



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:11 AM GMT

PDB ID : 3H59
Title : Hepatitis C virus polymerase NS5B with thiazine inhibitor 2
Authors : Harris, S.F.; Ghatge, M.
Deposited on : 2009-04-21
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>

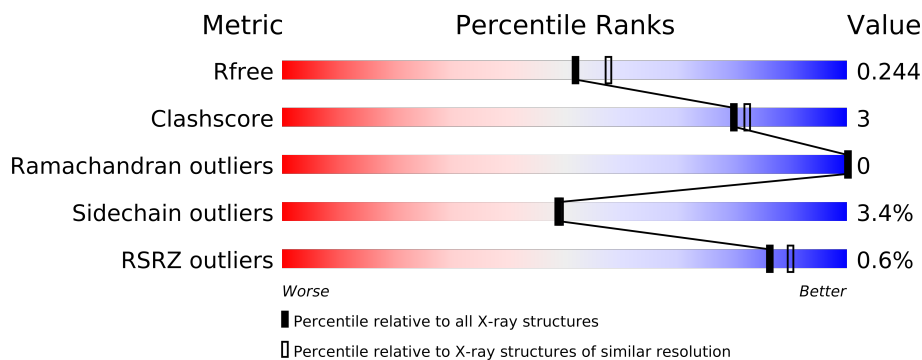
The following versions of software and data (see [references](#)) were used in the production of this report:

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 9582 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.

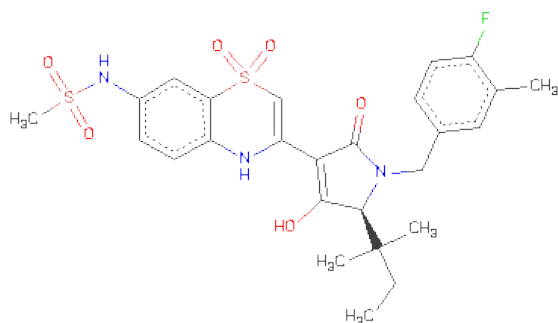
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	7	0
			4387	2767	775	810	35			
1	B	557	Total	C	N	O	S	0	6	0
			4381	2764	774	809	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP P26663
A	-4	HIS	-	EXPRESSION TAG	UNP P26663
A	-3	HIS	-	EXPRESSION TAG	UNP P26663
A	-2	HIS	-	EXPRESSION TAG	UNP P26663
A	-1	HIS	-	EXPRESSION TAG	UNP P26663
A	0	HIS	-	EXPRESSION TAG	UNP P26663
A	1	HIS	-	EXPRESSION TAG	UNP P26663
B	-5	MET	-	EXPRESSION TAG	UNP P26663
B	-4	HIS	-	EXPRESSION TAG	UNP P26663
B	-3	HIS	-	EXPRESSION TAG	UNP P26663
B	-2	HIS	-	EXPRESSION TAG	UNP P26663
B	-1	HIS	-	EXPRESSION TAG	UNP P26663
B	0	HIS	-	EXPRESSION TAG	UNP P26663
B	1	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is N-{3-[(5S)-5-(1,1-DIMETHYLPROPYL)-1-(4-FLUORO-3-METHYLBENZYL)-4-HYDROXY-2-OXO-2,5-DIHYDRO-1H-PYRROL-3-YL]-1,1-DIOXIDO-4H-1,4-BENZOTHAZIN-7-YL}METHANESULFONAMIDE (three-letter code: H59) (formula: C₂₆H₃₀FN₃O₆S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			38	26	1	3	6	2		
2	B	1	Total	C	F	N	O	S	0	0
			38	26	1	3	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	349	Total	O	0	0
			349	349		
3	B	389	Total	O	0	0
			389	389		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.86Å 106.42Å 127.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.10 49.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.09-2.10) 93.3 (49.09-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.246 0.196 , 0.244	Depositor DCC
R_{free} test set	3255 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 64784 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.72 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7893e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H59

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	0.59	1/4482 (0.0%)	0.67	0/6081
1	B	0.60	1/4476 (0.0%)	0.68	1/6073 (0.0%)
All	All	0.60	2/8958 (0.0%)	0.67	1/12154 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	CYS	CB-SG	-7.09	1.70	1.82
1	A	311	CYS	CB-SG	-6.95	1.70	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	VAL	CB-CA-C	-5.51	100.93	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	4387	0	4403	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4381	0	4399	26	0
2	A	38	0	29	2	0
2	B	38	0	29	1	0
3	A	349	0	0	6	1
3	B	389	0	0	5	1
All	All	9582	0	8860	59	1

