



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:01 PM UTC

PDB ID : 8BWK / pdb_00008bwk
Title : Metagenomic derived PL6 alginate lyase
Authors : Angen, E.F.; Wilkens, C.
Deposited on : 2022-12-06
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

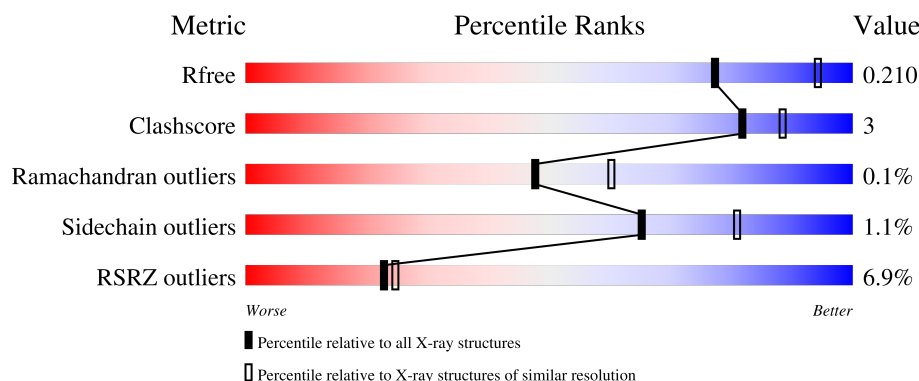
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	2% 95% 5%
1	B	728	3% 94% 6%
1	C	728	2% 92% 7%
1	D	728	20% 89% 8%

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	CL	B	806	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 45499 atoms, of which 22196 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 Alginate lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	725	Total	C	H	N	O	S	0	1	0
			11238	3554	5574	1005	1098	7			
1	B	725	Total	C	H	N	O	S	14	2	0
			11251	3558	5576	1009	1101	7			
1	C	727	Total	C	H	N	O	S	0	0	0
			11255	3558	5582	1008	1101	6			
1	D	708	Total	C	H	N	O	S	0	0	0
			10984	3480	5444	983	1071	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0P7DTY9
A	2	GLY	-	expression tag	UNP A0A0P7DTY9
A	340	ASP	ASN	conflict	UNP A0A0P7DTY9
A	355	SER	PRO	conflict	UNP A0A0P7DTY9
A	387	GLN	LYS	conflict	UNP A0A0P7DTY9
A	554	ASP	ASN	conflict	UNP A0A0P7DTY9
A	641	LYS	ASN	conflict	UNP A0A0P7DTY9
A	655	LYS	GLN	conflict	UNP A0A0P7DTY9
A	706	TYR	HIS	conflict	UNP A0A0P7DTY9
A	708	GLU	LYS	conflict	UNP A0A0P7DTY9
B	1	MET	-	initiating methionine	UNP A0A0P7DTY9
B	2	GLY	-	expression tag	UNP A0A0P7DTY9
B	340	ASP	ASN	conflict	UNP A0A0P7DTY9
B	355	SER	PRO	conflict	UNP A0A0P7DTY9
B	387	GLN	LYS	conflict	UNP A0A0P7DTY9
B	554	ASP	ASN	conflict	UNP A0A0P7DTY9
B	641	LYS	ASN	conflict	UNP A0A0P7DTY9
B	655	LYS	GLN	conflict	UNP A0A0P7DTY9
B	706	TYR	HIS	conflict	UNP A0A0P7DTY9
B	708	GLU	LYS	conflict	UNP A0A0P7DTY9
C	1	MET	-	initiating methionine	UNP A0A0P7DTY9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	GLY	-	expression tag	UNP A0A0P7DTY9
C	340	ASP	ASN	conflict	UNP A0A0P7DTY9
C	355	SER	PRO	conflict	UNP A0A0P7DTY9
C	387	GLN	LYS	conflict	UNP A0A0P7DTY9
C	554	ASP	ASN	conflict	UNP A0A0P7DTY9
C	641	LYS	ASN	conflict	UNP A0A0P7DTY9
C	655	LYS	GLN	conflict	UNP A0A0P7DTY9
C	706	TYR	HIS	conflict	UNP A0A0P7DTY9
C	708	GLU	LYS	conflict	UNP A0A0P7DTY9
D	1	MET	-	initiating methionine	UNP A0A0P7DTY9
D	2	GLY	-	expression tag	UNP A0A0P7DTY9
D	340	ASP	ASN	conflict	UNP A0A0P7DTY9
D	355	SER	PRO	conflict	UNP A0A0P7DTY9
D	387	GLN	LYS	conflict	UNP A0A0P7DTY9
D	554	ASP	ASN	conflict	UNP A0A0P7DTY9
D	641	LYS	ASN	conflict	UNP A0A0P7DTY9
D	655	LYS	GLN	conflict	UNP A0A0P7DTY9
D	706	TYR	HIS	conflict	UNP A0A0P7DTY9
D	708	GLU	LYS	conflict	UNP A0A0P7DTY9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	3	Total Cl 3 3	0	0
3	C	2	Total Cl 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

