



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2022 – 08:05 PM EST

PDB ID : 7S5R  
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibodies CV07-287 and COVA1-16  
Authors : Yuan, M.; Wilson, I.A.  
Deposited on : 2021-09-11  
Resolution : 2.45 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](mailto: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.

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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 : 2.27  
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) : 2.27

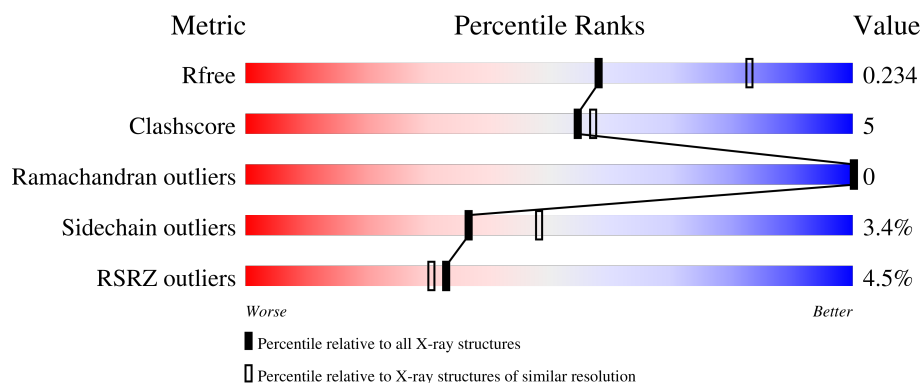
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	
2	H	232	
3	L	214	
4	B	226	
5	C	216	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8512 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	196	Total	C	N	O	S	0	0	0
			1554	997	260	289	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 COVA1-16 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1715	1081	292	334	8			

- Molecule 3 is a protein called COVA1-16 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1631	1019	272	336	4			

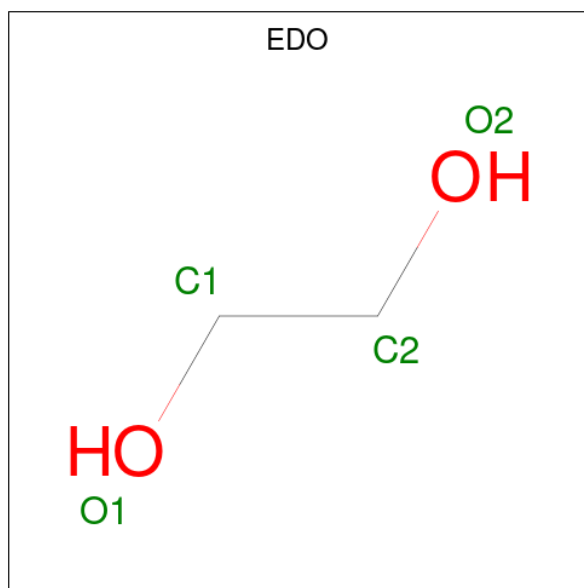
- Molecule 4 is a protein called CV07-287 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	219	Total	C	N	O	S	0	0	0
			1641	1032	274	325	10			

- Molecule 5 is a protein called CV07-287 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	214	Total	C	N	O	S	4	2	0
			1650	1034	278	333	5			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	H	1	Total O S 5 4 1	0	0
8	L	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0

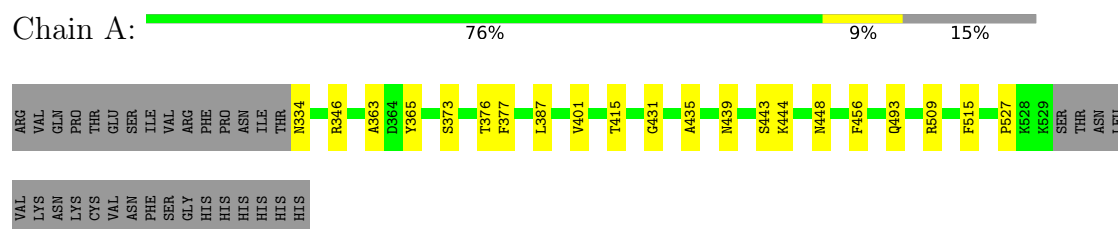
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	82	Total O 82 82	0	0
9	H	54	Total O 54 54	0	0
9	L	52	Total O 52 52	0	0
9	B	23	Total O 23 23	0	0
9	C	14	Total O 14 14	0	0

