



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:35 PM UTC

PDB ID : 8BSF / pdb_00008bsf
Title : CRYSTAL STRUCTURE OF SARS-COV-2 RECEPTOR BINDING DOMAIN (RBD-beta variant) in complex with 3D2 Fab
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Deposited on : 2022-11-25
Resolution : 2.20 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 : 4-5-2 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

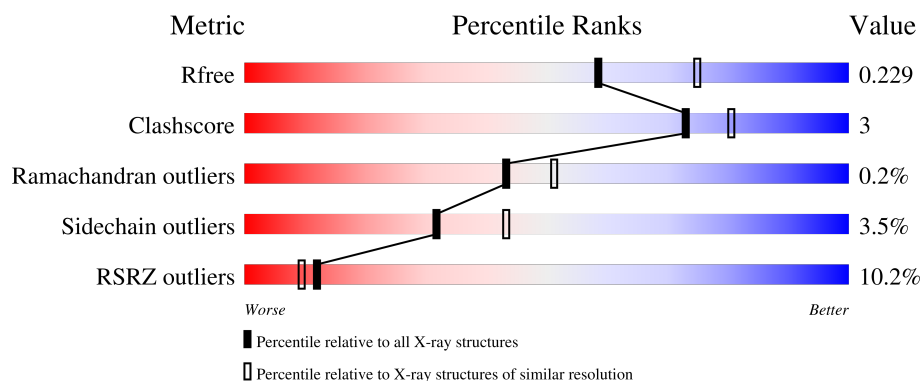
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	231	22% 63% 11% 26%
2	H	231	3% 86% 9% . .
3	L	216	2% 91% 7% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4789 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1369	879	227	255	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	ASN	LYS	engineered mutation	UNP P0DTC2
A	484	LYS	GLU	engineered mutation	UNP P0DTC2
A	501	TYR	ASN	engineered mutation	UNP P0DTC2
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 3D2 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1660	1057	273	324	6			

- Molecule 3 is a protein called 3D2 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	3	0
			1599	1002	263	330	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		

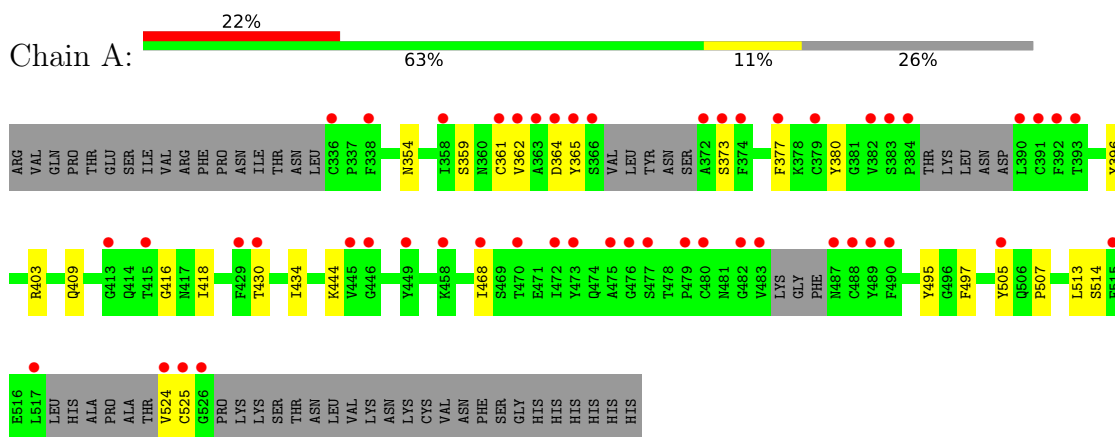
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	H	39	Total	O	0	0
			39	39		
6	L	66	Total	O	0	0
			66	66		

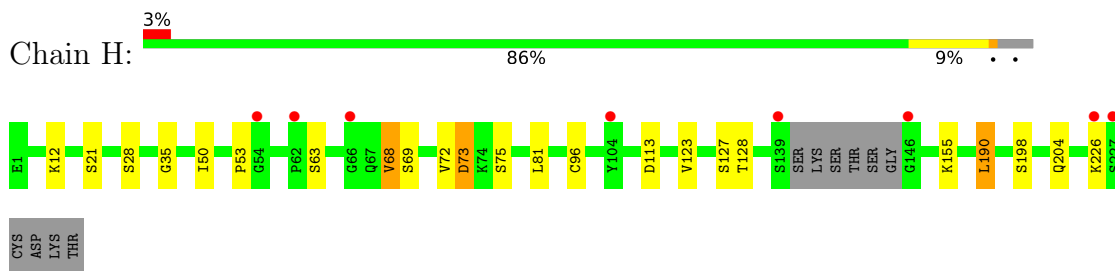
3 Residue-property plots [i](#)

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.

