



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 12:21 PM EDT

PDB ID : 7KMG
Title : LY-CoV555 neutralizing antibody against SARS-CoV-2
Authors : Hendle, J.; Pustilnik, A.; Sauder, J.M.; Coleman, K.A.; Boyles, J.S.; Dickinson, C.D.
Deposited on : 2020-11-02
Resolution : 2.16 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 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 : 2.23.1
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) : 2.23.1

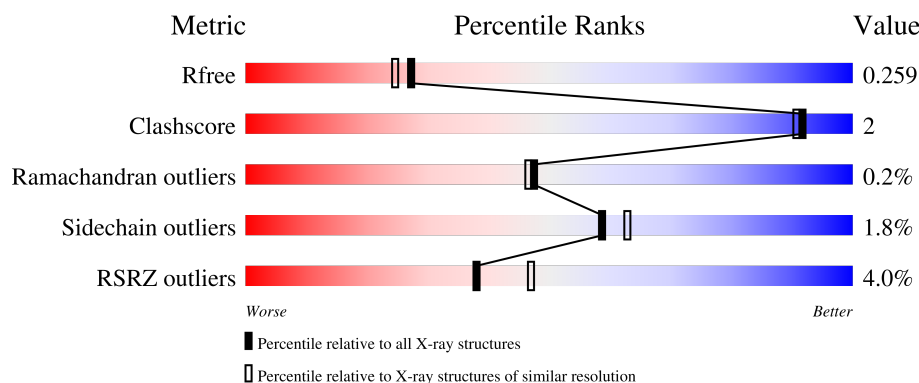
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	229	<div> <div>2%</div> <div>92%</div> <div>5% ..</div> </div>
1	D	229	<div> <div>2%</div> <div>92%</div> <div>5% .</div> </div>
2	B	212	<div> <div>%</div> <div>97%</div> <div>.</div> </div>
2	E	212	<div> <div>92%</div> <div>7% .</div> </div>
3	C	205	<div> <div>10%</div> <div>87%</div> <div>7% 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	205	<div> <div>9%</div> <div>87%</div> <div>6%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9614 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 LY-CoV555 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	3	0
			1668	1059	279	321	9			
1	D	222	Total	C	N	O	S	0	2	0
			1639	1043	272	315	9			

- Molecule 2 is a protein called LY-CoV555 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	3	0
			1615	1006	265	337	7			
2	E	212	Total	C	N	O	S	0	3	0
			1607	1003	263	334	7			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	193	Total	C	N	O	S	0	0	0
			1441	921	244	268	8			
3	F	191	Total	C	N	O	S	0	0	0
			1431	921	238	264	8			

There are 12 discrepancies between the modelled and reference sequences:

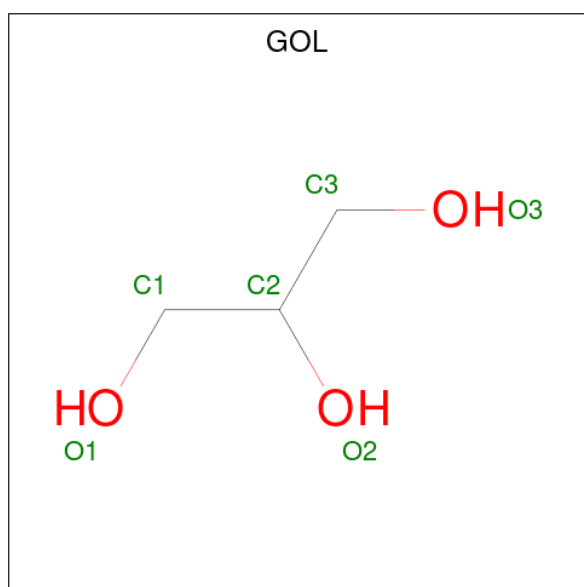
Chain	Residue	Modelled	Actual	Comment	Reference
C	528	HIS	-	expression tag	UNP P0DTC2
C	529	HIS	-	expression tag	UNP P0DTC2
C	530	HIS	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
F	528	HIS	-	expression tag	UNP P0DTC2
F	529	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	530	HIS	-	expression tag	UNP P0DTC2
F	531	HIS	-	expression tag	UNP P0DTC2
F	532	HIS	-	expression tag	UNP P0DTC2
F	533	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	2
			45	45		
5	B	49	Total	O	0	0
			49	49		
5	C	17	Total	O	0	0
			17	17		
5	D	32	Total	O	0	1
			33	33		
5	E	42	Total	O	0	1
			43	43		

Continued on next page...

