



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2016 – 12:08 PM EDT

PDB ID : 5J9W  
Title : Crystal structure of the NuA4 core complex  
Authors : Chen, Z.C.; Xu, P.  
Deposited on : 2016-04-11  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

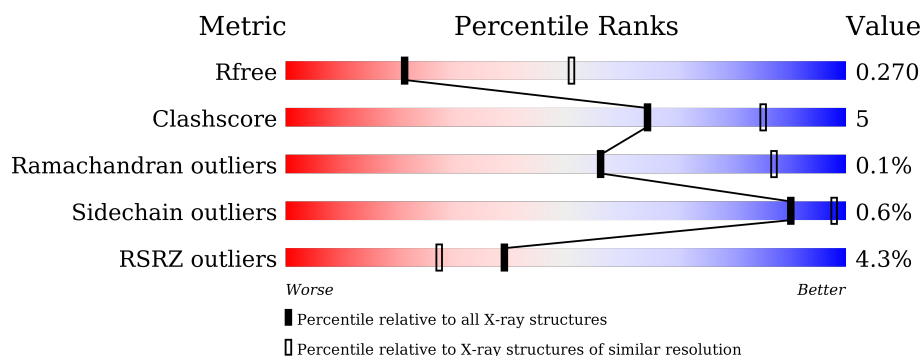
# 1 Overall quality at a glance

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.




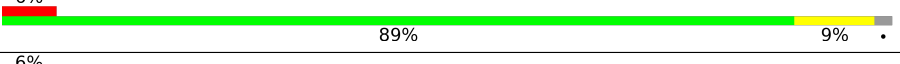
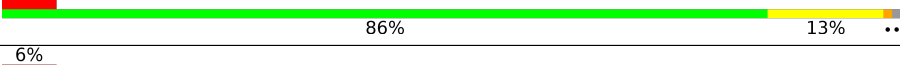

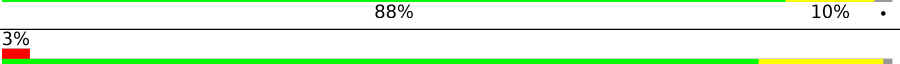
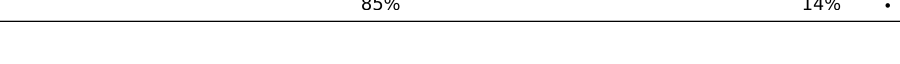
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	305	<div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
1	E	305	<div> <div>3%</div> <div>76%</div> <div>15%</div> <div>9%</div> </div>
1	I	305	<div> <div>5%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>
2	B	113	<div> <div>4%</div> <div>59%</div> <div>6%</div> <div>35%</div> </div>
2	F	113	<div> <div>4%</div> <div>56%</div> <div>•</div> <div>40%</div> </div>
2	J	113	<div> <div>3%</div> <div>54%</div> <div>8%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	280	 4% 79% 15% • 5%
3	G	280	 6% 89% 9% •
3	K	280	 6% 86% 13% ••
4	D	120	 6% 88% 11% •
4	H	120	 3% 88% 10% •
4	L	120	 3% 85% 14% •

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18691 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 ESA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			
1	A	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			
1	I	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	338	GLN	GLU	engineered mutation	UNP Q08649
A	338	GLN	GLU	engineered mutation	UNP Q08649
I	338	GLN	GLU	engineered mutation	UNP Q08649

- Molecule 2 is a protein called Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	68	Total	C	N	O		0	0	0
			570	355	96	119				
2	B	74	Total	C	N	O	S	0	0	0
			619	385	103	130	1			
2	J	70	Total	C	N	O		0	0	0
			587	367	99	121				

- Molecule 3 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	275	Total	C	N	O	S	0	0	0
			2307	1449	408	441	9			
3	C	267	Total	C	N	O	S	0	0	0
			2241	1410	392	430	9			

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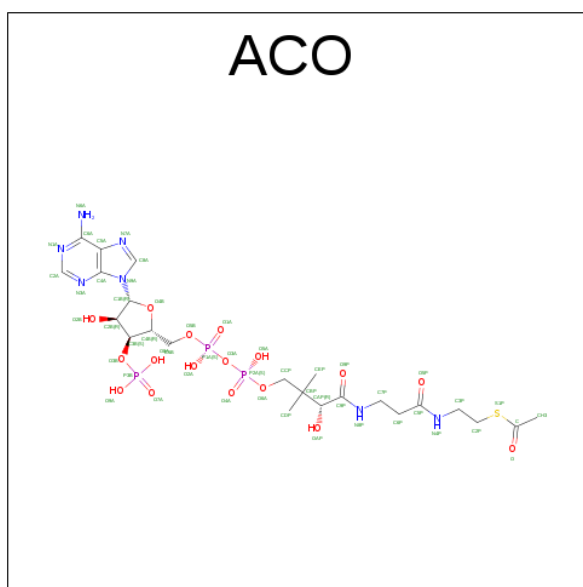
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	277	Total	C	N	O	S	0	0	0
			2321	1458	410	444	9			

- Molecule 4 is a protein called Chromatin modification-related protein YNG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	118	Total	C	N	O	S	0	0	0
			955	603	163	186	3			
4	D	119	Total	C	N	O	S	0	0	0
			962	608	164	187	3			
4	L	119	Total	C	N	O	S	0	0	0
			962	608	164	187	3			

- Molecule 5 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).