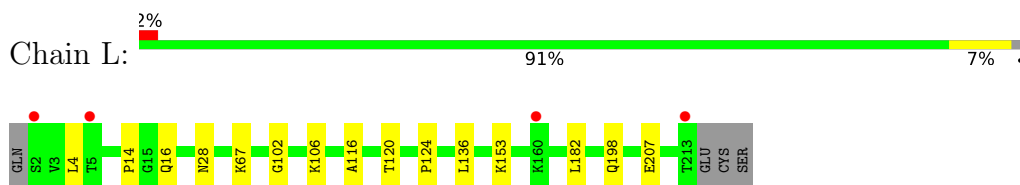
• Molecule 1: Spike protein S1



• Molecule 2: 3D2 FAB HEAVY CHAIN



• Molecule 3: 3D2 FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.69Å 71.20Å 121.25Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	48.07 – 2.20 48.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.07-2.20) 98.7 (48.07-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.229 0.201 , 0.229	Depositor DCC
R_{free} test set	2189 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4789	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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, NAG

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	1.07	1/1405 (0.1%)	1.30	1/1905 (0.1%)
2	H	1.02	0/1706	1.36	8/2325 (0.3%)
3	L	1.06	1/1638 (0.1%)	1.31	1/2242 (0.0%)
All	All	1.05	2/4749 (0.0%)	1.33	10/6472 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLY	C-O	5.56	1.27	1.23
3	L	14	PRO	C-O	-5.29	1.16	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	113	ASP	CA-CB-CG	7.58	120.18	112.60
2	H	128	THR	CB-CA-C	6.79	118.15	109.80
3	L	28	ASN	CA-C-O	-6.48	116.08	119.77
2	H	128	THR	CA-CB-OG1	-5.56	101.26	109.60
2	H	73	ASP	CA-C-N	5.37	128.22	120.38
2	H	73	ASP	C-N-CA	5.37	128.22	120.38
1	A	416	GLY	CA-C-O	-5.34	118.00	122.33
2	H	53	PRO	CA-C-N	5.34	126.02	119.99
2	H	53	PRO	C-N-CA	5.34	126.02	119.99
2	H	68	VAL	CA-C-O	-5.03	116.65	121.63

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	1369	0	1279	10	0
2	H	1660	0	1625	10	0
3	L	1599	0	1548	9	0
4	A	14	0	13	0	0
5	H	6	0	8	0	0
5	L	18	0	24	2	0
6	A	18	0	0	0	0
6	H	39	0	0	1	0
6	L	66	0	0	2	0
All	All	4789	0	4497	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 3.

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:H:68:VAL:HG11	2:H:81:LEU:HD11	1.66	0.77
2:H:155:LYS:NZ	6:H:401:HOH:O	2.19	0.73
2:H:190:LEU:C	2:H:190:LEU:HD12	2.17	0.69
2:H:68:VAL:CG1	2:H:81:LEU:HD11	2.26	0.64
3:L:4:LEU:HB2	3:L:102:GLY:HA2	1.84	0.59
3:L:124:PRO:HD3	3:L:136:LEU:HD23	1.85	0.57
3:L:153:LYS:NZ	6:L:402:HOH:O	2.37	0.57
3:L:124:PRO:HD3	3:L:136:LEU:CD2	2.36	0.56
2:H:35:GLY:HA3	2:H:50:ILE:HG22	1.89	0.54
2:H:190:LEU:C	2:H:190:LEU:CD1	2.84	0.50
2:H:73:ASP:OD1	2:H:75:SER:OG	2.31	0.48
3:L:120:THR:OG1	5:L:303:GOL:H31	2.12	0.48
1:A:505:TYR:CD1	1:A:505:TYR:O	2.68	0.47
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.50	0.46
1:A:468:ILE:HG22	1:A:468:ILE:O	2.16	0.45
3:L:198:GLN:NE2	3:L:207:GLU:OE2	2.48	0.45
1:A:396:TYR:O	1:A:513:LEU:HA	2.18	0.43
2:H:35:GLY:O	2:H:96:CYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:VAL:CG1	2:H:81:LEU:CD1	2.95	0.43
1:A:380:TYR:O	1:A:430:THR:HA	2.20	0.42
3:L:116:ALA:HA	5:L:302:GOL:O1	2.19	0.42
1:A:409:GLN:OE1	1:A:418:ILE:HB	2.20	0.42
1:A:362:VAL:HG13	1:A:525:CYS:O	2.21	0.41
3:L:16:GLN:NE2	6:L:408:HOH:O	2.53	0.41
2:H:12:LYS:O	2:H:123:VAL:HA	2.19	0.41
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.55	0.41
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.56	0.41
3:L:136:LEU:HD12	3:L:182:LEU:HD23	2.03	0.41
1:A:359:SER:O	1:A:524:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

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	162/231 (70%)	153 (94%)	8 (5%)	1 (1%)	21	23
2	H	217/231 (94%)	210 (97%)	7 (3%)	0	100	100
3	L	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
All	All	592/678 (87%)	571 (96%)	20 (3%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	CYS

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	148/203 (73%)	142 (96%)	6 (4%)	27	37
2	H	187/196 (95%)	177 (95%)	10 (5%)	20	26
3	L	181/182 (100%)	179 (99%)	2 (1%)	65	79
All	All	516/581 (89%)	498 (96%)	18 (4%)	32	43

