:C:123:TYR:CZ	1:C:127:ARG:HD2	2.41	0.56
1:A:198:GLU:HG2	1:A:201:LEU:HG	1.89	0.55
1:C:230:GLU:HB2	1:C:261:SER:HB3	1.88	0.55
2:D:397:LEU:HD12	2:D:632:VAL:HG23	1.89	0.54
2:B:338:MET:HB3	2:B:342:LEU:HD22	1.88	0.54
1:C:145:PHE:CE1	1:C:161:GLY:HA3	2.43	0.54
1:C:225:ILE:HG12	1:C:229:CYS:HB2	1.89	0.54
2:D:358:ILE:HD12	2:D:605:TYR:CD2	2.43	0.54
1:A:142:ALA:O	2:B:464:GLN:HG3	2.08	0.54
1:C:250:LEU:HD12	1:C:273:ILE:HB	1.89	0.53
2:D:335:ARG:NH2	2:D:368:ASN:OD1	2.41	0.53
2:D:396:ILE:HD13	2:D:605:TYR:HD1	1.74	0.53
2:B:381:VAL:O	2:B:385:VAL:HG13	2.09	0.53
2:B:593:ILE:HD13	2:B:597:VAL:HA	1.90	0.52
2:B:423:PHE:CD1	2:B:435:LEU:HD12	2.44	0.52
2:D:596:LYS:HE2	8:D:834:HOH:O	2.11	0.51
2:B:595:ASP:OD2	2:B:595:ASP:N	2.43	0.51
2:B:508:PHE:CZ	2:B:512:GLN:HG3	2.46	0.51
1:A:123:TYR:CZ	1:A:127:ARG:HD2	2.46	0.50
1:A:32:LEU:HD11	1:A:56:VAL:HG11	1.92	0.50
1:A:154:LYS:HE2	3:A:501:SO4:O4	2.10	0.50
1:A:250:LEU:HD12	1:A:273:ILE:HB	1.94	0.50
2:B:418:PRO:HD3	2:B:510:ARG:HG3	1.94	0.49
2:B:396:ILE:HD13	2:B:605:TYR:HD1	1.77	0.49
2:B:338:MET:O	2:B:342:LEU:HB2	2.12	0.49
1:C:138:ASP:OD2	8:C:601:HOH:O	2.20	0.49
2:B:563:LEU:HD13	2:B:607:THR:HG23	1.95	0.49
2:D:590:PHE:CZ	2:D:597:VAL:HG23	2.48	0.49
2:D:393:LEU:HD22	2:D:601:ILE:HG12	1.95	0.48
2:B:335:ARG:NH2	2:B:368:ASN:OD1	2.46	0.47
1:A:195:HIS:HD2	1:A:197:GLN:HG2	1.76	0.47
1:C:278:HIS:CE1	7:C:506:AMP:H2'	2.49	0.47
1:C:141:ARG:HB3	1:C:144:ALA:HB2	1.96	0.47
2:D:381:VAL:O	2:D:385:VAL:HG13	2.14	0.47
2:D:411:ASP:OD1	2:D:414:ARG:NH1	2.48	0.47
2:D:471:ARG:HG3	2:D:471:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:HG2	1:A:201:LEU:CG	2.45	0.47
1:C:202:PHE:HB3	1:C:239:LYS:HE3	1.96	0.47
2:D:580:ARG:CZ	2:D:580:ARG:HB3	2.45	0.46
1:A:286:LYS:HA	6:A:504:GOL:H32	1.96	0.46
2:D:563:LEU:HD22	2:D:607:THR:HG21	1.98	0.46
2:B:496:LYS:HB2	2:B:501:ILE:HD11	1.97	0.45
2:D:529:ALA:HB3	2:D:530:PRO:HD3	1.97	0.45
2:D:459:ALA:N	6:D:705:GOL:H12	2.29	0.45
1:A:87:VAL:HG21	1:A:291:ILE:HD11	1.97	0.45
2:D:637:LYS:HG3	2:D:638:ALA:N	2.31	0.45
2:B:401:ARG:H	2:B:401:ARG:HG2	1.62	0.45
2:D:348:HIS:NE2	2:D:638:ALA:HB2	2.32	0.45
2:D:577:GLN:HG2	8:D:827:HOH:O	2.17	0.45
2:B:529:ALA:HB3	2:B:530:PRO:HD3	1.98	0.45
1:A:134:LEU:O	1:A:159:PHE:HA	2.17	0.45
2:B:358:ILE:HG22	2:B:362:LEU:HD22	1.99	0.45
2:D:394:VAL:O	2:D:398:GLN:HG2	2.17	0.45
1:A:197:GLN:HE21	1:A:197:GLN:HB3	1.64	0.44
2:B:406:LEU:HD22	2:B:447:PHE:HE1	1.82	0.44
1:A:138:ASP:OD1	1:A:192:SER:HB3	2.18	0.44
2:B:426:VAL:HG22	8:B:818:HOH:O	2.17	0.44
