



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 04:08 AM EDT

PDB ID : 7NX8  
Title : Crystal structure of the K417T 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 : 1.95 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

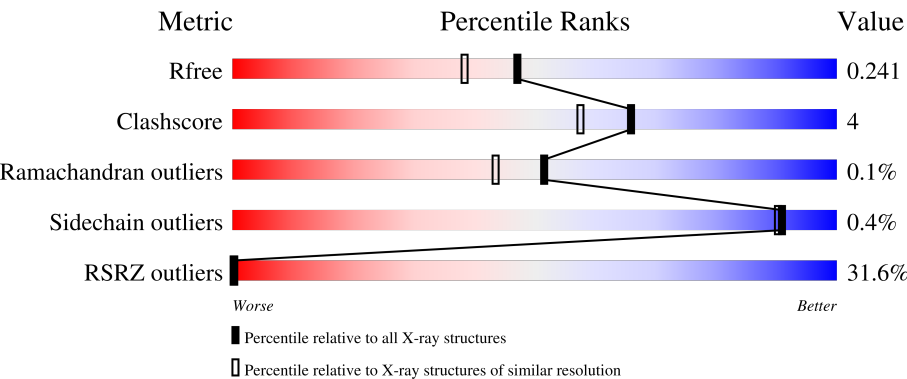
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	<div><div>64%</div><div><div></div><div></div><div></div><div></div></div><div>81%14%5%</div></div>
2	L	215	<div><div>57%</div><div><div></div><div></div><div></div><div></div></div><div>88%11%. </div></div>
3	E	205	<div><div>16%</div><div><div></div><div></div><div></div><div></div></div><div>89%5%5%</div></div>
4	A	224	<div><div>11%</div><div><div></div><div></div><div></div><div></div></div><div>88%8%. </div></div>
5	B	214	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>90%9%</div></div>

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
9	SO4	A	1211	-	-	-	X
9	SO4	B	310	-	-	X	X
9	SO4	B	312	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8474 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	215	Total	C	N	O	S	0	0	0
			1637	1041	273	317	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1618	1012	270	331	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	194	Total	C	N	O	S	0	1	0
			1540	986	258	288	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	THR	LYS	engineered mutation	UNP P0DTC2
E	527	LYS	PRO	conflict	UNP P0DTC2

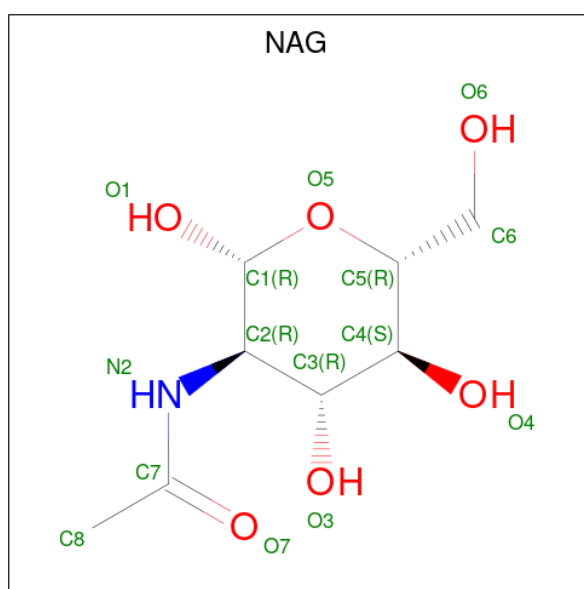
- Molecule 4 is a protein called COVOX-222 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	215	Total	C	N	O	S	0	0	0
			1583	998	264	315	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	1	0
			1637	1023	279	330	5			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



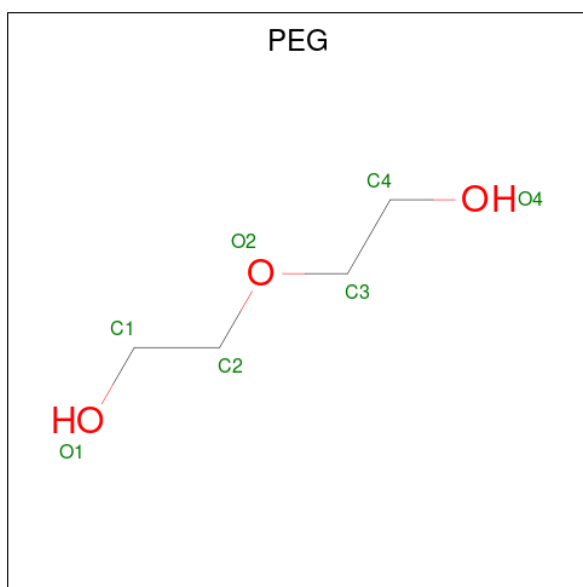
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O		0	0
			14	8	1	5			

- 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	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



