



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:44 am BST

PDB ID : 5J9Q  
Title : Crystal structure of the NuA4 core complex  
Authors : Chen, Z.C.; Xu, P.  
Deposited on : 2016-04-11  
Resolution : 3.25 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

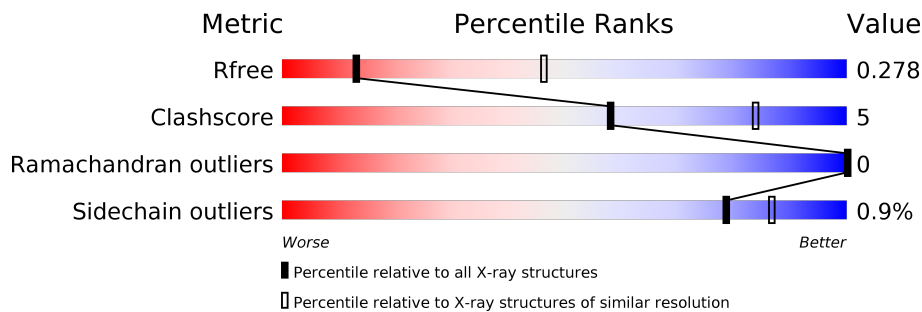
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	305	81% 15% .
1	E	305	84% 11% . .
1	I	305	80% 15% . .
2	B	113	61% 9% 30%
2	F	113	59% 7% 34%
2	J	113	55% 12% 33%
3	C	351	74% 9% 17%

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Mol	Chain	Length	Quality of chain
3	G	351	 73% 10% 16%
3	N	351	 69% 13% 18%
4	D	120	 92% 8%
4	H	120	 84% 15%
4	K	120	 84% 16%
5	L	10	 20% 20% 10% 50%
5	M	10	 10% 20% 10% 60%
5	O	10	 30% 70%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19671 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
			Total	C	N	O	S			
1	E	293	2479	1601	420	447	11	0	0	0
1	A	292	2470	1596	419	445	10	0	0	0
1	I	292	2470	1596	419	445	10	0	0	0

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
			Total	C	N	O	S			
2	F	75	622	389	99	133	1	0	0	0
2	B	79	660	413	108	138	1	0	0	0
2	J	76	627	392	100	134	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	295	2476	1562	437	469	8	0	0	0
3	N	289	2426	1533	424	461	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	293	Total	C	N	O	S	0	0	0
			2458	1554	429	467	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	120	Total	C	N	O	S	0	0	0
			969	613	165	188	3			
4	H	120	Total	C	N	O	S	0	0	0
			969	613	165	188	3			
4	K	120	Total	C	N	O	S	0	0	0
			969	613	165	188	3			

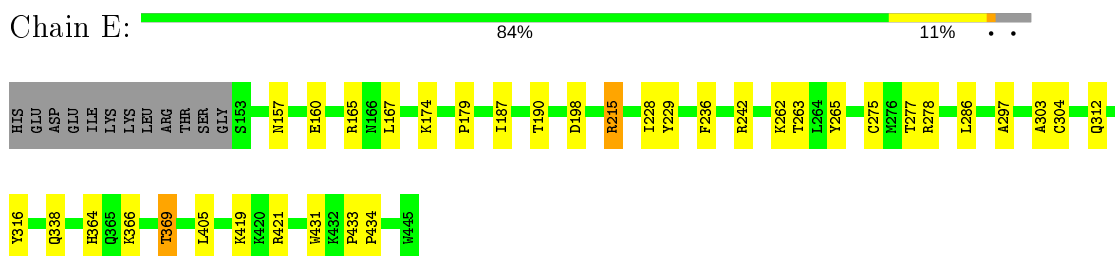
- Molecule 5 is a protein called Htz1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	5	Total	C	N	O	0	0	0
			32	18	6	8			
5	M	4	Total	C	N	O	0	0	0
			26	15	5	6			
5	O	3	Total	C	N	O	0	0	0
			18	11	4	3			

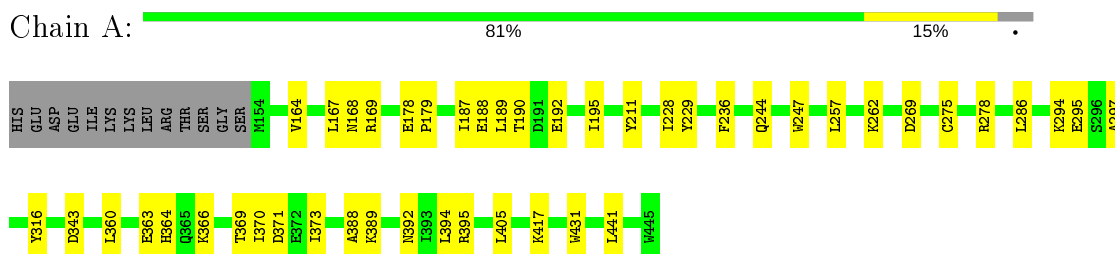
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