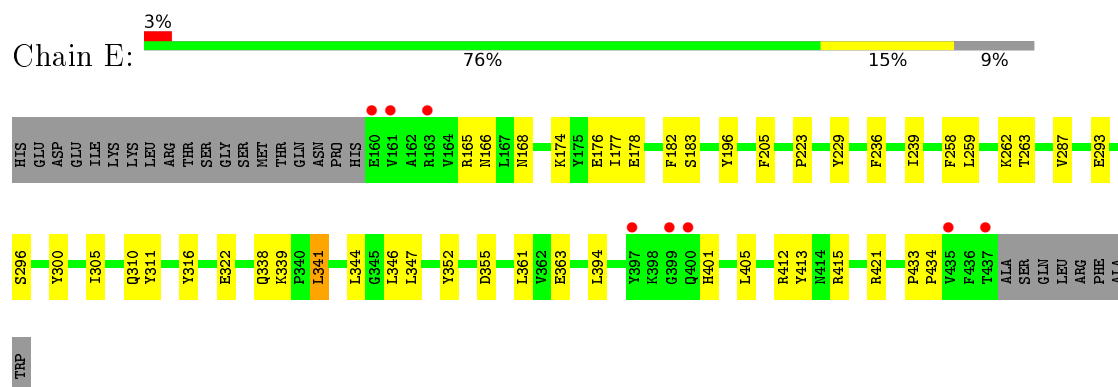


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

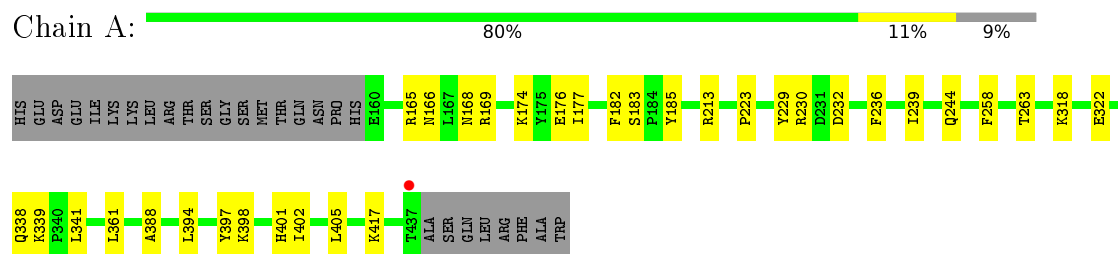
### 3 Residue-property plots [i](#)

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

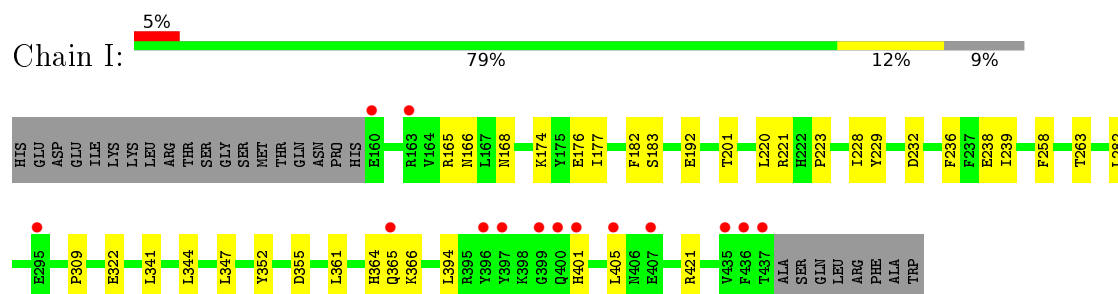
- Molecule 1: Histone acetyltransferase ESA1



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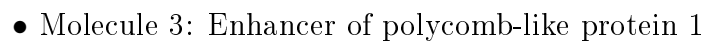
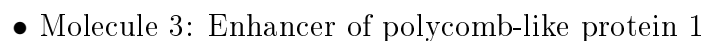
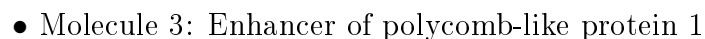


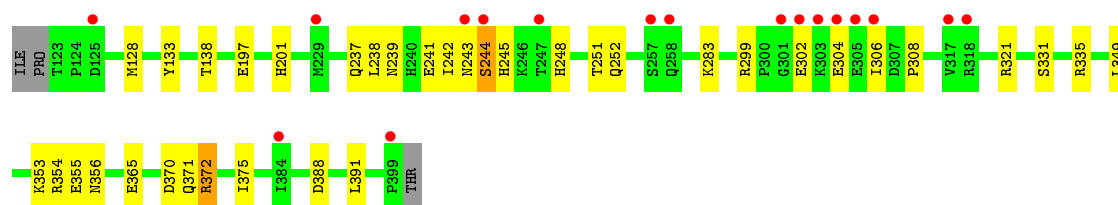
- Molecule 1: Histone acetyltransferase ESA1



