



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:27 AM GMT

PDB ID : 3IHG
Title : Crystal structure of a ternary complex of aklavinone-11 hydroxylase with FAD and aklavinone
Authors : Lindqvist, Y.; Koskiniemi, H.; Jansson, A.; Sandalova, T.; Schneider, G.
Deposited on : 2009-07-30
Resolution : 2.49 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

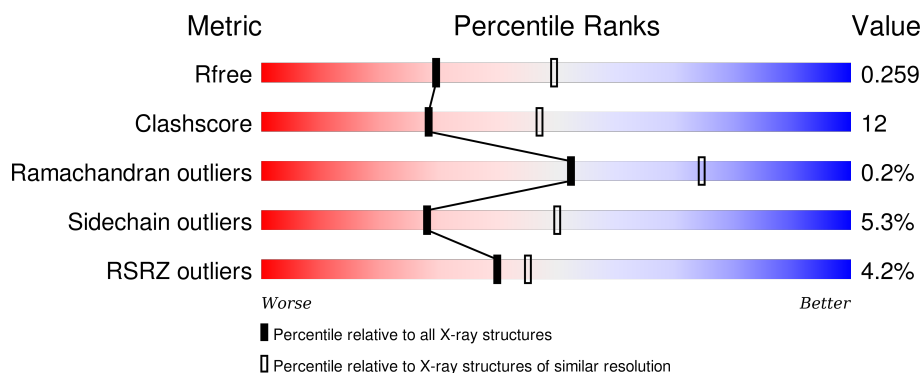
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 ≥ 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	535	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	B	535	<div> <div>4%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
1	C	535	<div> <div>5%</div> <div>79%</div> <div>18%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	542	-	-	X	-
4	SO4	A	545	-	-	X	-
4	SO4	C	541	-	-	-	X
4	SO4	C	542	-	-	X	-

2 Entry composition [i](#)

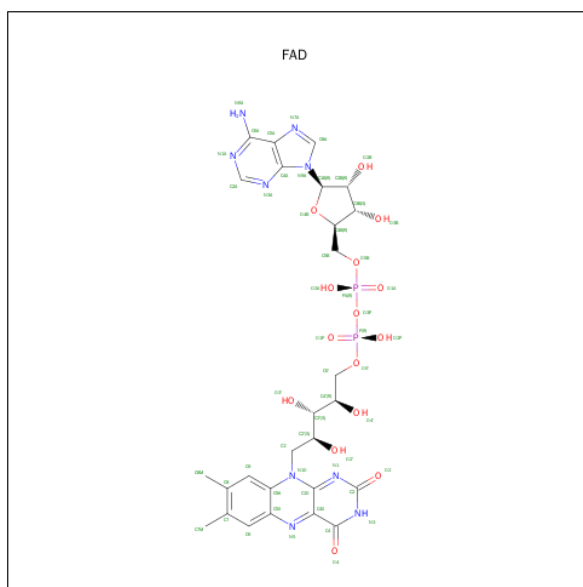
There are 5 unique types of molecules in this entry. The entry contains 12729 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RdmE.

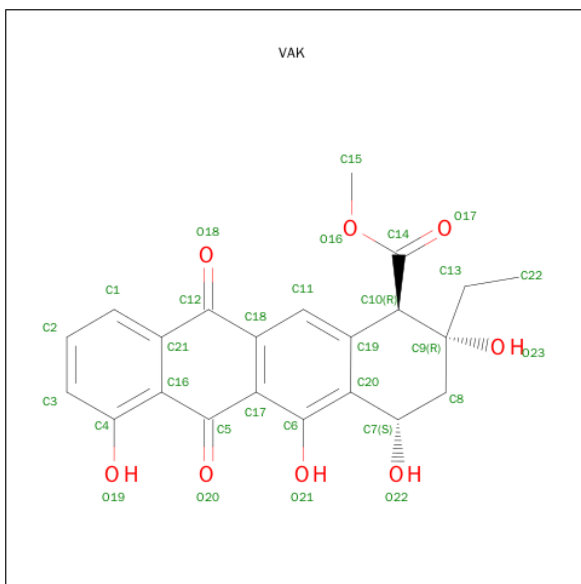
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	3	0
			4071	2547	735	776	13			
1	B	535	Total	C	N	O	S	0	1	0
			4053	2536	730	774	13			
1	C	535	Total	C	N	O	S	0	3	0
			4067	2545	735	774	13			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



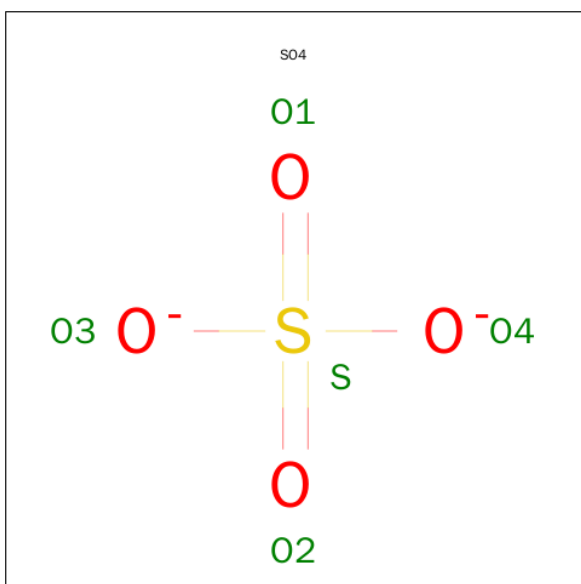
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is METHYL (1R,2R,4S)-2-ETHYL-2,4,5,7-TETRAHYDROXY-6,11-DIOXO-1,2,3,4,6,11-HEXAHYDROTETRACENE-1-CARBOXYLATE (three-letter code: VAK) (formula: $C_{22}H_{20}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			30	22	8		
3	B	1	Total	C	O	0	0
			30	22	8		
3	C	1	Total	C	O	0	0
			30	22	8		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	107	Total O 107 107	0	0
5	B	56	Total O 56 56	0	0

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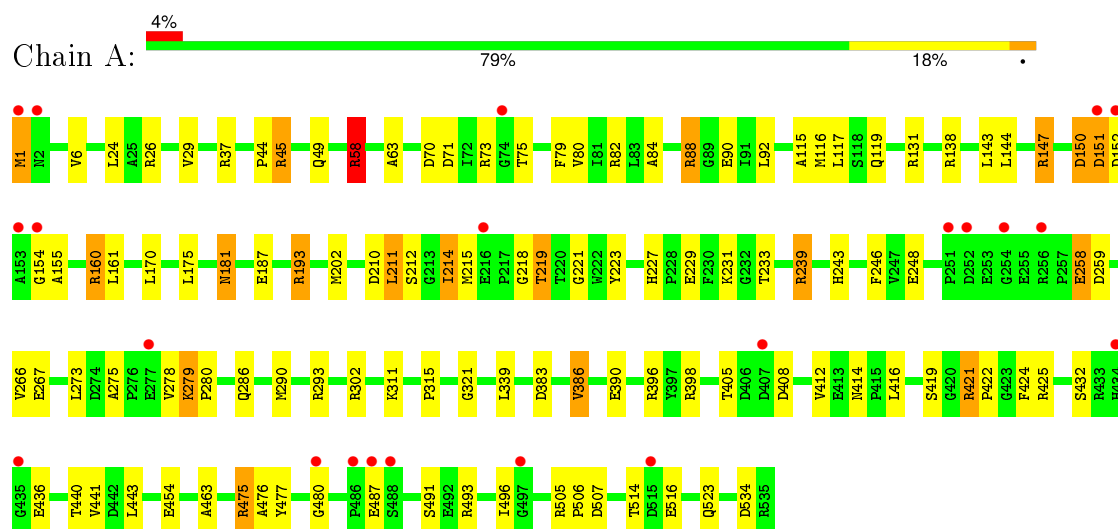
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	36	Total	O	0	0
			36	36		

