Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EB7
Title	:	Crystal Structure of Insecticidal Delta-Endotoxin Cry8Ea1 from Bacillus Thuringiensis at 2.2 Angstroms Resolution
Authors	:	Guo, S.; Ye, S.; Song, F.; Zhang, J.; Wei, L.; Shu, C.L.
Deposited on	:	2008-08-27
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

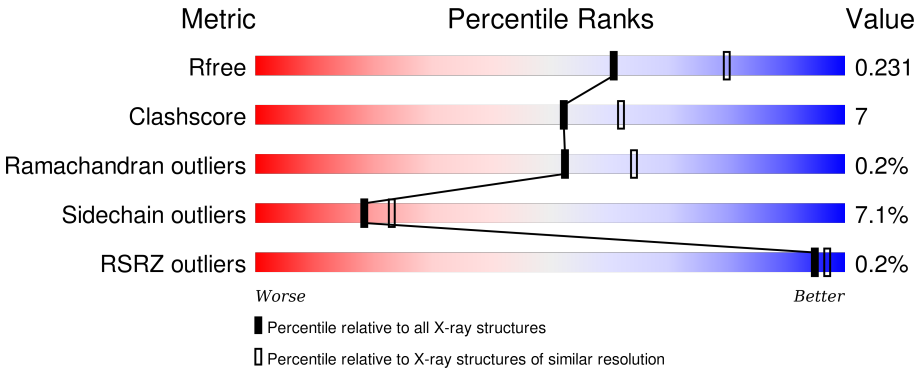
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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 <=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	589	84% 14% •
1	B	589	83% 15% •
1	C	589	79% 17% • •

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
2	SO4	A	2011	-	-	-	X
2	SO4	B	2006	-	-	-	X
2	SO4	B	2007	-	-	-	X
2	SO4	C	2009	-	-	-	X
2	SO4	C	2013	-	-	-	X
3	ACT	B	2015	-	-	-	X
3	ACT	C	2016	-	-	-	X

2 Entry composition

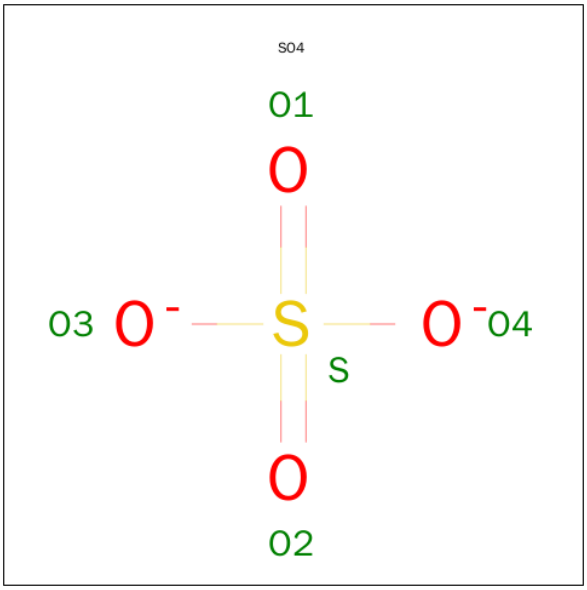
There are 4 unique types of molecules in this entry. The entry contains 15253 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Insecticidal Delta-Endotoxin Cry8Ea1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	2	0
			4701	3005	790	895	11			
1	B	589	Total	C	N	O	S	0	1	0
			4690	2999	786	894	11			
1	C	588	Total	C	N	O	S	0	1	0
			4684	2996	785	892	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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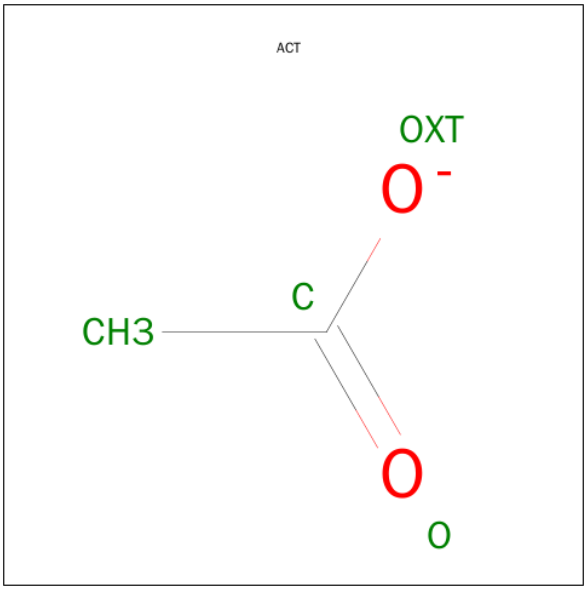
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

- Molecule 4 is water.

