Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2021 – 12:09 pm GMT

PDB ID	:	7PS0
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with beta-24 Fabs
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-09-22
Resolution	:	2.92 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 following versions of software and data (see references ⓘ) were used in the production of this report:

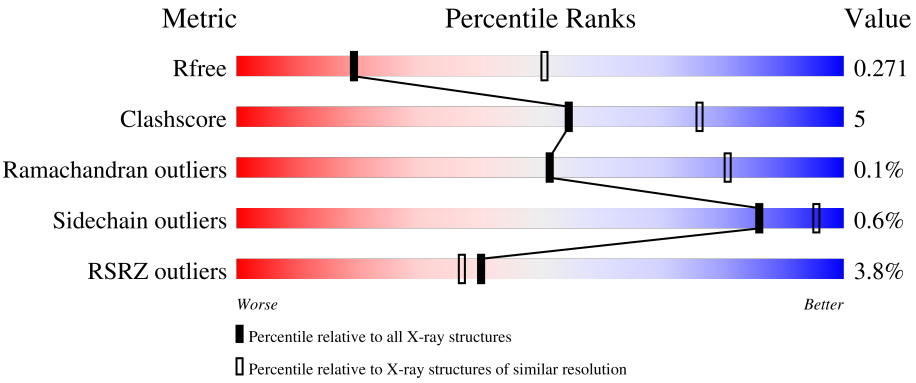
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	210	5% 71% 16% 13%
1	E	210	6% 82% 10% 7%
2	B	228	% 78% 18% .
2	H	228	% 85% 11% .
3	C	216	7% 87% 11% ..

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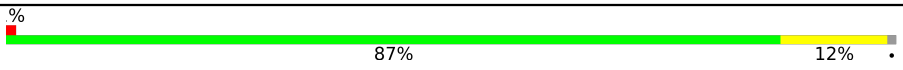
Mol	Chain	Length	Quality of chain
3	L	216	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9545 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	195	Total	C	N	O	S	0	0	0
			1544	991	257	288	8			
1	A	183	Total	C	N	O	S	0	0	0
			1465	943	242	273	7			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	319	MET	-	initiating methionine	UNP P0DTC2
E	320	GLY	-	expression tag	UNP P0DTC2
E	321	CYS	-	expression tag	UNP P0DTC2
E	322	VAL	-	expression tag	UNP P0DTC2
E	323	ALA	-	expression tag	UNP P0DTC2
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
A	319	MET	-	initiating methionine	UNP P0DTC2
A	320	GLY	-	expression tag	UNP P0DTC2
A	321	CYS	-	expression tag	UNP P0DTC2
A	322	VAL	-	expression tag	UNP P0DTC2
A	323	ALA	-	expression tag	UNP P0DTC2
A	324	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	THR	-	expression tag	UNP P0DTC2
A	326	GLY	-	expression tag	UNP P0DTC2
A	327	HIS	-	expression tag	UNP P0DTC2
A	328	HIS	-	expression tag	UNP P0DTC2
A	329	HIS	-	expression tag	UNP P0DTC2
A	330	HIS	-	expression tag	UNP P0DTC2
A	331	HIS	-	expression tag	UNP P0DTC2
A	332	HIS	-	expression tag	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	527	LYS	-	expression tag	UNP P0DTC2
A	528	LYS	-	expression tag	UNP P0DTC2

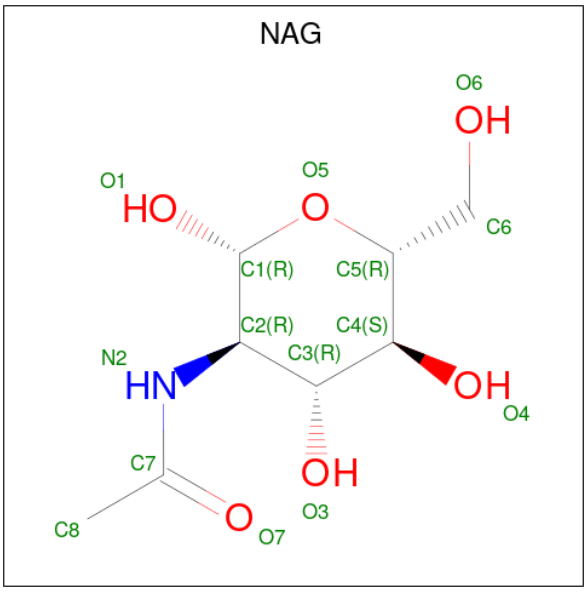
- Molecule 2 is a protein called Beta-24 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1655	1058	270	323	4			
2	B	219	Total	C	N	O	S	0	0	0
			1646	1052	268	322	4			

- Molecule 3 is a protein called Beta-24 light chain.

