



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 AM UTC

PDB ID : 7ZXU / pdb_00007zxu
Title : SARS-CoV-2 Omicron BA.4/5 RBD in complex with Beta-27 Fab and C1 nanobody
Authors : Huo, J.; Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2022-05-23
Resolution : 1.89 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

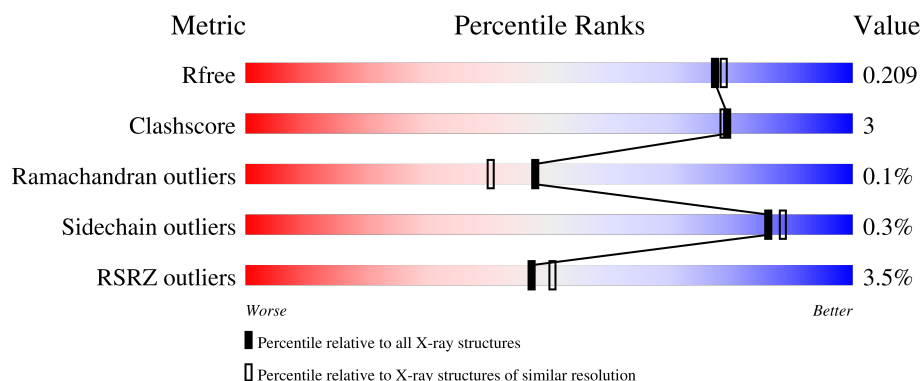
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	E	202	4% 90% 7% .
2	A	131	6% 87% 8% 5%
3	H	222	2% 91% 5% 5%
4	L	214	2% 95% .

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6491 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	E	197	Total	C	N	O	S	0	5	0
			1597	1027	275	287	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	452	ARG	LEU	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	486	VAL	PHE	conflict	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	527	LYS	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called Nanobody C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	124	Total	C	N	O	S	0	2	0
			978	615	170	189	4			

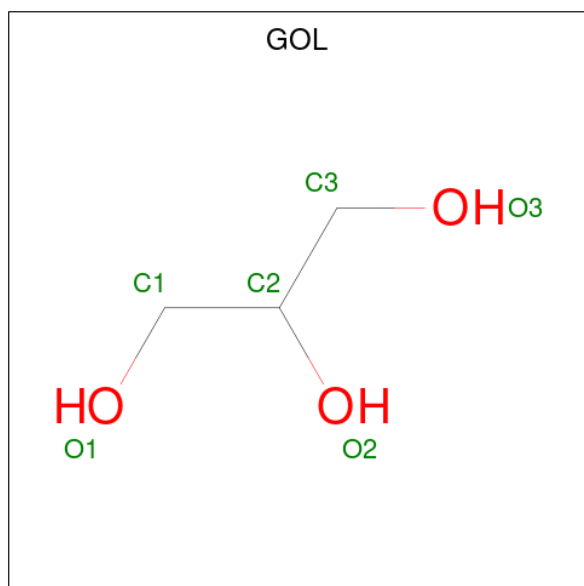
- Molecule 3 is a protein called Beta-27 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	1	0
			1583	1000	268	308	7			

- Molecule 4 is a protein called Beta-27 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	5	0
			1645	1023	279	338	5			

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



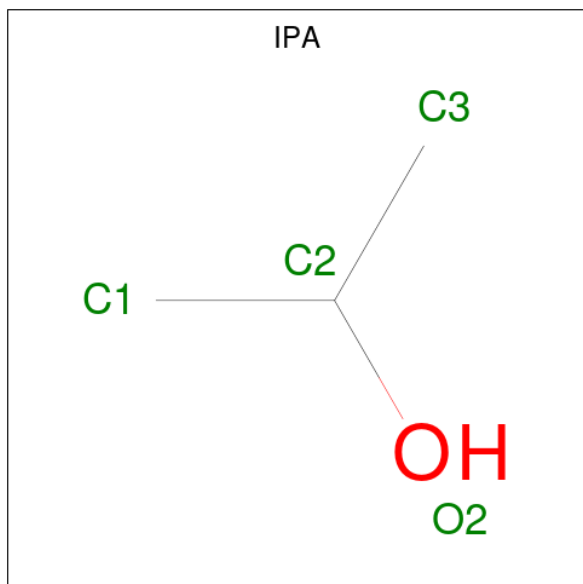
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

Continued on next page...

