Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:31 pm BST

PDB ID	:	2R0V
Title	:	Structure of the Rsc4 tandem bromodomain acetylated at K25
Authors	:	VanDemark, A.P.; Kasten, M.M.; Ferris, E.; Heroux, A.; Hill, C.P.; Cairns, B.R.
Deposited on	:	2007-08-21
Resolution	:	2.35 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:

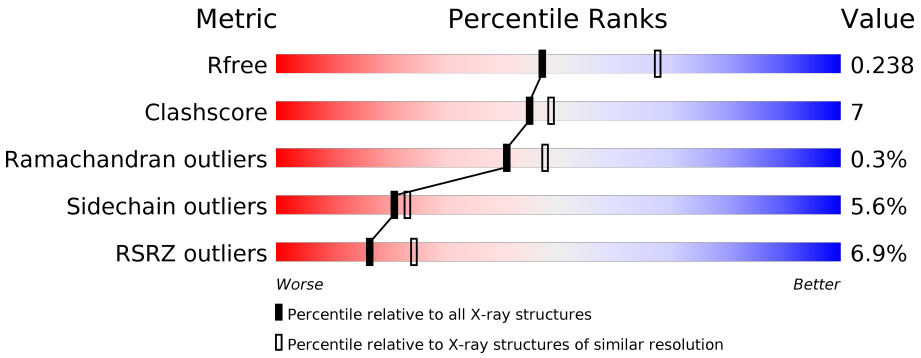
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	346	3% 73% 11% • 15%
1	B	346	5% 70% 11% • 17%
1	C	346	9% 69% 13% • 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7701 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.

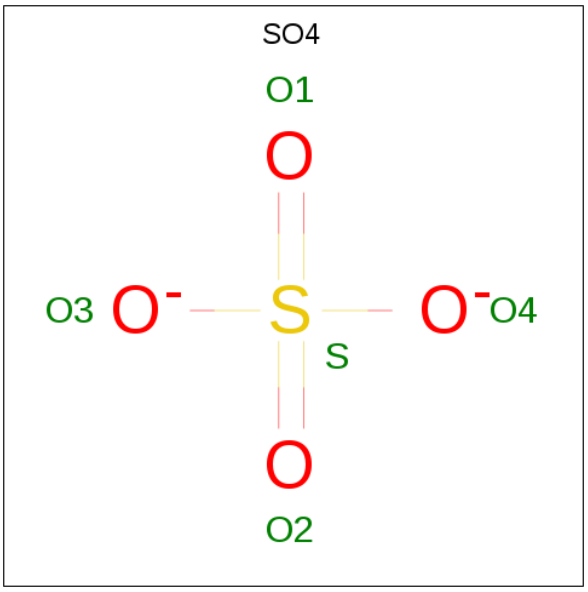
- Molecule 1 is a protein called Chromatin structure-remodeling complex protein RSC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2449	1596	388	458	7			
1	B	286	Total	C	N	O	S	0	0	0
			2387	1555	379	446	7			
1	C	291	Total	C	N	O	S	0	0	0
			2433	1585	386	455	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q02206
A	-4	ILE	-	EXPRESSION TAG	UNP Q02206
A	-3	ASP	-	EXPRESSION TAG	UNP Q02206
A	-2	PRO	-	EXPRESSION TAG	UNP Q02206
A	-1	PHE	-	EXPRESSION TAG	UNP Q02206
A	0	THR	-	EXPRESSION TAG	UNP Q02206
B	-5	GLY	-	EXPRESSION TAG	UNP Q02206
B	-4	ILE	-	EXPRESSION TAG	UNP Q02206
B	-3	ASP	-	EXPRESSION TAG	UNP Q02206
B	-2	PRO	-	EXPRESSION TAG	UNP Q02206
B	-1	PHE	-	EXPRESSION TAG	UNP Q02206
B	0	THR	-	EXPRESSION TAG	UNP Q02206
C	-5	GLY	-	EXPRESSION TAG	UNP Q02206
C	-4	ILE	-	EXPRESSION TAG	UNP Q02206
C	-3	ASP	-	EXPRESSION TAG	UNP Q02206
C	-2	PRO	-	EXPRESSION TAG	UNP Q02206
C	-1	PHE	-	EXPRESSION TAG	UNP Q02206
C	0	THR	-	EXPRESSION TAG	UNP Q02206