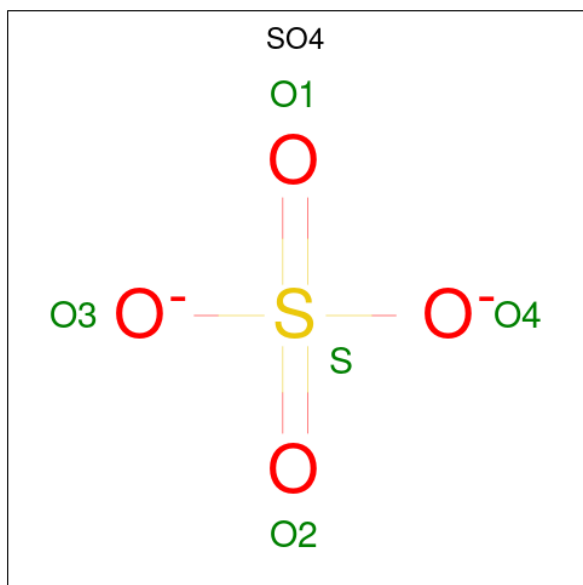
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



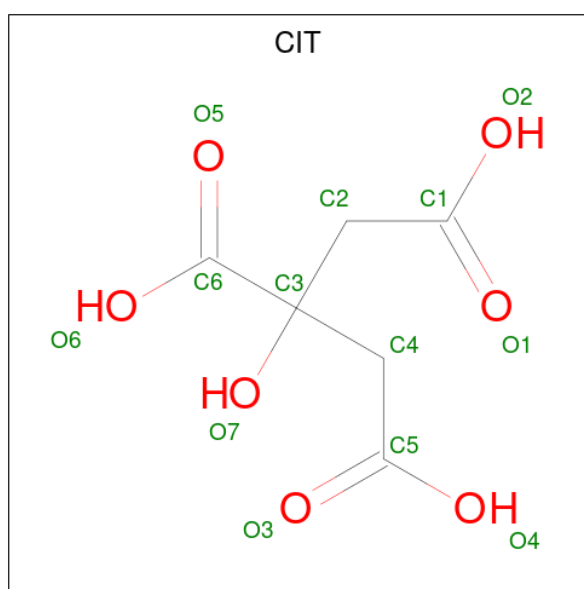
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 10 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



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

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	3	Total	Cl	0	0
			3	3		
11	B	4	Total	Cl	0	0
			4	4		

- Molecule 12 is water.

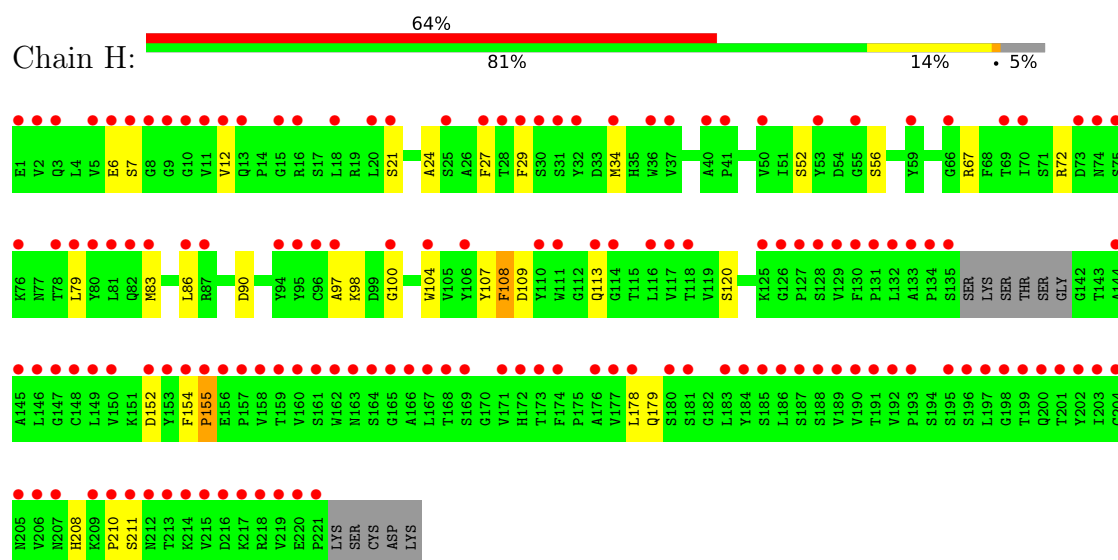


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	3	Total 3	O 3	0	0
12	L	7	Total 7	O 7	0	0
12	E	75	Total 75	O 75	0	0
12	A	122	Total 122	O 122	0	0
12	B	112	Total 112	O 112	0	0