Continued from previous page...

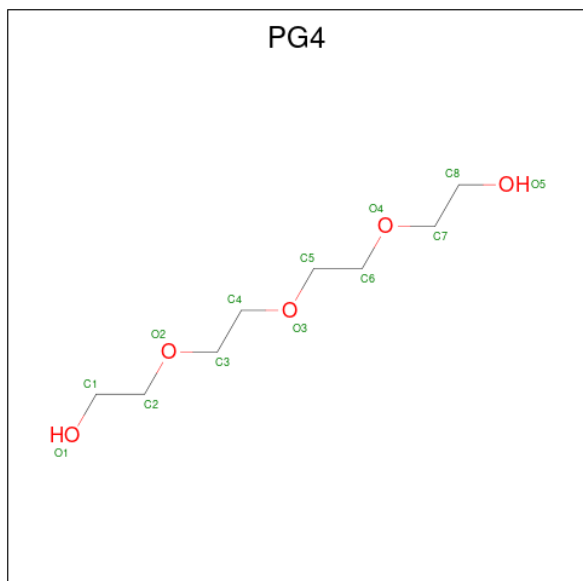
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			4	3	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			13	8	5		

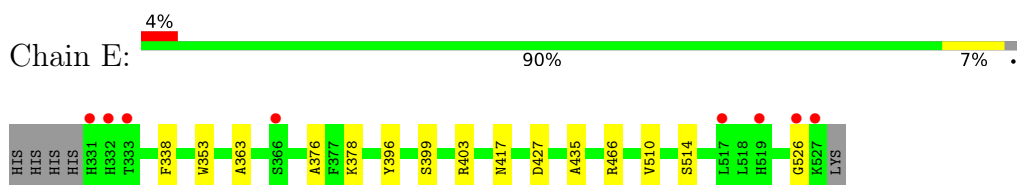
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	166	Total	O	0	0
			166	166		
9	A	73	Total	O	0	0
			73	73		
9	H	165	Total	O	0	0
			165	165		
9	L	173	Total	O	0	0
			173	173		

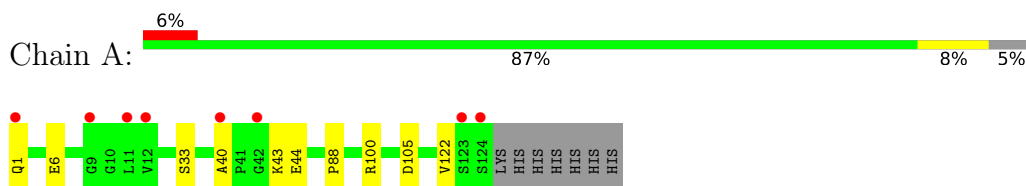
3 Residue-property plots [i](#)

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.

