Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:54 PM GMT

PDB ID	:	4DRU
Title	:	HCV NS5B in complex with macrocyclic INDOLE INHIBITOR
Authors	:	Cummings, M.D.; Vendeville, S.
Deposited on	:	2012-02-17
Resolution	:	2.10 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:

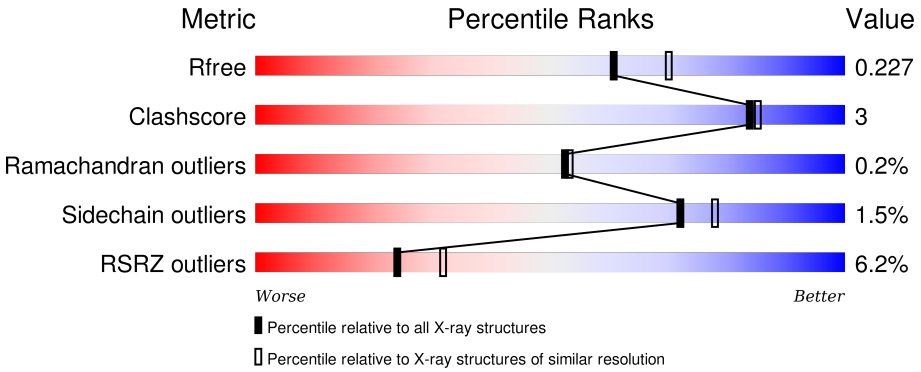
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	563	11% 88% 9%
1	B	563	% 93% 6%

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
3	SO4	A	603	-	-	-	X
3	SO4	A	605	-	-	-	X
3	SO4	B	602	-	-	-	X
3	SO4	B	607	-	-	-	X
3	SO4	B	609	-	-	-	X
3	SO4	B	610	-	-	-	X
3	SO4	B	611	-	-	-	X
4	GOL	A	606	-	-	-	X
4	GOL	A	607	-	-	-	X
4	GOL	B	613	-	-	-	X
4	GOL	B	614	-	-	-	X
4	GOL	B	616	-	-	-	X

2 Entry composition

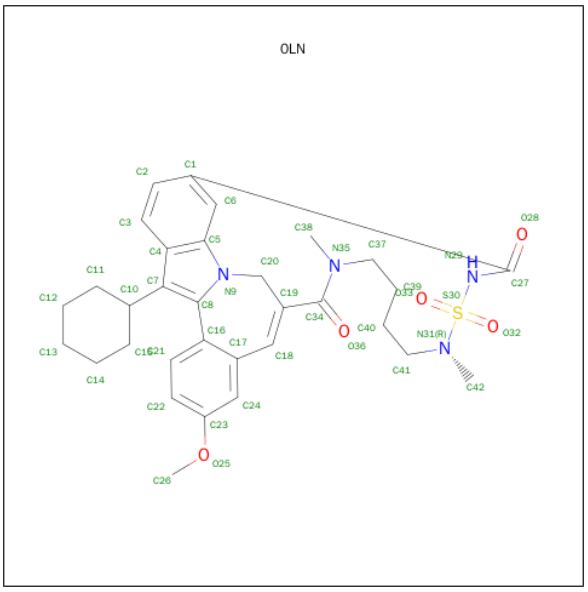
There are 5 unique types of molecules in this entry. The entry contains 9474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA-directed RNA polymerase.

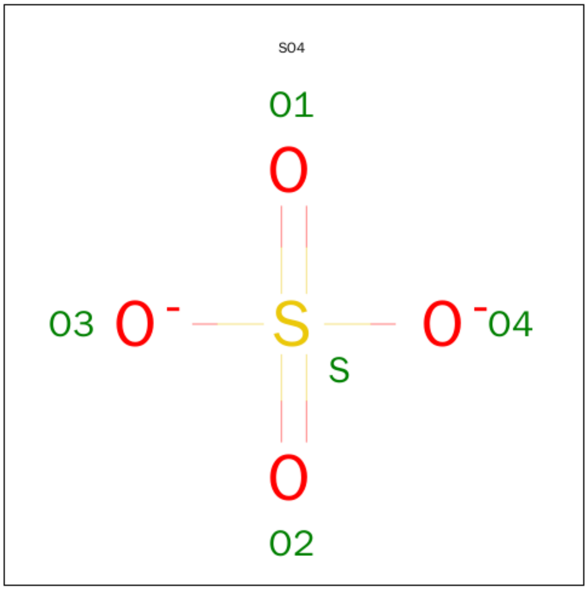
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	27	1	0
			4286	2698	756	800	32			
1	B	559	Total	C	N	O	S	14	6	0
			4403	2768	778	824	33			