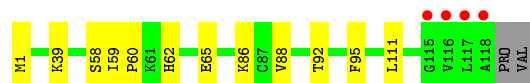
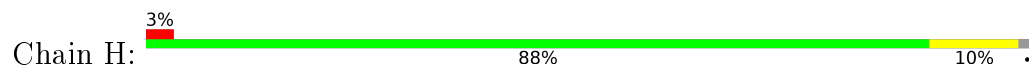
- Molecule 2: Chromatin modification-related protein EAF6



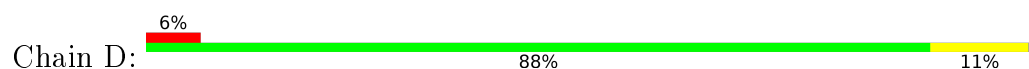




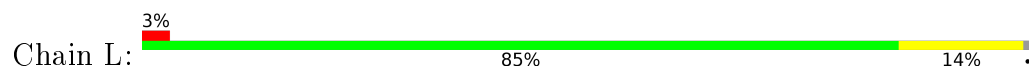
- Molecule 4: Chromatin modification-related protein YNG2



- Molecule 4: Chromatin modification-related protein YNG2



- Molecule 4: Chromatin modification-related protein YNG2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.26Å 138.57Å 167.87Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	29.88 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.6 (29.88-2.80) 75.8 (29.88-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.227 , 0.271 0.227 , 0.270	Depositor DCC
$R_{free}$ test set	1823 reflections (2.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, 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	0.26	0/2403	0.46	0/3246
1	E	0.28	0/2403	0.45	0/3246
1	I	0.27	0/2403	0.43	0/3246
2	B	0.26	0/626	0.42	0/834
2	F	0.25	0/577	0.37	0/769
2	J	0.25	0/594	0.40	0/791
3	C	0.26	0/2287	0.45	0/3080
3	G	0.27	0/2354	0.42	0/3168
3	K	0.29	0/2369	0.43	0/3190
4	D	0.25	0/974	0.38	0/1307
4	H	0.25	0/966	0.37	0/1295
4	L	0.25	0/974	0.38	0/1307
All	All	0.27	0/18930	0.43	0/25479

