



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:25 AM UTC

PDB ID : 3EB7 / pdb_00003eb7
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

<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

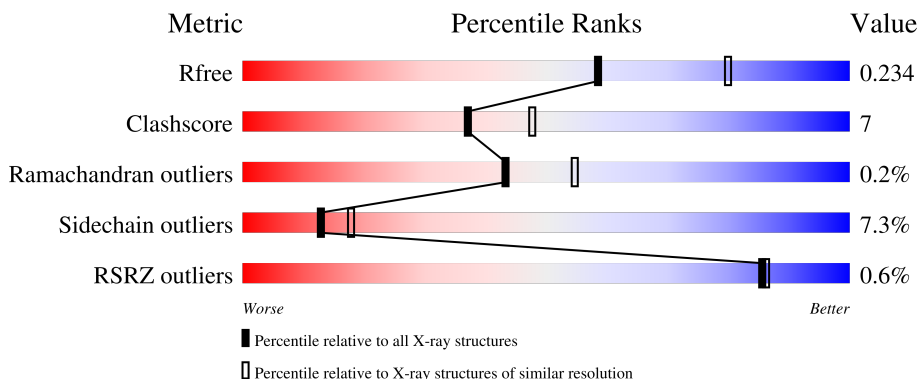
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	589	
1	B	589	
1	C	589	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	589	Total 4701	C 3005	N 790	O 895	S 11	0	2	0
1	B	589	Total 4690	C 2999	N 786	O 894	S 11	0	1	0
1	C	588	Total 4684	C 2996	N 785	O 892	S 11	0	1	0

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



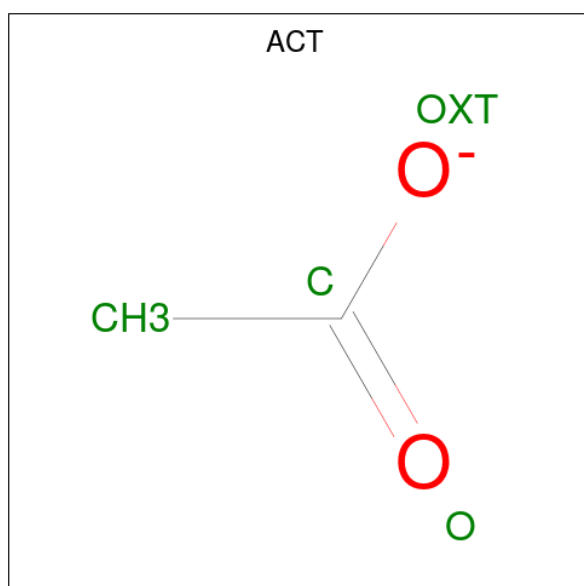
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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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 (CCD ID: ACT) (formula: C₂H₃O₂).



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	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

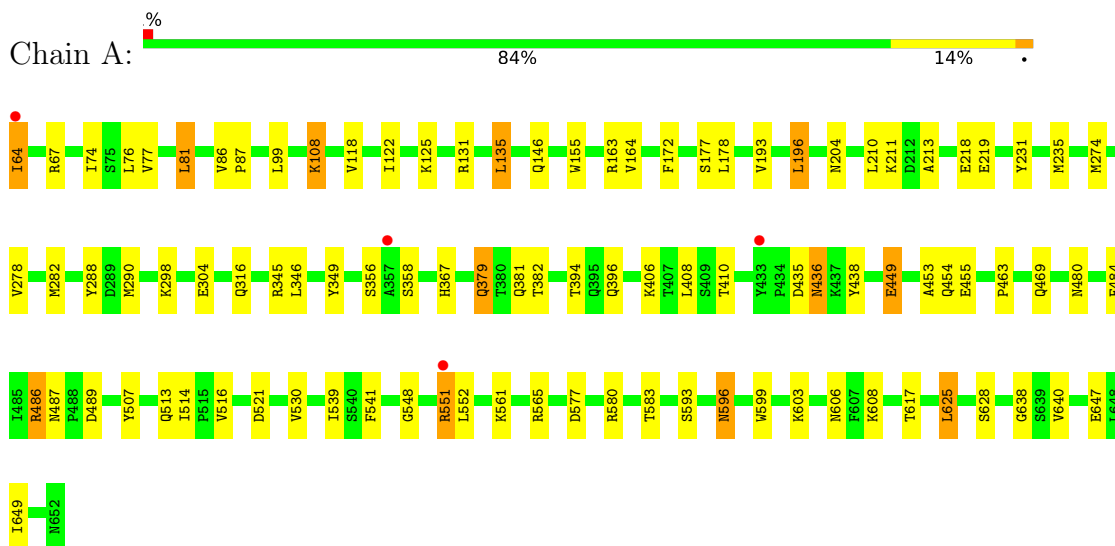
- Molecule 4 is water.