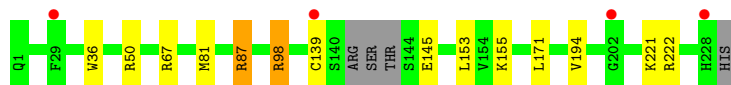
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	14	Total	O	0	0
			14	14		

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: LY-CoV555 Fab heavy chain



- Molecule 1: LY-CoV555 Fab heavy chain



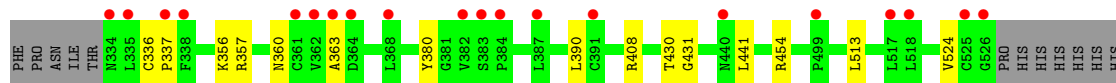
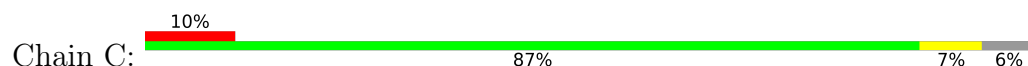
- Molecule 2: LY-CoV555 Fab light chain



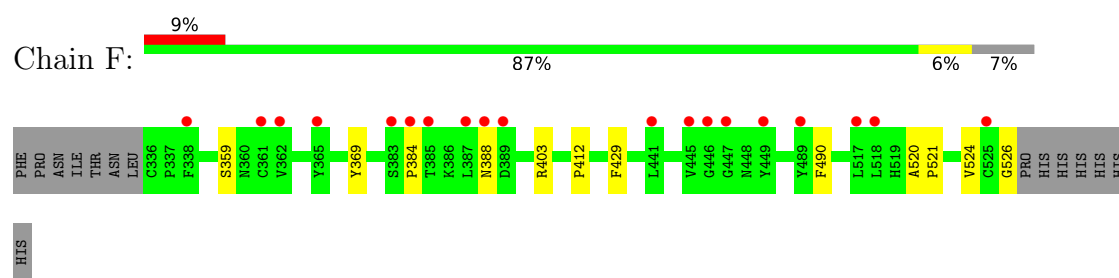
- Molecule 2: LY-CoV555 Fab light chain



- Molecule 3: Spike protein S1



- Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.32Å 280.36Å 68.91Å 90.00° 99.62° 90.00°	Depositor
Resolution (Å)	30.00 – 2.16 140.18 – 2.16	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.00-2.16) 91.7 (140.18-2.16)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.209 , 0.257 0.211 , 0.259	Depositor DCC
R_{free} test set	3764 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9614	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: GOL

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	0.30	0/1717	0.64	0/2341
1	D	0.29	0/1686	0.63	0/2303
2	B	0.30	0/1656	0.64	0/2251
2	E	0.29	0/1648	0.65	0/2243
3	C	0.28	0/1481	0.62	0/2023
3	F	0.28	0/1473	0.61	0/2012
All	All	0.29	0/9661	0.63	0/13173

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	A	0	3
1	D	0	2
3	C	0	3
3	F	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	ARG	Sidechain
1	A	87	ARG	Sidechain
1	A	98	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	357	ARG	Sidechain
3	C	408	ARG	Sidechain
3	C	454	ARG	Sidechain
1	D	38	ARG	Sidechain
1	D	87	ARG	Sidechain
3	F	403	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1668	0	1597	3	0
1	D	1639	0	1557	5	0
2	B	1615	0	1554	4	0
2	E	1607	0	1538	10	0
3	C	1441	0	1262	4	0
3	F	1431	0	1253	5	0
4	A	6	0	8	0	0
4	E	6	0	8	0	0
5	A	45	0	0	0	0
5	B	49	0	0	1	0
5	C	17	0	0	0	0
5	D	33	0	0	0	0
5	E	43	0	0	0	0
5	F	14	0	0	0	0
All	All	9614	0	8777	29	0

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 2.

All (29) 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:E:211:GLU:O	2:E:212:CYS:HB2	1.77	0.82
3:C:363:ALA:HB2	3:C:524:VAL:HG12	1.81	0.62
3:F:520:ALA:HB1	3:F:521:PRO:HD2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:22:THR:HG22	2:E:72:THR:HG22	1.89	0.54
3:F:359:SER:HA	3:F:524:VAL:HG22	1.90	0.53
3:F:388:ASN:HA	3:F:526:GLY:HA3	1.94	0.50
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.46	0.49
2:B:22:THR:HG22	2:B:72:THR:HG22	1.95	0.47
2:E:29:ILE:HA	2:E:92:TYR:CD2	2.50	0.47
2:E:21:ILE:HG12	2:E:102:THR:HG21	1.97	0.46
1:D:36:TRP:CE2	1:D:81:MET:HB2	2.51	0.45
1:D:221:LYS:NZ	2:E:123:GLU:OE1	2.45	0.44
1:D:52:ILE:HD13	3:F:490:PHE:CE1	2.52	0.44
2:E:136:LEU:HD11	2:E:146:VAL:HG22	2.00	0.44
2:E:166:GLN:HG3	2:E:173:TYR:CZ	2.53	0.43
1:D:190:LEU:HD12	1:D:190:LEU:C	2.39	0.43
3:F:412:PRO:HG3	3:F:429:PHE:HB3	2.01	0.43
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.01	0.42
2:E:208:ASN:HB3	2:E:211:GLU:HB3	2.01	0.42
2:E:37:GLN:HB2	2:E:47:LEU:HD11	2.01	0.42
2:B:136:LEU:HD11	2:B:146:VAL:HG22	2.02	0.42
1:D:158:PHE:HA	1:D:159:PRO:HA	1.84	0.41
3:C:431:GLY:HA3	3:C:513:LEU:O	2.21	0.41
2:E:211:GLU:O	2:E:212:CYS:CB	2.59	0.41
3:C:336:CYS:HA	3:C:337:PRO:HD3	1.92	0.41
1:A:153:LEU:HG	1:A:155:LYS:HG3	2.03	0.40
1:A:171:LEU:HD21	1:A:194:VAL:HG21	2.03	0.40
2:B:81[A]:GLU:HG3	5:B:310:HOH:O	2.22	0.40
3:C:380:TYR:O	3:C:430:THR:HA	2.22	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	224/229 (98%)	220 (98%)	4 (2%)	0	100	100
1	D	220/229 (96%)	212 (96%)	7 (3%)	1 (0%)	29	22
2	B	213/212 (100%)	204 (96%)	9 (4%)	0	100	100
2	E	213/212 (100%)	206 (97%)	7 (3%)	0	100	100
3	C	191/205 (93%)	179 (94%)	12 (6%)	0	100	100
3	F	189/205 (92%)	179 (95%)	9 (5%)	1 (0%)	29	22
All	All	1250/1292 (97%)	1200 (96%)	48 (4%)	2 (0%)	47	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	30	SER
3	F	384	PRO

