



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 PM UTC

PDB ID : 6XKP / pdb_00006xkp
Title : Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody CV07-270
Authors : Liu, H.; Yuan, M.; Zhu, X.; Wu, N.C.; Wilson, I.A.
Deposited on : 2020-06-26
Resolution : 2.72 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

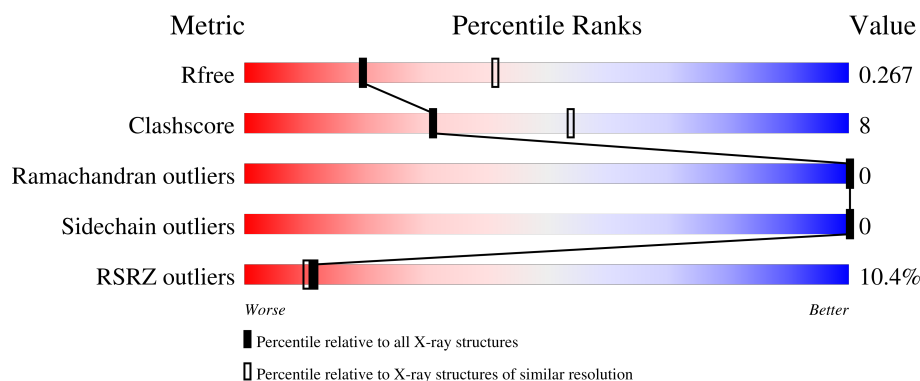
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	16% 67% 17% 16%
1	B	231	10% 67% 16% 16%
2	H	232	5% 75% 20% 5%
2	M	232	6% 81% 16% .
3	L	216	8% 89% 9% .

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Mol	Chain	Length	Quality of chain
3	N	216	12% 88% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9251 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	194	Total	C	N	O	S	0	0	0
			1438	921	242	267	8			
1	B	194	Total	C	N	O	S	0	0	0
			1492	958	248	278	8			

There are 16 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
B	542	SER	-	expression tag	UNP P0DTC2
B	543	GLY	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2

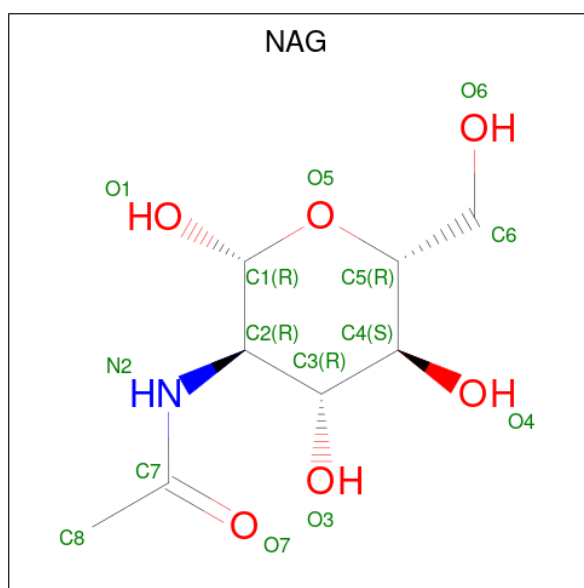
- Molecule 2 is a protein called CV07-270 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1643	1048	279	310	6			
2	M	224	Total	C	N	O	S	0	0	0
			1646	1049	278	313	6			

- Molecule 3 is a protein called CV07-270 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	1	0
			1502	941	248	307	6			
3	N	210	Total	C	N	O	S	0	0	0
			1462	913	240	303	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

