



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:29 PM UTC

PDB ID : 7NX8 / pdb_00007nx8
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

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

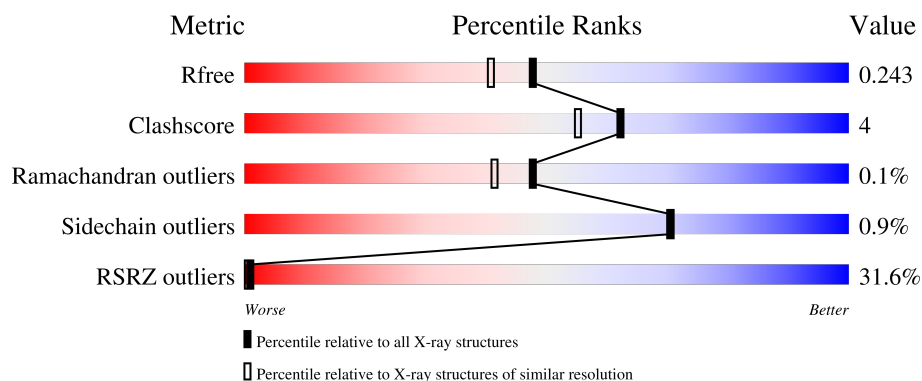
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 ≥ 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	65% 80% 15% 5%
2	L	215	58% 87% 12% .
3	E	205	17% 89% 6% 5%
4	A	224	6% 88% 8% .
5	B	214	5% 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
9	SO4	B	310	-	-	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

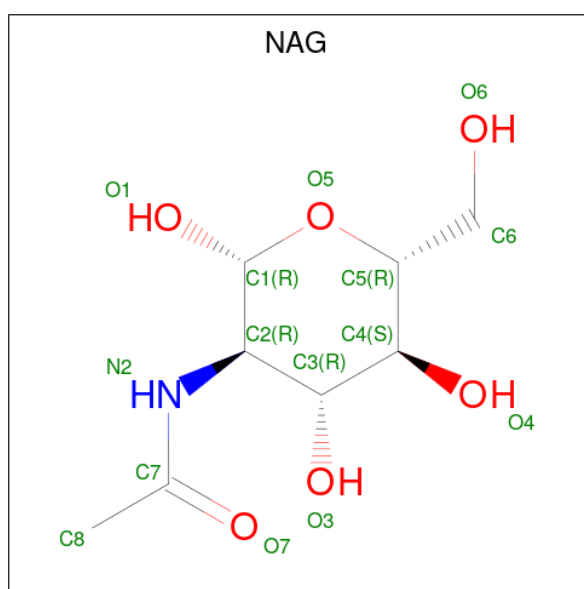
- Molecule 4 is a protein called COVOX-222 Fab heavy chain.

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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



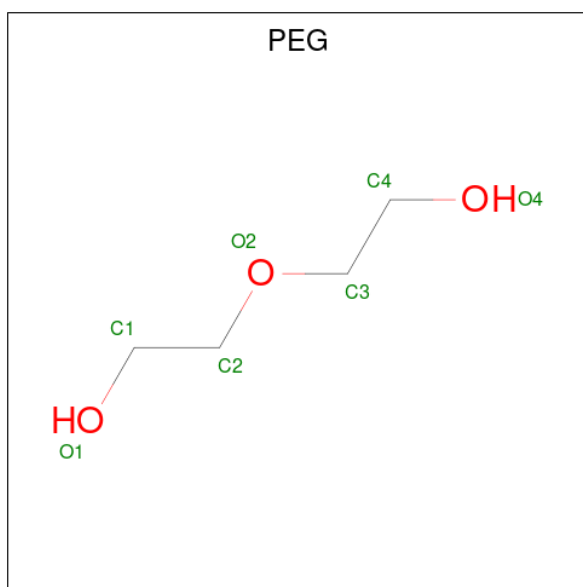
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 7 is GLYCEROL (CCD ID: 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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