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

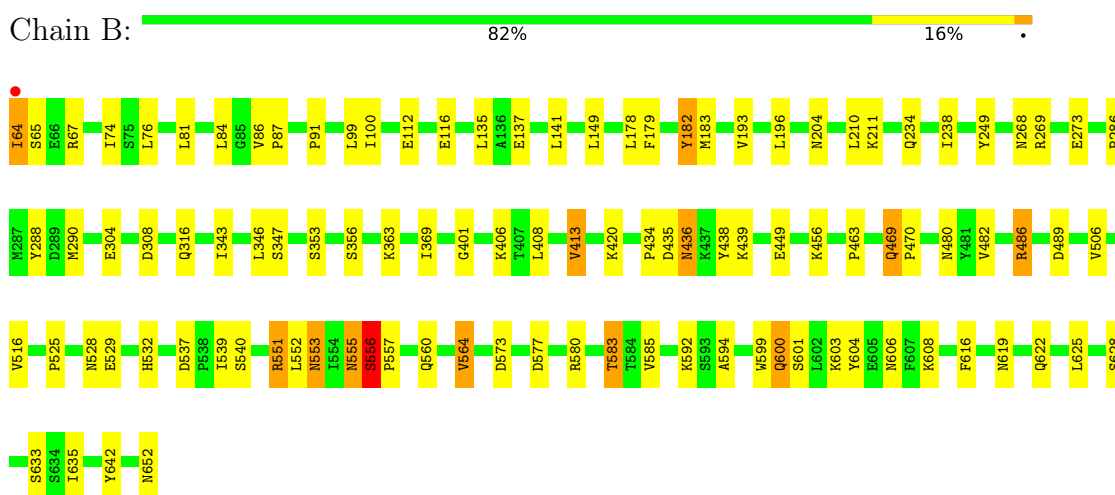
3 Residue-property plots i

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

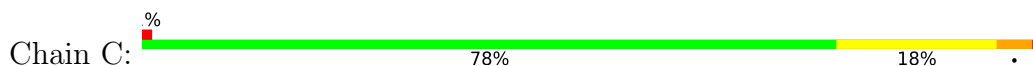
- Molecule 1: Insecticidal Delta-Endotoxin Cry8Ea1