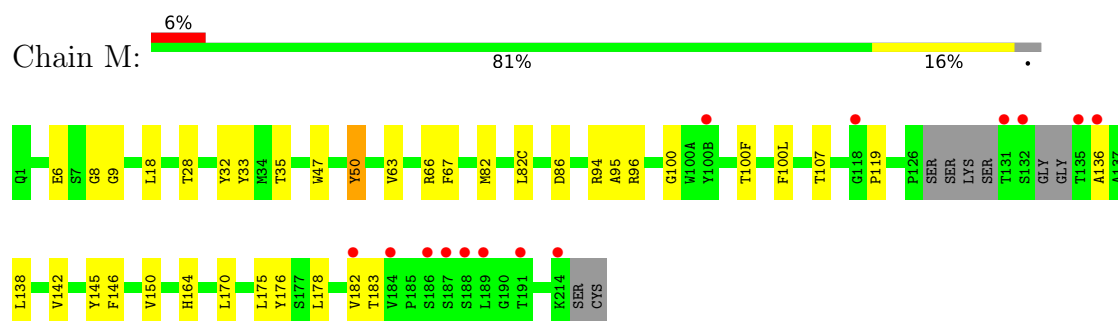


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

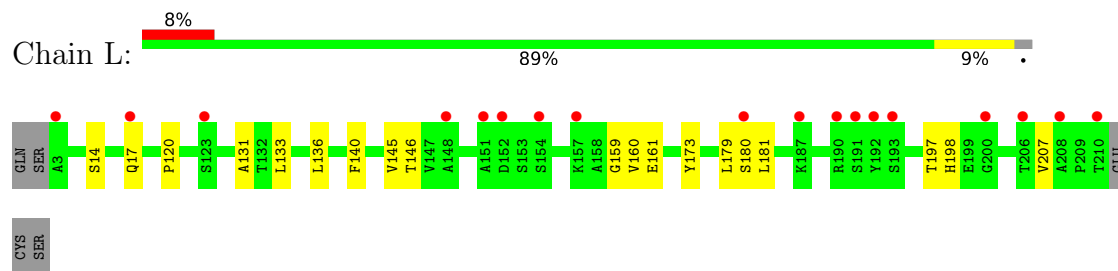
- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



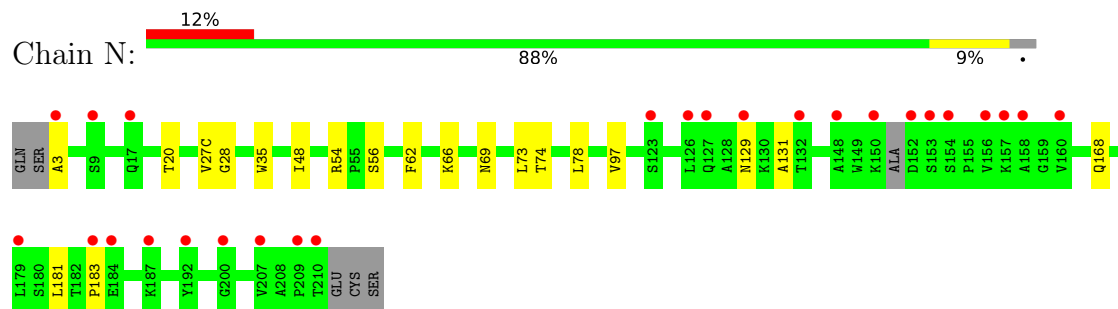
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		



• Molecule 3: CV07-270 Light Chain



• Molecule 3: CV07-270 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	175.02Å 151.78Å 66.02Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	49.73 – 2.72 49.73 – 2.72	Depositor EDS
% Data completeness (in resolution range)	89.9 (49.73-2.72) 90.2 (49.73-2.72)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.220 , 0.269 0.219 , 0.267	Depositor DCC
R_{free} test set	2055 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9251	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: SO4, 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	0.34	0/1479	0.59	0/2023
1	B	0.37	0/1536	0.68	3/2093 (0.1%)
2	H	0.36	0/1688	0.66	1/2303 (0.0%)
2	M	0.34	0/1690	0.65	1/2312 (0.0%)
3	L	0.32	0/1542	0.64	0/2118
3	N	0.30	0/1498	0.60	0/2057
All	All	0.34	0/9433	0.64	5/12906 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	LYS	CA-CB-CG	7.72	129.55	114.10
1	B	417	LYS	CB-CG-CD	-7.09	94.99	111.30
1	B	417	LYS	CG-CD-CE	5.28	123.43	111.30
2	H	50	TYR	CA-CB-CG	5.23	123.32	113.90
2	M	50	TYR	CA-CB-CG	5.14	123.16	113.90

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	1438	0	1249	29	1
1	B	1492	0	1350	26	0
2	H	1643	0	1561	38	0
2	M	1646	0	1527	32	0
3	L	1502	0	1375	11	0
3	N	1462	0	1279	11	1
4	A	14	0	13	1	0
4	B	14	0	13	0	0
5	H	15	0	0	1	0
5	L	10	0	0	0	0
5	M	10	0	0	1	0
5	N	5	0	0	1	0
All	All	9251	0	8367	143	1

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 8.