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
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLN	Peptide
2	B	4	GLU	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	2355	0	2343	23	0
1	E	2355	0	2343	36	0
1	I	2355	0	2343	25	0
2	B	619	0	584	5	0
2	F	570	0	531	4	0
2	J	587	0	555	9	0
3	C	2241	0	2182	40	0
3	G	2307	0	2255	29	0
3	K	2321	0	2269	32	0
4	D	962	0	994	15	0
4	H	955	0	987	14	0
4	L	962	0	994	16	0
5	E	51	0	34	5	0
5	I	51	0	34	3	0
All	All	18691	0	18448	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:GLU:HB3	3:G:125:ASP:HB3	1.59	0.82
1:E:176:GLU:HB3	3:G:128:MET:HB2	1.62	0.80
1:E:341:LEU:HD23	1:E:346:LEU:HA	1.63	0.79
4:L:62:HIS:HB3	4:L:65:GLU:HB2	1.65	0.79
1:I:165:ARG:NH2	1:I:168:ASN:O	2.18	0.75
3:C:379:LYS:NZ	4:D:58:SER:OG	2.20	0.75
1:E:412:ARG:HG2	1:E:415:ARG:HH21	1.55	0.72
1:I:364:HIS:CE1	1:I:366:LYS:HB2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ASN:ND2	1:I:183:SER:O	2.24	0.69
3:G:251:THR:HB	4:H:92:THR:HG22	1.75	0.68
1:A:397:TYR:HB3	1:A:402:ILE:HD13	1.75	0.68
3:K:299:ARG:NE	3:K:302:GLU:OE2	2.26	0.68
3:K:251:THR:HB	4:L:92:THR:HG22	1.75	0.67
1:A:361:LEU:HB3	1:A:405:LEU:HD21	1.77	0.65
4:H:62:HIS:HB3	4:H:65:GLU:HB2	1.80	0.64
1:A:398:LYS:H	4:L:114:ASP:HA	1.63	0.64
3:G:197:GLU:OE2	3:G:283:LYS:NZ	2.31	0.63
3:C:391:LEU:HD21	4:D:53:ILE:HB	1.81	0.62
1:I:394:LEU:HD11	1:I:401:HIS:HB3	1.80	0.62
1:A:165:ARG:NH2	1:A:168:ASN:O	2.28	0.62
3:K:197:GLU:OE2	3:K:283:LYS:NZ	2.32	0.62
1:I:344:LEU:HG	5:I:500:ACO:H133	1.83	0.61
3:C:197:GLU:OE2	3:C:283:LYS:NZ	2.33	0.61
1:I:361:LEU:HB3	1:I:405:LEU:HD21	1.83	0.60
1:E:300:TYR:OH	1:E:339:LYS:HD2	2.03	0.59
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.85	0.59
2:F:98:SER:HB2	3:G:354:ARG:HH22	1.68	0.59
1:E:165:ARG:NH2	1:E:168:ASN:O	2.30	0.58
1:I:355:ASP:OD2	1:I:421:ARG:NH1	2.37	0.58
4:L:1:MET:HB3	4:L:111:LEU:HD23	1.86	0.58
2:J:98:SER:HB2	3:K:354:ARG:HH22	1.68	0.57
2:B:22:ARG:NH1	3:C:365:GLU:OE2	2.36	0.57
1:E:394:LEU:HD11	1:E:401:HIS:HB3	1.86	0.57
3:C:370:ASP:OD2	4:D:73:LYS:NZ	2.38	0.56
3:G:299:ARG:NH2	3:G:302:GLU:HG3	2.20	0.56
3:C:252:GLN:H	4:D:92:THR:HG22	1.71	0.56
3:C:240:HIS:HB2	3:C:245:HIS:HE1	1.70	0.56
4:D:62:HIS:HB3	4:D:65:GLU:HB2	1.88	0.55
3:C:240:HIS:HB2	3:C:245:HIS:CE1	2.42	0.55
1:E:176:GLU:O	3:G:126:ALA:HA	2.06	0.55
1:I:176:GLU:HB3	3:K:128:MET:HB2	1.88	0.55
1:A:174:LYS:HB3	3:C:133:TYR:CG	2.42	0.55
3:G:379:LYS:NZ	4:H:58:SER:OG	2.34	0.55
3:G:237:GLN:NE2	3:G:241:GLU:OE2	2.39	0.55
4:H:1:MET:HB3	4:H:111:LEU:HD23	1.88	0.55
1:E:361:LEU:HB3	1:E:405:LEU:HD21	1.89	0.54
1:E:363:GLU:OE2	1:E:413:TYR:OH	2.16	0.54
2:J:15:LEU:HD11	3:K:372:ARG:HD2	1.88	0.54
3:K:237:GLN:NE2	3:K:241:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ILE:HD12	1:E:258:PHE:HZ	1.72	0.54
4:D:88:VAL:O	4:D:92:THR:HG23	2.08	0.54
3:K:335:ARG:NH2	4:L:112:GLU:OE2	2.41	0.53
3:C:392:ILE:O	3:C:392:ILE:HG23	2.09	0.53
2:B:98:SER:HB2	3:C:354:ARG:HH22	1.73	0.53
3:C:392:ILE:HG22	4:D:50:HIS:CD2	2.44	0.53
3:G:242:ILE:O	3:G:243:ASN:HB2	2.08	0.53
1:I:229:TYR:HB3	1:I:236:PHE:HB2	1.91	0.53
1:E:177:ILE:HG22	3:G:126:ALA:HB2	1.91	0.52
1:A:230:ARG:NH2	3:C:144:THR:O	2.42	0.52
1:E:177:ILE:HA	3:G:125:ASP:O	2.10	0.52