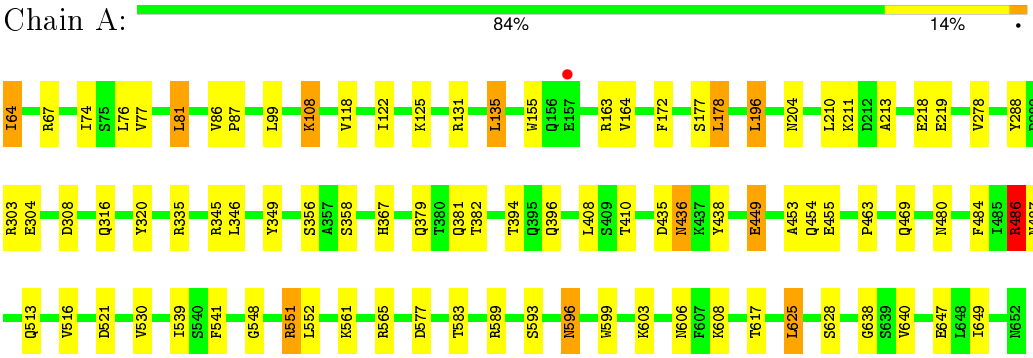
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	348	Total O 348 348	0	0
4	B	392	Total O 392 392	0	0
4	C	361	Total O 361 361	0	0

3 Residue-property plots (i)

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

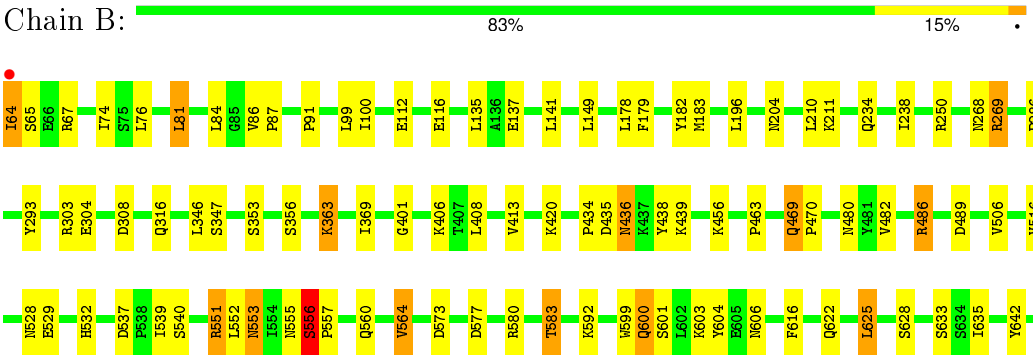
- Molecule 1: Insecticidal Delta-Endotoxin Cry8Ea1

Chain A:



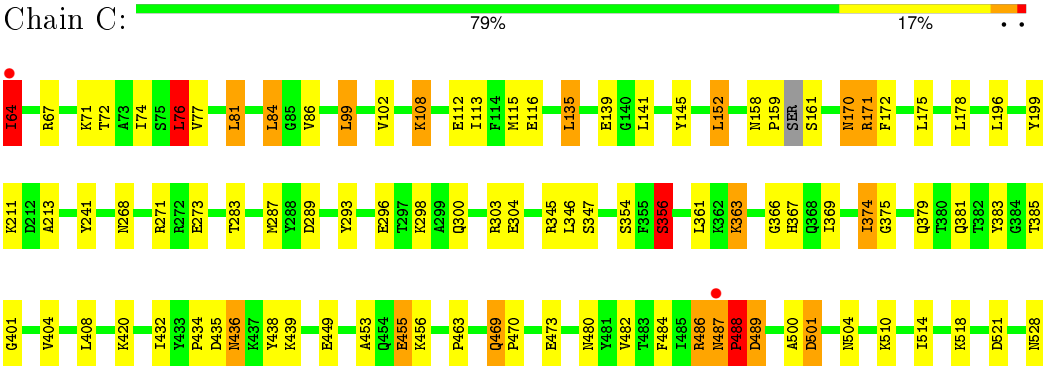
- Molecule 1: Insecticidal Delta-Endotoxin Cry8Ea1

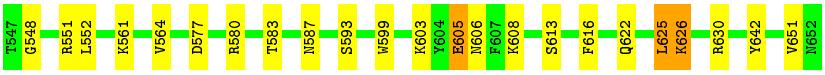
Chain B:



- Molecule 1: Insecticidal Delta-Endotoxin Cry8Ea1

Chain C:




T547
G548
R551
L552
K561
V564
D577
R580
T583
N587
S593
W599
K603
Y604
E605
N606
F607
K608
S613
F616
Q622
L625
K626
R630
Y642
V651
N652

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	407.28Å 47.96Å 103.12Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	43.20 – 2.30 43.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.20-2.30) 96.9 (43.20-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.162 , 0.230 0.162 , 0.231	Depositor DCC
R_{free} test set	8890 reflections (11.11%)	DCC
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.3	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 98913 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15253	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, ACT

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	0.81	0/4820	0.78	4/6550 (0.1%)
1	B	0.84	0/4809	0.82	6/6536 (0.1%)
1	C	0.81	3/4802 (0.1%)	0.82	10/6525 (0.2%)
All	All	0.82	3/14431 (0.0%)	0.81	20/19611 (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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	488	PRO	N-CD	8.10	1.59	1.47
1	C	273	GLU	CG-CD	5.38	1.60	1.51
1	C	605	GLU	CG-CD	5.26	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	488	PRO	N-CA-C	8.18	133.35	112.10
1	C	76	LEU	CA-CB-CG	7.07	131.57	115.30
1	C	487	ASN	N-CA-C	6.80	129.37	111.00
1	A	308	ASP	CB-CG-OD1	6.67	124.31	118.30
1	C	289	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	A	486	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	356	SER	CB-CA-C	6.16	121.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	152	LEU	CA-CB-CG	5.98	129.05	115.30
1	C	488	PRO	CA-N-CD	-5.90	103.23	111.50
1	A	335	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	413	VAL	CB-CA-C	-5.55	100.85	111.40
1	B	81	LEU	CA-CB-CG	5.39	127.71	115.30
1	B	250	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	C	289	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	269	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	489	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	501	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	521	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	178	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	625	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	64	ILE	Peptide

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	4701	0	4609	55	0
1	B	4690	0	4597	56	0
1	C	4684	0	4591	80	0
2	A	10	0	0	0	0
2	B	35	0	0	0	0
2	C	20	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
4	A	348	0	0	5	0
4	B	392	0	0	6	0
4	C	361	0	0	9	0
All	All	15253	0	13806	188	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 7.