1:C:32:LEU:HD11	1:C:56:VAL:HG11	1.99	0.44
1:A:198:GLU:HG3	1:A:201:LEU:H	1.83	0.44
2:B:500:GLY:O	2:B:504:GLU:HG3	2.17	0.44
2:D:619:THR:HG22	2:D:620:TYR:N	2.33	0.44
2:B:341:VAL:HG21	2:B:382:THR:HA	2.00	0.43
2:B:394:VAL:O	2:B:398:GLN:HG2	2.18	0.43
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.85	0.43
2:B:358:ILE:O	2:B:362:LEU:HB2	2.18	0.43
2:B:585:ILE:HD13	2:B:603:MET:HB3	2.01	0.43
1:C:149:LYS:HG3	1:C:159:PHE:CZ	2.53	0.43
1:A:141:ARG:HB3	1:A:144:ALA:HB2	2.00	0.42
1:A:114:LYS:NZ	4:A:502:GNP:O2B	2.51	0.42
2:B:456:THR:HG21	2:B:501:ILE:HD12	2.01	0.42
1:A:138:ASP:CG	1:A:192:SER:HB3	2.39	0.42
2:B:349:LEU:HD11	2:B:389:LEU:HD21	2.00	0.42
2:B:466:ARG:NH1	8:B:801:HOH:O	2.34	0.42
2:D:471:ARG:NH1	8:D:806:HOH:O	2.52	0.42
1:A:117:THR:HA	1:A:120:LYS:HB2	2.01	0.42
2:D:454:CYS:HB2	2:D:520:ASP:O	2.19	0.42
2:D:397:LEU:HD23	2:D:397:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:619:THR:HG22	2:D:621:CYS:H	1.84	0.42
2:B:393:LEU:HD22	2:B:601:ILE:HG12	2.01	0.42
2:B:431:LYS:HE2	8:B:805:HOH:O	2.19	0.42
2:B:426:VAL:HA	2:B:524:ARG:O	2.20	0.42
1:A:114:LYS:HE2	1:A:114:LYS:HB2	1.93	0.42
2:B:563:LEU:HD22	2:B:607:THR:HG21	2.01	0.42
2:D:342:LEU:HD21	2:D:367:ALA:HB2	2.02	0.42
2:D:585:ILE:HD13	2:D:603:MET:HB3	2.02	0.42
2:B:368:ASN:O	2:D:414:ARG:NH2	2.53	0.42
2:D:336:GLU:H	2:D:336:GLU:HG3	1.66	0.42
1:A:123:TYR:OH	1:A:127:ARG:HD2	2.20	0.41
1:C:25:GLU:O	1:C:29:ASN:ND2	2.43	0.41
2:B:336:GLU:H	2:B:336:GLU:HG3	1.63	0.41
2:D:443:LEU:HD23	2:D:447:PHE:O	2.20	0.41
2:D:595:ASP:OD2	2:D:637:LYS:HE2	2.20	0.41
1:A:101:GLN:OE1	1:A:180:LYS:HB2	2.20	0.41
1:C:138:ASP:OD1	1:C:192:SER:HB3	2.21	0.41
1:C:278:HIS:NE2	7:C:506:AMP:H2'	2.36	0.41
1:A:167:ASP:HA	1:A:168:PRO:HD2	1.89	0.41
2:D:423:PHE:CD1	2:D:435:LEU:HD12	2.56	0.41
2:B:570:LEU:HA	2:B:570:LEU:HD23	1.89	0.41
2:B:358:ILE:HD12	2:B:605:TYR:CD2	2.56	0.41
2:B:397:LEU:HD12	2:B:632:VAL:HG23	2.02	0.41
2:D:481:HIS:CG	2:D:486:MET:HG3	2.56	0.41
1:C:114:LYS:NZ	4:C:503:GNP:O2B	2.40	0.41
2:D:593:ILE:H	2:D:593:ILE:HG13	1.78	0.40
2:B:352:LYS:NZ	2:B:638:ALA:HB2	2.36	0.40
2:D:491:GLU:HG2	2:D:492:LYS:N	2.31	0.40
1:A:80:PHE:HE2	1:A:288:GLN:HE21	1.69	0.40
1:C:149:LYS:HG3	1:C:159:PHE:CE2	2.56	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	261/442 (59%)	259 (99%)	2 (1%)	0	100	100
1	C	261/442 (59%)	260 (100%)	1 (0%)	0	100	100
2	B	305/638 (48%)	293 (96%)	12 (4%)	0	100	100
2	D	305/638 (48%)	293 (96%)	12 (4%)	0	100	100
All	All	1132/2160 (52%)	1105 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	221/373 (59%)	209 (95%)	12 (5%)	27	68
