wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 01:41 PM GMT

PDB ID	:	2RS3
Title	:	STRUCTURAL ANALYSIS OF ANTIVIRAL AGENTS THAT INTERACT WITH THE CAPSID OF HUMAN RHINOVIRUSES
Authors	:	Badger, J.; Smith, T.J.; Rossmann, M.G.
Deposited on	:	1988-10-03
Resolution	:	3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
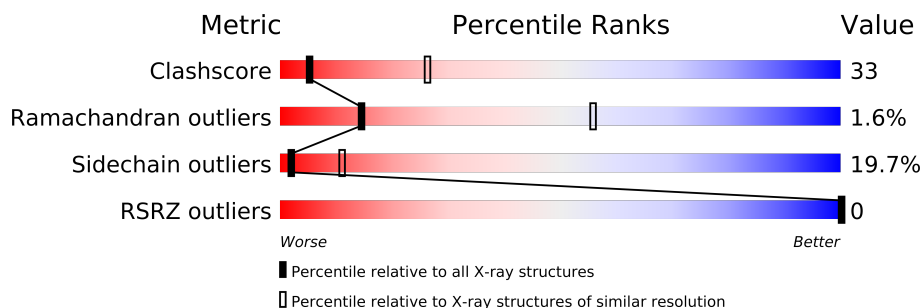A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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 3.00 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	Percentile Ranks	Value
Clashscore		33
Ramachandran outliers		1.6%
Sidechain outliers		19.7%
RSRZ outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	1	289	
2	2	262	
3	3	236	
4	4	68	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6299 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 HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total 2170	C 1373	N 375	O 414	S 8	0	0	0

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total 1952	C 1238	N 330	O 372	S 12	0	0	0

There is a discrepancy between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	CONFLICT	UNP P03303

- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total 1849	C 1184	N 305	O 353	S 7	0	0	0

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total 297	C 186	N 47	O 62	S 2	0	0	0

- Molecule 5 is 5-(7-(5-HYDRO-4-ETHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYLISOXAZOLE (three-letter code: W59) (formula: $C_{22}H_{30}N_2O_3$).
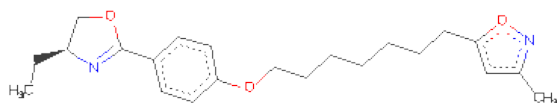
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	1	1	27	22	2	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	1	4	4	4	0	0

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.
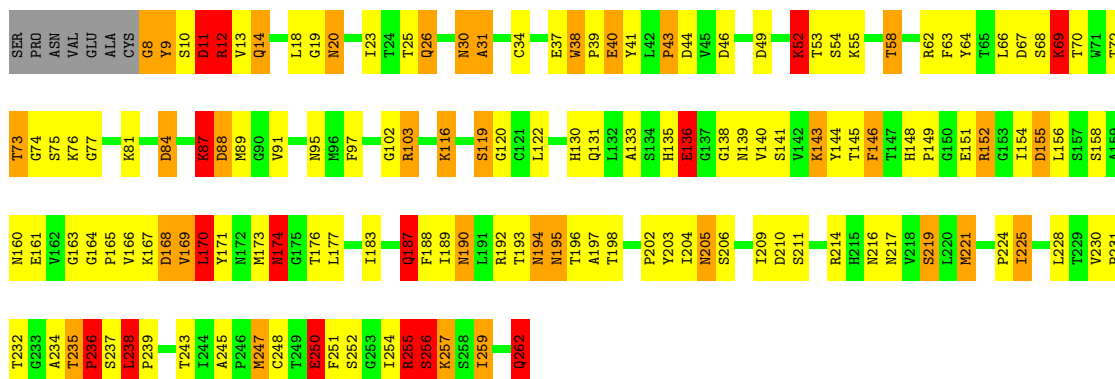
- Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