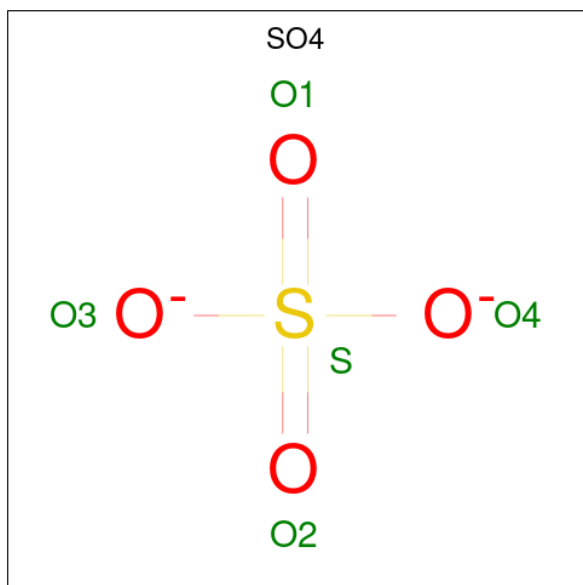
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

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 (CCD ID: SO4) (formula: O₄S).



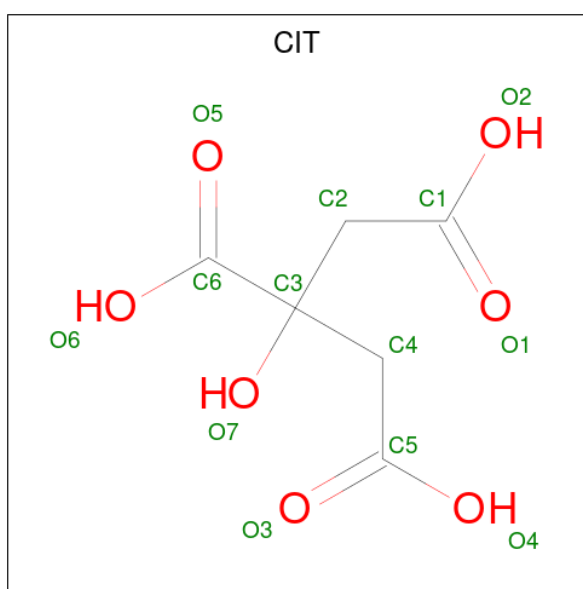
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: 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		

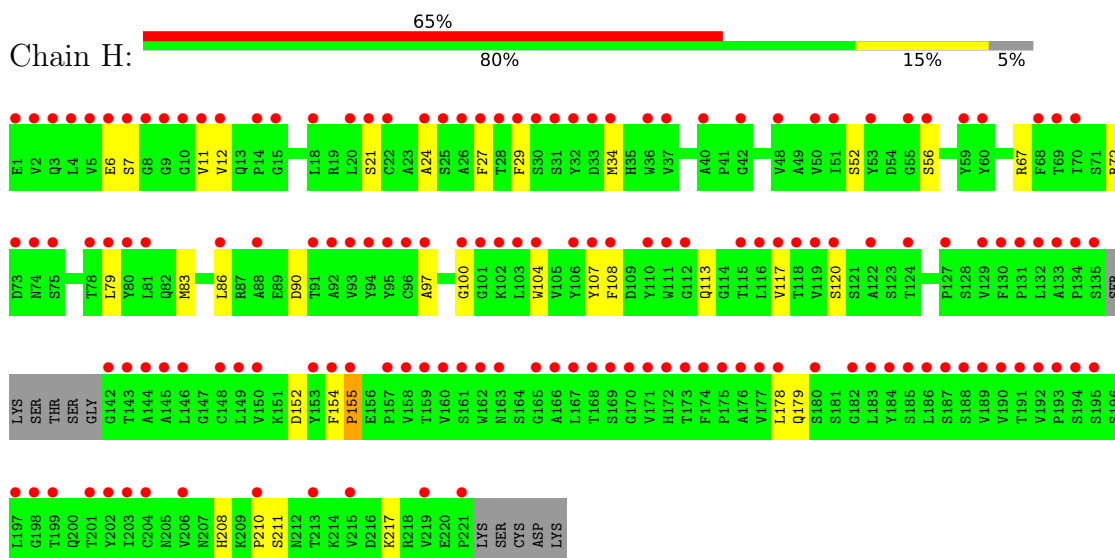
- Molecule 12 is water.

