



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:45 PM UTC

PDB ID : 7NX7 / pdb_00007nx7
Title : Crystal structure of the K417N mutant receptor binding domain of SARS-CoV-2 Spike glycoprotein in complex with COVOX-222 and EY6A Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.
Deposited on : 2021-03-17
Resolution : 2.30 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

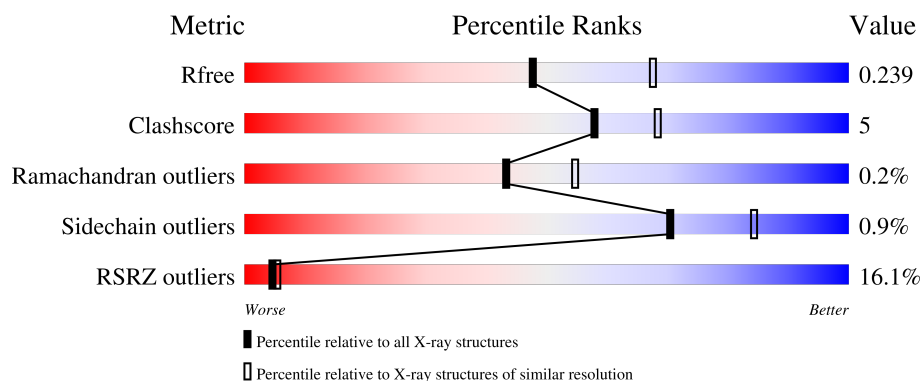
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	H	226	42% 81% 14% 5%
2	L	215	28% 85% 15%
3	E	205	4% 85% 9% 6%
4	A	224	2% 87% 8% .
5	B	214	% 86% 14%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8377 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	214	Total	C	N	O	S	0	0	0
			1631	1019	272	335	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
			1528	978	255	287	8			

There are 11 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	ASN	LYS	engineered mutation	UNP P0DTC2
E	527	LYS	PRO	conflict	UNP P0DTC2

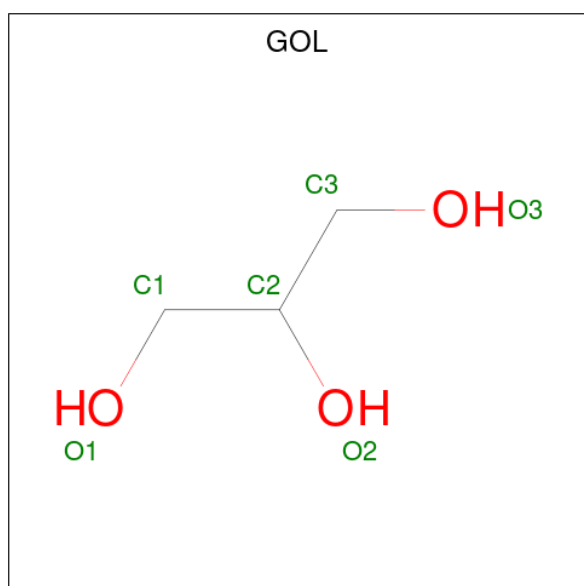
- Molecule 4 is a protein called COVOX-222 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	214	Total	C	N	O	S	0	0	0
			1577	995	263	313	6			

- 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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		

