



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:57 PM UTC

PDB ID : 7R6X / pdb_00007r6x
Title : SARS-CoV-2 spike receptor-binding domain (RBD) in complex with S2E12 Fab, S309 Fab, and S304 Fab
Authors : Snell, G.; Czudnochowski, N.; Croll, T.I.; Nix, J.C.; Corti, D.; Cameroni, E.; Pinto, D.; Beltramello, M.
Deposited on : 2021-06-23
Resolution : 2.95 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

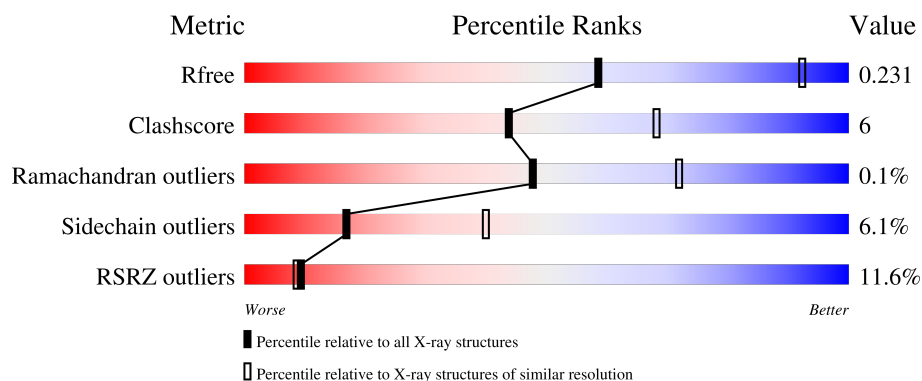
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



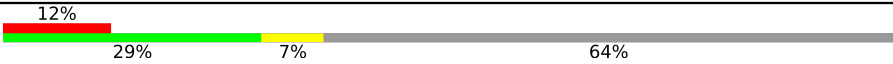
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	L	215	15% 59% 15% • 24%
2	H	223	13% 67% 14% • 17%
3	R	216	8% 79% 12% • 8%
4	B	214	2% 82% 16% •
5	A	230	3% 80% 17% ••

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Mol	Chain	Length	Quality of chain
6	D	216	
7	C	226	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	R	601	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9113 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 Monoclonal antibody S304 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	164	Total	C	N	O	S	0	0	0
			1241	781	200	256	4			

- Molecule 2 is a protein called Monoclonal antibody S304 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	186	Total	C	N	O	S	0	0	0
			1413	896	233	278	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	199	Total	C	N	O	S	0	0	0
			1575	1010	263	294	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	324	GLU	-	expression tag	UNP P0DTC2
R	325	THR	-	expression tag	UNP P0DTC2
R	326	GLY	-	expression tag	UNP P0DTC2
R	327	THR	-	expression tag	UNP P0DTC2
R	532	HIS	-	expression tag	UNP P0DTC2
R	533	HIS	-	expression tag	UNP P0DTC2
R	534	HIS	-	expression tag	UNP P0DTC2
R	535	HIS	-	expression tag	UNP P0DTC2
R	536	HIS	-	expression tag	UNP P0DTC2
R	537	HIS	-	expression tag	UNP P0DTC2
R	538	HIS	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is a protein called Monoclonal antibody S309 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			

- Molecule 5 is a protein called Monoclonal antibody S309 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	227	Total	C	N	O	S	0	0	0
			1713	1080	289	337	7			

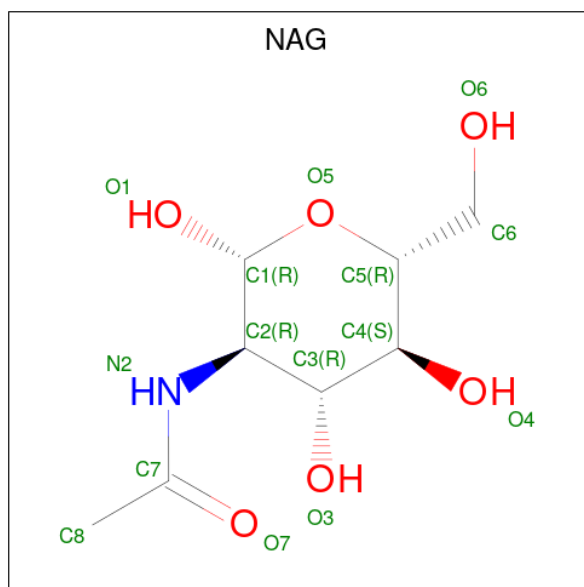
- Molecule 6 is a protein called Monoclonal antibody S2E12 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	78	Total	C	N	O	S	0	0	0
			595	376	101	116	2			

