



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:05 AM UTC

PDB ID : 7EDD / pdb\_00007edd  
Title : Crystal structure of a serine protease from Streptococcus pyogenes  
Authors : Jobichen, C.; Sivaraman, J.  
Deposited on : 2021-03-15  
Resolution : 2.90 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 : 4-5-2 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

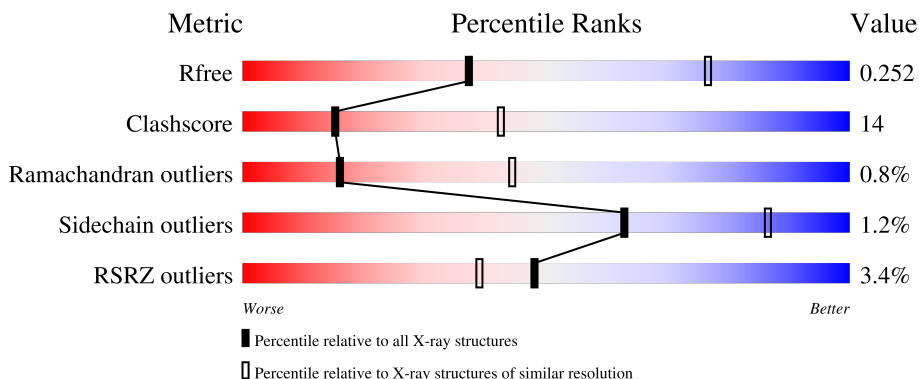
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	1519	

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
3	CA	A	1711	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1714	-	X	-	-
7	CL	A	1720	-	-	X	-
7	CL	A	1721	-	-	X	-

## 2 Entry composition [i](#)

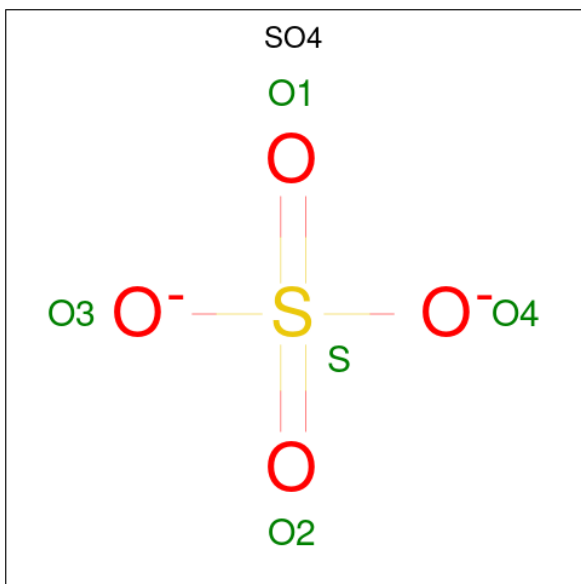
There are 8 unique types of molecules in this entry. The entry contains 10868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 C5a peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	1394	10731	6749	1835	2121	26	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total Ca 10 10	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

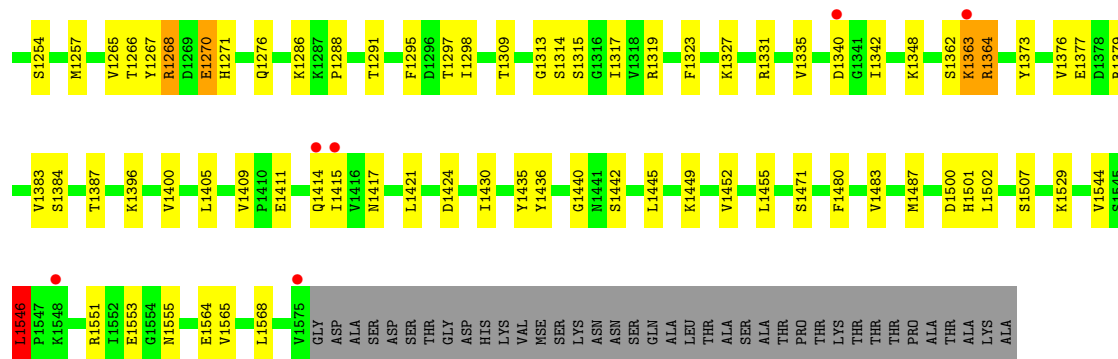
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	72	Total O 72 72	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.97Å 191.97Å 252.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 2.90 48.37 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.37-2.90) 99.0 (48.37-2.90)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.195 , 0.255 0.199 , 0.252	Depositor DCC
$R_{free}$ test set	3004 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: CA, PEG, MG, GOL, CL, 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	A	0.72	0/10917	0.96	22/14747 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	THR	N-CA-C	-10.04	101.02	113.38
1	A	403	GLY	N-CA-C	9.18	122.10	111.36
1	A	1032	THR	N-CA-C	-8.09	103.44	113.38
1	A	403	GLY	CA-C-N	6.77	128.12	120.06
1	A	403	GLY	C-N-CA	6.77	128.12	120.06
1	A	473	THR	N-CA-C	-6.24	103.66	108.78
1	A	474	ASP	N-CA-C	-6.23	104.89	113.18
1	A	473	THR	CB-CA-C	-6.04	108.37	117.07
1	A	382	GLU	CA-C-N	5.93	132.86	121.54
1	A	382	GLU	C-N-CA	5.93	132.86	121.54
1	A	1014	MSE	N-CA-C	5.86	119.06	108.69
1	A	402	VAL	CA-C-N	5.83	125.51	119.92
1	A	402	VAL	C-N-CA	5.83	125.51	119.92
1	A	710	MSE	N-CA-C	5.72	117.61	108.41
1	A	1030	PRO	N-CA-C	5.67	124.16	112.47
1	A	1270	GLU	N-CA-C	-5.58	101.11	109.15
1	A	321	MSE	N-CA-C	5.50	120.05	113.23
1	A	407	THR	CB-CA-C	-5.25	100.51	109.65
1	A	1270	GLU	CA-C-O	-5.24	114.38	120.62
1	A	655	MSE	N-CA-C	5.13	116.69	111.14