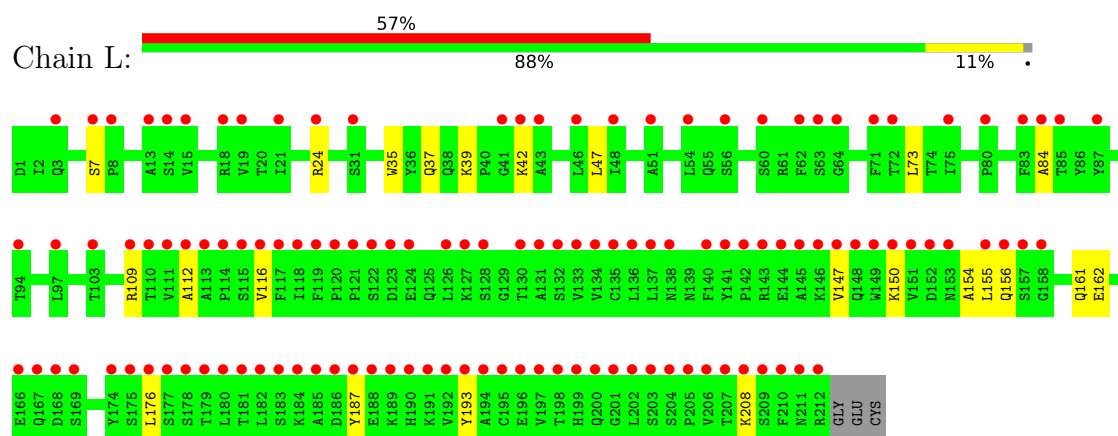
### 3 Residue-property plots

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.

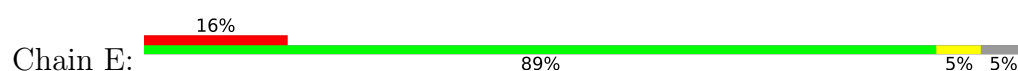
#### • Molecule 1: EY6A Fab heavy chain

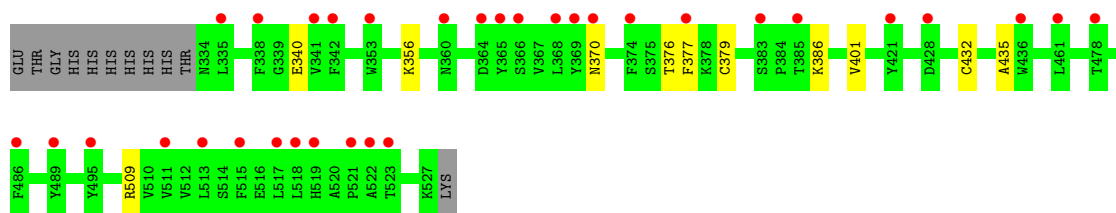


#### • Molecule 2: EY6A Fab light chain

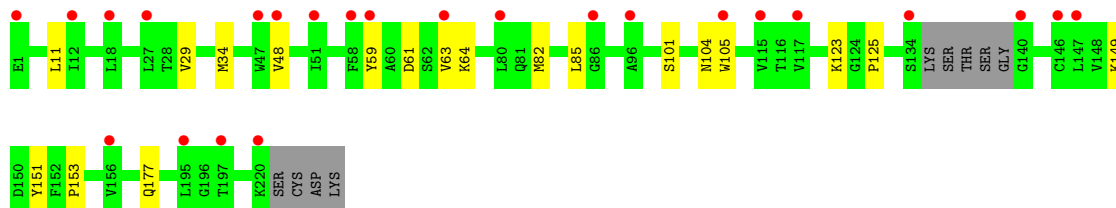
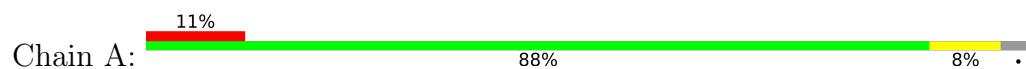


#### • Molecule 3: Spike protein S1

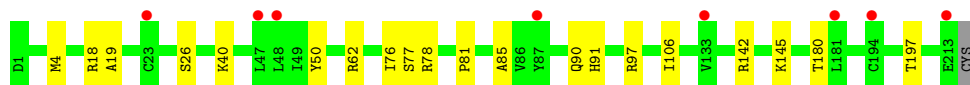
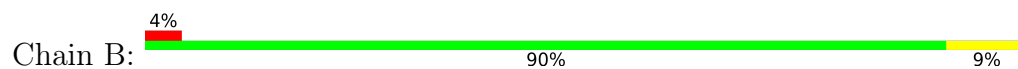




● Molecule 4: COVOX-222 Fab heavy chain



● 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, $\alpha$ , $\beta$ , $\gamma$	54.84Å 122.73Å 213.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.62 – 1.95 80.62 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.62-1.95) 99.9 (80.62-1.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.223 , 0.246 0.230 , 0.241	Depositor DCC
$R_{free}$ test set	5262 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, CL, GOL, CIT, NAG, SO4

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	0/1679	0.48	0/2288
2	L	0.25	0/1651	0.48	0/2241
3	E	0.25	0/1586	0.47	0/2159
4	A	0.25	0/1621	0.49	0/2211
5	B	0.24	0/1677	0.50	0/2279
All	All	0.25	0/8214	0.49	0/11178