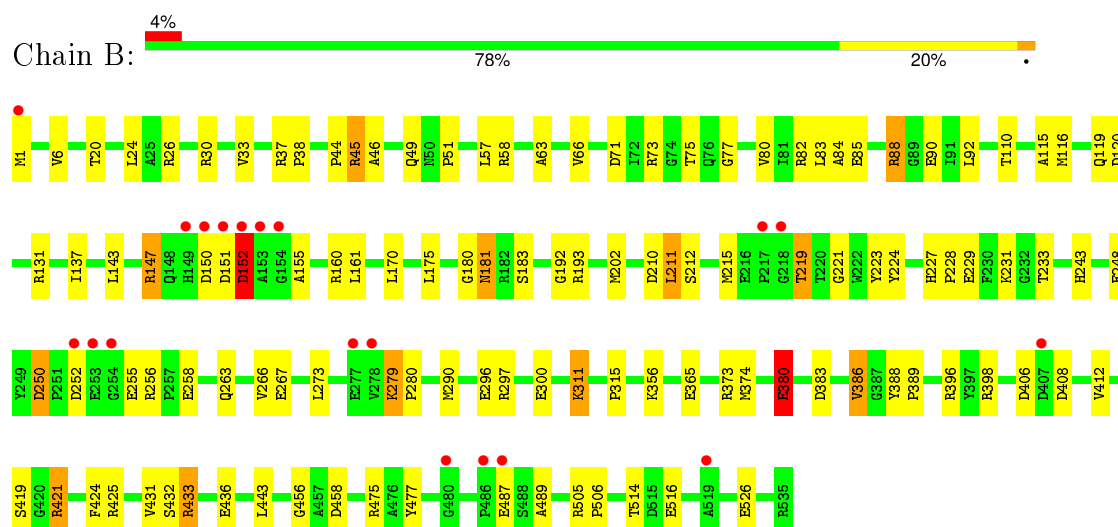
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

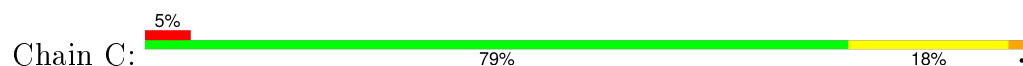
• Molecule 1: RdmE

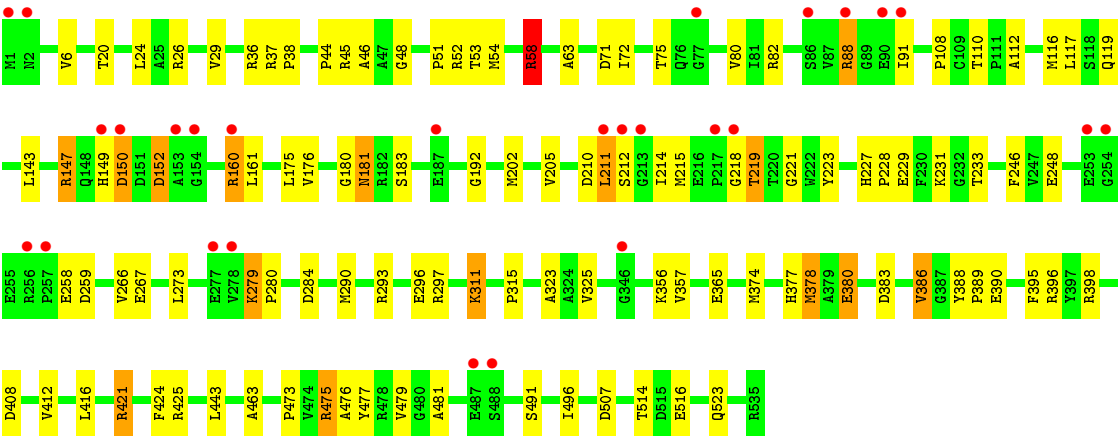


• Molecule 1: RdmE



• Molecule 1: RdmE





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	183.03 Å 183.03 Å 99.64 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.68 – 2.49 46.68 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.68-2.49) 97.9 (46.68-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.48 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.204 , 0.255 0.212 , 0.259	Depositor DCC
R_{free} test set	3319 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
Estimated twinning fraction	0.489 for H, K, L 0.511 for -H-K, K, -L 0.196 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.489 for H, K, L 0.511 for -H-K, K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 65119 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12729	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1804e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: VAK, SO4, FAD

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	0.96	6/4162 (0.1%)	1.05	20/5654 (0.4%)
1	B	0.90	2/4141 (0.0%)	0.97	15/5627 (0.3%)
1	C	0.91	2/4161 (0.0%)	1.00	7/5653 (0.1%)
All	All	0.92	10/12464 (0.1%)	1.01	42/16934 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	ARG	CZ-NH1	-7.60	1.23	1.33
1	A	193	ARG	CZ-NH2	-7.18	1.23	1.33
1	A	193	ARG	CZ-NH1	-6.55	1.24	1.33
1	B	380	GLU	CG-CD	-6.41	1.42	1.51
1	A	37	ARG	CZ-NH1	-6.08	1.25	1.33
1	C	246	PHE	CE2-CZ	5.94	1.48	1.37
1	A	151	ASP	CB-CG	5.86	1.64	1.51
1	A	58	ARG	CZ-NH2	-5.68	1.25	1.33
1	B	90	GLU	CG-CD	5.39	1.60	1.51
1	C	259	ASP	CG-OD1	-5.02	1.13	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	ASP	CB-CG-OD2	15.73	132.46	118.30
1	A	58	ARG	NE-CZ-NH2	14.90	127.75	120.30
1	C	259	ASP	CB-CG-OD1	-14.42	105.32	118.30
1	A	37	ARG	NE-CZ-NH2	12.96	126.78	120.30
1	A	160	ARG	NE-CZ-NH1	-12.17	114.22	120.30
1	A	152	ASP	CB-CG-OD2	12.16	129.25	118.30
1	C	160	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	C	160	ARG	NE-CZ-NH1	10.93	125.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	193	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	58	ARG	NH1-CZ-NH2	-8.45	110.10	119.40
1	C	421	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	B	1	MET	CB-CG-SD	-7.62	89.54	112.40
1	B	421	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	A	45	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	421	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	152	ASP	CB-CG-OD1	-7.11	111.91	118.30
1	B	160	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	193	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
1	A	160	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	B	458	ASP	CB-CG-OD1	7.02	124.61	118.30
1	A	259	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	259	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	A	425	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	B	421	ARG	NH1-CZ-NH2	-6.67	112.06	119.40
1	B	30	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	493	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	425	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	A	421	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	193	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	37	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
1	B	160	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	58	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	507	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	147	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	30	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	26	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	425	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	B	45	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	131	ARG	CG-CD-NE	5.39	123.13	111.80
1	B	193	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	152	ASP	CB-CG-OD2	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4071	0	3990	101	0
1	B	4053	0	3968	90	1
1	C	4067	0	3991	88	1
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
3	A	30	0	18	6	0
3	B	30	0	20	3	0
3	C	30	0	20	6	0
4	A	45	0	0	12	0
4	B	20	0	0	2	0
4	C	25	0	0	2	0
5	A	107	0	0	27	0
5	B	56	0	0	16	0
5	C	36	0	0	4	0
All	All	12729	0	12100	285	1

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 12.