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

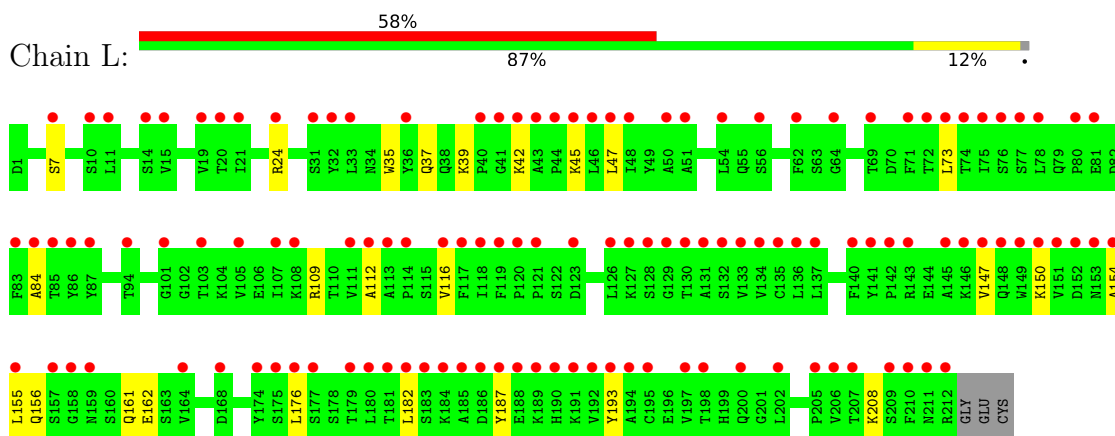
3 Residue-property plots [i](#)

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.

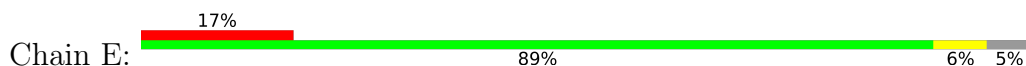
- Molecule 1: EY6A Fab heavy chain

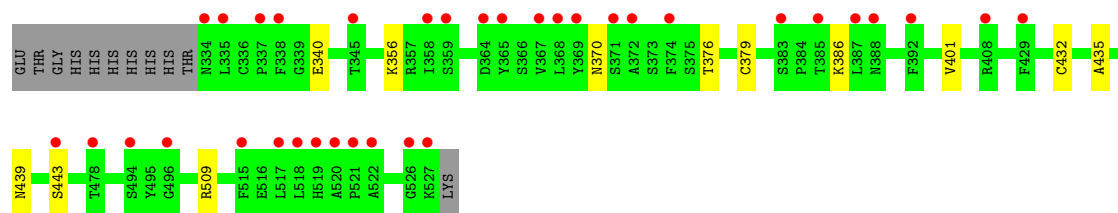


- Molecule 2: EY6A Fab light chain

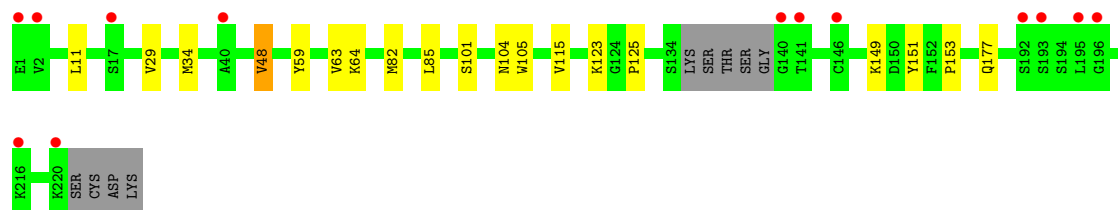
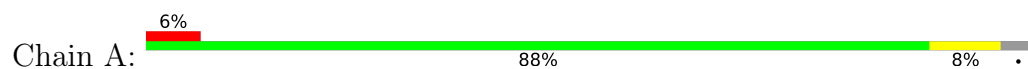


