



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:48 AM GMT

PDB ID : 3Q33
Title : Structure of the Rtt109-AcCoA/Vps75 Complex and Implications for
Chaperone-Mediated Histone Acetylation
Authors : Tang, Y.; Yuan, H.; Meeth, K.; Marmorstein, R.
Deposited on : 2010-12-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

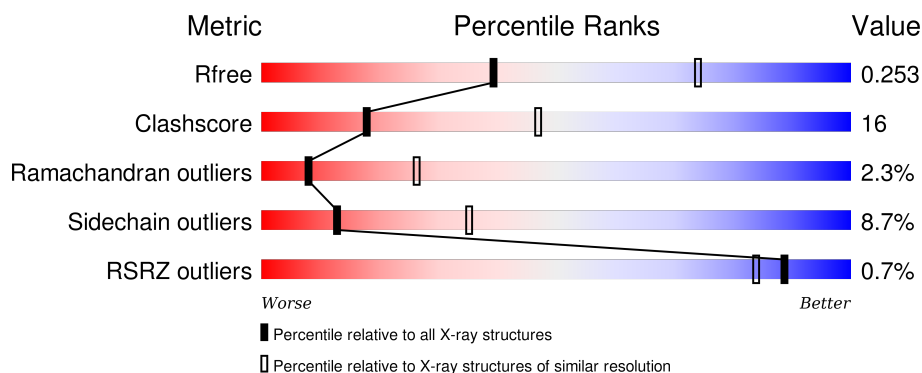
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 28%, green 58%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 58% 28% • • 10% </div> </div>
2	B	232	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 59%, yellow 28%, orange 1%, red 1%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 59% 28% • 8% </div> </div>
3	D	15	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 20%, yellow 7%, red 7%, grey 66%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 20% 7% 7% 67% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5077 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 Histone acetyltransferase RTT109.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3198	2058	539	592	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP A7A0Q4
A	0	SER	-	EXPRESSION TAG	UNP A7A0Q4

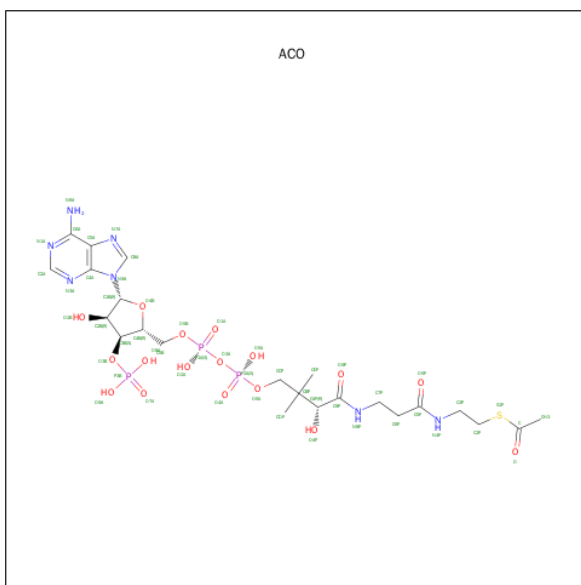
- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 75.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1776	1149	288	334	5			

- Molecule 3 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	1
			25	14	6	5			