All (188) 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:C:159:PRO:O	1:C:161:SER:HB3	1.45	1.16
1:B:556:SER:HB3	1:B:557:PRO:CD	1.72	1.16
1:B:556:SER:HB3	1:B:557:PRO:HD2	1.08	1.03
1:C:159:PRO:O	1:C:161:SER:CB	2.07	1.02
1:A:603:LYS:H	1:A:606:ASN:HD22	1.11	0.96
1:A:211:LYS:NZ	1:A:290:MET:SD	2.42	0.93
1:A:290:MET:SD	4:A:2287:HOH:O	2.31	0.89
1:C:408:LEU:HG	1:C:455:GLU:OE2	1.71	0.89
1:A:596:ASN:HD21	1:A:638:GLY:HA3	1.38	0.86
1:C:486:ARG:HD2	1:C:489:ASP:OD1	1.74	0.86
1:A:345:ARG:HH21	1:A:396:GLN:HE21	1.25	0.83
1:A:64:ILE:HG23	1:A:67:ARG:HD2	1.63	0.81
1:B:551:ARG:HH11	1:B:551:ARG:HG3	1.46	0.80
1:C:603:LYS:H	1:C:606:ASN:HD22	1.30	0.80
1:C:456:LYS:HE3	4:C:2109:HOH:O	1.80	0.80
1:A:603:LYS:H	1:A:606:ASN:ND2	1.80	0.80
1:B:211:LYS:NZ	1:B:290:MET:SD	2.55	0.79
1:B:603:LYS:H	1:B:606:ASN:HD22	1.30	0.78
1:C:469:GLN:HB2	1:C:470:PRO:HD2	1.65	0.78
1:C:486:ARG:CD	1:C:489:ASP:OD1	2.36	0.73
1:A:521:ASP:O	1:A:548:GLY:HA3	1.90	0.71
1:B:600:GLN:H	1:B:600:GLN:HE21	1.37	0.71
1:B:583:THR:HG22	4:B:2080:HOH:O	1.92	0.69
1:C:300:GLN:HG3	1:C:500:ALA:HA	1.74	0.69
1:C:593:SER:HB2	1:C:608:LYS:HD2	1.75	0.68
1:A:64:ILE:HG23	1:A:67:ARG:CD	2.24	0.67
1:C:159:PRO:C	1:C:161:SER:HB3	2.14	0.67
1:C:300:GLN:HE21	1:C:501:ASP:H	1.43	0.66
1:C:298:LYS:HD3	1:C:510:LYS:HD3	1.79	0.65
4:A:2092:HOH:O	1:C:108:LYS:HE2	1.96	0.64
1:C:593:SER:CB	1:C:608:LYS:HD2	2.28	0.63
1:A:487:ASN:HD21	1:B:622:GLN:HG3	1.62	0.63
1:A:379:GLN:CD	1:A:381:GLN:HE21	2.02	0.63
1:C:159:PRO:O	1:C:161:SER:OG	2.17	0.62
1:B:65:SER:OG	1:B:116:GLU:OE1	2.18	0.62
1:B:269:ARG:NH1	1:B:308:ASP:OD2	2.34	0.60
1:C:171:ARG:HD3	4:C:2302:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:GLN:NE2	1:C:501:ASP:H	1.99	0.60
1:A:436:ASN:C	1:A:436:ASN:HD22	2.05	0.60
1:B:100:ILE:HD12	1:B:149:LEU:HD22	1.82	0.59
1:B:556:SER:O	1:B:557:PRO:C	2.39	0.59
1:B:436:ASN:C	1:B:436:ASN:HD22	2.04	0.59
1:C:296:GLU:HG2	1:C:510:LYS:HG2	1.83	0.59
1:B:64:ILE:HG13	1:B:67:ARG:HD3	1.83	0.59
1:C:374:ILE:HD12	1:C:504:ASN:ND2	2.18	0.58
1:C:115:MET:CE	1:C:135:LEU:HD13	2.33	0.58
1:A:436:ASN:ND2	1:A:438:TYR:H	2.01	0.58
1:B:506:VAL:O	1:B:555:ASN:HB2	2.04	0.58
1:C:268:ASN:OD1	4:C:2132:HOH:O	2.17	0.58
1:A:345:ARG:HH21	1:A:396:GLN:NE2	2.00	0.57
1:B:86:VAL:HG11	1:B:91:PRO:HB2	1.87	0.57
1:A:298:LYS:HG3	1:A:507:TYR:CE1	2.38	0.57
1:C:436:ASN:ND2	1:C:438:TYR:H	2.02	0.57
1:B:556:SER:CB	1:B:557:PRO:CD	2.63	0.57
1:C:469:GLN:HB2	1:C:470:PRO:CD	2.35	0.56
1:A:436:ASN:HD22	1:A:438:TYR:H	1.54	0.56
1:A:408:LEU:HD12	4:A:2220:HOH:O	2.04	0.56
1:A:486:ARG:HD2	1:A:489:ASP:OD1	2.05	0.55
1:A:131:ARG:HG2	1:A:135:LEU:HD22	1.87	0.55
1:C:64:ILE:HG13	1:C:67:ARG:HD3	1.89	0.55
1:A:108:LYS:HD2	1:C:453:ALA:HB3	1.89	0.55
1:C:552:LEU:HD11	1:C:625:LEU:HD22	1.88	0.55
1:C:381:GLN:HG3	4:C:2101:HOH:O	2.08	0.54
1:B:564:VAL:HG22	1:B:616:PHE:HE2	1.72	0.54
1:B:583:THR:CG2	4:B:2080:HOH:O	2.51	0.54
1:B:363:LYS:NZ	1:B:489:ASP:OD2	2.33	0.54
1:C:300:GLN:NE2	1:C:518:LYS:NZ	2.56	0.54
1:A:551:ARG:HB2	4:A:2211:HOH:O	2.08	0.54
1:A:410:THR:HG23	1:A:453:ALA:HB1	1.90	0.54
1:B:286:PRO:HG3	1:B:604:TYR:HE1	1.73	0.53
1:C:170:ASN:HB2	4:C:2365:HOH:O	2.08	0.53
1:C:603:LYS:H	1:C:606:ASN:ND2	2.03	0.53
1:B:268:ASN:OD1	4:B:2217:HOH:O	2.19	0.53
1:C:199:TYR:HH	1:C:241:TYR:HD2	1.57	0.52
1:C:383:TYR:HB3	1:C:484:PHE:HB3	1.92	0.52
1:B:74:ILE:HD12	1:B:463:PRO:HD2	1.92	0.52
1:B:401:GLY:O	1:B:434:PRO:HD2	2.10	0.52
1:A:381:GLN:HG3	4:A:2157:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ASN:HD22	1:C:438:TYR:H	1.57	0.52
1:B:551:ARG:CG	1:B:551:ARG:HH11	2.21	0.52
1:B:179:PHE:O	1:B:183:MET:HG2	2.10	0.52
1:B:552:LEU:HD11	1:B:625:LEU:HD22	1.92	0.52
1:A:561:LYS:HD3	1:A:617:THR:CG2	2.41	0.51
1:A:304:GLU:OE2	1:A:480:ASN:ND2	2.43	0.51
1:C:436:ASN:C	1:C:436:ASN:HD22	2.14	0.51
1:B:486:ARG:HD2	1:B:489:ASP:OD1	2.10	0.51
1:C:77:VAL:O	1:C:81:LEU:HB2	2.11	0.50
1:C:170:ASN:CB	4:C:2365:HOH:O	2.59	0.50
1:A:552:LEU:HD11	1:A:625:LEU:HD22	1.94	0.50
1:C:564:VAL:HG23	1:C:616:PHE:HE2	1.75	0.50
1:C:521:ASP:O	1:C:548:GLY:HA3	2.12	0.50
1:B:540:SER:HB3	1:B:642:TYR:CD2	2.47	0.50
1:B:601:SER:O	1:B:603:LYS:HD3	2.12	0.49
1:A:516:VAL:HG23	1:A:539:ILE:HG12	1.94	0.49
1:B:64:ILE:CG1	1:B:67:ARG:HD3	2.42	0.49
1:C:300:GLN:CG	1:C:500:ALA:HA	2.42	0.48
1:A:449:GLU:HG3	1:C:139:GLU:OE2	2.13	0.48
1:C:540:SER:HB3	1:C:642:TYR:CD2	2.49	0.48
1:A:118:VAL:O	1:A:122:ILE:HG12	2.13	0.48
1:C:201:GLN:NE2	4:C:2050:HOH:O	2.42	0.48