- Molecule 2 is 13-CYCLOHEXYL-3-METHOXY-17,22-DIMETHYL-7H-10,6-(METHANOIMINOTHIOIMINOBUTANOIMINOMETHANO)INDOLO[2,1-A][2]BENZAZEPINE-14,23-DIONE 16,16-DIOXIDE (three-letter code: 0LN) (formula: $C_{32}H_{38}N_4O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			42	32	4	5	1		

- 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	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
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	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	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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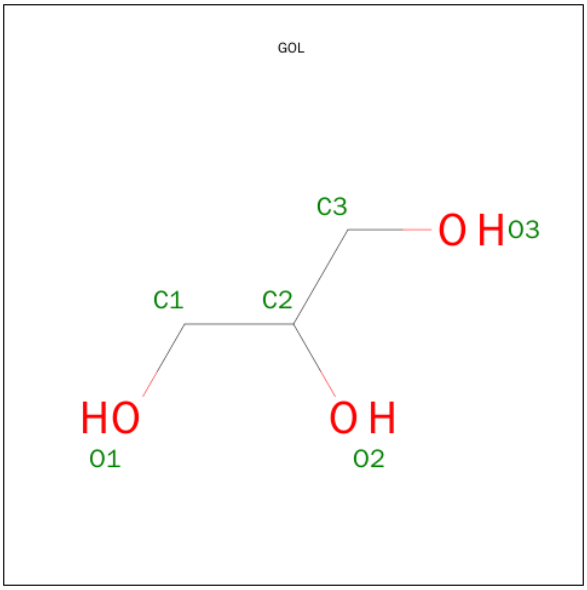
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	250	Total O 250 250	0	0

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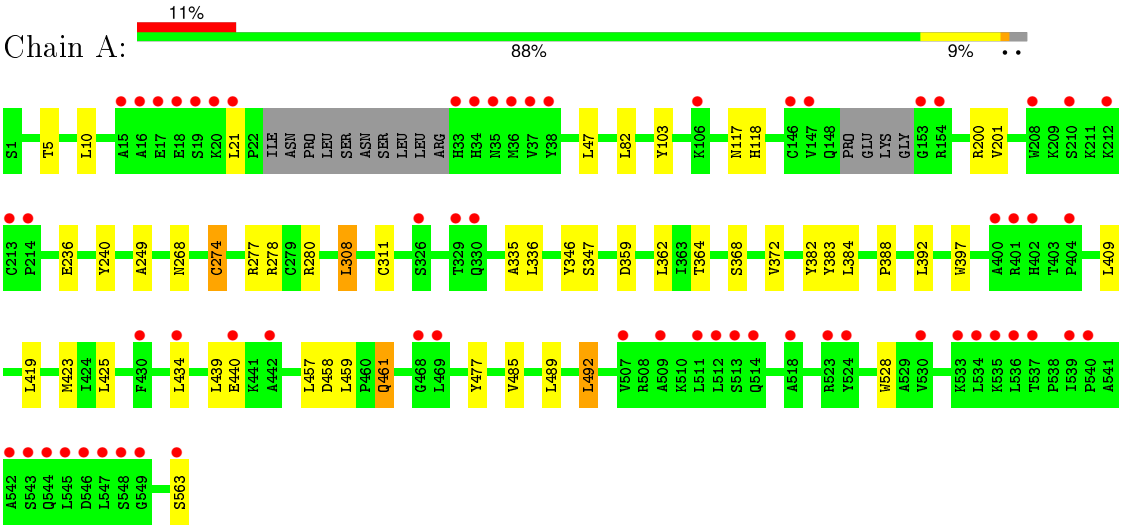
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	376	Total	O	0	0
			376	376		

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.