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	1637	0	1591	21	0
2	L	1618	0	1582	13	0
3	E	1540	0	1454	6	0
4	A	1583	0	1539	11	0
5	B	1637	0	1590	15	0
6	E	14	0	13	0	0
7	A	12	0	16	0	0
7	E	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	21	0	30	2	0
8	E	7	0	10	0	0
9	A	10	0	0	0	0
9	B	40	0	0	5	0
9	E	10	0	0	0	0
10	A	13	0	5	0	0
11	A	3	0	0	0	0
11	B	4	0	0	1	0
12	A	122	0	0	1	0
12	B	112	0	0	0	0
12	E	75	0	0	0	0
12	H	3	0	0	0	0
12	L	7	0	0	0	0
All	All	8474	0	7838	64	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 (64) 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)
8:A:1203:PEG:H22	5:B:180:THR:HG21	1.65	0.77
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.79	0.65
4:A:82:MET:HB3	4:A:85:LEU:HD21	1.78	0.63
1:H:208:HIS:HD1	1:H:211:SER:HG	1.46	0.62
5:B:18:ARG:NH2	9:B:310:SO4:O3	2.34	0.61
1:H:6:GLU:H	1:H:113:GLN:HE22	1.47	0.61
3:E:340:GLU:OE1	3:E:356:LYS:NZ	2.34	0.60
4:A:123:LYS:NZ	12:A:1303:HOH:O	2.35	0.59
5:B:26:SER:N	11:B:303:CL:CL	2.68	0.59
5:B:18:ARG:NH2	9:B:310:SO4:O4	2.36	0.58
1:H:56:SER:O	3:E:370:ASN:ND2	2.37	0.58
1:H:7:SER:OG	1:H:21:SER:OG	2.20	0.56
1:H:100:GLY:HA3	1:H:107:TYR:CZ	2.41	0.55
5:B:142:ARG:NH2	9:B:309:SO4:O2	2.40	0.55
5:B:4:MET:HG3	5:B:91:HIS:CE1	2.43	0.54
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.90	0.54
1:H:97:ALA:HB1	1:H:108:PHE:HB3	1.91	0.53
4:A:59:TYR:O	4:A:64:LYS:NZ	2.38	0.53
1:H:208:HIS:ND1	1:H:211:SER:OG	2.38	0.53
4:A:149:LYS:NZ	4:A:177:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:ARG:NH1	1:H:90:ASP:OD2	2.35	0.51
2:L:7:SER:HB3	2:L:24:ARG:HH22	1.75	0.51
1:H:12:VAL:HG11	1:H:86:LEU:HD13	1.93	0.51
5:B:19:ALA:HB3	5:B:76:ILE:HB	1.94	0.50
2:L:39:LYS:HB2	2:L:42:LYS:HB2	1.94	0.50
4:A:48:VAL:HG13	4:A:63:VAL:HG21	1.94	0.49
1:H:34:MET:HB3	1:H:79:LEU:HD22	1.95	0.49
2:L:147:VAL:HG21	2:L:176:LEU:HD22	1.93	0.49
4:A:11:LEU:HB2	4:A:153:PRO:HG3	1.95	0.48
5:B:18:ARG:NH2	9:B:310:SO4:S	2.85	0.48
2:L:154:ALA:O	2:L:156:GLN:NE2	2.43	0.48
5:B:78:ARG:NH1	9:B:312:SO4:O3	2.46	0.47
1:H:29:PHE:O	1:H:72:ARG:NH2	2.46	0.47
1:H:152:ASP:OD1	1:H:179:GLN:NE2	2.48	0.47
2:L:39:LYS:HD3	2:L:84:ALA:HB2	1.96	0.47
2:L:116:VAL:HB	2:L:208:LYS:HG3	1.97	0.47
4:A:105:TRP:CE2	5:B:50:TYR:HB2	2.51	0.46
2:L:187:TYR:O	2:L:193:TYR:OH	2.34	0.45
5:B:62:ARG:HB2	5:B:77:SER:O	2.16	0.45
1:H:154:PHE:HA	1:H:155:PRO:HA	1.77	0.45
3:E:376:THR:HB	3:E:435:ALA:HB3	1.97	0.45
1:H:52:SER:O	1:H:72:ARG:NH1	2.50	0.45
4:A:61:ASP:OD1	4:A:64:LYS:NZ	2.49	0.44
1:H:208:HIS:CD2	1:H:210:PRO:HD2	2.53	0.44
5:B:90:GLN:HG2	5:B:97:ARG:O	2.18	0.43
3:E:379:CYS:HA	3:E:432:CYS:HA	2.01	0.43
2:L:150:LYS:HG2	2:L:155:LEU:HD23	2.01	0.42
5:B:81:PRO:HA	5:B:106:ILE:HD13	2.01	0.42
1:H:24:ALA:HB1	1:H:27:PHE:CE1	2.54	0.42
1:H:104:TRP:HA	3:E:386:LYS:HG2	2.01	0.42
8:A:1206:PEG:H11	8:A:1206:PEG:H31	1.79	0.42
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.54	0.42
1:H:120:SER:HB3	1:H:154:PHE:CZ	2.55	0.42
2:L:162:GLU:HG2	2:L:176:LEU:HD21	2.01	0.41
5:B:145:LYS:HB3	5:B:197:THR:HB	2.02	0.41
3:E:401:VAL:HG22	3:E:509:ARG:HG2	2.02	0.41
2:L:109:ARG:NH1	2:L:112:ALA:HB2	2.35	0.41
1:H:6:GLU:H	1:H:113:GLN:NE2	2.16	0.41
1:H:98:LYS:NZ	1:H:109:ASP:OD2	2.42	0.41
4:A:101:SER:OG	4:A:104:ASN:HB3	2.21	0.41
5:B:40:LYS:HG2	5:B:85:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:29:VAL:HG13	4:A:34:MET:HG3	2.01	0.41
4:A:125:PRO:HB3	4:A:151:TYR:HB3	2.03	0.41
2:L:109:ARG:HH12	2:L:112:ALA:HB2	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	H	211/226 (93%)	201 (95%)	9 (4%)	1 (0%)	29	17
2	L	210/215 (98%)	200 (95%)	10 (5%)	0	100	100
3	E	193/205 (94%)	186 (96%)	7 (4%)	0	100	100
4	A	211/224 (94%)	204 (97%)	7 (3%)	0	100	100
5	B	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	1037/1084 (96%)	996 (96%)	40 (4%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	181/191 (95%)	179 (99%)	2 (1%)	73	71
2	L	186/188 (99%)	185 (100%)	1 (0%)	88	88
3	E	167/177 (94%)	166 (99%)	1 (1%)	86	85
4	A	177/186 (95%)	177 (100%)	0	100	100
5	B	185/185 (100%)	185 (100%)	0	100	100
All	All	896/927 (97%)	892 (100%)	4 (0%)	91	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	108	PHE
1	H	178	LEU
2	L	161	GLN
3	E	377	PHE