- Molecule 4 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

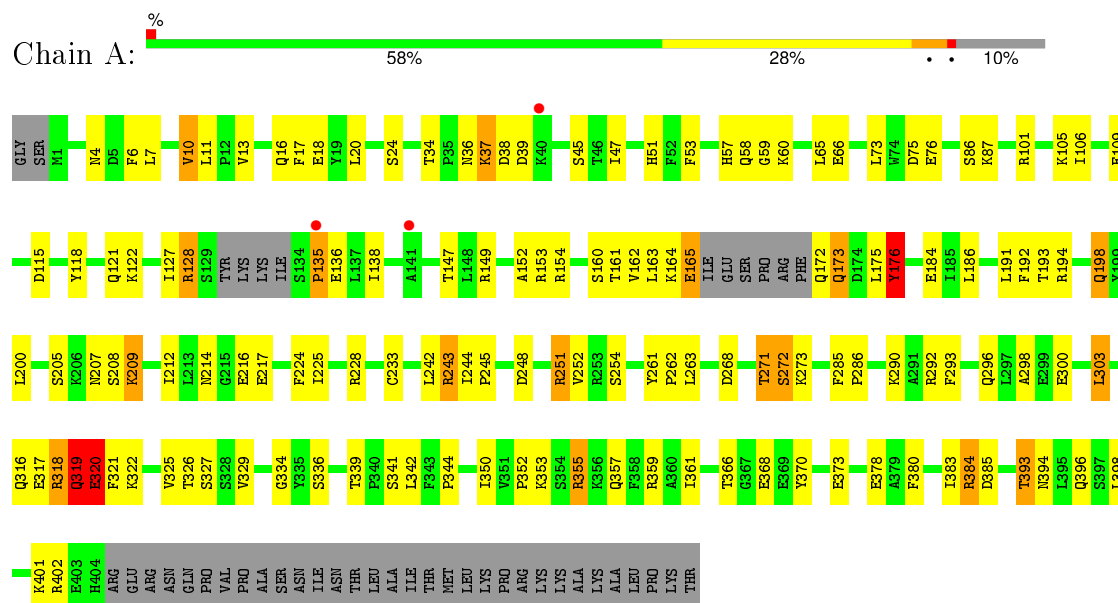
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total 14	O 14	0	0
6	B	9	Total 9	O 9	0	0

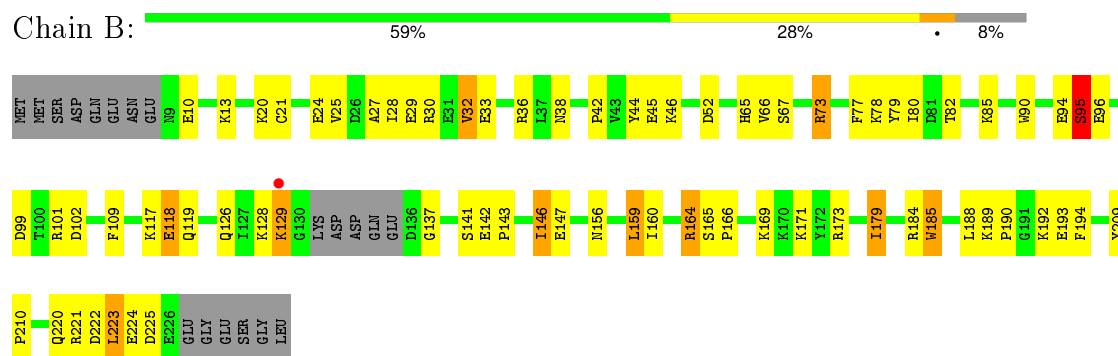
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Histone acetyltransferase RTT109



• Molecule 2: Vacuolar protein sorting-associated protein 75



• Molecule 3: HISTONE H3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.54Å 119.57Å 80.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.16 – 2.80 45.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.16-2.80) 96.0 (45.16-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.195 , 0.255 0.195 , 0.253	Depositor DCC
R_{free} test set	1167 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22889 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5077	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, 0.375 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: ALY, ACO, EDO, NH2

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	0.44	0/3255	0.61	0/4402
2	B	0.42	0/1823	0.57	0/2455
3	D	0.60	0/23	0.62	0/28
All	All	0.44	0/5101	0.59	0/6885

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	0	3239	103	0
2	B	1776	0	1721	55	0
3	D	25	0	25	2	0
4	A	51	0	34	0	0
5	A	4	0	6	2	0
6	A	14	0	0	0	0
6	B	9	0	0	1	0
All	All	5077	0	5025	159	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 16.