- Molecule 7 is a protein called Monoclonal antibody S2E12 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	122	Total	C	N	O	S	0	0	0
			933	580	163	183	7			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

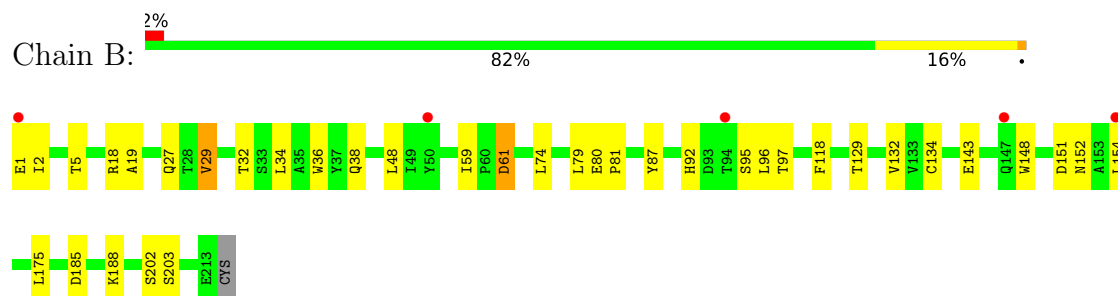
- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	R	1	Total 1	Cl 1	0	0
9	A	1	Total 1	Cl 1	0	0

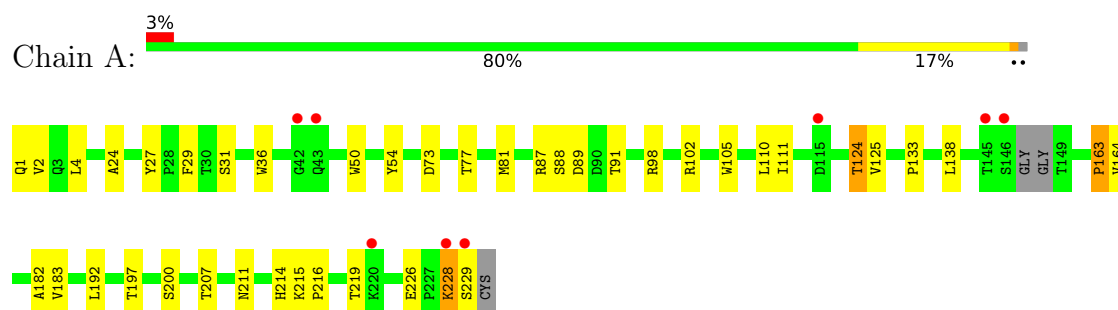
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	1	Total 1	O 1	0	0
10	A	2	Total 2	O 2	0	0

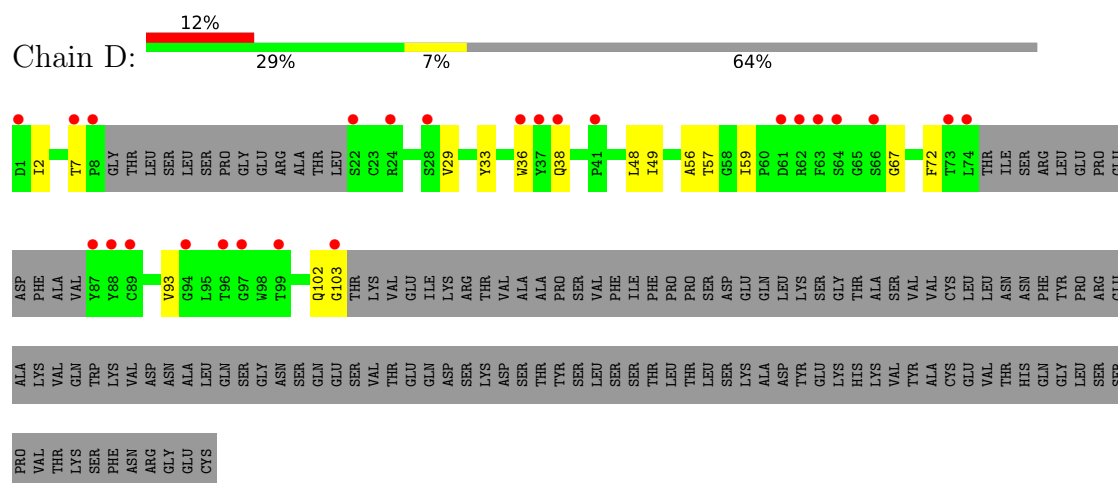
• Molecule 4: Monoclonal antibody S309 Fab light chain