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



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

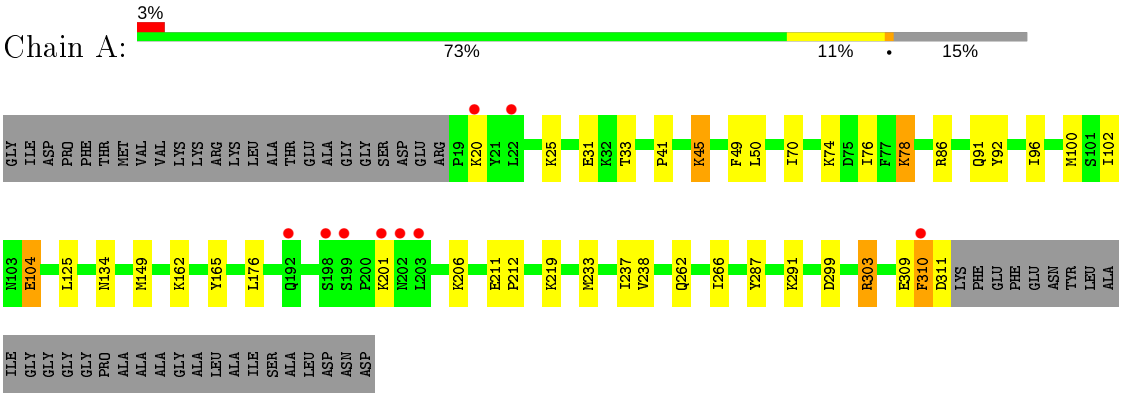
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	184	Total O 184 184	0	0
3	B	116	Total O 116 116	0	0
3	C	107	Total O 107 107	0	0

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 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.

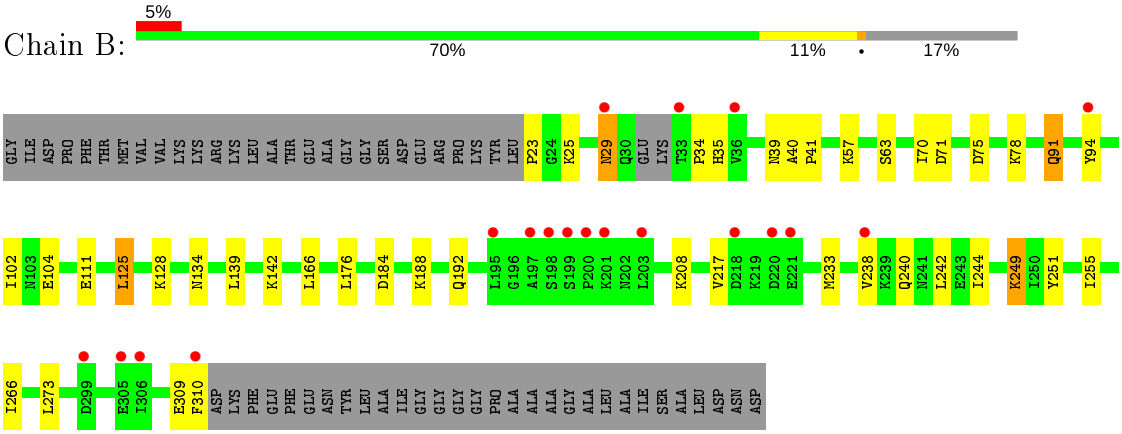
- Molecule 1: Chromatin structure-remodeling complex protein RSC4

Chain A:



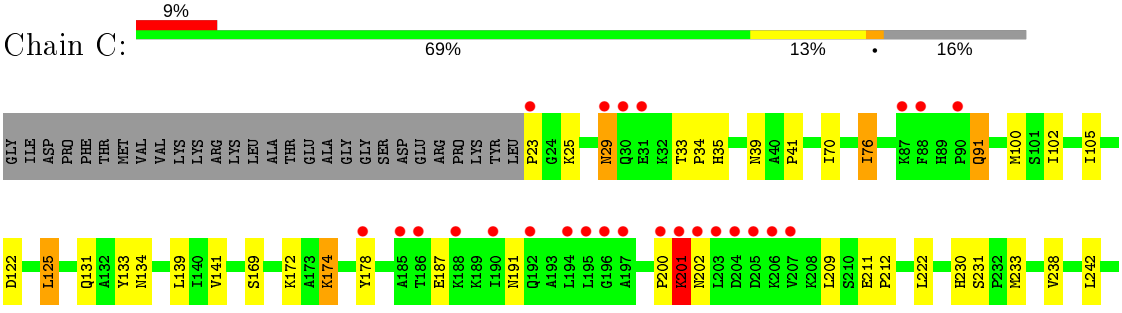
- Molecule 1: Chromatin structure-remodeling complex protein RSC4

