



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:16 am GMT

PDB ID : 4BC1  
Title : Structure of mouse acetylcholinesterase inhibited by CBDP (30-min soak): crystal-saligenin-phosphoserine adduct  
Authors : Carletti, E.; Colletier, J.-P.; Schopfer, L.M.; Santoni, G.; Masson, P.; Lockridge, O.; Nachon, F.; Weik, M.  
Deposited on : 2012-09-30  
Resolution : 2.95 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

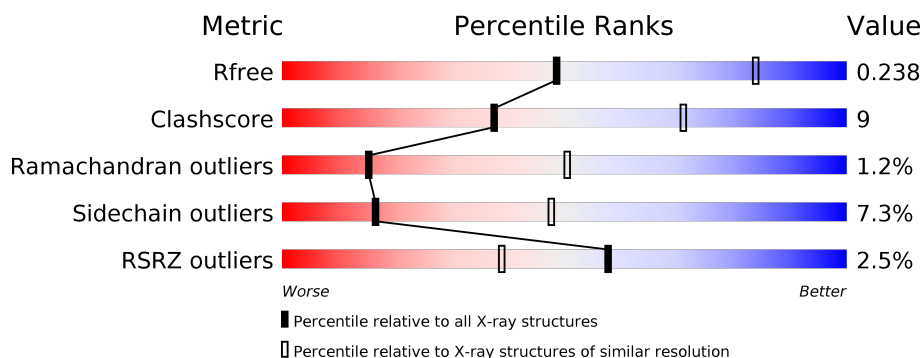
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	543	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	543	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	543	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	D	543	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TQV	C	600	-	-	X	X
3	NAG	B	702	-	-	-	X
4	CL	A	1544	-	-	X	-
5	SO4	A	1550	-	-	-	X
5	SO4	B	1546	-	-	-	X
5	SO4	C	1548	-	-	-	X

## 2 Entry composition [i](#)

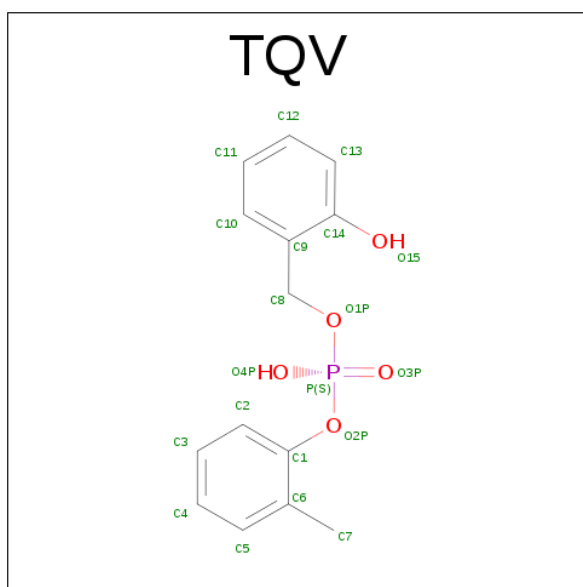
There are 6 unique types of molecules in this entry. The entry contains 17994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	3	0
			4224	2712	732	766	14			
1	B	539	Total	C	N	O	S	0	1	0
			4202	2698	728	762	14			
1	C	540	Total	C	N	O	S	0	4	0
			4230	2716	732	768	14			
1	D	540	Total	C	N	O	S	0	5	0
			4243	2723	741	765	14			

- Molecule 2 is O-CRESYL-SALIGENIN PHOSPHATE (three-letter code: TQV) (formula:  $C_{14}H_{15}O_5P$ ).



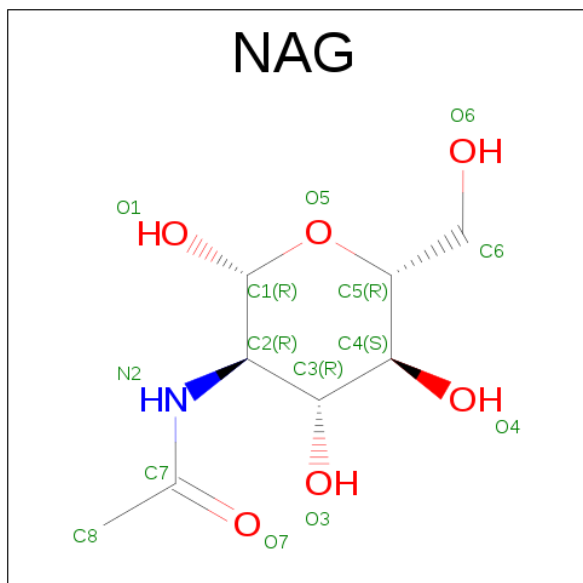
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			19	14	4	1		
2	B	1	Total	C	O	P	0	0
			19	14	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			19	14	4	1		
2	D	1	Total	C	O	P	0	0
			19	14	4	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

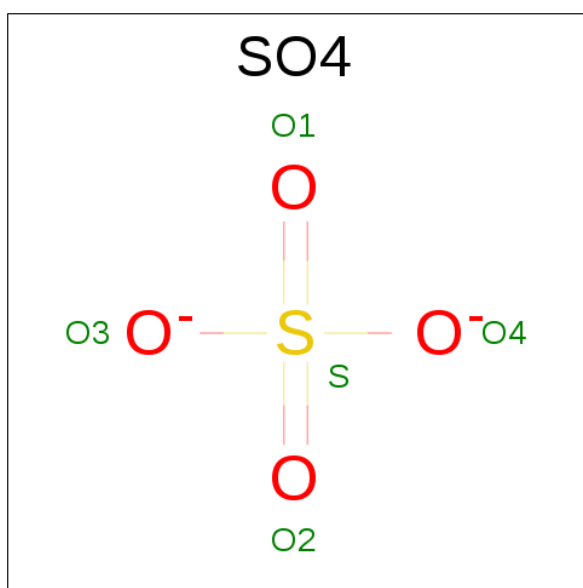


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	3	Total	Cl	0	0
			3	3		
4	D	3	Total	Cl	0	0
			3	3		
4	C	4	Total	Cl	0	0
			4	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