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

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

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

- Molecule 10 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	6	7		

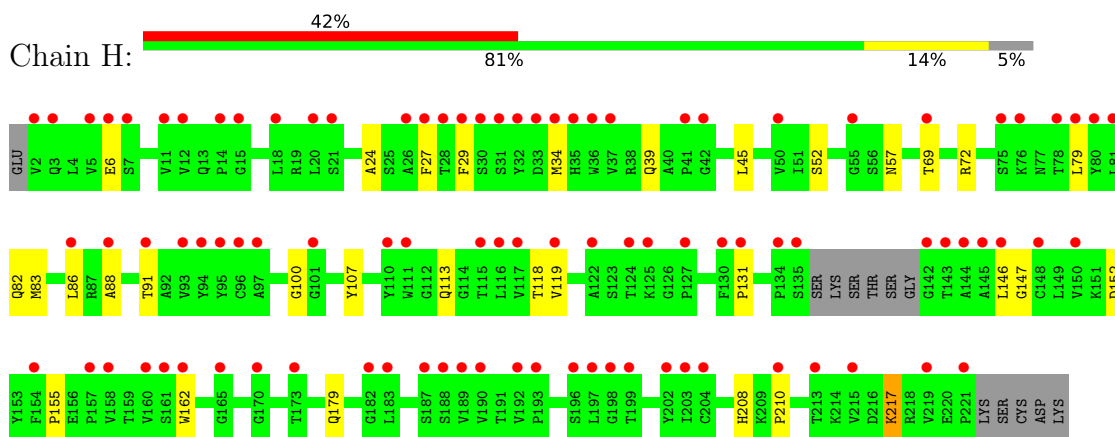
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	1	Total	O	0	0
			1	1		
11	L	13	Total	O	0	0
			13	13		
11	E	62	Total	O	0	0
			62	62		
11	A	95	Total	O	0	0
			95	95		
11	B	91	Total	O	0	0
			91	91		

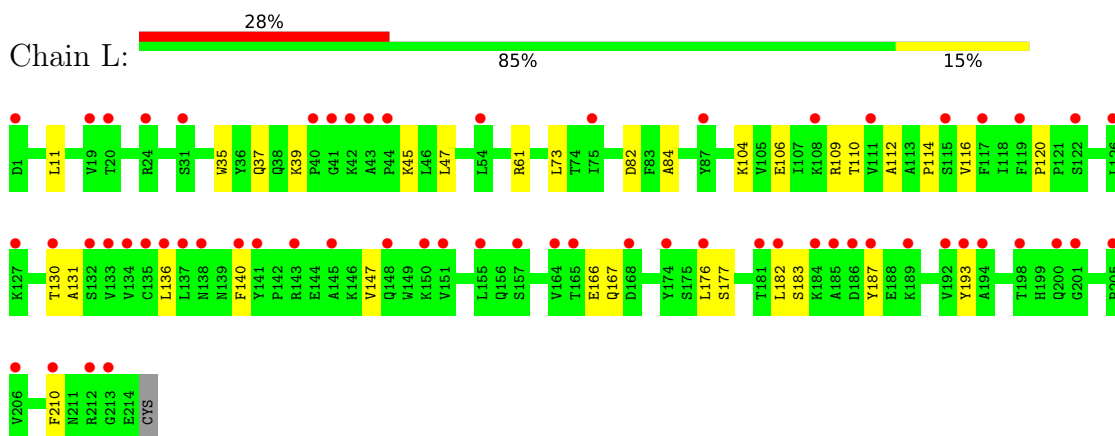
3 Residue-property plots [i](#)

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.

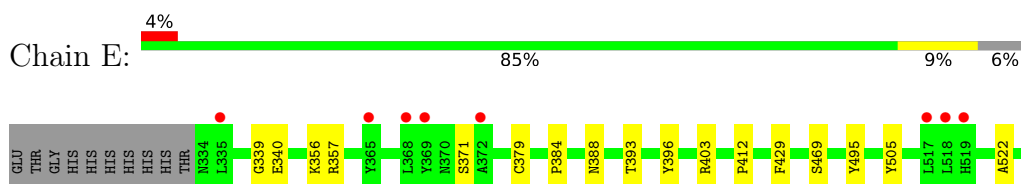
- Molecule 1: EY6A Fab heavy chain



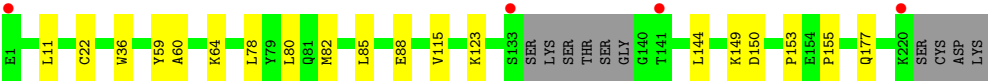
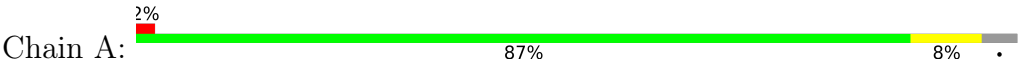
- Molecule 2: EY6A Fab light chain