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

Mol	Chain	Res	Type
1	H	57	ASN
3	E	370	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](#)

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	$\# Z  > 2$
7	GOL	A	1205	-	5,5,5	0.92	0	5,5,5	0.95	0
7	GOL	A	1201	-	5,5,5	0.91	0	5,5,5	0.97	0
10	CIT	A	1202	-	12,12,12	1.03	0	17,17,17	1.65	4 (23%)
9	SO4	A	1210	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	A	1211	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	B	312	-	4,4,4	0.14	0	6,6,6	0.05	0
8	PEG	A	1204	-	6,6,6	0.11	0	5,5,5	0.09	0
7	GOL	E	902	-	5,5,5	0.92	0	5,5,5	0.98	0
9	SO4	E	905	-	4,4,4	0.14	0	6,6,6	0.05	0
8	PEG	A	1206	-	6,6,6	0.12	0	5,5,5	0.09	0
8	PEG	A	1203	-	6,6,6	0.09	0	5,5,5	0.10	0
9	SO4	B	309	-	4,4,4	0.14	0	6,6,6	0.05	0
8	PEG	E	903	-	6,6,6	0.11	0	5,5,5	0.09	0
6	NAG	E	901	3	14,14,15	0.39	0	17,19,21	0.54	0
9	SO4	B	306	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.06	0
9	SO4	B	307	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	E	904	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	B	308	-	4,4,4	0.14	0	6,6,6	0.06	0
9	SO4	B	311	-	4,4,4	0.14	0	6,6,6	0.06	0
9	SO4	B	310	-	4,4,4	0.14	0	6,6,6	0.06	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	GOL	A	1205	-	-	2/4/4/4	-
8	PEG	A	1204	-	-	0/4/4/4	-
7	GOL	E	902	-	-	2/4/4/4	-
7	GOL	A	1201	-	-	0/4/4/4	-
8	PEG	A	1206	-	-	3/4/4/4	-
8	PEG	A	1203	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CIT	A	1202	-	-	5/16/16/16	-
8	PEG	E	903	-	-	2/4/4/4	-
6	NAG	E	901	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1202	CIT	O6-C6-C3	4.35	120.60	113.05
10	A	1202	CIT	C3-C4-C5	-2.14	108.64	113.81
10	A	1202	CIT	O4-C5-C4	2.10	121.10	114.35
10	A	1202	CIT	O2-C1-O1	-2.08	118.12	123.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1203	PEG	O1-C1-C2-O2
8	E	903	PEG	O2-C3-C4-O4
7	E	902	GOL	O1-C1-C2-C3
7	A	1205	GOL	O1-C1-C2-C3
8	A	1206	PEG	O1-C1-C2-O2
7	E	902	GOL	O1-C1-C2-O2
7	A	1205	GOL	O1-C1-C2-O2
10	A	1202	CIT	O7-C3-C4-C5
10	A	1202	CIT	C6-C3-C4-C5
8	A	1203	PEG	O2-C3-C4-O4
10	A	1202	CIT	C2-C3-C4-C5
10	A	1202	CIT	C2-C3-C6-O6
8	E	903	PEG	C1-C2-O2-C3
8	A	1203	PEG	C1-C2-O2-C3
6	E	901	NAG	O5-C5-C6-O6
10	A	1202	CIT	C2-C3-C6-O5
8	A	1206	PEG	C1-C2-O2-C3
8	A	1206	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	312	SO4	1	0
8	A	1206	PEG	1	0
8	A	1203	PEG	1	0
9	B	309	SO4	1	0
9	B	310	SO4	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	215/226 (95%)	3.55	144 (66%) 0 0	64, 127, 184, 210	0
2	L	212/215 (98%)	3.35	123 (58%) 0 0	49, 99, 172, 214	0
3	E	194/205 (94%)	1.38	33 (17%) 1 2	30, 48, 100, 130	0
4	A	215/224 (95%)	1.20	24 (11%) 5 8	30, 41, 66, 122	0
5	B	213/214 (99%)	0.99	8 (3%) 40 50	32, 44, 61, 89	0
All	All	1049/1084 (96%)	2.11	332 (31%) 0 0	30, 57, 164, 214	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	194	ALA	20.8
1	H	135	SER	16.0
1	H	130	PHE	14.2
1	H	160	VAL	14.1
2	L	185	ALA	13.0
1	H	168	THR	12.5
2	L	210	PHE	12.4
2	L	136	LEU	11.6
2	L	195	CYS	11.6
2	L	193	TYR	11.6
2	L	145	ALA	11.3
1	H	190	VAL	11.2
2	L	181	THR	10.7
1	H	215	VAL	10.5
2	L	117	PHE	10.0
2	L	192	VAL	9.6
2	L	183	SER	9.5
2	L	135	CYS	9.4
2	L	133	VAL	9.3
1	H	134	PRO	9.1

