



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:47 PM GMT

PDB ID : 4J08
Title : Crystal structure of hcv ns5b polymerase in complex with 2-[[[(4-METHYLPHENYL)SULFONYL]AMINO}-5-PHENOXYBENZOICACID
Authors : Coulombe,R.
Deposited on : 2013-01-30
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

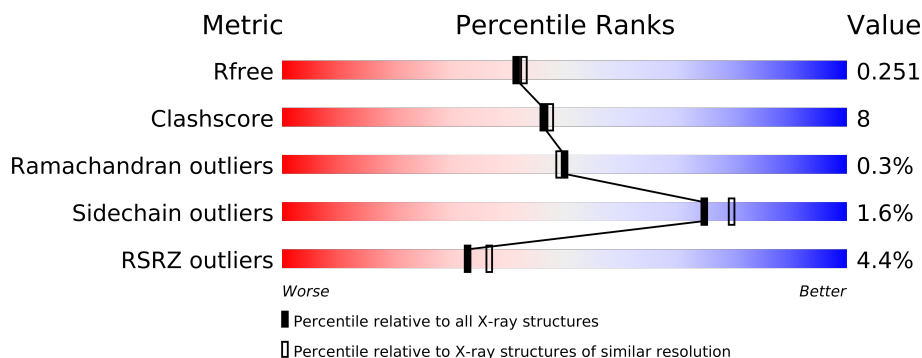
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9027 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

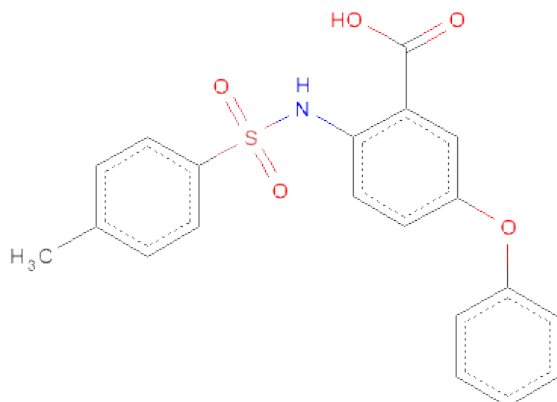
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	558	Total	C	N	O	S	0	0	0
			4346	2737	768	809	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is 2-[[[(4-METHYLPHENYL)SULFONYL]AMINO}-5-PHENOXYBENZOIC ACID (three-letter code: 1JH) (formula: C₂₀H₁₇NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	181	Total	O	0	0
			181	181		
3	B	115	Total	O	0	0
			115	115		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.83Å 107.68Å 135.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 41.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 99.6 (41.54-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.10Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.225 , 0.255 0.221 , 0.251	Depositor DCC
R_{free} test set	9100 reflections (11.10%)	DCC
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.8	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 91102 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: 1JH