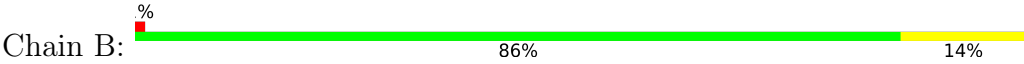
- Molecule 3: Spike protein S1



- Molecule 4: COVOX-222 Fab heavy chain



● Molecule 5: COVOX-222 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.71Å 122.36Å 213.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.49 – 2.30 80.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.49-2.30) 100.0 (80.49-2.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.207 , 0.239 0.207 , 0.239	Depositor DCC
R_{free} test set	3236 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8377	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, SO4, GOL, CIT

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	0.17	0/1670	0.31	0/2276
2	L	0.14	0/1664	0.32	0/2258
3	E	0.13	0/1571	0.30	0/2139
4	A	0.16	0/1615	0.35	0/2203
5	B	0.16	0/1683	0.37	0/2287
All	All	0.15	0/8203	0.33	0/11163

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 [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	H	1628	0	1582	15	0
2	L	1631	0	1591	19	0
3	E	1528	0	1438	9	0
4	A	1577	0	1534	11	0
5	B	1640	0	1594	17	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
6	E	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	14	0	13	1	0
8	A	15	0	0	0	0
8	B	35	0	0	1	0
8	E	15	0	0	0	0
9	A	1	0	0	1	0
10	B	13	0	5	2	0
11	A	95	0	0	1	0
11	B	91	0	0	2	0
11	E	62	0	0	0	0
11	H	1	0	0	0	0
11	L	13	0	0	0	0
All	All	8377	0	7781	72	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 (72) 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	1.69	0.74
1:H:6:GLU:H	1:H:113:GLN:HE22	1.36	0.72
4:A:22:CYS:HB3	4:A:78:LEU:HB3	1.75	0.68
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.74	0.67
3:E:340:GLU:OE1	3:E:356:LYS:NZ	2.30	0.65
4:A:149:LYS:NZ	4:A:177:GLN:OE1	2.30	0.65
5:B:1:ASP:N	11:B:501:HOH:O	2.29	0.64
5:B:4:MET:HE3	5:B:25:ALA:HB2	1.79	0.64
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.81	0.63
4:A:82:MET:HB3	4:A:85:LEU:HD21	1.81	0.63
5:B:169:LYS:HD2	6:B:401:GOL:H32	1.80	0.62
5:B:142:ARG:NH2	8:B:405:SO4:O2	2.36	0.58
1:H:100:GLY:HA3	1:H:107:TYR:CZ	2.38	0.58
3:E:339:GLY:HA3	7:E:702:NAG:H82	1.86	0.58
2:L:39:LYS:HD3	2:L:84:ALA:HB2	1.86	0.57
3:E:412:PRO:HG3	3:E:429:PHE:HB3	1.87	0.57
4:A:11:LEU:HB2	4:A:153:PRO:HG3	1.88	0.56
5:B:84:PHE:HB2	5:B:106:ILE:HD12	1.88	0.55
4:A:123:LYS:NZ	11:A:404:HOH:O	2.39	0.54
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.92	0.52
10:B:402:CIT:O4	10:B:402:CIT:O7	2.22	0.52
2:L:147:VAL:HG21	2:L:176:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:403:ARG:HD2	3:E:505:TYR:HA	1.91	0.51
