Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 04:59 AM EDT

PDB ID	:	7NXB
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 P.1 variant Spike glycoprotein in complex with COVOX-222 and EY6A Fabs
Authors	:	Zhou, D.; Ren, J.; Stuart, D.
Deposited on	:	2021-03-17
Resolution	:	2.67 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:

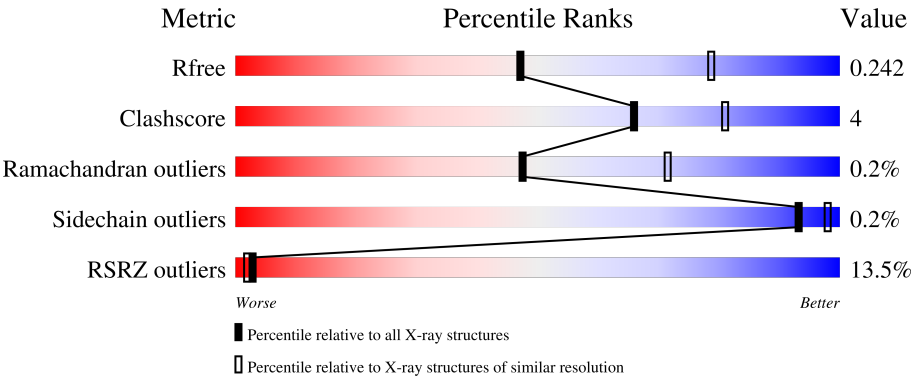
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	H	226	34% 79% 15% 5%
2	L	215	27% 90% 9%
3	E	205	% 86% 8% 6%
4	A	224	% 88% 9%
5	B	214	% 90% 9%

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
6	SO4	B	305	-	-	-	X
6	SO4	B	309	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 8202 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 EY6A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1628	1036	272	314	6			

- Molecule 2 is a protein called EY6A Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1622	1014	271	332	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	193	Total	C	N	O	S	0	0	0
			1531	984	254	285	8			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	THR	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	527	LYS	PRO	variant	UNP P0DTC2

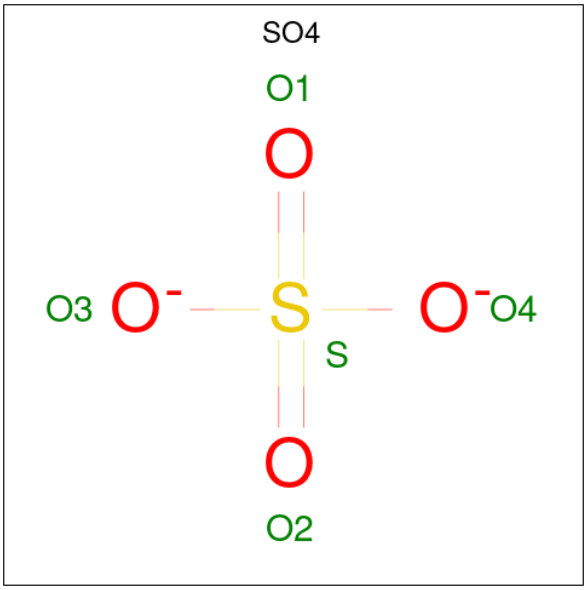
- Molecule 4 is a protein called COVOX-222 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	217	Total	C	N	O	S	0	0	0
			1595	1004	266	318	7			