1:I:168:ASN:ND2	1:I:192:GLU:O	2.42	0.52
4:L:56:GLN:HB3	4:L:60:PRO:HG2	1.92	0.52
1:A:394:LEU:HD11	1:A:401:HIS:HB3	1.92	0.52
3:C:366:LEU:HD12	4:D:76:LEU:HG	1.92	0.52
1:E:166:ASN:HB2	1:E:182:PHE:HA	1.91	0.51
3:G:252:GLN:H	4:H:92:THR:HG22	1.75	0.51
3:K:242:ILE:HB	3:K:244:SER:HB3	1.92	0.51
1:E:322:GLU:HG2	1:E:352:TYR:HE1	1.75	0.51
1:I:347:LEU:HD12	5:I:500:ACO:H1B	1.92	0.51
1:A:213:ARG:NH2	3:C:187:ASP:OD2	2.42	0.51
1:A:229:TYR:HB3	1:A:236:PHE:HB2	1.92	0.51
3:K:370:ASP:OD2	4:L:73:LYS:NZ	2.44	0.51
3:C:375:ILE:O	3:C:379:LYS:HG3	2.11	0.50
2:B:5:LEU:HD23	3:C:382:LEU:HD13	1.92	0.50
3:C:251:THR:HB	4:D:92:THR:HG22	1.93	0.50
1:I:201:THR:HG22	1:I:220:LEU:HD23	1.93	0.50
2:J:14:GLU:HA	2:J:17:LYS:HD3	1.93	0.49
3:K:239:ASN:HD21	3:K:248:HIS:HA	1.77	0.49
3:G:379:LYS:HZ2	4:H:58:SER:HG	1.60	0.49
1:I:341:LEU:HG	5:I:500:ACO:HH33	1.94	0.49
3:C:335:ARG:NH2	4:D:118:ALA:O	2.45	0.49
3:K:197:GLU:HG3	3:K:201:HIS:CE1	2.47	0.49
2:J:15:LEU:HD13	3:K:375:ILE:HD12	1.95	0.48
1:E:223:PRO:HB3	1:E:239:ILE:HD11	1.96	0.48
3:K:304:GLU:HG3	3:K:306:ILE:H	1.78	0.48
1:E:177:ILE:HG22	3:G:126:ALA:CB	2.44	0.48
1:E:300:TYR:CE2	1:E:338:GLN:HG3	2.49	0.48
3:K:355:GLU:OE2	4:L:86:LYS:HE2	2.14	0.47
3:K:331:SER:HB3	4:L:117:LEU:HD13	1.96	0.47
1:E:412:ARG:HG2	1:E:415:ARG:NH2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:242:ILE:O	3:K:243:ASN:HB2	2.15	0.47
2:J:15:LEU:HD12	3:K:371:GLN:HB3	1.95	0.47
3:C:307:ASP:HB3	3:C:310:VAL:HG23	1.95	0.47
3:C:379:LYS:HE2	3:C:379:LYS:HB3	1.61	0.47
1:A:166:ASN:ND2	1:A:183:SER:O	2.45	0.47
1:A:232:ASP:N	1:A:232:ASP:OD1	2.47	0.47
3:C:252:GLN:H	4:D:92:THR:CG2	2.27	0.47
2:F:26:GLU:HB3	3:G:398:ARG:NH1	2.30	0.47
3:K:197:GLU:HG3	3:K:201:HIS:HE1	1.78	0.47
2:F:22:ARG:O	2:F:26:GLU:HG3	2.14	0.46
3:G:249:PHE:HE2	4:H:95:PHE:HB2	1.80	0.46
3:G:252:GLN:H	4:H:92:THR:CG2	2.28	0.46
4:H:88:VAL:O	4:H:92:THR:HG23	2.16	0.46
1:A:223:PRO:HB3	1:A:239:ILE:HD11	1.98	0.46
3:G:361:TRP:CZ3	4:H:39:LYS:HE3	2.50	0.46
3:K:252:GLN:H	4:L:92:THR:CG2	2.28	0.46
3:K:252:GLN:H	4:L:92:THR:HG22	1.80	0.46
1:E:355:ASP:OD2	1:E:421:ARG:NH1	2.49	0.46
1:E:421:ARG:NH2	5:E:500:ACO:O9A	2.47	0.46
1:I:322:GLU:HG2	1:I:352:TYR:HE1	1.79	0.46
1:I:365:GLN:C	1:I:366:LYS:HG3	2.36	0.46
3:C:168:ASP:OD1	3:C:282:ARG:NH1	2.48	0.46
1:A:339:LYS:O	1:A:341:LEU:N	2.49	0.45
3:G:323:THR:HG23	3:G:326:ILE:H	1.80	0.45
4:L:88:VAL:O	4:L:92:THR:HG23	2.16	0.45
3:C:216:SER:HB3	3:C:219:GLU:HG3	1.98	0.45
1:E:347:LEU:HD12	5:E:500:ACO:H1B	1.98	0.45
1:E:344:LEU:HD23	5:E:500:ACO:HN8	1.80	0.45
3:K:238:LEU:O	3:K:242:ILE:HG13	2.16	0.45
1:I:174:LYS:HB3	3:K:133:TYR:CG	2.52	0.45
1:I:182:PHE:CE2	3:K:308:PRO:HB2	2.51	0.45
1:E:344:LEU:HG	5:E:500:ACO:H133	1.99	0.45
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.52	0.44
4:D:46:GLU:HG2	4:D:50:HIS:NE2	2.32	0.44
3:C:387:GLU:HG2	4:D:58:SER:OG	2.17	0.44
3:K:304:GLU:HA	3:K:304:GLU:OE1	2.17	0.44
1:I:232:ASP:N	1:I:232:ASP:OD1	2.50	0.44
1:E:305:ILE:HG23	5:E:500:ACO:H31	2.00	0.44
1:E:166:ASN:ND2	1:E:183:SER:O	2.49	0.44
1:E:310:GLN:HB3	3:G:126:ALA:HB1	2.00	0.44
3:C:391:LEU:HA	3:C:391:LEU:HD23	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:321:ARG:NH2	4:L:1:MET:O	2.51	0.43
1:A:169:ARG:NE	1:A:176:GLU:OE2	2.50	0.43
