



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 09:06 AM EST

PDB ID : 8DDL
Title : SARS-CoV-2 Main Protease (Mpro) H163A Mutant Apo Structure
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Deposited on : 2022-06-18
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

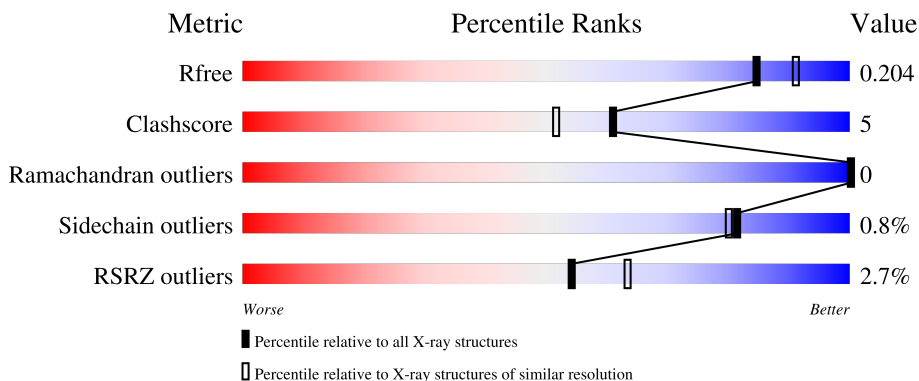
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	 5% 88% 9%
2	B	306	 5% 89% 10%

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
5	PEG	B	703	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5174 atoms, of which 30 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 ORF1a polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2353	1490	398	441	24	0	10	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ALA	HIS	engineered mutation	UNP A0A7U3EDN3

- Molecule 2 is a protein called ORF1a polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	302	2376	1508	398	445	25	0	11	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	163	ALA	HIS	engineered mutation	UNP A0A7U3EDN3

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

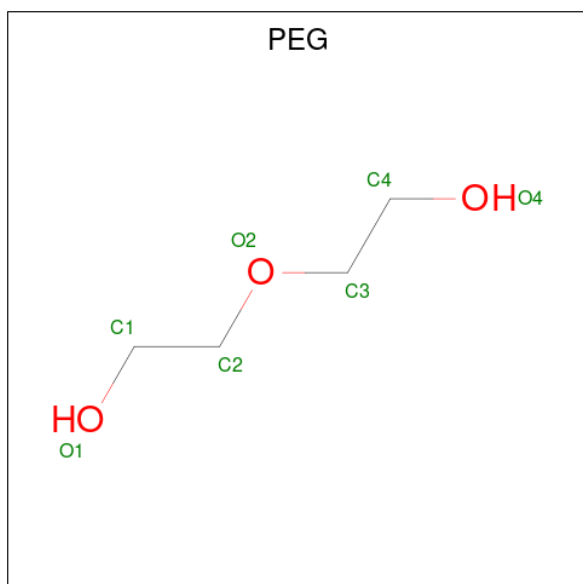


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 24 6 14 4	0	0
3	B	1	Total C O 10 6 4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O			
			7	4	3	0	0	
5	B	1	Total	C	H	O		
			17	4	10	3	0	

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O		
			10	2	6	2	0	

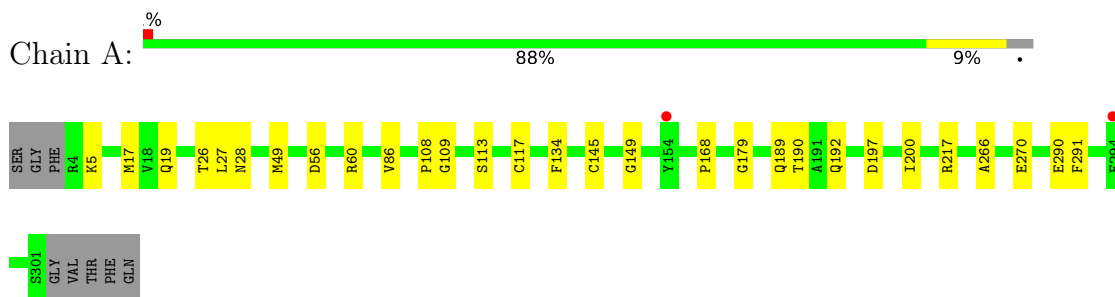
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	157	Total	O	0	0
			157	157		
7	B	219	Total	O	0	0
			219	219		