1:B:516:VAL:HG23	1:B:539:ILE:HG12	1.94	0.48
1:C:546:SER:HB3	1:C:626:LYS:HD3	1.94	0.48
1:B:204:ASN:ND2	1:B:288:TYR:OH	2.44	0.48
1:A:603:LYS:N	1:A:606:ASN:HD22	1.94	0.47
1:C:300:GLN:NE2	1:C:518:LYS:HZ2	2.11	0.47
1:C:112:GLU:OE2	1:C:116:GLU:OE2	2.31	0.47
1:C:347:SER:HA	1:C:395:GLN:O	2.15	0.47
1:A:577:ASP:OD1	1:A:628:SER:HB2	2.15	0.47
1:C:528:ASN:HB2	1:C:599:TRP:CD2	2.49	0.46
1:B:525:PRO:HB3	1:B:537:ASP:HB3	1.97	0.46
1:C:77:VAL:HG23	1:C:81:LEU:HD22	1.98	0.46
1:B:304:GLU:HG2	1:B:480:ASN:HD22	1.81	0.46
1:C:170:ASN:HB2	4:C:2281:HOH:O	2.14	0.46
1:C:304:GLU:HG2	1:C:480:ASN:HD22	1.80	0.46
1:C:469:GLN:HG3	1:C:473:GLU:HG3	1.97	0.46
1:B:112:GLU:OE2	1:B:116:GLU:OE2	2.34	0.46
1:C:605:GLU:H	1:C:605:GLU:CD	2.20	0.46
1:C:76:LEU:HD12	1:C:99:LEU:HD12	1.97	0.46
1:C:86:VAL:O	1:C:86:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ARG:HG2	1:A:649:ILE:HD11	1.99	0.45
1:A:211:LYS:HG3	1:A:290:MET:HG2	1.98	0.45
1:B:234:GLN:O	1:B:238:ILE:HG13	2.17	0.45
1:A:155:TRP:HA	1:A:164:VAL:HG11	1.99	0.45
1:C:375:GLY:HA3	1:C:551:ARG:HG3	1.97	0.45
1:C:115:MET:HE3	1:C:135:LEU:HD13	1.99	0.45
1:B:573:ASP:HB2	1:B:633:SER:HB3	1.99	0.45
1:B:577:ASP:OD1	1:B:628:SER:HB2	2.17	0.45
1:C:108:LYS:HE3	1:C:113:ILE:HG13	1.99	0.44
1:A:196:LEU:HD13	1:A:278:VAL:HG21	1.99	0.44
1:A:155:TRP:HA	1:A:164:VAL:CG1	2.48	0.44
1:B:316:GLN:O	1:B:420:LYS:HE2	2.18	0.44
1:A:561:LYS:HD3	1:A:617:THR:HG23	2.00	0.44
1:B:211:LYS:HG3	1:B:290:MET:HG2	1.99	0.44
1:B:603:LYS:H	1:B:606:ASN:ND2	2.09	0.44
1:C:72:THR:HG22	1:C:76:LEU:HD22	1.98	0.44
1:C:287:MET:HA	1:C:293:TYR:CD1	2.53	0.44
1:B:557:PRO:HG2	1:B:560:GLN:HB2	2.00	0.44
1:C:367:HIS:HE1	1:C:484:PHE:HB2	1.83	0.44
1:C:74:ILE:HD12	1:C:463:PRO:HD2	2.00	0.44
1:C:115:MET:HE1	1:C:135:LEU:HD13	2.00	0.43
1:C:76:LEU:HD13	1:C:102:VAL:HG11	2.00	0.43
1:A:530:VAL:CG2	1:A:599:TRP:HB2	2.49	0.43
1:A:486:ARG:CD	1:A:489:ASP:OD1	2.67	0.43
1:A:408:LEU:HD11	1:A:455:GLU:OE1	2.19	0.43
1:A:410:THR:CG2	1:A:453:ALA:HB1	2.49	0.43
1:C:432:ILE:HD12	1:C:439:LYS:HG2	2.00	0.43
1:C:108:LYS:HZ3	1:C:108:LYS:HB2	1.83	0.43
1:A:204:ASN:ND2	1:A:288:TYR:OH	2.50	0.43
1:A:596:ASN:ND2	1:A:638:GLY:HA3	2.19	0.43
1:C:603:LYS:HG3	1:C:605:GLU:HG2	2.01	0.42
1:C:580:ARG:HD2	1:C:580:ARG:C	2.38	0.42
1:B:137:GLU:HB3	1:B:182:TYR:CD1	2.54	0.42
1:B:529:GLU:HB3	1:B:532:HIS:CE1	2.55	0.42
1:B:369:ILE:HD13	1:B:482:VAL:H	1.83	0.42
1:B:469:GLN:HB2	1:B:470:PRO:HD2	2.02	0.42
1:C:283:THR:HG22	1:C:283:THR:O	2.19	0.42
1:C:366:GLY:HA3	1:C:385:THR:O	2.19	0.42
1:A:74:ILE:HD12	1:A:463:PRO:HD2	2.01	0.42
1:C:408:LEU:CG	1:C:455:GLU:OE2	2.56	0.42
1:B:456:LYS:HD2	4:B:2071:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HA	1:A:87:PRO:HD3	1.96	0.42
1:C:172:PHE:CZ	1:C:213:ALA:HB2	2.55	0.42
1:B:290:MET:HE2	1:B:293:TYR:O	2.20	0.42
1:B:353:SER:OG	1:B:363:LYS:HE2	2.20	0.42
1:B:580:ARG:C	1:B:580:ARG:HD2	2.40	0.42
1:A:172:PHE:CZ	1:A:213:ALA:HB2	2.54	0.42
1:C:84:LEU:HA	1:C:84:LEU:HD12	1.88	0.42
1:A:541:PHE:O	1:A:640:VAL:HA	2.20	0.42
1:A:521:ASP:C	1:A:521:ASP:OD2	2.58	0.41
1:C:300:GLN:HE21	1:C:501:ASP:N	2.15	0.41
1:A:593:SER:HB2	1:A:608:LYS:HG3	2.03	0.41
1:C:487:ASN:HA	1:C:488:PRO:HA	1.57	0.41
1:A:316:GLN:CD	1:A:316:GLN:H	2.23	0.41
1:C:455:GLU:HG3	4:C:2027:HOH:O	2.20	0.41
1:A:367:HIS:HE1	1:A:484:PHE:HB2	1.86	0.41
1:C:401:GLY:O	1:C:434:PRO:HD2	2.20	0.41
1:C:361:LEU:HG	1:C:363:LYS:HB3	2.04	0.41
1:C:369:ILE:HD13	1:C:482:VAL:H	1.86	0.40
1:B:528:ASN:HB2	1:B:599:TRP:CD2	2.55	0.40
1:B:439:LYS:NZ	4:B:2392:HOH:O	2.54	0.40
1:B:86:VAL:HA	1:B:87:PRO:HD3	1.86	0.40
1:B:553:ASN:ND2	4:B:2395:HOH:O	2.55	0.40
1:C:108:LYS:NZ	1:C:108:LYS:HB2	2.36	0.40
1:B:436:ASN:HD22	1:B:438:TYR:H	1.69	0.40
1:A:304:GLU:CG	1:A:480:ASN:HD22	2.35	0.40
1:A:77:VAL:O	1:A:81:LEU:HB2	2.22	0.40
1:A:513:GLN:HG2	1:A:647:GLU:HG2	2.04	0.40
1:A:349:TYR:CD2	1:A:394:THR:HG22	2.57	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	589/589 (100%)	574 (98%)	15 (2%)	0	100	100
1	B	588/589 (100%)	571 (97%)	15 (3%)	2 (0%)	46	57
1	C	585/589 (99%)	571 (98%)	13 (2%)	1 (0%)	52	64
All	All	1762/1767 (100%)	1716 (97%)	43 (2%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	556	SER
1	C	356	SER
1	B	435	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/514 (100%)	485 (94%)	31 (6%)	24	31
1	B	515/514 (100%)	486 (94%)	29 (6%)	26	35
1	C	514/514 (100%)	465 (90%)	49 (10%)	11	12
All	All	1545/1542 (100%)	1436 (93%)	109 (7%)	18	23

