



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9GI6 / pdb_00009gi6
Title : Structure of SARS-CoV-2 Main Protease (Mpro) with mutation of N214A
Authors : Creon, A.; Scheer, T.E.S.; Lane, T.J.; Rahmani Mashhour, A.; Guenther, S.; Reinke, P.Y.A.; Meents, A.; Chapman, H.N.
Deposited on : 2024-08-17
Resolution : 1.83 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

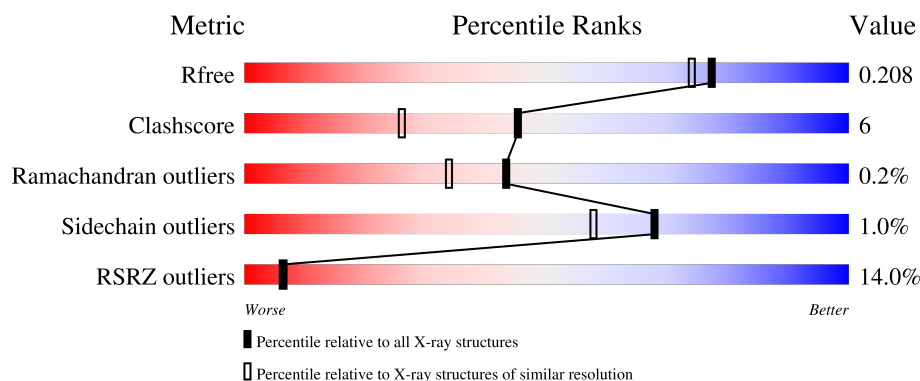
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	306	<div> <div>10%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	306	<div> <div>18%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

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
2	PEG	B	401	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5229 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.

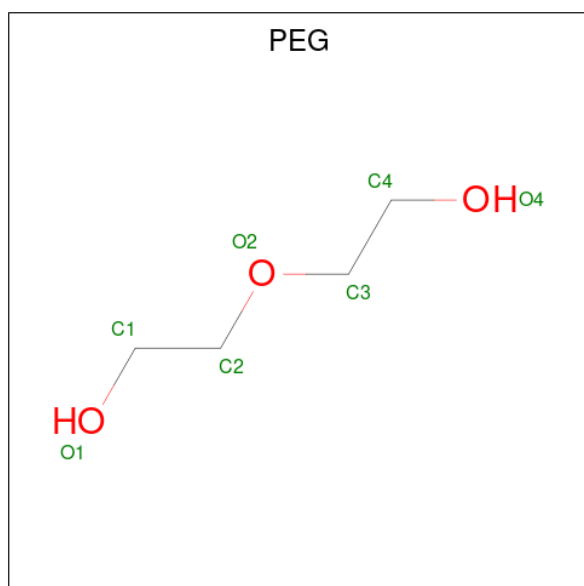
- Molecule 1 is a protein called Replicase polypeptide 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	10	0
			2383	1506	404	449	24			
1	B	301	Total	C	N	O	S	0	7	0
			2372	1503	404	443	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ALA	ASN	engineered mutation	UNP A0A6M4EPN9
B	214	ALA	ASN	engineered mutation	UNP A0A6M4EPN9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

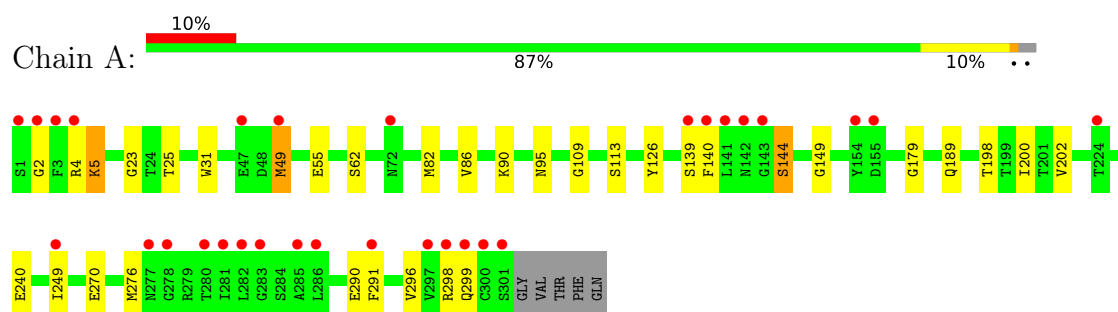
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	106	Total	O	0	0
			106	106		