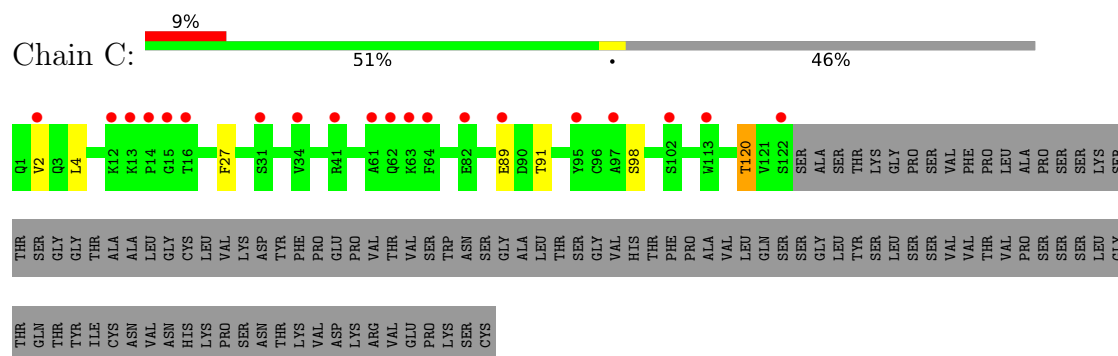
• Molecule 5: Monoclonal antibody S309 Fab heavy chain



• Molecule 6: Monoclonal antibody S2E12 Fab light chain



• Molecule 7: Monoclonal antibody S2E12 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	245.87Å 245.87Å 237.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.95 40.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.95) 99.0 (40.00-2.95)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.262 (Not available) , 0.231	Depositor DCC
R_{free} test set	3884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9113	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: CL, 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	L	0.48	0/1268	0.83	0/1726
2	H	0.47	0/1449	0.84	0/1971
3	R	0.44	0/1620	0.88	0/2205
4	B	0.48	0/1657	0.86	0/2250
5	A	0.47	0/1755	0.91	1/2390 (0.0%)
6	D	0.46	0/609	0.75	0/825
7	C	0.46	0/953	0.76	0/1292
All	All	0.47	0/9311	0.85	1/12659 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	163	PRO	N-CA-CB	-6.05	95.94	102.60

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	L	1241	0	1206	21	0
2	H	1413	0	1342	20	0
3	R	1575	0	1498	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1624	0	1582	19	0
5	A	1713	0	1671	21	0
6	D	595	0	563	9	0
7	C	933	0	895	3	0
8	R	14	0	13	8	0
9	A	1	0	0	0	0
9	R	1	0	0	0	0
10	A	2	0	0	0	0
10	H	1	0	0	0	0
All	All	9113	0	8770	109	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 6.