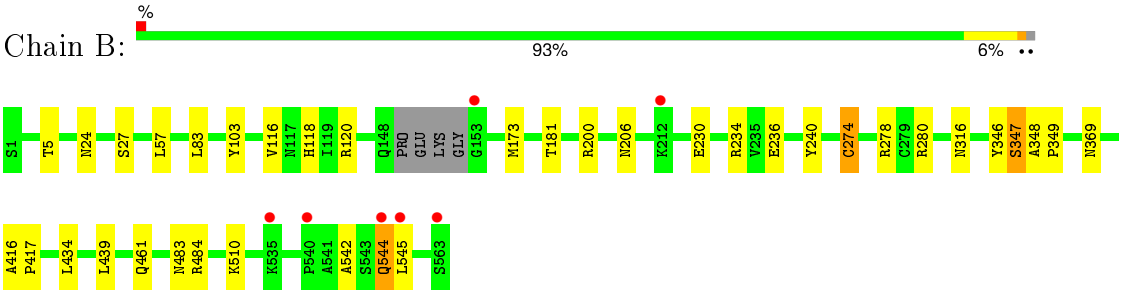
- Molecule 1: RNA-directed RNA polymerase

Chain A:



- Molecule 1: RNA-directed RNA polymerase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.13Å 106.64Å 133.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.63 – 2.10 41.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.63-2.10) 98.9 (41.63-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.226 0.194 , 0.227	Depositor DCC
R_{free} test set	990 reflections (1.15%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.5	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 86907 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9474	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.375 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: GOL, SO4, 0LN

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	0.53	1/4378 (0.0%)	0.63	2/5938 (0.0%)
1	B	0.60	1/4498 (0.0%)	0.69	2/6103 (0.0%)
All	All	0.57	2/8876 (0.0%)	0.66	4/12041 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	CYS	CB-SG	-8.96	1.67	1.82
1	A	274	CYS	CB-SG	-5.42	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	280	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	280	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	280	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	277	ARG	NE-CZ-NH2	5.09	122.84	120.30