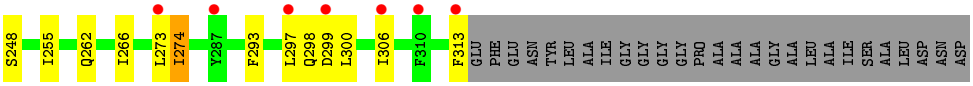
Chain B:



- Molecule 1: Chromatin structure-remodeling complex protein RSC4

Chain C:




S248
I255
Q262
I266
L273
I274
Y287
F293
L297
Q298
D299
L300
I306
F310
F313
GLU
PHE
GLU
ASN
TYR
LEU
ALA
ILE
GLY
GLY
GLY
GLY
PRO
ALA
ALA
ALA
GLY
ALA
LEU
ALA
ILE
SER
ALA
LEU
ASP
ASN
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.25Å 83.17Å 127.06Å 90.00° 109.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 46.64 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.35) 99.4 (46.64-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.230 0.198 , 0.238	Depositor DCC
R_{free} test set	2569 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.55	0/2497	0.61	0/3377
1	B	0.53	0/2432	0.57	0/3288
1	C	0.50	0/2480	0.57	0/3352
All	All	0.53	0/7409	0.58	0/10017

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	PHE	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	2449	0	2441	27	0
1	B	2387	0	2377	25	0
1	C	2433	0	2423	43	0
2	A	15	0	0	0	0
2	C	10	0	0	1	0
3	A	184	0	0	1	0
3	B	116	0	0	6	0
3	C	107	0	0	1	0
All	All	7701	0	7241	95	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 (95) 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:233:MET:HE3	1:A:237:ILE:HB	1.35	1.08
1:C:29:ASN:H	1:C:29:ASN:HD22	1.06	1.01
1:C:273:LEU:HD23	1:C:273:LEU:O	1.66	0.95
1:C:29:ASN:N	1:C:29:ASN:HD22	1.72	0.86
1:A:25:ALY:CH3	1:A:134:ASN:HD21	1.96	0.78
1:C:76:ILE:HG21	1:C:230:HIS:CD2	2.21	0.75
1:A:25:ALY:HH33	1:A:134:ASN:HD21	1.51	0.75
1:C:233:MET:HE2	1:C:238:VAL:HG22	1.66	0.75
1:C:100:MET:CE	1:C:105:ILE:HG12	2.16	0.74
1:A:233:MET:CE	1:A:237:ILE:HB	2.17	0.72
1:C:25:ALY:HH31	1:C:134:ASN:HD21	1.57	0.70
1:C:100:MET:CE	1:C:105:ILE:CG1	2.70	0.69
1:C:100:MET:HE2	1:C:105:ILE:HG12	1.73	0.69
1:B:142:LYS:HE3	1:B:266:ILE:O	1.92	0.68
1:C:273:LEU:C	1:C:273:LEU:HD23	2.13	0.68
1:A:233:MET:HE3	1:A:237:ILE:CB	2.18	0.67
1:C:300:LEU:HB3	1:C:306:ILE:HG12	1.76	0.67
1:A:262:GLN:O	1:A:266:ILE:HD13	1.96	0.66
1:C:293:PHE:CZ	1:C:297:LEU:HD11	2.30	0.66
1:C:25:ALY:HH32	3:C:447:HOH:O	1.93	0.66
1:C:100:MET:HE2	1:C:105:ILE:CG1	2.26	0.65
1:A:211:GLU:HB3	1:A:212:PRO:HD3	1.79	0.65
1:C:29:ASN:ND2	1:C:29:ASN:H	1.84	0.63
1:B:25:ALY:HH33	1:B:134:ASN:HD21	1.64	0.62
1:A:25:ALY:HH33	1:A:134:ASN:ND2	2.15	0.62
1:C:100:MET:HE3	1:C:105:ILE:CG1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:HIS:HE1	3:B:389:HOH:O	1.84	0.61
1:B:25:ALY:HH32	3:B:362:HOH:O	2.00	0.60
1:C:29:ASN:ND2	1:C:29:ASN:N	2.41	0.60
1:B:111:GLU:HG2	3:B:341:HOH:O	2.03	0.58
1:C:233:MET:HE2	1:C:238:VAL:CG2	2.33	0.57
1:A:233:MET:HE2	1:A:238:VAL:HG23	1.86	0.56
1:C:91:GLN:HA	1:C:91:GLN:HE21	1.71	0.56
1:C:33:THR:HB	1:C:34:PRO:HD2	1.88	0.56
1:A:299:ASP:O	1:A:303:ARG:HD2	2.06	0.56
1:C:100:MET:CE	1:C:105:ILE:HG13	2.36	0.55
1:C:100:MET:HE2	1:C:122:ASP:HB3	1.87	0.55