- Molecule 3: Spike protein S1

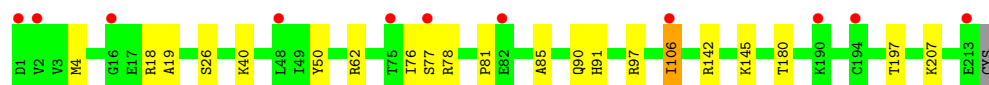
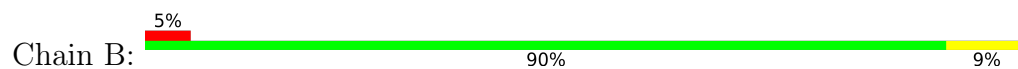




● Molecule 4: COVOX-222 Fab heavy chain



● 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	54.84Å 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
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.223 , 0.246 0.229 , 0.243	Depositor DCC
R_{free} test set	5265 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: PEG, CL, SO4, GOL, CIT, 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	H	0.08	0/1679	0.24	0/2288
2	L	0.08	0/1651	0.26	0/2241
3	E	0.07	0/1586	0.25	0/2159
4	A	0.09	0/1621	0.29	0/2211
5	B	0.09	0/1677	0.28	0/2279
All	All	0.08	0/8214	0.26	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	20	0
2	L	1618	0	1582	13	0
3	E	1540	0	1454	7	0
4	A	1583	0	1539	11	0
5	B	1637	0	1590	16	0
6	E	14	0	13	0	0
7	A	12	0	16	0	0
7	E	6	0	8	0	0

Continued on next page...

Continued from previous page...

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	1	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	65	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 (65) 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
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
4:A:59:TYR:O	4:A:64:LYS:NZ	2.38	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:208:HIS:ND1	1:H:211:SER:OG	2.38	0.54
1:H:97:ALA:HB1	1:H:108:PHE:HB3	1.91	0.53
4:A:149:LYS:NZ	4:A:177:GLN:OE1	2.42	0.52
1:H:67:ARG:NH1	1:H:90:ASP:OD2	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:207:LYS:NZ	12:B:406:HOH:O	2.47	0.46
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
4:A:82:MET:HE1	4:A:115:VAL:HG21	1.97	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:439:ASN:O	3:E:443:SER:OG	2.30	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
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:83:MET:HE1	1:H:117:VAL:HG21	2.02	0.41
1:H:6:GLU:H	1:H:113:GLN:NE2	2.16	0.41
4:A:101:SER:OG	4:A:104:ASN:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:40:LYS:HG2	5:B:85:ALA:HB2	2.03	0.41
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%)	24	16
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%)	48	41

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%)	178 (98%)	3 (2%)	53	49
2	L	186/188 (99%)	183 (98%)	3 (2%)	55	52
3	E	167/177 (94%)	167 (100%)	0	100	100
4	A	177/186 (95%)	176 (99%)	1 (1%)	78	79
5	B	185/185 (100%)	184 (100%)	1 (0%)	81	82
All	All	896/927 (97%)	888 (99%)	8 (1%)	70	70

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

Mol	Chain	Res	Type
1	H	11	VAL
1	H	178	LEU
1	H	217	LYS
2	L	45	LYS
2	L	161	GLN
2	L	182	LEU
4	A	48	VAL
5	B	106	ILE