All (109) 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:R:343:ASN:HD21	8:R:601:NAG:C1	0.89	1.49
3:R:343:ASN:ND2	8:R:601:NAG:C1	1.75	1.46
3:R:343:ASN:ND2	8:R:601:NAG:O5	2.05	0.89
3:R:343:ASN:CG	8:R:601:NAG:C1	2.59	0.74
4:B:32:THR:HB	5:A:111:ILE:HG12	1.72	0.72
6:D:38:GLN:HB2	6:D:48:LEU:HD11	1.71	0.70
1:L:6:GLN:HG3	1:L:101:PRO:HD2	1.75	0.69
3:R:343:ASN:HD21	8:R:601:NAG:C2	1.97	0.69
7:C:91:THR:HG23	7:C:120:THR:HA	1.77	0.67
1:L:94:SER:HB3	1:L:97:TYR:CE1	2.30	0.66
2:H:11:LEU:HD22	2:H:123:THR:HG22	1.78	0.65
5:A:228:LYS:HD2	5:A:229:SER:N	2.13	0.63
2:H:18:LEU:HD22	2:H:116:LEU:HD12	1.83	0.61
4:B:38:GLN:HG3	4:B:87:TYR:CE1	2.35	0.61
1:L:29:ILE:HD12	1:L:32:TYR:O	2.01	0.60
2:H:100:SER:HA	2:H:104:TYR:O	2.01	0.60
3:R:412:PRO:HG3	3:R:429:PHE:HB3	1.83	0.59
3:R:418:ILE:HA	3:R:422:ASN:HD22	1.68	0.59
4:B:151:ASP:O	4:B:152:ASN:HB2	2.04	0.58
2:H:162:ASN:O	2:H:163:SER:HB2	2.03	0.57
1:L:7:SER:HB3	1:L:22:THR:HG22	1.87	0.56
1:L:2:ILE:HD12	1:L:93:VAL:HG12	1.85	0.56
5:A:91:THR:HG23	5:A:124:THR:HA	1.87	0.56
4:B:92:HIS:HA	4:B:95:SER:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:185:ASP:HA	4:B:188:LYS:HE3	1.86	0.56
3:R:367:VAL:HG21	8:R:601:NAG:H81	1.86	0.56
2:H:90:THR:HG23	2:H:117:THR:HA	1.88	0.56
2:H:69:ILE:HD11	2:H:78:LEU:HD11	1.89	0.55
4:B:1:GLU:HG2	4:B:2:ILE:N	2.22	0.55
2:H:11:LEU:CD2	2:H:123:THR:HG22	2.37	0.54
1:L:94:SER:HB2	1:L:95:PRO:HA	1.89	0.54
3:R:429:PHE:HE1	3:R:514:SER:HB3	1.72	0.54
5:A:36:TRP:CE2	5:A:81:MET:HB2	2.43	0.53
5:A:1:GLN:HA	5:A:1:GLN:OE1	2.08	0.53
2:H:207:HIS:CD2	2:H:209:PRO:HD2	2.44	0.52
1:L:109:ARG:HG2	1:L:110:THR:N	2.24	0.52
5:A:27:TYR:CE2	5:A:98:ARG:HD2	2.45	0.51
5:A:192:LEU:C	5:A:192:LEU:HD12	2.36	0.51
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.92	0.51
5:A:4:LEU:HD23	5:A:24:ALA:HA	1.93	0.51
1:L:138:ASN:O	1:L:175:SER:OG	2.29	0.50
5:A:87:ARG:HG3	5:A:89:ASP:HB3	1.93	0.50
5:A:88:SER:HA	5:A:125:VAL:HB	1.94	0.49
1:L:160:SER:HA	1:L:179:THR:O	2.11	0.49
6:D:33:TYR:HB2	6:D:93:VAL:HG22	1.95	0.49
4:B:80:GLU:HB3	4:B:81:PRO:HD2	1.95	0.49
5:A:50:TRP:CZ2	5:A:102:ARG:HG2	2.47	0.49
5:A:182:ALA:HA	5:A:192:LEU:HB3	1.95	0.49
3:R:354:ASN:HD21	3:R:356:LYS:HZ3	1.61	0.49
6:D:56:ALA:HB3	6:D:59:ILE:HG13	1.95	0.48
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.78	0.48
4:B:48:LEU:HA	4:B:59:ILE:HG13	1.94	0.48
1:L:108:LYS:HA	1:L:141:TYR:OH	2.14	0.47
1:L:4:MET:HB2	1:L:100:GLY:HA2	1.95	0.47
4:B:134:CYS:HB2	4:B:148:TRP:CZ2	2.49	0.47
2:H:126:PRO:HB3	2:H:152:TYR:HB3	1.96	0.47
2:H:103:TYR:HB3	3:R:381:GLY:O	2.15	0.47
4:B:175:LEU:C	4:B:175:LEU:HD23	2.40	0.47
1:L:160:SER:CB	1:L:180:LEU:HA	2.46	0.46
2:H:121:ALA:HB3	2:H:153:PHE:CE2	2.50	0.46