1	C	221/373 (59%)	213 (96%)	8 (4%)	42	79
2	B	252/533 (47%)	240 (95%)	12 (5%)	31	72
2	D	252/533 (47%)	240 (95%)	12 (5%)	31	72
All	All	946/1812 (52%)	902 (95%)	44 (5%)	32	73

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	41	GLU
1	A	87	VAL
1	A	92	LYS
1	A	98	LYS
1	A	101	GLN
1	A	132	THR
1	A	154	LYS
1	A	197	GLN
1	A	200	SER

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Mol	Chain	Res	Type
1	A	206	LEU
1	A	240	VAL
2	B	341	VAL
2	B	342	LEU
2	B	362	LEU
2	B	401	ARG
2	B	402	ARG
2	B	449	VAL
2	B	487	VAL
2	B	491	GLU
2	B	510	ARG
2	B	555	VAL
2	B	595	ASP
2	B	606	ILE
1	C	41	GLU
1	C	97	THR
1	C	98	LYS
1	C	197	GLN
1	C	206	LEU
1	C	221	MET
1	C	240	VAL
1	C	288	GLN
2	D	341	VAL
2	D	342	LEU
2	D	362	LEU
2	D	385	VAL
2	D	449	VAL
2	D	466	ARG
2	D	487	VAL
2	D	491	GLU
2	D	575	MET
2	D	580	ARG
2	D	606	ILE
2	D	637	LYS

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 (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 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	SO4	A	501	-	4,4,4	0.26	0	6,6,6	0.22	0
4	GNP	A	502	5	29,34,34	2.58	9 (31%)	28,54,54	1.91	7 (25%)
6	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.62	0
7	AMP	A	505	-	22,25,25	0.97	1 (4%)	22,38,38	1.77	1 (4%)
3	SO4	B	701	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	B	702	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	B	703	-	4,4,4	0.21	0	6,6,6	0.16	0
3	SO4	B	704	-	4,4,4	0.21	0	6,6,6	0.11	0
4	GNP	B	705	5	29,34,34	2.66	10 (34%)	28,54,54	1.92	7 (25%)
6	GOL	B	707	-	5,5,5	0.28	0	5,5,5	0.69	0
3	SO4	C	501	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	C	502	-	4,4,4	0.21	0	6,6,6	0.14	0
4	GNP	C	503	5	29,34,34	2.80	10 (34%)	28,54,54	1.83	5 (17%)
6	GOL	C	505	-	5,5,5	0.35	0	5,5,5	0.30	0
7	AMP	C	506	-	22,25,25	1.03	1 (4%)	22,38,38	1.93	3 (13%)
3	SO4	D	701	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	D	702	-	4,4,4	0.21	0	6,6,6	0.15	0
4	GNP	D	703	5	29,34,34	2.78	11 (37%)	28,54,54	1.71	5 (17%)
6	GOL	D	705	-	5,5,5	0.32	0	5,5,5	0.37	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
4	GNP	A	502	5	-	0/16/38/38	0/3/3/3
6	GOL	A	504	-	-	0/4/4/4	0/0/0/0
7	AMP	A	505	-	-	0/6/26/26	0/3/3/3
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0
3	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	SO4	B	703	-	-	0/0/0/0	0/0/0/0
3	SO4	B	704	-	-	0/0/0/0	0/0/0/0
4	GNP	B	705	5	-	0/16/38/38	0/3/3/3
6	GOL	B	707	-	-	0/4/4/4	0/0/0/0
3	SO4	C	501	-	-	0/0/0/0	0/0/0/0