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Mol	Chain	Res	Type	RSRZ
2	L	151	VAL	9.0
1	H	161	SER	8.9
1	H	206	VAL	8.8
1	H	1	GLU	8.8
2	L	116	VAL	8.7
1	H	203	ILE	8.7
1	H	162	TRP	8.6
1	H	164	SER	8.5
2	L	137	LEU	8.4
1	H	205	ASN	8.4
1	H	204	CYS	8.4
1	H	219	VAL	8.4
2	L	189	LYS	8.2
1	H	192	VAL	8.2
1	H	166	ALA	8.0
3	E	518	LEU	7.8
2	L	119	PHE	7.8
1	H	171	VAL	7.6
1	H	131	PRO	7.5
2	L	132	SER	7.4
1	H	167	LEU	7.4
2	L	184	LYS	7.3
1	H	158	VAL	7.3
2	L	206	VAL	7.3
2	L	120	PRO	7.2
2	L	115	SER	7.1
1	H	165	GLY	7.1
1	H	199	THR	6.9
1	H	148	CYS	6.9
2	L	198	THR	6.9
1	H	181	SER	6.9
1	H	144	ALA	6.8
1	H	159	THR	6.8
1	H	210	PRO	6.6
2	L	209	SER	6.4
1	H	126	GLY	6.4
2	L	127	LYS	6.3
2	L	203	SER	6.3
2	L	128	SER	6.2
2	L	19	VAL	6.2
2	L	112	ALA	6.1
2	L	202	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	H	31	SER	6.0
1	H	133	ALA	5.9
2	L	208	LYS	5.9
1	H	150	VAL	5.9
1	H	81	LEU	5.8
2	L	141	TYR	5.8
1	H	201	THR	5.7
2	L	149	TRP	5.7
2	L	134	VAL	5.7
3	E	369	TYR	5.6
2	L	123	ASP	5.6
1	H	212	ASN	5.6
1	H	173	THR	5.6
1	H	188	SER	5.6
2	L	152	ASP	5.6
1	H	6	GLU	5.5
1	H	177	VAL	5.5
2	L	200	GLN	5.4
1	H	153	TYR	5.3
1	H	216	ASP	5.3
1	H	78	THR	5.3
2	L	188	GLU	5.3
2	L	122	SER	5.3
2	L	21	ILE	5.3
2	L	187	TYR	5.2
1	H	195	SER	5.2
2	L	147	VAL	5.2
1	H	27	PHE	5.1
1	H	220	GLU	5.1
1	H	75	SER	5.0
1	H	218	ARG	5.0
2	L	180	LEU	5.0
2	L	205	PRO	5.0
2	L	174	TYR	4.9
1	H	29	PHE	4.9
2	L	118	ILE	4.9
1	H	28	THR	4.9
2	L	182	LEU	4.9
1	H	76	LYS	4.8
2	L	130	THR	4.8
2	L	186	ASP	4.8
1	H	132	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	H	127	PRO	4.7
1	H	191	THR	4.7
1	H	111	TRP	4.7
1	H	196	SER	4.7
1	H	193	PRO	4.7
1	H	202	TYR	4.6
1	H	97	ALA	4.6
1	H	213	THR	4.6
1	H	187	SER	4.6
1	H	7	SER	4.5
2	L	190	HIS	4.5
2	L	142	PRO	4.5
1	H	80	TYR	4.4
1	H	129	VAL	4.4
1	H	221	PRO	4.4
1	H	146	LEU	4.4
1	H	176	ALA	4.4
1	H	11	VAL	4.4
3	E	521	PRO	4.4
4	A	1	GLU	4.3
2	L	204	SER	4.3
1	H	110	TYR	4.3
1	H	198	GLY	4.2
2	L	175	SER	4.2
1	H	157	PRO	4.2
2	L	111	VAL	4.2
3	E	335	LEU	4.1
2	L	156	GLN	4.1
1	H	125	LYS	4.1
1	H	163	ASN	4.1
2	L	153	ASN	4.1
2	L	87	TYR	4.1
1	H	207	ASN	4.0
2	L	207	THR	4.0
1	H	189	VAL	4.0
2	L	212	ARG	4.0
2	L	158	GLY	4.0
2	L	191	LYS	3.9
1	H	30	SER	3.9
3	E	519	HIS	3.9
2	L	150	LYS	3.9
2	L	197	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	75	ILE	3.9