3:G:299:ARG:HH21	3:G:302:GLU:HG3	1.82	0.43
1:E:310:GLN:HG2	1:E:311:TYR:CD2	2.54	0.43
1:A:230:ARG:HB3	3:C:147:TYR:CE1	2.54	0.43
3:G:379:LYS:NZ	4:H:58:SER:HG	2.16	0.43
1:A:166:ASN:HB2	1:A:182:PHE:HA	2.01	0.43
1:A:177:ILE:HD12	1:A:258:PHE:HZ	1.83	0.43
1:A:388:ALA:HB1	1:A:394:LEU:HB2	2.00	0.43
1:I:166:ASN:HB2	1:I:182:PHE:HA	2.01	0.43
2:J:22:ARG:NH1	3:K:365:GLU:OE1	2.48	0.43
3:C:221:LYS:O	3:C:225:ILE:HG12	2.19	0.43
2:B:8:TYR:HE1	3:C:379:LYS:HG2	1.83	0.43
3:C:379:LYS:HZ1	3:C:387:GLU:HG3	1.84	0.43
1:I:258:PHE:CE1	1:I:309:PRO:HG2	2.53	0.43
1:A:244:GLN:OE1	3:C:153:THR:HA	2.19	0.43
3:C:176:VAL:HG22	3:C:274:LYS:HE3	2.01	0.43
2:B:8:TYR:CE1	3:C:379:LYS:HG2	2.54	0.42
1:A:177:ILE:HD12	1:A:258:PHE:CZ	2.54	0.42
3:C:304:GLU:CD	3:C:313:ARG:HH12	2.22	0.42
4:L:76:LEU:HA	4:L:76:LEU:HD12	1.91	0.42
3:C:355:GLU:OE2	4:D:86:LYS:HE2	2.20	0.42
1:I:228:ILE:HD13	1:I:238:GLU:HB2	2.01	0.42
3:K:244:SER:HB2	3:K:356:ASN:ND2	2.34	0.42
3:K:349:LEU:HG	3:K:353:LYS:HE2	2.00	0.42
2:F:21:ASP:O	2:F:25:GLN:HG2	2.19	0.42
3:G:355:GLU:OE2	4:H:86:LYS:HE2	2.18	0.42
1:A:183:SER:O	1:A:185:TYR:N	2.51	0.42
1:A:417:LYS:HA	1:A:417:LYS:HD2	1.86	0.42
3:C:177:ASN:ND2	3:C:184:LEU:O	2.48	0.42
3:K:388:ASP:HA	3:K:391:LEU:HD23	2.02	0.42
3:C:203:ARG:HD2	3:C:223:THR:OG1	2.19	0.42
1:E:293:GLU:HB2	1:E:296:SER:HB2	2.02	0.41
3:G:250:ILE:HG23	4:H:88:VAL:HG22	2.02	0.41
3:G:302:GLU:OE1	3:G:302:GLU:HA	2.20	0.41
3:C:242:ILE:HG22	3:C:243:ASN:HD22	1.85	0.41
1:E:311:TYR:HB3	1:E:316:TYR:CD2	2.55	0.41
2:J:22:ARG:O	2:J:26:GLU:HG3	2.21	0.41
2:J:71:LYS:HD3	2:J:71:LYS:HA	1.84	0.41
1:I:221:ARG:NH2	3:K:138:THR:O	2.45	0.41
4:L:93:ALA:O	4:L:97:ILE:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:PRO:HB3	1:I:239:ILE:HD11	2.03	0.41
1:A:318:LYS:HE2	1:A:322:GLU:OE2	2.21	0.41
1:I:177:ILE:HD12	1:I:258:PHE:HZ	1.86	0.41
3:C:226:LYS:H	3:C:226:LYS:HG3	1.68	0.41
4:H:59:ILE:HB	4:H:60:PRO:HD3	2.03	0.41
1:I:221:ARG:HD3	1:I:282:LEU:O	2.21	0.41
2:J:21:ASP:O	2:J:25:GLN:HG2	2.21	0.40
1:E:196:TYR:HB2	1:E:205:PHE:HB2	2.02	0.40
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.98	0.40
3:G:203:ARG:HD2	3:G:223:THR:OG1	2.22	0.40
3:C:234:LEU:HD13	4:D:102:ASN:ND2	2.35	0.40
1:E:259:LEU:HD12	1:E:262:ALY:HG2	2.03	0.40
3:G:243:ASN:HA	3:G:245:HIS:CE1	2.56	0.40
3:K:372:ARG:HG3	3:K:391:LEU:HD13	2.02	0.40
1:E:287:VAL:HA	1:E:311:TYR:CD2	2.55	0.40
4:L:59:ILE:HB	4:L:60:PRO:HD3	2.04	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	275/305 (90%)	264 (96%)	11 (4%)	0	100	100
1	E	275/305 (90%)	265 (96%)	10 (4%)	0	100	100
1	I	275/305 (90%)	264 (96%)	11 (4%)	0	100	100
2	B	68/113 (60%)	65 (96%)	3 (4%)	0	100	100
2	F	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
2	J	64/113 (57%)	62 (97%)	2 (3%)	0	100	100
3	C	265/280 (95%)	255 (96%)	9 (3%)	1 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	273/280 (98%)	262 (96%)	10 (4%)	1 (0%)	39	74
3	K	275/280 (98%)	264 (96%)	11 (4%)	0	100	100
4	D	117/120 (98%)	117 (100%)	0	0	100	100
4	H	116/120 (97%)	116 (100%)	0	0	100	100
4	L	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
All	All	2182/2454 (89%)	2110 (97%)	70 (3%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	126	ALA
3	C	243	ASN