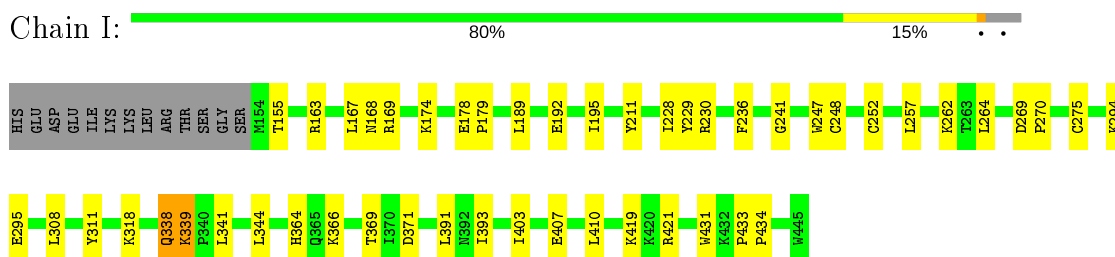
- Molecule 1: Histone acetyltransferase ESA1



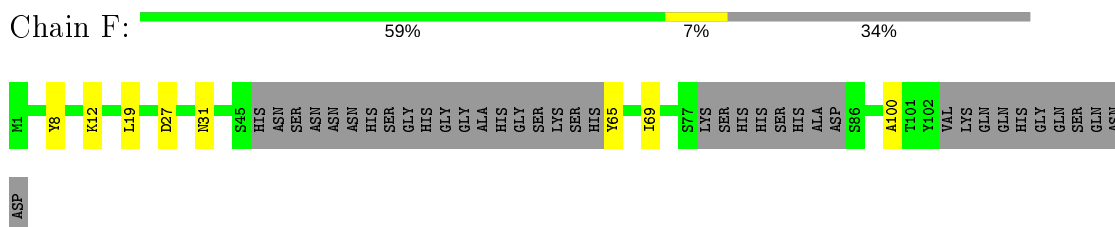
- Molecule 1: Histone acetyltransferase ESA1



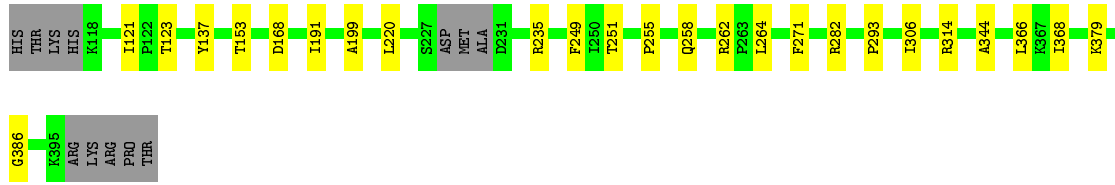
- Molecule 1: Histone acetyltransferase ESA1



- Molecule 2: Chromatin modification-related protein EAF6



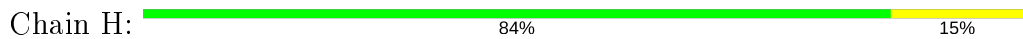




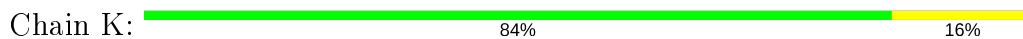
- Molecule 4: Chromatin modification-related protein YNG2



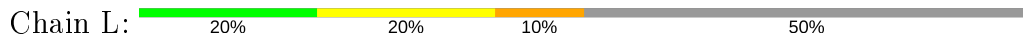
- Molecule 4: Chromatin modification-related protein YNG2