1	A	403	GLY	CA-C-O	-5.11	116.91	121.41
1	A	1546	LEU	N-CA-C	5.09	121.07	109.81

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10731	0	10467	284	0
2	A	15	0	0	1	0
3	A	10	0	0	0	0
4	A	30	0	39	4	0
5	A	1	0	0	1	0
6	A	7	0	10	0	0
7	A	2	0	0	6	0
8	A	72	0	0	6	0
All	All	10868	0	10516	290	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 14.

All (290) 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)
7:A:1720:CL:CL	8:A:1869:HOH:O	2.04	1.12
7:A:1720:CL:CL	8:A:1867:HOH:O	2.15	0.99
1:A:378:ALA:HB1	1:A:616:THR:HG23	1.40	0.98
1:A:1363:LYS:HG3	1:A:1364:ARG:H	1.28	0.98
1:A:349:THR:HB	1:A:404:SER:HB2	1.48	0.96
1:A:407:THR:HG22	1:A:585:THR:HG22	1.48	0.96
1:A:1268:ARG:HH11	1:A:1268:ARG:HG3	1.31	0.94
7:A:1721:CL:CL	8:A:1871:HOH:O	2.23	0.92
5:A:1718:MG:MG	7:A:1720:CL:CL	1.48	0.92
1:A:1223:HIS:ND1	1:A:1224:GLN:OE1	2.07	0.88
1:A:318:ASN:H	1:A:321:MSE:HE3	1.39	0.87
1:A:380:GLY:H	1:A:616:THR:HG21	1.38	0.87
1:A:869:ASN:HD22	1:A:874:THR:HG22	1.40	0.86
1:A:479:ALA:HB2	1:A:507:HIS:CD2	2.12	0.84
1:A:428:THR:HG22	1:A:442:LYS:HG2	1.59	0.84
1:A:1241:ILE:O	1:A:1244:THR:HG22	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ALA:HB2	1:A:507:HIS:HD2	1.44	0.83
1:A:1131:THR:OG1	1:A:1132:PRO:HD2	1.80	0.82
1:A:653:LEU:HD23	1:A:691:TYR:HB3	1.64	0.80
1:A:501:ILE:HG12	1:A:540:ILE:HG21	1.65	0.78
1:A:1101:LEU:HD23	1:A:1124:LEU:HD11	1.65	0.77
1:A:1143:GLN:HG3	4:A:1714:GOL:H11	1.67	0.77
1:A:1268:ARG:HG3	1:A:1268:ARG:NH1	2.00	0.77
1:A:394:ALA:HA	1:A:744:PHE:CE2	2.21	0.76
1:A:318:ASN:N	1:A:321:MSE:HE3	2.02	0.75
1:A:720:SER:HB2	1:A:722:LYS:HD3	1.68	0.74
1:A:311:MSE:HE3	1:A:340:ALA:HB2	1.69	0.74
1:A:406:SER:O	1:A:413:SER:HB2	1.87	0.73
1:A:693:THR:HG23	1:A:697:ASN:HA	1.70	0.72
1:A:721:ASN:OD1	1:A:764:ASN:ND2	2.22	0.71
1:A:349:THR:HB	1:A:404:SER:CB	2.21	0.71
1:A:959:ASN:HD21	1:A:970:THR:HG23	1.55	0.71
7:A:1720:CL:CL	8:A:1872:HOH:O	2.45	0.70
1:A:1186:ASP:OD1	1:A:1379:ARG:NH1	2.25	0.70
1:A:473:THR:O	1:A:503:LEU:HD21	1.92	0.69
1:A:617:SER:OG	2:A:1701:SO4:O1	2.10	0.68
1:A:383:ARG:HD2	1:A:578:HIS:O	1.94	0.68
1:A:633:TYR:O	1:A:637:THR:HG22	1.93	0.68
1:A:496:THR:HG23	1:A:499:GLU:H	1.59	0.68
1:A:526:MSE:HE3	1:A:540:ILE:HD13	1.75	0.68
1:A:482:VAL:CB	1:A:507:HIS:O	2.42	0.67
1:A:643:LYS:O	1:A:646:ILE:HG22	1.96	0.66
7:A:1720:CL:CL	7:A:1721:CL:CL	2.87	0.66
1:A:400:GLY:CA	1:A:583:GLY:HA3	2.25	0.66
1:A:1377:GLU:HG3	1:A:1383:VAL:HG22	1.78	0.65
1:A:407:THR:HG22	1:A:585:THR:CG2	2.26	0.65
1:A:504:ALA:C	1:A:509:ALA:HB2	2.22	0.65
1:A:400:GLY:HA3	1:A:583:GLY:HA3	1.78	0.65
1:A:1166:ALA:HB2	1:A:1178:SER:HB2	1.79	0.64