- Molecule 5 is a protein called COVOX-222 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	213	Total	C	N	O	S	0	2	0
			1640	1025	279	330	6			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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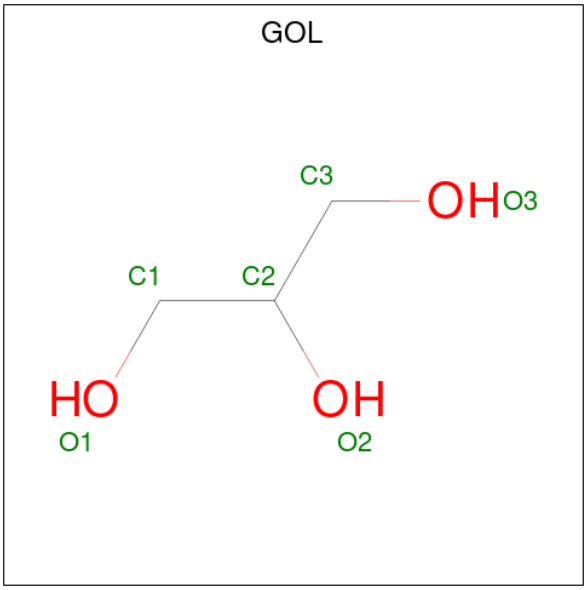
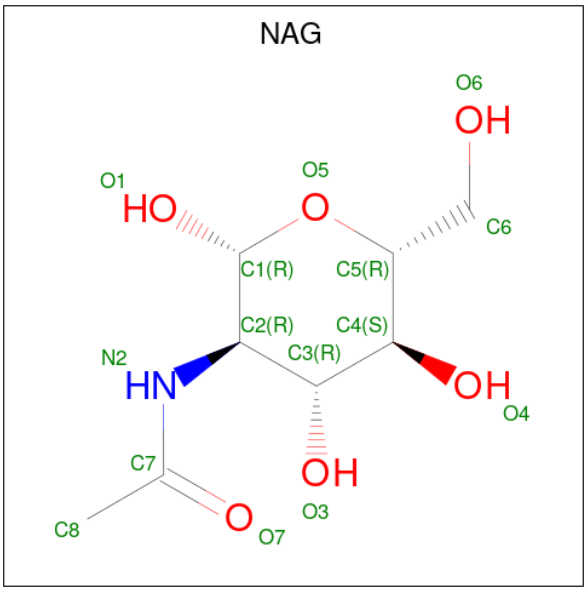
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



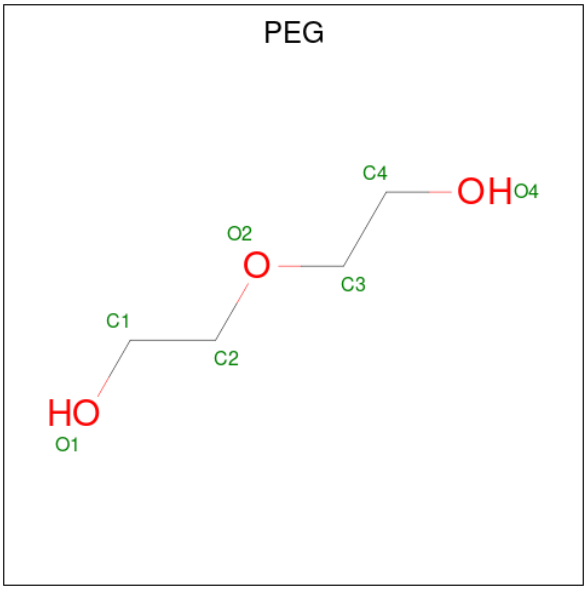
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0

- 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
8	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

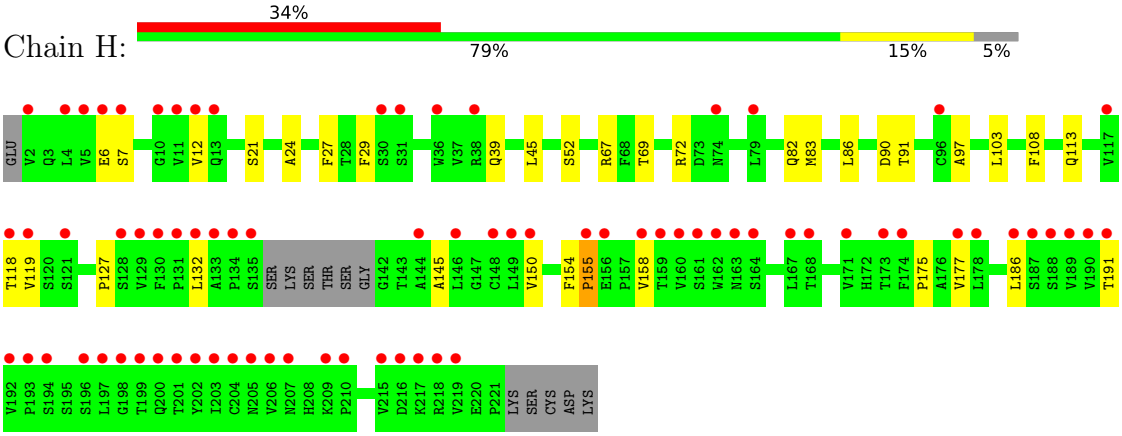
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	2	Total O 2 2	0	0
10	E	14	Total O 14 14	0	0
10	A	30	Total O 30 30	0	0
10	B	32	Total O 32 32	0	0

