



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:13 AM UTC

PDB ID : 2UVE / pdb_00002uve
Title : Structure of Yersinia enterocolitica Family 28 Exopolygalacturonase
Authors : Abbott, D.W.; Boraston, A.B.
Deposited on : 2007-03-09
Resolution : 2.19 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

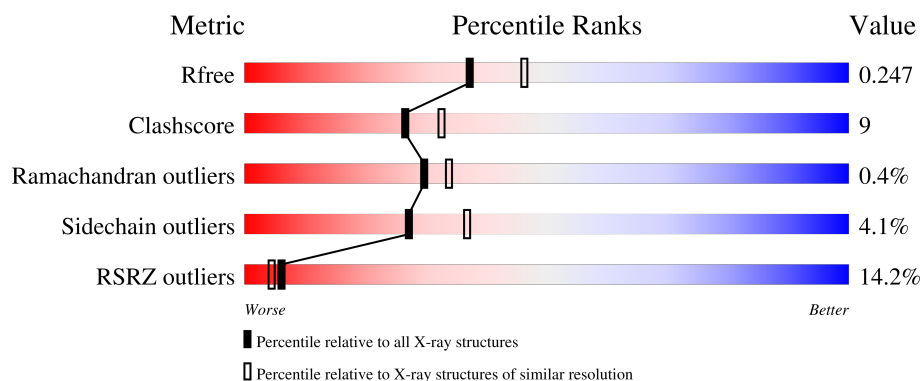
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	608	 14% 74% 18% •• 6%
1	B	608	 12% 76% 14% • 7%

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	SO4	A	1616	-	-	X	-
3	SO4	A	1621	-	-	X	-
3	SO4	B	1619	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9409 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 EXOPOLYGALACTURONASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	2	0
			4439	2784	776	864	15			
1	B	566	Total	C	N	O	S	0	1	0
			4399	2764	769	851	15			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ni	0	0
			4	4		
2	B	5	Total	Ni	0	0
			5	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

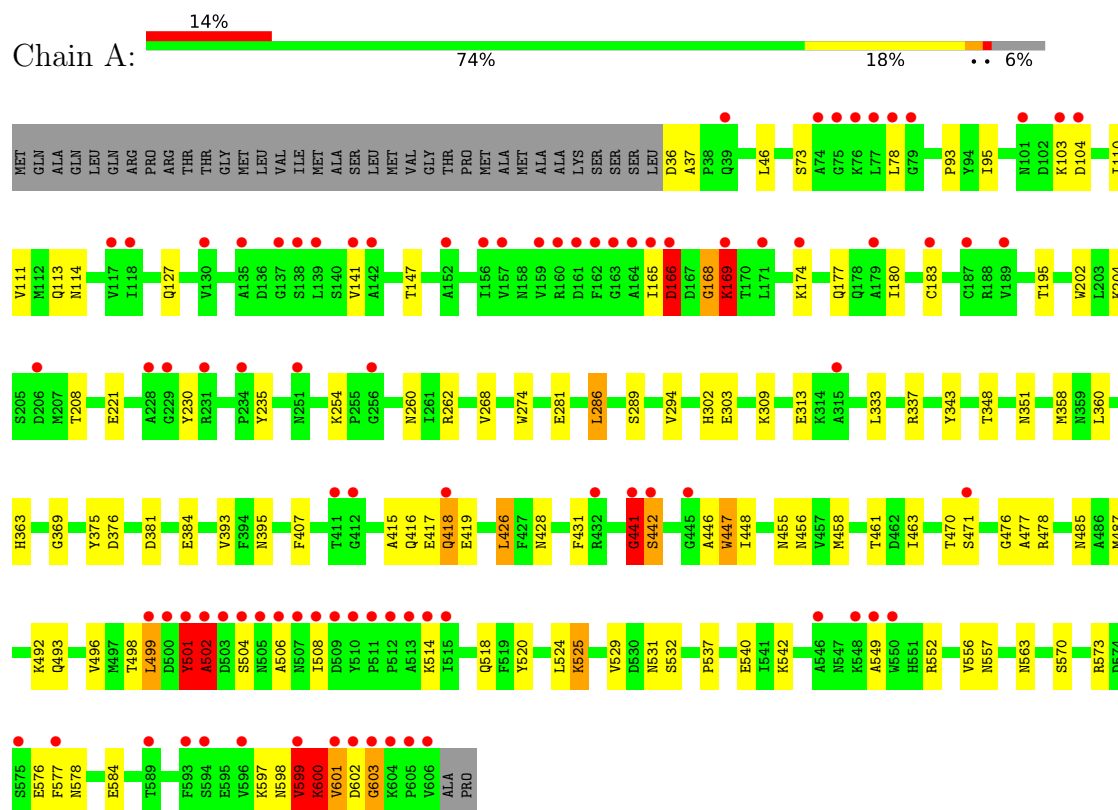
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	286	Total	O	0	0
			286	286		