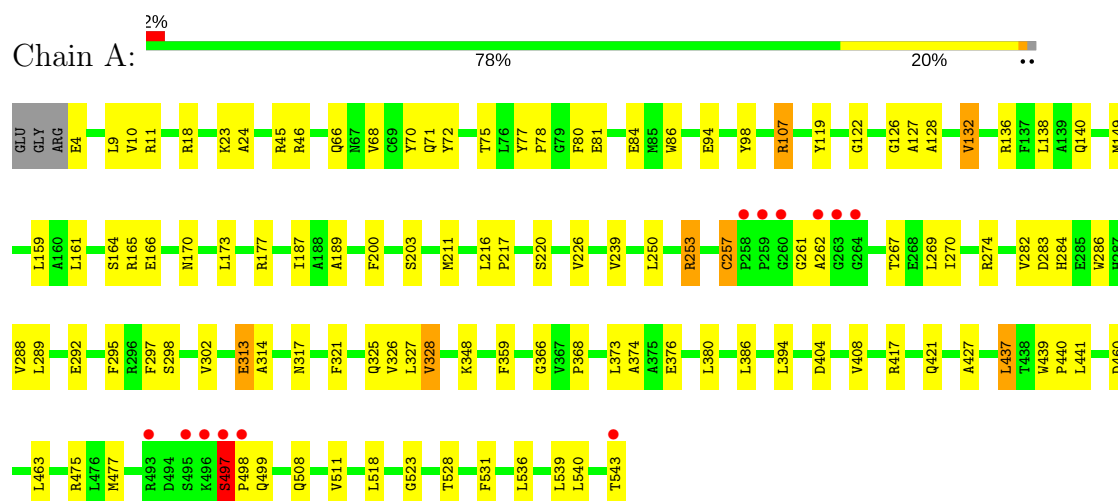
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		
6	B	144	Total	O	0	0
			144	144		
6	C	258	Total	O	0	0
			258	258		
6	D	186	Total	O	0	0
			186	186		

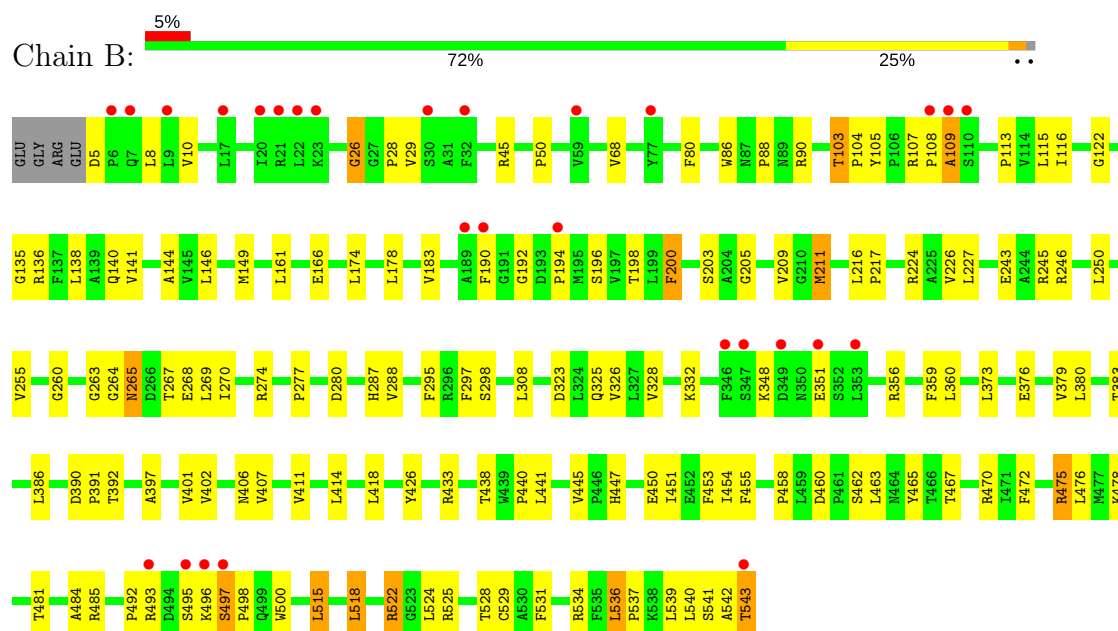
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: ACETYLCHOLINESTERASE