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	360	ASN
3	E	370	ASN
3	E	388	ASN
3	E	481	ASN
5	B	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 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	$\# Z > 2$
9	SO4	B	305	-	4,4,4	0.23	0	6,6,6	0.06	0
9	SO4	A	1210	-	4,4,4	0.23	0	6,6,6	0.05	0
9	SO4	E	905	-	4,4,4	0.24	0	6,6,6	0.08	0
9	SO4	A	1211	-	4,4,4	0.24	0	6,6,6	0.08	0
9	SO4	B	308	-	4,4,4	0.23	0	6,6,6	0.09	0
9	SO4	B	310	-	4,4,4	0.23	0	6,6,6	0.09	0
9	SO4	B	311	-	4,4,4	0.24	0	6,6,6	0.09	0
9	SO4	B	307	-	4,4,4	0.24	0	6,6,6	0.07	0
7	GOL	E	902	-	5,5,5	0.95	0	5,5,5	1.06	0
8	PEG	A	1204	-	6,6,6	0.11	0	5,5,5	0.09	0
9	SO4	B	312	-	4,4,4	0.24	0	6,6,6	0.08	0
8	PEG	A	1203	-	6,6,6	0.09	0	5,5,5	0.11	0
10	CIT	A	1202	-	12,12,12	1.08	0	17,17,17	1.53	3 (17%)
6	NAG	E	901	3	14,14,15	0.42	0	17,19,21	0.55	0
9	SO4	B	306	-	4,4,4	0.23	0	6,6,6	0.08	0
8	PEG	A	1206	-	6,6,6	0.12	0	5,5,5	0.09	0
8	PEG	E	903	-	6,6,6	0.11	0	5,5,5	0.09	0
7	GOL	A	1205	-	5,5,5	0.96	0	5,5,5	1.03	0
9	SO4	E	904	-	4,4,4	0.23	0	6,6,6	0.08	0
9	SO4	B	309	-	4,4,4	0.23	0	6,6,6	0.08	0
7	GOL	A	1201	-	5,5,5	0.95	0	5,5,5	1.04	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	E	902	-	-	2/4/4/4	-
8	PEG	E	903	-	-	2/4/4/4	-
8	PEG	A	1204	-	-	0/4/4/4	-
7	GOL	A	1205	-	-	2/4/4/4	-
8	PEG	A	1203	-	-	3/4/4/4	-
10	CIT	A	1202	-	-	5/16/16/16	-
6	NAG	E	901	3	-	1/6/23/26	0/1/1/1
8	PEG	A	1206	-	-	3/4/4/4	-
7	GOL	A	1201	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1202	CIT	O6-C6-C3	3.89	120.60	113.14
10	A	1202	CIT	O4-C5-C4	2.13	121.10	114.35
10	A	1202	CIT	O2-C1-O1	-2.02	118.12	123.33

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
7	E	902	GOL	O1-C1-C2-C3
7	A	1205	GOL	O1-C1-C2-C3
8	E	903	PEG	O2-C3-C4-O4
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	1206	PEG	O1-C1-C2-O2
8	A	1203	PEG	O2-C3-C4-O4
10	A	1202	CIT	C2-C3-C4-C5
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-O6
8	A	1206	PEG	C1-C2-O2-C3
8	A	1206	PEG	O2-C3-C4-O4
10	A	1202	CIT	C2-C3-C6-O5

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	310	SO4	3	0
9	B	312	SO4	1	0
8	A	1203	PEG	1	0
8	A	1206	PEG	1	0
9	B	309	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, 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	215/226 (95%)	2.71	147 (68%) 0 0	64, 127, 184, 210	0
2	L	212/215 (98%)	2.41	125 (58%) 0 0	49, 99, 172, 214	0
3	E	194/205 (94%)	1.16	35 (18%) 3 3	23, 48, 100, 130	1 (0%)
4	A	215/224 (95%)	0.76	13 (6%) 27 32	30, 41, 66, 122	0
5	B	213/214 (99%)	0.75	11 (5%) 33 38	26, 44, 61, 89	1 (0%)
All	All	1049/1084 (96%)	1.56	331 (31%) 1 0	23, 57, 164, 214	2 (0%)