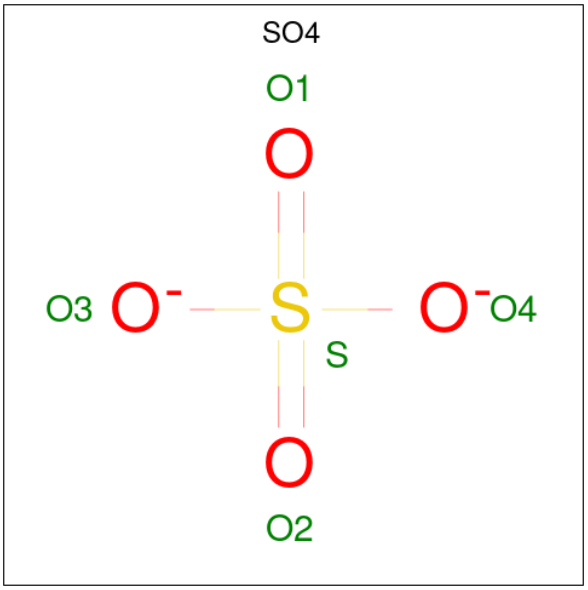
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1586	990	264	327	5			
3	C	214	Total	C	N	O	S	0	0	0
			1591	993	265	328	5			

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



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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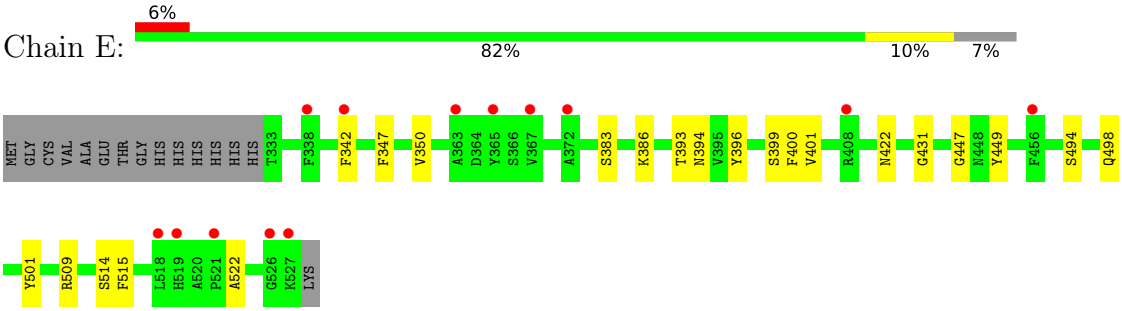
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

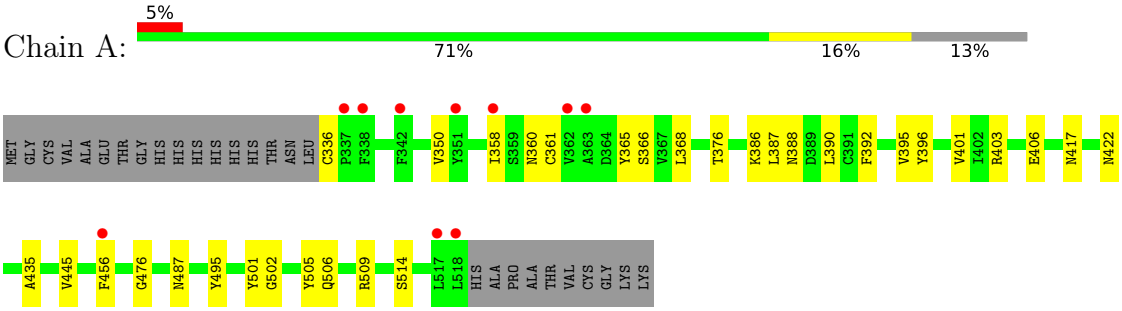
3 Residue-property plots (i)

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.