2:H:208:LYS:N	2:H:209:PRO:CD	2.79	0.45
3:R:367:VAL:CG2	8:R:601:NAG:C8	2.95	0.45
4:B:2:ILE:HG12	4:B:27:GLN:HG2	1.99	0.45
4:B:143:GLU:CD	4:B:143:GLU:N	2.74	0.45
6:D:2:ILE:HD13	6:D:29:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:19:ALA:HB2	4:B:79:LEU:HD11	1.98	0.45
3:R:345:THR:HG23	5:A:110:LEU:C	2.42	0.44
5:A:2:VAL:HG22	5:A:27:TYR:HB3	1.99	0.44
1:L:7:SER:HB3	1:L:22:THR:CG2	2.47	0.44
3:R:354:ASN:HD21	3:R:356:LYS:NZ	2.15	0.44
4:B:1:GLU:HG3	4:B:97:THR:HG21	1.98	0.44
3:R:337:PRO:HG3	5:A:105:TRP:CE3	2.52	0.44
4:B:61:ASP:OD1	4:B:61:ASP:N	2.51	0.44
6:D:38:GLN:HB2	6:D:48:LEU:CD1	2.44	0.44
4:B:36:TRP:CD2	4:B:74:LEU:HB2	2.52	0.44
1:L:162:GLU:HB3	1:L:176:LEU:HD21	1.99	0.43
4:B:2:ILE:HD13	4:B:29:VAL:HG23	2.00	0.43
2:H:22:CYS:HB3	2:H:78:LEU:HB3	2.00	0.43
3:R:367:VAL:CG2	8:R:601:NAG:H81	2.48	0.43
3:R:354:ASN:O	3:R:398:ASP:HA	2.18	0.43
2:H:18:LEU:CD2	2:H:116:LEU:HD12	2.48	0.43
6:D:56:ALA:HB3	6:D:59:ILE:CG1	2.48	0.43
3:R:337:PRO:HD2	3:R:358:ILE:HG23	2.00	0.43
6:D:67:GLY:HA3	6:D:72:PHE:HA	2.00	0.42
1:L:109:ARG:HG2	1:L:110:THR:H	1.82	0.42
3:R:391:CYS:HB3	3:R:522:ALA:HB1	2.02	0.42
6:D:102:GLN:HG2	6:D:103:GLY:N	2.34	0.42
2:H:112:GLN:H	2:H:112:GLN:HG3	1.64	0.42
2:H:30:SER:HB3	2:H:73:ASP:HB3	2.02	0.42
5:A:164:VAL:HG12	5:A:214:HIS:HB2	2.02	0.42
4:B:95:SER:OG	4:B:96:LEU:N	2.50	0.42
3:R:392:PHE:CD1	3:R:515:PHE:HB3	2.55	0.41
2:H:63:VAL:HG13	2:H:67:PHE:CG	2.55	0.41
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.02	0.41
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.02	0.41
7:C:4:LEU:HD11	7:C:98:SER:HB2	2.03	0.41
6:D:36:TRP:HB2	6:D:49:ILE:HB	2.02	0.41
1:L:94:SER:HB3	1:L:97:TYR:CZ	2.56	0.41
3:R:338:PHE:HE2	3:R:363:ALA:HB1	1.86	0.41
5:A:29:PHE:CE2	5:A:77:THR:HA	2.56	0.41
5:A:215:LYS:N	5:A:216:PRO:CD	2.84	0.41
1:L:29:ILE:HD11	1:L:33:LEU:HD23	2.03	0.41
1:L:160:SER:HB3	1:L:180:LEU:HA	2.02	0.41
5:A:54:TYR:CD2	5:A:105:TRP:HA	2.56	0.40
7:C:27:PHE:H	7:C:27:PHE:HD1	1.68	0.40
1:L:61:ARG:CZ	1:L:79:GLN:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:118:PHE:CD1	5:A:138:LEU:HB3	2.56	0.40
1:L:39:LYS:HE2	1:L:81:GLU:O	2.21	0.40
5:A:133:PRO:HD2	5:A:219:THR:HG21	2.02	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	L	160/215 (74%)	155 (97%)	5 (3%)	0	100	100
2	H	180/223 (81%)	175 (97%)	5 (3%)	0	100	100
3	R	197/216 (91%)	187 (95%)	10 (5%)	0	100	100
4	B	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
5	A	223/230 (97%)	215 (96%)	7 (3%)	1 (0%)	30	53
6	D	72/216 (33%)	66 (92%)	6 (8%)	0	100	100
7	C	120/226 (53%)	112 (93%)	8 (7%)	0	100	100
All	All	1163/1540 (76%)	1115 (96%)	47 (4%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	163	PRO