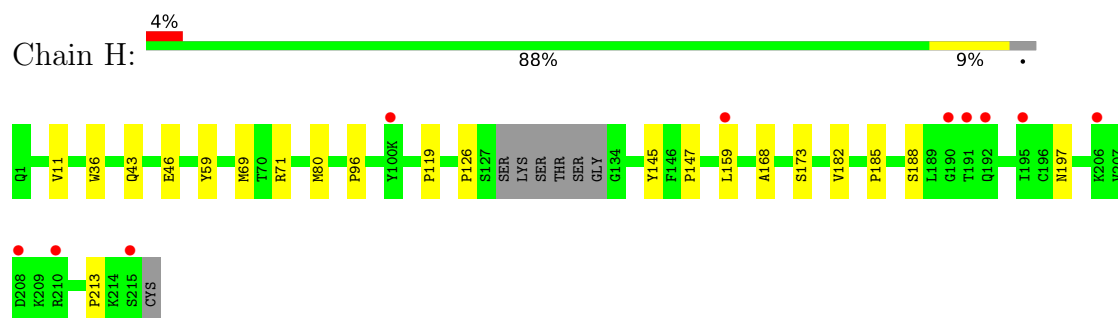
### 3 Residue-property plots

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.

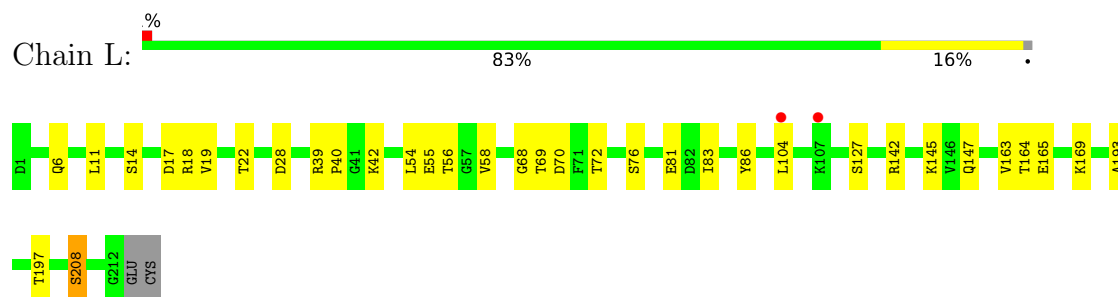
- Molecule 1: Spike protein S1



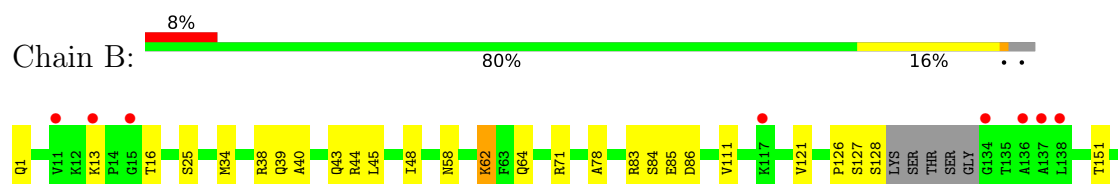
- Molecule 2: COVA1-16 Heavy chain

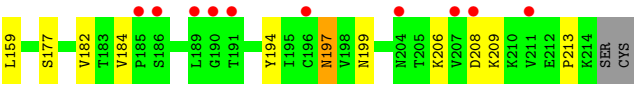


- Molecule 3: COVA1-16 Light chain

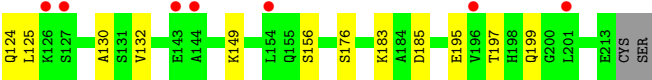
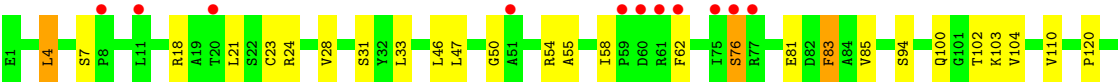
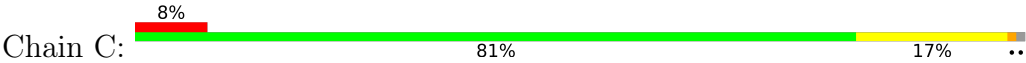


- Molecule 4: CV07-287 Heavy chain





● Molecule 5: CV07-287 Light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.63Å 121.48Å 136.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.53 – 2.45 40.53 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.53-2.45) 99.8 (40.53-2.45)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.207 , 0.237 0.204 , 0.234	Depositor DCC
$R_{free}$ test set	2728 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, SO4, 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	0.30	0/1598	0.53	0/2173
2	H	0.28	0/1759	0.54	0/2395
3	L	0.29	0/1666	0.53	0/2266
4	B	0.27	0/1679	0.54	0/2290
5	C	0.29	0/1693	0.52	0/2300
All	All	0.29	0/8395	0.53	0/11424

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	A	1554	0	1478	12	0
2	H	1715	0	1658	13	0
3	L	1631	0	1575	21	0
4	B	1641	0	1594	20	0
5	C	1650	0	1605	21	0
6	A	12	0	18	0	0
6	B	8	0	12	0	0
6	H	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	14	0	13	0	0
8	A	15	0	0	0	0
8	B	5	0	0	0	0
8	H	25	0	0	1	0
8	L	5	0	0	0	0
9	A	82	0	0	2	0
9	B	23	0	0	4	0
9	C	14	0	0	2	0
9	H	54	0	0	6	0
9	L	52	0	0	4	0
All	All	8512	0	7971	84	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 5.