### 5.3.2 Protein sidechains ⓘ

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	259/283 (92%)	258 (100%)	1 (0%)	93	98
1	E	259/283 (92%)	257 (99%)	2 (1%)	86	97
1	I	259/283 (92%)	258 (100%)	1 (0%)	93	98
2	B	69/100 (69%)	67 (97%)	2 (3%)	50	83
2	F	63/100 (63%)	63 (100%)	0	100	100
2	J	65/100 (65%)	65 (100%)	0	100	100
3	C	253/265 (96%)	250 (99%)	3 (1%)	78	95
3	G	260/265 (98%)	259 (100%)	1 (0%)	93	98
3	K	262/265 (99%)	259 (99%)	3 (1%)	80	95
4	D	110/111 (99%)	110 (100%)	0	100	100
4	H	109/111 (98%)	109 (100%)	0	100	100
4	L	110/111 (99%)	110 (100%)	0	100	100
All	All	2078/2277 (91%)	2065 (99%)	13 (1%)	90	98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	263	THR
1	E	341	LEU
3	G	247	THR
1	A	263	THR
2	B	1	MET
2	B	3	ASP
3	C	128	MET
3	C	261	THR
3	C	387	GLU
1	I	263	THR
3	K	244	SER
3	K	245	HIS
3	K	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	201	HIS
3	K	239	ASN
3	K	266	GLN
3	K	356	ASN

### 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	A	262	1	9,11,12	0.99	1 (11%)	10,12,14	0.88	1 (10%)
1	ALY	E	262	1	9,11,12	0.96	1 (11%)	10,12,14	0.93	0
1	ALY	I	262	1	9,11,12	1.02	1 (11%)	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	262	1	-	0/8/10/12	0/0/0/0
1	ALY	E	262	1	-	0/8/10/12	0/0/0/0
1	ALY	I	262	1	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	262	ALY	CH-NZ	2.02	1.39	1.33
1	A	262	ALY	CH-NZ	2.15	1.39	1.33
1	I	262	ALY	CH-NZ	2.28	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ALY	CD-CG-CB	-2.09	106.28	113.67
1	I	262	ALY	CD-CG-CB	-2.03	106.48	113.67

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
1	E	262	ALY	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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$
5	ACO	E	500	-	44,53,53	1.96	9 (20%)	54,79,79	1.91	3 (5%)
5	ACO	I	500	-	44,53,53	1.95	10 (22%)	54,79,79	2.08	8 (14%)