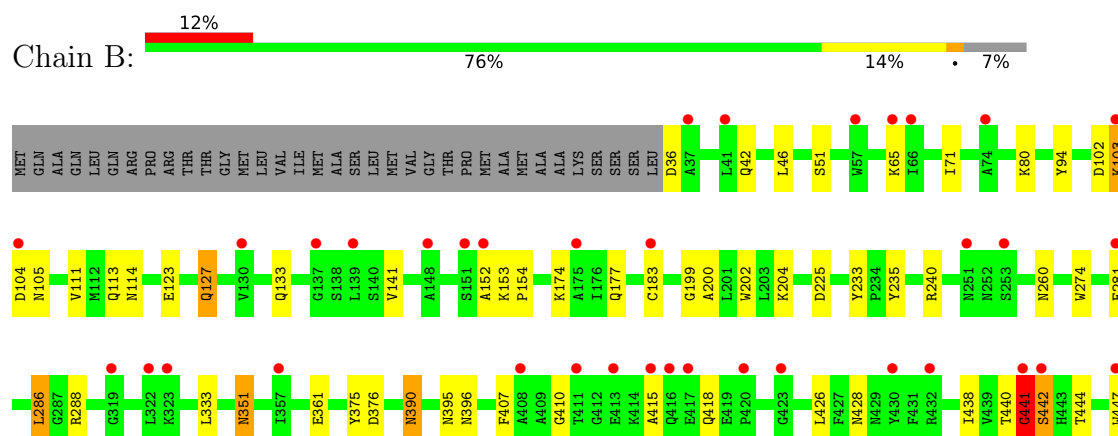
3 Residue-property plots

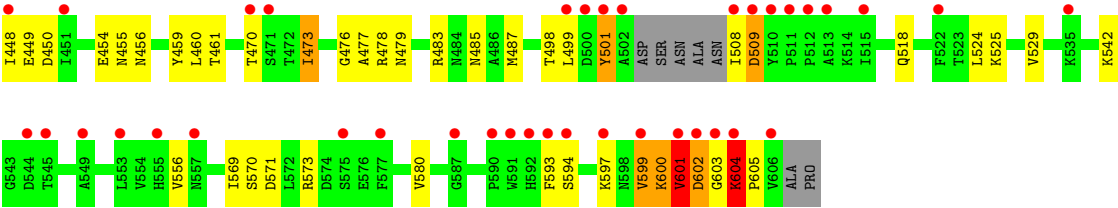
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: EXOPOLYGALACTURONASE



• Molecule 1: EXOPOLYGALACTURONASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.95Å 78.76Å 98.19Å 90.00° 103.61° 90.00°	Depositor
Resolution (Å)	34.42 – 2.19 34.42 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-2.19) 99.9 (34.42-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.228 0.246 , 0.247	Depositor DCC
R_{free} test set	4035 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.9	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	0.91	EDS
Total number of atoms	9409	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

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

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	1.08	1/4532 (0.0%)	1.03	7/6153 (0.1%)
1	B	1.17	9/4491 (0.2%)	1.09	11/6094 (0.2%)
All	All	1.12	10/9023 (0.1%)	1.06	18/12247 (0.1%)

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	A	0	8
1	B	0	7
All	All	0	15

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	601	VAL	CA-CB	8.23	1.62	1.53
1	B	351	ASN	C-O	-7.67	1.20	1.23
1	B	141	VAL	CA-CB	7.41	1.61	1.54
1	A	294	VAL	CA-CB	6.55	1.60	1.54
1	B	438	ILE	CA-CB	5.84	1.61	1.54
1	B	442	SER	N-CA	5.43	1.53	1.46
1	B	599	VAL	CA-CB	5.32	1.61	1.54
1	B	473	ILE	CA-CB	5.27	1.61	1.54
1	B	580	VAL	CA-CB	5.25	1.60	1.53
1	B	602	ASP	N-CA	-5.06	1.39	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	601	VAL	N-CA-C	18.16	133.16	107.37
1	B	441	GLY	CA-C-N	8.06	136.93	121.54
1	B	441	GLY	C-N-CA	8.06	136.93	121.54
1	A	166	ASP	CB-CA-C	7.02	119.86	111.22
1	B	604	LYS	CA-C-N	6.94	128.52	119.84
1	B	604	LYS	C-N-CA	6.94	128.52	119.84
1	A	599	VAL	N-CA-C	6.81	118.63	108.96
1	B	501	TYR	N-CA-C	-6.60	99.55	110.17
1	B	442	SER	N-CA-CB	6.18	120.93	110.49
1	A	502	ALA	N-CA-C	6.09	123.78	110.80
1	A	441	GLY	CA-C-N	5.76	132.55	121.54
1	A	441	GLY	C-N-CA	5.76	132.55	121.54
1	A	532	SER	N-CA-C	-5.53	98.08	107.91
1	A	501	TYR	N-CA-C	-5.46	101.65	110.32
1	B	240	ARG	CA-C-N	-5.40	114.69	120.03
1	B	240	ARG	C-N-CA	-5.40	114.69	120.03
1	B	200	ALA	N-CA-C	5.33	118.21	110.42
1	B	602	ASP	N-CA-CB	-5.01	104.30	111.91