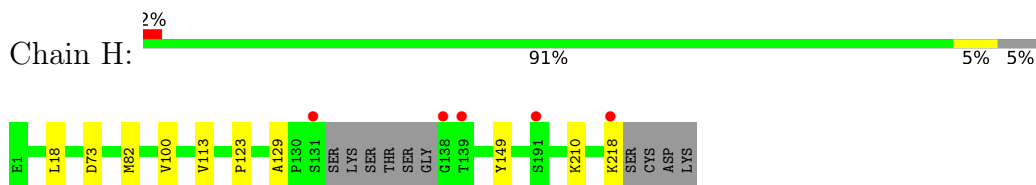
- Molecule 1: Spike protein S1



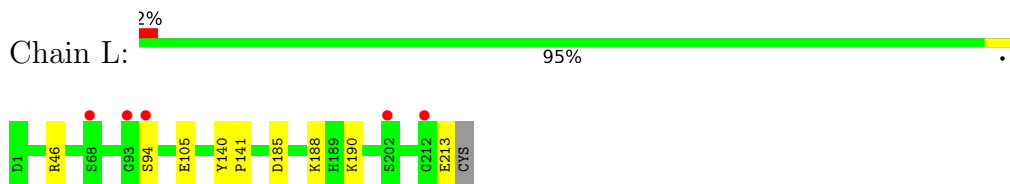
- Molecule 2: Nanobody C1



- Molecule 3: Beta-27 heavy chain



- Molecule 4: Beta-27 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.11Å 100.44Å 105.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.75 – 1.89 65.75 – 1.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.75-1.89) 99.9 (65.75-1.89)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.181 , 0.209 0.181 , 0.209	Depositor DCC
R_{free} test set	3761 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6491	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, IPA, PG4

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	E	0.10	0/1660	0.29	0/2257
2	A	0.10	0/1009	0.28	0/1372
3	H	0.11	0/1621	0.31	0/2208
4	L	0.10	0/1683	0.32	0/2283
All	All	0.10	0/5973	0.30	0/8120

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 [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	E	1597	0	1526	11	0
2	A	978	0	930	9	0
3	H	1583	0	1568	6	1
4	L	1645	0	1592	7	0
5	A	12	0	16	0	0
5	E	18	0	24	0	0
5	H	24	0	32	0	0
5	L	6	0	8	0	0
6	A	4	0	8	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	12	0	24	0	0
6	H	4	0	8	1	0
6	L	4	0	8	0	1
7	E	14	0	13	0	0
8	L	13	0	18	2	0
9	A	73	0	0	4	0
9	E	166	0	0	1	0
9	H	165	0	0	2	1
9	L	173	0	0	5	1
All	All	6491	0	5775	32	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 3.

All (32) 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)
3:H:73:ASP:H	6:H:304:IPA:H31	1.53	0.74
3:H:129:ALA:O	9:H:401:HOH:O	2.04	0.74
2:A:44:GLU:OE2	9:A:1501:HOH:O	2.08	0.70
4:L:94[B]:SER:O	9:L:401:HOH:O	2.10	0.69
1:E:403:ARG:HH12	8:L:301:PG4:H71	1.60	0.65
4:L:46:ARG:NH2	9:L:402:HOH:O	2.13	0.65
4:L:213:GLU:O	9:L:403:HOH:O	2.16	0.61
3:H:218:LYS:NZ	9:H:404:HOH:O	2.37	0.56
3:H:123:PRO:HB3	3:H:149:TYR:HB3	1.90	0.52
2:A:100[B]:ARG:HH12	6:A:1401:IPA:H31	1.76	0.50
2:A:100[B]:ARG:NH1	6:A:1401:IPA:H31	2.27	0.50
2:A:33:SER:HB3	9:A:1521:HOH:O	2.11	0.49
1:E:427:ASP:O	6:A:1401:IPA:H11	2.13	0.47
2:A:1:GLN:N	9:A:1505:HOH:O	2.46	0.47
4:L:185:ASP:HA	4:L:188:LYS:HD3	1.96	0.47
2:A:1:GLN:HB3	9:A:1517:HOH:O	2.14	0.47
1:E:396:TYR:HB2	1:E:514[A]:SER:OG	2.17	0.45
1:E:353:TRP:O	1:E:466[B]:ARG:NE	2.50	0.44
1:E:363:ALA:O	1:E:526:GLY:HA2	2.17	0.43
1:E:378:LYS:HD3	2:A:105:ASP:HB2	1.99	0.43
1:E:417:ASN:HB2	8:L:301:PG4:H32	2.00	0.43
2:A:88:PRO:HA	2:A:122:VAL:HB	2.01	0.43
1:E:399:SER:HA	1:E:510:VAL:O	2.20	0.42
3:H:82:MET:HE1	3:H:113:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:PHE:HE2	1:E:363:ALA:HB1	1.84	0.42
4:L:140:TYR:CG	4:L:141:PRO:HA	2.55	0.42
4:L:190:LYS:NZ	9:L:410:HOH:O	2.41	0.41
1:E:376:ALA:HB3	1:E:435:ALA:HB3	2.03	0.41
3:H:18:LEU:HB3	3:H:82:MET:HE3	2.03	0.41
1:E:403:ARG:HD2	9:E:758:HOH:O	2.20	0.40
2:A:40:ALA:HB3	2:A:43:LYS:HB2	2.03	0.40
4:L:46:ARG:HD2	9:L:431: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)
3:H:210:LYS:NZ	6:L:303:IPA:O2[4_444]	1.30	0.90
9:H:514:HOH:O	9:L:555:HOH:O[4_444]	2.05	0.15

