



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:10 AM GMT

PDB ID : 3CVK
Title : Crystal structure of HCV NS5B polymerase with a novel pyridazinone inhibitor
Authors : Zhao, Q.; Showalter, R.E.; Han, Q.; Kissinger, C.R.
Deposited on : 2008-04-18
Resolution : 2.31 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>

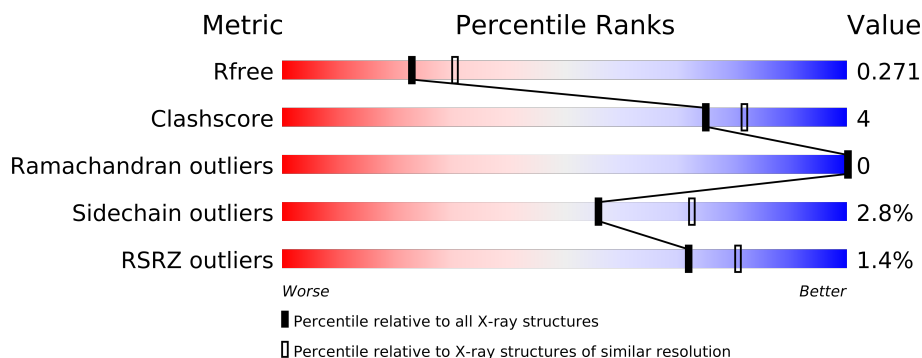
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.31 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	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (2.34-2.30)

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	578	
1	B	578	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9014 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.

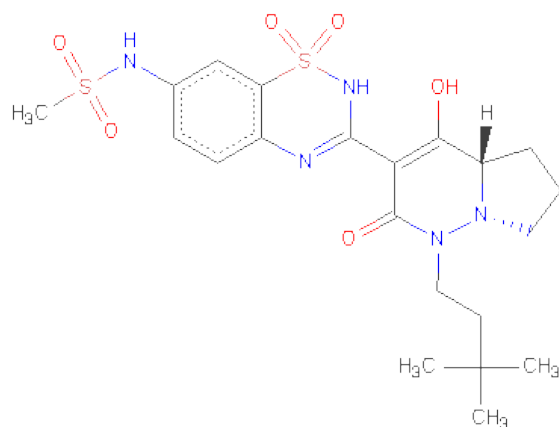
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4334	2735	764	804	31			
1	B	557	Total	C	N	O	S	0	0	0
			4334	2735	764	804	31			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLN	ARG	ENGINEERED	UNP P26663
A	571	LEU	-	EXPRESSION TAG	UNP P26663
A	572	GLU	-	EXPRESSION TAG	UNP P26663
A	573	HIS	-	EXPRESSION TAG	UNP P26663
A	574	HIS	-	EXPRESSION TAG	UNP P26663
A	575	HIS	-	EXPRESSION TAG	UNP P26663
A	576	HIS	-	EXPRESSION TAG	UNP P26663
A	577	HIS	-	EXPRESSION TAG	UNP P26663
A	578	HIS	-	EXPRESSION TAG	UNP P26663
B	544	GLN	ARG	ENGINEERED	UNP P26663
B	571	LEU	-	EXPRESSION TAG	UNP P26663
B	572	GLU	-	EXPRESSION TAG	UNP P26663
B	573	HIS	-	EXPRESSION TAG	UNP P26663
B	574	HIS	-	EXPRESSION TAG	UNP P26663
B	575	HIS	-	EXPRESSION TAG	UNP P26663
B	576	HIS	-	EXPRESSION TAG	UNP P26663
B	577	HIS	-	EXPRESSION TAG	UNP P26663
B	578	HIS	-	EXPRESSION TAG	UNP P26663