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLY	Peptide
1	A	441	GLY	Peptide
1	A	501	TYR	Peptide
1	A	502	ALA	Peptide
1	A	599	VAL	Peptide
1	A	600	LYS	Mainchain
1	A	601	VAL	Peptide
1	A	603	GLY	Peptide
1	B	102	ASP	Peptide
1	B	440	THR	Peptide
1	B	441	GLY	Peptide
1	B	501	TYR	Peptide
1	B	600	LYS	Peptide
1	B	601	VAL	Peptide
1	B	604	LYS	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	4439	0	4323	89	0
1	B	4399	0	4298	71	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	55	0	0	8	0
3	B	40	0	0	4	0
4	B	4	0	3	0	0
5	A	177	0	0	5	0
5	B	286	0	0	10	0
All	All	9409	0	8624	164	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 (164) 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:B:604:LYS:HB3	1:B:605:PRO:HD3	1.27	1.16
1:A:602:ASP:N	1:A:603:GLY:HA2	1.72	1.05
1:B:603:GLY:O	1:B:604:LYS:CG	2.05	1.04
1:B:604:LYS:CB	1:B:605:PRO:HD3	1.89	1.01
1:A:415:ALA:O	1:A:418:GLN:HG3	1.61	1.00
1:B:603:GLY:O	1:B:604:LYS:HG2	1.66	0.93
1:A:313:GLU:HG3	5:A:2094:HOH:O	1.67	0.91
3:A:1619:SO4:O1	5:A:2176:HOH:O	1.89	0.90
1:A:601:VAL:HG12	1:A:602:ASP:HB3	1.53	0.90
1:B:407:PHE:O	1:B:441:GLY:HA3	1.72	0.89
1:A:442:SER:OG	3:A:1621:SO4:O4	1.91	0.89
1:B:603:GLY:O	1:B:604:LYS:HG3	1.71	0.88
1:B:113:GLN:H	1:B:428:ASN:HD21	1.15	0.88
1:A:602:ASP:H	1:A:603:GLY:HA2	1.40	0.86
1:B:450:ASP:OD1	1:B:479:ASN:ND2	2.09	0.85
1:A:113:GLN:H	1:A:428:ASN:HD21	1.24	0.85
1:B:602:ASP:N	1:B:603:GLY:HA2	1.94	0.81
3:B:1619:SO4:S	5:B:2285:HOH:O	2.37	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:LYS:HZ2	1:B:604:LYS:HE2	1.45	0.81
1:A:418:GLN:OE1	5:A:2135:HOH:O	1.99	0.80
1:A:37:ALA:HB2	1:A:141:VAL:HG23	1.63	0.80
1:B:177:GLN:HE22	1:B:202:TRP:H	1.29	0.80
1:B:600:LYS:NZ	1:B:604:LYS:HE2	1.97	0.79
1:A:599:VAL:HG23	1:A:600:LYS:H	1.48	0.79
1:A:177:GLN:HE22	1:A:202:TRP:H	1.29	0.78
1:A:598:ASN:O	3:A:1616:SO4:O3	2.02	0.76
1:A:531[A]:ASN:HD22	1:A:563[A]:ASN:HB3	1.49	0.76
1:B:604:LYS:HB3	1:B:605:PRO:CD	2.14	0.75
1:A:577:PHE:O	1:A:602:ASP:HB2	1.86	0.75
1:A:602:ASP:N	1:A:603:GLY:CA	2.50	0.74
1:B:415:ALA:HA	1:B:418:GLN:HE21	1.51	0.74
1:A:600:LYS:HE2	3:A:1616:SO4:O2	1.87	0.74
1:A:506:ALA:HB1	1:A:508:ILE:HG12	1.68	0.73
1:A:281:GLU:OE1	1:A:289:SER:HB2	1.90	0.72
1:B:601:VAL:HG23	1:B:602:ASP:HB3	1.71	0.72
1:A:600:LYS:HD3	3:A:1616:SO4:O2	1.90	0.71
3:B:1619:SO4:O2	5:B:2285:HOH:O	2.07	0.71
1:B:288[A]:ARG:NH1	5:B:2157:HOH:O	2.06	0.69
1:A:168:GLY:O	1:A:169:LYS:HB3	1.92	0.69
1:A:600:LYS:CE	3:A:1616:SO4:O2	2.41	0.68
1:A:456:ASN:H	1:A:485:ASN:HD22	1.40	0.67
1:A:499:LEU:HD13	1:A:549:ALA:HB1	1.77	0.67
1:B:456:ASN:H	1:B:485:ASN:HD22	1.44	0.66
1:B:274:TRP:H	1:B:351:ASN:HD21	1.42	0.66
1:A:113:GLN:N	1:A:428:ASN:HD21	1.94	0.66
3:B:1613:SO4:O3	5:B:2282:HOH:O	2.10	0.65