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	4286	0	4285	24	0
1	B	4403	0	4394	28	0
2	A	42	0	38	1	0
3	A	20	0	0	0	0
3	B	55	0	0	0	0
4	A	12	0	16	1	0
4	B	30	0	40	0	0
5	A	250	0	0	1	0
5	B	376	0	0	5	0
All	All	9474	0	8773	52	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 (52) 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:B:369:ASN:HD21	1:B:484:ARG:HH22	1.26	0.80
1:B:236[B]:GLU:OE2	1:B:240:TYR:OH	2.11	0.67
1:A:117:ASN:HB3	5:A:909:HOH:O	1.95	0.66
1:A:21:LEU:HD21	1:A:397:TRP:HA	1.84	0.60
1:A:236[A]:GLU:OE1	1:A:240:TYR:OH	2.15	0.60
1:B:544:GLN:HA	1:B:544:GLN:HE21	1.69	0.58
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.45	0.57
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.89	0.55
1:B:103:TYR:OH	1:B:118[B]:HIS:HD2	1.91	0.54
1:B:230:GLU:HG3	1:B:234:ARG:HH11	1.74	0.53
1:A:103:TYR:OH	1:A:118:HIS:HD2	1.92	0.53
1:A:458:ASP:HA	1:A:461:GLN:HE22	1.74	0.53
1:B:542:ALA:O	1:B:545:LEU:HB2	2.09	0.52
1:B:200:ARG:HH12	1:B:316:ASN:HD21	1.58	0.50
1:B:544:GLN:CA	1:B:544:GLN:HE21	2.23	0.50
1:A:10:LEU:HD23	4:A:607:GOL:H11	1.93	0.50
1:B:230:GLU:HG3	1:B:234:ARG:NH1	2.27	0.49
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.54	0.48
1:B:483:ASN:HB3	5:B:1024:HOH:O	2.14	0.47
1:B:173:MET:CE	5:B:1074:HOH:O	2.62	0.47
1:B:347:SER:O	1:B:349:PRO:CD	2.63	0.47
1:B:116:VAL:O	1:B:120:ARG:HG3	2.15	0.47
1:B:200:ARG:HH12	1:B:316:ASN:ND2	2.14	0.46
1:B:346:TYR:O	1:B:347:SER:CB	2.63	0.46
1:B:206:ASN:HB3	5:B:995:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:GLU:CG	1:B:234:ARG:HH11	2.30	0.45
1:B:230:GLU:CG	1:B:234:ARG:NH1	2.80	0.45
1:B:483:ASN:ND2	5:B:1025:HOH:O	2.49	0.45
1:A:492:LEU:HG	2:A:601:0LN:H22	1.99	0.45
1:B:24:ASN:HB3	1:B:27:SER:OG	2.17	0.45
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.99	0.44
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.98	0.44
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.83	0.44
1:B:347:SER:O	1:B:349:PRO:HD3	2.17	0.43
1:B:236[B]:GLU:HG2	1:B:240:TYR:CZ	2.54	0.43
1:A:388:PRO:O	1:A:392:LEU:HG	2.18	0.42
1:A:372:VAL:HG22	1:A:382:TYR:CD1	2.54	0.42
1:B:5:THR:HG23	1:B:278:ARG:HH22	1.85	0.42
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.50	0.42
1:B:461:GLN:HB2	1:B:542:ALA:HA	2.01	0.42
1:B:181:THR:HG21	5:B:978:HOH:O	2.19	0.42
1:A:359:ASP:HB3	1:A:362:LEU:HD12	2.01	0.42
1:B:434:LEU:HD21	1:B:510:LYS:HB2	2.02	0.42
1:A:346:TYR:O	1:A:347:SER:CB	2.67	0.41
1:A:364:THR:HA	1:A:368:SER:O	2.20	0.41
1:A:383:TYR:HH	1:A:477:TYR:HD2	1.66	0.41
1:A:439:LEU:HB3	1:A:457:LEU:HD11	2.03	0.41
1:A:419:LEU:CD2	1:A:485:VAL:HG11	2.50	0.41
1:B:416:ALA:N	1:B:417:PRO:CD	2.84	0.41
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.54	0.41
1:A:409:LEU:HD11	1:A:459:LEU:HD11	2.02	0.41
1:B:83:LEU:HB2	1:B:173:MET:HA	2.03	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	544/563 (97%)	533 (98%)	11 (2%)	0	100	100
1	B	561/563 (100%)	546 (97%)	13 (2%)	2 (0%)	39	37
All	All	1105/1126 (98%)	1079 (98%)	24 (2%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	347	SER
1	B	348	ALA

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	467/479 (98%)	457 (98%)	10 (2%)	61	66
1	B	482/479 (101%)	478 (99%)	4 (1%)	86	91
All	All	949/958 (99%)	935 (98%)	14 (2%)	72	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	201	VAL
1	A	308	LEU
1	A	336	LEU
1	A	425	LEU
1	A	434	LEU
1	A	461	GLN
1	A	489	LEU
1	A	492	LEU
1	A	563	SER
1	B	57	LEU
1	B	274	CYS
1	B	439	LEU
1	B	544	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	118	HIS
1	A	194	GLN
1	A	316	ASN
1	A	461	GLN
1	A	514	GLN
1	B	110	ASN
1	B	194	GLN
1	B	316	ASN
1	B	369	ASN
1	B	483	ASN
1	B	544	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