All (285) 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:297:ARG:HD3	5:B:553:HOH:O	1.43	1.18
1:B:131:ARG:NH1	5:B:589:HOH:O	1.80	1.14
1:C:398:ARG:NH2	1:C:408:ASP:O	1.83	1.11
1:B:120:ASP:HA	5:B:585:HOH:O	1.51	1.08
1:A:231:LYS:HE2	1:A:248:GLU:OE1	1.57	1.04
1:A:214:ILE:HG23	5:A:620:HOH:O	1.61	1.00
1:C:181[A]:ASN:ND2	1:C:181[A]:ASN:H	1.51	0.99
1:B:398:ARG:NH2	1:B:408:ASP:O	1.97	0.97
1:A:181:ASN:HD22	1:A:181:ASN:H	1.09	0.96
1:A:398:ARG:NH2	1:A:408:ASP:O	2.01	0.94
1:B:231:LYS:HE2	1:B:248:GLU:OE1	1.71	0.91
1:B:514:THR:HG21	5:B:549:HOH:O	1.71	0.89
1:B:181:ASN:ND2	1:B:181:ASN:H	1.66	0.89
1:A:405:THR:HB	4:A:545:SO4:O2	1.76	0.86
1:A:138:ARG:NE	4:A:544:SO4:O4	2.09	0.85
1:C:215:MET:HG2	1:C:219:THR:CG2	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181[A]:ASN:H	1:C:181[A]:ASN:HD22	1.23	0.84
1:A:70:ASP:HA	5:A:581:HOH:O	1.80	0.82
1:B:215:MET:HG2	1:B:219:THR:CG2	2.11	0.81
1:C:227:HIS:CD2	1:C:229:GLU:H	1.99	0.80
1:A:88:ARG:HD3	1:A:273:LEU:O	1.81	0.80
1:C:202:MET:CE	3:C:537:VAK:H3	2.12	0.80
1:A:405:THR:CB	4:A:545:SO4:O2	2.29	0.80
1:C:514:THR:HG21	5:C:556:HOH:O	1.81	0.79
1:A:215:MET:HG2	1:A:219:THR:CG2	2.13	0.79
1:A:487:GLU:HA	5:A:622:HOH:O	1.83	0.78
1:A:154:GLY:HA3	5:A:566:HOH:O	1.84	0.78
1:C:202:MET:HE1	3:C:537:VAK:H3	1.66	0.78
1:A:202:MET:CE	3:A:537:VAK:H3	2.14	0.78
1:A:193:ARG:HD2	4:A:543:SO4:O3	1.85	0.77
1:A:181:ASN:H	1:A:181:ASN:ND2	1.82	0.77
1:C:231:LYS:HE2	1:C:248:GLU:OE1	1.84	0.77
1:A:202:MET:HE1	3:A:537:VAK:H3	1.66	0.75
1:B:192:GLY:O	1:B:296:GLU:HG3	1.86	0.75
1:C:231:LYS:HE3	1:C:374:MET:O	1.87	0.75
1:B:202:MET:HE1	3:B:537:VAK:H3	1.70	0.74
1:A:227:HIS:CD2	1:A:229:GLU:H	2.07	0.72
3:A:537:VAK:H11	5:A:629:HOH:O	1.90	0.72
1:B:456:GLY:HA2	5:B:552:HOH:O	1.88	0.72
1:A:239:ARG:HD2	4:A:546:SO4:O4	1.89	0.72
1:A:480:GLY:HA2	5:A:608:HOH:O	1.89	0.71
1:B:88:ARG:CG	1:B:273:LEU:O	2.37	0.71
1:B:152:ASP:OD1	1:B:152:ASP:N	2.20	0.71
1:C:227:HIS:HD2	1:C:229:GLU:H	1.37	0.71
1:A:386:VAL:CG1	1:A:412:VAL:HG21	2.21	0.71
1:C:290:MET:HG2	1:C:315:PRO:HD3	1.73	0.70
1:B:202:MET:CE	3:B:537:VAK:H3	2.20	0.70
1:A:88:ARG:CG	1:A:273:LEU:O	2.40	0.70
1:A:88:ARG:CD	1:A:273:LEU:O	2.40	0.70
1:B:227:HIS:CD2	1:B:229:GLU:H	2.11	0.68
1:C:396:ARG:HB2	1:C:424:PHE:CE1	2.28	0.68
1:B:228:PRO:HD3	5:B:561:HOH:O	1.94	0.68
1:C:88:ARG:CG	1:C:273:LEU:O	2.42	0.68
1:A:278:VAL:HA	5:A:580:HOH:O	1.94	0.67
1:A:227:HIS:HD2	1:A:229:GLU:H	1.42	0.66
1:C:297:ARG:NH1	5:C:570:HOH:O	2.28	0.65
1:A:193:ARG:NH2	1:A:293:ARG:HD2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HG21	1:A:82:ARG:NE	2.13	0.64
1:A:422:PRO:HD2	4:A:545:SO4:O1	1.97	0.64
1:B:252:ASP:HB2	5:B:577:HOH:O	1.96	0.64
1:B:300:GLU:HG3	5:B:553:HOH:O	1.96	0.64
1:C:357:VAL:HB	5:C:567:HOH:O	1.98	0.63
1:A:150:ASP:N	5:A:625:HOH:O	2.31	0.62
1:C:215:MET:HG2	1:C:219:THR:HG21	1.79	0.62
1:C:386:VAL:CG1	1:C:412:VAL:HG21	2.30	0.61
1:B:80:VAL:HG21	1:B:82:ARG:NE	2.14	0.61
1:A:386:VAL:O	1:A:390:GLU:HG3	2.00	0.61
1:B:256:ARG:HD3	5:B:597:HOH:O	2.01	0.60
1:B:88:ARG:HD3	1:B:273:LEU:O	2.02	0.59
1:A:90:GLU:O	5:A:565:HOH:O	2.17	0.59
1:A:73:ARG:NH2	5:A:592:HOH:O	2.34	0.59
1:A:151:ASP:HA	1:A:155:ALA:HB2	1.84	0.59
1:B:227:HIS:HD2	1:B:229:GLU:H	1.51	0.58
1:B:406:ASP:HB3	1:B:421:ARG:NH1	2.18	0.58
1:C:88:ARG:HD3	1:C:273:LEU:O	2.03	0.58
1:A:405:THR:OG1	4:A:545:SO4:O2	2.22	0.58
1:C:54:MET:HB2	1:C:112:ALA:HB1	1.85	0.58
1:B:505:ARG:HB3	1:B:506:PRO:CD	2.33	0.57
1:C:202:MET:HE3	3:C:537:VAK:H3	1.85	0.57
1:B:84:ALA:HA	1:B:92:LEU:HG	1.85	0.57
1:A:386:VAL:HG13	1:A:412:VAL:HG21	1.87	0.57
1:C:71:ASP:HB2	1:C:116:MET:HB2	1.87	0.57
1:B:433:ARG:NH1	5:B:573:HOH:O	2.37	0.56
1:B:71:ASP:HB2	1:B:116:MET:HB2	1.87	0.56
1:A:290:MET:HG2	1:A:315:PRO:HD3	1.87	0.56
1:A:279:LYS:HE2	5:A:594:HOH:O	2.05	0.56
1:C:386:VAL:HG13	1:C:412:VAL:HG21	1.86	0.56
1:B:49:GLN:HB2	1:B:115:ALA:HB3	1.87	0.56
1:C:152:ASP:N	1:C:152:ASP:OD1	2.38	0.56
3:C:537:VAK:O20	3:C:537:VAK:O19	2.16	0.56
1:C:149:HIS:CE1	5:C:562:HOH:O	2.59	0.55
1:C:51:PRO:HB3	1:C:110:THR:HG21	1.88	0.55
1:C:266:VAL:HG22	1:C:280:PRO:HG2	1.87	0.55
1:B:88:ARG:CD	1:B:273:LEU:O	2.54	0.55
