Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 10:56 AM EDT

PDB ID	:	7R6X
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:

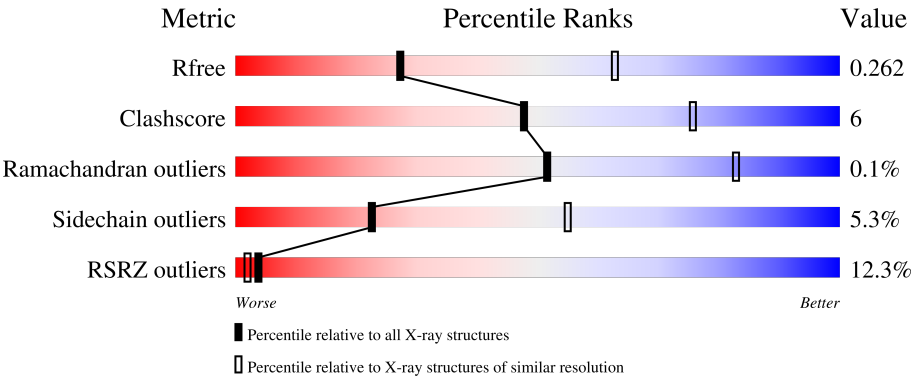
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	18% 59% 16% · 24%
2	H	223	18% 66% 15% · 17%
3	R	216	% 81% 10% · 8%
4	B	214	% 82% 16% ·
5	A	230	% 80% 17% ••

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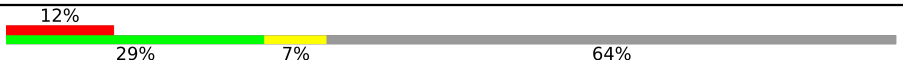
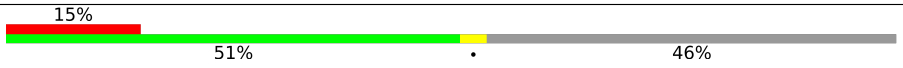
Mol	Chain	Length	Quality of chain
6	D	216	
7	C	226	

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 (i)

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
			Total	C	N	O	S			
4	B	213	1624	1011	277	332	4	0	0	0

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

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

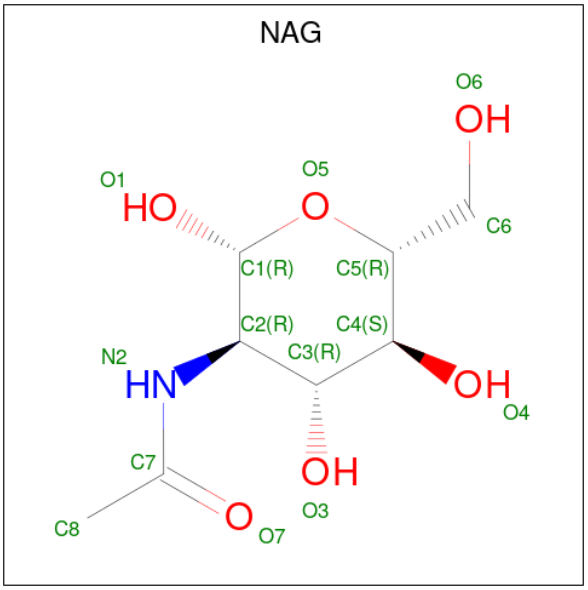
- Molecule 6 is a protein called Monoclonal antibody S2E12 Fab light chain.

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

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

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is water.

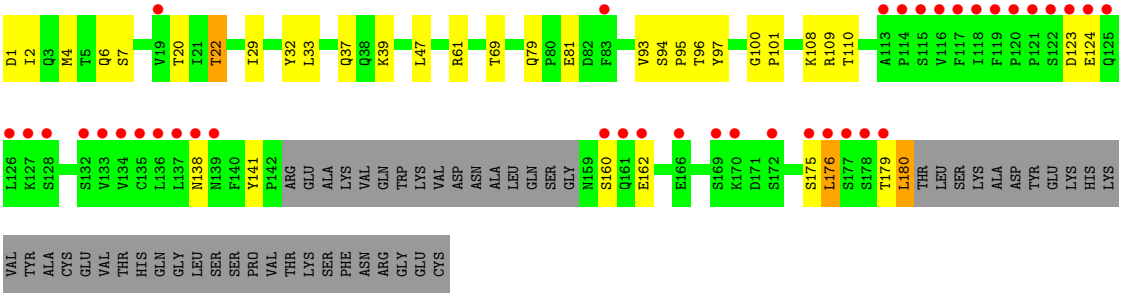
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total O 1 1	0	0
10	A	2	Total O 2 2	0	0

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.