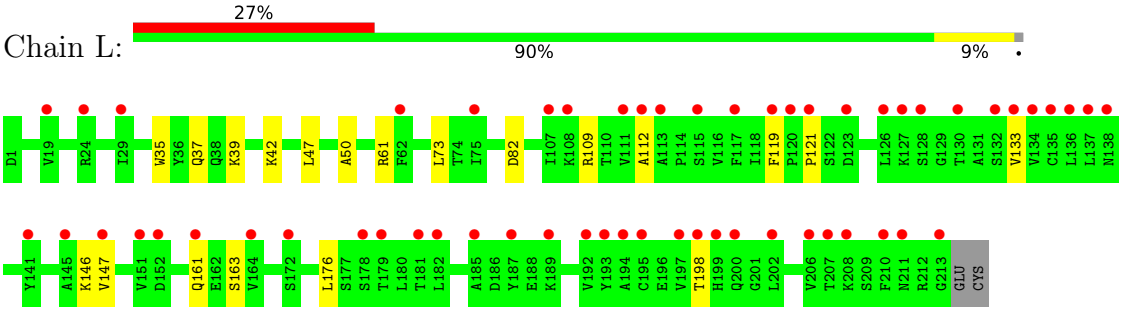
3 Residue-property plots (i)

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.

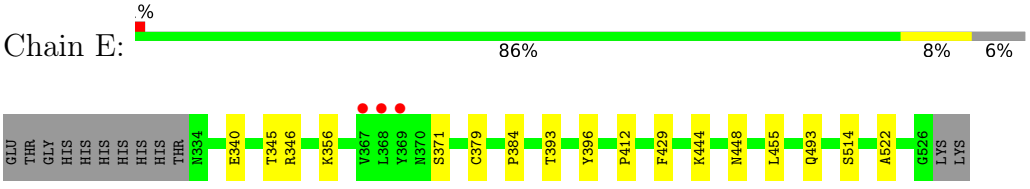
• Molecule 1: EY6A Fab heavy chain



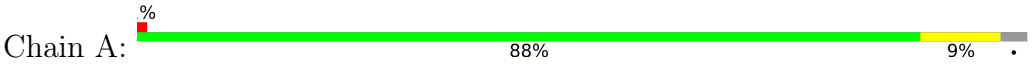
• Molecule 2: EY6A Fab light chain

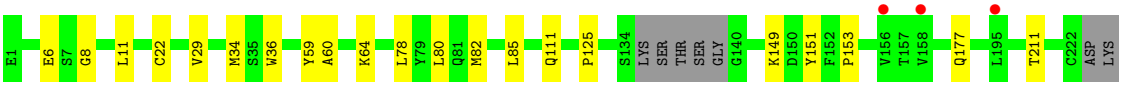


• Molecule 3: Spike protein S1



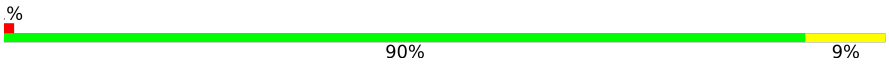
• Molecule 4: COVOX-222 Fab heavy chain





• Molecule 5: COVOX-222 Fab light chain

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.70Å 122.81Å 212.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.30 – 2.67 80.30 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.30-2.67) 99.9 (80.30-2.67)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.213 , 0.246 0.215 , 0.242	Depositor DCC
R_{free} test set	2106 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: PEG, NAG, SO4, GOL