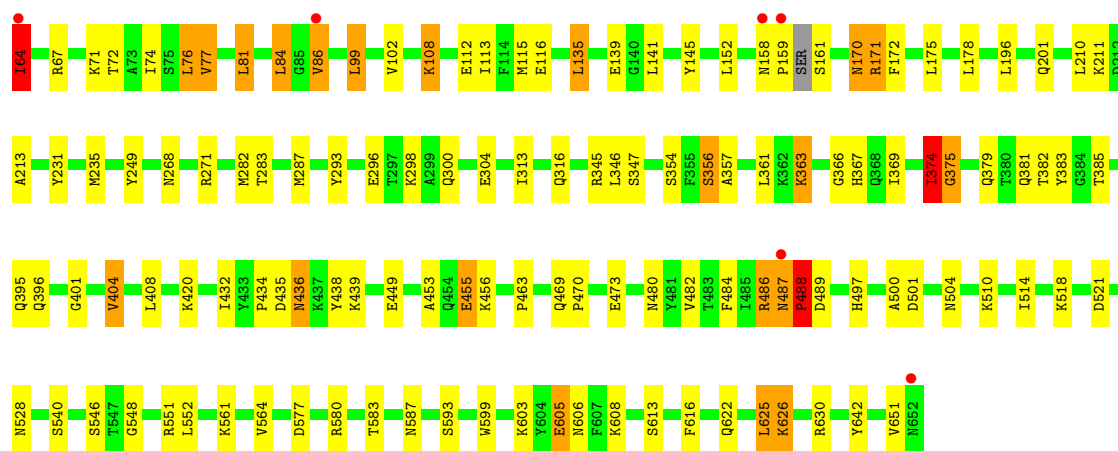


- Molecule 1: Insecticidal Delta-Endotoxin Cry8Ea1



- Molecule 1: Insecticidal Delta-Endotoxin Cry8Ea1





4 Data and refinement statistics

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 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.20-2.30) 99.0 (43.20-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.20Å)	Xtrriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.162 , 0.230 0.168 , 0.234	Depositor DCC
R_{free} test set	9895 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtrriage
Anisotropy	0.544	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15253	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.96	0/4820	0.97	2/6550 (0.0%)
1	B	1.00	3/4809 (0.1%)	1.03	9/6536 (0.1%)
1	C	0.95	1/4802 (0.0%)	1.04	10/6525 (0.2%)
All	All	0.97	4/14431 (0.0%)	1.01	21/19611 (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 (4) 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	B	343	ILE	CA-CB	5.51	1.59	1.54
1	B	193	VAL	CA-C	5.49	1.58	1.52
1	B	585	VAL	CA-CB	5.19	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	357	ALA	N-CA-C	-9.53	101.78	113.50
1	C	487	ASN	N-CA-C	8.85	129.37	109.81
1	C	488	PRO	N-CA-C	8.18	133.35	112.10
1	B	556	SER	CA-C-N	-7.46	110.52	119.84
1	B	556	SER	C-N-CA	-7.46	110.52	119.84
1	B	555	ASN	N-CA-C	6.90	118.88	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	GLU	N-CA-C	6.51	118.38	111.28
1	C	404	VAL	CB-CA-C	6.17	117.90	111.23
1	B	413	VAL	CB-CA-C	-5.97	100.85	110.28
1	C	488	PRO	CA-N-CD	-5.90	103.23	111.50
1	B	619	ASN	N-CA-C	5.88	118.92	111.69
1	C	356	SER	CB-CA-C	5.72	121.81	110.42
1	B	594	ALA	CA-C-N	5.64	125.62	120.21
1	B	594	ALA	C-N-CA	5.64	125.62	120.21
1	C	375	GLY	N-CA-C	-5.55	107.58	115.30
1	C	374	ILE	N-CA-CB	5.41	116.83	110.82
1	A	193	VAL	CA-C-N	-5.38	114.08	119.56
1	A	193	VAL	C-N-CA	-5.38	114.08	119.56
1	B	182	TYR	N-CA-C	5.20	118.79	112.23
1	C	497	HIS	CA-C-N	5.09	127.36	120.38
1	C	497	HIS	C-N-CA	5.09	127.36	120.38