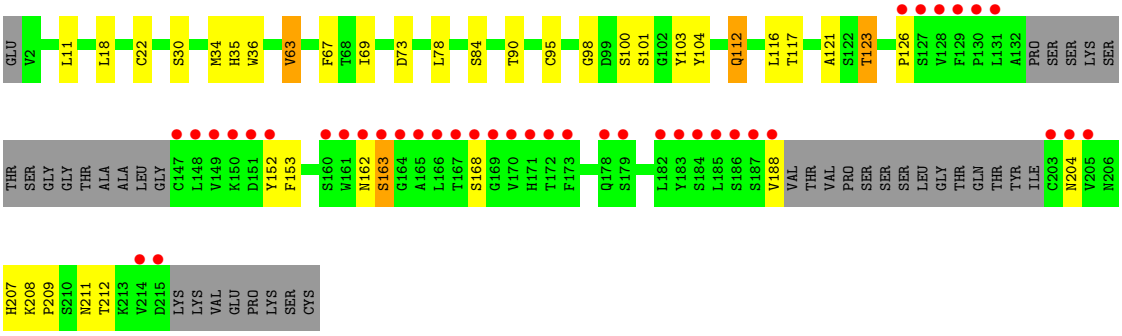
• Molecule 1: Monoclonal antibody S304 Fab light chain

Chain L:



• Molecule 2: Monoclonal antibody S304 Fab heavy chain

Chain H:

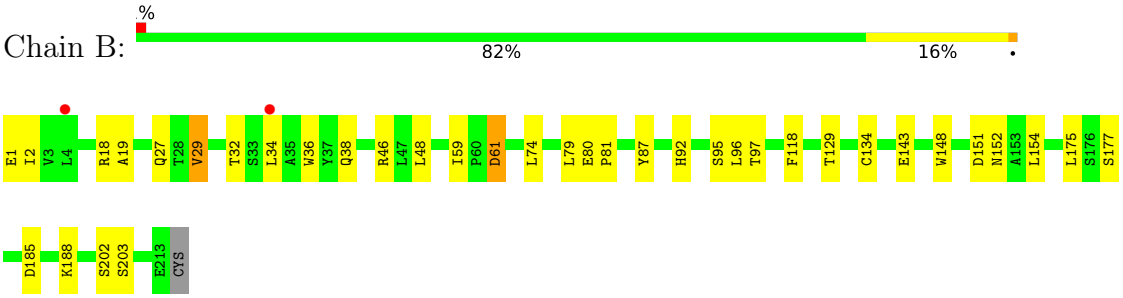


• Molecule 3: Spike protein S1

Chain R:

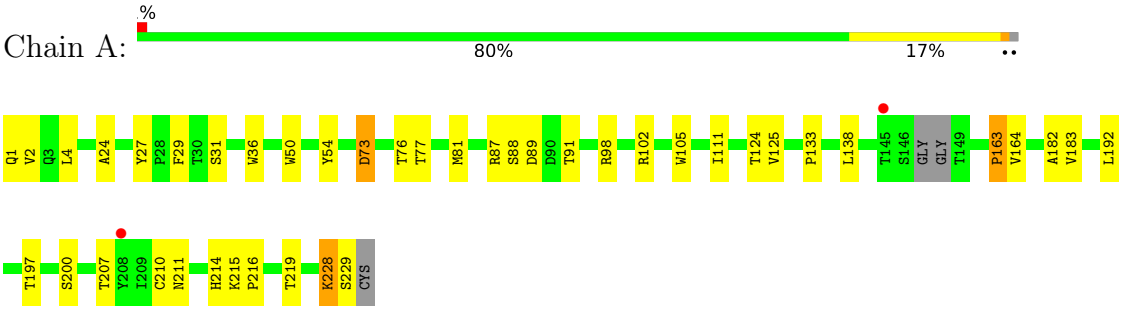
• Molecule 4: Monoclonal antibody S309 Fab light chain

Chain B:



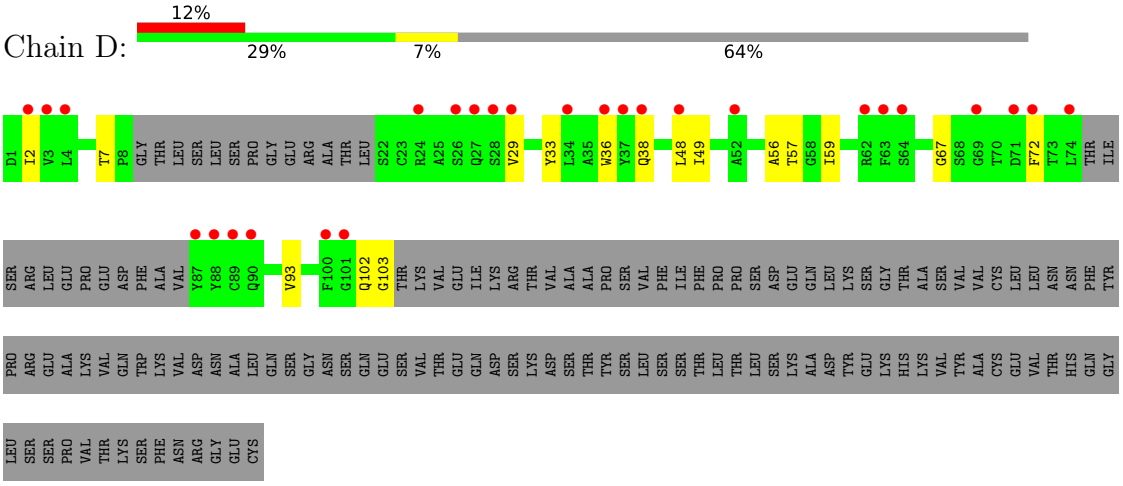
• Molecule 5: Monoclonal antibody S309 Fab heavy chain

Chain A:



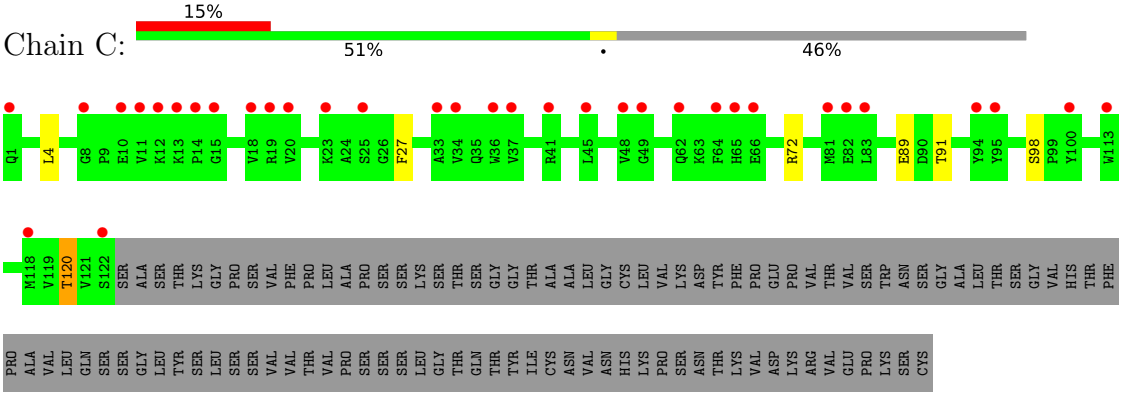
• Molecule 6: Monoclonal antibody S2E12 Fab light chain

Chain D:



• Molecule 7: Monoclonal antibody S2E12 Fab heavy chain

Chain C:



4 Data and refinement statistics (i)

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 49.00 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.95) 98.8 (49.00-2.93)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.262 0.233 , 0.262	Depositor DCC
R_{free} test set	3884 reflections (5.07%)	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)	0.30 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, CL

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	0.30	0/1268	0.56	0/1726
2	H	0.31	0/1449	0.58	0/1971
3	R	0.27	0/1620	0.58	0/2205
4	B	0.30	0/1657	0.59	0/2250
5	A	0.31	0/1755	0.65	1/2390 (0.0%)
6	D	0.31	0/609	0.52	0/825
7	C	0.27	0/953	0.52	0/1292
All	All	0.30	0/9311	0.58	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(^{o})	Ideal(^{o})
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