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

Mol	Chain	Res	Type
1	A	354	ASN
1	A	364	ASP
1	A	365	TYR
1	A	373	SER
1	A	444	LYS
1	A	514	SER
2	H	21	SER
2	H	28	SER
2	H	63	SER
2	H	69	SER
2	H	72	VAL
2	H	127	SER
2	H	190	LEU
2	H	198	SER
2	H	204	GLN
2	H	226	LYS
3	L	67	LYS
3	L	106	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
2	H	102	HIS
2	H	183	GLN

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Mol	Chain	Res	Type
2	H	204	GLN
3	L	39	GLN

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 ⓘ

5 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	$\# Z > 2$
5	GOL	H	301	-	5,5,5	0.19	0	5,5,5	0.43	0
5	GOL	L	302	-	5,5,5	0.23	0	5,5,5	0.40	0
5	GOL	L	303	-	5,5,5	0.21	0	5,5,5	0.49	0
4	NAG	A	601	1	14,14,15	1.17	2 (14%)	17,19,21	2.97	4 (23%)
5	GOL	L	301	-	5,5,5	0.12	0	5,5,5	0.38	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
5	GOL	H	301	-	-	4/4/4/4	-
5	GOL	L	302	-	-	0/4/4/4	-
5	GOL	L	303	-	-	2/4/4/4	-
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	GOL	L	301	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	2.21	1.47	1.43
4	A	601	NAG	O5-C5	2.17	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	10.27	125.95	112.19
4	A	601	NAG	C2-N2-C7	3.92	128.15	122.90
4	A	601	NAG	C1-C2-N2	2.15	113.82	110.43
4	A	601	NAG	O7-C7-N2	2.13	125.75	121.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	GOL	C1-C2-C3-O3
5	L	301	GOL	O1-C1-C2-C3
5	L	301	GOL	O2-C2-C3-O3
5	L	303	GOL	O1-C1-C2-C3
5	H	301	GOL	O1-C1-C2-C3
5	L	301	GOL	C1-C2-C3-O3
5	L	301	GOL	O1-C1-C2-O2
5	L	303	GOL	O1-C1-C2-O2
5	H	301	GOL	O2-C2-C3-O3
5	H	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	GOL	1	0
5	L	303	GOL	1	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

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	172/231 (74%)	1.45	50 (29%) 1 1	43, 73, 130, 151	0
2	H	221/231 (95%)	0.21	8 (3%) 46 43	34, 51, 76, 97	0
3	L	212/216 (98%)	-0.20	4 (1%) 66 63	20, 41, 61, 99	3 (1%)
All	All	605/678 (89%)	0.42	62 (10%) 12 9	20, 51, 110, 151	3 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	GLY	6.7
1	A	384	PRO	6.2
1	A	483	VAL	5.4
1	A	517	LEU	5.4
3	L	213	THR	5.2
1	A	390	LEU	5.1
1	A	372	ALA	5.1
1	A	365	TYR	4.7
1	A	366	SER	4.6
1	A	363	ALA	4.4
2	H	104	TYR	4.3
1	A	524	VAL	4.2
1	A	479	PRO	3.9
1	A	377	PHE	3.6
1	A	482	GLY	3.4
1	A	362	VAL	3.3
1	A	473	TYR	3.3
2	H	139	SER	3.3
1	A	489	TYR	3.3
1	A	336	CYS	3.3
1	A	475	ALA	3.2
1	A	458	LYS	3.1
1	A	468	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	445	VAL	3.0
1	A	525	CYS	2.9
1	A	382	VAL	2.9
1	A	505	TYR	2.8
3	L	160	LYS	2.8
1	A	429	PHE	2.8
1	A	449	TYR	2.7
1	A	515	PHE	2.7
1	A	487	ASN	2.7
1	A	392	PHE	2.6
3	L	2	SER	2.6
1	A	379	CYS	2.6
1	A	361	CYS	2.5
1	A	364	ASP	2.5
1	A	476	GLY	2.5
1	A	470	THR	2.4
1	A	480	CYS	2.4
1	A	358	ILE	2.4
1	A	490	PHE	2.4
1	A	488	CYS	2.3
1	A	415	THR	2.3
1	A	477	SER	2.3
2	H	227	SER	2.3
1	A	374	PHE	2.2
2	H	62	PRO	2.2
2	H	54	GLY	2.2
2	H	66	GLY	2.2
1	A	430	THR	2.2
1	A	391	CYS	2.2
1	A	446	GLY	2.2
1	A	373	SER	2.2
1	A	383	SER	2.2
3	L	5	THR	2.2
1	A	472	ILE	2.2
1	A	338	PHE	2.1
1	A	413	GLY	2.1
2	H	146	GLY	2.1
1	A	393	THR	2.0
2	H	226	LYS	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 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($\text{\AA}^2$)	Q<0.9
4	NAG	A	601	14/15	0.66	0.20	81,92,105,106	0
5	GOL	H	301	6/6	0.77	0.17	71,79,80,86	0
5	GOL	L	303	6/6	0.82	0.21	57,81,90,92	0
5	GOL	L	302	6/6	0.85	0.15	55,57,65,65	0
5	GOL	L	301	6/6	0.90	0.15	44,63,67,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.