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	62	0
1	B	4690	0	4597	58	0
1	C	4684	0	4591	82	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	361	0	0	9	0
All	All	15253	0	13806	199	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 (199) 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:HG3	1:B:551:ARG:HH11	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:231:TYR:CE2	1:C:235[A]:MET:HE3	2.22	0.74
1:C:486:ARG:CD	1:C:489:ASP:OD1	2.36	0.73
1:C:159:PRO:C	1:C:161:SER:HB3	2.14	0.72
1:A:521:ASP:O	1:A:548:GLY:HA3	1.90	0.71
1:B:600:GLN:HE21	1:B:600:GLN:H	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:379:GLN:CD	1:A:381:GLN:HE21	2.02	0.67
1:A:64:ILE:HG23	1:A:67:ARG:CD	2.24	0.67
1:C:300:GLN:HE21	1:C:501:ASP:H	1.43	0.66
1:A:436:ASN:C	1:A:436:ASN:HD22	2.05	0.65
1:C:298:LYS:HD3	1:C:510:LYS:HD3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:SER:O	1:B:557:PRO:C	2.39	0.64
4:A:2092:HOH:O	1:C:108:LYS:HE2	1.96	0.64
1:B:436:ASN:HD22	1:B:436:ASN:C	2.04	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: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
1:C:300:GLN:NE2	1:C:501:ASP:H	1.99	0.60
1:B:100:ILE:HD12	1:B:149:LEU:HD22	1.82	0.59
1:B:64:ILE:HG13	1:B:67:ARG:HD3	1.83	0.59
1:C:296:GLU:HG2	1:C:510:LYS:HG2	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:A:436:ASN:HD22	1:A:438:TYR:H	1.54	0.56
1:C:469:GLN:HB2	1:C:470:PRO:CD	2.35	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:C:436:ASN:C	1:C:436:ASN:HD22	2.14	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:363:LYS:NZ	1:B:489:ASP:OD2	2.33	0.54
1:B:583:THR:CG2	4:B:2080:HOH:O	2.51	0.54
1:A:551:ARG:HB2	4:A:2211:HOH:O	2.08	0.54
1:C:300:GLN:NE2	1:C:518:LYS:NZ	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:74:ILE:HD12	1:B:463:PRO:HD2	1.92	0.52
1:C:383:TYR:HB3	1:C:484:PHE:HB3	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
1:C:436:ASN:HD22	1:C:438:TYR:H	1.57	0.52
1:A:290:MET:HA	1:A:290:MET:HE2	1.90	0.52
1:B:179:PHE:O	1:B:183:MET:HG2	2.10	0.52
1:B:551:ARG:HH11	1:B:551:ARG:CG	2.21	0.52
1:B:552:LEU:HD11	1:B:625:LEU:HD22	1.92	0.52
1:A:304:GLU:OE2	1:A:480:ASN:ND2	2.43	0.51
1:A:561:LYS:HD3	1:A:617:THR:CG2	2.41	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:A:552:LEU:HD11	1:A:625:LEU:HD22	1.94	0.50
1:C:170:ASN:CB	4:C:2365:HOH:O	2.59	0.50
1:C:300:GLN:NE2	1:C:518:LYS:HZ2	2.08	0.50
1:C:605:GLU:H	1:C:605:GLU:CD	2.20	0.50
1:C:564:VAL:HG23	1:C:616:PHE:HE2	1.75	0.50
1:B:290:MET:HA	1:B:290:MET:HE2	1.94	0.50
1:B:540:SER:HB3	1:B:642:TYR:CD2	2.47	0.50
1:C:521:ASP:O	1:C:548:GLY:HA3	2.12	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:A:449:GLU:HG3	1:C:139:GLU:OE2	2.13	0.48
1:C:300:GLN:CG	1:C:500:ALA:HA	2.42	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:112:GLU:OE2	1:C:116:GLU:OE2	2.31	0.47
1:C:580:ARG:C	1:C:580:ARG:HD2	2.38	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:B:580:ARG:HD2	1:B:580:ARG:C	2.40	0.46
1:C:528:ASN:HB2	1:C:599:TRP:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:PRO:HB3	1:B:537:ASP:HB3	1.97	0.46
1:A:521:ASP:OD2	1:A:521:ASP:C	2.58	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:A:274:MET:HE3	1:A:278:VAL:HG21	1.97	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:A:316:GLN:H	1:A:316:GLN:CD	2.23	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:76:LEU:HD12	1:C:99:LEU:HD12	1.97	0.46
1:A:231:TYR:CE2	1:A:235[B]:MET:HE3	2.52	0.45
1:C:86:VAL:HG12	1:C:86:VAL:O	2.16	0.45
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:B:573:ASP:HB2	1:B:633:SER:HB3	1.99	0.45
1:C:115:MET:HE3	1:C:135:LEU:HD13	1.99	0.45
1:B:577:ASP:OD1	1:B:628:SER:HB2	2.17	0.45
1:A:196:LEU:HD13	1:A:278:VAL:HG21	1.99	0.44
1:A:282:MET:HE3	1:A:282:MET:HB3	1.87	0.44
1:C:108:LYS:HE3	1:C:113:ILE:HG13	1.99	0.44
1:C:249:TYR:CD2	1:C:249:TYR:C	2.96	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:74:ILE:HD12	1:C:463:PRO:HD2	2.00	0.44
1:C:367:HIS:HE1	1:C:484:PHE:HB2	1.83	0.44
1:B:436:ASN:C	1:B:436:ASN:ND2	2.75	0.44
1:C:115:MET:HE1	1:C:135:LEU:HD13	2.00	0.43
1:A:530:VAL:CG2	1:A:599:TRP:HB2	2.49	0.43
1:C:76:LEU:HD13	1:C:102:VAL:HG11	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLN:CD	1:A:381:GLN:NE2	2.75	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:A:580:ARG:HD2	1:A:580:ARG:C	2.44	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:B:249:TYR:CD2	1:B:249:TYR:C	2.96	0.42
1:C:603:LYS:HG3	1:C:605:GLU:HG2	2.01	0.42
1:B:137:GLU:HB3	1:B:182:TYR:CD1	2.54	0.42
1:B:369:ILE:HD13	1:B:482:VAL:H	1.83	0.42
1:B:529:GLU:HB3	1:B:532:HIS:CE1	2.55	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:B:456:LYS:HD2	4:B:2071:HOH:O	2.19	0.42
1:C:408:LEU:CG	1:C:455:GLU:OE2	2.56	0.42
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:A:172:PHE:CZ	1:A:213:ALA:HB2	2.54	0.42
1:A:316:GLN:CD	1:A:316:GLN:N	2.78	0.42
1:B:353:SER:OG	1:B:363:LYS:HE2	2.20	0.42
1:C:316:GLN:CD	1:C:316:GLN:H	2.28	0.42
1:A:541:PHE:O	1:A:640:VAL:HA	2.20	0.42
1:C:84:LEU:HD12	1:C:84:LEU:HA	1.88	0.42
1:A:593:SER:HB2	1:A:608:LYS:HG3	2.03	0.41
1:C:300:GLN:HE21	1:C:501:ASP:N	2.15	0.41
1:C:487:ASN:HA	1:C:488:PRO:HA	1.57	0.41
1:A:367:HIS:HE1	1:A:484:PHE:HB2	1.86	0.41
1:C:455:GLU:HG3	4:C:2027:HOH:O	2.20	0.41
1:C:401:GLY:O	1:C:434:PRO:HD2	2.20	0.41
1:C:282:MET:HB3	1:C:282:MET:HE3	1.84	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:439:LYS:NZ	4:B:2392:HOH:O	2.54	0.40
1:B:528:ASN:HB2	1:B:599:TRP:CD2	2.55	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:A:77:VAL:O	1:A:81:LEU:HB2	2.22	0.40
1:A:304:GLU:CG	1:A:480:ASN:HD22	2.35	0.40
1:A:513:GLN:HG2	1:A:647:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASN:HD22	1:B:438:TYR:H	1.69	0.40
1:C:108:LYS:HB2	1:C:108:LYS:NZ	2.36	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%)	36	46
1	C	585/589 (99%)	571 (98%)	13 (2%)	1 (0%)	43	55
All	All	1762/1767 (100%)	1716 (97%)	43 (2%)	3 (0%)	43	55