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	H	0.24	0/1670	0.48	0/2276
2	L	0.25	0/1655	0.47	0/2246
3	E	0.26	0/1575	0.46	0/2144
4	A	0.26	0/1633	0.49	0/2227
5	B	0.25	0/1683	0.50	0/2287
All	All	0.25	0/8216	0.48	0/11180

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	H	1628	0	1582	21	0
2	L	1622	0	1585	12	0
3	E	1531	0	1449	8	0
4	A	1595	0	1549	13	0
5	B	1640	0	1594	13	0
6	A	5	0	0	0	0
6	B	45	0	0	1	0
6	E	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	5	0	0	0	0
7	A	6	0	8	0	0
7	E	6	0	8	0	0
8	E	14	0	13	0	0
9	A	7	0	10	1	0
10	A	30	0	0	0	0
10	B	32	0	0	1	0
10	E	14	0	0	0	0
10	L	2	0	0	0	0
All	All	8202	0	7798	63	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 4.

All (63) 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)
5:B:81:PRO:HA	5:B:106:ILE:HD13	1.76	0.66
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.80	0.64
1:H:127:PRO:HB3	1:H:150:VAL:HG13	1.80	0.63
4:A:29:VAL:HG13	4:A:34:MET:HG3	1.81	0.62
5:B:24:ARG:NH1	6:B:303:SO4:O1	2.32	0.62
3:E:340:GLU:OE1	3:E:356:LYS:NZ	2.32	0.62
3:E:412:PRO:HG3	3:E:429:PHE:HB3	1.82	0.61
4:A:82:MET:HB3	4:A:85:LEU:HD21	1.82	0.61
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.83	0.60
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.86	0.58
3:E:455:LEU:HD22	3:E:493:GLN:HG3	1.86	0.58
4:A:8:GLY:H	9:A:301:PEG:H12	1.68	0.58
4:A:34:MET:HB3	4:A:78:LEU:HD22	1.86	0.58
4:A:6:GLU:H	4:A:111:GLN:HE22	1.50	0.57
5:B:185:ASP:HA	5:B:188:LYS:HD3	1.87	0.55
5:B:106:ILE:O	5:B:166:GLN:NE2	2.40	0.55
1:H:29:PHE:O	1:H:72:ARG:NH2	2.41	0.54
1:H:91:THR:HG23	1:H:118:THR:HA	1.90	0.54
4:A:22:CYS:HB3	4:A:78:LEU:HB3	1.88	0.54
1:H:97:ALA:HB1	1:H:108:PHE:HB3	1.90	0.53
1:H:67:ARG:NH1	1:H:90:ASP:OD2	2.36	0.53
2:L:121:PRO:HD3	2:L:133:VAL:HG22	1.90	0.52
4:A:11:LEU:HB2	4:A:153:PRO:HG3	1.92	0.52
1:H:150:VAL:HB	1:H:186:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:ARG:NE	2:L:82:ASP:OD2	2.43	0.51
2:L:39:LYS:HB2	2:L:42:LYS:HB2	1.93	0.51
5:B:10:THR:HG22	5:B:103:LYS:HB3	1.93	0.50
3:E:345:THR:HG23	3:E:346:ARG:HG2	1.93	0.50
4:A:59:TYR:HB2	4:A:64:LYS:HG2	1.93	0.50
5:B:84:PHE:HB2	5:B:106:ILE:HD12	1.94	0.50
2:L:146:LYS:HB3	2:L:198:THR:HB	1.94	0.49
2:L:147:VAL:HG21	2:L:176:LEU:HD22	1.95	0.48
1:H:6:GLU:H	1:H:113:GLN:HE22	1.59	0.48
1:H:103:LEU:HD11	2:L:50:ALA:HB2	1.95	0.48
1:H:177:VAL:HG11	2:L:161:GLN:HB3	1.96	0.48
5:B:210:ASN:ND2	10:B:404:HOH:O	2.47	0.48