1:C:290:MET:HG2	1:C:315:PRO:CD	2.35	0.55
1:A:266:VAL:HG22	1:A:280:PRO:HG2	1.88	0.55
1:A:73:ARG:CZ	5:A:592:HOH:O	2.54	0.55
1:C:514:THR:HG22	1:C:516:GLU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:O	1:B:221:GLY:HA3	2.07	0.54
1:B:388:TYR:HB3	1:B:389:PRO:HD3	1.89	0.54
1:A:248:GLU:HB3	5:A:621:HOH:O	2.07	0.54
1:B:252:ASP:CB	5:B:577:HOH:O	2.53	0.54
1:A:396:ARG:HB2	1:A:424:PHE:CE1	2.43	0.54
1:C:395:PHE:CD1	1:C:395:PHE:O	2.60	0.54
1:C:218:GLY:HA2	4:C:542:SO4:O2	2.07	0.54
1:B:290:MET:HG2	1:B:315:PRO:CD	2.37	0.54
1:C:88:ARG:CD	1:C:273:LEU:O	2.56	0.54
1:C:365:GLU:OE1	1:C:365:GLU:HA	2.08	0.54
1:B:386:VAL:CG1	1:B:412:VAL:HG21	2.38	0.53
1:B:181:ASN:N	1:B:181:ASN:ND2	2.47	0.53
1:A:75:THR:N	4:A:542:SO4:O3	2.41	0.53
1:B:514:THR:HG22	1:B:516:GLU:H	1.73	0.53
1:B:290:MET:HG2	1:B:315:PRO:HD3	1.90	0.53
1:A:419:SER:OG	1:A:421:ARG:HG3	2.09	0.53
1:C:72:ILE:CD1	3:C:537:VAK:H15A	2.38	0.53
1:B:33:VAL:O	1:B:137:ILE:HG13	2.09	0.53
1:A:279:LYS:N	5:A:580:HOH:O	2.35	0.53
1:A:258:GLU:OE1	1:A:258:GLU:N	2.42	0.53
1:A:24:LEU:HD22	1:A:29:VAL:HG11	1.91	0.53
1:A:80:VAL:HG21	1:A:82:ARG:CZ	2.40	0.52
1:B:20:THR:HG22	1:B:24:LEU:CD1	2.39	0.52
3:A:537:VAK:O20	3:A:537:VAK:O19	2.26	0.52
2:B:536:FAD:HM73	5:B:559:HOH:O	2.08	0.52
1:C:46:ALA:H	1:C:119:GLN:NE2	2.07	0.52
1:B:505:ARG:HB3	1:B:506:PRO:HD2	1.91	0.52
1:A:286[A]:GLN:NE2	5:A:612:HOH:O	2.43	0.52
1:B:443:LEU:HD22	1:B:477:TYR:CE2	2.44	0.52
1:A:422:PRO:HG2	4:A:545:SO4:O1	2.09	0.52
1:A:202:MET:HE3	3:A:537:VAK:H3	1.89	0.52
1:C:75:THR:N	4:C:542:SO4:O3	2.42	0.52
1:A:147[A]:ARG:HH12	1:A:160:ARG:HB2	1.74	0.52
1:B:75:THR:N	4:B:542:SO4:O3	2.41	0.52
1:B:223:TYR:O	1:B:233:THR:HA	2.09	0.52
1:B:71:ASP:OD2	1:B:73:ARG:NH2	2.42	0.52
1:C:52:ARG:NH2	1:C:507:ASP:O	2.37	0.52
1:B:396:ARG:HB2	1:B:424:PHE:CE1	2.45	0.51
1:C:147[A]:ARG:HH12	1:C:160:ARG:HB2	1.74	0.51
1:C:491:SER:HA	1:C:496:ILE:CG1	2.41	0.51
1:C:80:VAL:O	1:C:221:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:HB2	1:A:290:MET:HE3	1.93	0.50
1:C:443:LEU:HD22	1:C:477:TYR:CE2	2.46	0.50
1:B:432:SER:HA	1:B:436:GLU:O	2.10	0.50
1:B:250:ASP:O	1:B:255:GLU:HB2	2.12	0.50
1:A:279:LYS:HD3	5:A:594:HOH:O	2.11	0.50
1:B:386:VAL:HG13	1:B:412:VAL:HG21	1.93	0.50
1:B:80:VAL:HG21	1:B:82:ARG:CZ	2.41	0.50
1:A:223:TYR:O	1:A:233:THR:HA	2.11	0.50
1:C:192:GLY:O	1:C:296:GLU:HG3	2.12	0.50
1:B:143:LEU:HA	1:B:161:LEU:HD23	1.92	0.50
1:A:1:MET:HB3	5:A:628:HOH:O	2.10	0.49
1:B:252:ASP:N	5:B:577:HOH:O	2.20	0.49
1:B:83:LEU:HD21	1:B:373:ARG:HA	1.94	0.49
1:B:210:ASP:OD1	1:B:210:ASP:C	2.50	0.49
1:B:215:MET:HG2	1:B:219:THR:HG22	1.89	0.49
1:C:143:LEU:HA	1:C:161:LEU:HD23	1.94	0.49
1:A:71:ASP:HB2	1:A:116:MET:HB2	1.95	0.49
1:A:84:ALA:HA	1:A:92:LEU:HG	1.94	0.49
1:A:181:ASN:ND2	1:A:181:ASN:N	2.53	0.49
1:C:227:HIS:HD2	1:C:229:GLU:HB2	1.78	0.49
1:A:386:VAL:HG11	1:A:412:VAL:HG21	1.95	0.49
1:B:526:GLU:CD	5:B:584:HOH:O	2.51	0.49
1:A:80:VAL:O	1:A:221:GLY:HA3	2.12	0.49
1:C:475:ARG:NE	1:C:477:TYR:OH	2.46	0.48
1:C:150:ASP:HB2	1:C:152:ASP:OD1	2.13	0.48
1:C:293:ARG:O	1:C:311:LYS:HA	2.12	0.48
1:B:279:LYS:HE3	1:B:279:LYS:HB2	1.47	0.48
1:A:491:SER:HB2	5:A:597:HOH:O	2.13	0.48
1:A:218:GLY:HA2	4:A:542:SO4:O2	2.14	0.47
1:C:108:PRO:HG2	1:C:416:LEU:HD22	1.96	0.47
1:A:143:LEU:HA	1:A:161:LEU:HD23	1.96	0.47
1:B:85:GLU:HG2	5:B:561:HOH:O	2.14	0.47
1:B:475:ARG:NE	1:B:477:TYR:OH	2.47	0.47
1:B:26:ARG:NH1	4:B:541:SO4:O2	2.47	0.47
1:C:227:HIS:HD2	1:C:229:GLU:N	2.11	0.47
1:A:475:ARG:CD	5:A:589:HOH:O	2.63	0.47
1:C:215:MET:HG2	1:C:219:THR:HG22	1.93	0.47
1:B:181:ASN:HD22	1:B:181:ASN:H	1.58	0.47
1:C:279:LYS:HE3	1:C:279:LYS:HB2	1.52	0.47
1:A:321:GLY:N	5:A:550:HOH:O	2.48	0.47
1:C:386:VAL:O	1:C:390:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:H	1:B:119:GLN:NE2	2.12	0.46
1:B:311:LYS:O	1:B:311:LYS:HG3	2.14	0.46
1:B:88:ARG:HG2	1:B:273:LEU:O	2.13	0.46
1:B:58:ARG:HA	1:B:63:ALA:HB2	1.98	0.46
1:B:380:GLU:HG2	1:B:380:GLU:H	1.24	0.46
1:B:202:MET:HE3	3:B:537:VAK:H3	1.98	0.46
1:C:48:GLY:HA2	1:C:116:MET:HA	1.98	0.46
1:B:211:LEU:HD22	1:B:243:HIS:NE2	2.30	0.46
1:B:231:LYS:HE3	1:B:374:MET:O	2.15	0.46
1:A:155:ALA:C	5:A:566:HOH:O	2.54	0.46