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	369	TYR	7.8
1	H	160	VAL	6.7
2	L	145	ALA	6.6
2	L	192	VAL	6.2
1	H	187	SER	5.9
2	L	210	PHE	5.8
2	L	187	TYR	5.7
1	H	192	VAL	5.7
2	L	133	VAL	5.7
1	H	135	SER	5.5
1	H	215	VAL	5.4
2	L	126	LEU	5.4
1	H	97	ALA	5.3
3	E	368	LEU	5.3
2	L	193	TYR	5.2
1	H	167	LEU	5.2
2	L	134	VAL	5.1
2	L	184	LYS	5.0
2	L	120	PRO	5.0
1	H	159	THR	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	144	ALA	4.9
1	H	173	THR	4.9
2	L	185	ALA	4.9
1	H	197	LEU	4.8
2	L	206	VAL	4.8
1	H	219	VAL	4.8
1	H	28	THR	4.7
2	L	118	ILE	4.7
3	E	335	LEU	4.7
1	H	134	PRO	4.7
2	L	136	LEU	4.7
1	H	130	PHE	4.6
1	H	158	VAL	4.6
2	L	137	LEU	4.6
2	L	87	TYR	4.6
1	H	162	TRP	4.6
1	H	142	GLY	4.5
1	H	30	SER	4.5
2	L	31	SER	4.5
4	A	220	LYS	4.5
1	H	149	LEU	4.5
3	E	367	VAL	4.4
1	H	27	PHE	4.4
2	L	155	LEU	4.3
2	L	198	THR	4.3
3	E	527	LYS	4.3
2	L	202	LEU	4.2
2	L	164	VAL	4.2
2	L	117	PHE	4.2
1	H	133	ALA	4.1
1	H	81	LEU	4.1
2	L	54	LEU	4.1
1	H	111	TRP	4.1
2	L	195	CYS	4.1
1	H	177	VAL	4.1
1	H	110	TYR	4.1
1	H	116	LEU	4.0
1	H	26	ALA	4.0
1	H	37	VAL	4.0
3	E	522	ALA	4.0
1	H	31	SER	4.0
1	H	2	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	11	VAL	4.0
1	H	127	PRO	4.0
1	H	131	PRO	4.0
2	L	119	PHE	4.0
1	H	80	TYR	3.9
1	H	96	CYS	3.9
1	H	93	VAL	3.9
2	L	197	VAL	3.9
1	H	186	LEU	3.9
1	H	5	VAL	3.9
1	H	168	THR	3.8
1	H	68	PHE	3.8
2	L	20	THR	3.8
2	L	132	SER	3.8
1	H	221	PRO	3.8
2	L	75	ILE	3.8
1	H	79	LEU	3.7
2	L	19	VAL	3.7
2	L	62	PHE	3.7
1	H	4	LEU	3.7
4	A	195	LEU	3.7
1	H	203	ILE	3.7
1	H	143	THR	3.7
2	L	154	ALA	3.6
2	L	86	TYR	3.6
1	H	206	VAL	3.6
2	L	130	THR	3.6
1	H	161	SER	3.6
2	L	113	ALA	3.6
1	H	69	THR	3.6
2	L	24	ARG	3.6
1	H	18	LEU	3.6
1	H	118	THR	3.5
2	L	72	THR	3.5
4	A	141	THR	3.5
3	E	478	THR	3.5
1	H	190	VAL	3.5
2	L	77	SER	3.5
1	H	150	VAL	3.5
2	L	116	VAL	3.5
1	H	174	PHE	3.5
2	L	194	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	180	SER	3.4
1	H	193	PRO	3.4
1	H	95	TYR	3.4
2	L	21	ILE	3.4
2	L	107	ILE	3.4
2	L	127	LYS	3.4
2	L	131	ALA	3.4
1	H	146	LEU	3.4
3	E	496	GLY	3.4
2	L	212	ARG	3.4
3	E	521	PRO	3.4
2	L	135	CYS	3.3
1	H	171	VAL	3.3
1	H	40	ALA	3.3
1	H	132	LEU	3.3
2	L	108	LYS	3.3
3	E	337	PRO	3.3
1	H	154	PHE	3.3
3	E	383	SER	3.3
1	H	20	LEU	3.2
1	H	199	THR	3.2
1	H	53	TYR	3.2
1	H	148	CYS	3.2
1	H	24	ALA	3.2
1	H	32	TYR	3.2
1	H	78	THR	3.2
1	H	213	THR	3.2
2	L	182	LEU	3.2
1	H	36	TRP	3.1
1	H	166	ALA	3.1
2	L	121	PRO	3.1