3	E	385	THR	3.8
1	H	149	LEU	3.8
3	E	368	LEU	3.8
1	H	200	GLN	3.8
2	L	178	SER	3.8
1	H	12	VAL	3.8
1	H	79	LEU	3.8
2	L	176	LEU	3.8
1	H	116	LEU	3.7
1	H	209	LYS	3.7
1	H	10	GLY	3.7
2	L	121	PRO	3.6
1	H	53	TYR	3.6
2	L	167	GLN	3.6
2	L	155	LEU	3.6
1	H	174	PHE	3.6
1	H	5	VAL	3.6
2	L	179	THR	3.6
1	H	169	SER	3.5
1	H	36	TRP	3.5
2	L	114	PRO	3.5
1	H	186	LEU	3.4
2	L	131	ALA	3.4
2	L	64	GLY	3.4
2	L	62	PHE	3.4
2	L	103	THR	3.4
1	H	155	PRO	3.4
1	H	211	SER	3.3
1	H	118	THR	3.3
2	L	138	ASN	3.3
1	H	128	SER	3.3
2	L	80	PRO	3.3
2	L	110	THR	3.3
2	L	140	PHE	3.3
1	H	2	VAL	3.3
2	L	201	GLY	3.2
3	E	523	THR	3.2
1	H	50	VAL	3.2
1	H	178	LEU	3.1
2	L	31	SER	3.1
1	H	37	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	126	LEU	3.1
1	H	95	TYR	3.1
3	E	517	LEU	3.0
1	H	156	GLU	3.0
1	H	147	GLY	3.0
2	L	177	SER	3.0
1	H	117	VAL	3.0
4	A	220	LYS	2.9
2	L	8	PRO	2.9
2	L	18	ARG	2.9
2	L	84	ALA	2.9
2	L	148	GLN	2.9
2	L	169	SER	2.9
2	L	46	LEU	2.9
1	H	87	ARG	2.9
1	H	20	LEU	2.9
1	H	73	ASP	2.8
1	H	69	THR	2.8
2	L	94	THR	2.8
1	H	96	CYS	2.8
5	B	194	CYS	2.8
2	L	199	HIS	2.8
2	L	13	ALA	2.8
2	L	43	ALA	2.8
1	H	152	ASP	2.8
1	H	18	LEU	2.7
2	L	56	SER	2.7
4	A	48	VAL	2.7
2	L	24	ARG	2.7
1	H	40	ALA	2.7
1	H	66	GLY	2.7
1	H	41	PRO	2.7
1	H	217	LYS	2.7
2	L	113	ALA	2.6
1	H	184	TYR	2.6
3	E	360	ASN	2.6
1	H	34	MET	2.6
2	L	3	GLN	2.6
4	A	140	GLY	2.6
1	H	104	TRP	2.6
1	H	70	ILE	2.6
2	L	168	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	180	SER	2.5
1	H	114	GLY	2.5
1	H	59	TYR	2.5
1	H	83	MET	2.5
4	A	115	VAL	2.5
2	L	85	THR	2.5
1	H	82	GLN	2.5
1	H	74	ASN	2.5
1	H	214	LYS	2.5
1	H	16	ARG	2.5
1	H	21	SER	2.5
1	H	197	LEU	2.5
3	E	370	ASN	2.5
2	L	15	VAL	2.4
2	L	71	PHE	2.4
3	E	374	PHE	2.4
2	L	196	GLU	2.4
1	H	106	TYR	2.4
3	E	365	TYR	2.4
3	E	377	PHE	2.4
1	H	3	GLN	2.4
1	H	32	TYR	2.4
1	H	145	ALA	2.4
2	L	14	SER	2.3
5	B	181	LEU	2.3
3	E	489	TYR	2.3
2	L	166	GLU	2.3
2	L	63	SER	2.3
3	E	511	VAL	2.3
1	H	13	GLN	2.3
1	H	183	LEU	2.3
4	A	147	LEU	2.3
4	A	195	LEU	2.3
1	H	8	GLY	2.3
3	E	495	TYR	2.3
5	B	23	CYS	2.3
4	A	197	THR	2.3
3	E	383	SER	2.3
2	L	124	GLU	2.3
3	E	364	ASP	2.3
4	A	51	ILE	2.3
3	E	461	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	18	LEU	2.3
1	H	100	GLY	2.3
2	L	41	GLY	2.3
2	L	144	GLU	2.3
4	A	134	SER	2.3
1	H	154	PHE	2.2