All (143) 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:M:47:TRP:HZ2	2:M:50:TYR:HD1	1.10	0.98
2:H:47:TRP:HZ2	2:H:50:TYR:HD1	1.14	0.90
2:M:47:TRP:HZ2	2:M:50:TYR:CD1	1.92	0.88
2:H:47:TRP:HZ2	2:H:50:TYR:CD1	1.97	0.83
2:M:47:TRP:CZ2	2:M:50:TYR:HD1	2.02	0.74
2:H:47:TRP:CZ2	2:H:50:TYR:HD1	2.04	0.71
3:L:120:PRO:HA	3:L:133:LEU:HD23	1.71	0.70
2:H:56:THR:HG23	2:H:100(C):ARG:HD2	1.74	0.69
1:B:350:VAL:HG11	1:B:402:ILE:HG23	1.74	0.69
2:M:47:TRP:CZ2	2:M:50:TYR:CD1	2.79	0.67
2:H:47:TRP:CZ2	2:H:50:TYR:CD1	2.82	0.66
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.77	0.66
1:A:393:THR:HG23	1:A:517:LEU:HD12	1.77	0.66
2:H:32:TYR:CD1	2:H:94:ARG:HD2	2.31	0.65
3:L:131:ALA:HB3	3:L:181:LEU:O	1.96	0.65
3:N:131:ALA:HB3	3:N:181:LEU:O	1.98	0.63
2:H:71:ARG:HD3	2:H:73:ASN:OD1	1.99	0.62
1:A:350:VAL:HG21	1:A:402:ILE:HG22	1.80	0.61
2:M:35:THR:CG2	2:M:50:TYR:HB3	2.31	0.60
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.83	0.60
2:H:11:LEU:HD23	2:H:147:PRO:HG3	1.85	0.58
2:H:35:THR:HG22	2:H:50:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:HB3	1:B:396:TYR:HE1	1.69	0.58
1:A:392:PHE:HA	1:A:517:LEU:HD13	1.86	0.57
2:M:35:THR:HG22	2:M:50:TYR:HB3	1.86	0.57
1:B:350:VAL:HG11	1:B:402:ILE:CG2	2.35	0.56
2:H:35:THR:CG2	2:H:50:TYR:HB3	2.34	0.56
2:H:63:VAL:HG13	2:H:67:PHE:CG	2.41	0.56
1:B:444:LYS:HG2	1:B:448:ASN:HB2	1.87	0.56
1:B:357:ARG:HB3	1:B:396:TYR:CE1	2.41	0.55
2:H:126:PRO:HD3	2:H:138:LEU:HD23	1.89	0.55
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.38	0.55
2:M:32:TYR:CG	2:M:94:ARG:HD2	2.42	0.55
2:H:151:THR:HG22	2:H:199:ASN:HB3	1.88	0.55
3:N:27(C):VAL:O	3:N:66:LYS:NZ	2.39	0.55
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.89	0.54
1:B:388:ASN:HB3	1:B:527:PRO:HD2	1.89	0.54
2:M:9:GLY:H	2:M:107:THR:HG21	1.73	0.54
3:N:3:ALA:HB3	3:N:97:VAL:HG21	1.90	0.53
2:M:32:TYR:CD1	2:M:94:ARG:HD2	2.45	0.52
1:A:457:ARG:CZ	1:A:461:LEU:HD23	2.40	0.52
1:B:366:SER:HA	1:B:369:TYR:CE1	2.44	0.52
1:A:346:ARG:HG2	2:H:100(A):TRP:CZ2	2.45	0.51
1:B:431:GLY:HA3	1:B:513:LEU:O	2.10	0.51
2:H:27:PHE:CE2	2:H:94:ARG:HD3	2.46	0.51
2:H:94:ARG:HG3	2:H:95:ALA:N	2.26	0.51
3:L:145:VAL:HG12	3:L:198:HIS:HB2	1.93	0.51