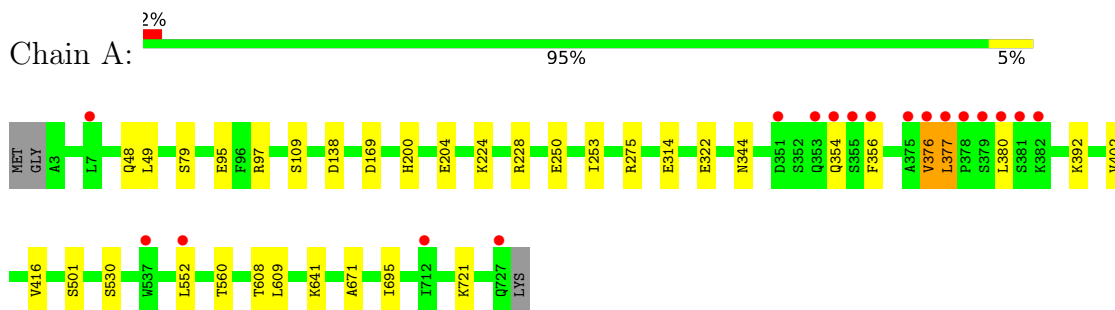
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total	O	0	0
			242	242		
5	B	205	Total	O	0	0
			205	205		
5	C	125	Total	O	0	0
			125	125		
5	D	94	Total	O	0	0
			94	94		

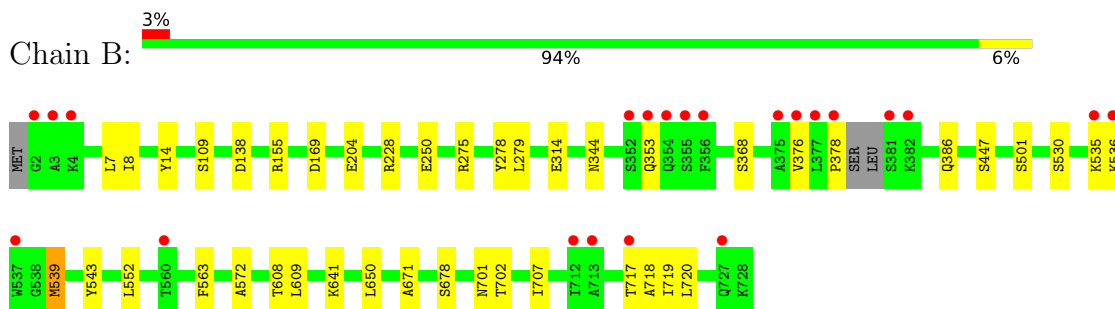
3 Residue-property plots [i](#)

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.