1:A:1065:THR:HG23	1:A:1080:ASN:OD1	1.98	0.64
1:A:380:GLY:N	1:A:616:THR:HG21	2.11	0.63
1:A:435:ARG:HG3	1:A:437:ASP:OD1	1.99	0.63
1:A:723:ASP:OD1	1:A:724:LYS:N	2.30	0.63
1:A:1502:LEU:HD23	1:A:1529:LYS:HG2	1.80	0.63
1:A:342:VAL:HG12	1:A:374:SER:HB2	1.81	0.63
1:A:1161:LEU:HD13	1:A:1183:MSE:HE2	1.81	0.63
1:A:1213:LEU:HD12	1:A:1267:TYR:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:LEU:HD22	1:A:1487:MSE:HE3	1.81	0.62
1:A:162:ARG:H	1:A:195:LYS:HD3	1.65	0.61
1:A:1430:ILE:HD12	1:A:1445:LEU:HD21	1.83	0.61
1:A:443:ALA:HB2	1:A:548:MSE:SE	2.52	0.60
1:A:458:LEU:HD23	1:A:464:HIS:CD2	2.36	0.60
1:A:869:ASN:ND2	1:A:874:THR:HG22	2.14	0.59
1:A:422:VAL:CG2	1:A:570:SER:HB2	2.33	0.59
1:A:869:ASN:HB2	1:A:874:THR:HG22	1.84	0.59
1:A:1031:GLU:OE2	1:A:1031:GLU:HA	2.02	0.58
1:A:177:MSE:O	1:A:180:ARG:N	2.36	0.58
1:A:275:LYS:C	1:A:277:GLU:H	2.10	0.58
1:A:1415:ILE:HG22	1:A:1417:ASN:H	1.67	0.58
1:A:156:PRO:HB3	1:A:196:VAL:HG21	1.86	0.58
1:A:311:MSE:CE	1:A:340:ALA:HB2	2.33	0.58
1:A:435:ARG:CG	1:A:435:ARG:HH11	2.17	0.57
1:A:1102:GLY:H	1:A:1120:LEU:HD11	1.69	0.57
1:A:1131:THR:OG1	1:A:1132:PRO:CD	2.51	0.57
1:A:797:ARG:HD3	1:A:797:ARG:N	2.19	0.57
1:A:1297:THR:O	1:A:1298:ILE:HD13	2.05	0.57
1:A:408:GLY:O	1:A:411:PRO:HD2	2.05	0.57
1:A:1314:SER:H	1:A:1379:ARG:HD2	1.70	0.56
1:A:385:TYR:HD2	1:A:958:LYS:HD3	1.69	0.56
1:A:438:LEU:HB3	1:A:548:MSE:HE2	1.88	0.55
1:A:1161:LEU:HD13	1:A:1183:MSE:CE	2.36	0.55
1:A:552:ASN:C	1:A:554:ASN:H	2.14	0.55
1:A:920:PHE:CD1	1:A:996:VAL:HG21	2.42	0.54
1:A:1551:ARG:NH1	1:A:1553:GLU:OE2	2.32	0.54
1:A:426:LEU:HD21	1:A:568:ALA:HB2	1.88	0.54
1:A:964:ILE:H	1:A:964:ILE:HD12	1.72	0.54
1:A:1152:LEU:HD12	1:A:1180:LEU:HD23	1.89	0.54
1:A:1295:PHE:O	1:A:1396:LYS:HE3	2.07	0.54
1:A:484:GLY:HA2	1:A:510:LEU:CD1	2.37	0.54
1:A:550:GLN:O	1:A:551:LEU:HD22	2.07	0.54
1:A:1023:LEU:HD13	1:A:1118:ALA:HB2	1.90	0.54
1:A:1363:LYS:CG	1:A:1364:ARG:H	2.05	0.54
1:A:1077:VAL:HG11	1:A:1342:ILE:HD12	1.90	0.53
1:A:426:LEU:HD23	1:A:442:LYS:HB3	1.89	0.53
1:A:516:ASN:HB3	1:A:545:GLY:HA2	1.91	0.53
1:A:290:ASN:ND2	1:A:306:PRO:O	2.42	0.53
1:A:547:ALA:O	1:A:548:MSE:HB2	2.09	0.53
1:A:1152:LEU:HD22	1:A:1182:LYS:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:CG	1:A:435:ARG:NH1	2.72	0.52
1:A:162:ARG:N	1:A:195:LYS:HD3	2.24	0.52
1:A:1152:LEU:CD1	1:A:1180:LEU:HD23	2.39	0.52
1:A:1168:LEU:HD22	1:A:1383:VAL:HB	1.90	0.52
1:A:754:TYR:CE2	1:A:773:MSE:HB3	2.44	0.52
1:A:821:GLU:HG2	1:A:822:ASN:N	2.25	0.52
1:A:435:ARG:NH1	1:A:435:ARG:HG2	2.23	0.52
1:A:533:MSE:O	1:A:536:PRO:HD3	2.10	0.52
1:A:1564:GLU:HG3	1:A:1565:VAL:N	2.24	0.52