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	0.34	0/4453	0.62	2/6044 (0.0%)
1	B	0.35	0/4440	0.60	1/6025 (0.0%)
All	All	0.34	0/8893	0.61	3/12069 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	351	GLY	N-CA-C	-5.22	100.04	113.10
1	A	351	GLY	N-CA-C	-5.13	100.27	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4358	0	4371	60	0
1	B	4346	0	4359	86	0
2	A	27	0	16	0	0
3	A	181	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	115	0	0	0	0
All	All	9027	0	8746	143	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:LYS:O	1:A:82:LEU:HB3	1.74	0.87
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.57	0.85
1:B:531:ARG:H	1:B:531:ARG:HH11	1.29	0.80
1:B:158:ARG:HG3	1:B:158:ARG:HH11	1.49	0.78
1:A:465:ARG:NH1	1:A:545:LEU:O	2.17	0.78
1:A:545:LEU:HB3	1:A:547:LEU:HD13	1.67	0.76
1:B:85:ILE:HD13	1:B:116:VAL:HG13	1.69	0.73
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.70	0.72
1:A:531:ARG:HH11	1:A:531:ARG:HB2	1.55	0.70
1:B:506:SER:O	1:B:510:LYS:HG3	1.92	0.69
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.75	0.68
1:B:51:LYS:HE2	1:B:223:CYS:SG	2.34	0.67
1:B:503:ARG:O	1:B:507:VAL:HG23	1.94	0.67
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.77	0.66
1:A:503:ARG:O	1:A:507:VAL:HG23	1.97	0.65
1:A:501:ARG:HD3	3:A:843:HOH:O	1.98	0.64
1:B:27:SER:OG	1:B:399:THR:HB	1.98	0.64
1:B:205:VAL:HG13	1:B:209:LYS:HE2	1.81	0.62
1:B:434:LEU:HD23	1:B:439:LEU:HD11	1.81	0.62
1:B:465:ARG:HG3	1:B:545:LEU:HB3	1.81	0.61
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.41	0.61
1:B:313:MET:SD	1:B:322:VAL:HG22	2.41	0.60
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.31	0.60
1:A:81:LYS:O	1:A:82:LEU:CB	2.46	0.60
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.32	0.59
1:A:531:ARG:HB2	1:A:531:ARG:NH1	2.19	0.57
1:A:434:LEU:HD12	1:A:507:VAL:HG13	1.86	0.57
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.33	0.56
1:B:361:GLU:HG2	1:B:370:VAL:O	2.05	0.56
1:B:531:ARG:HD2	1:B:532:THR:H	1.71	0.55
1:A:512:LEU:HD21	1:A:523:ARG:HG2	1.89	0.55
1:A:390:THR:HB	1:A:391:PRO:HD3	1.88	0.55
1:B:478:SER:O	1:B:482:ILE:HG13	2.06	0.55
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:LEU:HD12	1:B:31:LEU:O	2.07	0.54
1:B:27:SER:OG	1:B:396:ALA:O	2.24	0.54
1:B:118:HIS:O	1:B:122:VAL:HG23	2.07	0.54
1:B:374:HIS:O	1:B:474:LEU:HA	2.07	0.54
1:B:531:ARG:HD3	1:B:532:THR:HG23	1.90	0.54
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.39	0.53
1:B:531:ARG:HD2	1:B:532:THR:N	2.24	0.53
1:B:22:PRO:HD2	1:B:400:ALA:HB1	1.91	0.52
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.75	0.51
1:A:523:ARG:HD3	1:A:534:LEU:HD13	1.92	0.51
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.93	0.51
1:A:234:ARG:HD3	1:B:247:PRO:HG3	1.93	0.51
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.92	0.51
1:B:158:ARG:HG3	1:B:158:ARG:NH1	2.23	0.51
1:B:205:VAL:O	1:B:209:LYS:HG2	2.11	0.51
1:A:434:LEU:CD1	1:A:507:VAL:HG13	2.42	0.50
1:B:531:ARG:CD	1:B:532:THR:HG23	2.42	0.50
1:A:485:VAL:O	1:A:489:LEU:HG	2.12	0.50
1:B:158:ARG:CG	1:B:158:ARG:HH11	2.21	0.50
1:A:465:ARG:HG2	1:A:542:ALA:O	2.12	0.50
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.27	0.50
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.94	0.50
1:A:24:ASN:HB3	1:A:27:SER:OG	2.12	0.49
1:A:165:LEU:O	1:A:169:VAL:HG23	2.12	0.49
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.94	0.49
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.94	0.49
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.53	0.49
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.28	0.49
1:A:452:TYR:OH	1:A:562:HIS:HD2	1.96	0.49
1:A:73:ALA:O	1:A:76:SER:HB2	2.13	0.48