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	175/192 (91%)	168 (96%)	7 (4%)	31	29
1	D	171/192 (89%)	168 (98%)	3 (2%)	59	63
2	B	186/187 (100%)	186 (100%)	0	100	100
2	E	183/187 (98%)	180 (98%)	3 (2%)	62	67
3	C	137/178 (77%)	133 (97%)	4 (3%)	42	42
3	F	135/178 (76%)	134 (99%)	1 (1%)	84	89
All	All	987/1114 (89%)	969 (98%)	18 (2%)	59	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	87	ARG
1	A	98	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	CYS
1	A	145	GLU
1	A	221	LYS
1	A	222	ARG
3	C	356	LYS
3	C	360	ASN
3	C	390	LEU
3	C	441	LEU
1	D	50	ARG
1	D	145	GLU
1	D	190	LEU
2	E	27	GLN
2	E	211	GLU
2	E	212	CYS
3	F	369	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
2	E	152	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	GOL	A	301	-	5,5,5	0.30	0	5,5,5	0.18	0
4	GOL	E	301	-	5,5,5	0.35	0	5,5,5	0.27	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
4	GOL	A	301	-	-	0/4/4/4	-
4	GOL	E	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	225/229 (98%)	0.26	4 (1%) 68 75	23, 35, 75, 95	0
1	D	222/229 (96%)	0.26	4 (1%) 68 75	24, 40, 80, 130	0
2	B	212/212 (100%)	0.19	2 (0%) 84 88	23, 33, 51, 113	0
2	E	212/212 (100%)	0.18	1 (0%) 91 93	23, 41, 61, 98	0
3	C	193/205 (94%)	0.70	20 (10%) 6 9	29, 55, 109, 137	0
3	F	191/205 (93%)	0.61	19 (9%) 7 11	31, 52, 93, 125	0
All	All	1255/1292 (97%)	0.36	50 (3%) 38 47	23, 41, 87, 137	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	383	SER	7.5
1	D	203	THR	7.3
3	F	385	THR	6.3
3	C	335	LEU	5.5
3	C	363	ALA	5.2
2	B	212	CYS	5.1
3	F	388	ASN	4.8
3	C	391	CYS	4.5
3	C	384	PRO	4.3
3	C	364	ASP	4.2
3	C	382	VAL	4.1
2	E	212	CYS	3.8
3	F	525	CYS	3.7
3	C	368	LEU	3.6
3	F	338	PHE	3.6
3	C	526	GLY	3.5
3	F	446	GLY	3.4
3	C	518	LEU	3.1
3	F	384	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	362	VAL	3.1
3	F	362	VAL	3.0
1	D	29	PHE	2.9
3	C	525	CYS	2.9
3	F	518	LEU	2.9
3	F	387	LEU	2.8
3	C	361	CYS	2.8
1	A	202	GLY	2.8
1	A	139	CYS	2.7
3	F	365	TYR	2.6
3	C	334	ASN	2.6
3	F	441	LEU	2.5
3	F	445	VAL	2.4
3	C	517	LEU	2.4
1	D	26	GLY	2.4
1	A	228	HIS	2.4
3	C	338	PHE	2.4
3	F	361	CYS	2.4
3	C	440	ASN	2.3
1	A	29	PHE	2.3
3	F	517	LEU	2.3
3	F	383	SER	2.3
3	C	387	LEU	2.2
3	F	389	ASP	2.2
3	F	447	GLY	2.2
3	C	337	PRO	2.2
3	C	499	PRO	2.2
3	F	449	TYR	2.1
1	D	140	SER	2.0
3	F	489	TYR	2.0
2	B	76	THR	2.0

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 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(Å ²)	Q<0.9
4	GOL	E	301	6/6	0.96	0.14	27,30,39,45	0
4	GOL	A	301	6/6	0.97	0.15	25,32,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.