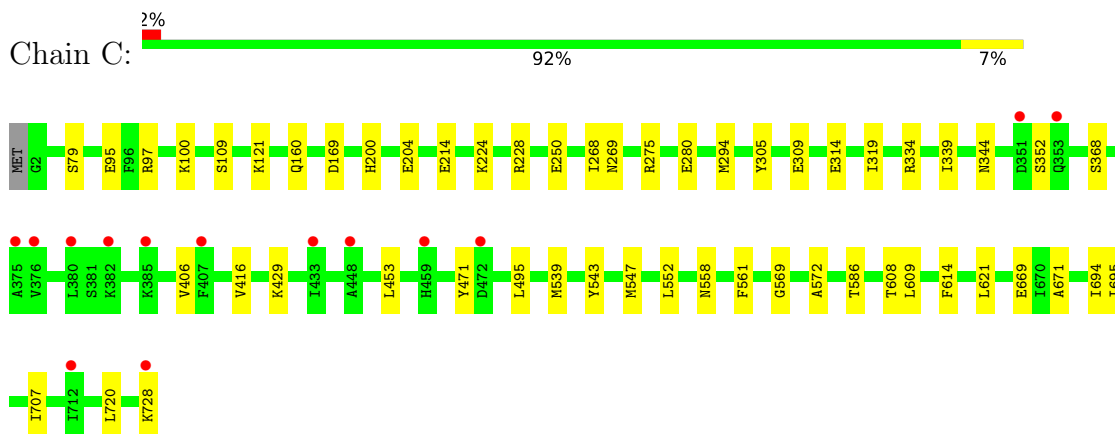
- Molecule 1: Alginate lyase



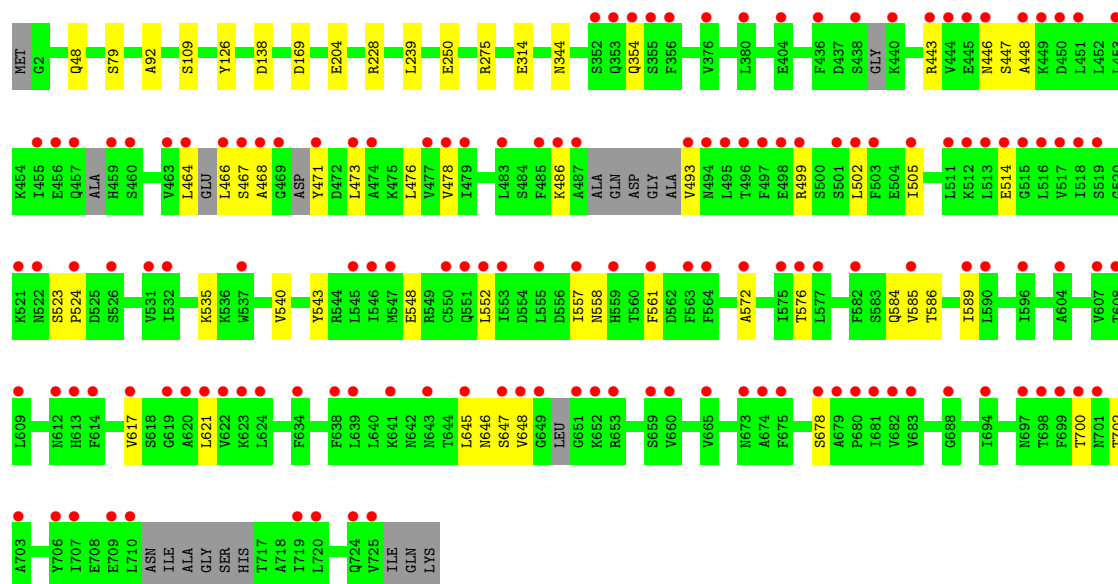
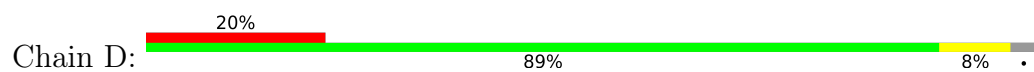
- Molecule 1: Alginate lyase



- Molecule 1: Alginate lyase



- Molecule 1: Alginate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.75Å 228.85Å 113.73Å 90.00° 101.86° 90.00°	Depositor
Resolution (Å)	63.86 – 2.29 63.86 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.9 (63.86-2.29) 98.0 (63.86-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.210 0.180 , 0.210	Depositor DCC
R_{free} test set	7888 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	45499	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, PEG

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	0.11	0/5771	0.31	0/7812
1	B	0.11	0/5779	0.30	0/7820
1	C	0.09	0/5777	0.28	0/7818
1	D	0.10	0/5636	0.29	0/7618
All	All	0.10	0/22963	0.29	0/31068

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	A	5664	5574	5574	21	0
1	B	5675	5576	5578	25	0
1	C	5673	5582	5581	29	0
1	D	5540	5444	5451	38	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	20	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	2	0
3	C	2	0	0	0	0
4	B	7	10	10	0	0
4	D	7	10	10	2	0
5	A	242	0	0	2	0
5	B	205	0	0	4	0
5	C	125	0	0	2	0
5	D	94	0	0	2	0
All	All	23303	22196	22204	114	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 3.