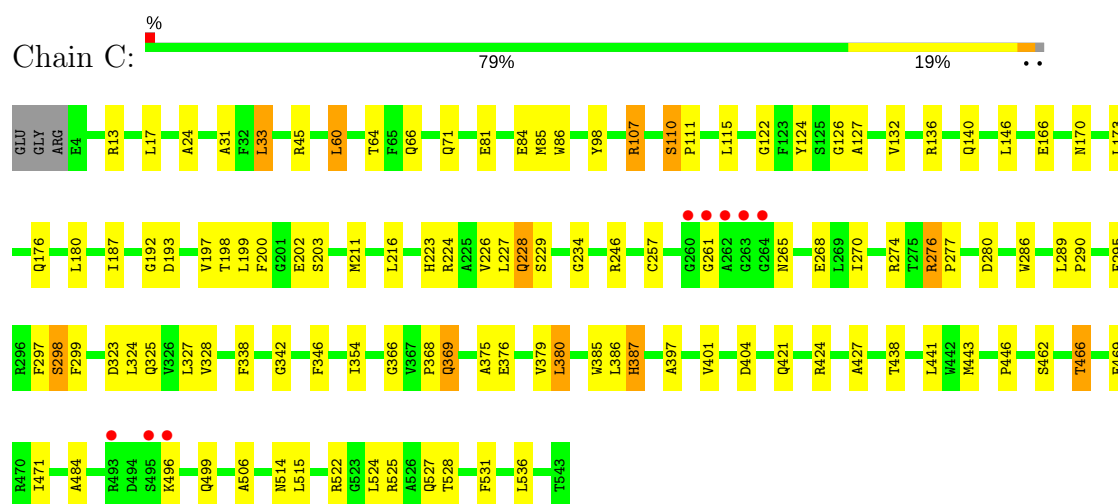


#### • Molecule 1: ACETYLCHOLINESTERASE

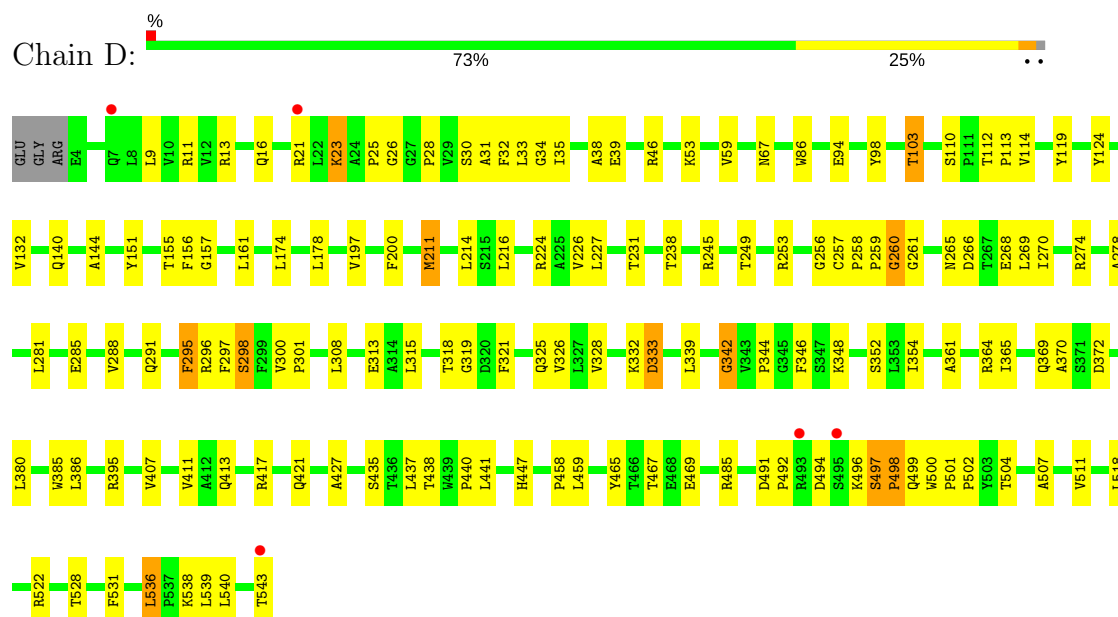


#### • Molecule 1: ACETYLCHOLINESTERASE





• Molecule 1: ACETYLCHOLINESTERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.54Å 173.25Å 224.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.28-2.95) 99.7 (49.75-2.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, $R_{free}$	0.186 , 0.238 0.185 , 0.238	Depositor DCC
$R_{free}$ test set	3343 reflections (3.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TQV, CL, SO4, 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	A	0.50	1/4358 (0.0%)	0.67	0/5955
1	B	0.41	1/4329 (0.0%)	0.60	0/5916
1	C	0.49	1/4367 (0.0%)	0.66	0/5968
1	D	0.45	0/4382	0.64	0/5984
All	All	0.46	3/17436 (0.0%)	0.64	0/23823

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SER	CB-OG	6.05	1.50	1.42
1	C	203	SER	CB-OG	5.34	1.49	1.42
1	B	203	SER	CB-OG	5.07	1.48	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	257	CYS	Peptide

## 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	4224	0	4111	64	0
1	B	4202	0	4089	80	0
1	C	4230	0	4116	66	0
1	D	4243	0	4146	88	0
2	A	19	0	12	4	0
2	B	19	0	11	3	0
2	C	19	0	12	7	0
2	D	19	0	12	4	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	42	0	39	0	0
4	A	3	0	0	2	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	1	0
5	A	30	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	1	0
5	D	15	0	0	0	0
6	A	247	0	0	18	0
6	B	144	0	0	6	0
6	C	258	0	0	9	0
6	D	186	0	0	12	0
All	All	17994	0	16600	296	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 9.

