



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:49 AM BST

PDB ID : 3WEE
Title : Structure of the full-length yeast Arp7-Arp9 Heterodimer
Authors : Lobsiger, J.; Richmond, T.J.
Deposited on : 2013-07-06
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

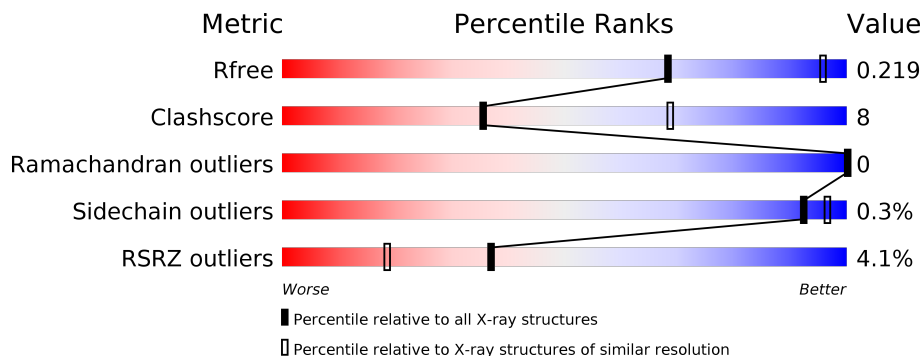
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	476	<p>4% 71% 17% 10%</p>
2	B	485	<p>3% 68% 16% 15%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	503	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6763 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 Actin-like protein ARP9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	Hg	N	O	S			
1	A	428	3432	2196	4	559	664	9	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP Q05123
A	-6	TYR	-	expression tag	UNP Q05123
A	-5	LYS	-	expression tag	UNP Q05123
A	-4	ASP	-	expression tag	UNP Q05123
A	-3	ASP	-	expression tag	UNP Q05123
A	-2	ASP	-	expression tag	UNP Q05123
A	-1	ASP	-	expression tag	UNP Q05123
A	0	LYS	-	expression tag	UNP Q05123
A	1	GLY	MET	engineered mutation	UNP Q05123

- Molecule 2 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	Hg	N	O	S			
2	B	412	3297	2117	3	542	619	16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	478	PRO	-	expression tag	UNP Q12406
B	479	HIS	-	expression tag	UNP Q12406
B	480	HIS	-	expression tag	UNP Q12406
B	481	HIS	-	expression tag	UNP Q12406
B	482	HIS	-	expression tag	UNP Q12406
B	483	HIS	-	expression tag	UNP Q12406
B	484	HIS	-	expression tag	UNP Q12406

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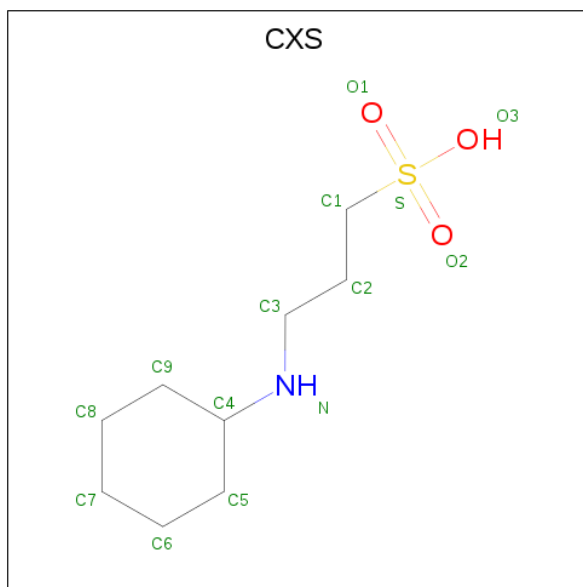
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	HIS	-	expression tag	UNP Q12406

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: C₉H₁₉NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	14	9	1	3	1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.77Å 103.77Å 184.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.73 – 3.10 29.73 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.73-3.10) 100.0 (29.73-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 3.11Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.199 , 0.220 0.198 , 0.219	Depositor DCC
R_{free} test set	2004 reflections (9.33%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6763	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: CXS, SO4, CMH