1:A:414:ASN:OD1	1:A:416:LEU:HB2	2.16	0.46
1:A:210:ASP:OD1	1:A:212:SER:HB2	2.16	0.46
1:A:279:LYS:HB2	1:A:279:LYS:HE3	1.51	0.45
1:B:57:LEU:HD13	1:B:66:VAL:HG21	1.97	0.45
1:C:311:LYS:HZ1	1:C:323:ALA:CB	2.30	0.45
3:C:537:VAK:O17	3:C:537:VAK:H8A	2.17	0.45
1:A:227:HIS:HD2	1:A:229:GLU:N	2.13	0.45
1:A:514:THR:HG22	1:A:516:GLU:H	1.80	0.45
1:A:181:ASN:HD22	1:A:181:ASN:N	1.91	0.45
1:C:46:ALA:H	1:C:119:GLN:HE21	1.64	0.45
1:C:37:ARG:HA	1:C:38:PRO:HD3	1.84	0.45
1:C:227:HIS:CD2	1:C:229:GLU:HB2	2.52	0.45
1:B:227:HIS:HD2	1:B:229:GLU:HB2	1.81	0.45
1:A:422:PRO:CD	4:A:545:SO4:O1	2.63	0.45
1:C:175:LEU:C	1:C:175:LEU:HD23	2.37	0.44
1:B:266:VAL:HG22	1:B:280:PRO:HG2	1.99	0.44
1:A:441:VAL:HG22	5:A:575:HOH:O	2.16	0.44
1:A:432:SER:HA	1:A:436:GLU:O	2.17	0.44
1:C:475:ARG:HG3	1:C:476:ALA:N	2.32	0.44
1:A:210:ASP:C	1:A:210:ASP:OD1	2.54	0.44
1:C:175:LEU:HD23	1:C:176:VAL:N	2.33	0.44
1:A:215:MET:HG2	1:A:219:THR:HG21	1.97	0.44
1:B:20:THR:HG22	1:B:24:LEU:HD11	2.00	0.44
1:B:180:GLY:O	1:B:183:SER:HB2	2.17	0.44
1:A:26:ARG:NH1	4:A:541:SO4:O2	2.50	0.44
1:A:45:ARG:NH1	1:A:119:GLN:OE1	2.50	0.44
1:A:463:ALA:CB	1:A:476:ALA:HB2	2.47	0.44
1:A:339:LEU:HD23	5:A:591:HOH:O	2.16	0.44
1:C:210:ASP:OD1	1:C:210:ASP:C	2.56	0.44
1:A:49:GLN:HB2	1:A:115:ALA:HB3	1.99	0.44
1:C:44:PRO:O	1:C:45:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:TYR:O	1:C:233:THR:HA	2.18	0.43
1:B:248:GLU:CD	5:B:565:HOH:O	2.57	0.43
1:A:202:MET:HG2	1:A:246:PHE:HB3	1.99	0.43
1:B:73:ARG:HD2	1:B:77:GLY:O	2.18	0.43
1:C:463:ALA:CB	1:C:476:ALA:HB2	2.49	0.43
1:C:80:VAL:HG21	1:C:82:ARG:NE	2.34	0.43
1:C:210:ASP:OD1	1:C:212:SER:HB2	2.17	0.43
1:C:227:HIS:CG	1:C:228:PRO:HD2	2.54	0.43
1:B:487:GLU:HG3	1:B:489:ALA:HB2	2.00	0.43
1:B:227:HIS:CD2	1:B:229:GLU:HB2	2.54	0.43
1:B:211:LEU:HD22	1:B:243:HIS:CE1	2.53	0.43
1:A:214:ILE:HG21	1:A:275:ALA:CB	2.49	0.43
1:C:82:ARG:HD3	1:C:91:ILE:HG12	2.01	0.43
1:C:37:ARG:HE	1:C:37:ARG:HB3	1.53	0.43
1:A:175:LEU:HD23	1:A:175:LEU:C	2.39	0.43
1:B:151[B]:ASP:HA	1:B:155:ALA:HB2	2.01	0.43
1:C:36:ARG:HG2	2:C:536:FAD:C4A	2.49	0.42
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.91	0.42
1:A:214:ILE:CG2	5:A:620:HOH:O	2.42	0.42
1:A:290:MET:HG2	1:A:315:PRO:CD	2.50	0.42
1:A:1:MET:CB	5:A:628:HOH:O	2.67	0.42
1:C:377:HIS:CD2	1:C:378:MET:HG2	2.54	0.42
1:A:505:ARG:HB3	1:A:506:PRO:CD	2.50	0.42
1:C:88:ARG:HG3	1:C:273:LEU:O	2.18	0.42
1:C:80:VAL:HG21	1:C:82:ARG:CZ	2.50	0.42
1:A:73:ARG:HG2	1:A:79:PHE:HB2	2.01	0.42
1:B:210:ASP:OD1	1:B:212:SER:HB2	2.19	0.42
1:C:395:PHE:CD1	1:C:395:PHE:C	2.93	0.42
1:B:175:LEU:C	1:B:175:LEU:HD23	2.40	0.42
1:C:205:VAL:HA	1:C:284:ASP:O	2.20	0.42
1:A:443:LEU:HD22	1:A:477:TYR:CE2	2.54	0.42
1:A:58:ARG:HA	1:A:63:ALA:HB2	2.02	0.42
1:A:534:ASP:HB2	5:A:616:HOH:O	2.18	0.42
1:B:83:LEU:HG	1:B:224:TYR:HB2	2.00	0.41
1:A:71:ASP:OD2	1:A:73:ARG:NH2	2.52	0.41
1:C:388:TYR:HB3	1:C:389:PRO:HD3	2.02	0.41
1:A:88:ARG:HG3	1:A:273:LEU:O	2.17	0.41
1:B:88:ARG:HG3	1:B:273:LEU:O	2.16	0.41
1:C:211:LEU:HG	1:C:214:ILE:HD11	2.03	0.41
1:C:24:LEU:HD22	1:C:29:VAL:HG11	2.01	0.41
1:B:365:GLU:OE1	1:B:365:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HB2	1:A:160:ARG:HG2	2.03	0.41
1:B:46:ALA:H	1:B:119:GLN:HE21	1.69	0.41
1:B:44:PRO:O	1:B:45:ARG:C	2.59	0.41
1:C:380:GLU:H	1:C:380:GLU:HG2	1.61	0.41
3:A:537:VAK:H8A	3:A:537:VAK:O17	2.21	0.41
1:A:211:LEU:HD22	1:A:243:HIS:CE1	2.56	0.41
1:C:53:THR:HG23	1:C:325:VAL:HG11	2.03	0.41
1:A:475:ARG:HD3	5:A:589:HOH:O	2.21	0.41
1:B:51:PRO:HB3	1:B:110:THR:HG21	2.02	0.41
1:C:479:VAL:C	1:C:481:ALA:H	2.23	0.41
1:A:491:SER:HA	1:A:496:ILE:CG1	2.51	0.40
1:C:58:ARG:HA	1:C:63:ALA:HB2	2.03	0.40
1:A:214:ILE:HG21	1:A:275:ALA:HB2	2.04	0.40
1:B:419:SER:HB2	1:B:421:ARG:HG3	2.02	0.40
1:A:44:PRO:O	1:A:45:ARG:C	2.58	0.40
1:C:311:LYS:HZ1	1:C:323:ALA:HB3	1.85	0.40
1:B:227:HIS:O	1:B:228:PRO:C	2.58	0.40
1:C:20:THR:HG22	1:C:24:LEU:HD11	2.04	0.40
1:A:302:ARG:HD3	1:A:302:ARG:HH11	1.68	0.40
1:C:491:SER:HA	1:C:496:ILE:HG13	2.03	0.40
1:C:180:GLY:O	1:C:183:SER:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLN:OE1	1:C:377:HIS:CB[4_665]	1.88	0.32