1:B:183:CYS:HB2	1:B:204:LYS:HE2	1.78	0.65
1:B:361:GLU:HG3	5:B:2190:HOH:O	1.94	0.65
1:A:363:HIS:NE2	1:A:419:GLU:OE1	2.21	0.65
1:B:600:LYS:HD3	1:B:604:LYS:HG2	1.79	0.64
1:A:601:VAL:CG1	1:A:602:ASP:HB3	2.26	0.63
1:B:603:GLY:C	1:B:604:LYS:CG	2.70	0.63
1:B:604:LYS:CB	1:B:605:PRO:CD	2.71	0.62
1:A:166:ASP:HB2	1:A:195:THR:O	1.99	0.62
1:B:508:ILE:N	5:B:2245:HOH:O	2.32	0.62
1:B:603:GLY:C	1:B:604:LYS:HG3	2.24	0.61
1:A:602:ASP:O	1:A:602:ASP:CG	2.37	0.61
1:A:578:ASN:HA	1:A:602:ASP:HB2	1.83	0.61
1:A:442:SER:CB	3:A:1621:SO4:O4	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:HG22	1:A:348:THR:HB	1.84	0.60
1:B:113:GLN:N	1:B:428:ASN:HD21	1.95	0.59
1:A:599:VAL:HG23	1:A:600:LYS:N	2.15	0.58
1:A:600:LYS:CD	3:A:1616:SO4:O2	2.51	0.58
1:A:73:SER:HB2	1:A:78:LEU:HD11	1.87	0.57
1:A:113:GLN:H	1:A:428:ASN:ND2	1.98	0.57
1:A:416:GLN:C	1:A:418:GLN:H	2.13	0.56
1:B:235:TYR:OH	1:B:418:GLN:NE2	2.40	0.55
1:A:531[A]:ASN:ND2	1:A:563[A]:ASN:HB3	2.21	0.55
1:A:576:GLU:HA	1:A:600:LYS:O	2.07	0.55
1:A:103:LYS:O	1:A:104:ASP:HB2	2.07	0.54
1:A:501:TYR:CD2	1:A:502:ALA:HA	2.42	0.54
1:B:390:ASN:HB2	5:B:2208:HOH:O	2.07	0.54
1:A:302:HIS:O	1:A:309:LYS:HE3	2.08	0.54
1:B:114:ASN:HD21	1:B:395:ASN:HD21	1.57	0.53
1:A:337:ARG:HA	1:A:360:LEU:O	2.09	0.53
1:B:274:TRP:N	1:B:351:ASN:HD21	2.07	0.52
1:A:93:PRO:HB2	1:A:286:LEU:HD21	1.92	0.52
1:A:563[A]:ASN:HA	1:A:584:GLU:O	2.09	0.52
1:A:506:ALA:HB1	1:A:508:ILE:CG1	2.40	0.52
1:B:602:ASP:O	1:B:602:ASP:CG	2.50	0.52
1:A:183:CYS:HB2	1:A:204:LYS:HE2	1.92	0.51
1:A:446:ALA:O	1:A:447:TRP:HB2	2.11	0.51
1:B:602:ASP:N	1:B:603:GLY:CA	2.72	0.51
1:B:454:GLU:HA	1:B:483:ARG:O	2.11	0.50
1:B:570:SER:HA	1:B:594:SER:O	2.12	0.50
1:A:537:PRO:HB2	1:A:540:GLU:HB2	1.94	0.50
1:B:103:LYS:HG3	1:B:104:ASP:HA	1.93	0.50
1:B:113:GLN:H	1:B:428:ASN:ND2	1.97	0.50
1:A:573:ARG:HA	1:A:597:LYS:O	2.13	0.49
1:B:470:THR:OG1	1:B:473:ILE:HG12	2.12	0.49
1:B:390:ASN:ND2	5:B:2208:HOH:O	2.45	0.49
1:A:114:ASN:HD21	1:A:395:ASN:HD21	1.61	0.49
1:A:525:LYS:HG3	1:A:557:ASN:HB2	1.95	0.49
1:B:508:ILE:HA	1:B:509:ASP:HA	1.42	0.48
1:B:51:SER:HB3	5:B:2068:HOH:O	2.12	0.48
1:B:199:GLY:HA3	1:B:225:ASP:HB3	1.94	0.48
1:A:456:ASN:H	1:A:485:ASN:ND2	2.10	0.48
1:A:46:LEU:HD11	1:A:260:ASN:HA	1.96	0.47
1:A:496:VAL:HG12	1:A:498:THR:HG23	1.96	0.47
1:A:578:ASN:OD1	1:A:602:ASP:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:OE1	1:A:289:SER:CB	2.61	0.47
1:A:407:PHE:O	1:A:441:GLY:HA3	2.13	0.47
1:A:599:VAL:CG2	1:A:600:LYS:N	2.78	0.47
1:A:499:LEU:HD12	5:A:2160:HOH:O	2.14	0.47
1:B:483:ARG:HA	1:B:525:LYS:O	2.15	0.47
1:A:274:TRP:H	1:A:351:ASN:HD21	1.62	0.47
1:A:111:VAL:H	1:A:455:ASN:ND2	2.13	0.46
1:A:463:ILE:HA	1:A:493:GLN:O	2.15	0.46