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	76	LEU
1	A	81	LEU
1	A	99	LEU
1	A	108	LYS
1	A	125	LYS
1	A	135	LEU
1	A	163	ARG
1	A	177	SER
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	210	LEU
1	A	218	GLU
1	A	219	GLU
1	A	303	ARG
1	A	320	TYR
1	A	346	LEU
1	A	356	SER
1	A	358	SER
1	A	382	THR
1	A	435	ASP
1	A	436	ASN
1	A	449	GLU
1	A	454	GLN
1	A	469	GLN
1	A	486	ARG
1	A	551	ARG
1	A	583	THR
1	A	589	ARG
1	A	596	ASN
1	A	625	LEU
1	B	64	ILE
1	B	76	LEU
1	B	81	LEU
1	B	84	LEU
1	B	99	LEU
1	B	135	LEU
1	B	141	LEU
1	B	178	LEU
1	B	196	LEU
1	B	210	LEU
1	B	303	ARG
1	B	346	LEU
1	B	347	SER
1	B	356	SER
1	B	363	LYS
1	B	406	LYS
1	B	408	LEU
1	B	436	ASN
1	B	469	GLN
1	B	486	ARG
1	B	551	ARG

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Mol	Chain	Res	Type
1	B	553	ASN
1	B	556	SER
1	B	564	VAL
1	B	583	THR
1	B	592	LYS
1	B	600	GLN
1	B	635	ILE
1	B	652	ASN
1	C	64	ILE
1	C	71	LYS
1	C	76	LEU
1	C	81	LEU
1	C	84	LEU
1	C	99	LEU
1	C	108	LYS
1	C	135	LEU
1	C	141	LEU
1	C	145	TYR
1	C	152	LEU
1	C	158	ASN
1	C	170	ASN
1	C	171	ARG
1	C	175	LEU
1	C	178	LEU
1	C	196	LEU
1	C	210	LEU
1	C	211	LYS
1	C	271	ARG
1	C	303	ARG
1	C	345	ARG
1	C	346	LEU
1	C	354	SER
1	C	356	SER
1	C	363	LYS
1	C	374	ILE
1	C	379	GLN
1	C	396	GLN
1	C	404	VAL
1	C	420	LYS
1	C	435	ASP
1	C	436	ASN
1	C	449	GLU