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	21	0
3	R	1575	0	1498	19	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
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
3:R:343:ASN:CG	8:R:601:NAG:C1	2.59	0.69
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
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
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
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
5:A:73:ASP:OD1	5:A:76:THR:OG1	2.15	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
5:A:192:LEU:C	5:A:192:LEU:HD12	2.36	0.47
1:L:138:ASN:O	1:L:175:SER:OG	2.29	0.46
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
6:D:2:ILE:HD13	6:D:29:VAL:HG22	1.97	0.45
4:B:19:ALA:HB2	4:B:79:LEU:HD11	1.98	0.45
5:A:2:VAL:HG22	5:A:27:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:95:SER:OG	4:B:96:LEU:N	2.50	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:35:HIS:HE2	2:H:98:GLY:HA3	1.85	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
4:B:175:LEU:C	4:B:175:LEU:HD23	2.40	0.42
5:A:164:VAL:HG12	5:A:214:HIS:HB2	2.02	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
4:B:143:GLU:CD	4:B:143:GLU:N	2.74	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%)	34	69
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%)	51	83

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%)	135 (94%)	9 (6%)	18 48
2	H	155/186 (83%)	143 (92%)	12 (8%)	13 39
3	R	172/188 (92%)	163 (95%)	9 (5%)	23 56
4	B	184/185 (100%)	174 (95%)	10 (5%)	22 54
5	A	191/192 (100%)	182 (95%)	9 (5%)	26 59
6	D	63/186 (34%)	61 (97%)	2 (3%)	39 71
7	C	103/193 (53%)	100 (97%)	3 (3%)	42 73
All	All	1012/1318 (77%)	958 (95%)	54 (5%)	22 55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	20	THR
1	L	22	THR
1	L	69	THR
1	L	96	THR
1	L	123	ASP
1	L	124	GLU
1	L	176	LEU
1	L	180	LEU
2	H	63	VAL
2	H	84	SER
2	H	95	CYS
2	H	101	SER
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
3	R	346	ARG
3	R	354	ASN
3	R	358	ILE
3	R	377	PHE
3	R	424	LYS