1:B:602:ASP:H	1:B:603:GLY:HA2	1.78	0.46
1:A:478:ARG:HA	1:A:520:TYR:O	2.16	0.46
1:B:487:MET:HE3	1:B:529:VAL:HG22	1.96	0.46
1:A:262:ARG:HG2	1:A:343:TYR:HB3	1.98	0.45
1:B:111:VAL:H	1:B:455:ASN:ND2	2.13	0.45
1:B:448:ILE:O	1:B:477:ALA:HA	2.16	0.45
1:B:524:LEU:O	1:B:556:VAL:HA	2.17	0.45
1:B:80:LYS:HE3	1:B:133:GLN:OE1	2.17	0.45
1:A:230:TYR:OH	1:A:358:MET:HE1	2.17	0.45
1:B:103:LYS:CG	1:B:104:ASP:HA	2.47	0.45
1:B:498:THR:HG22	1:B:542:LYS:HD3	1.99	0.44
1:B:114:ASN:ND2	1:B:395:ASN:HD21	2.16	0.44
1:B:573:ARG:HA	1:B:597:LYS:O	2.16	0.44
1:A:180:ILE:O	1:A:183:CYS:HB2	2.18	0.44
1:A:501:TYR:CG	1:A:502:ALA:HA	2.52	0.44
1:A:524:LEU:HB3	1:A:556:VAL:HG22	1.99	0.44
1:B:459:TYR:O	1:B:460:LEU:HB2	2.17	0.44
1:B:127:GLN:HE21	1:B:127:GLN:C	2.26	0.44
1:A:504:SER:C	1:A:506:ALA:H	2.24	0.43
1:B:94:TYR:CD1	1:B:286:LEU:HD22	2.53	0.43
1:B:103:LYS:HA	1:B:105:ASN:H	1.82	0.43
1:A:552:ARG:HA	1:A:573:ARG:O	2.19	0.43
1:B:444:THR:H	1:B:473:ILE:HG21	1.84	0.43
1:B:42:GLN:NE2	3:B:1616:SO4:O4	2.51	0.43
1:B:600:LYS:HB3	1:B:604:LYS:HA	2.01	0.43
1:A:416:GLN:C	1:A:418:GLN:N	2.73	0.43
1:B:71:ILE:HD12	1:B:71:ILE:N	2.33	0.43
1:A:476:GLY:HA3	1:A:518:GLN:O	2.19	0.43
1:A:487:MET:HE3	1:A:529:VAL:HG22	2.01	0.43
1:A:573:ARG:HD3	1:A:597:LYS:HB3	2.00	0.43
1:A:235:TYR:OH	1:A:418:GLN:NE2	2.53	0.42
1:A:448:ILE:O	1:A:477:ALA:HA	2.19	0.42
1:A:114:ASN:ND2	1:A:395:ASN:HD21	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:O	1:B:593:PHE:HA	2.20	0.42
1:A:114:ASN:ND2	5:A:2030:HOH:O	2.51	0.42
1:A:221:GLU:H	1:A:221:GLU:CD	2.27	0.42
1:B:274:TRP:H	1:B:351:ASN:ND2	2.12	0.41
1:B:46:LEU:HD11	1:B:260:ASN:HA	2.02	0.41
1:B:449:GLU:HA	1:B:478:ARG:O	2.20	0.41
1:A:563[B]:ASN:HA	1:A:584:GLU:O	2.19	0.41
1:B:103:LYS:CB	1:B:104:ASP:HA	2.50	0.41
1:B:390:ASN:CG	5:B:2208:HOH:O	2.63	0.41
1:A:492:LYS:C	1:A:493:GLN:HG3	2.45	0.41
1:B:233:TYR:CZ	1:B:410:GLY:HA2	2.56	0.41
1:B:375:TYR:HA	1:B:376:ASP:HA	1.84	0.41
1:A:369:GLY:HA2	1:A:395:ASN:O	2.20	0.40
1:A:375:TYR:HA	1:A:376:ASP:HA	1.79	0.40
1:A:381:ASP:OD2	1:A:384:GLU:OE2	2.39	0.40
1:A:431:PHE:HB2	1:A:458:MET:HG3	2.02	0.40
1:A:95:ILE:HG21	1:A:110:ILE:HD11	2.04	0.40
1:A:542:LYS:HA	1:A:570:SER:HB2	2.03	0.40
1:B:476:GLY:HA3	1:B:518:GLN:O	2.21	0.40
1:A:208:THR:HA	1:A:262:ARG:O	2.21	0.40
1:A:393:VAL:HB	1:A:426:LEU:HD12	2.02	0.40
1:B:123:GLU:HG3	1:B:152:ALA:HA	2.04	0.40
1:B:153:LYS:HD2	1:B:154:PRO:HD2	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	571/608 (94%)	526 (92%)	42 (7%)	3 (0%)	24 27
1	B	563/608 (93%)	526 (93%)	35 (6%)	2 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1134/1216 (93%)	1052 (93%)	77 (7%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	SER
1	A	169	LYS
1	A	417	GLU
1	B	447	TRP
1	A	447	TRP