23 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	0LN	A	601	-	41,47,47	1.19	5 (12%)	44,70,70	1.41	7 (15%)
3	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.39	0
3	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.33	0
3	SO4	A	604	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	A	605	-	4,4,4	0.21	0	6,6,6	0.25	0
4	GOL	A	606	-	5,5,5	0.45	0	5,5,5	0.53	0
4	GOL	A	607	-	5,5,5	0.47	0	5,5,5	1.17	1 (20%)
3	SO4	B	601	-	4,4,4	0.21	0	6,6,6	0.93	0
3	SO4	B	602	-	4,4,4	0.11	0	6,6,6	0.60	0
3	SO4	B	603	-	4,4,4	0.43	0	6,6,6	0.39	0
3	SO4	B	604	-	4,4,4	0.19	0	6,6,6	0.14	0
3	SO4	B	605	-	4,4,4	0.14	0	6,6,6	0.62	0
3	SO4	B	606	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	B	607	-	4,4,4	0.70	0	6,6,6	0.86	0
3	SO4	B	608	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	B	609	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	B	610	-	4,4,4	0.15	0	6,6,6	0.22	0
3	SO4	B	611	-	4,4,4	0.19	0	6,6,6	0.39	0
4	GOL	B	612	-	5,5,5	0.36	0	5,5,5	0.55	0
4	GOL	B	613	-	5,5,5	0.41	0	5,5,5	0.31	0
4	GOL	B	614	-	5,5,5	0.54	0	5,5,5	0.50	0
4	GOL	B	615	-	5,5,5	0.56	0	5,5,5	0.76	0
4	GOL	B	616	-	5,5,5	0.50	0	5,5,5	0.76	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	0LN	A	601	-	-	0/26/56/56	0/3/6/6
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	A	605	-	-	0/0/0/0	0/0/0/0
4	GOL	A	606	-	-	0/4/4/4	0/0/0/0
4	GOL	A	607	-	-	0/4/4/4	0/0/0/0
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	605	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	606	-	-	0/0/0/0	0/0/0/0
3	SO4	B	607	-	-	0/0/0/0	0/0/0/0
3	SO4	B	608	-	-	0/0/0/0	0/0/0/0
3	SO4	B	609	-	-	0/0/0/0	0/0/0/0
3	SO4	B	610	-	-	0/0/0/0	0/0/0/0
3	SO4	B	611	-	-	0/0/0/0	0/0/0/0
4	GOL	B	612	-	-	0/4/4/4	0/0/0/0
4	GOL	B	613	-	-	0/4/4/4	0/0/0/0
4	GOL	B	614	-	-	0/4/4/4	0/0/0/0
4	GOL	B	615	-	-	0/4/4/4	0/0/0/0
4	GOL	B	616	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	0LN	C7-C4	-2.69	1.37	1.40
2	A	601	0LN	C1-C27	-2.02	1.45	1.50
2	A	601	0LN	C18-C19	2.04	1.36	1.34
2	A	601	0LN	S30-N31	2.75	1.66	1.60
2	A	601	0LN	C20-C19	3.43	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	0LN	O36-C34-N35	-4.13	117.25	122.34
2	A	601	0LN	C42-N31-S30	-3.23	109.90	117.95
2	A	601	0LN	O36-C34-C19	-2.73	115.90	120.14
2	A	601	0LN	C11-C10-C7	-2.43	107.50	112.58
2	A	601	0LN	C38-N35-C34	-2.09	117.71	123.21
2	A	601	0LN	C39-C37-N35	2.02	119.97	112.53
4	A	607	GOL	O3-C3-C2	2.04	120.08	110.18
2	A	601	0LN	C37-N35-C34	2.40	125.68	119.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	0LN	1	0
4	A	607	GOL	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	A	549/563 (97%)	0.62	62 (11%) 7 9	19, 45, 94, 110	7 (1%)