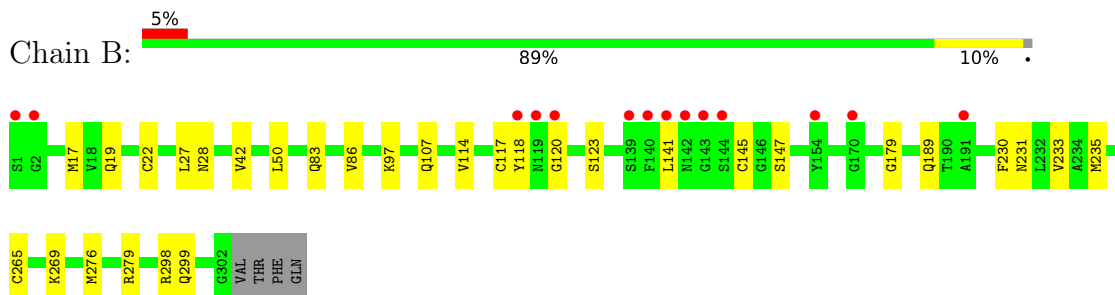
3 Residue-property plots [i](#)

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: ORF1a polyprotein



- Molecule 2: ORF1a polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.83Å 101.46Å 102.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.54 – 1.95 56.54 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (56.54-1.95) 99.5 (56.54-1.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.94Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.207 0.166 , 0.204	Depositor DCC
R_{free} test set	2661 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: CSO, NA, PEG, PGE, EDO

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	0.32	0/2433	0.56	0/3307
2	B	0.33	0/2452	0.57	0/3330
All	All	0.33	0/4885	0.57	0/6637

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	2353	0	2325	20	0
2	B	2376	0	2351	22	0
3	A	10	14	14	0	0
3	B	10	0	14	1	0
4	A	1	0	0	0	0
5	B	14	10	20	4	0
6	B	4	6	6	0	0
7	A	157	0	0	5	2
7	B	219	0	0	2	2
All	All	5144	30	4730	43	2

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 5.

All (43) 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)
2:B:97:LYS:HD2	5:B:703:PEG:H42	1.60	0.83
2:B:28[A]:ASN:OD1	2:B:117[A]:CYS:HB2	1.85	0.76
2:B:298:ARG:HH12	3:B:701:PGE:H6	1.52	0.75
1:A:217:ARG:HD2	7:A:646:HOH:O	1.88	0.74
2:B:118:TYR:OH	2:B:141:LEU:HD23	1.93	0.67
1:A:197:ASP:OD2	7:A:601:HOH:O	2.12	0.66
2:B:86[A]:VAL:HG23	2:B:179:GLY:HA2	1.77	0.66
1:A:49:MET:HB3	1:A:189:GLN:HB2	1.80	0.62
1:A:17:MET:HE3	1:A:117[B]:CYS:SG	2.39	0.62
1:A:5:LYS:HG2	1:A:291:PHE:CZ	2.35	0.61
2:B:17:MET:HE3	2:B:117[A]:CYS:SG	2.43	0.59
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.86	0.57
5:B:703:PEG:O1	7:B:801:HOH:O	2.17	0.56
2:B:233:VAL:HG11	2:B:269:LYS:HG3	1.87	0.56
2:B:118:TYR:OH	2:B:141:LEU:HA	2.06	0.56
1:A:28[B]:ASN:OD1	1:A:117[B]:CYS:HB2	2.07	0.55
1:A:56:ASP:O	1:A:60:ARG:HG2	2.06	0.54
2:B:231:ASN:O	2:B:235:MET:HG3	2.08	0.52
1:A:5:LYS:HG2	1:A:291:PHE:CE2	2.45	0.52
1:A:19[B]:GLN:HG3	1:A:26:THR:CG2	2.40	0.52
2:B:22:CSO:HB3	2:B:42:VAL:HG22	1.92	0.51
2:B:107:GLN:NE2	7:B:813:HOH:O	2.46	0.49
1:A:290:GLU:OE2	7:A:602:HOH:O	2.20	0.49
1:A:19[B]:GLN:HG3	1:A:26:THR:HG23	1.95	0.48
2:B:83:GLN:O	2:B:86[B]:VAL:HG12	2.14	0.48
1:A:190:THR:O	1:A:192:GLN:HG3	2.14	0.48
2:B:97:LYS:HD2	5:B:703:PEG:C4	2.41	0.47
2:B:114:VAL:HG13	2:B:147:SER:HB3	1.97	0.46
1:A:108:PRO:HG3	1:A:134:PHE:CE1	2.51	0.45
2:B:19[A]:GLN:NE2	2:B:120:GLY:HA2	2.31	0.45
1:A:86:VAL:HG23	1:A:179:GLY:HA2	1.98	0.44
2:B:298:ARG:NH2	2:B:299:GLN:HE21	2.16	0.44
2:B:97:LYS:NZ	5:B:703:PEG:O1	2.51	0.43
1:A:113:SER:O	1:A:149:GLY:HA2	2.18	0.43
1:A:266:ALA:O	1:A:270:GLU:HG2	2.19	0.42
1:A:28[B]:ASN:OD1	1:A:117[B]:CYS:CB	2.67	0.42
2:B:230:PHE:CD1	2:B:265:CYS:HB3	2.55	0.42
2:B:19[A]:GLN:HE22	2:B:120:GLY:HA2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19[B]:GLN:HG2	7:A:636:HOH:O	2.19	0.41
2:B:50:LEU:HD23	2:B:189:GLN:O	2.21	0.41
2:B:276:MET:HE2	2:B:279:ARG:O	2.20	0.41
2:B:118:TYR:HD2	2:B:123[B]:SER:OG	2.04	0.40
1:A:168:PRO:HD2	7:A:657:HOH:O	2.21	0.40