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	479/507 (94%)	457 (95%)	22 (5%)	24	32
1	B	474/507 (94%)	457 (96%)	17 (4%)	31	42
All	All	953/1014 (94%)	914 (96%)	39 (4%)	27	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	127	GLN
1	A	147	THR
1	A	165	ILE
1	A	166	ASP
1	A	169	LYS
1	A	174	LYS
1	A	254	LYS
1	A	286	LEU
1	A	303	GLU
1	A	333	LEU
1	A	418	GLN
1	A	426	LEU

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Mol	Chain	Res	Type
1	A	442	SER
1	A	461	THR
1	A	470	THR
1	A	471	SER
1	A	499	LEU
1	A	514	LYS
1	A	525	LYS
1	A	599	VAL
1	A	600	LYS
1	B	36	ASP
1	B	65	LYS
1	B	103	LYS
1	B	127	GLN
1	B	174	LYS
1	B	281	GLU
1	B	286	LEU
1	B	333	LEU
1	B	390	ASN
1	B	396	ASN
1	B	426	LEU
1	B	461	THR
1	B	499	LEU
1	B	509	ASP
1	B	571	ASP
1	B	599	VAL
1	B	601	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	114	ASN
1	A	127	GLN
1	A	177	GLN
1	A	324	ASN
1	A	351	ASN
1	A	390	ASN
1	A	418	GLN
1	A	428	ASN
1	A	435	HIS
1	A	455	ASN
1	A	485	ASN