1:A:576:MSE:HE2	1:A:675:GLN:HA	1.92	0.52
1:A:589:TYR:HD2	4:A:1716:GOL:H2	1.73	0.52
1:A:1028:PHE:CE2	1:A:1101:LEU:HD13	2.45	0.52
1:A:1202:PHE:H	1:A:1244:THR:HG23	1.75	0.52
1:A:1313:GLY:C	1:A:1315:SER:H	2.18	0.51
1:A:523:ASN:OD1	1:A:544:PHE:HA	2.10	0.51
1:A:165:ASP:O	1:A:168:THR:HG22	2.11	0.51
1:A:1079:ASP:HB2	1:A:1081:LYS:HG3	1.92	0.51
1:A:1449:LYS:HE2	1:A:1471:SER:HB2	1.91	0.51
1:A:1096:LEU:HD21	1:A:1101:LEU:HB2	1.93	0.51
1:A:1309:THR:HA	4:A:1717:GOL:H11	1.93	0.51
1:A:1123:HIS:CD2	1:A:1136:LYS:HD3	2.46	0.50
1:A:201:ASN:HA	1:A:314:ARG:HB3	1.94	0.50
1:A:552:ASN:C	1:A:554:ASN:N	2.68	0.50
1:A:1089:ASP:OD1	1:A:1091:SER:OG	2.23	0.50
1:A:428:THR:HG23	1:A:562:ASP:OD1	2.11	0.50
1:A:313:MSE:HG2	1:A:331:ALA:HB1	1.94	0.50
1:A:1335:VAL:HG13	1:A:1342:ILE:HG23	1.94	0.50
1:A:429:VAL:HG13	1:A:558:SER:O	2.11	0.50
1:A:383:ARG:HG2	1:A:384:VAL:HG22	1.94	0.50
1:A:192:ILE:HD12	1:A:192:ILE:N	2.27	0.50
1:A:422:VAL:HG21	1:A:570:SER:HB2	1.94	0.50
1:A:896:GLU:OE1	1:A:1049:ARG:NH1	2.42	0.49
1:A:177:MSE:HG2	1:A:191:TRP:HB2	1.93	0.49
1:A:407:THR:HA	1:A:591:LYS:HD2	1.94	0.49
1:A:147:VAL:HB	1:A:628:LEU:HD11	1.95	0.49
1:A:1036:LYS:HB2	1:A:1091:SER:HB3	1.94	0.49
1:A:1363:LYS:HG3	1:A:1364:ARG:N	2.11	0.49
1:A:759:VAL:HG11	1:A:769:VAL:CG1	2.43	0.49
1:A:377:VAL:HB	1:A:406:SER:HB3	1.95	0.49
1:A:1288:PRO:HG2	1:A:1384:SER:HB2	1.95	0.49
1:A:1507:SER:HB3	1:A:1546:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:THR:HB	1:A:675:GLN:NE2	2.28	0.49
1:A:1246:TRP:CZ2	1:A:1248:GLY:HA2	2.47	0.49
1:A:489:ILE:O	1:A:514:ILE:HA	2.13	0.48
1:A:720:SER:HB2	1:A:722:LYS:NZ	2.27	0.48
1:A:203:VAL:HG21	1:A:316:PHE:CD1	2.48	0.48
1:A:931:LEU:C	1:A:931:LEU:HD23	2.38	0.48
1:A:1188:PHE:O	1:A:1197:LYS:HE2	2.13	0.48
1:A:637:THR:O	1:A:638:GLN:HG2	2.12	0.48
1:A:1102:GLY:HA2	1:A:1121:GLY:N	2.28	0.48
1:A:1150:ASP:O	1:A:1151:ASN:HB2	2.12	0.48
1:A:199:ALA:HA	1:A:312:PHE:O	2.14	0.48
1:A:738:ASP:OD2	1:A:741:LYS:HB2	2.13	0.48
1:A:633:TYR:CE1	1:A:637:THR:HG21	2.49	0.48
1:A:721:ASN:HA	1:A:763:ALA:HB1	1.95	0.48
1:A:202:TYR:HB2	1:A:315:VAL:HG22	1.96	0.47
1:A:725:THR:HG23	1:A:760:THR:OG1	2.15	0.47
1:A:316:PHE:O	1:A:321:MSE:HE1	2.15	0.47
1:A:204:GLU:CB	1:A:206:SER:HB2	2.45	0.47
1:A:426:LEU:HD22	1:A:566:SER:HB2	1.97	0.47
1:A:718:ASN:HB2	1:A:761:VAL:HG12	1.95	0.47
1:A:380:GLY:HA3	1:A:581:ASN:ND2	2.30	0.47
1:A:1327:LYS:HA	1:A:1331:ARG:O	2.15	0.47
1:A:1421:LEU:HB2	1:A:1455:LEU:HD11	1.97	0.47
1:A:313:MSE:HE2	1:A:335:ALA:HB2	1.97	0.47
1:A:1377:GLU:HG3	1:A:1383:VAL:CG2	2.45	0.47
1:A:1291:THR:HG22	1:A:1480:PHE:CD2	2.50	0.46
1:A:715:THR:HG22	1:A:717:HIS:NE2	2.30	0.46