All (159) 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)
2:B:164:ARG:HG3	2:B:164:ARG:HH11	1.12	1.06
2:B:164:ARG:HH11	2:B:164:ARG:CG	1.90	0.83
2:B:184:ARG:HH11	2:B:184:ARG:HG3	1.44	0.83
2:B:209:TYR:HB3	2:B:210:PRO:HD3	1.62	0.80
2:B:164:ARG:HG3	2:B:164:ARG:NH1	1.82	0.80
1:A:115:ASP:HB2	1:A:341:SER:HA	1.62	0.79
2:B:25:VAL:HA	2:B:28:ILE:HD12	1.70	0.73
2:B:189:LYS:HB3	2:B:192:LYS:HD2	1.70	0.72
1:A:214:ASN:ND2	1:A:217:GLU:HG3	2.04	0.72
1:A:138:ILE:HG21	1:A:147:THR:HG23	1.72	0.71
1:A:316:GLN:HG3	1:A:317:GLU:OE1	1.91	0.71
2:B:165:SER:HB2	2:B:166:PRO:HD2	1.77	0.67
1:A:47:ILE:N	1:A:47:ILE:HD12	2.11	0.66
2:B:129:LYS:HD2	2:B:129:LYS:H	1.59	0.66
1:A:244:ILE:HD12	1:A:252:VAL:HG12	1.78	0.66
1:A:6:PHE:HB3	1:A:106:ILE:HG23	1.78	0.65
2:B:119:GLN:HE22	2:B:147:GLU:HB2	1.61	0.65
2:B:119:GLN:NE2	2:B:147:GLU:HB2	2.11	0.65
1:A:173:GLN:OE1	1:A:173:GLN:HA	1.97	0.65
1:A:325:VAL:HG12	1:A:326:THR:H	1.63	0.64
1:A:319:GLN:O	1:A:321:PHE:N	2.31	0.64
1:A:184:GLU:HB2	1:A:339:THR:HG23	1.80	0.64
2:B:221:ARG:HG3	2:B:221:ARG:HH11	1.63	0.64
2:B:10:GLU:OE2	2:B:13:LYS:HD2	1.98	0.64
2:B:184:ARG:CG	2:B:184:ARG:HH11	2.11	0.63
2:B:156:ASN:HB3	2:B:159:LEU:HB2	1.79	0.63
2:B:94:GLU:O	2:B:95:SER:HB3	1.97	0.63
1:A:384:ARG:HG3	1:A:385:ASP:N	2.13	0.62
1:A:384:ARG:HG3	1:A:385:ASP:H	1.64	0.62
1:A:6:PHE:HB3	1:A:106:ILE:CG2	2.30	0.61
1:A:118:TYR:CE1	1:A:344:PRO:HD2	2.36	0.61
2:B:52:ASP:OD1	2:B:85:LYS:HE2	2.01	0.61
3:D:13:GLY:O	3:D:14:LYS:CB	2.48	0.60
1:A:105:LYS:HB2	1:A:225:ILE:HG23	1.84	0.60
1:A:303:LEU:H	1:A:303:LEU:HD12	1.68	0.59
1:A:368:GLU:HB3	1:A:370:TYR:CE2	2.37	0.58
2:B:65:HIS:CE1	2:B:67:SER:HB3	2.39	0.58
2:B:222:ASP:O	2:B:223:LEU:HB2	2.05	0.57
1:A:154:ARG:CZ	1:A:163:LEU:HD11	2.34	0.57
1:A:251:ARG:NH1	1:A:251:ARG:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:C	1:A:191:LEU:HD12	2.25	0.57
2:B:221:ARG:HG3	2:B:221:ARG:NH1	2.18	0.56
2:B:65:HIS:HE1	2:B:67:SER:HB3	1.71	0.56
1:A:292:ARG:NH1	1:A:320:GLU:HG2	2.19	0.56
2:B:189:LYS:N	2:B:189:LYS:HD2	2.21	0.56
1:A:325:VAL:HG12	1:A:326:THR:N	2.20	0.56
1:A:101:ARG:HD3	1:A:224:PHE:CD2	2.41	0.56
1:A:128:ARG:HH22	1:A:176:TYR:HE1	1.55	0.55
1:A:154:ARG:NH2	1:A:163:LEU:HD11	2.22	0.55
2:B:142:GLU:HG3	2:B:143:PRO:HD2	1.89	0.55
2:B:21:CYS:O	2:B:25:VAL:HG23	2.07	0.54
2:B:33:GLU:OE1	2:B:36:ARG:NH1	2.41	0.54
1:A:162:VAL:HG12	1:A:163:LEU:H	1.71	0.54
1:A:66:GLU:HG2	1:A:86:SER:HB3	1.90	0.54
1:A:214:ASN:HD21	1:A:217:GLU:HG3	1.71	0.54
1:A:20:LEU:O	1:A:53:PHE:HA	2.07	0.54
1:A:318:ARG:HH11	1:A:318:ARG:HG3	1.73	0.53
1:A:13:VAL:HG12	1:A:401:LYS:HA	1.91	0.53
2:B:94:GLU:O	2:B:95:SER:CB	2.57	0.53
1:A:193:THR:O	1:A:194:ARG:HG3	2.10	0.52
1:A:243:ARG:NH1	1:A:268:ASP:OD2	2.43	0.52
2:B:27:ALA:HB2	6:B:306:HOH:O	2.10	0.52
1:A:18:GLU:HA	1:A:396:GLN:O	2.10	0.52
2:B:184:ARG:CG	2:B:184:ARG:NH1	2.71	0.51
2:B:24:GLU:O	2:B:28:ILE:HG13	2.10	0.51
2:B:223:LEU:O	2:B:224:GLU:C	2.48	0.51
1:A:109:GLU:HG2	1:A:233:CYS:SG	2.51	0.51
2:B:109:PHE:O	2:B:118:GLU:HG2	2.11	0.51
1:A:290:ALY:HH33	1:A:329:VAL:CG1	2.41	0.51
2:B:78:LYS:HD3	2:B:79:TYR:CE1	2.46	0.51
1:A:298:ALA:HA	1:A:303:LEU:HD21	1.92	0.50
1:A:207:ASN:OD1	1:A:209:LYS:HD2	2.10	0.50
1:A:136:GLU:HG3	1:A:136:GLU:O	2.12	0.50
1:A:393:THR:HG22	1:A:394:ASN:H	1.77	0.50
1:A:13:VAL:HG13	1:A:402:ARG:C	2.32	0.49
1:A:319:GLN:HA	1:A:322:LYS:HB3	1.93	0.49
2:B:179:ILE:HD13	2:B:179:ILE:O	2.12	0.49
1:A:198:GLN:HE21	1:A:198:GLN:C	2.16	0.49
1:A:7:LEU:O	1:A:10:VAL:HG23	2.13	0.48
1:A:244:ILE:CD1	1:A:252:VAL:HG12	2.42	0.48