All (114) 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)
1:D:486:LYS:HG2	1:D:514:GLU:HB2	1.53	0.89
1:D:535:LYS:N	5:D:901:HOH:O	2.11	0.84
3:B:806:CL:CL	5:B:1049:HOH:O	2.40	0.77
1:D:621:LEU:HD11	1:D:645:LEU:HD21	1.67	0.76
1:C:728:LYS:O	5:C:901:HOH:O	2.08	0.72
1:A:322:GLU:OE1	5:A:901:HOH:O	2.09	0.70
1:D:478:VAL:HG22	4:D:802:PEG:H42	1.72	0.70
1:C:558:ASN:O	1:C:586:THR:HG21	1.95	0.66
1:D:466:LEU:N	1:D:471:TYR:HH	1.95	0.64
1:C:471:TYR:HB2	1:C:495:LEU:HD23	1.81	0.62
1:C:561:PHE:H	1:C:586:THR:HG23	1.65	0.62
1:D:514:GLU:HA	1:D:548:GLU:O	2.01	0.61
3:B:806:CL:CL	5:B:1099:HOH:O	2.54	0.59
1:D:621:LEU:CD1	1:D:645:LEU:HD21	2.35	0.56
1:A:608:THR:C	1:A:609:LEU:HD12	2.31	0.56
1:A:48:GLN:C	1:A:49:LEU:HD22	2.32	0.55
1:D:505:ILE:O	5:D:901:HOH:O	2.18	0.54
1:B:155:ARG:NH2	5:B:904:HOH:O	2.39	0.54
1:B:278:TYR:C	1:B:279:LEU:HD12	2.34	0.53
1:B:719:ILE:C	1:B:720:LEU:HD23	2.34	0.53
1:D:476:LEU:O	4:D:802:PEG:O1	2.17	0.53
1:D:486:LYS:CG	1:D:514:GLU:HB2	2.31	0.52
1:D:585:VAL:HB	1:D:617:VAL:HG13	1.93	0.51
1:C:543:TYR:CZ	1:C:572:ALA:HB2	2.46	0.51
1:D:543:TYR:CZ	1:D:572:ALA:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:VAL:O	1:D:48:GLN:NE2	2.44	0.50
1:C:204:GLU:HA	1:C:228:ARG:O	2.12	0.50
1:C:344:ASN:HA	1:C:368:SER:O	2.12	0.49
1:C:608:THR:C	1:C:609:LEU:HD12	2.36	0.49
1:B:169:ASP:HA	1:B:204:GLU:O	2.13	0.49
1:B:275:ARG:HA	1:B:314:GLU:O	2.13	0.49
1:B:608:THR:C	1:B:609:LEU:HD12	2.37	0.49
5:A:1021:HOH:O	1:B:717:THR:HG23	2.14	0.48
1:B:204:GLU:HA	1:B:228:ARG:O	2.13	0.48
1:D:468:ALA:O	1:D:493:VAL:HG22	2.13	0.48
1:D:464:LEU:C	1:D:466:LEU:HD22	2.38	0.47
1:A:169:ASP:HA	1:A:204:GLU:O	2.14	0.47
1:A:275:ARG:HA	1:A:314:GLU:O	2.15	0.47
1:D:446:ASN:HB2	1:D:468:ALA:HB1	1.96	0.47
1:A:501:SER:HA	1:A:530:SER:O	2.14	0.47
1:B:7:LEU:HD13	1:B:7:LEU:C	2.39	0.47
1:D:576:THR:O	1:D:576:THR:HG23	2.15	0.47
1:A:204:GLU:HA	1:A:228:ARG:O	2.15	0.47
1:A:695:ILE:HD12	1:A:721:LYS:HB3	1.96	0.47
1:B:8:ILE:HG21	1:B:14:TYR:HB2	1.97	0.47
1:C:294:MET:HE1	1:C:305:TYR:CE1	2.50	0.47
1:D:275:ARG:HA	1:D:314:GLU:O	2.14	0.47
1:D:448:ALA:HB1	1:D:473:LEU:HD13	1.97	0.47
1:C:169:ASP:HA	1:C:204:GLU:O	2.15	0.46
1:A:356:PHE:CG	1:A:376:VAL:HG13	2.50	0.46
1:B:707:ILE:HD13	1:B:718:ALA:CB	2.45	0.46
1:D:558:ASN:O	1:D:586:THR:HG21	2.15	0.46
1:A:376:VAL:HG12	1:A:377:LEU:N	2.31	0.46
1:D:250:GLU:HA	1:D:275:ARG:O	2.17	0.45
1:D:169:ASP:HA	1:D:204:GLU:O	2.17	0.45
1:D:204:GLU:HA	1:D:228:ARG:O	2.17	0.45
1:A:253:ILE:HD13	1:A:416:VAL:HG22	1.99	0.44
1:B:543:TYR:CZ	1:B:572:ALA:HB2	2.53	0.44
1:C:707:ILE:HD12	1:C:720:LEU:HD11	1.99	0.44
1:A:392:LYS:HB2	1:A:402:VAL:HG22	1.98	0.44
1:B:717:THR:O	1:B:717:THR:HG22	2.17	0.44