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	0.37	0/3464	0.52	1/4687 (0.0%)
2	B	0.36	0/3339	0.49	0/4509
All	All	0.37	0/6803	0.50	1/9196 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	231	SER	N-CA-C	-7.38	91.07	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	SER	Peptide
1	A	273	ASN	Peptide
1	A	393	ALA	Peptide
2	B	321	ASP	Peptide
2	B	322	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3432	0	3419	60	0
2	B	3297	0	3299	53	0
3	A	5	0	0	1	0
3	B	15	0	0	2	0
4	B	14	0	19	4	0
All	All	6763	0	6737	109	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 8.

All (109) 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:A:230:SER:HB2	1:A:231:SER:HB2	1.63	0.78
2:B:341:GLY:HA2	2:B:384:VAL:HG21	1.67	0.76
1:A:280:GLU:HG2	1:A:281:PHE:CD1	2.25	0.71
2:B:344:ILE:HG21	2:B:384:VAL:HG11	1.74	0.69
2:B:51:THR:HB	4:B:501:CXS:H31	1.80	0.64
1:A:453:LYS:NZ	1:A:464:ASP:OD2	2.31	0.63
1:A:40:GLN:HB2	1:A:64:LEU:HD11	1.82	0.62
2:B:398:THR:O	2:B:401:ILE:HG13	2.01	0.61
2:B:51:THR:O	2:B:55:ILE:HG13	2.01	0.61
2:B:147:LEU:HD23	2:B:443:MET:HG2	1.83	0.60
1:A:9:ILE:H	1:A:24:GLY:HA2	1.66	0.60
2:B:341:GLY:HA3	2:B:385:TYR:HE1	1.67	0.59
1:A:282:ASN:OD1	1:A:283:THR:N	2.35	0.58
1:A:10:LEU:HD13	1:A:23:PHE:HD1	1.68	0.58
1:A:120:SER:HB3	2:B:96:LYS:HD2	1.84	0.58
2:B:341:GLY:HA2	2:B:384:VAL:CG2	2.35	0.57
1:A:318:ASP:HA	1:A:403[B]:CMH:CM	2.35	0.56
1:A:190:GLY:O	1:A:193:SER:OG	2.23	0.56
2:B:164:CYS:H	2:B:182:SER:HB3	1.70	0.55
2:B:381:PRO:O	2:B:384:VAL:HG22	2.07	0.55
2:B:140:ILE:HG22	2:B:142:PRO:HD2	1.87	0.55
1:A:250:GLU:HG2	1:A:293:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HB	1:A:291:GLU:HB3	1.90	0.53
2:B:316:PRO:O	2:B:319:ILE:HG12	2.09	0.52
1:A:416:PHE:N	1:A:417:PRO:HD3	2.25	0.52
1:A:202:LEU:HD21	1:A:297:GLN:HG2	1.92	0.52
2:B:411:GLU:HG3	2:B:415:ARG:NH1	2.26	0.51
1:A:168:HIS:ND1	3:A:501:SO4:O2	2.36	0.51
2:B:16:ARG:NH2	3:B:503:SO4:O4	2.30	0.51
1:A:157:GLN:HG2	1:A:176:ASP:HA	1.93	0.50
2:B:190:ASP:OD1	2:B:232:LYS:NZ	2.33	0.50
2:B:52:TYR:O	2:B:53:ASN:HB2	2.10	0.50
1:A:123:ASP:O	1:A:127:ILE:HG12	2.11	0.49
2:B:112:ASN:OD1	2:B:113:GLY:N	2.45	0.49
1:A:9:ILE:O	1:A:24:GLY:N	2.45	0.49
2:B:151:LYS:HE3	2:B:424:PHE:CE2	2.47	0.49
2:B:30:ILE:HG22	4:B:501:CXS:H51	1.93	0.49