- Molecule 4: Chromatin modification-related protein YNG2



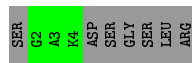
- Molecule 5: Htz1



- Molecule 5: Htz1



- Molecule 5: Htz1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.86Å 190.99Å 172.35Å 90.00° 113.56° 90.00°	Depositor
Resolution (Å)	30.00 – 3.25 46.74 – 3.25	Depositor EDS
% Data completeness (in resolution range)	78.9 (30.00-3.25) 78.7 (46.74-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.25Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.250 , 0.273 0.252 , 0.278	Depositor DCC
$R_{free}$ test set	2000 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.1	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 26.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	19671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/2523	0.43	0/3411
1	E	0.27	0/2532	0.41	0/3422
1	I	0.31	1/2523 (0.0%)	0.43	0/3411
2	B	0.27	0/669	0.39	0/893
2	F	0.26	0/630	0.39	0/841
2	J	0.27	0/635	0.41	0/848
3	C	0.27	0/2509	0.41	0/3379
3	G	0.26	0/2528	0.42	0/3404
3	N	0.26	0/2477	0.40	0/3335
4	D	0.27	0/981	0.39	0/1317
4	H	0.27	0/981	0.38	0/1317
4	K	0.27	0/981	0.39	0/1317
5	L	0.33	0/31	0.81	0/39
5	M	0.29	0/25	0.92	0/31
5	O	0.24	0/17	0.45	0/20
All	All	0.28	1/20042 (0.0%)	0.41	0/26985