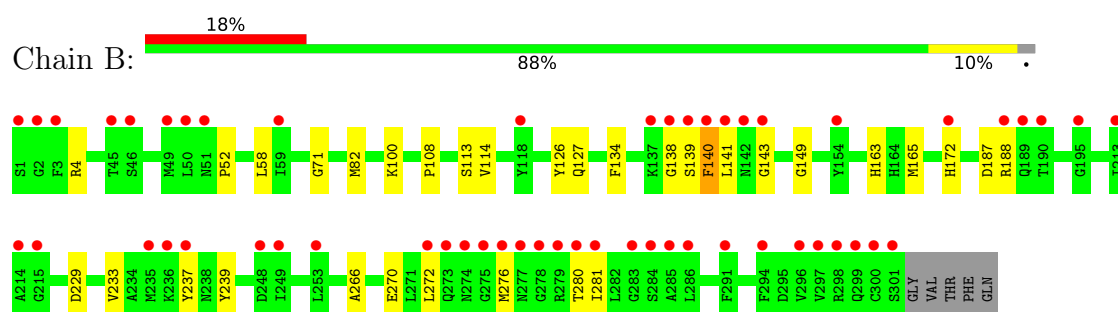
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Replicase polypeptide 1a



• Molecule 1: Replicase polypeptide 1a



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.81Å 100.57Å 102.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.28 – 1.83 55.28 – 1.83	Depositor EDS
% Data completeness (in resolution range)	68.9 (55.28-1.83) 68.9 (55.28-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.174 , 0.207 0.174 , 0.208	Depositor DCC
R_{free} test set	2011 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5229	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, PEG, CL

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	0.33	0/2435	0.52	0/3310
1	B	0.30	0/2426	0.48	0/3297
All	All	0.32	0/4861	0.50	0/6607

There are no bond length outliers.

There are no bond angle outliers.

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	2383	0	2321	28	1
1	B	2372	0	2315	30	0
2	A	98	0	140	8	0
2	B	63	0	90	11	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	204	0	0	4	0
5	B	106	0	0	2	1
All	All	5229	0	4866	58	1

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 6.

The worst 5 of 58 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:100[B]:LYS:HG3	2:B:404:PEG:H32	1.66	0.78
2:A:404:PEG:HO1	2:A:408:PEG:HO1	1.31	0.77
1:B:140:PHE:HA	2:B:402:PEG:H31	1.69	0.73
1:A:49:MET:HB3	1:A:189:GLN:HG3	1.75	0.67
1:A:55[B]:GLU:OE2	5:A:501:HOH:O	2.13	0.66

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:OE2	5:B:547:HOH:O[2_555]	2.15	0.05

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	307/306 (100%)	292 (95%)	15 (5%)	0	100	100
1	B	304/306 (99%)	296 (97%)	7 (2%)	1 (0%)	36	25
All	All	611/612 (100%)	588 (96%)	22 (4%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	LEU

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	266/262 (102%)	262 (98%)	4 (2%)	57	42
1	B	263/262 (100%)	262 (100%)	1 (0%)	84	78
All	All	529/524 (101%)	524 (99%)	5 (1%)	68	60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	49	MET
1	A	62	SER
1	A	144	SER
1	B	140	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	B	69	GLN
1	B	244	GLN
1	B	180	ASN
1	A	163	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 3 are monoatomic - leaving 23 for Mogul analysis.