1:B:350:VAL:CG1	1:B:402:ILE:HG23	2.40	0.50
1:A:393:THR:HG21	1:A:518:LEU:H	1.77	0.50
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.93	0.50
3:L:180:SER:O	3:L:181:LEU:HD23	2.12	0.50
2:M:150:VAL:HG13	2:M:178:LEU:HD21	1.91	0.50
1:A:490:PHE:HZ	2:H:100(D):ILE:HD11	1.76	0.50
1:A:393:THR:OG1	1:A:516:GLU:O	2.27	0.50
3:L:133:LEU:HD22	3:L:207:VAL:HG11	1.93	0.50
2:M:63:VAL:HG13	2:M:67:PHE:HB2	1.92	0.49
1:A:346:ARG:HG2	2:H:100(A):TRP:CH2	2.47	0.49
1:A:376:THR:HB	1:A:435:ALA:HB3	1.93	0.49
2:M:9:GLY:HA3	2:M:107:THR:HG22	1.94	0.49
2:H:181:VAL:CG2	3:L:136:LEU:HD13	2.43	0.49
2:M:164:HIS:NE2	3:N:168:GLN:OE1	2.45	0.49
2:H:9:GLY:H	2:H:107:THR:HG21	1.77	0.49
2:H:143:LYS:HD2	2:H:177:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:O	1:B:398:ASP:HA	2.14	0.48
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.96	0.48
2:M:66:ARG:NH2	2:M:86:ASP:OD1	2.47	0.48
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.95	0.47
1:A:354:ASN:O	1:A:398:ASP:HA	2.15	0.47
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.48	0.47
2:M:8:GLY:O	2:M:18:LEU:HD11	2.14	0.47
1:A:403:ARG:HD3	1:A:495:TYR:CE1	2.49	0.47
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.95	0.47
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.50	0.47
2:M:94:ARG:HG3	2:M:95:ALA:N	2.29	0.47
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.95	0.47
2:H:32:TYR:CG	2:H:94:ARG:HD2	2.49	0.46
3:L:160:VAL:O	3:L:161:GLU:HG2	2.15	0.46
3:L:146:THR:OG1	3:L:197:THR:HB	2.15	0.46
2:M:82:MET:HB3	2:M:82(C):LEU:HD21	1.97	0.46
2:H:195:ILE:HD11	2:H:210:LYS:HD3	1.97	0.46
2:M:63:VAL:HG13	2:M:67:PHE:CG	2.51	0.46
2:H:35:THR:HG21	2:H:100(L):PHE:CZ	2.51	0.46
1:A:368:LEU:O	1:A:374:PHE:HE2	2.00	0.45
2:H:105:GLN:H	2:H:105:GLN:CD	2.24	0.45
2:H:33:TYR:CD1	2:H:100:GLY:HA2	2.51	0.45
1:A:396:TYR:HB2	1:A:514:SER:HB2	1.98	0.45
4:A:1001:NAG:H83	4:A:1001:NAG:H3	1.98	0.45
2:H:150:VAL:HG12	2:H:178:LEU:HD21	1.99	0.44
2:M:170:LEU:HD13	2:M:176:TYR:CZ	2.52	0.44
3:N:48:ILE:HD13	3:N:54:ARG:HG2	1.99	0.44
1:B:417:LYS:NZ	1:B:455:LEU:HD13	2.32	0.44
2:M:136:ALA:O	2:M:183:THR:HA	2.18	0.44
1:A:431:GLY:HA3	1:A:513:LEU:O	2.17	0.44
1:B:350:VAL:O	1:B:353:TRP:HD1	2.00	0.44