1:B:228:ARG:HA	1:B:250:GLU:O	2.17	0.44
1:A:560:THR:HG22	1:A:560:THR:O	2.18	0.43
1:D:646:ASN:C	1:D:647:SER:HG	2.22	0.43
1:A:79:SER:HA	1:A:109:SER:O	2.18	0.43
1:C:547:MET:HE1	1:C:552:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:589:ILE:HD12	1:D:621:LEU:HA	2.00	0.43
1:C:608:THR:O	1:C:609:LEU:HD12	2.19	0.43
1:D:617:VAL:HB	1:D:648:VAL:HG13	2.00	0.43
1:B:552:LEU:HD22	1:B:563:PHE:CD1	2.54	0.43
1:C:453:LEU:C	1:C:453:LEU:HD23	2.44	0.43
1:B:250:GLU:HA	1:B:275:ARG:O	2.19	0.43
1:C:228:ARG:HA	1:C:250:GLU:O	2.19	0.42
1:C:275:ARG:HA	1:C:314:GLU:O	2.19	0.42
1:A:200:HIS:HA	1:A:224:LYS:O	2.19	0.42
1:A:228:ARG:HA	1:A:250:GLU:O	2.19	0.42
1:D:523:SER:HB3	1:D:524:PRO:HD2	2.01	0.42
1:C:671:ALA:HA	1:C:695:ILE:O	2.20	0.42
1:D:92:ALA:HA	1:D:126:TYR:O	2.19	0.42
1:B:641:LYS:HA	1:B:671:ALA:O	2.20	0.42
1:B:717:THR:HG21	5:B:1082:HOH:O	2.19	0.42
1:D:678:SER:O	1:D:702:THR:HG23	2.19	0.42
1:A:641:LYS:HA	1:A:671:ALA:O	2.20	0.42
1:B:344[B]:ASN:HA	1:B:368:SER:O	2.20	0.42
1:B:535:LYS:HB2	1:B:539:MET:HG3	2.01	0.42
1:D:138:ASP:HA	1:D:169:ASP:O	2.20	0.42
1:A:95:GLU:OE2	1:A:97:ARG:NE	2.43	0.42
1:A:314:GLU:HA	1:A:344:ASN:O	2.20	0.41
1:B:678:SER:O	1:B:702:THR:HG23	2.20	0.41
1:D:228:ARG:HA	1:D:250:GLU:O	2.20	0.41
1:D:514:GLU:HG2	1:D:548:GLU:HB2	2.01	0.41
1:D:561:PHE:H	1:D:586:THR:HG23	1.84	0.41
1:C:250:GLU:HA	1:C:275:ARG:O	2.19	0.41
1:B:501:SER:HA	1:B:530:SER:O	2.20	0.41
1:D:109:SER:HA	1:D:138:ASP:O	2.21	0.41
1:B:138:ASP:HA	1:B:169:ASP:O	2.21	0.41
1:C:280:GLU:HA	1:C:319:ILE:O	2.21	0.41
1:C:561:PHE:HB3	1:C:586:THR:HG22	2.03	0.41
1:B:109:SER:HA	1:B:138:ASP:O	2.20	0.41
1:C:614:PHE:CG	1:C:621:LEU:HD21	2.55	0.41
1:D:239:LEU:C	1:D:239:LEU:HD23	2.46	0.41
1:A:377:LEU:HD23	1:A:380:LEU:HB2	2.03	0.41
1:B:376:VAL:HG13	1:B:386:GLN:HB2	2.02	0.41
1:C:200:HIS:HA	1:C:224:LYS:O	2.21	0.40
1:D:473:LEU:HD22	1:D:473:LEU:H	1.85	0.40
1:C:268:ILE:HG22	1:C:269:ASN:N	2.36	0.40
1:C:79:SER:HA	1:C:109:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLU:OE2	1:C:97:ARG:NH2	2.55	0.40
1:A:138:ASP:HA	1:A:169:ASP:O	2.21	0.40
1:C:121:LYS:NZ	1:C:569:GLY:O	2.48	0.40
1:C:694:ILE:C	1:C:695:ILE:HD12	2.46	0.40
1:D:443:ARG:NH1	1:D:467:SER:OG	2.54	0.40
1:C:429:LYS:NZ	5:C:908:HOH:O	2.48	0.40
1:D:79:SER:HA	1:D:109:SER:O	2.21	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	724/728 (100%)	698 (96%)	24 (3%)	2 (0%)	36	46
1	B	725/728 (100%)	699 (96%)	25 (3%)	1 (0%)	48	60
1	C	725/728 (100%)	694 (96%)	30 (4%)	1 (0%)	48	60
1	D	692/728 (95%)	658 (95%)	34 (5%)	0	100	100
All	All	2866/2912 (98%)	2749 (96%)	113 (4%)	4 (0%)	48	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	B	378	PRO
1	C	352	SER
1	A	376	VAL