1:C:187:GLU:O	1:C:191:ASN:ND2	2.36	0.55
1:C:100:MET:HE3	1:C:105:ILE:HG13	1.87	0.55
1:C:262:GLN:O	1:C:266:ILE:HG12	2.06	0.55
1:C:70:ILE:HD11	1:C:102:ILE:HG21	1.90	0.53
1:A:100:MET:SD	1:A:104:GLU:HG2	2.49	0.52
1:A:25:ALY:HH31	1:A:134:ASN:HD21	1.73	0.51
1:C:100:MET:CE	1:C:122:ASP:HB3	2.41	0.51
1:C:273:LEU:C	1:C:273:LEU:CD2	2.79	0.50
1:A:287:TYR:O	1:A:291:LYS:HB2	2.11	0.50
1:C:133:TYR:OH	2:C:341:SO4:O4	2.24	0.48
1:C:233:MET:CE	1:C:238:VAL:CG2	2.90	0.48
1:C:300:LEU:CB	1:C:306:ILE:HG12	2.44	0.48
1:C:174:LYS:O	1:C:178:TYR:HD2	1.97	0.47
1:B:166:LEU:HD12	1:B:309:GLU:HB2	1.97	0.47
1:C:233:MET:CE	1:C:238:VAL:HG22	2.42	0.47
1:A:45:LYS:HD2	1:A:50:LEU:HD11	1.96	0.47
1:B:111:GLU:CG	3:B:341:HOH:O	2.62	0.47
1:A:211:GLU:N	1:A:212:PRO:HD2	2.31	0.46
1:B:70:ILE:HD11	1:B:102:ILE:HG21	1.98	0.45
1:C:172:LYS:HD2	1:C:242:LEU:O	2.16	0.45
1:C:211:GLU:HB3	1:C:212:PRO:HD3	1.98	0.45
1:C:274:ILE:O	1:C:274:ILE:HG12	2.16	0.45
1:A:149:MET:SD	1:A:262:GLN:HG2	2.56	0.45
1:B:125:LEU:HA	1:B:125:LEU:HD12	1.78	0.45
1:B:25:ALY:CH3	1:B:134:ASN:HD21	2.30	0.45
1:A:92:TYR:CZ	1:A:96:ILE:HG13	2.52	0.45
1:C:39:ASN:O	1:C:41:PRO:HD3	2.17	0.45
1:B:75:ASP:HA	1:B:78:LYS:HD2	1.98	0.45
1:A:41:PRO:HB3	1:A:49:PHE:CE2	2.52	0.44
1:B:25:ALY:HE2	1:B:25:ALY:HH31	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HD12	1:C:125:LEU:HA	1.77	0.44
1:A:162:LYS:O	1:A:310:PHE:HZ	2.01	0.44
1:B:23:PRO:HA	1:B:139:LEU:HD23	2.00	0.44
1:A:74:LYS:O	1:A:78:LYS:HB3	2.18	0.44
1:B:35:HIS:CE1	3:B:389:HOH:O	2.63	0.43
1:C:293:PHE:CZ	1:C:297:LEU:CD1	2.99	0.43
1:B:184:ASP:HA	1:B:208:LYS:HD3	2.00	0.43
1:B:40:ALA:O	1:B:128:LYS:NZ	2.47	0.43
1:B:29:ASN:H	1:B:29:ASN:ND2	2.16	0.43
1:A:211:GLU:N	1:A:212:PRO:CD	2.82	0.43
1:C:200:PRO:O	1:C:201:LYS:C	2.57	0.42
1:B:233:MET:CE	1:B:238:VAL:HG22	2.49	0.42
1:B:91:GLN:HG3	1:B:91:GLN:H	1.54	0.42
1:B:249:LYS:NZ	3:B:398:HOH:O	2.52	0.42
1:C:23:PRO:HA	1:C:139:LEU:HD23	2.02	0.42
1:A:309:GLU:HG3	3:A:357:HOH:O	2.19	0.42
1:B:251:TYR:O	1:B:255:ILE:HG12	2.19	0.42
1:A:70:ILE:HD11	1:A:102:ILE:HG21	2.02	0.42
1:B:240:GLN:O	1:B:244:ILE:HG12	2.20	0.41
1:A:45:LYS:HD2	1:A:45:LYS:HA	1.81	0.41
1:B:39:ASN:O	1:B:41:PRO:HD3	2.21	0.41
1:B:233:MET:HE3	1:B:238:VAL:CG2	2.51	0.41
1:B:176:LEU:HD23	1:B:242:LEU:HD23	2.03	0.41
1:A:25:ALY:CH3	1:A:134:ASN:ND2	2.73	0.40
1:C:131:GLN:HG2	1:C:141:VAL:HG13	2.04	0.40
1:A:165:TYR:HA	1:A:309:GLU:O	2.21	0.40
1:A:162:LYS:O	1:A:310:PHE:CZ	2.75	0.40
1:C:209:LEU:O	1:C:212:PRO:HD2	2.21	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	290/346 (84%)	287 (99%)	3 (1%)	0	100	100
1	B	281/346 (81%)	277 (99%)	2 (1%)	2 (1%)	22	23
1	C	288/346 (83%)	283 (98%)	4 (1%)	1 (0%)	41	47
All	All	859/1038 (83%)	847 (99%)	9 (1%)	3 (0%)	41	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	LYS
1	B	34	PRO
1	B	217	VAL