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Mol	Chain	Res	Type
1	C	455	GLU
1	C	469	GLN
1	C	486	ARG
1	C	488	PRO
1	C	514	ILE
1	C	561	LYS
1	C	577	ASP
1	C	583	THR
1	C	587	ASN
1	C	613	SER
1	C	622	GLN
1	C	625	LEU
1	C	626	LYS
1	C	630	ARG
1	C	651	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	117	GLN
1	A	124	GLN
1	A	201	GLN
1	A	204	ASN
1	A	372	GLN
1	A	381	GLN
1	A	396	GLN
1	A	436	ASN
1	A	480	ASN
1	A	487	ASN
1	A	586	ASN
1	A	596	ASN
1	A	606	ASN
1	B	110	GLN
1	B	117	GLN
1	B	170	ASN
1	B	201	GLN
1	B	204	ASN
1	B	372	GLN
1	B	396	GLN
1	B	436	ASN
1	B	480	ASN

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Mol	Chain	Res	Type
1	B	553	ASN
1	B	600	GLN
1	B	606	ASN
1	B	622	GLN
1	B	652	ASN
1	C	117	GLN
1	C	124	GLN
1	C	201	GLN
1	C	204	ASN
1	C	240	GLN
1	C	300	GLN
1	C	368	GLN
1	C	372	GLN
1	C	396	GLN
1	C	436	ASN
1	C	480	ASN
1	C	586	ASN
1	C	606	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 carbohydrates in this entry.