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	536/535 (100%)	512 (96%)	22 (4%)	2 (0%)	39	61
1	B	534/535 (100%)	501 (94%)	32 (6%)	1 (0%)	52	75
1	C	536/535 (100%)	511 (95%)	25 (5%)	0	100	100
All	All	1606/1605 (100%)	1524 (95%)	79 (5%)	3 (0%)	52	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	THR
1	A	454	GLU
1	B	431	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	408/405 (101%)	385 (94%)	23 (6%)	26	47
1	B	406/405 (100%)	387 (95%)	19 (5%)	32	56
1	C	408/405 (101%)	381 (93%)	27 (7%)	21	38
All	All	1222/1215 (101%)	1153 (94%)	69 (6%)	28	47

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	VAL
1	A	58	ARG
1	A	88	ARG
1	A	117	LEU
1	A	147[A]	ARG
1	A	147[B]	ARG
1	A	150	ASP
1	A	170	LEU
1	A	181	ASN

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Mol	Chain	Res	Type
1	A	187	GLU
1	A	211	LEU
1	A	214	ILE
1	A	219	THR
1	A	239	ARG
1	A	258	GLU
1	A	267	GLU
1	A	279	LYS
1	A	311	LYS
1	A	383	ASP
1	A	386	VAL
1	A	475	ARG
1	A	523	GLN
1	B	6	VAL
1	B	88	ARG
1	B	147	ARG
1	B	150	ASP
1	B	152	ASP
1	B	170	LEU
1	B	181	ASN
1	B	211	LEU
1	B	219	THR
1	B	250	ASP
1	B	258	GLU
1	B	267	GLU
1	B	279	LYS
1	B	311	LYS
1	B	356	LYS
1	B	380	GLU
1	B	383	ASP
1	B	386	VAL
1	B	433	ARG
1	C	6	VAL
1	C	58	ARG
1	C	88	ARG
1	C	117	LEU
1	C	147[A]	ARG
1	C	147[B]	ARG
1	C	150	ASP
1	C	152	ASP
1	C	181[A]	ASN
1	C	181[B]	ASN