1:H:52:SER:O	1:H:72:ARG:NH1	2.47	0.47
1:H:150:VAL:HG11	1:H:158:VAL:HG21	1.96	0.47
5:B:11:LEU:O	5:B:105:ASP:N	2.43	0.47
3:E:393:THR:HA	3:E:522:ALA:HA	1.96	0.47
4:A:149:LYS:NZ	4:A:177:GLN:OE1	2.46	0.47
4:A:125:PRO:HD2	4:A:211:THR:HG21	1.95	0.47
1:H:132:LEU:HB3	2:L:119:PHE:CG	2.49	0.47
3:E:444:LYS:HG3	3:E:448:ASN:HB2	1.99	0.45
1:H:175:PRO:HD2	2:L:163:SER:HB2	2.00	0.44
5:B:62:ARG:HB2	5:B:77:SER:O	2.18	0.43
2:L:109:ARG:HH12	2:L:112:ALA:HB2	1.83	0.43
3:E:379:CYS:SG	3:E:384:PRO:HG3	2.57	0.43
1:H:7:SER:OG	1:H:21:SER:OG	2.36	0.43
4:A:125:PRO:HB3	4:A:151:TYR:HB3	1.99	0.43
3:E:396:TYR:HB2	3:E:514:SER:HB2	2.01	0.42
1:H:154:PHE:HA	1:H:155:PRO:HA	1.82	0.42
1:H:12:VAL:HG13	1:H:119:VAL:HG22	2.02	0.42
1:H:69:THR:HB	1:H:82:GLN:HB3	2.01	0.42
1:H:145:ALA:HB2	1:H:191:THR:HG22	2.01	0.42
5:B:4:MET:SD	5:B:25:ALA:HB2	2.60	0.42
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.55	0.41
5:B:145:LYS:HB3	5:B:197:THR:OG1	2.21	0.41
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.56	0.41
4:A:60:ALA:O	4:A:64:LYS:HG3	2.21	0.41
5:B:197:THR:HG22	5:B:204:PRO:HB3	2.03	0.40
4:A:36:TRP:NE1	4:A:80:LEU:HB2	2.37	0.40
5:B:34:LEU:HD22	5:B:34:LEU:HA	1.91	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	H	210/226 (93%)	200 (95%)	9 (4%)	1 (0%)	29 52
2	L	211/215 (98%)	200 (95%)	11 (5%)	0	100 100
3	E	191/205 (93%)	184 (96%)	6 (3%)	1 (0%)	29 52
4	A	213/224 (95%)	207 (97%)	6 (3%)	0	100 100
5	B	213/214 (100%)	202 (95%)	11 (5%)	0	100 100
All	All	1038/1084 (96%)	993 (96%)	43 (4%)	2 (0%)	47 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	371	SER
1	H	155	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	H	180/191 (94%)	180 (100%)	0	100 100
2	L	186/188 (99%)	186 (100%)	0	100 100
3	E	166/177 (94%)	166 (100%)	0	100 100
4	A	179/186 (96%)	179 (100%)	0	100 100
5	B	186/185 (100%)	184 (99%)	2 (1%)	73 89
All	All	897/927 (97%)	895 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	34	LEU
5	B	93	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	E	705	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	B	304	-	4,4,4	0.13	0	6,6,6	0.06	0
6	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	E	706	-	4,4,4	0.13	0	6,6,6	0.09	0
6	SO4	E	703	-	4,4,4	0.13	0	6,6,6	0.06	0
6	SO4	B	309	-	4,4,4	0.14	0	6,6,6	0.06	0
7	GOL	E	701	-	5,5,5	0.93	0	5,5,5	1.01	0