- Molecule 2 is N-{3-[1-(3,3-DIMETHYL-BUTYL)-4-HYDROXY-2-OXO-1,2,4A,5,6,7-HEXAHYDRO-PYRROLO[1,2-B]PYRIDAZIN-3-YL]-1,1-DIOXO-1,2-DIHYDRO-1LAMBDA6-BENZO[1,2,4]THIADIAZIN-7-YL}-METHANESULFONAMIDE (three-letter code: N34) (formula: C₂₁H₂₉N₅O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	21	5	6	2		
2	B	1	Total	C	N	O	S	0	0
			34	21	5	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	125	Total	O	0	0
			125	125		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.30Å 106.26Å 126.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.12 – 2.31 38.11 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.12-2.31) 98.9 (38.11-2.31)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.272 0.210 , 0.271	Depositor DCC
R_{free} test set	2606 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	4 of 51041 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 42.26 % 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 2.0939e-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: N34

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	0/4428	0.59	0/6009
1	B	0.45	0/4428	0.57	0/6009
All	All	0.45	0/8856	0.58	0/12018

There are no bond length outliers.

There are no bond angle outliers.

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	4334	0	4352	28	0
1	B	4334	0	4354	42	0
2	A	34	0	29	2	0
2	B	34	0	29	1	0
3	A	153	0	0	6	0
3	B	125	0	0	3	0
All	All	9014	0	8764	69	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 4.