1:A:160:SER:OG	1:A:161:THR:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLN:O	1:A:300:GLU:HG2	2.13	0.48
1:A:136:GLU:HA	1:A:136:GLU:OE2	2.14	0.48
1:A:318:ARG:CZ	1:A:318:ARG:HB2	2.44	0.48
1:A:248:ASP:O	1:A:251:ARG:HB2	2.14	0.48
1:A:4:ASN:HD21	1:A:396:GLN:HB3	1.78	0.48
1:A:245:PRO:HD2	1:A:327:SER:O	2.14	0.47
1:A:11:LEU:HD13	1:A:17:PHE:CD1	2.50	0.47
1:A:165:GLU:O	1:A:172:GLN:HA	2.14	0.47
2:B:188:LEU:C	2:B:190:PRO:HD3	2.34	0.47
1:A:65:LEU:HD12	1:A:87:LYS:O	2.14	0.47
2:B:102:ASP:OD1	2:B:126:GLN:HA	2.15	0.47
3:D:13:GLY:O	3:D:14:LYS:HB3	2.15	0.47
1:A:115:ASP:H	1:A:342:LEU:H	1.62	0.46
1:A:318:ARG:O	1:A:319:GLN:HG3	2.16	0.46
1:A:378:GLU:OE1	2:B:73:ARG:HD3	2.15	0.46
1:A:293:PHE:O	1:A:293:PHE:CD1	2.68	0.46
1:A:57:HIS:NE2	1:A:58:GLN:NE2	2.63	0.46
1:A:128:ARG:NH2	1:A:176:TYR:HE1	2.14	0.46
1:A:298:ALA:CB	1:A:303:LEU:HD21	2.46	0.46
1:A:16:GLN:HA	1:A:398:LEU:O	2.15	0.46
2:B:156:ASN:O	2:B:160:ILE:HG13	2.15	0.46
2:B:30:ARG:NH2	2:B:96:GLU:HA	2.31	0.45
1:A:118:TYR:CD1	1:A:344:PRO:HD2	2.51	0.45
1:A:186:LEU:HD12	1:A:334:GLY:O	2.16	0.45
2:B:141:SER:OG	2:B:142:GLU:N	2.50	0.45
1:A:59:GLY:HA2	1:A:380:PHE:CD2	2.52	0.45
1:A:318:ARG:HH11	1:A:318:ARG:CG	2.29	0.45
1:A:290:ALY:HH33	1:A:329:VAL:HG13	1.97	0.45
1:A:86:SER:O	5:A:502:EDO:H12	2.16	0.45
1:A:271:THR:HG22	1:A:272:SER:N	2.32	0.45
1:A:194:ARG:NH1	5:A:502:EDO:O2	2.49	0.44
1:A:342:LEU:O	1:A:344:PRO:HD3	2.18	0.44
1:A:17:PHE:C	1:A:18:GLU:HG3	2.36	0.44
1:A:361:ILE:HG23	1:A:383:ILE:HD13	1.98	0.44
1:A:261:TYR:CD1	1:A:262:PRO:HD2	2.52	0.44
2:B:29:GLU:HA	2:B:32:VAL:CG2	2.48	0.44
1:A:53:PHE:N	1:A:53:PHE:CD2	2.85	0.44
1:A:149:ARG:O	1:A:152:ALA:HB3	2.17	0.44
2:B:82:THR:O	2:B:109:PHE:HA	2.17	0.44
2:B:77:PHE:HA	2:B:80:ILE:HB	1.99	0.44
1:A:350:ILE:O	1:A:352:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:N	1:A:47:ILE:CD1	2.81	0.44
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.82	0.44
2:B:146:ILE:HG13	2:B:147:GLU:N	2.33	0.43
1:A:242:LEU:HG	1:A:243:ARG:N	2.34	0.43
1:A:325:VAL:CG1	1:A:326:THR:H	2.30	0.43
1:A:75:ASP:OD1	1:A:76:GLU:N	2.50	0.43
1:A:51:HIS:HB3	1:A:53:PHE:CE2	2.53	0.43
2:B:169:LYS:O	2:B:173:ARG:HG2	2.18	0.43
2:B:29:GLU:HA	2:B:32:VAL:HG22	2.01	0.42
1:A:45:SER:OG	1:A:73:LEU:HD12	2.19	0.42
1:A:60:LYS:NZ	1:A:373:GLU:OE1	2.48	0.42
2:B:193:GLU:O	2:B:194:PHE:C	2.57	0.42
1:A:200:LEU:O	1:A:366:THR:HA	2.19	0.42
2:B:38:ASN:O	2:B:42:PRO:HD2	2.20	0.42
1:A:261:TYR:HA	1:A:262:PRO:HD3	1.69	0.42
1:A:212:ILE:HD12	1:A:212:ILE:N	2.34	0.42
1:A:394:ASN:N	1:A:394:ASN:OD1	2.52	0.42
1:A:398:LEU:HA	1:A:398:LEU:HD23	1.81	0.42
1:A:13:VAL:HG13	1:A:402:ARG:N	2.35	0.41
1:A:36:ASN:ND2	1:A:39:ASP:HB2	2.34	0.41
2:B:128:LYS:O	2:B:137:GLY:HA2	2.20	0.41
2:B:171:LYS:HD3	2:B:171:LYS:HA	1.87	0.41
1:A:163:LEU:HD12	1:A:163:LEU:N	2.36	0.41
2:B:129:LYS:HE3	2:B:129:LYS:HB3	1.87	0.41
2:B:42:PRO:O	2:B:46:LYS:HG2	2.21	0.41
1:A:285:PHE:HB3	1:A:286:PRO:HD2	2.01	0.41
1:A:271:THR:O	1:A:272:SER:O	2.39	0.41
2:B:184:ARG:O	2:B:185:TRP:C	2.59	0.41
2:B:25:VAL:HA	2:B:28:ILE:CD1	2.44	0.41
1:A:318:ARG:O	1:A:319:GLN:C	2.59	0.41
2:B:44:TYR:HE2	2:B:90:TRP:CH2	2.39	0.41
1:A:138:ILE:HD13	1:A:147:THR:HG23	2.03	0.40
2:B:99:ASP:C	2:B:101:ARG:N	2.74	0.40
1:A:135:PRO:O	1:A:136:GLU:HB3	2.21	0.40
1:A:353:LYS:HG2	1:A:357:GLN:OE1	2.21	0.40
1:A:298:ALA:HB2	1:A:303:LEU:HD21	2.02	0.40
1:A:355:ARG:O	1:A:359:ARG:HG3	2.22	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	387/438 (88%)	340 (88%)	37 (10%)	10 (3%)	7	22
2	B	209/232 (90%)	193 (92%)	13 (6%)	3 (1%)	14	42
3	D	3/15 (20%)	2 (67%)	0	1 (33%)	0	0
All	All	599/685 (87%)	535 (89%)	50 (8%)	14 (2%)	8	26