2	L	142	PRO	3.1
1	H	178	LEU	3.1
1	H	117	VAL	3.1
1	H	210	PRO	3.1
3	E	520	ALA	3.1
4	A	193	SER	3.1
1	H	7	SER	3.1
2	L	43	ALA	3.1
2	L	176	LEU	3.0
2	L	147	VAL	3.0
2	L	94	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	191	LYS	3.0
2	L	44	PRO	3.0
2	L	84	ALA	3.0
2	L	48	ILE	3.0
1	H	86	LEU	2.9
1	H	185	SER	2.9
2	L	179	THR	2.9
1	H	1	GLU	2.9
2	L	149	TRP	2.9
2	L	33	LEU	2.9
3	E	518	LEU	2.9
1	H	189	VAL	2.9
2	L	181	THR	2.9
1	H	22	CYS	2.9
1	H	55	GLY	2.9
2	L	140	PHE	2.9
1	H	70	ILE	2.9
1	H	100	GLY	2.9
4	A	140	GLY	2.9
2	L	103	THR	2.8
3	E	334	ASN	2.8
2	L	151	VAL	2.8
1	H	157	PRO	2.8
1	H	184	TYR	2.8
1	H	88	ALA	2.8
1	H	101	GLY	2.8
2	L	159	ASN	2.8
2	L	148	GLN	2.8
1	H	129	VAL	2.8
1	H	92	ALA	2.8
2	L	211	ASN	2.8
1	H	42	GLY	2.8
2	L	158	GLY	2.8
1	H	91	THR	2.8
2	L	150	LYS	2.8
5	B	190	LYS	2.8
2	L	141	TYR	2.8
1	H	188	SER	2.8
1	H	195	SER	2.8
1	H	3	GLN	2.8
1	H	165	GLY	2.8
1	H	170	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	75	SER	2.7
4	A	2	VAL	2.7
2	L	45	LYS	2.7
3	E	372	ALA	2.7
4	A	146	CYS	2.7
1	H	119	VAL	2.7
2	L	105	VAL	2.7
2	L	111	VAL	2.7
1	H	106	TYR	2.7
2	L	69	THR	2.7
1	H	183	LEU	2.7
2	L	14	SER	2.7
4	A	17	SER	2.7
2	L	50	ALA	2.6
1	H	108	PHE	2.6
2	L	209	SER	2.6
2	L	205	PRO	2.6
1	H	103	LEU	2.6
1	H	198	GLY	2.6
2	L	112	ALA	2.6
2	L	143	ARG	2.6
2	L	188	GLU	2.6
4	A	1	GLU	2.6
5	B	106	ILE	2.6
1	H	34	MET	2.6
2	L	64	GLY	2.6
1	H	50	VAL	2.6
1	H	122	ALA	2.6
2	L	175	SER	2.6
2	L	46	LEU	2.6
2	L	80	PRO	2.5
1	H	29	PHE	2.5
2	L	83	PHE	2.5
3	E	374	PHE	2.5
2	L	78	LEU	2.5
1	H	21	SER	2.5
3	E	494	SER	2.5
5	B	213	GLU	2.5
1	H	94	TYR	2.5
2	L	189	LYS	2.5
1	H	74	ASN	2.5
1	H	194	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	40	PRO	2.5
2	L	47	LEU	2.5
2	L	153	ASN	2.5
1	H	6	GLU	2.5
1	H	155	PRO	2.5
1	H	8	GLY	2.4
1	H	112	GLY	2.4
3	E	365	TYR	2.4
3	E	517	LEU	2.4
1	H	169	SER	2.4
2	L	128	SER	2.4
3	E	358	ILE	2.4
2	L	74	THR	2.4
2	L	123	ASP	2.4
2	L	186	ASP	2.4
1	H	10	GLY	2.4
1	H	59	TYR	2.4
2	L	73	LEU	2.4
3	E	392	PHE	2.4
2	L	146	LYS	2.4
1	H	124	THR	2.4
2	L	207	THR	2.4
1	H	145	ALA	2.4
1	H	9	GLY	2.4
2	L	129	GLY	2.4
1	H	204	CYS	2.4
3	E	345	THR	2.4
1	H	172	HIS	2.4
2	L	76	SER	2.4
1	H	102	LYS	2.4
5	B	194	CYS	2.4
5	B	75	THR	2.3
3	E	388	ASN	2.3
1	H	182	GLY	2.3
1	H	12	VAL	2.3
1	H	25	SER	2.3
1	H	33	ASP	2.3
5	B	82	GLU	2.3
3	E	387	LEU	2.3
1	H	176	ALA	2.3
2	L	51	ALA	2.3
2	L	41	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	85	THR	2.3