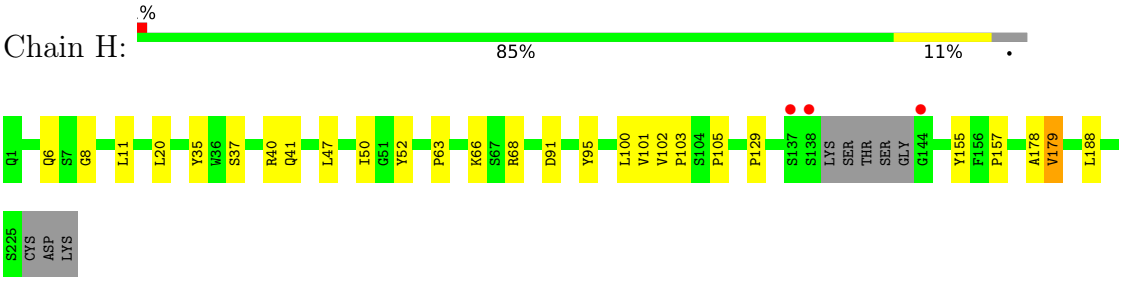
• Molecule 1: Spike protein S1



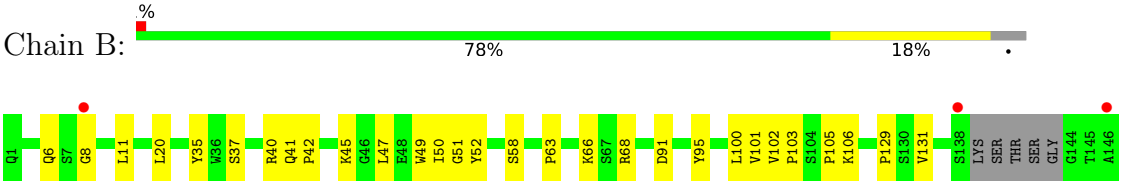
• Molecule 1: Spike protein S1

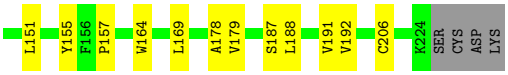


• Molecule 2: Beta-24 heavy chain



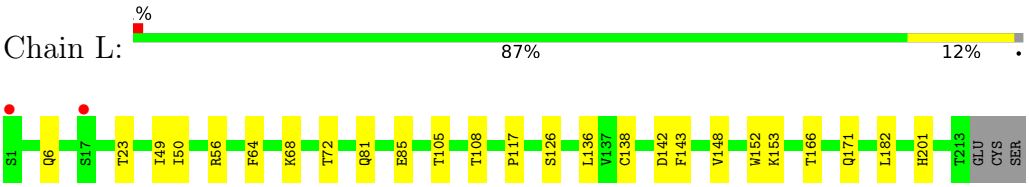
• Molecule 2: Beta-24 heavy chain





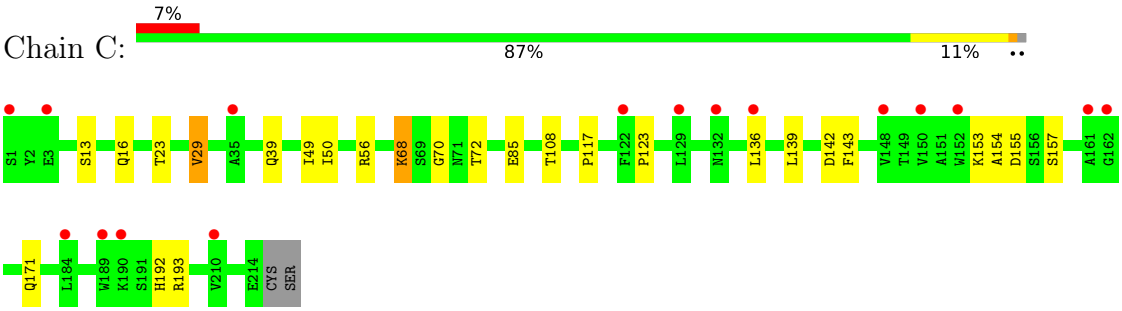
• Molecule 3: Beta-24 light chain

Chain L:



• Molecule 3: Beta-24 light chain

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.82Å 110.83Å 85.36Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	65.25 – 2.92 66.57 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.6 (65.25-2.92) 99.7 (66.57-2.92)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.222 , 0.271 0.223 , 0.271	Depositor DCC
R_{free} test set	1497 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9545	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: 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	0.26	0/1507	0.47	0/2049
1	E	0.25	0/1588	0.47	0/2162
2	B	0.25	0/1692	0.48	0/2317
2	H	0.25	0/1701	0.49	0/2328
3	C	0.25	0/1629	0.47	0/2224
3	L	0.26	0/1624	0.48	0/2217
All	All	0.25	0/9741	0.48	0/13297