All (296) 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)
4:A:1544:CL:CL	6:A:2034:HOH:O	2.19	0.98
2:C:600:TQV:H8	2:C:600:TQV:H2	1.47	0.95
1:D:112:THR:HG21	1:D:144:ALA:HA	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:HG22	1:D:253:ARG:HH21	1.44	0.82
1:A:126:GLY:HA2	6:A:2086:HOH:O	1.82	0.79
1:C:387[A]:HIS:ND1	6:C:2216:HOH:O	2.16	0.78
2:C:600:TQV:H2	2:C:600:TQV:C8	2.15	0.77
1:A:72:TYR:O	6:A:2052:HOH:O	2.02	0.77
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.67	0.77
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.67	0.77
1:C:387[A]:HIS:ND1	6:C:2215:HOH:O	2.19	0.75
1:D:227:LEU:HB2	1:D:328:VAL:HG12	1.70	0.73
1:D:39:GLU:OE2	6:D:2019:HOH:O	2.07	0.72
1:A:4:GLU:N	6:A:2001:HOH:O	2.23	0.71
1:C:387[B]:HIS:ND1	6:C:2214:HOH:O	2.22	0.71
1:B:138:LEU:HD21	1:B:455:PHE:HA	1.72	0.70
1:D:155:THR:O	6:D:2080:HOH:O	2.09	0.70
1:B:265:ASN:HB3	1:B:268:GLU:HB2	1.73	0.70
1:C:227:LEU:HB2	1:C:328:VAL:HG12	1.72	0.70
1:C:122:GLY:N	2:C:600:TQV:O3P	2.24	0.70
1:A:165:ARG:NH2	4:A:1544:CL:CL	2.62	0.69
1:C:86:TRP:CD2	2:C:600:TQV:H5	2.28	0.68
1:C:274:ARG:NH1	6:C:2041:HOH:O	2.17	0.68
1:D:86:TRP:CD2	2:D:600:TQV:H5	2.31	0.66
1:B:10:VAL:HG22	1:B:107:ARG:HH21	1.62	0.65
1:A:508:GLN:NE2	6:A:2228:HOH:O	2.18	0.65
1:A:4:GLU:OE1	1:A:18:ARG:NH1	2.28	0.64
1:A:161:LEU:HD11	1:A:269:LEU:HD23	1.78	0.64
1:B:103:THR:HG21	1:B:190:PHE:O	1.97	0.64
1:D:259:PRO:HB2	6:D:2124:HOH:O	1.99	0.63
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.81	0.62
1:D:265:ASN:HB3	1:D:268:GLU:HB2	1.82	0.62
1:B:528:THR:O	1:B:531:PHE:HB3	1.99	0.62
1:D:380:LEU:HA	1:D:385:TRP:HZ2	1.65	0.62
1:C:265:ASN:HB3	1:C:268:GLU:H	1.66	0.61
1:D:380:LEU:HB3	6:D:2154:HOH:O	1.98	0.61
1:C:86:TRP:CE3	2:C:600:TQV:H5	2.36	0.61
1:B:122:GLY:N	2:B:600:TQV:O3P	2.33	0.61
1:C:366:GLY:O	1:C:368:PRO:HD3	2.00	0.61
1:B:166:GLU:HG2	1:B:274:ARG:HH22	1.66	0.60
1:A:46:ARG:O	1:A:274:ARG:NH1	2.34	0.60
1:C:107:ARG:HH11	1:C:107:ARG:HG2	1.65	0.60
1:D:214:LEU:HD22	1:D:315:LEU:HB3	1.84	0.60
1:A:250:LEU:HG	1:A:288:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLY:O	1:A:368:PRO:HD3	2.04	0.58
1:D:348:LYS:O	1:D:440:PRO:HG3	2.03	0.58
1:B:541:SER:O	1:B:543:THR:N	2.36	0.58
1:D:86:TRP:CE3	2:D:600:TQV:H5	2.38	0.58
1:C:197:VAL:H	1:C:223:HIS:HD2	1.51	0.58
1:D:332:LYS:HB3	1:D:333:ASP:OD1	2.04	0.58
1:C:380:LEU:HA	1:C:385:TRP:HZ2	1.69	0.57
1:B:166:GLU:OE1	1:B:267:THR:HG22	2.05	0.57
1:D:497:SER:OG	6:D:2169:HOH:O	2.07	0.57
1:B:260:GLY:HA2	1:C:286:TRP:CG	2.39	0.57
1:B:498:PRO:HD2	1:B:518:LEU:HB3	1.87	0.57
1:A:107:ARG:NH2	6:A:2010:HOH:O	2.28	0.56
1:D:224:ARG:HG2	1:D:325:GLN:HB2	1.87	0.56
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.87	0.56
1:B:263:GLY:O	1:B:265:ASN:N	2.38	0.56
1:A:68:VAL:HG13	1:A:127:ALA:HB2	1.88	0.56
1:B:113:PRO:HG3	1:B:485:ARG:HB3	1.88	0.55
1:C:71:GLN:NE2	1:C:126:GLY:O	2.37	0.55
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.87	0.55
1:C:466:THR:HG23	1:C:469:GLU:OE1	2.07	0.55
1:B:475:ARG:NH2	6:B:2131:HOH:O	2.30	0.54
1:A:321:PHE:HD2	1:A:421:GLN:HB3	1.73	0.54
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.89	0.54
1:B:260:GLY:HA2	1:C:286:TRP:CD1	2.42	0.54
1:C:180:LEU:HD21	1:C:199:LEU:HD21	1.90	0.54
1:B:450:GLU:OE1	6:B:2061:HOH:O	2.18	0.54
1:A:177:ARG:NH2	1:A:217:PRO:HG2	2.23	0.54
1:A:497:SER:H	1:A:498:PRO:HA	1.73	0.54
1:D:30:SER:HB2	1:D:103:THR:HG23	1.90	0.54
1:D:333:ASP:OD1	1:D:333:ASP:N	2.40	0.53
1:D:256:GLY:O	1:D:259:PRO:HB3	2.09	0.53
1:D:266:ASP:O	1:D:270:ILE:HG12	2.09	0.53
1:A:348:LYS:HA	1:A:440:PRO:HG3	1.91	0.53
1:B:525:ARG:O	1:B:529:CYS:HB2	2.08	0.53
1:C:115:LEU:HD23	1:C:198:THR:HB	1.90	0.53
1:D:39:GLU:HG2	1:D:53:LYS:HA	1.91	0.53
1:D:370:ALA:HA	1:D:540:LEU:HD11	1.91	0.53
1:A:226:VAL:HG13	1:A:327:LEU:HB3	1.90	0.53
1:A:71:GLN:HA	6:A:2050:HOH:O	2.09	0.53
1:B:348:LYS:O	1:B:440:PRO:HG3	2.09	0.53
1:C:200:PHE:HB2	1:C:226:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:TYR:O	1:D:151:TYR:OH	2.21	0.52
1:C:115:LEU:HD21	1:C:484:ALA:HB2	1.91	0.52
1:C:187:ILE:HG13	1:C:192:GLY:HA3	1.91	0.52
1:D:38:ALA:HB2	1:D:178:LEU:HD23	1.91	0.52
1:A:122:GLY:N	2:A:600:TQV:O3P	2.36	0.52
1:C:246:ARG:NH2	1:C:290:PRO:HG3	2.25	0.52
1:C:298:SER:HB3	1:C:299:PHE:CD2	2.44	0.52
1:D:249:THR:HG22	1:D:253:ARG:NH2	2.20	0.52
1:D:511:VAL:HB	1:D:518:LEU:HD22	1.91	0.52
1:B:28:PRO:HG2	1:B:105:TYR:HB3	1.92	0.52
1:B:356:ARG:O	1:B:360:LEU:HG	2.10	0.51
1:B:373:LEU:HD23	1:B:539:LEU:HD11	1.92	0.51
1:B:323:ASP:N	1:B:323:ASP:OD1	2.43	0.51
1:D:214:LEU:HD22	1:D:315:LEU:CB	2.41	0.51
1:B:534:ARG:NH1	6:B:2141:HOH:O	2.33	0.51