All (2) 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)
7:A:730:HOH:O	7:B:961:HOH:O[3_554]	2.14	0.06
7:A:751:HOH:O	7:B:991:HOH:O[3_654]	2.16	0.04

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	306/306 (100%)	301 (98%)	5 (2%)	0	100	100
2	B	310/306 (101%)	302 (97%)	8 (3%)	0	100	100
All	All	616/612 (101%)	603 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	264 (99%)	2 (1%)	81	80
2	B	268/261 (103%)	266 (99%)	2 (1%)	84	82
All	All	534/523 (102%)	530 (99%)	4 (1%)	81	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	145	CYS
2	B	27	LEU
2	B	145	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	107	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue 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	CSO	B	22	2	3,6,7	0.69	0	0,6,8	-	-

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	CSO	B	22	2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	22	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	22	CSO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
3	PGE	B	701	-	9,9,9	0.34	0	8,8,8	0.29	0
3	PGE	A	501	-	9,9,9	0.30	0	8,8,8	0.35	0
5	PEG	B	703	-	6,6,6	0.18	0	5,5,5	0.06	0
6	EDO	B	704	-	3,3,3	0.49	0	2,2,2	0.28	0
5	PEG	B	702	-	6,6,6	0.12	0	5,5,5	0.09	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
3	PGE	B	701	-	-	1/7/7/7	-
3	PGE	A	501	-	-	4/7/7/7	-
5	PEG	B	703	-	-	1/4/4/4	-
6	EDO	B	704	-	-	0/1/1/1	-
5	PEG	B	702	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	702	PEG	C4-C3-O2-C2
5	B	702	PEG	O2-C3-C4-O4
3	A	501	PGE	O1-C1-C2-O2
5	B	703	PEG	O1-C1-C2-O2
5	B	702	PEG	O1-C1-C2-O2
3	A	501	PGE	O2-C3-C4-O3
3	B	701	PGE	C4-C3-O2-C2
3	A	501	PGE	C4-C3-O2-C2
3	A	501	PGE	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	PGE	1	0
5	B	703	PEG	4	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	298/306 (97%)	-0.11	2 (0%) 87 92	19, 33, 58, 82	6 (2%)
2	B	301/306 (98%)	0.00	14 (4%) 31 41	19, 30, 63, 94	5 (1%)
All	All	599/612 (97%)	-0.05	16 (2%) 54 63	19, 31, 61, 94	11 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	142	ASN	4.3
2	B	143	GLY	4.0
1	A	154	TYR	4.0
2	B	141	LEU	3.6
2	B	120	GLY	3.5
2	B	154	TYR	3.4
2	B	118	TYR	3.3
2	B	191	ALA	3.2
2	B	144	SER	3.0
2	B	119	ASN	2.8
2	B	2	GLY	2.7
2	B	170	GLY	2.5
2	B	140	PHE	2.4
2	B	139	SER	2.0
1	A	294	PHE	2.0
2	B	1	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	CSO	B	22	7/8	0.90	0.10	28,41,48,49	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	PGE	A	501	10/10	0.78	0.18	50,74,89,89	0
5	PEG	B	703	7/7	0.83	0.23	43,57,68,69	0
5	PEG	B	702	7/7	0.90	0.15	39,43,49,57	0
3	PGE	B	701	10/10	0.91	0.13	36,43,59,64	0
6	EDO	B	704	4/4	0.92	0.37	39,50,64,78	0
4	NA	A	502	1/1	0.94	0.13	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.