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.53	0.44
1:A:369:TYR:HA	1:A:377:PHE:HE2	1.82	0.44
3:N:28:GLY:HA3	3:N:69:ASN:OD1	2.17	0.44
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.53	0.43
1:B:359:SER:HB3	1:B:394:ASN:OD1	2.18	0.43
2:M:28:THR:HG23	5:M:302:SO4:O1	2.18	0.43
1:A:384:PRO:O	1:A:387:LEU:HB2	2.17	0.43
1:B:350:VAL:HG12	1:B:400:PHE:CD1	2.53	0.43
1:A:425:LEU:HD21	1:A:512:VAL:HG11	2.01	0.43
2:H:63:VAL:CG1	2:H:67:PHE:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:35:TRP:CD2	3:N:73:LEU:HB2	2.53	0.43
2:H:63:VAL:HG13	2:H:67:PHE:CD2	2.54	0.43
2:H:85:GLU:H	2:H:85:GLU:CD	2.26	0.43
1:B:362:VAL:HA	1:B:525:CYS:O	2.19	0.42
1:B:388:ASN:HA	1:B:526:GLY:HA3	1.99	0.42
1:B:401:VAL:HB	1:B:451:TYR:CD1	2.53	0.42
3:L:14:SER:O	3:L:17[B]:GLN:HG2	2.19	0.42
1:A:403:ARG:HB2	1:A:406:GLU:HG3	2.01	0.42
2:M:96:ARG:NH2	5:N:301:SO4:S	2.92	0.42
1:B:518:LEU:O	1:B:520:ALA:N	2.53	0.42
2:M:35:THR:HG23	2:M:50:TYR:HB3	2.00	0.42
2:H:121:VAL:O	2:H:209:LYS:HE3	2.19	0.42
2:M:35:THR:HG21	2:M:100(L):PHE:CZ	2.55	0.42
2:M:142:VAL:HG11	2:M:150:VAL:HG21	2.01	0.42
1:A:456:PHE:HB3	1:A:473:TYR:CG	2.55	0.42
1:B:391:CYS:SG	1:B:525:CYS:CB	3.06	0.41
1:B:472:ILE:HD12	1:B:484:GLU:HG2	2.01	0.41
1:A:403:ARG:HD3	1:A:495:TYR:HE1	1.85	0.41
1:B:336:CYS:O	1:B:338:PHE:N	2.51	0.41
2:H:100(G):ARG:O	2:H:100(J):ASN:ND2	2.53	0.41
3:N:54:ARG:HD3	3:N:62:PHE:O	2.21	0.41
3:N:20:THR:HG23	3:N:74:THR:HG22	2.03	0.41
2:H:96:ARG:NH2	5:H:302:SO4:O3	2.53	0.41
3:L:140:PHE:CE1	3:L:173:TYR:HB2	2.56	0.41
2:M:138:LEU:HG	2:M:182:VAL:HG12	2.03	0.41
2:M:6:GLU:H	2:M:6:GLU:HG2	1.74	0.41
2:M:150:VAL:CG1	2:M:178:LEU:HD21	2.51	0.41
1:A:350:VAL:HG12	1:A:422:ASN:HB3	2.03	0.40
1:B:502:GLY:O	1:B:506:GLN:HG3	2.21	0.40
2:M:50:TYR:OH	2:M:100(F):THR:HB	2.21	0.40
3:N:129:ASN:HA	3:N:183:PRO:HG2	2.03	0.40
1:A:350:VAL:CG2	1:A:402:ILE:HG22	2.48	0.40
2:H:171:GLN:NE2	2:H:177:SER:OG	2.55	0.40
1:A:393:THR:CG2	1:A:518:LEU:H	2.35	0.40
1:B:472:ILE:CD1	1:B:484:GLU:HG2	2.52	0.40
3:L:159:GLY:O	3:L:179:LEU:HD12	2.22	0.40
2:M:33:TYR:CD1	2:M:100:GLY:HA2	2.57	0.40
2:M:146:PHE:HB2	2:M:175:LEU:HD23	2.03	0.40
3:N:78:LEU:HA	3:N:78:LEU:HD23	1.74	0.40