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	PEG	B	409	-	6,6,6	0.16	0	5,5,5	0.09	0
2	PEG	B	404	-	6,6,6	0.14	0	5,5,5	0.11	0
2	PEG	A	403	-	6,6,6	0.16	0	5,5,5	0.20	0
2	PEG	A	409	-	6,6,6	0.16	0	5,5,5	0.09	0
2	PEG	A	405	-	6,6,6	0.18	0	5,5,5	0.11	0
2	PEG	B	406	-	6,6,6	0.19	0	5,5,5	0.11	0
2	PEG	A	410	-	6,6,6	0.14	0	5,5,5	0.11	0
2	PEG	B	403	-	6,6,6	0.17	0	5,5,5	0.08	0
2	PEG	A	401	-	6,6,6	0.26	0	5,5,5	0.08	0
2	PEG	A	404	-	6,6,6	0.18	0	5,5,5	0.07	0
2	PEG	A	414	-	6,6,6	0.15	0	5,5,5	0.08	0
2	PEG	B	405	-	6,6,6	0.16	0	5,5,5	0.08	0
2	PEG	A	411	-	6,6,6	0.17	0	5,5,5	0.08	0
2	PEG	B	407	-	6,6,6	0.19	0	5,5,5	0.08	0
2	PEG	A	406	-	6,6,6	0.19	0	5,5,5	0.12	0
2	PEG	A	408	-	6,6,6	0.19	0	5,5,5	0.07	0
2	PEG	A	402	-	6,6,6	0.18	0	5,5,5	0.07	0
2	PEG	A	412	-	6,6,6	0.18	0	5,5,5	0.07	0
2	PEG	B	401	-	6,6,6	0.37	0	5,5,5	0.13	0
2	PEG	A	413	-	6,6,6	0.23	0	5,5,5	0.09	0
2	PEG	B	408	-	6,6,6	0.18	0	5,5,5	0.14	0
2	PEG	A	407	-	6,6,6	0.24	0	5,5,5	0.09	0
2	PEG	B	402	-	6,6,6	0.14	0	5,5,5	0.08	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	PEG	B	409	-	-	2/4/4/4	-
2	PEG	B	404	-	-	2/4/4/4	-
2	PEG	A	403	-	-	1/4/4/4	-
2	PEG	A	409	-	-	1/4/4/4	-
2	PEG	A	405	-	-	2/4/4/4	-
2	PEG	B	406	-	-	2/4/4/4	-
2	PEG	A	410	-	-	3/4/4/4	-
2	PEG	B	403	-	-	3/4/4/4	-
2	PEG	A	401	-	-	4/4/4/4	-
2	PEG	A	404	-	-	3/4/4/4	-
2	PEG	A	414	-	-	1/4/4/4	-
2	PEG	B	405	-	-	2/4/4/4	-
2	PEG	A	411	-	-	3/4/4/4	-
2	PEG	B	407	-	-	1/4/4/4	-
2	PEG	A	406	-	-	2/4/4/4	-
2	PEG	A	408	-	-	3/4/4/4	-
2	PEG	A	402	-	-	3/4/4/4	-
2	PEG	A	412	-	-	3/4/4/4	-
2	PEG	B	401	-	-	1/4/4/4	-
2	PEG	A	413	-	-	2/4/4/4	-
2	PEG	B	408	-	-	2/4/4/4	-
2	PEG	A	407	-	-	3/4/4/4	-
2	PEG	B	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	406	PEG	C4-C3-O2-C2
2	A	408	PEG	O2-C3-C4-O4
2	B	401	PEG	C1-C2-O2-C3
2	A	413	PEG	O2-C3-C4-O4
2	B	403	PEG	O2-C3-C4-O4

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	409	PEG	1	0
2	B	404	PEG	2	0
2	B	403	PEG	1	0
2	A	401	PEG	1	0
2	A	404	PEG	1	0
2	A	408	PEG	3	0
2	A	402	PEG	2	0
2	A	412	PEG	2	0
2	B	401	PEG	5	0
2	B	402	PEG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	301/306 (98%)	0.19	30 (9%) 12 13	11, 28, 62, 109	8 (2%)
1	B	301/306 (98%)	0.79	54 (17%) 3 3	14, 36, 80, 137	5 (1%)
All	All	602/612 (98%)	0.49	84 (13%) 6 6	11, 30, 74, 137	13 (2%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	PHE	9.5
1	B	294[A]	PHE	7.1
1	A	3	PHE	6.8
1	B	141	LEU	6.5
1	B	3	PHE	6.3

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 oligosaccharides 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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	B	405	7/7	0.75	0.20	63,71,74,76	0
2	PEG	B	402	7/7	0.79	0.21	66,71,75,78	0
2	PEG	A	410	7/7	0.80	0.15	50,52,66,67	0
2	PEG	B	406	7/7	0.81	0.16	44,49,57,59	0
2	PEG	A	407	7/7	0.82	0.16	49,55,66,67	0
2	PEG	A	413	7/7	0.83	0.17	47,50,63,63	0
2	PEG	A	406	7/7	0.83	0.15	50,51,56,59	0
2	PEG	A	405	7/7	0.84	0.15	43,48,59,65	0
2	PEG	A	412	7/7	0.84	0.17	40,46,53,59	0
2	PEG	A	409	7/7	0.84	0.20	63,64,66,67	0
2	PEG	A	401	7/7	0.85	0.11	28,33,42,44	0
2	PEG	A	408	7/7	0.85	0.15	50,54,57,61	0
2	PEG	A	414	7/7	0.85	0.15	51,59,60,65	0
2	PEG	B	403	7/7	0.86	0.14	44,47,55,58	0
2	PEG	B	407	7/7	0.87	0.13	45,50,56,61	0
2	PEG	B	408	7/7	0.87	0.13	36,38,50,53	0
2	PEG	B	409	7/7	0.87	0.13	44,51,64,67	0
2	PEG	A	404	7/7	0.88	0.13	43,48,56,59	0
2	PEG	A	403	7/7	0.88	0.13	41,47,52,59	0
2	PEG	B	404	7/7	0.88	0.13	35,40,49,52	0
2	PEG	B	401	7/7	0.88	0.11	32,32,39,42	0
2	PEG	A	411	7/7	0.91	0.10	37,42,56,56	0
2	PEG	A	402	7/7	0.93	0.09	35,39,44,51	0
4	NA	B	410	1/1	0.97	0.07	33,33,33,33	0
4	NA	A	416	1/1	0.99	0.06	27,27,27,27	0
3	CL	A	415	1/1	1.00	0.03	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.