1	B	559/563 (99%)	0.08	7 (1%) 79 84	19, 29, 53, 78	4 (0%)
All	All	1108/1126 (98%)	0.35	69 (6%) 24 32	19, 34, 85, 110	11 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	6.5
1	A	34	HIS	6.2
1	A	535	LYS	6.0
1	A	16	ALA	5.1
1	A	534	LEU	4.7
1	A	33	HIS	4.6
1	A	542	ALA	4.6
1	A	21	LEU	4.5
1	B	544	GLN	4.1
1	A	547	LEU	4.1
1	A	540	PRO	4.0
1	A	518	ALA	4.0
1	A	19	SER	3.9
1	A	563	SER	3.9
1	A	442	ALA	3.8
1	A	536	LEU	3.8
1	A	147	VAL	3.8
1	A	35	ASN	3.7
1	A	549	GLY	3.6
1	A	404	PRO	3.5
1	A	543	SER	3.4
1	B	153	GLY	3.4
1	A	18	GLU	3.4
1	A	507	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	MET	3.2
1	A	512	LEU	3.0
1	A	402	HIS	3.0
1	A	537	THR	2.9
1	A	469	LEU	2.9
1	A	530	VAL	2.9
1	A	213	CYS	2.9
1	A	548	SER	2.9
1	A	212	LYS	2.9
1	A	20	LYS	2.8
1	A	511	LEU	2.8
1	A	513	SER	2.8
1	A	509	ALA	2.8
1	B	540	PRO	2.8
1	A	146	CYS	2.8
1	A	430	PHE	2.7
1	A	37	VAL	2.7
1	A	17	GLU	2.7
1	A	523	ARG	2.7
1	B	535	LYS	2.6
1	B	545	LEU	2.5
1	A	154	ARG	2.5
1	A	106	LYS	2.5
1	A	539	ILE	2.4
1	B	212	LYS	2.4
1	A	330	GLN	2.4
1	A	401	ARG	2.4
1	A	546	ASP	2.3
1	A	38	TYR	2.3
1	A	208	TRP	2.3
1	A	514	GLN	2.3
1	B	563	SER	2.2
1	A	15	ALA	2.2
1	A	434	LEU	2.2
1	A	545	LEU	2.2
1	A	468	GLY	2.2
1	A	533	LYS	2.1
1	A	326	SER	2.1
1	A	544	GLN	2.1
1	A	210	SER	2.1
1	A	524	TYR	2.0
1	A	214	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	2.0
1	A	329	THR	2.0
1	A	440	GLU	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
4	GOL	A	607	6/6	0.80	0.26	12.90	47,58,63,65	0
3	SO4	B	607	5/5	0.81	0.26	8.64	40,59,65,75	0
4	GOL	B	616	6/6	0.78	0.29	8.51	41,45,53,53	0
3	SO4	B	611	5/5	0.80	0.21	4.62	56,65,79,83	0
4	GOL	B	613	6/6	0.83	0.23	4.52	56,61,65,65	0
3	SO4	B	609	5/5	0.86	0.21	3.82	85,88,91,91	0
3	SO4	B	610	5/5	0.89	0.29	3.17	74,79,83,84	0
3	SO4	B	602	5/5	0.98	0.17	2.94	37,42,48,53	0
3	SO4	A	603	5/5	0.91	0.19	2.80	68,76,80,85	0
4	GOL	B	614	6/6	0.85	0.26	2.65	44,53,59,60	0
3	SO4	A	605	5/5	0.90	0.20	2.50	88,92,94,98	0
4	GOL	A	606	6/6	0.78	0.19	2.44	48,58,59,68	0
4	GOL	B	615	6/6	0.85	0.17	1.18	44,56,59,61	0
2	0LN	A	601	42/42	0.81	0.31	1.18	75,91,104,107	0
4	GOL	B	612	6/6	0.96	0.12	1.02	29,34,40,42	0
3	SO4	A	602	5/5	0.95	0.13	0.79	59,60,64,64	0
3	SO4	B	605	5/5	0.96	0.14	0.14	49,55,62,62	0
3	SO4	B	601	5/5	0.96	0.12	-0.02	37,39,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	603	5/5	0.95	0.13	-3.11	42,53,63,69	0
3	SO4	A	604	5/5	0.87	0.17	-	92,96,97,99	0
3	SO4	B	604	5/5	0.90	0.26	-	79,83,90,93	0
3	SO4	B	606	5/5	0.91	0.23	-	104,104,106,107	0
3	SO4	B	608	5/5	0.92	0.17	-	56,60,69,76	0

6.5 Other polymers

There are no such residues in this entry.