All (1) 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)
1:A:501:ASN:ND2	3:N:56:SER:OG[1_554]	2.14	0.06

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	192/231 (83%)	184 (96%)	8 (4%)	0	100	100
1	B	192/231 (83%)	184 (96%)	8 (4%)	0	100	100
2	H	216/232 (93%)	210 (97%)	6 (3%)	0	100	100
2	M	218/232 (94%)	212 (97%)	6 (3%)	0	100	100
3	L	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
3	N	206/216 (95%)	201 (98%)	5 (2%)	0	100	100
All	All	1234/1358 (91%)	1196 (97%)	38 (3%)	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	134/203 (66%)	134 (100%)	0	100	100
1	B	150/203 (74%)	150 (100%)	0	100	100
2	H	171/193 (89%)	171 (100%)	0	100	100
2	M	166/193 (86%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	156/182 (86%)	156 (100%)	0	100	100
3	N	144/182 (79%)	144 (100%)	0	100	100
All	All	921/1156 (80%)	921 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	B	501	ASN
2	H	164	HIS
2	H	171	GLN
3	L	60	ASN
3	N	39	HIS

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 ⓘ

10 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	SO4	L	302	-	4,4,4	0.24	0	6,6,6	0.17	0
5	SO4	M	301	-	4,4,4	0.24	0	6,6,6	0.23	0
5	SO4	M	302	-	4,4,4	0.21	0	6,6,6	0.21	0
5	SO4	L	301	-	4,4,4	0.26	0	6,6,6	0.19	0
5	SO4	H	302	-	4,4,4	0.21	0	6,6,6	0.11	0
5	SO4	H	303	-	4,4,4	0.23	0	6,6,6	0.11	0
4	NAG	A	1001	1	14,14,15	2.31	2 (14%)	17,19,21	2.61	3 (17%)
5	SO4	H	301	-	4,4,4	0.24	0	6,6,6	0.26	0
5	SO4	N	301	-	4,4,4	0.25	0	6,6,6	0.26	0
4	NAG	B	1001	1	14,14,15	0.94	1 (7%)	17,19,21	1.25	1 (5%)