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%)	484 (94%)	32 (6%)	16	24
1	B	515/514 (100%)	485 (94%)	30 (6%)	18	26
1	C	514/514 (100%)	463 (90%)	51 (10%)	7	9
All	All	1545/1542 (100%)	1432 (93%)	113 (7%)	13	18

All (113) 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	146	GLN
1	A	163	ARG
1	A	177	SER
1	A	178	LEU
1	A	196	LEU
1	A	210	LEU
1	A	218	GLU
1	A	219	GLU
1	A	346	LEU
1	A	356	SER
1	A	358	SER
1	A	379	GLN
1	A	382	THR
1	A	406	LYS
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	514	ILE
1	A	551	ARG
1	A	583	THR
1	A	596	ASN
1	A	625	LEU
1	B	64	ILE
1	B	76	LEU

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Mol	Chain	Res	Type
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	346	LEU
1	B	347	SER
1	B	356	SER
1	B	406	LYS
1	B	408	LEU
1	B	413	VAL
1	B	436	ASN
1	B	449	GLU
1	B	469	GLN
1	B	486	ARG
1	B	551	ARG
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	608	LYS
1	B	635	ILE
1	B	652	ASN
1	C	64	ILE
1	C	71	LYS
1	C	76	LEU
1	C	77	VAL
1	C	81	LEU
1	C	84	LEU
1	C	86	VAL
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