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
4	GNP	C	503	5	-	0/16/38/38	0/3/3/3
6	GOL	C	505	-	-	0/4/4/4	0/0/0/0
7	AMP	C	506	-	-	0/6/26/26	0/3/3/3
3	SO4	D	701	-	-	0/0/0/0	0/0/0/0
3	SO4	D	702	-	-	0/0/0/0	0/0/0/0
4	GNP	D	703	5	-	0/16/38/38	0/3/3/3
6	GOL	D	705	-	-	0/4/4/4	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	703	GNP	C4-N9	-8.20	1.36	1.47
4	C	503	GNP	C4-N9	-7.93	1.37	1.47
4	B	705	GNP	C4-N9	-7.65	1.37	1.47
4	A	502	GNP	C4-N9	-7.25	1.38	1.47
4	B	705	GNP	C5-C6	-6.60	1.41	1.53
4	D	703	GNP	C5-C6	-6.38	1.41	1.53
4	C	503	GNP	C5-C6	-6.31	1.41	1.53
4	A	502	GNP	C5-C6	-6.21	1.41	1.53
4	C	503	GNP	PB-O3A	-5.34	1.52	1.59
4	D	703	GNP	PB-O3A	-4.72	1.53	1.59
4	A	502	GNP	PB-O3A	-4.09	1.54	1.59
4	B	705	GNP	PB-O3A	-4.03	1.54	1.59
4	D	703	GNP	PB-O2B	-3.34	1.47	1.56
4	C	503	GNP	PB-O2B	-3.33	1.47	1.56
4	B	705	GNP	PB-O2B	-3.09	1.48	1.56
4	A	502	GNP	PB-O2B	-3.09	1.48	1.56
4	A	502	GNP	C8-N9	-2.91	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	GNP	C8-N9	-2.81	1.38	1.47
4	C	503	GNP	C8-N9	-2.79	1.38	1.47
4	C	503	GNP	C2-N3	-2.70	1.32	1.43
4	D	703	GNP	C8-N9	-2.69	1.38	1.47
4	D	703	GNP	C2-N3	-2.61	1.32	1.43
4	B	705	GNP	C2-N3	-2.44	1.33	1.43
4	B	705	GNP	PG-O3G	-2.29	1.50	1.56
4	A	502	GNP	C2-N3	-2.26	1.34	1.43
4	D	703	GNP	PG-O3G	-2.13	1.51	1.56
4	C	503	GNP	PG-O2G	-2.10	1.51	1.56
4	A	502	GNP	PG-O3G	-2.05	1.51	1.56
4	D	703	GNP	PG-O2G	-2.04	1.51	1.56
4	D	703	GNP	C1'-N9	2.04	1.46	1.42
4	C	503	GNP	C1'-N9	2.19	1.46	1.42
4	B	705	GNP	C1'-N9	2.21	1.46	1.42
7	A	505	AMP	C5-C4	3.25	1.47	1.40
4	B	705	GNP	C6-N1	3.50	1.39	1.33
7	C	506	AMP	C5-C4	3.53	1.48	1.40
4	D	703	GNP	C6-N1	3.54	1.39	1.33
4	C	503	GNP	C6-N1	3.78	1.39	1.33
4	A	502	GNP	C6-N1	4.18	1.40	1.33
4	B	705	GNP	PG-O1G	4.50	1.51	1.46
4	D	703	GNP	PG-O1G	4.92	1.51	1.46
4	A	502	GNP	PG-O1G	5.13	1.51	1.46
4	C	503	GNP	PG-O1G	5.24	1.51	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	506	AMP	N3-C2-N1	-7.49	122.98	128.87
7	A	505	AMP	N3-C2-N1	-7.00	123.37	128.87
4	A	502	GNP	O3G-PG-O1G	-3.22	105.11	113.58
4	B	705	GNP	O3G-PG-O1G	-3.18	105.20	113.58
4	C	503	GNP	PA-O3A-PB	-2.95	122.00	132.71
7	C	506	AMP	C1'-N9-C4	-2.75	123.74	126.81
4	C	503	GNP	O6-C6-N1	-2.73	119.22	122.80
4	A	502	GNP	C3'-C2'-C1'	-2.63	96.16	101.44
4	D	703	GNP	PA-O3A-PB	-2.57	123.38	132.71
4	B	705	GNP	O6-C6-N1	-2.54	119.46	122.80
4	D	703	GNP	O6-C6-N1	-2.49	119.53	122.80
4	B	705	GNP	PA-O3A-PB	-2.02	125.40	132.71
7	C	506	AMP	C2-N1-C6	2.25	122.78	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	705	GNP	O3G-PG-O2G	2.55	115.07	107.67