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	L	144/188 (77%)	132 (92%)	12 (8%)	10	27
2	H	155/186 (83%)	142 (92%)	13 (8%)	10	26
3	R	172/188 (92%)	160 (93%)	12 (7%)	14	34
4	B	184/185 (100%)	174 (95%)	10 (5%)	20	44
5	A	191/192 (100%)	181 (95%)	10 (5%)	21	46
6	D	63/186 (34%)	61 (97%)	2 (3%)	34	59
7	C	103/193 (53%)	100 (97%)	3 (3%)	37	61
All	All	1012/1318 (77%)	950 (94%)	62 (6%)	17	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	15	VAL
1	L	17	ASP
1	L	20	THR
1	L	22	THR
1	L	33	LEU
1	L	69	THR
1	L	74	THR
1	L	93	VAL
1	L	96	THR
1	L	124	GLU
1	L	176	LEU
1	L	180	LEU
2	H	18	LEU
2	H	63	VAL
2	H	84	SER
2	H	95	CYS
2	H	112	GLN
2	H	123	THR
2	H	163	SER
2	H	168	SER
2	H	188	VAL
2	H	204	ASN
2	H	211	ASN
2	H	212	THR
2	H	214	VAL
3	R	346	ARG

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Mol	Chain	Res	Type
3	R	354	ASN
3	R	358	ILE
3	R	424	LYS
3	R	434	ILE
3	R	462	LYS
3	R	471	GLU
3	R	483	VAL
3	R	498	GLN
3	R	503	VAL
3	R	514	SER
3	R	517	LEU
4	B	5	THR
4	B	18	ARG
4	B	29	VAL
4	B	34	LEU
4	B	61	ASP
4	B	129	THR
4	B	132	VAL
4	B	154	LEU
4	B	202	SER
4	B	203	SER
5	A	31	SER
5	A	73	ASP
5	A	124	THR
5	A	183	VAL
5	A	197	THR
5	A	200	SER
5	A	207	THR
5	A	211	ASN
5	A	226	GLU
5	A	228	LYS
6	D	7	THR
6	D	57	THR
7	C	2	VAL
7	C	89	GLU
7	C	120	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	138	ASN