2:L:109:ARG:NH1	2:L:110:THR:O	2.44	0.51
3:E:388:ASN:HA	3:E:526:GLY:HA3	1.93	0.50
5:B:31:SER:HB2	10:B:402:CIT:H41	1.93	0.50
1:H:91:THR:HG23	1:H:118:THR:HA	1.94	0.50
2:L:104:LYS:NZ	2:L:166:GLU:OE1	2.40	0.49
2:L:120:PRO:HB3	2:L:210:PHE:CE2	2.47	0.49
1:H:152:ASP:OD1	1:H:179:GLN:NE2	2.46	0.49
2:L:187:TYR:O	2:L:193:TYR:OH	2.30	0.49
2:L:131:ALA:HB3	2:L:182:LEU:HD12	1.95	0.48
2:L:61:ARG:NE	2:L:82:ASP:OD2	2.41	0.48
2:L:109:ARG:HH12	2:L:112:ALA:HB2	1.79	0.47
3:E:379:CYS:SG	3:E:384:PRO:HG3	2.55	0.47
4:A:82:MET:HE1	4:A:115:VAL:HG21	1.97	0.46
3:E:393:THR:HA	3:E:522:ALA:HA	1.97	0.46
5:B:55:ARG:HG2	5:B:59:ILE:HB	1.96	0.46
3:E:403:ARG:HG3	3:E:495:TYR:CE1	2.52	0.45
4:A:155:PRO:HA	9:A:305:CL:CL	2.53	0.45
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.99	0.45
2:L:114:PRO:HB3	2:L:140:PHE:CD2	2.52	0.45
4:A:149:LYS:HG2	4:A:150:ASP:CG	2.42	0.45
4:A:59:TYR:HB2	4:A:64:LYS:HG2	1.98	0.45
1:H:29:PHE:O	1:H:72:ARG:NH2	2.50	0.45
4:A:36:TRP:CE2	4:A:80:LEU:HB2	2.52	0.44
1:H:208:HIS:CD2	1:H:210:PRO:HD2	2.53	0.44
1:H:131:PRO:HD3	1:H:217:LYS:HD3	2.00	0.43
5:B:120:PRO:HD3	5:B:132:VAL:HG22	1.99	0.43
5:B:90:GLN:HG2	5:B:97:ARG:O	2.18	0.43
4:A:60:ALA:O	4:A:64:LYS:HG3	2.19	0.43
1:H:88:ALA:HA	1:H:119:VAL:HB	2.00	0.43
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.54	0.43
5:B:93:ASP:OD1	5:B:94:THR:N	2.45	0.43
2:L:130:THR:HA	2:L:183:SER:HA	2.00	0.43
2:L:106:GLU:HB2	2:L:167:GLN:OE1	2.19	0.42
2:L:109:ARG:HG3	2:L:110:THR:O	2.18	0.42
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.55	0.42
5:B:145:LYS:HB3	5:B:197:THR:OG1	2.20	0.42
5:B:210:ASN:HB2	5:B:213:GLU:HB2	2.01	0.42
2:L:116:VAL:HA	2:L:136:LEU:O	2.20	0.41
2:L:11:LEU:O	2:L:106:GLU:HG2	2.19	0.41
2:L:131:ALA:N	2:L:182:LEU:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:62:ARG:HB2	5:B:77:SER:O	2.20	0.41
5:B:91:HIS:HD2	11:B:584:HOH:O	2.03	0.41
5:B:48:LEU:HB3	5:B:49:ILE:HD12	2.02	0.41
3:E:357:ARG:HG3	3:E:396:TYR:CE1	2.55	0.41
5:B:19:ALA:HB3	5:B:76:ILE:HB	2.02	0.41
1:H:147:GLY:HA2	1:H:162:TRP:CZ2	2.56	0.41
1:H:52:SER:HB3	1:H:57:ASN:HB2	2.04	0.40
1:H:69:THR:HB	1:H:82:GLN:HB3	2.03	0.40
2:L:176:LEU:HD23	2:L:177:SER:N	2.36	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%)	201 (96%)	8 (4%)	1 (0%)	24	31
2	L	212/215 (99%)	200 (94%)	12 (6%)	0	100	100
3	E	191/205 (93%)	186 (97%)	4 (2%)	1 (0%)	24	31
4	A	210/224 (94%)	203 (97%)	7 (3%)	0	100	100
5	B	213/214 (100%)	206 (97%)	7 (3%)	0	100	100
All	All	1036/1084 (96%)	996 (96%)	38 (4%)	2 (0%)	43	55