All (84) 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:L:55:GLU:OE2	9:L:401:HOH:O	2.00	0.78
4:B:159:LEU:HD11	4:B:182:VAL:HG21	1.65	0.78
2:H:46:GLU:HB2	6:H:303:EDO:H21	1.70	0.73
5:C:149:LYS:NZ	5:C:195:GLU:OE1	2.23	0.71
5:C:18:ARG:HG3	5:C:76:SER:HA	1.73	0.71
2:H:168:ALA:O	9:H:401:HOH:O	2.07	0.71
2:H:11:VAL:HB	2:H:147:PRO:HG3	1.73	0.69
1:A:456:PHE:O	9:A:701:HOH:O	2.13	0.67
4:B:197:ASN:ND2	4:B:208:ASP:OD2	2.25	0.67
1:A:334:ASN:ND2	9:A:704:HOH:O	2.29	0.66
5:C:124:GLN:OE1	9:C:301:HOH:O	2.15	0.65
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.78	0.65
2:H:126:PRO:O	9:H:403:HOH:O	2.15	0.65
4:B:127:SER:OG	9:B:401:HOH:O	2.12	0.64
3:L:40:PRO:HB3	3:L:165:GLU:HG3	1.80	0.64
4:B:38:ARG:HB3	4:B:48:ILE:HD11	1.77	0.64
4:B:151:THR:HG22	4:B:199:ASN:HB3	1.80	0.64
3:L:22:THR:HG22	3:L:72:THR:HG22	1.79	0.63
3:L:6:GLN:NE2	3:L:86:TYR:O	2.31	0.63
5:C:46:LEU:O	9:C:302:HOH:O	2.15	0.63
5:C:4:LEU:HG	5:C:23:CYS:SG	2.38	0.62
5:C:47:LEU:HD12	5:C:58:ILE:HD12	1.81	0.62
4:B:83:ARG:NH1	9:B:402:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:GLN:O	9:H:404:HOH:O	2.16	0.61
4:B:85:GLU:N	4:B:85:GLU:OE2	2.35	0.59
4:B:64:GLN:NE2	9:B:404:HOH:O	2.36	0.59
3:L:169:LYS:NZ	4:B:1:GLN:O	2.36	0.57
1:A:334:ASN:N	1:A:334:ASN:OD1	2.37	0.57
3:L:40:PRO:O	9:L:402:HOH:O	2.17	0.57
3:L:14:SER:OG	9:L:403:HOH:O	2.18	0.56
5:C:120:PRO:HD3	5:C:132:VAL:HG22	1.88	0.55
4:B:13:LYS:O	4:B:16:THR:OG1	2.25	0.55
5:C:31:SER:HA	5:C:50:GLY:HA2	1.88	0.55
3:L:145:LYS:HB3	3:L:197:THR:HB	1.89	0.54
2:H:185:PRO:O	2:H:188:SER:OG	2.25	0.54
4:B:58:ASN:ND2	5:C:94:SER:OG	2.36	0.54
5:C:85:VAL:HG22	5:C:103:LYS:HG2	1.90	0.52
2:H:173:SER:OG	9:H:402:HOH:O	2.07	0.52
1:A:376:THR:HB	1:A:435:ALA:HB3	1.91	0.51
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.91	0.51
3:L:142:ARG:HH21	3:L:163:VAL:HG11	1.76	0.51
4:B:126:PRO:HG2	4:B:213:PRO:HB3	1.92	0.50
3:L:164:THR:O	9:L:404:HOH:O	2.20	0.50
4:B:40:ALA:HB3	4:B:43:GLN:HB2	1.94	0.49
2:H:96:PRO:O	9:H:406:HOH:O	2.20	0.49
5:C:81:GLU:H	5:C:81:GLU:CD	2.16	0.48
4:B:34:MET:SD	4:B:78:ALA:HB3	2.53	0.48
4:B:39:GLN:HB2	4:B:45:LEU:HD23	1.94	0.48
3:L:11:LEU:HD11	3:L:19:VAL:HG13	1.96	0.48
4:B:44:ARG:HE	5:C:100:GLN:HA	1.78	0.48
2:H:126:PRO:HD2	2:H:213:PRO:HA	1.95	0.47
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.50	0.47