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	619/620 (100%)	617 (100%)	2 (0%)	86	93
1	B	619/620 (100%)	613 (99%)	6 (1%)	68	82
1	C	619/620 (100%)	610 (98%)	9 (2%)	57	75
1	D	607/620 (98%)	597 (98%)	10 (2%)	55	73
All	All	2464/2480 (99%)	2437 (99%)	27 (1%)	65	81

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	A	552	LEU
1	B	353	GLN
1	B	447	SER
1	B	536	LYS
1	B	539	MET
1	B	650	LEU
1	B	701	ASN
1	C	100	LYS
1	C	160	GLN
1	C	214	GLU
1	C	309	GLU
1	C	334	ARG
1	C	339	ILE
1	C	406	VAL
1	C	539	MET
1	C	669	GLU
1	D	344	ASN
1	D	354	GLN
1	D	447	SER
1	D	499	ARG
1	D	502	LEU
1	D	540	VAL
1	D	552	LEU

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Mol	Chain	Res	Type
1	D	557	ILE
1	D	584	GLN
1	D	700	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	30	GLN
1	A	193	HIS
1	A	205	ASN
1	A	210	GLN
1	A	229	ASN
1	B	12	GLN
1	B	105	ASN
1	B	163	GLN
1	B	315	ASN
1	B	323	HIS
1	B	325	GLN
1	B	345	ASN
1	B	350	ASN
1	B	369	ASN
1	B	387	GLN
1	B	489	GLN
1	B	603	ASN
1	B	611	ASN
1	B	701	ASN
1	B	722	ASN
1	C	44	GLN
1	C	66	GLN
1	C	160	GLN
1	C	200	HIS
1	C	205	ASN
1	C	210	GLN
1	C	243	HIS
1	C	306	HIS
1	C	494	ASN
1	C	529	ASN
1	D	66	GLN
1	D	74	GLN
1	D	134	HIS
1	D	210	GLN