1:A:166:GLU:HB3	1:A:274:ARG:HH22	1.75	0.51
1:A:380:LEU:HB3	6:A:2246:HOH:O	2.11	0.51
1:A:528:THR:O	1:A:531:PHE:HB3	2.10	0.51
1:D:157:GLY:O	6:D:2081:HOH:O	2.20	0.51
1:A:292:GLU:HB2	1:D:249:THR:HG21	1.93	0.51
1:C:166:GLU:N	1:C:166:GLU:OE1	2.40	0.51
1:D:297[A]:PHE:CG	1:D:298:SER:N	2.79	0.50
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.46	0.50
1:B:5:ASP:OD2	1:B:105:TYR:OH	2.23	0.50
1:D:21:ARG:HH11	1:D:28:PRO:HB3	1.76	0.50
1:A:128:ALA:HB3	6:A:2072:HOH:O	2.10	0.50
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.47	0.50
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.93	0.50
1:B:454:ILE:HD12	1:B:476:LEU:HD13	1.94	0.49
1:C:31:ALA:HB1	1:C:33:LEU:HD21	1.93	0.49
1:D:313:GLU:HG2	1:D:417[B]:ARG:HH12	1.76	0.49
1:D:342:GLY:O	1:D:344:PRO:HD3	2.11	0.49
1:D:407:VAL:O	1:D:411:VAL:HG23	2.11	0.49
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.48	0.49
1:B:243:GLU:OE2	1:B:246:ARG:NH2	2.42	0.49
1:C:404:ASP:OD2	1:C:525:ARG:NH2	2.45	0.49
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.95	0.49
1:C:424:ARG:HD2	6:C:2225:HOH:O	2.12	0.49
1:D:34:GLY:HA2	1:D:98:TYR:HB3	1.94	0.49
1:B:113:PRO:HA	1:B:196:SER:HB3	1.94	0.49
1:B:332:LYS:HB3	1:B:445:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:O	1:D:253:ARG:NH1	2.45	0.48
1:A:286:TRP:CG	1:D:260:GLY:HA2	2.49	0.48
1:B:379:VAL:O	1:B:383:THR:OG1	2.15	0.48
1:D:326:VAL:HG12	1:D:328:VAL:HG13	1.95	0.48
1:A:475:ARG:NH2	6:A:2220:HOH:O	2.47	0.48
1:D:16:GLN:HB2	1:D:59:VAL:HG22	1.96	0.48
1:B:116:ILE:HD11	1:B:183:VAL:HG11	1.95	0.48
1:D:211:MET:HG2	1:D:308:LEU:HD21	1.95	0.48
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.94	0.48
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.96	0.47
1:D:67:ASN:ND2	6:D:2041:HOH:O	2.46	0.47
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.79	0.47
1:B:407:VAL:O	1:B:411:VAL:HG23	2.15	0.47
1:B:200:PHE:CB	1:B:226:VAL:HB	2.44	0.47
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.96	0.47
1:D:528:THR:O	1:D:531:PHE:HB3	2.14	0.47
1:B:103:THR:HG22	1:B:104:PRO:HD2	1.96	0.47
1:D:497:SER:N	1:D:498:PRO:HA	2.29	0.47
1:D:174:LEU:HD23	1:D:174:LEU:HA	1.74	0.47
1:B:115:LEU:HD23	1:B:198:THR:HB	1.97	0.47
1:C:346:PHE:CZ	1:C:354:ILE:HD13	2.49	0.47
1:D:156:PHE:CZ	1:D:278:ALA:HB1	2.50	0.47
1:D:435:SER:OG	1:D:469:GLU:OE1	2.29	0.47
1:C:24:ALA:HB3	1:C:140:GLN:HG3	1.97	0.47
1:C:338:PHE:CE2	2:C:600:TQV:H8A	2.49	0.47
1:C:197:VAL:H	1:C:223:HIS:CD2	2.31	0.47
1:A:373:LEU:HD23	1:A:539:LEU:HD11	1.97	0.46
1:B:447:HIS:HD2	2:B:600:TQV:C2	2.28	0.46
1:B:522:ARG:HB3	6:B:2138:HOH:O	2.15	0.46
1:B:543:THR:O	1:B:543:THR:OG1	2.29	0.46
1:C:528:THR:O	1:C:531:PHE:HB3	2.15	0.46
1:D:339:LEU:HD13	1:D:346:PHE:CE2	2.50	0.46
1:A:75:THR:O	1:A:78:PRO:HD3	2.15	0.46
1:D:124:TYR:HB3	1:D:297[A]:PHE:CD2	2.50	0.46
1:D:32:PHE:HB3	1:D:35:ILE:HD11	1.97	0.46
1:A:11:ARG:N	6:A:2011:HOH:O	2.35	0.46
1:B:297[A]:PHE:CG	1:B:298:SER:N	2.82	0.46
1:A:86:TRP:CD2	2:A:600:TQV:H5	2.50	0.46
1:B:109:ALA:HB3	6:B:2035:HOH:O	2.15	0.46
1:B:26:GLY:HA3	1:B:140:GLN:OE1	2.16	0.46
1:C:124:TYR:HB3	1:C:297[A]:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:CG2	1:D:253:ARG:HH21	2.22	0.46
1:C:289:LEU:HA	1:C:290:PRO:HD3	1.78	0.46
1:A:239:VAL:HG23	1:A:302:VAL:HG23	1.98	0.46
1:B:216:LEU:HB3	1:B:217:PRO:HD3	1.98	0.46
1:B:397:ALA:O	1:B:401:VAL:HG23	2.16	0.46
1:A:536:LEU:HD23	6:A:2240:HOH:O	2.16	0.46
1:C:111:PRO:HB2	1:C:193:ASP:HB2	1.98	0.46
1:C:276:ARG:N	1:C:276:ARG:HD2	2.29	0.46
1:C:66:GLN:HG3	1:C:98:TYR:CD2	2.51	0.46
1:D:300:VAL:HB	1:D:301:PRO:HD2	1.97	0.46
1:D:328:VAL:O	1:D:427:ALA:HA	2.15	0.46
1:C:270:ILE:O	1:C:274:ARG:HG3	2.16	0.45
1:D:113:PRO:HG3	1:D:485:ARG:HG2	1.97	0.45
1:D:369:GLN:HB2	6:D:2139:HOH:O	2.17	0.45
1:A:166:GLU:HG2	6:A:2144:HOH:O	2.15	0.45
1:B:414:LEU:O	1:B:418:LEU:HG	2.17	0.45
1:C:346:PHE:HZ	1:C:354:ILE:HD13	1.81	0.45
1:D:114:VAL:HB	1:D:197:VAL:HG22	1.97	0.45
1:D:245:ARG:NH2	1:D:266:ASP:OD1	2.50	0.45
1:B:192:GLY:O	1:B:194:PRO:HD3	2.16	0.45
1:C:443:MET:HB3	1:C:446:PRO:HG3	1.98	0.45
1:D:31:ALA:HB1	1:D:33:LEU:HD21	1.99	0.45
1:A:499:GLN:HB3	6:A:2223:HOH:O	2.15	0.45
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.97	0.45
1:B:86:TRP:CD2	2:B:600:TQV:H5	2.52	0.45
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.72	0.45
1:A:46:ARG:HD2	1:A:274:ARG:HG2	1.99	0.44
1:C:81:GLU:HG3	6:C:2076:HOH:O	2.17	0.44
1:D:161:LEU:HD11	1:D:269:LEU:HD23	1.99	0.44
1:D:231:THR:HG21	1:D:411:VAL:HA	1.99	0.44
1:B:426:TYR:HB3	1:B:500:TRP:NE1	2.33	0.44
1:D:112:THR:CG2	1:D:144:ALA:HA	2.40	0.44
1:D:539:LEU:O	1:D:543:THR:HG22	2.17	0.44