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	E	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
2	A	124/131 (95%)	122 (98%)	2 (2%)	0	100	100
3	H	209/222 (94%)	206 (99%)	2 (1%)	1 (0%)	24	16
4	L	216/214 (101%)	210 (97%)	6 (3%)	0	100	100
All	All	749/769 (97%)	734 (98%)	14 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	100	VAL

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	E	173/174 (99%)	173 (100%)	0	100	100
2	A	105/110 (96%)	104 (99%)	1 (1%)	68	70
3	H	178/187 (95%)	178 (100%)	0	100	100
4	L	187/184 (102%)	186 (100%)	1 (0%)	81	84
All	All	643/655 (98%)	641 (100%)	2 (0%)	86	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	GLU
4	L	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	39	GLN
2	A	73	HIS
2	A	77	ASN
2	A	82	GLN
2	A	84	ASN
3	H	39	GLN
4	L	39	GLN
4	L	160	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	302	-	5,5,5	0.92	0	5,5,5	1.10	0
6	IPA	E	606	-	3,3,3	0.54	0	3,3,3	0.31	0
8	PG4	L	301	-	12,12,12	0.12	0	11,11,11	0.63	0
5	GOL	H	303	-	5,5,5	0.90	0	5,5,5	1.07	0
6	IPA	E	604	-	3,3,3	0.54	0	3,3,3	0.32	0
6	IPA	E	603	-	3,3,3	0.53	0	3,3,3	0.31	0
5	GOL	H	305	-	5,5,5	0.91	0	5,5,5	1.05	0
6	IPA	H	304	-	3,3,3	0.53	0	3,3,3	0.31	0
5	GOL	E	602	-	5,5,5	0.87	0	5,5,5	1.10	1 (20%)
5	GOL	A	1402	-	5,5,5	0.95	0	5,5,5	1.07	0
5	GOL	H	301	-	5,5,5	0.89	0	5,5,5	1.11	0
5	GOL	E	607	-	5,5,5	1.02	0	5,5,5	1.05	0
6	IPA	A	1401	-	3,3,3	0.51	0	3,3,3	0.43	0
7	NAG	E	605	1	14,14,15	0.28	0	17,19,21	0.35	0
5	GOL	A	1403	-	5,5,5	0.92	0	5,5,5	1.09	0
5	GOL	E	601	-	5,5,5	0.92	0	5,5,5	1.07	0
6	IPA	L	303	-	3,3,3	0.54	0	3,3,3	0.36	0
5	GOL	L	302	-	5,5,5	0.94	0	5,5,5	1.09	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
5	GOL	H	302	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PG4	L	301	-	-	8/10/10/10	-
5	GOL	H	303	-	-	4/4/4/4	-
5	GOL	H	305	-	-	2/4/4/4	-
7	NAG	E	605	1	-	0/6/23/26	0/1/1/1
5	GOL	E	602	-	-	2/4/4/4	-
5	GOL	A	1402	-	-	2/4/4/4	-
5	GOL	H	301	-	-	2/4/4/4	-
5	GOL	E	607	-	-	2/4/4/4	-
5	GOL	A	1403	-	-	0/4/4/4	-
5	GOL	E	601	-	-	0/4/4/4	-
5	GOL	L	302	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	602	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	303	GOL	C1-C2-C3-O3
5	E	602	GOL	O1-C1-C2-O2
5	H	303	GOL	O2-C2-C3-O3
5	E	602	GOL	O1-C1-C2-C3
5	E	607	GOL	O1-C1-C2-C3
5	A	1402	GOL	O1-C1-C2-C3
5	H	301	GOL	O1-C1-C2-C3
5	H	303	GOL	O1-C1-C2-C3
5	H	305	GOL	C1-C2-C3-O3
8	L	301	PG4	O3-C5-C6-O4
5	H	303	GOL	O1-C1-C2-O2
5	E	607	GOL	O1-C1-C2-O2
5	H	305	GOL	O2-C2-C3-O3
8	L	301	PG4	O4-C7-C8-O5
5	H	301	GOL	O1-C1-C2-O2
5	A	1402	GOL	O1-C1-C2-O2
5	L	302	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	301	PG4	C5-C6-O4-C7
8	L	301	PG4	C4-C3-O2-C2
8	L	301	PG4	O1-C1-C2-O2
8	L	301	PG4	C8-C7-O4-C6
8	L	301	PG4	C1-C2-O2-C3
8	L	301	PG4	O2-C3-C4-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	301	PG4	2	0
6	H	304	IPA	1	0
6	A	1401	IPA	3	0
6	L	303	IPA	0	1