All (69) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:303:CYS:CB	1:B:311:CYS:HG	2.06	0.68
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.79	0.64
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.64	0.62
1:B:429:PHE:O	1:B:433:LEU:HG	2.01	0.61
1:A:373:ALA:HB3	1:A:474:LEU:HD13	1.83	0.60
1:B:141:LYS:HG2	1:B:160:ILE:HD11	1.83	0.60
1:B:308:LEU:CD2	1:B:335:SER:HB3	2.32	0.59
1:B:202:GLU:HG3	3:B:695:HOH:O	2.04	0.57
1:B:227:THR:HB	1:B:347:SER:O	2.05	0.56
1:B:86:GLU:O	1:B:90:LYS:HG2	2.05	0.55
1:B:12:THR:HG21	1:B:270:LYS:HE2	1.87	0.55
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.89	0.54
1:A:523:LYS:HG3	1:A:534:LEU:HD23	1.88	0.54
1:B:466:LEU:HD22	1:B:551:PHE:CE2	2.42	0.54
1:A:141:LYS:NZ	1:A:158:ARG:HH21	2.05	0.53
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.74	0.53
1:B:308:LEU:HD23	1:B:335:SER:HB3	1.91	0.52
1:B:414:MET:HG3	2:B:579:N34:H12A	1.92	0.52
1:A:455:GLU:HB3	3:A:717:HOH:O	2.10	0.52
1:B:201:VAL:HG13	1:B:384:LEU:HG	1.91	0.52
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.50	0.52
1:B:455:GLU:HB3	3:B:667:HOH:O	2.11	0.51
1:B:346:TYR:O	1:B:347:SER:HB3	2.10	0.51
1:A:110:ASN:HD22	1:A:110:ASN:C	2.15	0.50
1:A:414:MET:HG3	2:A:579:N34:H12A	1.93	0.49
1:A:233:ILE:HA	1:A:236:GLU:HG2	1.95	0.48
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.14	0.47
1:B:313:MET:HG2	1:B:320:LEU:HD11	1.97	0.47
2:A:579:N34:O27	2:A:579:N34:N22	2.47	0.47
1:B:197:PRO:O	1:B:201:VAL:HG23	2.15	0.47
1:B:308:LEU:HD21	1:B:335:SER:HB3	1.95	0.46
1:B:197:PRO:O	1:B:201:VAL:CG2	2.64	0.46
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.97	0.46
1:A:192:GLY:HA3	1:A:316:ASN:OD1	2.16	0.46
1:A:538:PRO:HG2	1:B:270:LYS:O	2.16	0.45
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.57	0.45
1:B:303:CYS:HB3	1:B:311:CYS:SG	2.57	0.45
1:A:184:GLN:HB3	3:A:612:HOH:O	2.17	0.45
1:A:448:TYR:CE2	1:A:551:PHE:HD1	2.35	0.45
1:B:197:PRO:HD2	1:B:466:LEU:HB3	1.99	0.45
1:B:264:GLY:HA3	3:B:600:HOH:O	2.17	0.44
1:B:67:VAL:HG11	1:B:300:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.99	0.44
1:B:426:MET:O	1:B:430:PHE:HB2	2.17	0.44
1:B:201:VAL:HG22	1:B:384:LEU:HD12	2.01	0.43
1:A:346:TYR:O	1:A:347:SER:HB3	2.19	0.43
1:B:113:SER:O	1:B:117:ASN:HB2	2.18	0.43
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.36	0.43
1:A:128:GLU:HG3	3:A:724:HOH:O	2.18	0.43
1:B:5:THR:O	1:B:275:GLY:HA3	2.19	0.43
1:A:77:THR:O	1:B:24:ASN:HB2	2.19	0.43
1:A:404:PRO:HA	3:A:727:HOH:O	2.19	0.43
1:A:314:LEU:HB3	1:A:321:VAL:HG13	2.01	0.43
1:A:28:ASN:ND2	3:A:710:HOH:O	2.52	0.42
1:A:79:LYS:HA	1:A:244:ASP:HB3	2.02	0.42
1:B:411:ASN:O	1:B:415:TYR:HB2	2.19	0.42
1:A:257:THR:HA	1:A:261:TYR:HB2	2.00	0.42
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.49	0.42
1:B:220:ASP:O	1:B:350:PRO:HA	2.19	0.42
1:B:230:GLU:HG3	1:B:262:ILE:HG23	2.02	0.42
1:B:309:GLN:HB2	1:B:325:GLU:HB2	2.02	0.42
1:A:141:LYS:HZ1	1:A:158:ARG:HH21	1.68	0.41
1:A:154:ARG:N	3:A:722:HOH:O	2.53	0.41
1:B:96:SER:OG	1:B:168:ARG:NH2	2.53	0.41
1:B:466:LEU:CD2	1:B:551:PHE:HE2	2.33	0.41
1:B:129:ASP:O	1:B:255:SER:OG	2.39	0.41
1:A:375:ASP:O	1:A:475:HIS:CD2	2.73	0.41
1:B:90:LYS:HA	1:B:90:LYS:HD2	1.97	0.40
1:B:461:GLN:HG2	1:B:541:ALA:HB3	2.03	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	553/578 (96%)	541 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	553/578 (96%)	541 (98%)	12 (2%)	0	100	100
All	All	1106/1156 (96%)	1082 (98%)	24 (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	475/493 (96%)	465 (98%)	10 (2%)	66	82
1	B	475/493 (96%)	458 (96%)	17 (4%)	47	62
All	All	950/986 (96%)	923 (97%)	27 (3%)	56	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	50	LYS
1	A	56	ARG
1	A	110	ASN
1	A	148	GLN
1	A	308	LEU
1	A	335	SER
1	A	440	GLU
1	A	487	SER
1	A	532	THR
1	B	14	CYS
1	B	31	LEU
1	B	43	ARG
1	B	106	LYS
1	B	141	LYS
1	B	148	GLN
1	B	201	VAL
1	B	213	ASN
1	B	237	GLU
1	B	255	SER

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Mol	Chain	Res	Type
1	B	313	MET
1	B	330	GLN
1	B	336	LEU
1	B	461	GLN
1	B	473	SER
1	B	544	GLN
1	B	547	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	117	ASN
1	A	120	HIS
1	A	142	ASN
1	A	330	GLN
1	B	117	ASN
1	B	148	GLN
1	B	231	ASN
1	B	446	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 ⓘ

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	N34	A	579	-	37,37,37	1.99	6 (16%)	59,59,59	1.76	16 (27%)
2	N34	B	579	-	37,37,37	1.87	5 (13%)	59,59,59	1.83	11 (18%)