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 3.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:MET:SD	3:A:661:HOH:O	2.23	0.94
1:B:329:THR:HG23	3:B:638:HOH:O	1.68	0.93
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.58	0.86
1:A:182:LEU:HD23	1:A:182:LEU:C	1.96	0.86
1:A:403:THR:HG22	3:A:720:HOH:O	1.81	0.80
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.68	0.74
1:A:182:LEU:HD23	1:A:182:LEU:O	1.90	0.71
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.75	0.69
1:B:82:LEU:CD1	1:B:249:ALA:HB2	2.23	0.68
1:B:440:GLU:OE2	1:B:457:LEU:HD12	1.93	0.68
1:A:527:ASN:HD21	1:A:534:LEU:H	1.41	0.68
1:B:154:ARG:N	3:B:645:HOH:O	2.26	0.68
2:B:571:H59:H37A	2:B:571:H59:H31A	1.78	0.65
2:A:571:H59:H37A	2:A:571:H59:H31A	1.79	0.65
1:B:461:GLN:H	1:B:461:GLN:HE21	1.46	0.63
1:A:12:THR:O	1:A:139:MET:HE3	1.98	0.63
1:A:201:VAL:HG22	1:A:384:LEU:HG	1.80	0.62
1:B:103:TYR:OH	1:B:118:HIS:HD2	1.85	0.60
1:A:182:LEU:CD2	1:A:182:LEU:C	2.69	0.59
1:A:103:TYR:OH	1:A:118:HIS:HD2	1.85	0.59
1:B:306:ALA:HB3	1:B:308:LEU:HD13	1.85	0.59
1:A:178:VAL:HG23	3:A:657:HOH:O	2.03	0.58
1:B:197:PRO:O	1:B:201:VAL:HG23	2.05	0.57
1:A:201:VAL:HG22	1:A:384:LEU:CD1	2.35	0.57
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.87	0.56
1:A:36[B]:MET:SD	1:A:491:LYS:O	2.64	0.55
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.90	0.54
1:A:197:PRO:O	1:A:201:VAL:HG23	2.08	0.54
2:A:571:H59:H36A	3:A:822:HOH:O	2.08	0.53
1:A:217:PHE:CE2	1:A:336:LEU:HD21	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.92	0.51
1:B:306:ALA:CB	1:B:308:LEU:HD13	2.41	0.51
1:A:523:LYS:HG3	1:A:534:LEU:HD23	1.91	0.50
1:A:80:ALA:HB3	1:A:245:LEU:CD2	2.41	0.49
1:A:46:GLY:HA2	1:A:49:GLN:HE21	1.77	0.49
1:A:12:THR:O	1:A:139:MET:CE	2.60	0.49
1:B:182:LEU:HD13	1:B:243:CYS:SG	2.53	0.49
1:A:296:TYR:CD2	1:A:313:MET:CE	2.96	0.48
1:B:262[A]:ILE:HD11	3:B:946:HOH:O	2.14	0.47
1:B:440:GLU:OE2	1:B:457:LEU:CD1	2.60	0.47
1:A:201:VAL:HG22	1:A:384:LEU:CG	2.43	0.47
1:A:77:THR:O	1:B:24:ASN:HB2	2.16	0.46
1:B:372:VAL:HG13	3:B:766:HOH:O	2.16	0.45
1:B:532:THR:HG23	3:B:585:HOH:O	2.16	0.45
1:B:527:ASN:HD21	1:B:534:LEU:H	1.64	0.45
1:A:217:PHE:CD2	1:A:336:LEU:HD21	2.53	0.44
1:B:523:LYS:HG3	1:B:534:LEU:HD23	1.99	0.44
1:A:503:ARG:O	1:A:507:VAL:HG23	2.19	0.42
1:B:411:ASN:O	1:B:415:TYR:HB2	2.20	0.42
1:A:22:PRO:HG2	1:A:401:ARG:HG3	2.01	0.42
1:A:306:ALA:CB	1:A:308:LEU:HD13	2.50	0.42
1:A:412:ILE:O	1:A:416:ALA:HB2	2.20	0.42
1:B:374:HIS:O	1:B:474:LEU:HA	2.20	0.42
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.60	0.42
1:B:52:VAL:HG12	1:B:223[B]:CYS:SG	2.61	0.41
1:A:154:ARG:N	3:A:731:HOH:O	2.53	0.41
1:A:222:ARG:HD3	3:A:764:HOH:O	2.20	0.41
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.04	0.40
1:B:36[A]:MET:O	1:B:147:VAL:HG13	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:737:HOH:O	3:B:853:HOH:O[4_445]	2.19	0.01

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	560/576 (97%)	552 (99%)	8 (1%)	0	100	100
1	B	559/576 (97%)	545 (98%)	14 (2%)	0	100	100
All	All	1119/1152 (97%)	1097 (98%)	22 (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	482/491 (98%)	465 (96%)	17 (4%)	48	48
1	B	481/491 (98%)	466 (97%)	15 (3%)	52	54
All	All	963/982 (98%)	931 (97%)	32 (3%)	49	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	82	LEU
1	A	90	LYS
1	A	159	LEU
1	A	182	LEU
1	A	311	CYS
1	A	321	VAL
1	A	355	GLN
1	A	381	VAL
1	A	439	LEU
1	A	461	GLN
1	A	473	SER
1	A	510	ARG
1	A	527	ASN
1	A	532	THR
1	A	536	LEU
1	A	547	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	57	LEU
1	B	82	LEU
1	B	159	LEU
1	B	222	ARG
1	B	321	VAL
1	B	381	VAL
1	B	419	LEU
1	B	439	LEU
1	B	461	GLN
1	B	492	LEU
1	B	527	ASN
1	B	532	THR
1	B	536	LEU
1	B	545	LEU
1	B	547	LEU