1:A:400:GLY:HA2	1:A:583:GLY:HA3	1.97	0.46
1:A:836:GLN:HG3	1:A:838:LYS:HD2	1.98	0.46
1:A:196:VAL:HA	1:A:310:VAL:O	2.15	0.46
1:A:1555:ASN:O	1:A:1568:LEU:HD23	2.15	0.46
1:A:401:LEU:HD11	1:A:960:PHE:HB2	1.98	0.46
1:A:126:ILE:HG23	1:A:597:PRO:HG2	1.98	0.46
1:A:201:ASN:HB3	1:A:206:SER:HB3	1.98	0.46
1:A:132:THR:HG21	1:A:136:TRP:CE2	2.51	0.45
1:A:204:GLU:HB2	1:A:206:SER:HB2	1.99	0.45
1:A:535:ILE:O	1:A:535:ILE:HG13	2.16	0.45
1:A:782:LEU:HD23	1:A:785:GLN:HE21	1.82	0.45
1:A:1024:SER:HB2	1:A:1038:GLU:HG3	1.98	0.45
1:A:341:ASP:OD1	1:A:631:LYS:NZ	2.36	0.45
1:A:451:PHE:CZ	1:A:537:SER:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:HA	1:A:500:MSE:HE3	1.97	0.45
1:A:643:LYS:HB2	1:A:643:LYS:HE2	1.79	0.45
1:A:720:SER:HB2	1:A:722:LYS:CD	2.43	0.45
1:A:1052:SER:HB2	1:A:1107:MSE:HB3	1.97	0.45
1:A:1435:TYR:CD1	1:A:1440:GLY:HA2	2.51	0.45
1:A:177:MSE:HE3	1:A:197:VAL:O	2.16	0.45
1:A:275:LYS:HB2	1:A:277:GLU:HG3	1.98	0.45
1:A:799:ARG:HD2	1:A:804:ASP:HB2	1.98	0.45
1:A:1409:VAL:HG23	1:A:1414:GLN:HG2	1.98	0.45
1:A:283:VAL:HG13	1:A:621:PRO:HG3	1.98	0.45
1:A:191:TRP:C	1:A:192:ILE:HD12	2.42	0.45
1:A:479:ALA:CB	1:A:507:HIS:HB3	2.46	0.45
1:A:487:ALA:O	1:A:512:VAL:HG23	2.15	0.45
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.84	0.45
1:A:1202:PHE:H	1:A:1244:THR:CG2	2.29	0.45
1:A:1249:ILE:HA	1:A:1254:SER:O	2.17	0.45
1:A:1340:ASP:OD1	1:A:1340:ASP:N	2.47	0.45
1:A:501:ILE:CD1	1:A:540:ILE:HG12	2.47	0.45
1:A:606:ASN:O	1:A:609:HIS:HB2	2.17	0.45
1:A:544:PHE:CB	1:A:571:GLN:HE22	2.31	0.44
1:A:1400:VAL:O	1:A:1480:PHE:HA	2.18	0.44
1:A:469:VAL:O	1:A:489:ILE:HD13	2.17	0.44
1:A:1107:MSE:HE3	1:A:1109:GLU:OE2	2.17	0.44
1:A:725:THR:OG1	1:A:760:THR:HG23	2.17	0.44
1:A:959:ASN:HD21	1:A:970:THR:CG2	2.28	0.44
1:A:1023:LEU:HD23	1:A:1023:LEU:HA	1.76	0.44
1:A:1544:VAL:HG12	1:A:1546:LEU:HD13	2.00	0.44
1:A:451:PHE:CE2	1:A:537:SER:HA	2.53	0.44
1:A:1373:TYR:CE2	1:A:1387:THR:HG22	2.52	0.44
1:A:484:GLY:HA2	1:A:510:LEU:HD11	1.98	0.44
1:A:559:LEU:HD12	1:A:559:LEU:C	2.43	0.44
1:A:637:THR:C	1:A:638:GLN:HG2	2.43	0.44
1:A:1268:ARG:NH1	1:A:1268:ARG:CG	2.73	0.43
1:A:1362:SER:OG	1:A:1363:LYS:HG2	2.18	0.43
1:A:468:TYR:CD2	1:A:551:LEU:HD11	2.54	0.43
1:A:195:LYS:NZ	1:A:308:ALA:O	2.45	0.43
1:A:384:VAL:O	1:A:387:SER:HB3	2.18	0.43
1:A:395:THR:HG22	1:A:787:PRO:HG2	2.00	0.43
1:A:407:THR:CG2	1:A:585:THR:HG22	2.35	0.43
1:A:655:MSE:HE2	1:A:699:GLY:C	2.44	0.43
1:A:1500:ASP:HB3	1:A:1501:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLY:HA2	1:A:538:ALA:O	2.18	0.43
1:A:1405:LEU:HD22	1:A:1487:MSE:CE	2.47	0.43