5.6 Ligand geometry

16 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	SO4	A	2008	-	4,4,4	0.10	0	6,6,6	0.23	0
2	SO4	A	2011	-	4,4,4	0.13	0	6,6,6	0.24	0
3	ACT	A	2014	-	1,3,3	1.68	0	0,3,3	0.00	-
2	SO4	B	2001	-	4,4,4	0.53	0	6,6,6	0.28	0
2	SO4	B	2002	-	4,4,4	0.57	0	6,6,6	0.44	0
2	SO4	B	2005	-	4,4,4	0.16	0	6,6,6	0.39	0
2	SO4	B	2006	-	4,4,4	0.14	0	6,6,6	0.47	0
2	SO4	B	2007	-	4,4,4	0.31	0	6,6,6	0.31	0
2	SO4	B	2010	-	4,4,4	0.18	0	6,6,6	0.62	0
2	SO4	B	2012	-	4,4,4	0.17	0	6,6,6	0.33	0
3	ACT	B	2015	-	1,3,3	2.00	0	0,3,3	0.00	-
2	SO4	C	2003	-	4,4,4	0.27	0	6,6,6	0.80	0
2	SO4	C	2004	-	4,4,4	0.46	0	6,6,6	0.41	0
2	SO4	C	2009	-	4,4,4	0.06	0	6,6,6	0.66	0
2	SO4	C	2013	-	4,4,4	0.15	0	6,6,6	0.27	0
3	ACT	C	2016	-	1,3,3	1.70	0	0,3,3	0.00	-

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	SO4	A	2008	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2011	-	-	0/0/0/0	0/0/0/0
3	ACT	A	2014	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2005	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2007	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2010	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2012	-	-	0/0/0/0	0/0/0/0
3	ACT	B	2015	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2009	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2013	-	-	0/0/0/0	0/0/0/0
3	ACT	C	2016	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	589/589 (100%)	-0.52	1 (0%)	95	97	14, 25, 38, 56	0
1	B	589/589 (100%)	-0.59	1 (0%)	95	97	12, 23, 34, 53	0
1	C	588/589 (99%)	-0.45	2 (0%)	94	96	15, 26, 39, 57	0
All	All	1766/1767 (99%)	-0.52	4 (0%)	95	97	12, 25, 38, 57	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	ILE	3.9
1	B	64	ILE	2.7
1	C	487	ASN	2.5
1	A	157	GLU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	ACT	B	2015	4/4	0.78	0.20	10.75	53,54,54,54	0
3	ACT	C	2016	4/4	0.70	0.23	5.08	50,50,51,51	0
2	SO4	A	2011	5/5	0.92	0.14	4.83	75,75,76,76	0
2	SO4	C	2013	5/5	0.86	0.22	4.32	77,77,79,79	0
2	SO4	B	2006	5/5	0.96	0.25	3.58	50,52,54,55	0
2	SO4	C	2009	5/5	0.95	0.23	2.29	66,67,67,68	0
2	SO4	B	2007	5/5	0.92	0.19	2.16	63,63,64,65	0
3	ACT	A	2014	4/4	0.92	0.13	1.64	38,38,39,39	0
2	SO4	B	2010	5/5	0.93	0.12	1.04	66,66,66,67	0
2	SO4	A	2008	5/5	0.90	0.14	0.89	74,74,75,76	0
2	SO4	B	2001	5/5	0.98	0.10	-0.36	29,29,30,35	0
2	SO4	B	2005	5/5	0.98	0.09	-0.63	40,41,42,44	0
2	SO4	C	2004	5/5	0.99	0.09	-0.86	46,46,47,47	0
2	SO4	C	2003	5/5	0.98	0.09	-0.90	46,47,48,49	0
2	SO4	B	2002	5/5	0.99	0.07	-1.48	33,33,35,37	0
2	SO4	B	2012	5/5	0.91	0.27	-	61,61,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.