3	E	513	LEU	2.2
5	B	47	LEU	2.2
5	B	48	LEU	2.2
1	H	9	GLY	2.2
2	L	211	ASN	2.2
2	L	51	ALA	2.2
4	A	80	LEU	2.2
4	A	156	VAL	2.2
4	A	27	LEU	2.2
3	E	342	PHE	2.2
3	E	522	ALA	2.2
4	A	146	CYS	2.2
1	H	55	GLY	2.2
2	L	109	ARG	2.2
2	L	97	LEU	2.2
4	A	63	VAL	2.2
2	L	60	SER	2.1
2	L	72	THR	2.1
2	L	83	PHE	2.1
3	E	515	PHE	2.1
4	A	58	PHE	2.1
1	H	185	SER	2.1
2	L	7	SER	2.1
2	L	157	SER	2.1
3	E	341	VAL	2.1
3	E	478	THR	2.1
2	L	54	LEU	2.1
3	E	436	TRP	2.1
4	A	59	TYR	2.1
3	E	486	PHE	2.1
4	A	117	VAL	2.1
1	H	15	GLY	2.1
3	E	428	ASP	2.1
3	E	421	TYR	2.1
5	B	87	TYR	2.1
3	E	353	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	113	GLN	2.1
1	H	172	HIS	2.1
2	L	48	ILE	2.1
1	H	86	LEU	2.1
4	A	86	GLY	2.1
2	L	143	ARG	2.0
1	H	94	TYR	2.0
3	E	338	PHE	2.0
4	A	105	TRP	2.0
2	L	42	LYS	2.0
1	H	25	SER	2.0
2	L	146	LYS	2.0
5	B	133	VAL	2.0
4	A	96	ALA	2.0
5	B	213	GLU	2.0
4	A	47	TRP	2.0
4	A	12	ILE	2.0
3	E	366	SER	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SO4	B	310	5/5	0.53	0.44	87,87,93,110	0
9	SO4	E	905	5/5	0.56	0.34	110,112,116,117	0
6	NAG	E	901	14/15	0.67	0.33	93,104,109,111	0
7	GOL	A	1201	6/6	0.67	0.28	44,45,63,65	0
9	SO4	A	1211	5/5	0.70	0.45	64,76,79,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	PEG	E	903	7/7	0.77	0.31	36,65,70,75	0
9	SO4	B	312	5/5	0.80	0.51	74,80,91,98	0
9	SO4	B	305	5/5	0.81	0.23	47,57,75,80	0
9	SO4	B	308	5/5	0.81	0.42	49,67,86,89	0
7	GOL	E	902	6/6	0.83	0.18	52,57,61,66	0
8	PEG	A	1204	7/7	0.83	0.25	51,62,67,75	0
10	CIT	A	1202	13/13	0.84	0.21	43,57,64,70	0
8	PEG	A	1206	7/7	0.86	0.32	45,56,65,66	0
8	PEG	A	1203	7/7	0.87	0.39	46,55,69,73	0
7	GOL	A	1205	6/6	0.87	0.15	39,62,72,74	0
11	CL	B	301	1/1	0.89	0.11	54,54,54,54	0
11	CL	A	1209	1/1	0.90	0.19	60,60,60,60	0
9	SO4	B	309	5/5	0.91	0.41	65,71,75,84	0
9	SO4	B	307	5/5	0.91	0.20	57,64,77,78	0
9	SO4	B	306	5/5	0.91	0.36	61,78,83,91	0
9	SO4	E	904	5/5	0.92	0.28	51,56,75,80	0
9	SO4	B	311	5/5	0.92	0.39	46,48,73,75	0
11	CL	B	303	1/1	0.92	0.06	59,59,59,59	0
11	CL	B	302	1/1	0.93	0.20	64,64,64,64	0
9	SO4	A	1210	5/5	0.95	0.12	38,43,50,52	0
11	CL	A	1207	1/1	0.95	0.18	69,69,69,69	0
11	CL	B	304	1/1	0.95	0.14	58,58,58,58	0
11	CL	A	1208	1/1	0.97	0.09	37,37,37,37	0

## 6.5 Other polymers

There are no such residues in this entry.