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%)	178 (99%)	2 (1%)	65	81
2	L	187/188 (100%)	186 (100%)	1 (0%)	81	90
3	E	166/177 (94%)	165 (99%)	1 (1%)	78	89
4	A	176/186 (95%)	174 (99%)	2 (1%)	65	81
5	B	186/185 (100%)	184 (99%)	2 (1%)	65	81
All	All	895/927 (96%)	887 (99%)	8 (1%)	70	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	146	LEU
1	H	217	LYS
2	L	45	LYS
3	E	469	SER
4	A	88	GLU
4	A	144	LEU
5	B	26	SER
5	B	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	354	ASN
3	E	394	ASN
3	E	501	ASN
5	B	138	ASN
5	B	160	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	SO4	E	704	-	4,4,4	0.25	0	6,6,6	0.12	0
7	NAG	E	702	3	14,14,15	0.37	0	17,19,21	0.60	0
8	SO4	B	405	-	4,4,4	0.25	0	6,6,6	0.09	0
8	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	B	403	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.10	0
8	SO4	E	703	-	4,4,4	0.25	0	6,6,6	0.08	0
10	CIT	B	402	-	12,12,12	1.13	0	17,17,17	1.34	2 (11%)
6	GOL	A	301	-	5,5,5	0.94	0	5,5,5	1.02	0
8	SO4	E	705	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	A	304	-	4,4,4	0.26	0	6,6,6	0.08	0
8	SO4	B	404	-	4,4,4	0.25	0	6,6,6	0.09	0
8	SO4	B	408	-	4,4,4	0.26	0	6,6,6	0.07	0
6	GOL	E	701	-	5,5,5	0.91	0	5,5,5	1.10	0
8	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.09	0
8	SO4	B	406	-	4,4,4	0.24	0	6,6,6	0.05	0
6	GOL	B	401	-	5,5,5	0.89	0	5,5,5	1.15	0
8	SO4	B	407	-	4,4,4	0.25	0	6,6,6	0.07	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
7	NAG	E	702	3	-	2/6/23/26	0/1/1/1
6	GOL	A	301	-	-	4/4/4/4	-
6	GOL	E	701	-	-	2/4/4/4	-
10	CIT	B	402	-	-	9/16/16/16	-
6	GOL	B	401	-	-	3/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	402	CIT	O6-C6-C3	3.20	119.29	113.14
10	B	402	CIT	O4-C5-C4	2.10	120.99	114.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	701	GOL	O1-C1-C2-C3
10	B	402	CIT	O7-C3-C6-O5
10	B	402	CIT	O7-C3-C6-O6
10	B	402	CIT	C4-C3-C6-O5
10	B	402	CIT	C4-C3-C6-O6
7	E	702	NAG	O5-C5-C6-O6
6	A	301	GOL	O1-C1-C2-C3
6	A	301	GOL	C1-C2-C3-O3
6	B	401	GOL	O1-C1-C2-C3
6	B	401	GOL	C1-C2-C3-O3
6	E	701	GOL	O1-C1-C2-O2
6	A	301	GOL	O1-C1-C2-O2
6	B	401	GOL	O2-C2-C3-O3
7	E	702	NAG	C4-C5-C6-O6
6	A	301	GOL	O2-C2-C3-O3
10	B	402	CIT	C6-C3-C4-C5
10	B	402	CIT	O7-C3-C4-C5
10	B	402	CIT	C3-C4-C5-O4