6	SO4	B	302	-	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	$\#\|Z\|>2$
6	SO4	B	308	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	E	704	-	4,4,4	0.13	0	6,6,6	0.06	0
7	GOL	A	302	-	5,5,5	0.92	0	5,5,5	0.92	0
6	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	B	306	-	4,4,4	0.13	0	6,6,6	0.06	0
8	NAG	E	702	3	14,14,15	0.30	0	17,19,21	0.45	0
6	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.05	0
9	PEG	A	301	-	6,6,6	0.12	0	5,5,5	0.07	0
6	SO4	B	307	-	4,4,4	0.15	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
8	NAG	E	702	3	-	0/6/23/26	0/1/1/1
9	PEG	A	301	-	-	3/4/4/4	-
7	GOL	E	701	-	-	2/4/4/4	-
7	GOL	A	302	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	701	GOL	O1-C1-C2-C3
7	E	701	GOL	O1-C1-C2-O2
9	A	301	PEG	C1-C2-O2-C3
9	A	301	PEG	O2-C3-C4-O4
9	A	301	PEG	O1-C1-C2-O2
7	A	302	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	SO4	1	0
9	A	301	PEG	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	H	214/226 (94%)	2.06	77 (35%) 0 0	75, 149, 208, 244	0
2	L	213/215 (99%)	1.59	57 (26%) 0 0	65, 115, 183, 221	0
3	E	193/205 (94%)	0.49	3 (1%) 72 73	47, 64, 110, 152	0
4	A	217/224 (96%)	0.43	3 (1%) 75 76	45, 55, 91, 143	0
5	B	213/214 (99%)	0.51	2 (0%) 84 85	47, 62, 83, 128	0
All	All	1050/1084 (96%)	1.02	142 (13%) 3 2	45, 74, 181, 244	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	192	VAL	15.9
1	H	135	SER	11.0
2	L	193	TYR	10.7
2	L	136	LEU	10.7
1	H	206	VAL	9.7
2	L	132	SER	8.4
1	H	204	CYS	8.3
2	L	145	ALA	8.2
1	H	162	TRP	8.2
2	L	194	ALA	8.1
1	H	202	TYR	7.8
2	L	127	LYS	7.7
1	H	203	ILE	7.6
2	L	181	THR	7.5
1	H	167	LEU	7.5
1	H	161	SER	7.4
1	H	215	VAL	7.3
2	L	210	PHE	6.8
1	H	117	VAL	6.6
2	L	137	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	H	160	VAL	6.4
2	L	197	VAL	6.4
3	E	369	TYR	6.3
1	H	159	THR	6.3
1	H	146	LEU	6.1
1	H	134	PRO	6.1
1	H	144	ALA	6.1
2	L	198	THR	6.1
2	L	200	GLN	6.1
1	H	133	ALA	5.9
1	H	216	ASP	5.7
2	L	126	LEU	5.6
1	H	129	VAL	5.5
1	H	79	LEU	5.5
1	H	210	PRO	5.5
2	L	147	VAL	5.3
1	H	205	ASN	5.3
1	H	193	PRO	5.3
2	L	121	PRO	5.2
1	H	155	PRO	5.2
1	H	30	SER	5.1
1	H	207	ASN	5.0
1	H	130	PHE	5.0
1	H	132	LEU	4.9
1	H	218	ARG	4.9
2	L	206	VAL	4.8
1	H	173	THR	4.7
1	H	119	VAL	4.7
1	H	201	THR	4.6
2	L	133	VAL	4.6
2	L	117	PHE	4.5
2	L	120	PRO	4.4
2	L	134	VAL	4.4
2	L	164	VAL	4.3
2	L	208	LYS	4.3
1	H	219	VAL	4.1
1	H	188	SER	4.0
1	H	164	SER	4.0
2	L	185	ALA	3.9
1	H	168	THR	3.8