1:A:301:PHE:C	1:A:302:LEU:HD23	2.43	0.43
1:A:377:VAL:HB	1:A:406:SER:CB	2.48	0.43
1:A:422:VAL:HG23	1:A:570:SER:HB2	2.00	0.43
1:A:675:GLN:OE1	1:A:678:GLY:HA2	2.19	0.43
1:A:677:ALA:HA	1:A:812:PRO:HG3	2.01	0.43
1:A:1211:ASN:HB2	1:A:1268:ARG:O	2.19	0.43
1:A:1455:LEU:HA	1:A:1455:LEU:HD23	1.71	0.43
1:A:782:LEU:HD23	1:A:782:LEU:HA	1.82	0.43
1:A:287:VAL:HG23	1:A:625:GLY:N	2.34	0.43
1:A:1124:LEU:HD23	1:A:1124:LEU:HA	1.81	0.43
1:A:275:LYS:C	1:A:277:GLU:N	2.75	0.42
1:A:590:LEU:O	1:A:591:LYS:HG2	2.19	0.42
1:A:707:THR:C	1:A:709:THR:H	2.27	0.42
1:A:1163:THR:OG1	1:A:1164:ASN:N	2.51	0.42
1:A:591:LYS:HA	1:A:592:PRO:O	2.18	0.42
1:A:728:TYR:HA	1:A:797:ARG:O	2.19	0.42
1:A:1098:LYS:HD3	1:A:1098:LYS:HA	1.86	0.42
1:A:526:MSE:H	1:A:526:MSE:HG2	1.72	0.42
1:A:177:MSE:C	1:A:179:ALA:N	2.77	0.42
1:A:352:GLY:HA3	1:A:404:SER:HA	2.00	0.42
1:A:693:THR:CG2	1:A:697:ASN:HA	2.43	0.42
1:A:550:GLN:C	1:A:551:LEU:HD22	2.45	0.42
1:A:559:LEU:HD12	1:A:560:GLU:N	2.35	0.42
1:A:1250:THR:O	1:A:1251:ALA:C	2.62	0.42
1:A:1257:MSE:SE	1:A:1409:VAL:HA	2.70	0.42
1:A:501:ILE:HD13	1:A:540:ILE:HG12	2.02	0.42
1:A:657:ASN:O	1:A:681:ASN:HB3	2.20	0.42
1:A:722:LYS:O	1:A:763:ALA:HB2	2.20	0.42
1:A:1025:GLN:HB2	1:A:1135:LEU:O	2.19	0.42
1:A:200:HIS:HB3	1:A:202:TYR:CE1	2.55	0.42
1:A:297:THR:HG21	1:A:423:ILE:HD13	2.02	0.41
1:A:1286:LYS:HD3	1:A:1411:GLU:HG2	2.01	0.41
1:A:897:LYS:HD3	1:A:901:GLY:O	2.21	0.41
1:A:203:VAL:HG21	1:A:316:PHE:CE1	2.55	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.87	0.41
1:A:867:GLU:O	4:A:1714:GOL:H2	2.20	0.41
1:A:1102:GLY:HA2	1:A:1121:GLY:CA	2.51	0.41
1:A:378:ALA:HB2	1:A:617:SER:HA	2.03	0.41
1:A:1215:VAL:HG22	1:A:1265:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:THR:HG22	1:A:1276:GLN:HB2	2.02	0.41
1:A:281:MSE:HG3	1:A:604:THR:O	2.21	0.41
1:A:418:ASN:ND2	1:A:572:LYS:HD2	2.36	0.41
1:A:551:LEU:HD13	1:A:551:LEU:HA	1.74	0.41
1:A:707:THR:O	1:A:709:THR:N	2.54	0.41
1:A:1362:SER:HB3	1:A:1364:ARG:NH2	2.36	0.41
1:A:1452:VAL:HG11	1:A:1483:VAL:HG11	2.02	0.41
1:A:182:LYS:N	8:A:1802:HOH:O	2.54	0.41
1:A:351:ASN:ND2	1:A:958:LYS:HE3	2.35	0.41
1:A:1323:PHE:CD2	1:A:1348:LYS:HG2	2.56	0.41
1:A:1424:ASP:OD1	1:A:1424:ASP:C	2.64	0.41
1:A:854:VAL:HB	1:A:881:HIS:HA	2.03	0.41
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.46	0.41
1:A:1436:TYR:HB3	1:A:1442:SER:HB3	2.03	0.41
1:A:1564:GLU:HG3	1:A:1565:VAL:H	1.84	0.41
1:A:863:THR:OG1	1:A:915:GLN:HA	2.21	0.41
1:A:304:ILE:N	1:A:304:ILE:HD12	2.36	0.40
1:A:408:GLY:C	1:A:411:PRO:HD2	2.45	0.40
1:A:617:SER:C	1:A:618:MSE:HE3	2.46	0.40
1:A:132:THR:CG2	1:A:136:TRP:CE2	3.04	0.40