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	E	197/202 (97%)	0.09	8 (4%)	41	44	16, 32, 64, 108	5 (2%)
2	A	124/131 (94%)	0.32	8 (6%)	25	26	22, 43, 73, 84	2 (1%)
3	H	212/222 (95%)	0.03	5 (2%)	59	63	24, 35, 59, 84	1 (0%)
4	L	213/214 (99%)	0.07	5 (2%)	61	65	18, 36, 56, 85	5 (2%)
All	All	746/769 (97%)	0.10	26 (3%)	47	50	16, 36, 65, 108	13 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	527	LYS	4.0
4	L	94[A]	SER	4.0
1	E	333	THR	3.8
3	H	131	SER	3.1
1	E	519	HIS	3.1
2	A	40	ALA	2.9
2	A	1	GLN	2.8
1	E	332	HIS	2.8
2	A	42	GLY	2.7
4	L	212	GLY	2.7
1	E	526	GLY	2.7
3	H	218	LYS	2.6
3	H	138	GLY	2.6
2	A	12	VAL	2.4
4	L	93[A]	GLY	2.4
2	A	123	SER	2.4
4	L	68	SER	2.3
1	E	366	SER	2.3
2	A	11[A]	LEU	2.3
2	A	124	SER	2.2
4	L	202	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	331	HIS	2.1
3	H	139	THR	2.1
3	H	191	SER	2.1
2	A	9	GLY	2.1
1	E	517	LEU	2.1

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
7	NAG	E	605	14/15	0.30	0.19	82,98,104,104	0
6	IPA	L	303	4/4	0.66	0.24	47,52,61,79	0
6	IPA	E	606	4/4	0.75	0.20	48,53,57,58	0
6	IPA	A	1401	4/4	0.75	0.21	38,52,53,53	0
8	PG4	L	301	13/13	0.80	0.17	42,48,63,64	0
5	GOL	H	303	6/6	0.81	0.15	53,58,62,64	0
5	GOL	A	1402	6/6	0.82	0.14	57,62,66,69	0
5	GOL	H	301	6/6	0.82	0.16	41,51,57,59	0
5	GOL	H	302	6/6	0.83	0.13	53,57,61,71	0
5	GOL	A	1403	6/6	0.84	0.18	50,53,57,60	0
5	GOL	L	302	6/6	0.86	0.14	54,58,64,72	0
5	GOL	H	305	6/6	0.86	0.13	39,53,59,61	0
6	IPA	E	604	4/4	0.87	0.16	36,40,47,54	0
5	GOL	E	607	6/6	0.87	0.15	42,54,63,63	0
6	IPA	H	304	4/4	0.88	0.15	44,49,56,61	0
5	GOL	E	601	6/6	0.88	0.15	38,44,54,55	0
5	GOL	E	602	6/6	0.89	0.12	43,46,51,53	0
6	IPA	E	603	4/4	0.90	0.14	47,51,57,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.