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Mol	Chain	Res	Type
1	L	139	ASN
2	H	83	ASN
3	R	343	ASN
3	R	354	ASN
3	R	460	ASN
4	B	199	GLN
5	A	65	GLN
6	D	27	GLN
6	D	38	GLN
7	C	65	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 ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
8	NAG	R	601	-	14,14,15	0.32	0	17,19,21	0.98	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
8	NAG	R	601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	601	NAG	O5-C1-C2	-2.04	108.13	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	601	NAG	8	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	L	164/215 (76%)	1.08	33 (20%) 3 2	69, 116, 206, 226	0
2	H	186/223 (83%)	0.75	30 (16%) 4 4	67, 107, 203, 234	0
3	R	199/216 (92%)	0.40	17 (8%) 16 15	62, 87, 164, 187	0
4	B	213/214 (99%)	0.03	5 (2%) 61 53	67, 88, 114, 134	0
5	A	227/230 (98%)	0.06	8 (3%) 47 40	63, 81, 134, 172	0
6	D	78/216 (36%)	1.59	25 (32%) 1 1	167, 196, 223, 233	0
7	C	122/226 (53%)	1.05	20 (16%) 4 4	130, 167, 216, 224	0
All	All	1189/1540 (77%)	0.56	138 (11%) 9 8	62, 97, 205, 234	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	8	PRO	7.6
3	R	330	PRO	7.4
2	H	132	ALA	7.1
1	L	142	PRO	6.6
1	L	138	ASN	6.2
2	H	148	LEU	6.1
1	L	180	LEU	5.8
7	C	122	SER	5.7
1	L	114	PRO	5.3
1	L	111	VAL	5.2
7	C	63	LYS	5.0
6	D	87	TYR	5.0
2	H	188	VAL	5.0
6	D	103	GLY	4.9
2	H	177	LEU	4.8
6	D	37	TYR	4.6
2	H	215	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	H	167	THR	4.5
3	R	478	THR	4.5
1	L	127	LYS	4.5
2	H	166	LEU	4.5
6	D	28	SER	4.5
1	L	179	THR	4.4
1	L	1	ASP	4.3
7	C	13	LYS	4.2
2	H	168	SER	4.1
2	H	208	LYS	4.1
7	C	113	TRP	4.0
1	L	118	ILE	4.0
1	L	159	ASN	3.9
6	D	74	LEU	3.9
1	L	113	ALA	3.9
2	H	181	GLY	3.8
2	H	124	LYS	3.8
2	H	186	SER	3.7
5	A	229	SER	3.7
2	H	172	THR	3.7
5	A	228	LYS	3.7
7	C	97	ALA	3.6
1	L	164	VAL	3.6
6	D	63	PHE	3.6
2	H	203	CYS	3.5
2	H	150	LYS	3.5
7	C	14	PRO	3.5
1	L	131	ALA	3.4
5	A	42	GLY	3.4
1	L	162	GLU	3.4
1	L	120	PRO	3.4
1	L	115	SER	3.4
3	R	487	ASN	3.3
2	H	213	LYS	3.3
2	H	147	CYS	3.3
2	H	165	ALA	3.3
1	L	160	SER	3.3
3	R	334	ASN	3.2
2	H	131	LEU	3.2
2	H	173	PHE	3.2
1	L	137	LEU	3.2
5	A	220	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	3.0
5	A	115	ASP	3.0
6	D	97	GLY	3.0
6	D	22	SER	3.0
6	D	88	TYR	3.0
7	C	41	ARG	3.0
1	L	3	GLN	3.0
1	L	116	VAL	2.9
6	D	41	PRO	2.9
5	A	146	SER	2.9
6	D	66	SER	2.8
2	H	43	LYS	2.8
7	C	62	GLN	2.8
1	L	178	SER	2.8
6	D	7	THR	2.8
3	R	528	LYS	2.8
1	L	170	LYS	2.8
2	H	187	SER	2.7
3	R	458	LYS	2.7
3	R	405	ASP	2.7
2	H	128	VAL	2.7
7	C	82	GLU	2.7
1	L	83	PHE	2.6
6	D	36	TRP	2.6
7	C	95	TYR	2.6
4	B	1	GLU	2.6
1	L	175	SER	2.6
7	C	15	GLY	2.6
2	H	212	THR	2.6
3	R	483	VAL	2.5
6	D	62	ARG	2.5
1	L	42	LYS	2.5
3	R	486	PHE	2.5
6	D	1	ASP	2.5
1	L	117	PHE	2.5
3	R	476	GLY	2.4
6	D	24	ARG	2.4
7	C	61	ALA	2.4
1	L	135	CYS	2.4
6	D	96	THR	2.4
4	B	154	LEU	2.4
6	D	38	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	110	THR	2.3
2	H	112	GLN	2.3
3	R	408	ARG	2.3
3	R	367	VAL	2.3
6	D	89	CYS	2.3
7	C	89	GLU	2.2
7	C	2	VAL	2.2
3	R	482	GLY	2.2
1	L	108	LYS	2.2
5	A	43	GLN	2.2
3	R	445	VAL	2.2
6	D	61	ASP	2.2
5	A	145	THR	2.2
2	H	169	GLY	2.2
6	D	94	GLY	2.2
7	C	12	LYS	2.2
1	L	172	SER	2.2
7	C	31	SER	2.2
7	C	64	PHE	2.2
2	H	214	VAL	2.1
7	C	34	VAL	2.1
4	B	50	TYR	2.1
6	D	64	SER	2.1
1	L	39	LYS	2.1
3	R	470	THR	2.1
2	H	162	ASN	2.1
2	H	161	TRP	2.1
1	L	130	THR	2.1
3	R	333	THR	2.1
7	C	16	THR	2.1
4	B	147	GLN	2.0
1	L	128	SER	2.0
7	C	102	SER	2.0
3	R	450	ASN	2.0
4	B	94	THR	2.0
6	D	73	THR	2.0
6	D	99	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
8	NAG	R	601	14/15	0.89	0.18	119,124,129,132	0
9	CL	A	301	1/1	0.91	0.18	92,92,92,92	0
9	CL	R	602	1/1	0.92	0.18	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.