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
5	ACO	E	500	-	-	0/47/67/67	0/3/3/3
5	ACO	I	500	-	-	0/47/67/67	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	500	ACO	C2B-C1B	-5.10	1.45	1.53
5	E	500	ACO	C2B-C1B	-5.00	1.45	1.53
5	I	500	ACO	C2B-C3B	-4.20	1.43	1.53
5	E	500	ACO	C2B-C3B	-4.17	1.43	1.53
5	E	500	ACO	CEP-CBP	-2.29	1.48	1.53
5	E	500	ACO	C3B-C4B	-2.28	1.46	1.52
5	I	500	ACO	CEP-CBP	-2.27	1.48	1.53
5	I	500	ACO	C3B-C4B	-2.26	1.46	1.52
5	I	500	ACO	C5B-C4B	-2.00	1.45	1.51
5	I	500	ACO	C2A-N3A	2.25	1.36	1.32
5	E	500	ACO	C2A-N3A	2.30	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	500	ACO	C6A-N6A	2.49	1.44	1.34
5	I	500	ACO	C6A-N6A	2.49	1.44	1.34
5	I	500	ACO	O4B-C1B	4.01	1.47	1.41
5	E	500	ACO	O4B-C1B	4.11	1.47	1.41
5	I	500	ACO	C9P-N8P	4.75	1.43	1.33
5	E	500	ACO	C9P-N8P	4.84	1.43	1.33
5	I	500	ACO	C5P-N4P	6.14	1.48	1.33
5	E	500	ACO	C5P-N4P	6.22	1.48	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	500	ACO	N3A-C2A-N1A	-11.22	120.06	128.87
5	I	500	ACO	N3A-C2A-N1A	-11.19	120.08	128.87
5	I	500	ACO	C4B-O4B-C1B	-5.93	103.35	109.64
5	E	500	ACO	C4B-O4B-C1B	-4.74	104.61	109.64
5	I	500	ACO	C1B-N9A-C4A	-2.65	123.85	126.81
5	I	500	ACO	O9P-C9P-N8P	-2.29	118.48	123.04
5	I	500	ACO	O4B-C1B-N9A	2.04	111.97	108.11
5	I	500	ACO	C6P-C5P-N4P	2.24	120.35	116.46
5	I	500	ACO	CEP-CBP-CAP	2.37	113.49	109.17
5	E	500	ACO	C3B-C2B-C1B	2.38	105.24	100.06
5	I	500	ACO	C3B-C2B-C1B	2.39	105.26	100.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	500	ACO	5	0
5	I	500	ACO	3	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/305 (90%)	-0.35	1 (0%) 93 90	21, 40, 73, 96	0
1	E	277/305 (90%)	-0.09	8 (2%) 55 43	26, 52, 91, 111	0
1	I	277/305 (90%)	0.05	14 (5%) 32 21	29, 56, 110, 141	0
2	B	74/113 (65%)	0.11	5 (6%) 20 12	33, 52, 91, 129	0
2	F	68/113 (60%)	0.18	5 (7%) 17 9	32, 63, 105, 124	0
2	J	70/113 (61%)	0.20	3 (4%) 39 27	37, 57, 96, 104	0
3	C	267/280 (95%)	-0.01	11 (4%) 41 29	20, 56, 98, 130	0
3	G	275/280 (98%)	-0.02	17 (6%) 24 15	26, 55, 99, 116	0
3	K	277/280 (98%)	0.05	17 (6%) 25 15	32, 61, 100, 132	0
4	D	119/120 (99%)	-0.21	7 (5%) 26 16	23, 41, 100, 130	0
4	H	118/120 (98%)	-0.09	4 (3%) 49 36	34, 55, 92, 112	0
4	L	119/120 (99%)	-0.13	3 (2%) 61 48	26, 52, 100, 107	0
All	All	2218/2454 (90%)	-0.05	95 (4%) 39 27	20, 53, 99, 141	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	107	HIS	6.3
3	C	259	MET	6.0
4	D	118	ALA	5.0
3	C	258	GLN	4.8
2	J	107	HIS	4.5
2	B	66	SER	4.4
4	D	115	GLY	4.4
3	K	306	ILE	4.4
3	C	317	VAL	4.3
3	C	306	ILE	4.3
1	I	160	GLU	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	119	PRO	4.2
2	F	107	HIS	4.2
4	L	119	PRO	4.2
3	G	385	SER	4.1
1	I	397	TYR	4.0
4	H	118	ALA	4.0
3	G	305	GLU	3.9
4	D	114	ASP	3.9
3	G	306	ILE	3.8
3	G	257	SER	3.8
2	J	66	SER	3.5
1	I	295	GLU	3.5
1	E	163	ARG	3.5
3	G	383	ASN	3.5
1	E	437	THR	3.4
1	I	437	THR	3.4
3	K	304	GLU	3.4
4	H	115	GLY	3.4
3	C	305	GLU	3.3
1	E	435	VAL	3.3
1	I	435	VAL	3.3
4	L	118	ALA	3.3
4	D	117	LEU	3.2
1	I	365	GLN	3.2
3	K	303	LYS	3.1
3	K	317	VAL	3.1
1	I	163	ARG	3.1
3	K	305	GLU	3.1
3	G	258	GLN	3.1
1	E	160	GLU	3.1
1	E	397	TYR	3.1
2	B	105	GLN	3.1
3	K	247	THR	3.0
4	H	116	VAL	3.0
3	G	318	ARG	3.0
3	C	301	GLY	3.0
1	E	399	GLY	2.9
4	D	1	MET	2.9
3	G	386	GLY	2.8
2	J	8	TYR	2.8
1	I	399	GLY	2.8
3	G	300	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	88	PHE	2.7
3	C	304	GLU	2.7
3	G	247	THR	2.6
1	A	437	THR	2.6
3	C	318	ARG	2.6
4	H	117	LEU	2.6
3	G	316	GLU	2.5
3	G	303	LYS	2.5
3	K	399	PRO	2.5
3	G	127	SER	2.5
1	I	407	GLU	2.5
4	D	116	VAL	2.5
3	K	302	GLU	2.4
3	G	125	ASP	2.4
3	C	316	GLU	2.4
1	I	401	HIS	2.3
1	I	400	GLN	2.3
4	L	117	LEU	2.3
1	I	396	TYR	2.3
3	K	243	ASN	2.3
3	G	301	GLY	2.3
3	C	260	ASN	2.2
2	B	104	LYS	2.2
3	K	257	SER	2.2
3	K	384	ILE	2.2
2	F	106	GLN	2.2
1	E	400	GLN	2.2
2	F	12	LYS	2.2
3	K	229	MET	2.2
3	K	125	ASP	2.2
1	I	436	PHE	2.2
1	E	161	VAL	2.2
3	G	259	MET	2.1
1	I	405	LEU	2.1
3	C	300	PRO	2.1
3	K	244	SER	2.1
3	K	301	GLY	2.1
2	B	67	GLY	2.0
3	G	128	MET	2.0
3	K	258	GLN	2.0
2	F	74	ASP	2.0
3	K	318	ARG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	ALY	A	262	12/13	0.96	0.16	-	23,36,42,51	0
1	ALY	E	262	12/13	0.97	0.15	-	29,38,51,57	0
1	ALY	I	262	12/13	0.94	0.20	-	35,46,54,56	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	ACO	I	500	51/51	0.90	0.22	0.33	42,78,105,112	0
5	ACO	E	500	51/51	0.93	0.17	-0.37	38,69,95,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.