3	E	515	PHE	2.3
2	L	157	SER	2.3
3	E	364	ASP	2.3
1	H	191	THR	2.3
2	L	42	LYS	2.3
1	H	104	TRP	2.2
2	L	114	PRO	2.2
4	A	196	GLY	2.2
3	E	443	SER	2.2
2	L	168	ASP	2.2
5	B	2	VAL	2.2
1	H	163	ASN	2.2
5	B	48	LEU	2.2
2	L	10	SER	2.2
2	L	101	GLY	2.2
3	E	371	SER	2.2
2	L	32	TYR	2.2
2	L	71	PHE	2.2
2	L	190	HIS	2.2
2	L	180	LEU	2.2
1	H	73	ASP	2.2
1	H	120	SER	2.2
1	H	202	TYR	2.2
2	L	174	TYR	2.2
2	L	15	VAL	2.2
3	E	385	THR	2.2
1	H	15	GLY	2.2
2	L	11	LEU	2.2
1	H	48	VAL	2.1
1	H	115	THR	2.1
2	L	152	ASP	2.1
2	L	56	SER	2.1
1	H	14	PRO	2.1
1	H	175	PRO	2.1
4	A	216	LYS	2.1
4	A	40	ALA	2.1
2	L	200	GLN	2.1
2	L	177	SER	2.1
2	L	183	SER	2.1
5	B	16	GLY	2.1
2	L	81	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	519	HIS	2.1
3	E	429	PHE	2.1
1	H	60	TYR	2.1
1	H	107	TYR	2.1
1	H	56	SER	2.1
5	B	77	SER	2.1
3	E	338	PHE	2.0
3	E	359	SER	2.0
2	L	36	TYR	2.0
3	E	526	GLY	2.0
5	B	1	ASP	2.0
2	L	7	SER	2.0
4	A	192	SER	2.0
1	H	51	ILE	2.0
1	H	201	THR	2.0
1	H	153	TYR	2.0
3	E	408	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 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SO4	B	312	5/5	0.41	0.18	74,80,91,98	0
9	SO4	E	905	5/5	0.47	0.16	110,112,116,117	0
6	NAG	E	901	14/15	0.51	0.17	93,104,109,111	0
9	SO4	A	1211	5/5	0.54	0.17	64,76,79,104	0
9	SO4	B	310	5/5	0.57	0.13	87,87,93,110	0
9	SO4	B	305	5/5	0.59	0.19	47,57,75,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SO4	B	308	5/5	0.63	0.17	49,67,86,89	0
9	SO4	B	309	5/5	0.64	0.14	65,71,75,84	0
7	GOL	A	1201	6/6	0.69	0.22	44,45,63,65	0
8	PEG	E	903	7/7	0.71	0.25	36,65,70,75	0
9	SO4	B	307	5/5	0.73	0.13	57,64,77,78	0
8	PEG	A	1203	7/7	0.75	0.21	46,55,69,73	0
8	PEG	A	1204	7/7	0.75	0.17	51,62,67,75	0
9	SO4	B	306	5/5	0.77	0.14	61,78,83,91	0
9	SO4	E	904	5/5	0.77	0.12	51,56,75,80	0
9	SO4	B	311	5/5	0.81	0.12	46,48,73,75	0
8	PEG	A	1206	7/7	0.82	0.19	45,56,65,66	0
7	GOL	E	902	6/6	0.84	0.14	52,57,61,66	0
10	CIT	A	1202	13/13	0.86	0.13	43,57,64,70	0
11	CL	A	1207	1/1	0.89	0.20	69,69,69,69	0
11	CL	B	303	1/1	0.90	0.13	59,59,59,59	0
11	CL	B	302	1/1	0.91	0.30	64,64,64,64	0
7	GOL	A	1205	6/6	0.91	0.12	39,62,72,74	0
11	CL	A	1209	1/1	0.92	0.29	60,60,60,60	0
11	CL	B	301	1/1	0.93	0.13	54,54,54,54	0
9	SO4	A	1210	5/5	0.95	0.09	38,43,50,52	0
11	CL	B	304	1/1	0.96	0.14	58,58,58,58	0
11	CL	A	1208	1/1	0.97	0.17	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.