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.94	0.48
1:B:273:ASN:ND2	1:B:275:GLY:H	2.10	0.48
1:B:160:ILE:HA	1:B:282:SER:OG	2.13	0.48
1:B:431:SER:HB2	1:B:507:VAL:HG21	1.96	0.48
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.78	0.48
1:A:251:GLN:NE2	1:B:254:ARG:HG2	2.29	0.48
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.47
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.96	0.47
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.97	0.47
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.80	0.47
1:B:11:ILE:HD13	1:B:159:LEU:HD22	1.96	0.47
1:B:512:LEU:O	1:B:515:GLY:N	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:459:LEU:O	1:B:463:ILE:HG13	2.14	0.46
1:B:83:LEU:HB2	1:B:173:MET:HA	1.97	0.46
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.30	0.46
1:B:459:LEU:N	1:B:460:PRO:CD	2.78	0.46
1:B:546:ASP:C	1:B:547:LEU:HD23	2.36	0.46
1:A:248:GLU:HG3	3:A:747:HOH:O	2.14	0.46
1:B:489:LEU:HD22	1:B:494:VAL:HG11	1.97	0.46
1:A:523:ARG:HD3	1:A:534:LEU:CD1	2.46	0.46
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.98	0.46
1:A:32:ARG:HD3	1:A:493:GLY:O	2.16	0.46
1:A:508:ARG:HG2	1:A:508:ARG:NH1	2.30	0.45
1:B:346:TYR:O	1:B:347:SER:HB3	2.16	0.45
1:B:51:LYS:HG2	1:B:223:CYS:SG	2.56	0.45
1:B:233:ILE:HD13	1:B:261:TYR:O	2.16	0.45
1:A:444:ASP:HA	1:A:452:TYR:O	2.16	0.45
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.99	0.45
1:A:346:TYR:O	1:A:347:SER:HB3	2.16	0.45
1:B:22:PRO:O	1:B:25:PRO:HG3	2.17	0.45
1:A:184:GLN:HG3	3:A:880:HOH:O	2.16	0.45
1:B:211:LYS:HE3	1:B:323:ILE:HG22	1.98	0.44
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.58	0.44
1:B:372:VAL:HG22	1:B:373:ALA:N	2.33	0.44
1:A:545:LEU:HD22	1:A:547:LEU:HD11	2.00	0.44
1:B:300:THR:HA	1:B:313:MET:HE2	2.00	0.44
1:B:458:ASP:OD1	1:B:461:GLN:OE1	2.36	0.44
1:A:102:GLY:HA3	1:A:114:ARG:HE	1.82	0.44
1:B:408:TRP:O	1:B:412:ILE:HG13	2.18	0.44
1:A:314:LEU:HB3	1:A:321:VAL:HG13	2.00	0.43
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.94	0.43
1:B:508:ARG:HG3	1:B:522:GLY:O	2.19	0.43
1:B:418:THR:O	1:B:422:ARG:HG3	2.18	0.43
1:B:7:THR:HG23	1:B:275:GLY:HA2	2.01	0.43
1:B:309:GLN:HA	1:B:309:GLN:HE21	1.83	0.43
1:B:531:ARG:HG3	1:B:531:ARG:HH11	1.83	0.43
1:B:31:LEU:HD12	1:B:31:LEU:C	2.39	0.43
1:B:309:GLN:O	1:B:324:CYS:HB2	2.19	0.43
1:A:85:ILE:HG12	1:A:173:MET:SD	2.59	0.43
1:B:309:GLN:CA	1:B:309:GLN:HE21	2.33	0.42
1:A:22:PRO:HG3	1:A:401:ARG:NH2	2.34	0.42
1:B:158:ARG:NH1	1:B:158:ARG:CG	2.79	0.42
1:A:531:ARG:HH11	1:A:531:ARG:CB	2.29	0.42
1:B:531:ARG:NH1	1:B:531:ARG:HG3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:434:LEU:CD2	1:B:439:LEU:HD11	2.49	0.42
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.54	0.42
1:B:434:LEU:HD12	1:B:507:VAL:HG13	2.01	0.42
1:B:102:GLY:O	1:B:114:ARG:HD3	2.18	0.42
1:A:535:LYS:HA	1:A:535:LYS:HD3	1.89	0.42
1:B:222:ARG:O	1:B:223:CYS:C	2.58	0.42
1:B:431:SER:HB2	1:B:507:VAL:CG2	2.49	0.42
1:A:48:ARG:NH1	3:A:825:HOH:O	2.51	0.42
1:B:18:GLU:HA	1:B:18:GLU:OE2	2.19	0.42
1:A:300:THR:HA	1:A:313:MET:CE	2.49	0.41
1:A:36:MET:O	1:A:146:CYS:HA	2.20	0.41
1:A:84:SER:OG	1:A:87:GLU:HG3	2.20	0.41
1:B:85:ILE:CD1	1:B:116:VAL:HG13	2.43	0.41
1:B:489:LEU:HD22	1:B:494:VAL:CG1	2.51	0.41
1:A:257:THR:O	1:A:262:ILE:HG23	2.21	0.41
1:B:530:VAL:O	1:B:533:LYS:NZ	2.45	0.41
1:B:512:LEU:O	1:B:513:SER:C	2.59	0.41
1:B:137:THR:O	1:B:161:VAL:HA	2.21	0.41
1:A:57:LEU:HD23	1:A:57:LEU:C	2.41	0.41
1:A:233:ILE:HD13	1:A:261:TYR:O	2.20	0.41
1:B:93:PRO:HG3	1:B:561:TYR:HB2	2.03	0.41
1:B:385:THR:OG1	1:B:386:ARG:N	2.53	0.41
1:A:375:ASP:OD1	1:A:375:ASP:C	2.60	0.41
1:A:501:ARG:O	1:A:505:ARG:HG3	2.22	0.40
1:A:374:HIS:O	1:A:474:LEU:HA	2.22	0.40