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Mol	Chain	Res	Type
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	313	ILE
1	C	345	ARG
1	C	346	LEU
1	C	354	SER
1	C	363	LYS
1	C	374	ILE
1	C	379	GLN
1	C	382	THR
1	C	396	GLN
1	C	404	VAL
1	C	420	LYS
1	C	435	ASP
1	C	436	ASN
1	C	449	GLU
1	C	455	GLU
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	605	GLU
1	C	613	SER
1	C	622	GLN
1	C	625	LEU
1	C	626	LYS
1	C	630	ARG
1	C	651	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	156	GLN
1	A	170	ASN
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	396	GLN
1	B	436	ASN
1	B	480	ASN
1	B	513	GLN
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	146	GLN
1	C	201	GLN
1	C	204	ASN
1	C	228	ASN
1	C	300	GLN
1	C	368	GLN
1	C	396	GLN
1	C	436	ASN
1	C	480	ASN
1	C	487	ASN
1	C	504	ASN
1	C	591	ASN

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Mol	Chain	Res	Type
1	C	606	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	2005	-	4,4,4	0.25	0	6,6,6	0.38	0
2	SO4	B	2006	-	4,4,4	0.23	0	6,6,6	0.43	0
2	SO4	B	2007	-	4,4,4	0.26	0	6,6,6	0.34	0
2	SO4	B	2010	-	4,4,4	0.34	0	6,6,6	0.46	0
2	SO4	B	2001	-	4,4,4	0.33	0	6,6,6	0.42	0
2	SO4	C	2003	-	4,4,4	0.25	0	6,6,6	0.54	0
2	SO4	C	2013	-	4,4,4	0.34	0	6,6,6	0.17	0
3	ACT	A	2014	-	3,3,3	0.80	0	3,3,3	1.13	0
3	ACT	B	2015	-	3,3,3	0.97	0	3,3,3	1.20	0
2	SO4	B	2012	-	4,4,4	0.34	0	6,6,6	0.49	0
2	SO4	C	2009	-	4,4,4	0.28	0	6,6,6	0.40	0
2	SO4	A	2008	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	A	2011	-	4,4,4	0.22	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	C	2016	-	3,3,3	0.95	0	3,3,3	1.31	0
2	SO4	B	2002	-	4,4,4	0.20	0	6,6,6	0.70	0
2	SO4	C	2004	-	4,4,4	0.17	0	6,6,6	0.41	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	589/589 (100%)	-0.38	4 (0%) 84 85	8, 25, 38, 56	2 (0%)
1	B	589/589 (100%)	-0.45	1 (0%) 91 91	12, 23, 34, 53	1 (0%)
1	C	588/589 (99%)	-0.33	6 (1%) 79 80	15, 26, 39, 57	1 (0%)
All	All	1766/1767 (99%)	-0.38	11 (0%) 85 86	8, 25, 38, 57	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	PRO	3.7
1	C	64	ILE	3.5
1	B	64	ILE	3.1
1	C	487	ASN	2.9
1	A	551	ARG	2.3
1	C	86	VAL	2.3
1	A	64	ILE	2.2
1	A	433	TYR	2.2
1	C	158	ASN	2.1
1	A	357	ALA	2.0
1	C	652	ASN	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

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
3	ACT	B	2015	4/4	0.63	0.26	53,54,54,54	0
3	ACT	C	2016	4/4	0.63	0.19	50,50,51,51	0
2	SO4	C	2013	5/5	0.78	0.11	77,77,79,79	0
3	ACT	A	2014	4/4	0.80	0.15	38,38,39,39	0
2	SO4	B	2010	5/5	0.82	0.17	66,66,66,67	0
2	SO4	B	2012	5/5	0.83	0.21	61,61,62,62	0
2	SO4	C	2009	5/5	0.86	0.16	66,67,67,68	0
2	SO4	A	2008	5/5	0.88	0.11	74,74,75,76	0
2	SO4	B	2007	5/5	0.91	0.16	63,63,64,65	0
2	SO4	A	2011	5/5	0.91	0.10	75,75,76,76	0
2	SO4	B	2006	5/5	0.93	0.18	50,52,54,55	0
2	SO4	C	2003	5/5	0.94	0.09	46,47,48,49	0
2	SO4	B	2005	5/5	0.95	0.13	40,41,42,44	0
2	SO4	C	2004	5/5	0.96	0.07	46,46,47,47	0
2	SO4	B	2002	5/5	0.97	0.06	33,33,35,37	0
2	SO4	B	2001	5/5	0.98	0.06	29,29,30,35	0

6.5 Other polymers

There are no such residues in this entry.