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	I	0	1
3	G	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	339	LYS	C-N	6.50	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	62	VAL	Peptide
1	I	338	GLN	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2470	0	2446	30	0
1	E	2479	0	2458	25	0
1	I	2470	0	2445	35	0
2	B	660	0	619	7	0
2	F	622	0	579	7	0
2	J	627	0	581	15	0
3	C	2458	0	2414	27	0
3	G	2476	0	2427	26	0
3	N	2426	0	2374	36	0
4	D	969	0	1003	9	0
4	H	969	0	1003	15	0
4	K	969	0	1003	14	0
5	L	32	0	32	3	0
5	M	26	0	24	3	0
5	O	18	0	20	0	0
All	All	19671	0	19428	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:I:407:GLU:HG2	3:C:63:LYS:HG3	1.67	0.74
1:E:338:GLN:NE2	5:L:2:GLY:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:379:LYS:NZ	3:G:386:GLY:O	2.18	0.71
2:J:41:THR:HG22	2:J:93:ARG:HH22	1.55	0.71
4:D:14:VAL:HG22	4:D:100:HIS:HD2	1.57	0.69
3:N:344:ALA:HB1	2:J:69:ILE:HD11	1.75	0.68
4:H:62:HIS:HB3	4:H:65:GLU:HB2	1.76	0.67
1:I:338:GLN:HE21	5:M:4:LYS:HB2	1.58	0.67
3:N:392:ILE:HG23	4:K:50:HIS:HB3	1.76	0.66
1:I:391:LEU:HB2	1:I:393:ILE:HG12	1.78	0.66
1:I:318:LYS:HE2	1:I:421:ARG:HH21	1.62	0.63
1:I:229:TYR:HB3	1:I:236:PHE:HB2	1.80	0.63
1:I:252:CYS:HB3	1:I:264:LEU:HD11	1.80	0.62
3:G:191:ILE:HG22	3:G:264:LEU:HD23	1.80	0.62
3:G:379:LYS:NZ	3:G:388:ASP:OD1	2.33	0.62
4:K:62:HIS:HB3	4:K:65:GLU:HB2	1.81	0.62
3:N:73:ASP:HB2	3:N:123:THR:HB	1.81	0.61
4:K:10:THR:HG21	4:K:104:LEU:HD13	1.83	0.60
1:A:211:TYR:HH	3:C:137:TYR:HH	1.49	0.60
4:K:103:LYS:HD3	4:K:106:LYS:HE3	1.84	0.59
3:C:235:ARG:HG3	3:C:249:PHE:HB3	1.84	0.59
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.84	0.59
1:E:419:LYS:HG2	1:E:421:ARG:HG3	1.85	0.59
3:N:368:ILE:HD13	2:J:19:LEU:HD23	1.84	0.58
4:D:62:HIS:HB3	4:D:65:GLU:HB2	1.85	0.58
1:I:269:ASP:O	1:I:294:LYS:NZ	2.30	0.58
3:N:191:ILE:HG22	3:N:264:LEU:HD13	1.84	0.58
3:C:366:LEU:HD12	4:D:76:LEU:HG	1.86	0.57
1:E:312:GLN:NE2	3:G:124:PRO:O	2.36	0.57
3:G:65:HIS:C	3:G:65:HIS:ND1	2.58	0.57
3:N:199:ALA:HB1	3:N:220:LEU:HD11	1.86	0.57
2:F:19:LEU:HD23	3:G:368:ILE:HD13	1.85	0.56
3:N:366:LEU:HD13	4:K:76:LEU:HB3	1.87	0.56
1:I:407:GLU:HG2	3:C:63:LYS:CG	2.35	0.56
4:H:111:LEU:HB3	4:H:117:LEU:HB2	1.88	0.56
3:G:161:ASN:N	3:G:161:ASN:OD1	2.38	0.56
3:N:365:GLU:OE2	2:J:22:ARG:NH1	2.38	0.56
1:I:371:ASP:HB2	3:C:72:ASN:HB2	1.86	0.56
1:A:179:PRO:HB3	1:A:257:LEU:HD22	1.86	0.55
2:J:100:ALA:N	4:K:32:ASP:OD2	2.34	0.55
1:I:228:ILE:HB	1:I:431:TRP:HB2	1.88	0.55
1:A:168:ASN:ND2	1:A:192:GLU:O	2.40	0.55
4:D:32:ASP:OD2	2:B:100:ALA:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:ILE:HG22	3:C:264:LEU:HD13	1.90	0.54
1:E:165:ARG:O	1:E:190:THR:OG1	2.26	0.54
1:I:211:TYR:HH	3:N:137:TYR:HH	1.52	0.54
3:N:392:ILE:HD13	4:K:54:ARG:HG3	1.88	0.54
3:N:347:LEU:HD11	2:J:39:LYS:HB3	1.90	0.54
3:G:70:LEU:HD23	3:G:73:ASP:HA	1.89	0.54
3:G:321:ARG:NH1	1:I:155:THR:HG21	2.22	0.54
3:N:344:ALA:CB	2:J:69:ILE:HD11	2.37	0.54
3:C:251:THR:HB	4:D:92:THR:HG22	1.90	0.53
3:N:390:ASP:HB3	2:J:15:LEU:HD22	1.90	0.53
3:G:119:ASP:HA	1:A:389:LYS:HD2	1.90	0.53
1:I:179:PRO:HB3	1:I:257:LEU:HD22	1.90	0.53
3:C:344:ALA:CB	2:B:69:ILE:HD11	2.39	0.53
1:A:388:ALA:HB1	1:A:394:LEU:HD13	1.90	0.53
1:I:338:GLN:NE2	5:M:2:GLY:O	2.35	0.52
3:N:177:ASN:HD21	3:N:184:LEU:H	1.58	0.52
3:N:372:ARG:HG3	2:J:15:LEU:HD11	1.90	0.52
1:I:167:LEU:HB2	1:I:179:PRO:HG2	1.92	0.52
2:F:65:TYR:HE2	3:G:340:GLU:HG3	1.76	0.51
3:N:304:GLU:O	3:N:313:ARG:NH1	2.44	0.51