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

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	1465	0	1385	21	0
1	E	1544	0	1457	14	0
2	B	1646	0	1622	25	0
2	H	1655	0	1635	19	0
3	C	1591	0	1535	16	0
3	L	1586	0	1533	14	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	14	0	13	1	0
5	B	5	0	0	0	0
5	C	10	0	0	1	0
5	H	5	0	0	0	0
5	L	10	0	0	1	0
All	All	9545	0	9193	98	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 (98) 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:H:11:LEU:HB2	2:H:157:PRO:HG3	1.65	0.79
3:C:49:ILE:HG22	3:C:50:ILE:HG12	1.66	0.78
1:A:366:SER:HB2	1:A:388:ASN:HD21	1.49	0.76
2:H:179:VAL:HG23	3:L:166:THR:HG22	1.70	0.73
1:A:336:CYS:N	1:A:361:CYS:SG	2.65	0.70
3:L:49:ILE:HG22	3:L:50:ILE:HG12	1.73	0.68
2:B:178:ALA:HA	2:B:188:LEU:HB3	1.76	0.67
3:L:81:GLN:HB3	1:A:386:LYS:HE3	1.79	0.65
2:B:41:GLN:HB2	2:B:47:LEU:HD23	1.80	0.64
2:H:41:GLN:HB2	2:H:47:LEU:HD23	1.79	0.63
1:E:383:SER:HB3	1:E:386:LYS:HB3	1.81	0.62
2:B:101:VAL:HG12	2:B:103:PRO:HD3	1.82	0.62
2:H:178:ALA:HA	2:H:188:LEU:HB3	1.80	0.61
1:E:501:TYR:HE1	2:H:102:VAL:HG12	1.65	0.61
2:H:35:TYR:HB2	2:H:100:LEU:HB3	1.83	0.61
2:B:129:PRO:HB3	2:B:155:TYR:HB3	1.83	0.59
2:B:11:LEU:HB2	2:B:157:PRO:HG3	1.86	0.58
1:A:387:LEU:HA	1:A:390:LEU:HD12	1.86	0.57
2:B:42:PRO:HB2	2:B:45:LYS:HD2	1.86	0.56
2:H:101:VAL:HG12	2:H:103:PRO:HD3	1.88	0.56
3:C:39:GLN:HB2	3:C:49:ILE:HD11	1.86	0.55
2:B:169:LEU:HD21	2:B:192:VAL:HG21	1.89	0.54
1:A:445:VAL:HG11	2:B:58:SER:HB3	1.90	0.54
2:B:35:TYR:HB2	2:B:100:LEU:HB3	1.90	0.54
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.25	0.53
2:H:6:GLN:NE2	2:H:95:TYR:O	2.29	0.53
1:A:501:TYR:HE1	2:B:102:VAL:HG12	1.74	0.51
3:L:142:ASP:OD1	3:L:171:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:148:VAL:HG12	3:L:201:HIS:HB2	1.91	0.50
3:C:155:ASP:OD1	3:C:192:HIS:HB3	2.11	0.50
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.94	0.50
2:H:63:PRO:HA	2:H:66:LYS:HB2	1.93	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.50
1:A:376:THR:HB	1:A:435:ALA:HB3	1.94	0.49
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.93	0.49
2:H:40:ARG:HB3	2:H:50:ILE:HD11	1.94	0.49
2:H:37:SER:HA	2:H:52:TYR:HA	1.94	0.49
1:A:417:ASN:O	1:A:422:ASN:ND2	2.45	0.49
1:A:390:LEU:HD13	1:A:392:PHE:HZ	1.78	0.48
2:B:40:ARG:HB3	2:B:50:ILE:HD11	1.94	0.48
1:E:350:VAL:HA	1:E:400:PHE:HB2	1.95	0.48
3:C:50:ILE:HD13	3:C:56:ARG:HG2	1.95	0.48
3:L:50:ILE:HD13	3:L:56:ARG:HG2	1.94	0.47
1:A:365:TYR:HA	1:A:368:LEU:HD12	1.96	0.47
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.95	0.47
2:B:37:SER:HA	2:B:52:TYR:HA	1.96	0.47
2:B:68:ARG:HH22	2:B:91:ASP:CG	2.17	0.47
3:L:6:GLN:NE2	3:L:105:THR:OG1	2.47	0.47