10	B	402	CIT	C1-C2-C3-O7
10	B	402	CIT	C3-C4-C5-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	702	NAG	1	0
8	B	405	SO4	1	0
10	B	402	CIT	2	0
6	B	401	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	214/226 (94%)	1.95	94 (43%) 0 0	72, 142, 188, 207	0
2	L	214/215 (99%)	1.54	61 (28%) 1 1	57, 117, 179, 199	0
3	E	193/205 (94%)	0.35	8 (4%) 41 43	39, 57, 117, 145	0
4	A	214/224 (95%)	0.11	4 (1%) 66 68	39, 50, 81, 127	0
5	B	213/214 (99%)	0.15	2 (0%) 81 82	32, 54, 75, 111	2 (0%)
All	All	1048/1084 (96%)	0.83	169 (16%) 4 5	32, 67, 176, 207	2 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	136	LEU	5.7
3	E	369	TYR	5.4
1	H	11	VAL	5.2
2	L	192	VAL	5.1
1	H	31	SER	4.6
1	H	2	VAL	4.3
1	H	135	SER	4.1
2	L	193	TYR	4.1
2	L	117	PHE	4.1
1	H	3	GLN	4.0
2	L	145	ALA	3.9
1	H	144	ALA	3.9
2	L	194	ALA	3.8
1	H	27	PHE	3.8
1	H	26	ALA	3.7
2	L	155	LEU	3.7
1	H	215	VAL	3.7
2	L	151	VAL	3.6
2	L	130	THR	3.6
1	H	30	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	192	VAL	3.6
1	H	28	THR	3.6
2	L	181	THR	3.6
1	H	79	LEU	3.5
1	H	124	THR	3.5
2	L	206	VAL	3.5
2	L	40	PRO	3.5
1	H	162	TRP	3.5
1	H	110	TYR	3.5
1	H	117	VAL	3.4
1	H	80	TYR	3.4
2	L	87	TYR	3.4
1	H	199	THR	3.4
1	H	50	VAL	3.3
4	A	220	LYS	3.3
5	B	1	ASP	3.3
1	H	116	LEU	3.3
1	H	160	VAL	3.3
2	L	164	VAL	3.3
1	H	122	ALA	3.2
2	L	54	LEU	3.2
3	E	368	LEU	3.2
1	H	134	PRO	3.2
1	H	15	GLY	3.2
2	L	137	LEU	3.2
2	L	134	VAL	3.2
2	L	210	PHE	3.1
2	L	41	GLY	3.1
1	H	173	THR	3.1
1	H	197	LEU	3.1
1	H	189	VAL	3.0
1	H	91	THR	3.0
2	L	108	LYS	3.0
1	H	12	VAL	3.0
2	L	31	SER	3.0
1	H	130	PHE	2.9
2	L	43	ALA	2.9
1	H	111	TRP	2.9
2	L	111	VAL	2.9
2	L	127	LYS	2.9
2	L	182	LEU	2.9
1	H	219	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	221	PRO	2.9
1	H	20	LEU	2.8
1	H	182	GLY	2.8
4	A	133	SER	2.8
1	H	81	LEU	2.8
1	H	146	LEU	2.8
1	H	5	VAL	2.8
2	L	213	GLY	2.8
1	H	193	PRO	2.8
2	L	20	THR	2.7
4	A	141	THR	2.7
1	H	183	LEU	2.7
1	H	97	ALA	2.7
2	L	165	THR	2.7
1	H	35	HIS	2.7
2	L	119	PHE	2.7
2	L	198	THR	2.7
1	H	127	PRO	2.7
4	A	1	GLU	2.7
1	H	36	TRP	2.7
1	H	154	PHE	2.7
1	H	158	VAL	2.7
1	H	148	CYS	2.7
2	L	126	LEU	2.7
1	H	55	GLY	2.6
1	H	101	GLY	2.6
3	E	335	LEU	2.6
2	L	185	ALA	2.6
1	H	190	VAL	2.6
2	L	133	VAL	2.6
1	H	21	SER	2.6
1	H	203	ILE	2.6