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	276/312 (88%)	260 (94%)	16 (6%)	20	22
1	B	269/312 (86%)	256 (95%)	13 (5%)	25	30
1	C	274/312 (88%)	257 (94%)	17 (6%)	18	19
All	All	819/936 (88%)	773 (94%)	46 (6%)	21	23

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	31	GLU
1	A	33	THR
1	A	45	LYS
1	A	76	ILE
1	A	78	LYS
1	A	86	ARG
1	A	91	GLN
1	A	104	GLU
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	176	LEU
1	A	201	LYS
1	A	206	LYS
1	A	219	LYS
1	A	303	ARG
1	A	311	ASP
1	B	29	ASN
1	B	57	LYS
1	B	63	SER
1	B	71	ASP
1	B	91	GLN
1	B	94	TYR
1	B	104	GLU
1	B	125	LEU
1	B	188	LYS
1	B	192	GLN
1	B	249	LYS
1	B	273	LEU
1	B	310	PHE
1	C	29	ASN
1	C	35	HIS
1	C	76	ILE
1	C	91	GLN
1	C	125	LEU
1	C	169	SER
1	C	174	LYS
1	C	201	LYS
1	C	202	ASN
1	C	222	LEU
1	C	231	SER
1	C	248	SER
1	C	255	ILE
1	C	274	ILE
1	C	298	GLN
1	C	299	ASP
1	C	313	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	180	ASN
1	A	263	ASN
1	B	29	ASN
1	B	54	HIS
1	B	98	GLN
1	B	192	GLN
1	B	265	HIS
1	C	29	ASN
1	C	89	HIS
1	C	91	GLN
1	C	103	ASN
1	C	192	GLN
1	C	202	ASN
1	C	263	ASN
1	C	265	HIS
1	C	298	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
1	ALY	C	25	1	10,11,12	0.63	0	7,12,14	1.38	1 (14%)
1	ALY	A	25	1	10,11,12	0.51	0	7,12,14	2.36	3 (42%)
1	ALY	B	25	1	10,11,12	0.43	0	7,12,14	0.45	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
1	ALY	C	25	1	-	2/9/10/12	-
1	ALY	A	25	1	-	4/9/10/12	-
1	ALY	B	25	1	-	4/9/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ALY	CE-NZ-CH	5.21	130.56	122.56
1	C	25	ALY	CE-NZ-CH	2.63	126.59	122.56
1	A	25	ALY	CH3-CH-NZ	2.13	119.86	116.09
1	A	25	ALY	CD-CG-CB	-2.05	106.39	113.62