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TYR
1	A	272	SER
1	A	121	GLN
1	A	175	LEU
1	A	320	GLU
2	B	95	SER
3	D	14	LYS
1	A	135	PRO
1	A	271	THR
2	B	185	TRP
1	A	37	LYS
1	A	127	ILE
1	A	319	GLN
2	B	225	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	359/398 (90%)	327 (91%)	32 (9%)	12	34
2	B	190/207 (92%)	175 (92%)	15 (8%)	15	40
3	D	2/10 (20%)	1 (50%)	1 (50%)	0	0
All	All	551/615 (90%)	503 (91%)	48 (9%)	13	35

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	24	SER
1	A	34	THR
1	A	37	LYS
1	A	38	ASP
1	A	122	LYS
1	A	128	ARG
1	A	153	ARG
1	A	164	LYS
1	A	165	GLU
1	A	173	GLN
1	A	176	TYR
1	A	192	PHE
1	A	198	GLN
1	A	205	SER
1	A	208	SER
1	A	209	LYS
1	A	216	GLU
1	A	228	ARG
1	A	243	ARG
1	A	251	ARG
1	A	254	SER
1	A	263	LEU
1	A	273	LYS
1	A	303	LEU
1	A	318	ARG
1	A	319	GLN
1	A	320	GLU
1	A	336	SER
1	A	355	ARG
1	A	384	ARG
1	A	393	THR
2	B	20	LYS
2	B	32	VAL