4:B:184:VAL:HG11	4:B:194:TYR:CE1	2.50	0.47
5:C:47:LEU:HA	5:C:58:ILE:HD12	1.97	0.46
1:A:415:THR:O	3:L:56:THR:HG21	2.15	0.46
4:B:62:LYS:NZ	9:B:405:HOH:O	2.38	0.46
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.98	0.45
5:C:4:LEU:HD12	5:C:4:LEU:HA	1.71	0.45
8:H:306:SO4:O2	9:H:405:HOH:O	2.18	0.45
5:C:110:VAL:HG11	5:C:199:GLN:HG2	1.98	0.45
5:C:21:LEU:HD23	5:C:102:THR:HB	1.99	0.45
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.53	0.43
3:L:54:LEU:HD21	3:L:58:VAL:O	2.18	0.43
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:28:ASP:OD1	3:L:68:GLY:HA2	2.17	0.43
5:C:83:PHE:HA	5:C:104:VAL:O	2.17	0.43
3:L:39:ARG:HB2	3:L:42:LYS:HD3	2.01	0.43
5:C:55:ALA:HB3	5:C:58:ILE:HG13	2.00	0.43
4:B:38:ARG:NH1	4:B:86:ASP:HA	2.34	0.42
4:B:121:VAL:HG12	4:B:209:LYS:HE3	2.00	0.42
2:H:159:LEU:HD21	2:H:182:VAL:HG21	2.01	0.42
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.55	0.42
3:L:83:ILE:HD12	3:L:104:LEU:O	2.19	0.42
2:H:59:TYR:HE1	2:H:69:MET:HB2	1.85	0.41
1:A:439:ASN:O	1:A:443:SER:HB2	2.20	0.41
3:L:69:THR:HG22	3:L:70:ASP:OD1	2.21	0.41
1:A:363:ALA:O	1:A:527:PRO:HD3	2.21	0.41
5:C:125:LEU:HD23	5:C:125:LEU:HA	1.89	0.41
3:L:81:GLU:CD	3:L:81:GLU:H	2.24	0.40
3:L:193:ALA:CB	3:L:208:SER:HB3	2.49	0.40
3:L:18:ARG:HG2	3:L:76:SER:HA	2.02	0.40
5:C:54:ARG:NH1	5:C:62:PHE:O	2.51	0.40
1:A:444:LYS:HG3	1:A:448:ASN:HB2	2.03	0.40
5:C:120:PRO:HG3	5:C:130:ALA:HB1	2.04	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	194/231 (84%)	187 (96%)	7 (4%)	0	100	100
2	H	221/232 (95%)	212 (96%)	9 (4%)	0	100	100
3	L	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
4	B	215/226 (95%)	209 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	214/216 (99%)	208 (97%)	6 (3%)	0	100	100
All	All	1054/1119 (94%)	1018 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	169/203 (83%)	165 (98%)	4 (2%)	49	61
2	H	190/198 (96%)	188 (99%)	2 (1%)	73	82
3	L	187/189 (99%)	183 (98%)	4 (2%)	53	66
4	B	186/194 (96%)	177 (95%)	9 (5%)	25	33
5	C	187/187 (100%)	175 (94%)	12 (6%)	17	21
All	All	919/971 (95%)	888 (97%)	31 (3%)	37	48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	ARG
1	A	373	SER
1	A	377	PHE
1	A	493	GLN
2	H	71	ARG
2	H	197	ASN
3	L	17	ASP
3	L	127	SER
3	L	147	GLN
3	L	208	SER
4	B	25	SER
4	B	62	LYS
4	B	71	ARG
4	B	84	SER