1	H	196	SER	3.8
1	H	190	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	128	SER	3.8
1	H	6	GLU	3.7
1	H	217	LYS	3.7
2	L	112	ALA	3.7
2	L	119	PHE	3.7
1	H	131	PRO	3.7
1	H	189	VAL	3.6
2	L	135	CYS	3.6
1	H	150	VAL	3.6
2	L	189	LYS	3.5
1	H	2	VAL	3.5
3	E	368	LEU	3.5
1	H	12	VAL	3.5
2	L	202	LEU	3.5
1	H	7	SER	3.4
1	H	209	LYS	3.4
2	L	151	VAL	3.4
2	L	213	GLY	3.4
1	H	4	LEU	3.4
1	H	118	THR	3.3
1	H	11	VAL	3.3
2	L	138	ASN	3.2
2	L	211	ASN	3.2
1	H	197	LEU	3.2
2	L	182	LEU	3.2
1	H	191	THR	3.1
1	H	5	VAL	3.1
1	H	156	GLU	3.1
2	L	115	SER	3.0
2	L	172	SER	3.0
1	H	96	CYS	3.0
1	H	31	SER	2.9
1	H	187	SER	2.8
2	L	123	ASP	2.8
1	H	158	VAL	2.8
1	H	199	THR	2.8
2	L	19	VAL	2.8
2	L	152	ASP	2.7
2	L	130	THR	2.7
2	L	195	CYS	2.7
1	H	178	LEU	2.7
1	H	148	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	10	GLY	2.6
2	L	141	TYR	2.6
2	L	187	TYR	2.6
2	L	207	THR	2.6
4	A	195	LEU	2.6
2	L	111	VAL	2.6
1	H	13	GLN	2.5
2	L	128	SER	2.5
2	L	75	ILE	2.5
1	H	174	PHE	2.5
1	H	163	ASN	2.5
4	A	158	VAL	2.5
2	L	179	THR	2.5
1	H	36	TRP	2.5
1	H	186	LEU	2.4
2	L	192	VAL	2.4
2	L	199	HIS	2.4
1	H	74	ASN	2.4
2	L	62	PHE	2.4
1	H	121	SER	2.3
2	L	29	ILE	2.3
2	L	161	GLN	2.3
1	H	177	VAL	2.2
2	L	113	ALA	2.2
1	H	194	SER	2.2
2	L	24	ARG	2.2
1	H	171	VAL	2.2
4	A	156	VAL	2.2
1	H	198	GLY	2.2
1	H	200	GLN	2.1
3	E	367	VAL	2.1
5	B	13	LEU	2.1
1	H	149	LEU	2.1
2	L	107	ILE	2.1
2	L	108	LYS	2.1
2	L	178	SER	2.0
5	B	11	LEU	2.0
1	H	38	ARG	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
6	SO4	E	706	5/5	0.65	0.21	100,110,118,142	0
6	SO4	H	301	5/5	0.70	0.24	136,141,148,221	0
6	SO4	B	305	5/5	0.72	0.52	107,116,128,145	0
6	SO4	B	301	5/5	0.74	0.15	122,124,155,157	0
6	SO4	A	303	5/5	0.76	0.23	101,109,135,153	0
6	SO4	B	309	5/5	0.76	0.53	84,100,108,179	0
8	NAG	E	702	14/15	0.76	0.26	98,107,120,122	0
6	SO4	B	303	5/5	0.81	0.19	123,124,140,227	0
7	GOL	A	302	6/6	0.82	0.31	60,71,77,92	0
6	SO4	B	308	5/5	0.83	0.17	136,138,148,217	0
6	SO4	B	306	5/5	0.84	0.46	88,89,124,137	0
6	SO4	E	704	5/5	0.85	0.29	84,95,134,136	0
6	SO4	B	302	5/5	0.87	0.11	94,101,106,121	0
6	SO4	E	705	5/5	0.87	0.13	90,94,110,197	0
6	SO4	B	304	5/5	0.87	0.28	110,114,128,141	0
9	PEG	A	301	7/7	0.89	0.22	67,79,84,84	0
7	GOL	E	701	6/6	0.92	0.15	64,69,77,82	0
6	SO4	E	703	5/5	0.93	0.14	70,81,99,100	0
6	SO4	B	307	5/5	0.93	0.28	107,113,133,139	0

6.5 Other polymers (i)

There are no such residues in this entry.