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Mol	Chain	Res	Type
1	A	562	ASN
1	A	592	HIS
1	B	42	GLN
1	B	85	ASN
1	B	127	GLN
1	B	177	GLN
1	B	178	GLN
1	B	210	ASN
1	B	292	GLN
1	B	324	ASN
1	B	351	ASN
1	B	364	ASN
1	B	387	ASN
1	B	390	ASN
1	B	395	ASN
1	B	418	GLN
1	B	428	ASN
1	B	455	ASN
1	B	485	ASN
1	B	518	GLN
1	B	531	ASN
1	B	536	ASN
1	B	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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	$\# Z > 2$
3	SO4	A	1619	-	4,4,4	0.44	0	6,6,6	0.46	0
3	SO4	A	1612	-	4,4,4	0.37	0	6,6,6	0.31	0
3	SO4	A	1620	-	4,4,4	0.44	0	6,6,6	0.37	0
3	SO4	A	1618	-	4,4,4	0.53	0	6,6,6	0.80	0
3	SO4	B	1612	-	4,4,4	0.56	0	6,6,6	0.87	0
3	SO4	A	1616	-	4,4,4	0.57	0	6,6,6	0.55	0
3	SO4	B	1618	-	4,4,4	0.50	0	6,6,6	0.81	0
3	SO4	A	1614	-	4,4,4	0.40	0	6,6,6	0.40	0
3	SO4	B	1615	-	4,4,4	0.54	0	6,6,6	0.22	0
3	SO4	A	1615	-	4,4,4	0.58	0	6,6,6	1.05	0
3	SO4	A	1613	-	4,4,4	0.29	0	6,6,6	0.33	0
3	SO4	B	1614	-	4,4,4	0.34	0	6,6,6	0.29	0
3	SO4	B	1617	-	4,4,4	0.48	0	6,6,6	0.64	0
3	SO4	B	1613	-	4,4,4	0.26	0	6,6,6	0.51	0
3	SO4	A	1611	-	4,4,4	0.43	0	6,6,6	0.53	0
3	SO4	A	1617	-	4,4,4	0.56	0	6,6,6	0.73	0
3	SO4	B	1619	-	4,4,4	1.04	0	6,6,6	1.38	1 (16%)
3	SO4	B	1616	-	4,4,4	0.52	0	6,6,6	0.31	0
3	SO4	A	1621	-	4,4,4	1.05	0	6,6,6	1.39	1 (16%)
4	ACT	B	1620	-	3,3,3	1.04	0	3,3,3	0.97	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1621	SO4	O4-S-O3	3.06	125.39	108.54
3	B	1619	SO4	O4-S-O3	3.05	125.36	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1619	SO4	1	0
3	A	1616	SO4	5	0
3	B	1613	SO4	1	0
3	B	1619	SO4	2	0
3	B	1616	SO4	1	0
3	A	1621	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	571/608 (93%)	1.19	87 (15%) 5 4	2, 26, 45, 79	4 (0%)
1	B	566/608 (93%)	1.25	74 (13%) 7 5	2, 19, 33, 57	2 (0%)
All	All	1137/1216 (93%)	1.22	161 (14%) 6 4	2, 22, 41, 79	6 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	ILE	8.9
1	A	502	ALA	6.6
1	A	508	ILE	6.5
1	A	603	GLY	6.0
1	A	231	ARG	5.7
1	B	502	ALA	4.8
1	A	504	SER	4.4
1	A	432	ARG	4.3
1	A	606	VAL	4.3
1	A	549	ALA	4.2
1	B	148	ALA	4.2
1	B	510	TYR	4.2
1	A	187	CYS	4.2
1	B	432	ARG	4.2
1	A	602	ASP	4.2
1	B	441	GLY	4.1
1	A	501	TYR	3.7
1	A	505	ASN	3.6
1	A	157	VAL	3.6
1	A	104	ASP	3.6
1	A	141	VAL	3.6
1	A	604	LYS	3.5
1	A	507	ASN	3.5
1	B	594	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	501	TYR	3.4
1	B	603	GLY	3.4
1	B	545	THR	3.3
1	A	166	ASP	3.3
1	A	503	ASP	3.3
1	A	546	ALA	3.3
1	B	103	LYS	3.3
1	B	417	GLU	3.2
1	A	169	LYS	3.2
1	A	593	PHE	3.2
1	B	512	PRO	3.2
1	A	506	ALA	3.2
1	B	416	GLN	3.1
1	B	602	ASP	3.1
1	A	510	TYR	3.1
1	A	152	ALA	3.0
1	A	256	GLY	3.0
1	A	605	PRO	3.0
1	A	509	ASP	3.0
1	A	162	PHE	3.0
1	A	118	ILE	3.0
1	A	163	GLY	3.0
1	B	575	SER	2.9
1	B	65	LYS	2.9
1	B	599	VAL	2.9
1	B	509	ASP	2.9
1	B	522	PHE	2.9
1	A	442	SER	2.9
1	A	135	ALA	2.9
1	B	515	ILE	2.9
1	A	171	LEU	2.8
1	B	413	GLU	2.8
1	A	251	ASN	2.8
1	A	513	ALA	2.8
1	A	103	LYS	2.8
1	A	79	GLY	2.8
1	A	164	ALA	2.8
1	A	159	VAL	2.8
1	A	511	PRO	2.8
1	A	515	ILE	2.8
1	B	577	PHE	2.8