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Mol	Chain	Res	Type
2	B	45	GLU
2	B	66	VAL
2	B	73	ARG
2	B	95	SER
2	B	117	LYS
2	B	118	GLU
2	B	129	LYS
2	B	146	ILE
2	B	159	LEU
2	B	164	ARG
2	B	179	ILE
2	B	220	GLN
2	B	223	LEU
3	D	14	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	198	GLN
1	A	275	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	A	290	1	10,11,12	0.35	0	10,12,14	0.92	1 (10%)

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	A	290	1	-	2/8/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ALY	O-C-CA	-2.02	120.22	125.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	290	ALY	CH3-CH-NZ-CE
1	A	290	ALY	OH-CH-NZ-CE

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	290	ALY	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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
4	ACO	A	501	-	43,53,53	0.92	2 (4%)	55,79,79	1.94	10 (18%)
5	EDO	A	502	-	3,3,3	0.57	0	2,2,2	0.52	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	ACO	A	501	-	-	0/47/67/67	0/3/3/3
5	EDO	A	502	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	ACO	C5A-N7A	-2.06	1.32	1.39
4	A	501	ACO	C5A-C4A	3.00	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	ACO	N3A-C2A-N1A	-7.37	123.25	128.89
4	A	501	ACO	C4A-C5A-N7A	-4.39	105.44	109.48
4	A	501	ACO	C2P-C3P-N4P	-3.67	105.01	112.36
4	A	501	ACO	C1B-N9A-C4A	-3.27	122.00	126.94
4	A	501	ACO	O3A-P1A-O5B	-2.62	96.00	102.94
4	A	501	ACO	C3P-N4P-C5P	2.17	127.06	122.79
4	A	501	ACO	C6P-C7P-N8P	2.84	118.11	111.88
4	A	501	ACO	C2P-S1P-C	3.18	121.53	101.83
4	A	501	ACO	CAP-C9P-N8P	3.26	123.69	116.47
4	A	501	ACO	O3A-P2A-O6A	3.41	111.98	102.94

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
5	A	502	EDO	2	0

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 [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	393/438 (89%)	-0.23	3 (0%) 87 81	42, 78, 132, 162	0
2	B	213/232 (91%)	-0.20	1 (0%) 91 88	57, 84, 118, 158	0
3	D	4/15 (26%)	0.01	0 100 100	62, 69, 103, 116	0
All	All	610/685 (89%)	-0.22	4 (0%) 89 84	42, 81, 130, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	PRO	3.3
2	B	129	LYS	3.1
1	A	40	LYS	2.4
1	A	141	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	ALY	A	290	12/13	0.97	0.17	-	40,52,64,64	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ACO	A	501	51/51	0.96	0.16	-0.15	47,79,119,121	0
5	EDO	A	502	4/4	0.91	0.16	-0.40	72,76,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.