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	25	ALY	OH-CH-NZ-CE
1	A	25	ALY	CH3-CH-NZ-CE
1	B	25	ALY	OH-CH-NZ-CE
1	B	25	ALY	CH3-CH-NZ-CE
1	A	25	ALY	CA-CB-CG-CD
1	B	25	ALY	CE-CD-CG-CB
1	C	25	ALY	CA-CB-CG-CD
1	C	25	ALY	N-CA-CB-CG
1	B	25	ALY	C-CA-CB-CG
1	A	25	ALY	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	25	ALY	2	0
1	A	25	ALY	5	0
1	B	25	ALY	4	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
2	SO4	A	342	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	343	-	4,4,4	0.18	0	6,6,6	0.50	0
2	SO4	A	341	-	4,4,4	0.16	0	6,6,6	0.32	0
2	SO4	C	341	-	4,4,4	0.18	0	6,6,6	0.33	0
2	SO4	C	342	-	4,4,4	0.15	0	6,6,6	0.20	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	341	SO4	1	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, 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	292/346 (84%)	0.20	9 (3%) 49 61	27, 45, 80, 128	0
1	B	285/346 (82%)	0.46	19 (6%) 17 26	37, 52, 94, 144	0
1	C	290/346 (83%)	0.69	32 (11%) 5 8	34, 55, 107, 142	0
All	All	867/1038 (83%)	0.45	60 (6%) 16 24	27, 51, 99, 144	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	LEU	7.9
1	B	33	THR	6.4
1	C	29	ASN	6.0
1	A	202	ASN	5.8
1	C	313	PHE	5.7
1	C	207	VAL	5.4
1	B	310	PHE	5.2
1	C	192	GLN	5.2
1	B	197	ALA	5.2
1	C	306	ILE	4.8
1	C	31	GLU	4.8
1	C	87	LYS	4.8
1	C	200	PRO	4.8
1	C	188	LYS	4.6
1	B	306	ILE	4.6
1	C	310	PHE	4.6
1	C	88	PHE	4.5
1	A	20	LYS	4.4
1	A	199	SER	4.1
1	C	206	LYS	4.1
1	C	194	LEU	4.1
1	B	94	TYR	4.0
1	C	197	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	3.9
1	B	200	PRO	3.8
1	A	203	LEU	3.8
1	C	297	LEU	3.8
1	C	195	LEU	3.7
1	C	186	THR	3.6
1	A	198	SER	3.6
1	B	198	SER	3.6
1	B	203	LEU	3.2
1	B	29	ASN	3.1
1	A	201	LYS	3.1
1	C	190	ILE	3.0
1	C	204	ASP	3.0
1	C	287	TYR	2.9
1	B	201	LYS	2.9
1	B	305	GLU	2.8
1	C	299	ASP	2.6
1	A	22	LEU	2.6
1	B	218	ASP	2.6
1	C	273	LEU	2.5
1	B	36	VAL	2.5
1	A	192	GLN	2.4
1	C	30	GLN	2.4
1	C	90	PRO	2.4
1	C	178	TYR	2.3
1	C	201	LYS	2.3
1	B	199	SER	2.3
1	C	196	GLY	2.2
1	A	310	PHE	2.2
1	C	205	ASP	2.2
1	B	220	ASP	2.2
1	B	299	ASP	2.1
1	B	221	GLU	2.1
1	C	202	ASN	2.1
1	B	238	VAL	2.1
1	C	23	PRO	2.1
1	C	185	ALA	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, 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	B-factors(Å^2)	Q<0.9
1	ALY	C	25	12/13	0.88	0.18	56,64,69,72	0
1	ALY	B	25	12/13	0.92	0.16	58,68,78,79	0
1	ALY	A	25	12/13	0.96	0.15	40,47,50,51	0

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. 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	B-factors(Å^2)	Q<0.9
2	SO4	A	343	5/5	0.83	0.21	70,71,74,75	0
2	SO4	C	342	5/5	0.87	0.24	111,112,112,112	0
2	SO4	C	341	5/5	0.90	0.19	92,92,93,94	0
2	SO4	A	342	5/5	0.92	0.25	108,109,109,109	0
2	SO4	A	341	5/5	0.94	0.16	67,68,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.