1	B	587	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	2.7
1	A	512	PRO	2.7
1	B	592	HIS	2.7
1	A	315	ALA	2.7
1	B	152	ALA	2.7
1	B	513	ALA	2.7
1	B	447	TRP	2.7
1	A	514	LYS	2.7
1	B	511	PRO	2.7
1	B	591	TRP	2.7
1	A	77	LEU	2.6
1	B	423	GLY	2.6
1	A	74	ALA	2.6
1	B	499	LEU	2.6
1	B	544	ASP	2.6
1	A	137	GLY	2.6
1	B	251	ASN	2.6
1	A	234	PRO	2.6
1	A	165	ILE	2.6
1	A	76	LYS	2.6
1	B	57	TRP	2.6
1	A	156	ILE	2.5
1	A	550	TRP	2.5
1	A	130	VAL	2.5
1	A	601	VAL	2.5
1	B	535	LYS	2.5
1	A	418	GLN	2.5
1	A	499	LEU	2.5
1	A	596	VAL	2.5
1	A	139	LEU	2.5
1	B	130	VAL	2.4
1	B	601	VAL	2.4
1	A	411	THR	2.4
1	B	604	LYS	2.4
1	B	137	GLY	2.4
1	A	117	VAL	2.4
1	B	151	SER	2.4
1	A	75	GLY	2.4
1	B	357	ILE	2.4
1	A	575	SER	2.4
1	B	411	THR	2.4
1	B	470	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	430	TYR	2.3
1	B	37	ALA	2.3
1	B	175	ALA	2.3
1	A	229	GLY	2.3
1	A	599	VAL	2.3
1	B	442	SER	2.3
1	A	142	ALA	2.3
1	A	138	SER	2.3
1	B	606	VAL	2.3
1	A	589	THR	2.3
1	B	420	PRO	2.3
1	A	183	CYS	2.3
1	B	104	ASP	2.3
1	B	553	LEU	2.3
1	B	323	LYS	2.3
1	B	597	LYS	2.3
1	B	253	SER	2.2
1	B	549	ALA	2.2
1	A	471	SER	2.2
1	A	594	SER	2.2
1	B	593	PHE	2.2
1	B	451	ILE	2.2
1	B	281	GLU	2.2
1	A	174	LYS	2.2
1	B	408	ALA	2.2
1	A	78	LEU	2.2
1	B	183	CYS	2.2
1	B	471	SER	2.2
1	A	101	ASN	2.2
1	A	577	PHE	2.1
1	A	189	VAL	2.1
1	A	39	GLN	2.1
1	B	41	LEU	2.1
1	A	500	ASP	2.1
1	B	448	ILE	2.1
1	B	322	LEU	2.1
1	B	557	ASN	2.1
1	B	500	ASP	2.1
1	A	441	GLY	2.1
1	A	445	GLY	2.1
1	A	161	ASP	2.1
1	A	206	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	160	ARG	2.1
1	A	412	GLY	2.1
1	A	179	ALA	2.1
1	B	415	ALA	2.1
1	B	590	PRO	2.0
1	B	66	ILE	2.0
1	A	228	ALA	2.0
1	B	74	ALA	2.0
1	B	555	HIS	2.0
1	A	548	LYS	2.0
1	B	319	GLY	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	NI	B	1611	1/1	0.29	0.31	136,136,136,136	0
3	SO4	A	1612	5/5	0.63	0.16	74,75,76,77	0
3	SO4	B	1615	5/5	0.72	0.32	49,53,53,56	0
3	SO4	B	1616	5/5	0.73	0.33	55,57,60,60	0
3	SO4	A	1616	5/5	0.74	0.33	50,51,53,54	0
3	SO4	B	1618	5/5	0.74	0.21	43,49,51,53	0
3	SO4	A	1611	5/5	0.75	0.23	50,50,55,55	0
3	SO4	A	1615	5/5	0.76	0.32	45,45,49,52	0
3	SO4	B	1613	5/5	0.79	0.19	58,60,60,62	0
4	ACT	B	1620	4/4	0.79	0.24	20,20,20,20	0
3	SO4	B	1614	5/5	0.80	0.19	51,52,54,55	0
3	SO4	A	1617	5/5	0.80	0.29	47,48,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1618	5/5	0.80	0.32	52,55,57,57	0
3	SO4	B	1617	5/5	0.80	0.17	51,53,54,56	0
3	SO4	A	1620	5/5	0.80	0.32	43,46,50,50	0
3	SO4	B	1619	5/5	0.80	0.29	20,20,20,20	0
3	SO4	A	1613	5/5	0.80	0.21	62,63,64,64	0
3	SO4	B	1612	5/5	0.82	0.20	33,46,46,46	0
3	SO4	A	1619	5/5	0.82	0.24	46,47,47,49	0
3	SO4	A	1621	5/5	0.82	0.29	20,20,20,20	0
2	NI	A	1609	1/1	0.84	0.18	92,92,92,92	0
2	NI	A	1610	1/1	0.86	0.27	93,93,93,93	0
2	NI	A	1608	1/1	0.87	0.23	41,41,41,41	0
3	SO4	A	1614	5/5	0.88	0.13	38,38,41,41	0
2	NI	B	1608	1/1	0.92	0.14	29,29,29,29	0
2	NI	A	1607	1/1	0.92	0.13	33,33,33,33	0
2	NI	B	1610	1/1	0.94	0.08	35,35,35,35	0
2	NI	B	1609	1/1	0.94	0.24	38,38,38,38	0
2	NI	B	1607	1/1	0.98	0.13	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.