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	49	GLN
1	A	118	HIS
1	A	273	ASN
1	A	374	HIS
1	A	461	GLN
1	A	483	ASN
1	A	527	ASN
1	B	35	ASN
1	B	49	GLN
1	B	118	HIS
1	B	446	GLN
1	B	461	GLN
1	B	527	ASN

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 ⓘ

2 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	H59	A	571	-	41,41,41	1.31	5 (12%)	65,65,65	2.18	18 (27%)
2	H59	B	571	-	41,41,41	1.47	4 (9%)	65,65,65	2.32	15 (23%)

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	H59	A	571	-	-	0/18/57/57	0/2/4/4
2	H59	B	571	-	-	0/18/57/57	0/2/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	571	H59	C21-S20	6.06	1.78	1.71
2	B	571	H59	C18-N19	4.53	1.41	1.35
2	A	571	H59	C21-S20	3.87	1.76	1.71
2	A	571	H59	C9-N10	3.80	1.49	1.46
2	A	571	H59	C18-N19	3.64	1.40	1.35
2	A	571	H59	C12-S20	2.89	1.80	1.76
2	B	571	H59	O22-S20	-2.57	1.41	1.44
2	B	571	H59	C26-S25	2.21	1.81	1.75
2	A	571	H59	C26-S25	2.19	1.81	1.75

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	571	H59	C31-N10-C9	7.17	128.68	121.52
2	A	571	H59	C31-N10-C9	6.94	128.45	121.52
2	B	571	H59	C26-S25-N24	-6.78	98.38	106.80
2	B	571	H59	C2-C3-C4	5.82	120.08	116.12
2	A	571	H59	C2-C3-C4	5.49	119.85	116.12
2	A	571	H59	C5-C4-C3	-5.42	118.45	123.79
2	B	571	H59	C18-C21-S20	-5.14	119.93	123.19
2	A	571	H59	C8-C9-N10	4.84	104.78	101.38
2	B	571	H59	C1-C31-N10	-4.82	104.49	113.39
2	B	571	H59	O22-S20-C21	-4.81	105.37	109.91
2	B	571	H59	C8-C9-N10	4.77	104.74	101.38
2	A	571	H59	C1-C31-N10	-4.71	104.69	113.39
2	B	571	H59	C5-C4-C3	-4.70	119.16	123.79
2	A	571	H59	C9-N10-C11	-4.61	107.72	113.13
2	A	571	H59	C18-C21-S20	-4.03	120.63	123.19
2	B	571	H59	C9-N10-C11	-3.93	108.52	113.13
2	B	571	H59	C9-C8-C7	-3.66	106.75	113.60
2	A	571	H59	O29-C8-C9	3.61	126.55	118.21
2	A	571	H59	O30-C11-C7	-3.22	122.60	130.04
2	A	571	H59	C9-C8-C7	-3.16	107.69	113.60
2	B	571	H59	C21-C18-C7	-2.94	117.25	124.00
2	B	571	H59	O29-C8-C9	2.79	124.65	118.21
2	B	571	H59	O28-S25-N24	2.76	113.06	107.15
2	A	571	H59	C21-C18-C7	-2.69	117.83	124.00
2	A	571	H59	O23-S20-C12	-2.60	105.97	108.73
2	B	571	H59	O30-C11-C7	-2.60	124.03	130.04
2	A	571	H59	C16-C17-C12	2.52	122.00	119.42
2	A	571	H59	C26-S25-N24	-2.51	103.68	106.80
2	A	571	H59	C6-C5-C4	2.28	121.52	118.95
2	B	571	H59	O22-S20-C12	2.10	110.95	108.73
2	A	571	H59	O27-S25-N24	-2.07	102.72	107.15
2	A	571	H59	O22-S20-C12	2.04	110.89	108.73
2	A	571	H59	O28-S25-O27	2.03	122.15	118.74

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	557/576 (96%)	-0.17	3 (0%) 88 91	13, 24, 35, 42	0
1	B	557/576 (96%)	-0.17	4 (0%) 84 88	13, 22, 34, 47	0
All	All	1114/1152 (96%)	-0.17	7 (0%) 86 90	13, 23, 34, 47	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	GLN	2.7
1	A	102	GLY	2.6
1	B	531	LYS	2.5
1	B	376	ALA	2.2
1	B	95	HIS	2.2
1	B	542	ALA	2.1
1	A	16	ALA	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	H59	A	571	38/38	0.10	0.35	12,18,22,26	0
2	H59	B	571	38/38	0.09	-0.49	11,17,20,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.