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	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	5/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAG	O5-C1	6.77	1.55	1.43
4	A	1001	NAG	C1-C2	5.16	1.59	1.52
4	B	1001	NAG	O5-C1	-2.82	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAG	C1-O5-C5	9.29	124.64	112.19
4	A	1001	NAG	C2-N2-C7	4.32	128.69	122.90
4	B	1001	NAG	C3-C4-C5	3.98	117.44	110.23
4	A	1001	NAG	C3-C4-C5	-2.12	106.39	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1001	NAG	C8-C7-N2-C2
4	A	1001	NAG	O7-C7-N2-C2
4	B	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	A	1001	NAG	C1-C2-N2-C7
4	A	1001	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	302	SO4	1	0
5	H	302	SO4	1	0
4	A	1001	NAG	1	0
5	N	301	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, 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	194/231 (83%)	0.77	37 (19%) 3 3	18, 47, 84, 100	0
1	B	194/231 (83%)	0.41	23 (11%) 9 8	17, 38, 80, 89	0
2	H	220/232 (94%)	0.04	12 (5%) 30 27	16, 34, 80, 99	0
2	M	224/232 (96%)	0.26	14 (6%) 26 23	16, 38, 69, 83	0
3	L	211/216 (97%)	0.30	18 (8%) 16 14	13, 36, 78, 94	1 (0%)
3	N	210/216 (97%)	0.70	26 (12%) 8 7	20, 52, 81, 99	0
All	All	1253/1358 (92%)	0.40	130 (10%) 11 10	13, 40, 81, 100	1 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	ALA	5.6
1	B	391	CYS	5.2
3	L	152	ASP	4.8
2	M	187	SER	4.5
2	H	189	LEU	4.2
2	M	132	SER	3.9
1	A	334	ASN	3.8
3	N	156	VAL	3.8
3	N	192	TYR	3.8
1	A	519	HIS	3.8
1	B	383	SER	3.7
2	M	188	SER	3.7
3	L	208	ALA	3.7
1	A	372	ALA	3.7
1	A	477	SER	3.7
3	N	153	SER	3.6
1	B	384	PRO	3.6
1	A	486	PHE	3.6
3	L	191	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	M	184	VAL	3.5
2	M	186	SER	3.5
2	H	191	THR	3.5
1	B	481	ASN	3.5
3	L	180	SER	3.4
3	N	154	SER	3.4
1	A	391	CYS	3.4
1	A	478	THR	3.3
2	M	100(B)	TYR	3.3
1	B	519	HIS	3.3
3	N	157	LYS	3.3
1	A	522	ALA	3.2
1	A	388	ASN	3.2
1	B	334	ASN	3.2
1	A	521	PRO	3.2
1	A	371	SER	3.2
1	A	393	THR	3.2
1	B	385	THR	3.2
1	B	390	LEU	3.2
3	L	17[A]	GLN	3.2
2	M	135	THR	3.2
1	A	383	SER	3.1
1	A	394	ASN	3.1
2	M	118	GLY	3.1
3	L	206	THR	3.1
2	H	186	SER	3.1
3	N	210	THR	3.0
1	A	385	THR	2.9
3	N	160	VAL	2.9
2	M	189	LEU	2.9
3	L	210	THR	2.9
3	N	3	ALA	2.9
2	H	126	PRO	2.9
2	H	188	SER	2.9
2	H	193	THR	2.9
1	A	479	PRO	2.8
2	H	185	PRO	2.8
3	L	193	SER	2.8
1	B	518	LEU	2.8
1	B	520	ALA	2.8
3	L	123	SER	2.7
3	L	200	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	151	ALA	2.7
1	A	517	LEU	2.7
3	N	187	LYS	2.7
3	L	190	ARG	2.7
1	A	367	VAL	2.7
3	N	150	LYS	2.7
3	N	207	VAL	2.7
1	A	516	GLU	2.6
1	A	382	VAL	2.6
2	M	136	ALA	2.6
1	A	360	ASN	2.6
1	B	521	PRO	2.6
1	B	393	THR	2.6
3	N	200	GLY	2.6
1	A	525	CYS	2.5
3	N	9	SER	2.5
1	A	370	ASN	2.5
2	H	212	GLU	2.5
3	N	184	GLU	2.4
1	A	377	PHE	2.4
3	L	154	SER	2.4
3	N	209	PRO	2.4
1	A	392	PHE	2.4
1	A	524	VAL	2.4
1	B	382	VAL	2.4
1	B	417	LYS	2.3
1	A	381	GLY	2.3
1	A	502	GLY	2.3
3	N	158	ALA	2.3
3	L	192	TYR	2.3
3	N	152	ASP	2.3
3	L	148	ALA	2.3
1	B	371	SER	2.3
1	B	381	GLY	2.3
3	N	127	GLN	2.3
3	N	179	LEU	2.3
2	M	191	THR	2.3
3	N	123	SER	2.3
3	N	183	PRO	2.3
1	A	387	LEU	2.3
1	A	483	VAL	2.3
3	L	187	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	N	132	THR	2.2
1	A	515	PHE	2.2
1	A	335	LEU	2.2
2	H	214	LYS	2.2
2	M	214	LYS	2.2
2	H	121	VAL	2.2
1	A	369	TYR	2.2
1	B	370	ASN	2.2
1	B	526	GLY	2.2
2	M	131	THR	2.1
3	L	157	LYS	2.1
3	N	17	GLN	2.1
1	A	518	LEU	2.1
1	B	387	LEU	2.1
1	B	389	ASP	2.1
2	H	187	SER	2.1
3	N	126	LEU	2.1
1	A	480	CYS	2.1
1	B	362	VAL	2.1
2	M	182	VAL	2.1
3	N	148	ALA	2.1
1	A	523	THR	2.1
1	A	520	ALA	2.0
1	B	359	SER	2.0
3	L	3	ALA	2.0
3	N	129	ASN	2.0
2	H	184	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 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	1001	14/15	0.71	0.21	73,82,91,104	0
4	NAG	B	1001	14/15	0.77	0.15	55,71,79,84	0
5	SO4	L	302	5/5	0.79	0.17	63,71,83,93	0
5	SO4	N	301	5/5	0.93	0.10	44,46,49,68	0
5	SO4	M	301	5/5	0.94	0.13	50,52,69,81	0
5	SO4	L	301	5/5	0.94	0.13	60,66,91,92	0
5	SO4	M	302	5/5	0.95	0.16	51,55,57,67	0
5	SO4	H	303	5/5	0.95	0.13	48,51,63,71	0
5	SO4	H	301	5/5	0.96	0.10	45,45,62,63	0
5	SO4	H	302	5/5	0.97	0.09	33,39,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.