1:A:6:GLN:N	1:A:7:ASP:HA	2.27	0.49
1:A:87:PHE:CE2	1:A:135:LEU:HD13	2.47	0.49
2:B:238:VAL:HG22	2:B:310:ALA:HB1	1.94	0.49
1:A:25:LEU:HD11	1:A:433:GLN:HG3	1.94	0.49
2:B:54:MET:HE2	2:B:221:TRP:CZ2	2.48	0.48
1:A:401:VAL:HG23	2:B:234:THR:HB	1.95	0.48
1:A:435:VAL:O	1:A:439:ILE:HG23	2.13	0.48
2:B:347:MET:C	2:B:348:LYS:HG2	2.34	0.47
2:B:76:LEU:HD13	2:B:119:ILE:HD13	1.95	0.47
1:A:447:PHE:HE2	1:A:467:PHE:CE1	2.31	0.47
1:A:330:TRP:CD2	1:A:404:PRO:HG3	2.49	0.47
1:A:330:TRP:CE2	1:A:404:PRO:HG3	2.50	0.47
1:A:323:ILE:HG13	1:A:403[B]:CMH:SG	2.54	0.47
2:B:315:LYS:HE2	2:B:318:LEU:HD11	1.96	0.47
1:A:9:ILE:N	1:A:24:GLY:HA2	2.30	0.47
1:A:25:LEU:HD21	1:A:433:GLN:HG3	1.97	0.46
1:A:285:TRP:CH2	1:A:291:GLU:HB2	2.50	0.46
1:A:398:ILE:HG23	2:B:289:ASN:ND2	2.30	0.46
1:A:43:ARG:NH2	1:A:63:GLU:OE1	2.44	0.46
2:B:154:ALA:O	2:B:169:ILE:N	2.46	0.46
1:A:404:PRO:HG2	1:A:407:ILE:HD11	1.97	0.46
1:A:86:ILE:O	1:A:90:ILE:HG12	2.16	0.46
2:B:191:PHE:O	2:B:195:GLU:HG2	2.16	0.46
2:B:159:ILE:HD11	2:B:408:ILE:HD11	1.98	0.46
1:A:146:SER:HB2	1:A:174:ILE:HD11	1.97	0.45
1:A:280:GLU:HG2	1:A:281:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HD12	1:A:312:ARG:HG3	1.98	0.45
1:A:314:GLY:HA3	1:A:357:HIS:CE1	2.52	0.45
1:A:41:ILE:HD11	1:A:53:TYR:HB3	1.99	0.45
2:B:387:LEU:O	2:B:390:THR:HG22	2.17	0.45
2:B:170:ILE:O	2:B:173:ILE:HG13	2.15	0.45
2:B:237:GLN:HG2	2:B:402:GLU:HB3	1.99	0.44
2:B:394:ILE:HD12	2:B:405:GLU:HG3	1.99	0.44
1:A:274:VAL:HG22	1:A:275:LYS:H	1.83	0.44
2:B:239:SER:O	2:B:407:ARG:HD3	2.17	0.44
2:B:30:ILE:O	4:B:501:CXS:H12	2.17	0.44
1:A:141:ILE:HG12	1:A:448:TYR:HB3	1.99	0.44
1:A:7:ASP:HB2	1:A:25:LEU:HB3	1.99	0.43
1:A:9:ILE:HG22	1:A:25:LEU:HB2	1.99	0.43
1:A:157:GLN:HG3	1:A:177:TYR:CE2	2.53	0.43
1:A:283:THR:CG2	1:A:291:GLU:HG3	2.49	0.43
1:A:401:VAL:HG21	2:B:235:MET:HG2	2.00	0.43
1:A:393:ALA:HB1	1:A:394:PHE:HA	2.01	0.43
1:A:53:TYR:CD1	1:A:81:GLN:HG3	2.53	0.43
2:B:116:ASP:O	2:B:120:LEU:HG	2.19	0.43
1:A:230:SER:CB	1:A:231:SER:HB2	2.40	0.42
1:A:368:LYS:HD3	1:A:368:LYS:HA	1.84	0.42
2:B:161:ALA:HA	2:B:186:GLY:H	1.83	0.42
1:A:371:GLU:OE1	1:A:382:LYS:NZ	2.52	0.42
1:A:393:ALA:HB3	1:A:394:PHE:HD1	1.83	0.42
1:A:9:ILE:HD12	1:A:110:PRO:O	2.20	0.42
1:A:149:ALA:O	1:A:152:SER:OG	2.28	0.42