1	H	96	CYS	2.6
1	H	37	VAL	2.6
1	H	187	SER	2.6
1	H	196	SER	2.6
2	L	42	LYS	2.6
1	H	75	SER	2.6
1	H	34	MET	2.5
2	L	184	LYS	2.5
2	L	174	TYR	2.5
1	H	29	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	125	LYS	2.5
1	H	6	GLU	2.5
1	H	161	SER	2.4
3	E	519	HIS	2.4
1	H	42	GLY	2.4
2	L	143	ARG	2.4
2	L	205	PRO	2.4
1	H	143	THR	2.4
2	L	132	SER	2.4
2	L	187	TYR	2.4
1	H	131	PRO	2.4
1	H	210	PRO	2.4
2	L	150	LYS	2.4
2	L	141	TYR	2.4
1	H	14	PRO	2.3
1	H	76	LYS	2.3
2	L	157	SER	2.3
2	L	19	VAL	2.3
1	H	18	LEU	2.3
1	H	88	ALA	2.3
2	L	212	ARG	2.3
1	H	93	VAL	2.3
1	H	142	GLY	2.3
3	E	365	TYR	2.3
1	H	115	THR	2.3
1	H	213	THR	2.3
2	L	135	CYS	2.2
1	H	95	TYR	2.2
1	H	7	SER	2.2
1	H	119	VAL	2.2
2	L	186	ASP	2.2
2	L	24	ARG	2.2
1	H	94	TYR	2.2
1	H	41	PRO	2.2
3	E	517	LEU	2.2
2	L	140	PHE	2.2
2	L	44	PRO	2.2
1	H	165	GLY	2.2
1	H	145	ALA	2.2
3	E	372	ALA	2.2
1	H	202	TYR	2.1
2	L	176	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	518	LEU	2.1
1	H	150	VAL	2.1
1	H	69	THR	2.1
2	L	75	ILE	2.1
2	L	168	ASP	2.1
1	H	170	GLY	2.1
1	H	198	GLY	2.1
1	H	188	SER	2.1
2	L	189	LYS	2.1
2	L	200	GLN	2.1
2	L	122	SER	2.1
2	L	148	GLN	2.1
1	H	32	TYR	2.1
5	B	16	GLY	2.1
2	L	115	SER	2.0
1	H	33	ASP	2.0
1	H	86	LEU	2.0
2	L	1	ASP	2.0
2	L	138	ASN	2.0
2	L	201	GLY	2.0
1	H	78	THR	2.0
1	H	204	CYS	2.0
1	H	157	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	E	702	14/15	0.49	0.19	108,117,124,126	0
8	SO4	E	704	5/5	0.53	0.15	105,117,121,130	0
8	SO4	E	705	5/5	0.57	0.11	114,121,139,175	0
8	SO4	B	409	5/5	0.61	0.17	98,109,140,141	0
8	SO4	B	403	5/5	0.66	0.10	112,115,137,153	0
8	SO4	B	405	5/5	0.70	0.11	86,99,107,125	0
8	SO4	E	703	5/5	0.71	0.13	83,87,123,134	0
8	SO4	B	408	5/5	0.72	0.11	140,144,153,194	0
8	SO4	A	304	5/5	0.74	0.12	94,101,113,167	0
6	GOL	B	401	6/6	0.75	0.18	76,88,90,91	0
8	SO4	B	407	5/5	0.78	0.10	115,122,163,164	0
10	CIT	B	402	13/13	0.78	0.17	74,89,124,125	0
8	SO4	B	404	5/5	0.81	0.11	73,85,101,103	0
8	SO4	B	406	5/5	0.81	0.13	84,89,122,161	0
6	GOL	A	301	6/6	0.87	0.17	50,58,62,77	0
8	SO4	A	303	5/5	0.88	0.12	81,83,87,160	0
6	GOL	E	701	6/6	0.90	0.13	64,68,75,83	0
9	CL	A	305	1/1	0.94	0.12	64,64,64,64	0
8	SO4	A	302	5/5	0.94	0.08	64,74,82,84	0

6.5 Other polymers

There are no such residues in this entry.