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Mol	Chain	Res	Type
3	R	462	LYS
3	R	483	VAL
3	R	498	GLN
3	R	514	SER
4	B	18	ARG
4	B	29	VAL
4	B	34	LEU
4	B	46	ARG
4	B	61	ASP
4	B	129	THR
4	B	154	LEU
4	B	177	SER
4	B	202	SER
4	B	203	SER
5	A	31	SER
5	A	73	ASP
5	A	183	VAL
5	A	197	THR
5	A	200	SER
5	A	207	THR
5	A	210	CYS
5	A	211	ASN
5	A	228	LYS
6	D	7	THR
6	D	57	THR
7	C	72	ARG
7	C	89	GLU
7	C	120	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	139	ASN
3	R	343	ASN
3	R	354	ASN
4	B	90	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	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
8	NAG	R	601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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, 95^{th} 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%)	1.23	38 (23%) 0 0	69, 116, 206, 226	0
2	H	186/223 (83%)	0.95	40 (21%) 0 0	67, 107, 203, 234	0
3	R	199/216 (92%)	0.29	3 (1%) 73 57	62, 87, 164, 187	0
4	B	213/214 (99%)	0.32	2 (0%) 84 71	67, 88, 114, 134	0
5	A	227/230 (98%)	0.34	2 (0%) 84 71	63, 81, 134, 172	0
6	D	78/216 (36%)	1.57	27 (34%) 0 0	167, 196, 223, 233	0
7	C	122/226 (53%)	1.11	34 (27%) 0 0	130, 167, 216, 224	0
All	All	1189/1540 (77%)	0.71	146 (12%) 4 2	62, 97, 205, 234	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	138	ASN	8.1
2	H	187	SER	8.0
1	L	179	THR	7.7
2	H	168	SER	7.6
1	L	136	LEU	7.5
2	H	167	THR	7.4
6	D	37	TYR	7.1
1	L	124	GLU	7.0
2	H	129	PHE	6.3
2	H	128	VAL	6.3
1	L	123	ASP	5.8
6	D	87	TYR	5.5
2	H	173	PHE	5.3
1	L	127	LYS	5.2
7	C	45	LEU	5.2
1	L	115	SER	5.0
1	L	121	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	L	134	VAL	5.0
2	H	166	LEU	4.9
1	L	132	SER	4.8
6	D	29	VAL	4.8
6	D	63	PHE	4.8
1	L	126	LEU	4.7
1	L	120	PRO	4.7
2	H	188	VAL	4.6
6	D	64	SER	4.5
1	L	133	VAL	4.5
6	D	89	CYS	4.4
1	L	160	SER	4.4
2	H	130	PRO	4.4
6	D	52	ALA	4.3
2	H	185	LEU	4.2
7	C	34	VAL	4.1
1	L	117	PHE	4.1
1	L	128	SER	4.0
1	L	114	PRO	4.0
2	H	183	TYR	4.0
7	C	81	MET	4.0
1	L	175	SER	4.0
2	H	149	VAL	4.0
6	D	101	GLY	4.0
2	H	172	THR	4.0
1	L	83	PHE	3.9
2	H	165	ALA	3.9
6	D	62	ARG	3.8
1	L	113	ALA	3.8
6	D	100	PHE	3.8
7	C	83	LEU	3.8
7	C	65	HIS	3.8
1	L	177	SER	3.8
2	H	186	SER	3.7
6	D	36	TRP	3.7
2	H	203	CYS	3.7
6	D	72	PHE	3.7
7	C	113	TRP	3.7
7	C	95	TYR	3.6
2	H	204	ASN	3.6
1	L	137	LEU	3.6
6	D	74	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	116	VAL	3.5
7	C	12	LYS	3.5
2	H	147	CYS	3.5
2	H	161	TRP	3.5
1	L	118	ILE	3.5
1	L	178	SER	3.4
6	D	4	LEU	3.4
6	D	38	GLN	3.3
6	D	48	LEU	3.3
2	H	163	SER	3.3
2	H	160	SER	3.3
1	L	135	CYS	3.3
2	H	127	SER	3.3
1	L	119	PHE	3.2
7	C	41	ARG	3.2
2	H	171	HIS	3.1
1	L	162	GLU	3.1
2	H	162	ASN	3.1
6	D	90	GLN	3.1
7	C	19	ARG	3.1
7	C	18	VAL	3.1
5	A	145	THR	3.1
2	H	151	ASP	3.0
7	C	82	GLU	3.0
1	L	139	ASN	3.0
6	D	34	LEU	3.0
1	L	122	SER	3.0
6	D	88	TYR	3.0
7	C	48	VAL	3.0
6	D	2	ILE	2.9
7	C	49	GLY	2.8
7	C	37	VAL	2.8
1	L	176	LEU	2.7
2	H	205	VAL	2.7
2	H	169	GLY	2.7
6	D	24	ARG	2.7
7	C	13	LYS	2.7
1	L	169	SER	2.7
7	C	8	GLY	2.7
6	D	26	SER	2.7
1	L	172	SER	2.6
1	L	161	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	164	GLY	2.6
7	C	14	PRO	2.6
7	C	33	ALA	2.6
7	C	122	SER	2.5
2	H	184	SER	2.5
6	D	28	SER	2.5
7	C	62	GLN	2.5
2	H	214	VAL	2.5
6	D	71	ASP	2.4
2	H	148	LEU	2.3
4	B	4	LEU	2.3
7	C	23	LYS	2.3
1	L	125	GLN	2.3
2	H	170	VAL	2.3
2	H	178	GLN	2.3
2	H	131	LEU	2.3
7	C	1	GLN	2.3
7	C	10	GLU	2.3
7	C	20	VAL	2.3
2	H	182	LEU	2.3
7	C	11	VAL	2.2
4	B	34	LEU	2.2
7	C	25	SER	2.2
3	R	367	VAL	2.2
6	D	27	GLN	2.2
2	H	150	LYS	2.2
6	D	69	GLY	2.1
7	C	36	TRP	2.1
5	A	208	TYR	2.1
2	H	215	ASP	2.1
6	D	3	VAL	2.1
7	C	118	MET	2.1
7	C	100	TYR	2.1
2	H	179	SER	2.1
7	C	64	PHE	2.1
7	C	15	GLY	2.1
1	L	166	GLU	2.1
3	R	332	ILE	2.1
3	R	489	TYR	2.1
1	L	170	LYS	2.1
2	H	126	PRO	2.1
7	C	66	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	19	VAL	2.0
7	C	94	TYR	2.0
2	H	152	TYR	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^{th} 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^2)	Q<0.9
9	CL	R	602	1/1	0.64	0.21	119,119,119,119	0
8	NAG	R	601	14/15	0.86	0.32	119,124,129,132	0
9	CL	A	301	1/1	0.97	0.26	92,92,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.