3:L:23:THR:HA	3:L:72:THR:HG22	1.97	0.47
3:C:154:ALA:N	3:C:157:SER:O	2.40	0.47
3:L:117:PRO:HB3	3:L:143:PHE:HB3	1.96	0.46
3:C:85:GLU:HG3	3:C:108:THR:HA	1.96	0.46
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.98	0.46
1:A:501:TYR:CE2	2:B:105:PRO:HD3	2.51	0.46
2:B:191:VAL:HG11	3:C:139:LEU:HD13	1.97	0.46
1:E:396:TYR:HB2	1:E:514:SER:HB2	1.97	0.46
1:E:342:PHE:HB2	4:E:601:NAG:H82	1.98	0.45
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.96	0.45
2:B:63:PRO:HA	2:B:66:LYS:HB2	1.96	0.45
3:C:142:ASP:OD1	3:C:171:GLN:NE2	2.45	0.45
3:C:68:LYS:HG3	3:C:70:GLY:H	1.81	0.45
2:B:68:ARG:NH2	2:B:91:ASP:OD2	2.48	0.45
2:H:68:ARG:HH22	2:H:91:ASP:CG	2.20	0.45
1:A:358:ILE:HB	1:A:395:VAL:HB	1.97	0.45
1:E:498:GLN:NE2	2:H:102:VAL:HG11	2.32	0.45
1:A:505:TYR:OH	2:B:106:LYS:HE3	2.17	0.45
3:L:85:GLU:HG3	3:L:108:THR:HA	1.98	0.44
1:E:449:TYR:HD2	1:E:494:SER:HG	1.66	0.44
3:C:13:SER:HB2	3:C:16:GLN:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:PHE:CE2	1:E:399:SER:HB2	2.53	0.44
1:E:447:GLY:HA2	1:E:498:GLN:HG3	1.99	0.43
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.44	0.43
3:C:23:THR:HA	3:C:72:THR:HG22	1.99	0.43
3:C:155:ASP:OD1	3:C:193:ARG:HG2	2.17	0.43
2:B:178:ALA:HB2	2:B:188:LEU:HD23	2.00	0.43
1:E:393:THR:HA	1:E:522:ALA:HA	2.00	0.42
3:L:126:SER:N	5:L:302:SO4:O4	2.46	0.42
2:B:131:VAL:HA	2:B:151:LEU:O	2.20	0.42
1:E:401:VAL:HG22	1:E:509:ARG:HG2	2.00	0.42
2:B:179:VAL:HG12	2:B:187:SER:O	2.20	0.42
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.55	0.42
1:A:456:PHE:CE2	3:C:29:VAL:HG11	2.55	0.41
2:H:37:SER:HB3	2:H:52:TYR:HB3	2.02	0.41
3:L:56:ARG:HD3	3:L:64:PHE:O	2.20	0.41
2:B:6:GLN:NE2	2:B:95:TYR:O	2.33	0.41
3:L:136:LEU:HB2	3:L:182:LEU:HB3	2.03	0.41
1:A:502:GLY:O	1:A:506:GLN:HG3	2.20	0.41
3:C:123:PRO:HA	3:C:136:LEU:HD23	2.01	0.41
1:A:396:TYR:HB2	1:A:514:SER:HB2	2.02	0.41
1:E:431:GLY:HA2	1:E:515:PHE:HD2	1.86	0.41
2:B:164:TRP:CH2	2:B:206:CYS:HB3	2.56	0.41
3:C:117:PRO:HB3	3:C:143:PHE:HB3	2.03	0.41
1:E:501:TYR:CE2	2:H:105:PRO:HD3	2.56	0.40
2:H:11:LEU:HD22	2:H:157:PRO:HD3	2.03	0.40
3:L:138:CYS:HB2	3:L:152:TRP:CH2	2.57	0.40
2:B:49:TRP:CZ2	2:B:51:GLY:HA2	2.56	0.40
3:C:153:LYS:NZ	5:C:302:SO4:O2	2.54	0.40
1:A:476:GLY:H	1:A:487:ASN:HB3	1.87	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	181/210 (86%)	167 (92%)	13 (7%)	1 (1%)	25 57
1	E	193/210 (92%)	181 (94%)	12 (6%)	0	100 100
2	B	215/228 (94%)	209 (97%)	6 (3%)	0	100 100
2	H	216/228 (95%)	210 (97%)	6 (3%)	0	100 100
3	C	212/216 (98%)	201 (95%)	11 (5%)	0	100 100
3	L	211/216 (98%)	200 (95%)	11 (5%)	0	100 100
All	All	1228/1308 (94%)	1168 (95%)	59 (5%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	ASN