2:B:16:ARG:NH2	3:B:503:SO4:S	2.93	0.42
1:A:416:PHE:H	1:A:417:PRO:HD3	1.85	0.42
1:A:417:PRO:HA	1:A:418:GLU:HA	1.61	0.42
2:B:54:MET:HE2	2:B:221:TRP:CH2	2.54	0.42
2:B:320:SER:OG	2:B:321:ASP:N	2.53	0.42
2:B:10:ILE:O	2:B:106:ILE:HA	2.20	0.42
2:B:112:ASN:O	2:B:176:LYS:HB3	2.20	0.41
1:A:173:PRO:HD2	1:A:184:VAL:HG22	2.02	0.41
2:B:5:ARG:HD3	2:B:5:ARG:HA	1.91	0.41
2:B:319:ILE:HG13	2:B:320:SER:N	2.35	0.41
2:B:344:ILE:HD12	2:B:344:ILE:HA	1.96	0.41
2:B:40:ASP:OD1	2:B:62:ARG:NH1	2.43	0.41
1:A:325:LYS:O	1:A:329:VAL:HG23	2.21	0.41
2:B:300:THR:O	2:B:301:LEU:HD23	2.20	0.41
1:A:15:ARG:NH2	1:A:18:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:SER:O	2:B:384:VAL:HG13	2.21	0.40
2:B:458:GLU:N	2:B:458:GLU:OE1	2.52	0.40
2:B:51:THR:OG1	4:B:501:CXS:H4	2.22	0.40
1:A:335:ILE:HD13	1:A:349:LEU:HD23	2.03	0.40
2:B:91:TYR:CE1	2:B:99:PRO:HA	2.56	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	417/476 (88%)	399 (96%)	18 (4%)	0	100	100
2	B	401/485 (83%)	387 (96%)	14 (4%)	0	100	100
All	All	818/961 (85%)	786 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	386/428 (90%)	384 (100%)	2 (0%)	88	94
2	B	360/425 (85%)	360 (100%)	0	100	100
All	All	746/853 (88%)	744 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	TYR
1	A	448	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	CMH	B	306	2	5,7,8	4.15	1 (20%)	1,7,9	0.55	0
1	CMH	A	403[B]	1	5,7,8	3.45	1 (20%)	1,7,9	1.73	0
2	CMH	B	29	2	5,7,8	3.90	1 (20%)	1,7,9	0.29	0
2	CMH	B	7	2	5,7,8	3.91	1 (20%)	1,7,9	0.05	0
1	CMH	A	302	1	5,7,8	3.87	1 (20%)	1,7,9	1.06	0
1	CMH	A	403[A]	1	5,7,8	3.74	1 (20%)	1,7,9	1.09	0
1	CMH	A	159	1	5,7,8	4.10	1 (20%)	1,7,9	0.72	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	CMH	B	306	2	-	0/0/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CMH	A	403[B]	1	-	0/0/6/8	-
2	CMH	B	29	2	-	0/0/6/8	-
2	CMH	B	7	2	-	0/0/6/8	-
1	CMH	A	302	1	-	0/0/6/8	-
1	CMH	A	403[A]	1	-	0/0/6/8	-
1	CMH	A	159	1	-	0/0/6/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	306	CMH	CM-HG	9.08	2.36	2.08
1	A	159	CMH	CM-HG	9.06	2.36	2.08
2	B	7	CMH	CM-HG	8.58	2.35	2.08
2	B	29	CMH	CM-HG	8.55	2.35	2.08
1	A	302	CMH	CM-HG	8.49	2.34	2.08
1	A	403[A]	CMH	CM-HG	8.15	2.33	2.08
1	A	403[B]	CMH	CM-HG	7.44	2.31	2.08