1:A:179:ALA:C	8:A:1802:HOH:O	2.64	0.40
1:A:634:LEU:HD11	1:A:649:ILE:HG22	2.03	0.40
1:A:1317:ILE:HD12	1:A:1376:VAL:HB	2.04	0.40
1:A:152:THR:O	1:A:314:ARG:HG3	2.21	0.40
1:A:368:ALA:HB1	1:A:373:VAL:HB	2.04	0.40
1:A:377:VAL:CG1	1:A:406:SER:HB3	2.51	0.40
1:A:728:TYR:HB3	1:A:798:PHE:CD1	2.57	0.40
1:A:484:GLY:HA2	1:A:510:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1390/1519 (92%)	1261 (91%)	118 (8%)	11 (1%)	16 44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	GLY
1	A	536	PRO
1	A	1128	LEU
1	A	1271	HIS
1	A	405	PRO
1	A	537	SER
1	A	1130	LYS
1	A	544	PHE
1	A	1363	LYS
1	A	1546	LEU
1	A	1364	ARG

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1158/1257 (92%)	1144 (99%)	14 (1%)	63 86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	ILE
1	A	213	GLN
1	A	275	LYS
1	A	402	VAL
1	A	404	SER
1	A	407	THR
1	A	435	ARG
1	A	474	ASP
1	A	480	GLN
1	A	1031	GLU

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Mol	Chain	Res	Type
1	A	1249	ILE
1	A	1268	ARG
1	A	1270	GLU
1	A	1319	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	200	HIS
1	A	282	HIS
1	A	480	GLN
1	A	494	ASN
1	A	507	HIS
1	A	574	ASN
1	A	810	ASN
1	A	878	ASN
1	A	915	GLN
1	A	929	GLN
1	A	1156	GLN
1	A	1262	GLN
1	A	1278	GLN
1	A	1284	ASN
1	A	1536	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

Of 22 ligands modelled in this entry, 13 are monoatomic - leaving 9 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
2	SO4	A	1703	-	4,4,4	0.55	0	6,6,6	0.68	0
4	GOL	A	1716	-	5,5,5	1.29	1 (20%)	5,5,5	1.31	0
4	GOL	A	1714	-	5,5,5	2.98	3 (60%)	5,5,5	0.97	0
4	GOL	A	1713	-	5,5,5	1.44	1 (20%)	5,5,5	1.13	0
6	PEG	A	1719	-	6,6,6	0.75	0	5,5,5	0.98	0
4	GOL	A	1717	-	5,5,5	2.53	2 (40%)	5,5,5	1.40	1 (20%)
2	SO4	A	1701	-	4,4,4	0.62	0	6,6,6	0.72	0
4	GOL	A	1715	-	5,5,5	2.04	3 (60%)	5,5,5	0.70	0
2	SO4	A	1702	-	4,4,4	0.26	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1716	-	-	2/4/4/4	-
4	GOL	A	1714	-	-	4/4/4/4	-
4	GOL	A	1713	-	-	1/4/4/4	-
6	PEG	A	1719	-	-	3/4/4/4	-
4	GOL	A	1717	-	-	2/4/4/4	-
4	GOL	A	1715	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1717	GOL	C1-C2	4.70	1.69	1.51
4	A	1714	GOL	C3-C2	4.56	1.69	1.51
4	A	1714	GOL	C1-C2	3.99	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1716	GOL	O2-C2	-2.69	1.35	1.43
4	A	1715	GOL	C1-C2	2.52	1.61	1.51
4	A	1713	GOL	C1-C2	2.44	1.61	1.51
4	A	1714	GOL	O1-C1	2.31	1.52	1.42
4	A	1717	GOL	C3-C2	2.30	1.60	1.51
4	A	1715	GOL	C3-C2	2.15	1.60	1.51
4	A	1715	GOL	O1-C1	2.04	1.51	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1717	GOL	O2-C2-C1	2.09	117.84	109.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1714	GOL	O1-C1-C2-O2