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	555/576 (96%)	538 (97%)	16 (3%)	1 (0%)	56	57
1	B	554/576 (96%)	528 (95%)	24 (4%)	2 (0%)	43	39
All	All	1109/1152 (96%)	1066 (96%)	40 (4%)	3 (0%)	50	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	B	541	ALA
1	B	515	GLY

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	477/491 (97%)	468 (98%)	9 (2%)	69	73
1	B	475/491 (97%)	469 (99%)	6 (1%)	80	85
All	All	952/982 (97%)	937 (98%)	15 (2%)	75	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	32	ARG
1	A	160	ILE
1	A	184	GLN
1	A	307	LYS
1	A	336	LEU
1	A	381	VAL
1	A	402	HIS
1	A	465	ARG
1	B	182	LEU
1	B	309	GLN
1	B	310	ASP
1	B	313	MET
1	B	465	ARG
1	B	531	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	ASN
1	A	374	HIS
1	A	438	GLN
1	A	514	GLN
1	A	544	GLN
1	A	562	HIS
1	B	24	ASN
1	B	251	GLN
1	B	273	ASN
1	B	309	GLN
1	B	411	ASN
1	B	461	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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	1JH	A	601	-	29,29,29	2.65	20 (68%)	41,41,41	1.15	5 (12%)

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	1JH	A	601	-	-	0/19/19/19	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1JH	S7-N10	6.68	1.74	1.63
2	A	601	1JH	O18-C17	4.20	1.36	1.23
2	A	601	1JH	C22-C21	3.36	1.45	1.38
2	A	601	1JH	O20-C21	3.13	1.47	1.39
2	A	601	1JH	C26-C21	3.06	1.45	1.38
2	A	601	1JH	O9-S7	2.94	1.46	1.43
2	A	601	1JH	C5-C6	2.91	1.43	1.38
2	A	601	1JH	C11-N10	2.76	1.47	1.42
2	A	601	1JH	O8-S7	2.74	1.46	1.43
2	A	601	1JH	C12-C11	2.67	1.45	1.41
2	A	601	1JH	O19-C17	-2.46	1.22	1.30
2	A	601	1JH	C23-C24	2.44	1.45	1.37
2	A	601	1JH	C5-C4	2.34	1.43	1.38
2	A	601	1JH	C15-C14	2.31	1.43	1.38
2	A	601	1JH	C1-C6	2.29	1.42	1.38
2	A	601	1JH	C25-C24	2.23	1.44	1.37
2	A	601	1JH	C6-S7	2.21	1.79	1.76
2	A	601	1JH	C25-C26	2.15	1.44	1.39
2	A	601	1JH	C1-C2	2.07	1.42	1.38
2	A	601	1JH	C23-C22	2.06	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1JH	O18-C17-C12	-3.14	113.94	121.82
2	A	601	1JH	O19-C17-C12	2.78	123.78	115.47
2	A	601	1JH	O9-S7-C6	-2.60	104.66	107.98
2	A	601	1JH	O8-S7-N10	2.42	112.92	106.72
2	A	601	1JH	O20-C14-C15	2.33	127.93	119.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	559/576 (97%)	-0.05	12 (2%) 60 65	20, 31, 48, 57	0
1	B	558/576 (96%)	0.33	37 (6%) 18 20	22, 39, 54, 60	0
All	All	1117/1152 (96%)	0.14	49 (4%) 33 37	20, 35, 52, 60	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	5.6
1	B	543	SER	5.0
1	B	542	ALA	4.7
1	A	149	PRO	4.3
1	B	541	ALA	4.2
1	B	24	ASN	4.2
1	B	531	ARG	4.2
1	B	535	LYS	4.1
1	B	532	THR	3.8
1	B	27	SER	3.7
1	B	379	LYS	3.7
1	B	25	PRO	3.6
1	B	376	ALA	3.6
1	B	540	PRO	3.5
1	B	545	LEU	3.4
1	B	530	VAL	3.3
1	A	535	LYS	3.3
1	B	26	LEU	3.3
1	B	22	PRO	3.2
1	A	543	SER	3.2
1	B	153	GLY	3.2
1	B	539	ILE	3.1
1	B	21	LEU	3.0
1	A	86	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	534	LEU	2.9
1	B	507	VAL	2.8
1	B	546	ASP	2.7
1	B	402	HIS	2.7
1	B	213	CYS	2.6
1	B	34	HIS	2.5
1	A	544	GLN	2.5
1	B	563	SER	2.3
1	A	212	LYS	2.3
1	B	523	ARG	2.2
1	B	330	GLN	2.2
1	B	378	GLY	2.2
1	B	106	LYS	2.2
1	B	331	GLU	2.2
1	A	534	LEU	2.1
1	B	434	LEU	2.1
1	B	544	GLN	2.1
1	A	148	GLN	2.1
1	A	402	HIS	2.1
1	B	19	SER	2.1
1	A	546	ASP	2.1
1	B	440	GLU	2.1
1	A	545	LEU	2.0
1	B	537	THR	2.0
1	A	309	GLN	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	1JH	A	601	27/27	0.14	1.78	37,44,46,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.