1:A:45:ARG:NH1	6:A:2034:HOH:O	2.48	0.44
1:A:77:TYR:O	1:A:80:PHE:HB3	2.18	0.44
1:B:166:GLU:HB3	1:B:274:ARG:HH12	1.83	0.44
1:C:170:ASN:O	1:C:173:LEU:HB2	2.18	0.44
1:D:346:PHE:CE1	1:D:354:ILE:HG21	2.53	0.44
1:D:447:HIS:HD2	2:D:600:TQV:C2	2.30	0.44
1:D:522[B]:ARG:H	1:D:522[B]:ARG:HE	1.66	0.44
1:C:274:ARG:HD3	6:C:2041:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:HG3	1:A:314:ALA:N	2.32	0.44
1:C:527:GLN:N	5:C:1547:SO4:O3	2.44	0.44
1:C:536:LEU:HA	1:C:536:LEU:HD23	1.74	0.44
1:C:173:LEU:O	1:C:176:GLN:HB2	2.18	0.44
1:C:338:PHE:HE2	2:C:600:TQV:H8A	1.83	0.44
1:D:238:THR:HG22	1:D:301:PRO:HB2	2.00	0.44
1:B:402:VAL:O	1:B:406:ASN:HB2	2.18	0.43
1:C:297[A]:PHE:CG	1:C:298:SER:N	2.86	0.43
1:C:81:GLU:O	1:C:85:MET:HG2	2.18	0.43
1:D:504:THR:OG1	1:D:507:ALA:HB3	2.17	0.43
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.86	0.43
1:B:390:ASP:HA	1:B:391:PRO:HD2	1.84	0.43
1:D:23:LYS:HG3	6:D:2012:HOH:O	2.18	0.43
1:D:313:GLU:HG3	6:D:2160:HOH:O	2.18	0.43
1:C:202:GLU:HA	1:C:228:GLN:O	2.19	0.43
1:C:328:VAL:O	1:C:427:ALA:HA	2.17	0.43
1:B:265:ASN:OD1	1:B:267:THR:OG1	2.36	0.43
1:A:404:ASP:HA	1:A:408:VAL:HB	2.00	0.43
1:D:501:PRO:HA	1:D:502:PRO:HD3	1.95	0.43
1:A:282:VAL:O	1:A:284:HIS:N	2.52	0.43
1:A:107:ARG:NH1	1:A:189:ALA:O	2.52	0.43
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.99	0.43
2:A:600:TQV:H2	2:A:600:TQV:O1P	2.18	0.43
1:B:115:LEU:HD21	1:B:484:ALA:HB2	2.00	0.43
1:B:531:PHE:CE1	1:B:536:LEU:HG	2.54	0.43
1:C:234:GLY:O	6:C:2150:HOH:O	2.21	0.43
1:C:277:PRO:O	1:C:280:ASP:HB3	2.18	0.43
1:A:253:ARG:NH2	4:D:1991:CL:CL	2.89	0.43
1:B:458:PRO:HG3	1:B:465:TYR:CD2	2.54	0.43
1:D:352:SER:O	1:D:395:ARG:HG3	2.19	0.43
1:D:492:PRO:O	1:D:494:ASP:N	2.44	0.43
1:C:397:ALA:O	1:C:401:VAL:HG23	2.19	0.42
1:D:46:ARG:O	1:D:274:ARG:HD3	2.19	0.42
1:C:200:PHE:CB	1:C:226:VAL:HB	2.48	0.42
1:A:119:TYR:CE1	1:A:126:GLY:HA3	2.55	0.42
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.42
1:A:460:ASP:HB3	1:A:463:LEU:HD12	1.99	0.42
1:D:200:PHE:CB	1:D:226:VAL:HB	2.49	0.42
1:D:296:ARG:N	2:D:600:TQV:H12	2.33	0.42
1:C:45:ARG:HA	1:C:45:ARG:HD2	1.78	0.42
1:D:46:ARG:NH2	1:D:94:GLU:OE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:HA	6:B:2037:HOH:O	2.20	0.42
1:B:68:VAL:HG23	1:B:90:ARG:HB2	2.02	0.42
1:C:17:LEU:HB3	1:C:60:LEU:HB3	2.02	0.42
1:B:537:PRO:C	1:B:539:LEU:H	2.23	0.42
1:D:200:PHE:HB2	1:D:226:VAL:HB	2.02	0.42
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.01	0.42
1:C:369[A]:GLN:HG2	6:C:2152:HOH:O	2.20	0.42
1:D:361:ALA:O	1:D:365:ILE:HG13	2.20	0.42
1:B:433:ARG:HH12	1:B:441:LEU:HA	1.83	0.42
1:B:359:PHE:HD2	1:B:360:LEU:HD23	1.84	0.41
1:B:467:THR:HG22	1:B:470:ARG:NH2	2.34	0.41
1:D:258:PRO:HD2	1:D:259:PRO:HA	2.01	0.41
1:D:494:ASP:HB2	6:D:2172:HOH:O	2.20	0.41
1:A:94:GLU:HA	6:A:2016:HOH:O	2.20	0.41
1:D:295:PHE:O	1:D:296:ARG:HD3	2.19	0.41
1:C:376:GLU:OE1	1:D:538:LYS:HD2	2.21	0.41
1:C:375:ALA:O	1:C:379:VAL:HG23	2.21	0.41
1:D:531:PHE:CZ	1:D:536:LEU:HD23	2.56	0.41
1:A:297[A]:PHE:CG	1:A:298:SER:N	2.88	0.41
1:A:374:ALA:HA	1:A:539:LEU:HD23	2.02	0.41
1:A:86:TRP:HB3	6:A:2061:HOH:O	2.21	0.41
1:B:277:PRO:HG2	1:B:280:ASP:CG	2.41	0.41
1:A:138:LEU:HA	1:A:477:MET:HE3	2.03	0.41
1:A:86:TRP:CE2	2:A:600:TQV:H5	2.56	0.41
1:C:224:ARG:HG2	1:C:325:GLN:HB2	2.01	0.41
1:D:26:GLY:N	6:D:2013:HOH:O	2.31	0.41
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.91	0.41
1:D:288:VAL:HG23	1:D:298:SER:HB3	2.03	0.41
1:B:205:GLY:O	1:B:209:VAL:HG23	2.21	0.41
1:C:33:LEU:HB2	1:C:64:THR:O	2.20	0.41
1:A:437:LEU:HD12	1:A:439:TRP:H	1.86	0.41
1:B:104:PRO:HG2	1:B:108:PRO:HD3	2.02	0.41
1:B:50:PRO:HB2	1:B:178:LEU:HD22	2.03	0.41
1:B:515:LEU:H	1:B:515:LEU:HG	1.58	0.41
1:C:66:GLN:HG3	1:C:98:TYR:CG	2.56	0.41
1:D:500:TRP:HA	1:D:501:PRO:HD2	1.92	0.41
1:A:132:VAL:HG22	6:A:2060:HOH:O	2.21	0.41
1:A:359:PHE:CG	1:A:394:LEU:HD22	2.56	0.40
1:A:511:VAL:HB	1:A:518:LEU:HD22	2.03	0.40
1:C:324:LEU:HA	1:C:324:LEU:HD12	1.91	0.40
1:D:319:GLY:HA3	1:D:321:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ASP:OD2	1:B:462:SER:OG	2.35	0.40
1:B:481:THR:O	1:B:485:ARG:HG2	2.21	0.40
1:B:80:PHE:CD1	1:B:348:LYS:HE2	2.57	0.40
1:A:170:ASN:HB3	1:A:173:LEU:HD12	2.03	0.40
1:B:250:LEU:HG	1:B:288:VAL:HG12	2.03	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	541/543 (100%)	500 (92%)	35 (6%)	6 (1%)	17	53
1	B	538/543 (99%)	485 (90%)	45 (8%)	8 (2%)	12	45
1	C	542/543 (100%)	500 (92%)	36 (7%)	6 (1%)	17	53
1	D	543/543 (100%)	503 (93%)	34 (6%)	6 (1%)	17	53
All	All	2164/2172 (100%)	1988 (92%)	150 (7%)	26 (1%)	15	50