Chain 1:
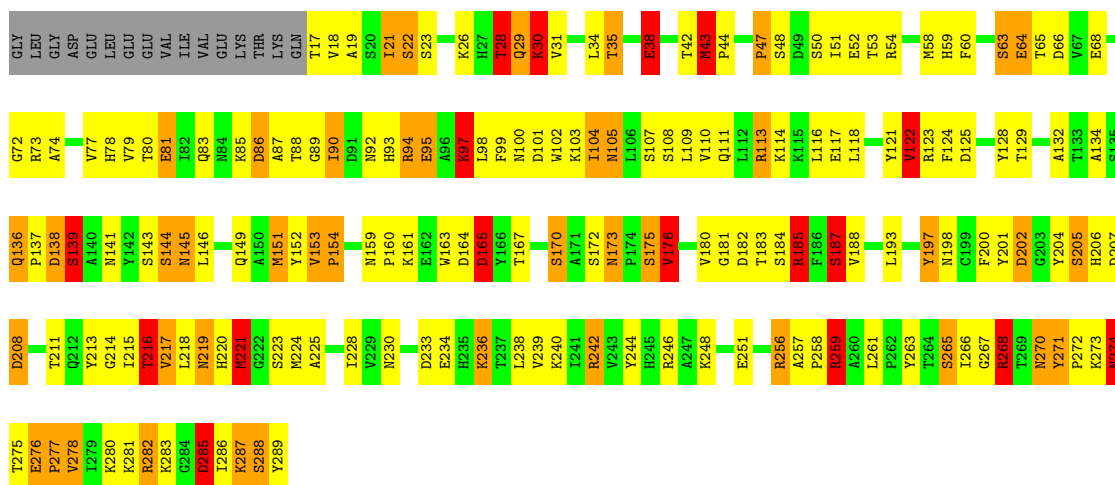
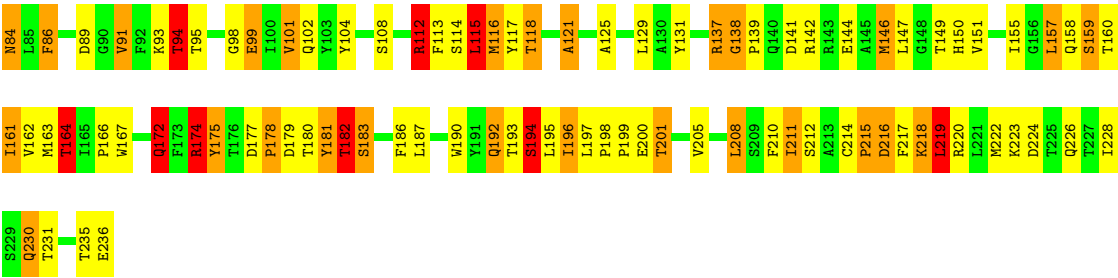- Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

Chain 2:

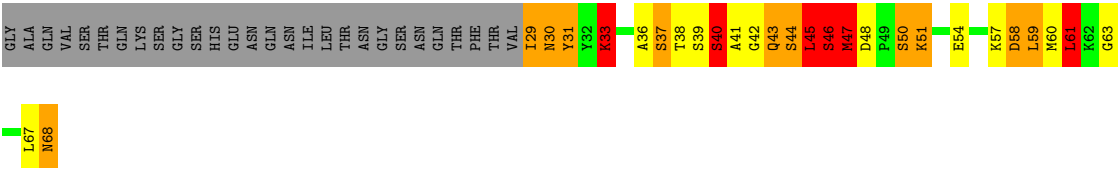- Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3:

N84 L85 F86 D89 G90 V91 F92 K93 T94 T95 G98 E99 I100 V101 Q102 Y103 Y104 S108 R112 F113 S114 L115 M116 Y117 T118 A121 A125 L129 A130 Y131 R137 G138 P139 Q140 D141 R142 R143 E144 A145 M146 L147 G148 T149 H150 V151 I155 G156 L157 Q158 S159 T160

I161 V162 M163 T164 I165 P166 W167 Q172 F173 R174 Y175 T176 D177 P178 D179 T180 Y181 T182 S183 F186 L187 W190 Y191 Q192 T193 S194 L195 I196 L197 P198 P199 E200 T201 V205 L208 S209 F210 I211 S212 A213 C214 P215 D216 F217 K218 L219 R220 L221 M222 K223 D224 T225 Q226 T227 I228

S229 Q230 T231 T235 E236

• Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)

Chain 4:

GLY ALA GLN VAL SER THR GLN LYS SER GLY SER HIS GLU ASN GLN ASN ILE LEU THR ASN GLY SER ASN GLN THR PHE THR VAL I29 N30 Y31 Y32 M33 A36 S37 T38 S39 S40 A41 G42 Q43 S44 L45 S46 M47 D48 P49 S50 K51 E54 K57 D58 L59 M60 L61 K62 G63

L67 N68

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00 39.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00) 15.1 (39.19-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 3.01Å)	Xtriage
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	(Not available) , (Not available) 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 127.2	EDS
Estimated twinning fraction	0.148 for l,-k,h	Xtriage
L-test for twinning	$< |L| > = 0.32, < L^2 > = 0.15$	Xtriage
Outliers	0 of 87288 reflections	Xtriage
F_o,F_c correlation	0.07	EDS
Total number of atoms	6299	wwPDB-VP
Average B, all atoms (Å^2)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: W59