4	A	502	GNP	O3G-PG-O2G	2.73	115.59	107.67
4	D	703	GNP	O2B-PB-O1B	2.73	115.40	110.02
4	A	502	GNP	O2B-PB-O1B	2.80	115.53	110.02
4	A	502	GNP	O3A-PB-N3B	3.10	114.62	106.07
4	B	705	GNP	O2B-PB-O1B	3.23	116.39	110.02
4	A	502	GNP	O6-C6-C5	3.36	126.11	119.69
4	C	503	GNP	O2B-PB-O1B	3.52	116.95	110.02
4	B	705	GNP	O6-C6-C5	4.53	128.36	119.69
4	D	703	GNP	O6-C6-C5	4.58	128.44	119.69
4	C	503	GNP	O6-C6-C5	4.67	128.61	119.69
4	C	503	GNP	C4-C5-N7	5.30	110.94	102.67
4	A	502	GNP	C4-C5-N7	5.48	111.22	102.67
4	D	703	GNP	C4-C5-N7	5.63	111.46	102.67
4	B	705	GNP	C4-C5-N7	5.77	111.67	102.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SO4	1	0
4	A	502	GNP	1	0
6	A	504	GOL	2	0
7	A	505	AMP	2	0
3	B	702	SO4	1	0
4	C	503	GNP	1	0
7	C	506	AMP	2	0
6	D	705	GOL	2	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	A	265/442 (59%)	0.14	0 100 100	35, 54, 115, 151	0
1	C	265/442 (59%)	0.58	5 (1%) 70 55	49, 72, 123, 163	0
2	B	307/638 (48%)	-0.00	0 100 100	31, 49, 86, 126	0
2	D	307/638 (48%)	0.05	1 (0%) 94 93	31, 49, 91, 122	0
All	All	1144/2160 (52%)	0.18	6 (0%) 91 87	31, 55, 106, 163	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	VAL	3.1
1	C	93	ALA	2.4
2	D	332	SER	2.3
1	C	277	GLU	2.3
1	C	187	ILE	2.2
1	C	87	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
6	GOL	B	707	6/6	0.77	1.07	14.35	99,101,101,102	0
6	GOL	D	705	6/6	0.94	1.11	10.90	110,111,112,113	0
7	AMP	A	505	23/23	0.71	0.70	7.12	55,78,192,192	23
3	SO4	B	704	5/5	0.78	0.63	6.29	180,180,181,181	0
7	AMP	C	506	23/23	0.73	0.61	3.30	55,90,168,169	23
4	GNP	B	705	32/32	0.99	0.23	-0.57	26,36,42,55	0
4	GNP	D	703	32/32	0.99	0.23	-0.67	22,36,42,57	0
4	GNP	A	502	32/32	0.99	0.23	-0.95	27,37,43,47	0
4	GNP	C	503	32/32	0.99	0.24	-1.25	33,45,49,53	0
5	MG	D	704	1/1	0.99	0.08	-3.36	24,24,24,24	0
5	MG	A	503	1/1	1.00	0.10	-3.63	30,30,30,30	0
5	MG	B	706	1/1	0.99	0.10	-3.69	28,28,28,28	0
3	SO4	C	501	5/5	0.80	0.21	-	151,152,152,152	0
3	SO4	D	702	5/5	0.81	0.34	-	147,148,148,149	0
3	SO4	B	701	5/5	0.89	0.31	-	157,157,157,157	0
3	SO4	D	701	5/5	0.92	0.29	-	135,135,136,137	0
5	MG	C	504	1/1	0.99	0.08	-	40,40,40,40	0
6	GOL	C	505	6/6	0.73	0.25	-	107,108,110,110	0
3	SO4	A	501	5/5	0.85	0.81	-	165,165,165,166	0
3	SO4	C	502	5/5	0.86	0.50	-	155,155,156,156	0
3	SO4	B	702	5/5	0.85	0.40	-	155,156,156,156	0
3	SO4	B	703	5/5	0.91	0.33	-	131,133,133,134	0
6	GOL	A	504	6/6	0.76	0.29	-	95,98,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.