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	GLY
1	B	495	SER
1	B	542	ALA
1	D	497	SER
1	A	283	ASP
1	C	496	LYS
1	D	260	GLY
1	A	257	CYS
1	A	261	GLY
1	A	497	SER

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Mol	Chain	Res	Type
1	C	127	ALA
1	A	262	ALA
1	B	109	ALA
1	B	492	PRO
1	B	497	SER
1	C	110	SER
1	C	342	GLY
1	D	25	PRO
1	D	261	GLY
1	B	26	GLY
1	C	261	GLY
1	C	506	ALA
1	A	523	GLY
1	D	342	GLY
1	B	255	VAL
1	D	498	PRO

### 5.3.2 Protein sidechains ⓘ

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	444/443 (100%)	411 (93%)	33 (7%)	16	47
1	B	441/443 (100%)	408 (92%)	33 (8%)	16	46
1	C	445/443 (100%)	410 (92%)	35 (8%)	14	43
1	D	446/443 (101%)	416 (93%)	30 (7%)	19	52
All	All	1776/1772 (100%)	1645 (93%)	131 (7%)	16	47

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	VAL
1	A	23	LYS
1	A	70	TYR
1	A	81	GLU

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Mol	Chain	Res	Type
1	A	84	GLU
1	A	107	ARG
1	A	132	VAL
1	A	136	ARG
1	A	149	MET
1	A	159	LEU
1	A	164	SER
1	A	200	PHE
1	A	211	MET
1	A	216	LEU
1	A	220	SER
1	A	253	ARG
1	A	257	CYS
1	A	267	THR
1	A	295	PHE
1	A	313	GLU
1	A	317	ASN
1	A	325	GLN
1	A	326	VAL
1	A	328	VAL
1	A	376	GLU
1	A	386	LEU
1	A	417	ARG
1	A	437	LEU
1	A	441	LEU
1	A	497	SER
1	A	540	LEU
1	A	543	THR
1	B	8	LEU
1	B	29	VAL
1	B	45	ARG
1	B	103	THR
1	B	136	ARG
1	B	141	VAL
1	B	149	MET
1	B	200	PHE
1	B	211	MET
1	B	245	ARG
1	B	265	ASN
1	B	287	HIS
1	B	295	PHE
1	B	351	GLU

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Mol	Chain	Res	Type
1	B	376	GLU
1	B	380	LEU
1	B	386	LEU
1	B	392	THR
1	B	438	THR
1	B	451	ILE
1	B	472	PHE
1	B	475	ARG
1	B	478	LYS
1	B	493	ARG
1	B	496	LYS
1	B	497	SER
1	B	515	LEU
1	B	518	LEU
1	B	522	ARG
1	B	524	LEU
1	B	536	LEU
1	B	540	LEU
1	B	543	THR
1	C	13	ARG
1	C	33	LEU
1	C	60	LEU
1	C	84	GLU
1	C	107	ARG
1	C	110	SER
1	C	132	VAL
1	C	136	ARG
1	C	146	LEU
1	C	211	MET
1	C	216	LEU
1	C	228	GLN
1	C	229	SER
1	C	257	CYS
1	C	276	ARG
1	C	295	PHE
1	C	298	SER
1	C	323	ASP
1	C	327	LEU
1	C	369[A]	GLN
1	C	369[B]	GLN
1	C	380	LEU
1	C	386	LEU

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Mol	Chain	Res	Type
1	C	387[A]	HIS
1	C	387[B]	HIS
1	C	421	GLN
1	C	438	THR
1	C	441	LEU
1	C	462	SER
1	C	466	THR
1	C	471	ILE
1	C	499	GLN
1	C	514	ASN
1	C	522	ARG
1	C	524	LEU
1	D	9	LEU
1	D	11	ARG
1	D	13	ARG
1	D	23	LYS
1	D	103	THR
1	D	110	SER
1	D	132	VAL
1	D	140	GLN
1	D	211	MET
1	D	216	LEU
1	D	281	LEU
1	D	285	GLU
1	D	291	GLN
1	D	295	PHE
1	D	298	SER
1	D	318	THR
1	D	333	ASP
1	D	364	ARG
1	D	372	ASP
1	D	386	LEU
1	D	413	GLN
1	D	437	LEU
1	D	438	THR
1	D	441	LEU
1	D	459	LEU
1	D	467	THR
1	D	491	ASP
1	D	496	LYS
1	D	499	GLN
1	D	536	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	223	HIS
1	D	67	ASN
1	D	228	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 11 are monoatomic - leaving 26 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	$\# Z  > 2$
5	SO4	A	1545	-	4,4,4	0.19	0	6,6,6	0.25	0
5	SO4	A	1546	-	4,4,4	0.15	0	6,6,6	0.09	0
5	SO4	A	1547	-	4,4,4	0.19	0	6,6,6	0.31	0
5	SO4	A	1548	-	4,4,4	0.17	0	6,6,6	0.21	0
5	SO4	A	1549	-	4,4,4	0.19	0	6,6,6	0.24	0
5	SO4	A	1550	-	4,4,4	0.17	0	6,6,6	0.20	0
2	TQV	A	600	1	17,20,21	1.14	1 (5%)	22,26,29	1.10	2 (9%)
3	NAG	A	701	1	14,14,15	0.45	0	15,19,21	1.05	1 (6%)
5	SO4	B	1545	-	4,4,4	0.17	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	1546	-	4,4,4	0.13	0	6,6,6	0.13	0
5	SO4	B	1547	-	4,4,4	0.17	0	6,6,6	0.12	0
2	TQV	B	600	1	17,20,21	1.14	2 (11%)	22,26,29	1.34	5 (22%)
3	NAG	B	701	1	14,14,15	0.46	0	15,19,21	1.65	3 (20%)
3	NAG	B	702	1	14,14,15	0.48	0	15,19,21	2.17	1 (6%)
5	SO4	C	1547	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	C	1548	-	4,4,4	0.26	0	6,6,6	0.34	0
5	SO4	C	1549	-	4,4,4	0.19	0	6,6,6	0.15	0
2	TQV	C	600	1	17,20,21	0.99	1 (5%)	22,26,29	1.46	2 (9%)
3	NAG	C	701	1	14,14,15	0.44	0	15,19,21	1.31	1 (6%)
5	SO4	D	1545	-	4,4,4	0.17	0	6,6,6	0.15	0
5	SO4	D	1546	-	4,4,4	0.13	0	6,6,6	0.19	0
5	SO4	D	1547	-	4,4,4	0.15	0	6,6,6	0.08	0
2	TQV	D	600	1	17,20,21	1.30	2 (11%)	22,26,29	1.37	3 (13%)
3	NAG	D	701	1	14,14,15	0.38	0	15,19,21	2.07	2 (13%)
3	NAG	D	702	1	14,14,15	0.53	0	15,19,21	2.03	2 (13%)
3	NAG	D	703	1	14,14,15	0.61	0	15,19,21	1.43	2 (13%)