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	N34	A	579	-	-	0/11/60/60	0/0/4/4
2	N34	B	579	-	-	0/11/60/60	0/0/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	N34	S33-N23	7.93	1.70	1.62
2	B	579	N34	S33-N23	6.93	1.69	1.62
2	A	579	N34	S34-N26	5.72	1.71	1.63
2	B	579	N34	S34-N26	5.04	1.70	1.63
2	B	579	N34	C10-N24	3.44	1.39	1.37
2	B	579	N34	C7-C10	3.07	1.51	1.44
2	A	579	N34	C10-N24	2.97	1.39	1.37
2	A	579	N34	C9-N23	2.81	1.43	1.38
2	A	579	N34	C7-C10	2.69	1.50	1.44
2	A	579	N34	C14-C8	2.46	1.53	1.50
2	B	579	N34	C9-N23	2.20	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	N34	C8-C14-N25	5.62	113.04	107.99
2	B	579	N34	O29-S33-N23	5.51	111.78	108.17
2	A	579	N34	C8-C14-N25	5.39	112.84	107.99
2	B	579	N34	C9-N23-S33	4.47	122.58	117.18
2	A	579	N34	C18-S34-N26	-4.39	101.34	106.80
2	B	579	N34	O29-S33-C6	-4.02	103.51	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	N34	O27-C10-N24	3.97	123.95	120.48
2	A	579	N34	C19-C20-N24	-3.53	103.97	114.47
2	B	579	N34	C18-S34-N26	-3.47	102.49	106.80
2	A	579	N34	C9-N23-S33	3.43	121.33	117.18
2	A	579	N34	O27-C10-C7	-3.10	118.09	125.19
2	A	579	N34	C7-C10-N24	3.09	117.77	114.69
2	A	579	N34	O29-S33-N23	2.96	110.11	108.17
2	B	579	N34	O31-S34-N26	2.87	113.28	107.15
2	A	579	N34	C9-C7-C8	2.79	124.99	119.47
2	A	579	N34	O29-S33-C6	-2.77	105.28	109.22
2	B	579	N34	C19-C20-N24	-2.77	106.23	114.47
2	B	579	N34	C12-C14-C8	-2.74	114.77	117.45
2	A	579	N34	C7-C9-N23	-2.72	114.93	117.43
2	B	579	N34	O27-C10-N24	2.59	122.75	120.48
2	A	579	N34	O29-S33-O28	2.56	121.07	118.85
2	B	579	N34	C7-C9-N23	-2.26	115.35	117.43
2	B	579	N34	O32-C8-C14	-2.22	112.20	115.56
2	A	579	N34	O31-S34-N26	2.13	111.71	107.15
2	A	579	N34	C4-N22-C9	2.10	121.75	117.85
2	A	579	N34	C10-C7-C9	-2.02	116.74	120.69
2	A	579	N34	O30-S34-C18	-2.01	104.61	108.44

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	557/578 (96%)	-0.13	6 (1%) 77 85	32, 45, 62, 89	0
1	B	557/578 (96%)	-0.06	10 (1%) 65 75	34, 48, 67, 84	0
All	All	1114/1156 (96%)	-0.10	16 (1%) 72 81	32, 46, 65, 89	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	4.3
1	A	541	ALA	3.6
1	A	544	GLN	3.5
1	A	543	SER	3.4
1	B	544	GLN	3.2
1	B	16	ALA	2.9
1	B	309	GLN	2.9
1	A	545	LEU	2.8
1	B	43	ARG	2.5
1	B	541	ALA	2.4
1	B	543	SER	2.3
1	B	331	GLU	2.2
1	B	110	ASN	2.2
1	B	212	LYS	2.2
1	A	540	PRO	2.1
1	B	535	LYS	2.1

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	N34	A	579	34/34	0.15	1.50	35,37,39,41	0
2	N34	B	579	34/34	0.13	0.71	35,39,42,42	0

6.5 Other polymers

There are no such residues in this entry.