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	159/180 (88%)	159 (100%)	0	100 100
1	E	167/180 (93%)	166 (99%)	1 (1%)	86 95
2	B	191/200 (96%)	191 (100%)	0	100 100
2	H	192/200 (96%)	191 (100%)	1 (0%)	88 96
3	C	179/182 (98%)	177 (99%)	2 (1%)	73 91
3	L	179/182 (98%)	177 (99%)	2 (1%)	73 91
All	All	1067/1124 (95%)	1061 (99%)	6 (1%)	86 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	394	ASN
2	H	179	VAL
3	L	68	LYS
3	L	153	LYS

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Mol	Chain	Res	Type
3	C	29	VAL
3	C	68	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	498	GLN
1	A	388	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	C	301	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	NAG	A	601	1	14,14,15	0.32	0	17,19,21	0.42	0
5	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	601	1	14,14,15	0.27	0	17,19,21	0.50	0
5	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.05	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
4	NAG	E	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	SO4	1	0
4	E	601	NAG	1	0
5	C	302	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^{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	A	183/210 (87%)	0.38	10 (5%)	25	22	55, 85, 140, 166	0
1	E	195/210 (92%)	0.38	13 (6%)	17	14	57, 78, 148, 183	0
2	B	219/228 (96%)	0.17	3 (1%)	75	76	43, 62, 91, 125	0
2	H	220/228 (96%)	0.14	3 (1%)	75	76	44, 62, 94, 140	0
3	C	214/216 (99%)	0.38	16 (7%)	14	11	49, 75, 111, 134	0
3	L	213/216 (98%)	-0.02	2 (0%)	84	84	47, 65, 97, 119	0
All	All	1244/1308 (95%)	0.23	47 (3%)	40	37	43, 70, 122, 183	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	VAL	5.2
2	B	138	SER	5.0
1	E	521	PRO	4.9
1	E	338	PHE	4.8
1	A	337	PRO	4.5
1	A	338	PHE	4.5
3	L	1	SER	4.1
2	H	137	SER	3.9
1	E	363	ALA	3.9
3	C	184	LEU	3.7
2	H	138	SER	3.7
3	C	1	SER	3.3
1	A	517	LEU	3.3
3	C	162	GLY	3.2
1	A	342	PHE	3.1
3	C	148	VAL	3.1
1	E	527	LYS	3.0
1	E	367	VAL	2.9
1	E	519	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	351	TYR	2.7
3	C	190	LYS	2.7
1	A	456	PHE	2.7
3	L	17	SER	2.6
1	E	518	LEU	2.5
3	C	161	ALA	2.4
1	A	363	ALA	2.4
3	C	129	LEU	2.4
2	H	144	GLY	2.4
3	C	210	VAL	2.3
1	E	372	ALA	2.3
3	C	152	TRP	2.3
3	C	136	LEU	2.3
1	E	526	GLY	2.3
2	B	8	GLY	2.3
3	C	189	TRP	2.3
3	C	122	PHE	2.2
3	C	35	ALA	2.2
1	A	518	LEU	2.2
1	E	365	TYR	2.1
1	E	342	PHE	2.1
1	E	456	PHE	2.1
2	B	146	ALA	2.1
1	E	408	ARG	2.1
3	C	132	ASN	2.1
3	C	3	GLU	2.0
3	C	150	VAL	2.0
1	A	358	ILE	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
5	SO4	H	301	5/5	0.75	0.19	94,95,116,186	0
4	NAG	A	601	14/15	0.77	0.18	82,112,123,124	0
4	NAG	E	601	14/15	0.79	0.25	78,99,104,115	0
5	SO4	L	302	5/5	0.83	0.33	88,98,122,143	0
5	SO4	B	301	5/5	0.85	0.18	118,130,149,230	0
5	SO4	C	302	5/5	0.88	0.15	106,108,125,128	0
5	SO4	L	301	5/5	0.89	0.13	71,83,110,115	0
5	SO4	C	301	5/5	0.93	0.16	89,91,105,115	0

6.5 Other polymers (i)

There are no such residues in this entry.