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Mol	Chain	Res	Type
1	D	261	HIS
1	D	442	HIS
1	D	457	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	D	805	-	4,4,4	0.25	0	6,6,6	0.08	0
4	PEG	B	803	-	6,6,6	0.12	0	5,5,5	0.10	0
2	SO4	A	802	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	801	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	804	-	4,4,4	0.24	0	6,6,6	0.08	0
4	PEG	D	802	-	6,6,6	0.12	0	5,5,5	0.10	0
2	SO4	D	801	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	802	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	803	-	4,4,4	0.25	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	801	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	D	803	-	4,4,4	0.24	0	6,6,6	0.08	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	PEG	B	803	-	-	3/4/4/4	-
4	PEG	D	802	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	802	PEG	O1-C1-C2-O2
4	D	802	PEG	C1-C2-O2-C3
4	D	802	PEG	O2-C3-C4-O4
4	B	803	PEG	O2-C3-C4-O4
4	B	803	PEG	O1-C1-C2-O2
4	B	803	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	802	PEG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	725/728 (99%)	-0.26	18 (2%) 58 60	23, 42, 72, 145	1 (0%)
1	B	724/728 (99%)	-0.12	22 (3%) 52 54	21, 47, 78, 180	1 (0%)
1	C	727/728 (99%)	0.11	14 (1%) 66 68	34, 60, 93, 141	0
1	D	708/728 (97%)	0.85	144 (20%) 3 3	37, 71, 128, 202	0
All	All	2884/2912 (99%)	0.14	198 (6%) 23 25	21, 52, 109, 202	2 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	469	GLY	6.7
1	B	377	LEU	6.2
1	C	376	VAL	6.0
1	B	378	PRO	5.8
1	A	377	LEU	5.4
1	D	725	VAL	5.2
1	D	552	LEU	5.1
1	D	467	SER	5.1
1	D	449	LYS	5.1
1	D	468	ALA	5.0
1	D	582	PHE	5.0
1	A	356	PHE	4.9
1	B	375	ALA	4.9
1	D	710	LEU	4.8
1	D	487	ALA	4.7
1	D	700	THR	4.6
1	B	537	TRP	4.6
1	A	380	LEU	4.6
1	B	376	VAL	4.5
1	A	355	SER	4.5
1	D	546	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	596	ILE	4.4
1	D	516	LEU	4.3
1	D	485	PHE	4.2
1	D	607	VAL	4.2
1	A	354	GLN	4.1
1	D	649	GLY	4.1
1	D	448	ALA	3.9
1	D	455	ILE	3.9
1	D	513	LEU	3.8
1	D	466	LEU	3.8
1	A	376	VAL	3.8
1	D	707	ILE	3.8
1	D	496	THR	3.7
1	D	621	LEU	3.7
1	A	712	ILE	3.7
1	D	608	THR	3.7
1	D	451	LEU	3.6
1	D	474	ALA	3.6
1	D	679	ALA	3.6
1	D	674	ALA	3.6
1	A	727	GLN	3.6
1	D	498	GLU	3.5
1	D	497	PHE	3.5
1	D	675	PHE	3.5
1	D	473	LEU	3.5
1	D	609	LEU	3.5
1	D	709	GLU	3.5
1	D	698	THR	3.4
1	D	521	LYS	3.4
1	B	3	ALA	3.4
1	D	494	ASN	3.4
1	D	517	VAL	3.4
1	D	459	HIS	3.4
1	B	712	ILE	3.4
1	D	376	VAL	3.4
1	D	493	VAL	3.4
1	B	381	SER	3.3
1	D	645	LEU	3.3
1	D	518	ILE	3.3
1	D	647	SER	3.3
1	D	653	ARG	3.3
1	A	379	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	660	VAL	3.3
1	D	589	ILE	3.2
1	D	641	LYS	3.2
1	D	511	LEU	3.2
1	D	614	PHE	3.2
1	D	464	LEU	3.2
1	D	483	LEU	3.2
1	D	550	CYS	3.2
1	B	382	LYS	3.1
1	D	585	VAL	3.1
1	D	719	ILE	3.1
1	D	436	PHE	3.1
1	A	7	LEU	3.1
1	D	673	ASN	3.1
1	B	354	GLN	3.1
1	B	2	GLY	3.1
1	D	638	PHE	3.1
1	D	651	GLY	3.0
1	D	486	LYS	3.0
1	C	353	GLN	3.0
1	D	720	LEU	3.0
1	D	353	GLN	3.0
1	B	352	SER	3.0
1	D	619	GLY	3.0
1	D	680	PRO	2.9