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
5	SO4	A	1545	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1546	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1547	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1548	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1549	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1550	-	-	0/0/0/0	0/0/0/0
2	TQV	A	600	1	-	0/6/9/11	0/2/2/2
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	SO4	B	1545	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1546	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1547	-	-	0/0/0/0	0/0/0/0
2	TQV	B	600	1	-	0/6/9/11	0/2/2/2
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
5	SO4	C	1547	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1548	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1549	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TQV	C	600	1	-	0/6/9/11	0/2/2/2
3	NAG	C	701	1	-	0/6/23/26	0/1/1/1
5	SO4	D	1545	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1546	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1547	-	-	0/0/0/0	0/0/0/0
2	TQV	D	600	1	-	0/6/9/11	0/2/2/2
3	NAG	D	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1	-	0/6/23/26	0/1/1/1
3	NAG	D	703	1	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	TQV	C8-C9	-4.16	1.39	1.50
2	D	600	TQV	C8-C9	-4.14	1.39	1.50
2	B	600	TQV	C8-C9	-4.03	1.39	1.50
2	C	600	TQV	C8-C9	-3.87	1.40	1.50
2	D	600	TQV	O1P-C8	-3.00	1.40	1.44
2	B	600	TQV	O1P-C8	-2.05	1.42	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	NAG	C4-C3-C2	-2.40	107.50	111.02
2	B	600	TQV	O2P-C1-C6	-2.32	116.45	118.43
2	D	600	TQV	C7-C6-C1	-2.22	117.55	120.94
2	D	600	TQV	O2P-C1-C6	-2.21	116.54	118.43
3	B	701	NAG	O7-C7-C8	-2.04	118.34	122.06
3	D	702	NAG	C3-C4-C5	2.05	113.82	110.22
2	A	600	TQV	C10-C9-C14	2.09	120.50	118.18
2	B	600	TQV	O1P-C8-C9	2.13	113.53	109.33
2	B	600	TQV	O2P-C1-C2	2.16	124.24	120.37
2	C	600	TQV	P-O2P-C1	2.20	133.61	121.82
2	B	600	TQV	C10-C9-C14	2.21	120.63	118.18
3	D	703	NAG	C1-C2-N2	2.59	114.92	110.49
2	D	600	TQV	C10-C9-C14	2.62	121.09	118.18
2	B	600	TQV	P-O2P-C1	2.66	136.04	121.82
2	A	600	TQV	P-O2P-C1	2.69	136.22	121.82
3	B	701	NAG	C1-O5-C5	3.11	116.45	112.17
3	A	701	NAG	C1-O5-C5	3.60	117.13	112.17
3	D	703	NAG	C1-O5-C5	3.90	117.54	112.17
3	B	701	NAG	C2-N2-C7	3.93	128.68	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	TQV	O1P-C8-C9	4.41	118.04	109.33
3	C	701	NAG	C1-O5-C5	4.41	118.25	112.17
3	D	701	NAG	C1-O5-C5	6.87	121.63	112.17
3	D	702	NAG	C1-O5-C5	7.03	121.86	112.17
3	B	702	NAG	C1-O5-C5	7.40	122.37	112.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	703	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TQV	4	0
2	B	600	TQV	3	0
5	C	1547	SO4	1	0
2	C	600	TQV	7	0
2	D	600	TQV	4	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	540/543 (99%)	-0.32	12 (2%) 62 43	14, 33, 69, 138	0
1	B	539/543 (99%)	-0.06	28 (5%) 28 17	26, 61, 107, 165	0
1	C	540/543 (99%)	-0.47	8 (1%) 74 55	14, 32, 72, 133	0
1	D	540/543 (99%)	-0.35	5 (0%) 84 69	21, 43, 79, 146	0
All	All	2159/2172 (99%)	-0.30	53 (2%) 58 39	14, 41, 94, 165	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	4.7
1	B	543	THR	4.6
1	D	493	ARG	4.4
1	A	259	PRO	4.3
1	C	493	ARG	4.2
1	A	497	SER	4.1
1	B	493	ARG	3.8
1	A	264	GLY	3.6
1	B	21	ARG	3.6
1	A	495	SER	3.5
1	A	263	GLY	3.5
1	C	495	SER	3.4
1	B	30	SER	3.3
1	B	59	VAL	3.3
1	C	263	GLY	3.2
1	C	264	GLY	3.1
1	D	21	ARG	3.1
1	A	260	GLY	3.0
1	B	9	LEU	3.0
1	B	495	SER	2.9
1	C	261	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	32	PHE	2.9
1	B	77	TYR	2.8
1	A	493	ARG	2.8
1	B	6	PRO	2.7
1	B	349	ASP	2.7
1	B	109	ALA	2.6
1	B	351	GLU	2.6
1	B	496	LYS	2.5
1	C	260	GLY	2.4
1	B	7	GLN	2.4
1	B	190	PHE	2.4
1	B	17	LEU	2.4
1	D	543	THR	2.3
1	C	496	LYS	2.3
1	B	110	SER	2.3
1	D	495	SER	2.3
1	A	262	ALA	2.3
1	B	20	ILE	2.3
1	A	543	THR	2.3
1	B	347	SER	2.3
1	C	262	ALA	2.2
1	A	496	LYS	2.2
1	B	189	ALA	2.2
1	D	7	GLN	2.1
1	B	353	LEU	2.1
1	B	346	PHE	2.1
1	A	498	PRO	2.1
1	A	258	PRO	2.1
1	B	194	PRO	2.1
1	B	23	LYS	2.0
1	B	22	LEU	2.0
1	B	108	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	1550	5/5	0.84	0.50	6.67	122,123,127,131	0
5	SO4	B	1546	5/5	0.78	0.35	4.74	166,166,167,169	0
5	SO4	C	1548	5/5	0.96	0.20	2.51	54,56,62,66	0
2	TQV	C	600	19/20	0.97	0.21	2.13	22,49,83,83	8
3	NAG	B	702	14/15	0.76	0.49	1.98	68,106,117,120	0
2	TQV	D	600	19/20	0.94	0.23	1.71	34,46,116,118	8
2	TQV	B	600	19/20	0.94	0.23	1.63	42,60,97,97	8
2	TQV	A	600	19/20	0.97	0.20	1.32	27,44,57,59	8
5	SO4	A	1548	5/5	0.93	0.21	1.24	92,93,96,100	0
5	SO4	D	1545	5/5	0.97	0.17	0.25	68,69,72,79	0
4	CL	C	1545	1/1	0.98	0.07	-2.42	35,35,35,35	0
4	CL	A	1990	1/1	0.91	0.07	-3.24	59,59,59,59	0
4	CL	A	1544	1/1	0.98	0.06	-	67,67,67,67	0
5	SO4	C	1547	5/5	0.96	0.13	-	75,82,83,87	0
4	CL	C	1990	1/1	0.97	0.12	-	50,50,50,50	0
3	NAG	D	703	14/15	0.74	0.36	-	109,127,137,141	0
5	SO4	D	1547	5/5	0.93	0.36	-	138,139,141,144	0
4	CL	C	1544	1/1	0.82	0.15	-	55,55,55,55	0
3	NAG	D	702	14/15	0.78	0.33	-	60,102,109,110	0
5	SO4	B	1547	5/5	0.91	0.16	-	119,122,123,128	0
3	NAG	D	701	14/15	0.76	0.24	-	77,101,115,121	0
4	CL	A	1991	1/1	0.78	0.13	-	66,66,66,66	0
5	SO4	B	1545	5/5	0.95	0.14	-	75,90,92,97	0
4	CL	D	1544	1/1	0.77	0.20	-	84,84,84,84	0
3	NAG	A	701	14/15	0.80	0.35	-	96,119,122,123	0
4	CL	D	1991	1/1	0.72	0.12	-	82,82,82,82	0
3	NAG	B	701	14/15	0.79	0.18	-	98,103,107,110	0
5	SO4	A	1545	5/5	0.97	0.12	-	70,73,74,75	0
5	SO4	D	1546	5/5	0.87	0.32	-	116,119,120,123	0
4	CL	D	1990	1/1	0.94	0.11	-	57,57,57,57	0
5	SO4	A	1546	5/5	0.96	0.10	-	110,110,112,115	0
5	SO4	A	1549	5/5	0.81	0.21	-	106,116,120,121	0
4	CL	C	1546	1/1	0.84	0.13	-	72,72,72,72	0
5	SO4	A	1547	5/5	0.95	0.16	-	59,60,71,72	0
3	NAG	C	701	14/15	0.72	0.35	-	120,126,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	C	1549	5/5	0.94	0.29	-	113,116,118,119	0
4	CL	B	1544	1/1	0.88	0.17	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.