4	A	1714	GOL	O1-C1-C2-C3
4	A	1714	GOL	C1-C2-C3-O3
4	A	1714	GOL	O2-C2-C3-O3
6	A	1719	PEG	C4-C3-O2-C2
4	A	1716	GOL	C1-C2-C3-O3
4	A	1717	GOL	C1-C2-C3-O3
4	A	1716	GOL	O2-C2-C3-O3
4	A	1717	GOL	O2-C2-C3-O3
6	A	1719	PEG	O1-C1-C2-O2
6	A	1719	PEG	C1-C2-O2-C3
4	A	1713	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1716	GOL	1	0
4	A	1714	GOL	2	0
4	A	1717	GOL	1	0
2	A	1701	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	A	1367/1519 (89%)	-0.14	47 (3%) 48 39	25, 50, 87, 120	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	SER	6.2
1	A	1575	VAL	6.0
1	A	551	LEU	5.3
1	A	275	LYS	4.6
1	A	478	ASN	4.5
1	A	535	ILE	4.2
1	A	484	GLY	4.2
1	A	483	LYS	4.0
1	A	481	ASP	3.9
1	A	117	ALA	3.4
1	A	477	TYR	3.4
1	A	549	SER	3.3
1	A	485	LYS	3.3
1	A	1129	GLY	3.3
1	A	213	GLN	3.2
1	A	1128	LEU	3.1
1	A	492	ASP	3.1
1	A	532	GLY	3.0
1	A	480	GLN	3.0
1	A	1127	THR	2.9
1	A	538	ALA	2.9
1	A	536	PRO	2.8
1	A	1126	GLN	2.8
1	A	531	ASN	2.7
1	A	534	GLY	2.7
1	A	276	TYR	2.7
1	A	1131	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	476	GLY	2.6
1	A	547	ALA	2.6
1	A	1414	GLN	2.5
1	A	553	GLY	2.5
1	A	540	ILE	2.4
1	A	723	ASP	2.3
1	A	1031	GLU	2.3
1	A	406	SER	2.3
1	A	1415	ILE	2.2
1	A	544	PHE	2.2
1	A	1340	ASP	2.2
1	A	473	THR	2.2
1	A	539	PHE	2.2
1	A	1130	LYS	2.2
1	A	555	GLY	2.1
1	A	543	GLU	2.1
1	A	1363	LYS	2.0
1	A	550	GLN	2.0
1	A	405	PRO	2.0
1	A	1548	LYS	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, 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(Å <sup>2</sup> )	Q<0.9
3	CA	A	1711	1/1	0.64	0.46	94,94,94,94	0
3	CA	A	1704	1/1	0.65	0.14	114,114,114,114	0
3	CA	A	1722	1/1	0.66	0.25	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	A	1708	1/1	0.73	0.24	99,99,99,99	0
3	CA	A	1710	1/1	0.76	0.20	98,98,98,98	0
2	SO4	A	1702	5/5	0.79	0.09	93,94,99,111	0
3	CA	A	1705	1/1	0.80	0.24	111,111,111,111	0
4	GOL	A	1714	6/6	0.84	0.28	56,61,62,65	0
6	PEG	A	1719	7/7	0.87	0.19	41,46,61,61	0
4	GOL	A	1717	6/6	0.88	0.15	38,51,53,58	0
4	GOL	A	1713	6/6	0.89	0.15	59,67,72,72	0
3	CA	A	1709	1/1	0.89	0.20	89,89,89,89	0
2	SO4	A	1703	5/5	0.90	0.28	60,69,103,114	0
2	SO4	A	1701	5/5	0.90	0.16	51,56,99,101	0
4	GOL	A	1715	6/6	0.94	0.12	38,40,43,45	0
4	GOL	A	1716	6/6	0.96	0.09	39,44,45,48	0
7	CL	A	1721	1/1	0.96	0.19	60,60,60,60	0
3	CA	A	1712	1/1	0.98	0.02	45,45,45,45	0
5	MG	A	1718	1/1	0.99	0.11	11,11,11,11	0
3	CA	A	1707	1/1	0.99	0.03	41,41,41,41	0
3	CA	A	1706	1/1	0.99	0.02	39,39,39,39	0
7	CL	A	1720	1/1	1.00	0.07	10,10,10,10	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.