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Mol	Chain	Res	Type
1	C	211	LEU
1	C	219	THR
1	C	258	GLU
1	C	267	GLU
1	C	279	LYS
1	C	311	LYS
1	C	356	LYS
1	C	378	MET
1	C	380	GLU
1	C	383	ASP
1	C	386	VAL
1	C	421	ARG
1	C	425	ARG
1	C	473	PRO
1	C	475	ARG
1	C	523[A]	GLN
1	C	523[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	181	ASN
1	A	201	HIS
1	A	227	HIS
1	A	263	GLN
1	B	119	GLN
1	B	181	ASN
1	B	201	HIS
1	B	227	HIS
1	B	523	GLN
1	C	119	GLN
1	C	201	HIS
1	C	227	HIS
1	C	263	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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	FAD	A	536	-	48,58,58	1.27	7 (14%)	54,89,89	2.22	11 (20%)
3	VAK	A	537	-	31,33,33	2.18	9 (29%)	43,52,52	1.55	4 (9%)
4	SO4	A	538	-	4,4,4	0.63	0	6,6,6	0.88	0
4	SO4	A	539	-	4,4,4	0.54	0	6,6,6	1.02	1 (16%)
4	SO4	A	540	-	4,4,4	0.20	0	6,6,6	0.43	0
4	SO4	A	541	-	4,4,4	0.54	0	6,6,6	0.35	0
4	SO4	A	542	-	4,4,4	0.41	0	6,6,6	0.39	0
4	SO4	A	543	-	4,4,4	0.73	0	6,6,6	1.51	2 (33%)
4	SO4	A	544	-	4,4,4	0.46	0	6,6,6	0.59	0
4	SO4	A	545	-	4,4,4	0.46	0	6,6,6	0.91	0
4	SO4	A	546	-	4,4,4	0.64	0	6,6,6	0.39	0
2	FAD	B	536	-	48,58,58	1.15	4 (8%)	54,89,89	2.06	10 (18%)
3	VAK	B	537	-	31,33,33	2.08	8 (25%)	43,52,52	1.51	6 (13%)
4	SO4	B	538	-	4,4,4	0.39	0	6,6,6	0.90	0
4	SO4	B	539	-	4,4,4	0.76	0	6,6,6	0.52	0
4	SO4	B	541	-	4,4,4	0.17	0	6,6,6	0.73	0
4	SO4	B	542	-	4,4,4	0.57	0	6,6,6	0.21	0
2	FAD	C	536	-	48,58,58	1.16	5 (10%)	54,89,89	2.42	12 (22%)
3	VAK	C	537	-	31,33,33	2.16	8 (25%)	43,52,52	1.68	7 (16%)
4	SO4	C	538	-	4,4,4	0.52	0	6,6,6	1.00	0
4	SO4	C	539	-	4,4,4	0.29	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	540	-	4,4,4	0.23	0	6,6,6	0.25	0
4	SO4	C	541	-	4,4,4	0.40	0	6,6,6	0.49	0
4	SO4	C	542	-	4,4,4	0.58	0	6,6,6	0.30	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
2	FAD	A	536	-	-	0/30/50/50	0/6/6/6
3	VAK	A	537	-	-	0/9/44/44	0/4/4/4
4	SO4	A	538	-	-	0/0/0/0	0/0/0/0
4	SO4	A	539	-	-	0/0/0/0	0/0/0/0
4	SO4	A	540	-	-	0/0/0/0	0/0/0/0
4	SO4	A	541	-	-	0/0/0/0	0/0/0/0
4	SO4	A	542	-	-	0/0/0/0	0/0/0/0
4	SO4	A	543	-	-	0/0/0/0	0/0/0/0
4	SO4	A	544	-	-	0/0/0/0	0/0/0/0
4	SO4	A	545	-	-	0/0/0/0	0/0/0/0
4	SO4	A	546	-	-	0/0/0/0	0/0/0/0
2	FAD	B	536	-	-	0/30/50/50	0/6/6/6
3	VAK	B	537	-	-	0/9/44/44	0/4/4/4
4	SO4	B	538	-	-	0/0/0/0	0/0/0/0
4	SO4	B	539	-	-	0/0/0/0	0/0/0/0
4	SO4	B	541	-	-	0/0/0/0	0/0/0/0
4	SO4	B	542	-	-	0/0/0/0	0/0/0/0
2	FAD	C	536	-	-	0/30/50/50	0/6/6/6
3	VAK	C	537	-	-	0/9/44/44	0/4/4/4
4	SO4	C	538	-	-	0/0/0/0	0/0/0/0
4	SO4	C	539	-	-	0/0/0/0	0/0/0/0
4	SO4	C	540	-	-	0/0/0/0	0/0/0/0
4	SO4	C	541	-	-	0/0/0/0	0/0/0/0
4	SO4	C	542	-	-	0/0/0/0	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	537	VAK	C21-C12	-4.27	1.39	1.48
3	C	537	VAK	C21-C12	-4.16	1.39	1.48
3	C	537	VAK	C18-C12	-4.11	1.39	1.48
3	B	537	VAK	C21-C12	-4.07	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	537	VAK	C16-C5	-3.81	1.38	1.47
3	B	537	VAK	C16-C5	-3.60	1.38	1.47
3	A	537	VAK	C18-C12	-3.40	1.41	1.48
3	B	537	VAK	C17-C5	-3.37	1.39	1.47
3	A	537	VAK	C17-C5	-3.18	1.39	1.47
3	A	537	VAK	C16-C5	-3.11	1.39	1.47
3	B	537	VAK	C18-C12	-3.04	1.41	1.48
3	C	537	VAK	C19-C10	-2.99	1.46	1.51
3	A	537	VAK	C19-C10	-2.81	1.47	1.51
2	A	536	FAD	P-O2P	-2.77	1.43	1.54
3	C	537	VAK	C17-C5	-2.66	1.41	1.47
3	B	537	VAK	C19-C10	-2.30	1.48	1.51
2	A	536	FAD	C1'-N10	-2.28	1.46	1.48
2	B	536	FAD	C4A-N3A	-2.14	1.32	1.35
2	B	536	FAD	C9A-C5X	-2.03	1.38	1.42
2	A	536	FAD	C4X-N5	2.02	1.36	1.33
2	A	536	FAD	C2A-N1A	2.13	1.37	1.33
2	A	536	FAD	C2A-N3A	2.15	1.36	1.32
2	C	536	FAD	O4B-C1B	2.17	1.43	1.41
3	B	537	VAK	O18-C12	2.30	1.27	1.22
3	C	537	VAK	O20-C5	2.31	1.27	1.22
2	B	536	FAD	O4B-C1B	2.39	1.44	1.41
3	A	537	VAK	O18-C12	2.39	1.27	1.22
2	C	536	FAD	C9A-N10	2.46	1.42	1.38
2	C	536	FAD	C4X-N5	2.51	1.37	1.33
3	A	537	VAK	O20-C5	3.20	1.28	1.22
2	B	536	FAD	C4-C4X	3.26	1.47	1.41
2	A	536	FAD	C10-N10	3.33	1.43	1.39
2	C	536	FAD	C10-N10	3.34	1.43	1.39
2	C	536	FAD	C4-C4X	3.66	1.48	1.41
2	A	536	FAD	C4-C4X	3.91	1.49	1.41
3	C	537	VAK	O16-C14	4.26	1.44	1.33
3	B	537	VAK	O16-C14	4.87	1.45	1.33
3	A	537	VAK	O16-C14	5.23	1.46	1.33
3	A	537	VAK	C20-C19	5.69	1.49	1.40
3	B	537	VAK	C20-C19	5.79	1.49	1.40
3	C	537	VAK	C20-C19	6.15	1.49	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	536	FAD	N3A-C2A-N1A	-9.09	121.93	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	536	FAD	N3A-C2A-N1A	-8.63	122.28	128.89
2	A	536	FAD	N3A-C2A-N1A	-7.90	122.85	128.89
2	C	536	FAD	C4X-C10-N10	-5.86	117.06	120.52
2	A	536	FAD	C4X-C10-N10	-4.88	117.64	120.52
2	C	536	FAD	C4-C4X-C10	-4.66	116.96	119.94
2	B	536	FAD	C4X-C4-N3	-3.97	118.17	123.59
2	C	536	FAD	O4'-C4'-C5'	-3.96	101.56	110.19
2	A	536	FAD	C4X-C4-N3	-3.93	118.21	123.59
3	C	537	VAK	O16-C14-O17	-3.91	115.72	123.79
2	A	536	FAD	C4A-C5A-N7A	-3.68	106.09	109.48
3	B	537	VAK	O16-C14-O17	-3.63	116.29	123.79
2	C	536	FAD	P-O3P-PA	-3.57	122.70	132.73