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Mol	Chain	Res	Type
4	B	111	VAL
4	B	128	SER
4	B	177	SER
4	B	197	ASN
4	B	206	LYS
5	C	4	LEU
5	C	7	SER
5	C	24	ARG
5	C	28	VAL
5	C	33	LEU
5	C	76	SER
5	C	83	PHE
5	C	156	SER
5	C	176	SER
5	C	183	LYS
5	C	185	ASP
5	C	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
4	B	43	GLN
4	B	58	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

19 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	$\# Z  > 2$
7	NAG	A	604	1	14,14,15	0.46	0	17,19,21	0.57	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.09	0
8	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.07	0
6	EDO	A	602	-	3,3,3	0.54	0	2,2,2	0.23	0
8	SO4	H	304	-	4,4,4	0.15	0	6,6,6	0.16	0
8	SO4	H	308	-	4,4,4	0.14	0	6,6,6	0.13	0
8	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.15	0
6	EDO	H	303	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	H	301	-	3,3,3	0.45	0	2,2,2	0.35	0
6	EDO	H	302	-	3,3,3	0.46	0	2,2,2	0.48	0
8	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.08	0
8	SO4	H	306	-	4,4,4	0.13	0	6,6,6	0.12	0
6	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.36	0
6	EDO	A	601	-	3,3,3	0.44	0	2,2,2	0.41	0
6	EDO	B	301	-	3,3,3	0.47	0	2,2,2	0.34	0
8	SO4	A	607	-	4,4,4	0.12	0	6,6,6	0.14	0
8	SO4	H	305	-	4,4,4	0.12	0	6,6,6	0.10	0
8	SO4	H	307	-	4,4,4	0.13	0	6,6,6	0.06	0
6	EDO	B	302	-	3,3,3	0.52	0	2,2,2	0.24	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
6	EDO	A	602	-	-	0/1/1/1	-
6	EDO	A	603	-	-	1/1/1/1	-
6	EDO	A	601	-	-	0/1/1/1	-
6	EDO	B	301	-	-	0/1/1/1	-
7	NAG	A	604	1	-	0/6/23/26	0/1/1/1
6	EDO	H	301	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	302	-	-	0/1/1/1	-
6	EDO	H	303	-	-	1/1/1/1	-
6	EDO	B	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	EDO	O1-C1-C2-O2
6	H	303	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	303	EDO	1	0
8	H	306	SO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/231 (84%)	0.02	0 100 100	26, 40, 58, 74	0
2	H	225/232 (96%)	0.20	10 (4%) 34 32	33, 53, 93, 112	0