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	1	1.88	41/2228 (1.8%)	2.38	119/3031 (3.9%)
2	2	1.85	32/2001 (1.6%)	2.17	78/2735 (2.9%)
3	3	1.77	21/1898 (1.1%)	2.18	75/2597 (2.9%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.86	107/6429 (1.7%)	2.26	293/8769 (3.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
2	2	0	2
All	All	0	4

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	170	SER	CB-OG	-14.31	1.23	1.42
1	1	285	ASP	CA-CB	11.82	1.79	1.53
4	4	42	GLY	N-CA	11.70	1.63	1.46
4	4	40	SER	CB-OG	10.74	1.56	1.42
2	2	256	SER	CB-OG	10.20	1.55	1.42

The worst 5 of 293 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	246	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	1	256	ARG	NE-CZ-NH2	20.38	130.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	123	ARG	NE-CZ-NH1	19.14	129.87	120.30
2	2	255	ARG	NE-CZ-NH2	-18.62	110.99	120.30
2	2	87	LYS	CA-CB-CG	17.62	152.17	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	Sidechain

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	1	2170	0	2106	182	0
2	2	1952	0	1926	127	0
3	3	1849	0	1831	150	0
4	4	297	0	294	35	0
5	1	27	0	30	6	0
6	1	4	0	0	2	0
All	All	6299	0	6187	411	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 33.

The worst 5 of 411 close contacts within the same asymmetric unit are listed below:

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:4:33:LYS:NZ	4:4:33:LYS:CE	1.67	1.57
3:3:57:ASN:CA	3:3:57:ASN:CB	1.75	1.55
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
2:2:52:LYS:CE	2:2:52:LYS:NZ	1.68	1.53
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.13

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	1	271/289 (94%)	242 (89%)	21 (8%)	8 (3%)	7	34
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	27	76
3	3	234/236 (99%)	217 (93%)	15 (6%)	2 (1%)	25	73
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	8	39
All	All	796/855 (93%)	726 (91%)	57 (7%)	13 (2%)	14	56

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	139	SER
3	3	57	ASN
3	3	77	ASN
1	1	108	SER
1	1	165	ASP

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	1	239/253 (94%)	195 (82%)	44 (18%)	2	13
2	2	223/229 (97%)	179 (80%)	44 (20%)	2	11
3	3	209/209 (100%)	171 (82%)	38 (18%)	2	13
4	4	33/57 (58%)	20 (61%)	13 (39%)	0	0
All	All	704/748 (94%)	565 (80%)	139 (20%)	2	11

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	141	SER
2	2	221	MET
4	4	40	SER
2	2	152	ARG
2	2	187	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	187	GLN
2	2	205	ASN
3	3	192	GLN
2	2	190	ASN
2	2	195	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 ⓘ

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
5	W59	1	900	-	29,29,29	3.67	4 (13%)	37,37,37	2.77	8 (21%)

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
5	W59	1	900	-	-	0/16/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	900	W59	C4A-N3A	-13.82	1.36	1.48
5	1	900	W59	C2A-N3A	13.08	1.43	1.26
5	1	900	W59	O1A-C5A	-3.63	1.38	1.45
5	1	900	W59	O1A-C2A	-2.18	1.32	1.36

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	900	W59	O1A-C2A-N3A	-8.75	108.83	118.19
5	1	900	W59	CM1-C4A-N3A	8.17	132.42	111.95
5	1	900	W59	O1A-C2A-C4B	7.70	123.64	115.61
5	1	900	W59	O1A-C5A-C4A	6.12	112.20	104.53
5	1	900	W59	C1C-C5-C4	3.20	135.47	128.51

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(Å²)	Q<0.9
1	1	273/289 (94%)	-0.35	0	100	100	1, 1, 1, 1	0
2	2	255/262 (97%)	-0.31	0	100	100	1, 1, 1, 1	0
3	3	236/236 (100%)	-0.33	0	100	100	1, 1, 1, 1	0
4	4	40/68 (58%)	-0.36	0	100	100	1, 1, 1, 1	0
All	All	804/855 (94%)	-0.33	0	100	100	1, 1, 1, 1	0

There are no RSRZ outliers to report.

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(Å²)	Q<0.9
5	W59	1	900	27/27	0.24	-	1,1,1,1	0

6.5 Other polymers ⓘ

There are no such residues in this entry.