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	403[B]	CMH	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
3	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.41	0
4	CXS	B	501	-	14,14,14	2.39	2 (14%)	18,18,18	6.70	6 (33%)
3	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	B	504	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	B	503	-	4,4,4	0.19	0	6,6,6	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CXS	B	501	-	-	4/8/16/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	CXS	C1-S	-7.51	1.66	1.77
4	B	501	CXS	O3-S	4.51	1.63	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	CXS	O1-S-C1	-19.81	83.07	106.92
4	B	501	CXS	O2-S-C1	-13.89	90.19	106.92
4	B	501	CXS	O3-S-C1	-13.43	84.05	105.77
4	B	501	CXS	O3-S-O2	3.78	120.52	111.27
4	B	501	CXS	O3-S-O1	3.75	120.43	111.27
4	B	501	CXS	C3-N-C4	2.49	119.03	114.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	CXS	C2-C1-S-O1
4	B	501	CXS	C2-C1-S-O2
4	B	501	CXS	C2-C1-S-O3
4	B	501	CXS	C1-C2-C3-N

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	CXS	4	0
3	A	501	SO4	1	0
3	B	503	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	425/476 (89%)	-0.03	18 (4%) 36 18	34, 60, 138, 193	0
2	B	409/485 (84%)	-0.04	16 (3%) 39 20	39, 61, 128, 170	0
All	All	834/961 (86%)	-0.04	34 (4%) 37 18	34, 60, 136, 193	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	THR	4.8
1	A	419	TRP	4.4
1	A	392	THR	4.1
1	A	254	SER	3.8
1	A	28	GLU	3.8
2	B	468	LYS	3.8
2	B	352	SER	3.5
1	A	60	ASN	3.5
1	A	420	LYS	3.3
2	B	350	ASN	3.1
1	A	47	GLN	3.1
2	B	44	GLU	3.0
2	B	345	ASN	3.0
2	B	347	MET	3.0
2	B	203	GLU	2.9
2	B	41	GLU	2.9
1	A	94	ARG	2.8
2	B	349	ALA	2.8
1	A	273	ASN	2.7
2	B	278	GLY	2.6
2	B	277	THR	2.5
1	A	256	ARG	2.5
1	A	274	VAL	2.4
1	A	253	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	42	GLY	2.3
1	A	417	PRO	2.3
2	B	215	LYS	2.3
1	A	26	ASN	2.3
1	A	31	THR	2.3
1	A	59	ASP	2.2
2	B	43	GLY	2.2
1	A	278	ASP	2.1
2	B	260	GLN	2.1
2	B	351	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CMH	A	403[B]	8/9	0.95	0.15	78,80,82,82	8
1	CMH	A	403[A]	8/9	0.95	0.15	78,81,85,87	8
2	CMH	B	7	8/9	0.99	0.13	59,60,62,63	1
2	CMH	B	306	8/9	0.99	0.14	59,61,62,63	2
1	CMH	A	159	8/9	0.99	0.14	63,64,65,65	2
2	CMH	B	29	8/9	1.00	0.14	50,51,51,51	1
1	CMH	A	302	8/9	1.00	0.14	64,65,68,70	1

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	504	5/5	0.92	0.22	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	503	5/5	0.94	0.17	97,97,97,97	0
3	SO4	B	502	5/5	0.95	0.28	76,76,76,76	0
3	SO4	A	501	5/5	0.97	0.17	62,62,62,62	0
4	CXS	B	501	14/14	0.98	0.15	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.