3	L	212/214 (99%)	0.19	2 (0%) 84 85	35, 55, 73, 78	0
4	B	219/226 (96%)	0.44	18 (8%) 11 8	44, 71, 98, 106	0
5	C	214/216 (99%)	0.54	18 (8%) 11 8	55, 74, 88, 101	0
All	All	1066/1119 (95%)	0.28	48 (4%) 33 30	26, 59, 91, 112	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	196	CYS	5.7
5	C	76	SER	5.1
2	H	215	SER	4.9
4	B	185	PRO	4.5
2	H	191	THR	3.8
4	B	117	LYS	3.7
4	B	189	LEU	3.6
5	C	201	LEU	3.5
5	C	11	LEU	3.3
2	H	206	LYS	3.2
5	C	51	ALA	3.1
5	C	196	VAL	3.0
5	C	154	LEU	3.0
5	C	59	PRO	3.0
2	H	210	ARG	2.9
5	C	8	PRO	2.9
5	C	77	ARG	2.8
2	H	208	ASP	2.8
4	B	136	ALA	2.7
5	C	127	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	104	LEU	2.7
5	C	20	THR	2.7
4	B	204	ASN	2.7
5	C	61	ARG	2.7
4	B	191	THR	2.6
5	C	143	GLU	2.6
4	B	15	GLY	2.5
4	B	186	SER	2.5
4	B	211	VAL	2.5
2	H	159	LEU	2.5
2	H	192	GLN	2.4
2	H	195	ILE	2.4
4	B	208	ASP	2.4
4	B	13	LYS	2.3
5	C	75	ILE	2.3
3	L	107	LYS	2.3
2	H	190	GLY	2.2
4	B	137	ALA	2.2
4	B	138	LEU	2.2
4	B	11	VAL	2.2
5	C	60	ASP	2.1
2	H	100(K)	TYR	2.1
4	B	190	GLY	2.1
5	C	62	PHE	2.1
4	B	134	GLY	2.1
5	C	126	LYS	2.1
5	C	144	ALA	2.0
4	B	207	VAL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	A	604	14/15	0.78	0.29	69,90,99,99	0
6	EDO	B	302	4/4	0.83	0.21	60,61,64,69	0
8	SO4	H	307	5/5	0.85	0.22	74,75,87,94	5
8	SO4	L	301	5/5	0.86	0.32	66,80,95,96	5
8	SO4	B	303	5/5	0.87	0.24	57,59,72,76	5
6	EDO	H	302	4/4	0.89	0.16	63,63,65,78	0
8	SO4	H	306	5/5	0.91	0.26	52,55,68,79	5
6	EDO	A	602	4/4	0.91	0.17	41,42,44,46	0
6	EDO	B	301	4/4	0.91	0.16	58,63,74,75	0
8	SO4	A	606	5/5	0.91	0.19	67,69,73,86	5
8	SO4	A	607	5/5	0.92	0.35	43,48,54,61	5
8	SO4	H	305	5/5	0.92	0.23	43,47,54,58	5
6	EDO	H	303	4/4	0.92	0.17	45,61,62,65	0
6	EDO	A	603	4/4	0.93	0.23	50,57,62,66	0
8	SO4	H	304	5/5	0.95	0.35	35,40,50,55	5
8	SO4	H	308	5/5	0.95	0.22	45,45,52,55	5
6	EDO	A	601	4/4	0.96	0.22	35,37,41,44	0
6	EDO	H	301	4/4	0.97	0.22	40,47,50,54	0
8	SO4	A	605	5/5	0.98	0.13	58,59,66,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.