1	D	440	LYS	2.9
1	D	515	GLY	2.9
1	D	643	ASN	2.9
1	D	613	HIS	2.9
1	D	502	LEU	2.9
1	D	576	THR	2.9
1	D	697	ASN	2.9
1	A	353	GLN	2.8
1	D	354	GLN	2.8
1	D	445	GLU	2.8
1	D	648	VAL	2.8
1	D	537	TRP	2.8
1	D	706	TYR	2.8
1	C	728	LYS	2.8
1	C	712	ILE	2.7
1	B	356	PHE	2.7
1	C	472	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	575	ILE	2.7
1	B	355	SER	2.7
1	D	352	SER	2.7
1	B	4	LYS	2.7
1	D	503	PHE	2.7
1	A	537	TRP	2.7
1	A	351	ASP	2.6
1	D	477	VAL	2.6
1	A	378	PRO	2.6
1	D	526	SER	2.6
1	D	457	GLN	2.6
1	D	380	LEU	2.6
1	D	522	ASN	2.6
1	D	471	TYR	2.6
1	D	532	ILE	2.6
1	D	463	VAL	2.5
1	C	433	ILE	2.5
1	D	505	ILE	2.5
1	D	499	ARG	2.5
1	D	446	ASN	2.5
1	D	356	PHE	2.5
1	B	713	ALA	2.5
1	D	659	SER	2.5
1	D	545	LEU	2.5
1	D	577	LEU	2.5
1	B	727	GLN	2.5
1	D	438	SER	2.4
1	D	557	ILE	2.4
1	D	501	SER	2.4
1	D	561	PHE	2.4
1	C	385	LYS	2.4
1	D	404	GLU	2.4
1	C	448	ALA	2.4
1	D	634	PHE	2.4
1	D	450	ASP	2.3
1	D	524	PRO	2.3
1	D	623	LYS	2.3
1	D	678	SER	2.3
1	D	617	VAL	2.3
1	D	694	ILE	2.3
1	A	552	LEU	2.3
1	D	724	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	572	ALA	2.3
1	D	620	ALA	2.3
1	D	622	VAL	2.3
1	C	382	LYS	2.3
1	D	612	ASN	2.3
1	C	375	ALA	2.3
1	D	547	MET	2.3
1	D	559	HIS	2.3
1	B	353	GLN	2.3
1	D	682	VAL	2.3
1	D	639	LEU	2.3
1	D	444	VAL	2.3
1	D	699	PHE	2.2
1	D	355	SER	2.2
1	D	460	SER	2.2
1	C	380	LEU	2.2
1	D	555	LEU	2.2
1	D	590	LEU	2.2
1	D	478	VAL	2.2
1	D	564	PHE	2.2
1	D	443	ARG	2.2
1	D	512	LYS	2.2
1	D	553	ILE	2.2
1	D	456	GLU	2.2
1	B	560	THR	2.2
1	D	604	ALA	2.2
1	D	624	LEU	2.1
1	D	681	ILE	2.1
1	C	351	ASP	2.1
1	D	683	VAL	2.1
1	D	563	PHE	2.1
1	D	688	GLY	2.1
1	A	381	SER	2.1
1	A	382	LYS	2.1
1	D	453	LEU	2.1
1	D	479	ILE	2.1
1	D	652	LYS	2.1
1	C	407	PHE	2.1
1	D	495	LEU	2.1
1	D	701	ASN	2.1
1	D	531	VAL	2.1
1	D	665	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	535	LYS	2.0
1	B	717	THR	2.0
1	D	519	SER	2.0
1	D	514	GLU	2.0
1	C	459	HIS	2.0
1	A	375	ALA	2.0
1	D	703	ALA	2.0
1	D	551	GLN	2.0
1	B	536	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, 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(Å ²)	Q<0.9
2	SO4	D	803	5/5	0.54	0.15	107,111,119,122	0
2	SO4	B	804	5/5	0.67	0.13	72,72,74,87	0
2	SO4	D	805	5/5	0.67	0.14	82,83,93,101	0
2	SO4	B	801	5/5	-	-	81,85,89,89	5
4	PEG	D	802	7/7	0.72	0.19	82,102,106,107	0
2	SO4	C	803	5/5	0.74	0.11	65,82,87,90	0
2	SO4	C	801	5/5	0.78	0.11	73,74,89,90	0
2	SO4	A	803	5/5	0.79	0.14	63,64,79,95	0
2	SO4	D	801	5/5	0.81	0.10	60,79,81,81	0
3	CL	B	807	1/1	0.81	0.30	96,96,96,96	0
4	PEG	B	803	7/7	0.81	0.19	52,62,71,74	0
2	SO4	D	804	5/5	0.81	0.15	73,77,93,100	0
2	SO4	A	802	5/5	0.84	0.12	57,62,93,97	0
2	SO4	C	802	5/5	0.88	0.13	59,61,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	805	1/1	0.88	0.29	101,101,101,101	0
2	SO4	B	802	5/5	0.92	0.13	45,60,68,77	0
2	SO4	A	801	5/5	0.94	0.14	37,57,63,73	0
3	CL	B	806	1/1	0.94	0.21	81,81,81,81	0
3	CL	A	804	1/1	0.99	0.03	37,37,37,37	0
3	CL	B	805	1/1	0.99	0.03	36,36,36,36	0
3	CL	C	804	1/1	0.99	0.06	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.