2	B	536	FAD	C4X-C10-N10	-3.39	118.52	120.52
2	B	536	FAD	O4'-C4'-C5'	-3.37	102.85	110.19
2	C	536	FAD	C4A-C5A-N7A	-3.33	106.42	109.48
3	B	537	VAK	C8-C7-C20	-3.32	107.23	111.93
3	A	537	VAK	C22-C13-C9	-3.24	109.39	115.00
2	A	536	FAD	C4-C4X-C10	-3.20	117.89	119.94
3	A	537	VAK	O16-C14-O17	-3.17	117.24	123.79
2	B	536	FAD	P-O3P-PA	-3.17	123.84	132.73
2	A	536	FAD	O4'-C4'-C5'	-2.88	103.91	110.19
2	C	536	FAD	C4X-C4-N3	-2.84	119.71	123.59
2	B	536	FAD	C4-C4X-C10	-2.72	118.20	119.94
3	C	537	VAK	C4-C16-C5	-2.59	115.90	120.55
3	C	537	VAK	O23-C9-C8	-2.56	104.77	108.92
3	B	537	VAK	C22-C13-C9	-2.52	110.64	115.00
2	A	536	FAD	P-O3P-PA	-2.52	125.66	132.73
3	C	537	VAK	C8-C7-C20	-2.19	108.83	111.93
2	C	536	FAD	C9A-C5X-N5	-2.05	119.33	122.36
2	A	536	FAD	O2P-P-O1P	2.00	123.38	112.53
3	B	537	VAK	C21-C16-C4	2.13	120.50	118.42
4	A	539	SO4	O2-S-O1	2.16	116.33	109.50
2	B	536	FAD	O2A-PA-O1A	2.16	124.22	112.53
2	C	536	FAD	O2A-PA-O1A	2.30	124.97	112.53
3	B	537	VAK	C15-O16-C14	2.33	121.45	115.99
4	A	543	SO4	O4-S-O3	2.34	118.50	108.98
3	C	537	VAK	C15-O16-C14	2.46	121.76	115.99
2	B	536	FAD	C5X-C9A-N10	2.48	119.51	117.62
3	A	537	VAK	C15-O16-C14	2.52	121.90	115.99
4	A	543	SO4	O2-S-O1	2.61	117.78	109.50
2	B	536	FAD	C4X-N5-C5X	3.23	120.48	116.76
3	C	537	VAK	C21-C16-C4	3.45	121.79	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	536	FAD	C4X-N5-C5X	3.63	120.94	116.76
2	C	536	FAD	C5X-C9A-N10	4.00	120.66	117.62
2	A	536	FAD	C5X-C9A-N10	4.10	120.73	117.62
2	C	536	FAD	C4X-N5-C5X	4.35	121.77	116.76
3	B	537	VAK	O16-C14-C10	5.22	120.09	111.17
3	A	537	VAK	O16-C14-C10	5.36	120.34	111.17
2	B	536	FAD	C4-N3-C2	5.61	120.10	115.25
3	C	537	VAK	O16-C14-C10	5.83	121.13	111.17
2	C	536	FAD	C4-N3-C2	7.54	121.77	115.25
2	A	536	FAD	C4-N3-C2	7.57	121.79	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	537	VAK	6	0
4	A	541	SO4	1	0
4	A	542	SO4	2	0
4	A	543	SO4	1	0
4	A	544	SO4	1	0
4	A	545	SO4	6	0
4	A	546	SO4	1	0
2	B	536	FAD	1	0
3	B	537	VAK	3	0
4	B	541	SO4	1	0
4	B	542	SO4	1	0
2	C	536	FAD	1	0
3	C	537	VAK	6	0
4	C	542	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	535/535 (100%)	0.35	22 (4%)	41 46	2, 21, 35, 42	0
1	B	535/535 (100%)	0.08	19 (3%)	46 51	3, 22, 35, 42	0
1	C	535/535 (100%)	0.11	27 (5%)	32 37	2, 22, 35, 42	0
All	All	1605/1605 (100%)	0.18	68 (4%)	40 45	2, 22, 35, 42	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	154	GLY	5.5
1	A	154	GLY	5.3
1	B	1	MET	5.2
1	C	154	GLY	4.1
1	C	217	PRO	4.1
1	C	254	GLY	4.1
1	A	252	ASP	4.0
1	B	151[A]	ASP	3.7
1	A	277	GLU	3.7
1	C	278	VAL	3.7
1	C	212	SER	3.7
1	A	407	ASP	3.7
1	A	1	MET	3.6
1	B	254	GLY	3.5
1	A	152	ASP	3.5
1	C	88	ARG	3.4
1	B	153	ALA	3.3
1	B	407	ASP	3.2
1	C	86	SER	3.2
1	C	77	GLY	3.1
1	B	277	GLU	3.1
1	A	435	GLY	3.1
1	B	278	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	218	GLY	2.9
1	A	2	ASN	2.9
1	B	149	HIS	2.9
1	C	346	GLY	2.8
1	A	151	ASP	2.8
1	C	487	GLU	2.7
1	A	488	SER	2.7
1	A	487	GLU	2.7
1	C	488	SER	2.7
1	A	480	GLY	2.6
1	C	213	GLY	2.6
1	B	486	PRO	2.6
1	B	253	GLU	2.6
1	A	434	HIS	2.6
1	A	216	GLU	2.5
1	B	217	PRO	2.5
1	A	486	PRO	2.4
1	C	277	GLU	2.4
1	A	251	PRO	2.4
1	B	218	GLY	2.4
1	C	150	ASP	2.4
1	C	153	ALA	2.4
1	B	480	GLY	2.3
1	A	515	ASP	2.3
1	B	519	ALA	2.3
1	C	257	PRO	2.3
1	C	2	ASN	2.3
1	A	254	GLY	2.3
1	B	152	ASP	2.3
1	C	91	ILE	2.2
1	A	497	GLY	2.2
1	C	256	ARG	2.2
1	B	150	ASP	2.2
1	B	487	GLU	2.2
1	C	149	HIS	2.2
1	C	211	LEU	2.1
1	A	153	ALA	2.1
1	B	252	ASP	2.1
1	C	90	GLU	2.1
1	A	74	GLY	2.1
1	C	1	MET	2.1
1	C	187	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	253	GLU	2.1
1	C	160	ARG	2.0
1	A	256	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	C	541	5/5	0.91	0.21	5.88	36,37,38,41	0
4	SO4	C	539	5/5	0.95	0.16	0.63	36,36,38,39	0
4	SO4	A	542	5/5	0.93	0.22	0.36	32,33,36,38	0
4	SO4	B	542	5/5	0.92	0.23	0.13	33,34,36,38	0
3	VAK	B	537	30/30	0.94	0.15	0.01	21,23,25,26	0
4	SO4	C	542	5/5	0.96	0.25	-0.03	33,34,36,39	0
3	VAK	C	537	30/30	0.92	0.15	-0.08	21,23,25,26	0
3	VAK	A	537	30/30	0.93	0.17	-0.17	21,23,24,26	0
4	SO4	B	541	5/5	0.95	0.14	-0.26	36,37,38,40	0
2	FAD	C	536	53/53	0.96	0.12	-0.56	13,19,25,26	0
2	FAD	B	536	53/53	0.97	0.13	-0.61	12,19,25,26	0
2	FAD	A	536	53/53	0.96	0.16	-0.81	13,18,25,26	0
4	SO4	A	545	5/5	0.98	0.14	-1.12	29,33,36,38	0
4	SO4	A	539	5/5	0.98	0.14	-1.28	36,37,37,38	0
4	SO4	A	546	5/5	0.98	0.16	-1.44	27,28,29,30	0
4	SO4	B	539	5/5	0.98	0.13	-1.50	36,36,37,38	0
4	SO4	A	541	5/5	0.95	0.13	-1.59	35,38,38,41	0
4	SO4	A	543	5/5	0.94	0.14	-1.78	17,25,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	544	5/5	0.91	0.20	-	34,37,41,43	0
4	SO4	A	540	5/5	0.95	0.16	-	41,41,43,43	0
4	SO4	C	540	5/5	0.92	0.30	-	76,77,77,77	0
4	SO4	C	538	5/5	0.92	0.17	-	42,42,44,45	0
4	SO4	B	538	5/5	0.93	0.21	-	42,43,44,45	0
4	SO4	A	538	5/5	0.97	0.16	-	42,42,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.