1:A:278:ARG:HD2	1:A:316:TYR:OH	2.10	0.51
1:I:168:ASN:ND2	1:I:192:GLU:O	2.43	0.51
3:G:199:ALA:HB1	3:G:220:LEU:HD11	1.91	0.51
1:E:405:LEU:HB2	3:N:64:GLN:O	2.11	0.51
1:I:174:LYS:HB3	3:N:133:TYR:CG	2.46	0.51
2:F:100:ALA:N	4:H:32:ASP:OD2	2.39	0.50
3:N:247:THR:OG1	3:N:248:HIS:N	2.44	0.50
3:N:375:ILE:HD12	2:J:15:LEU:HD13	1.94	0.50
4:K:111:LEU:HB3	4:K:117:LEU:HB2	1.94	0.50
1:A:229:TYR:HB3	1:A:236:PHE:HB2	1.93	0.50
3:C:73:ASP:HB2	3:C:123:THR:HB	1.95	0.49
3:C:199:ALA:HB1	3:C:220:LEU:HD11	1.93	0.49
1:A:188:GLU:HB2	3:C:293:PRO:HG3	1.95	0.49
3:N:296:LYS:HB3	3:N:309:TYR:O	2.13	0.49
1:A:247:TRP:HH2	1:A:275:CYS:HG	1.60	0.49
3:C:168:ASP:OD1	3:C:282:ARG:NH1	2.44	0.49
4:H:83:GLN:HA	4:H:86:LYS:HZ3	1.77	0.49
3:C:366:LEU:CD1	4:D:76:LEU:HG	2.41	0.49
1:A:275:CYS:HB3	1:A:286:LEU:HD13	1.95	0.49
1:E:303:ALA:HA	1:E:338:GLN:HG3	1.95	0.48
1:E:157:ASN:HB3	1:E:160:GLU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HB	1:A:431:TRP:HB2	1.95	0.48
1:I:262:ALY:HH31	1:I:262:ALY:HE2	1.57	0.48
3:C:368:ILE:HD13	2:B:19:LEU:HD23	1.94	0.48
3:C:344:ALA:HB1	2:B:69:ILE:HD11	1.96	0.48
1:A:364:HIS:O	1:A:366:LYS:N	2.45	0.48
3:G:64:GLN:O	1:A:405:LEU:HB2	2.13	0.48
3:G:76:HIS:CE1	3:G:120:TYR:HA	2.48	0.48
3:N:70:LEU:HD23	3:N:73:ASP:HA	1.96	0.48
3:N:374:LYS:HE2	2:J:11:LEU:HD11	1.95	0.48
1:E:304:CYS:SG	5:L:4:LYS:HD3	2.54	0.47
1:A:167:LEU:HB2	1:A:179:PRO:HG2	1.96	0.47
1:A:370:ILE:HD12	1:A:370:ILE:H	1.79	0.47
3:C:70:LEU:HD23	3:C:73:ASP:HA	1.96	0.47
5:M:4:LYS:O	5:M:5:ASP:HB2	2.15	0.47
4:D:14:VAL:HG22	4:D:100:HIS:CD2	2.44	0.47
1:A:269:ASP:O	1:A:294:LYS:NZ	2.46	0.47
3:C:379:LYS:HE3	3:C:386:GLY:H	1.80	0.47
1:E:265:TYR:HA	3:G:313:ARG:HH21	1.79	0.47
1:A:363:GLU:OE2	1:A:417:LYS:NZ	2.47	0.46
3:G:187:ASP:O	3:G:191:ILE:HG12	2.15	0.46
3:G:255:PRO:HG2	3:G:258:GLN:HG2	1.97	0.46
1:E:228:ILE:HB	1:E:431:TRP:HB2	1.97	0.46
1:E:263:THR:HG21	5:L:5:ASP:HB2	1.96	0.46
3:N:197:GLU:OE2	3:N:283:LYS:NZ	2.41	0.46
3:N:380:ARG:HG2	4:K:59:ILE:HA	1.97	0.46
4:H:112:GLU:HG3	4:H:117:LEU:HD23	1.97	0.46
1:E:187:ILE:O	1:E:190:THR:HG22	2.16	0.46
1:I:364:HIS:O	1:I:366:LYS:N	2.47	0.46
4:K:112:GLU:HG3	4:K:117:LEU:HD23	1.97	0.46
3:N:187:ASP:O	3:N:191:ILE:HG12	2.15	0.46
1:A:244:GLN:OE1	3:C:153:THR:HA	2.16	0.46
1:E:198:ASP:OD1	1:E:215:ARG:NE	2.49	0.45
1:I:247:TRP:HH2	1:I:275:CYS:HG	1.63	0.45
2:F:100:ALA:HB2	4:H:33:LEU:HD22	1.97	0.45
1:I:403:ILE:O	3:C:65:HIS:HB2	2.17	0.45
1:E:364:HIS:O	1:E:366:LYS:N	2.43	0.45
3:G:241:GLU:O	3:G:353:LYS:NZ	2.34	0.45
4:H:56:GLN:HB3	4:H:60:PRO:HG2	1.98	0.45
3:G:308:PRO:HB3	1:A:297:ALA:HB2	1.98	0.45
3:N:71:PRO:O	3:N:125:ASP:HB3	2.17	0.45
1:A:369:THR:HG22	1:A:371:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ALY:HH31	1:A:262:ALY:HE2	1.74	0.44
4:H:114:ASP:HB2	4:H:116:VAL:HG22	2.00	0.44
1:A:189:LEU:HD13	1:A:195:ILE:HD13	2.00	0.44
3:G:252:GLN:HG3	4:H:92:THR:HG21	1.99	0.44
3:N:182:ASP:OD2	3:N:262:ARG:NH1	2.45	0.44
1:E:369:THR:HB	3:N:71:PRO:HD2	1.98	0.44
3:C:368:ILE:HG23	2:B:15:LEU:HD11	1.98	0.44
1:I:241:GLY:HA2	1:I:248:CYS:SG	2.58	0.44
4:K:25:LEU:HD23	4:K:28:ILE:HD12	2.00	0.44
1:E:278:ARG:HD2	1:E:316:TYR:OH	2.18	0.43
2:F:27:ASP:O	2:F:31:ASN:ND2	2.51	0.43
1:A:164:VAL:HG23	1:I:295:GLU:HB3	1.98	0.43
4:D:112:GLU:HG3	4:D:117:LEU:HD23	1.99	0.43
1:I:169:ARG:NH1	1:I:178:GLU:HB2	2.33	0.43
2:J:70:ILE:HG21	2:J:92:ASP:HB3	2.00	0.43
4:D:10:THR:O	4:D:14:VAL:HG23	2.18	0.43
1:E:277:THR:HG22	1:E:286:LEU:HA	1.99	0.43
1:I:189:LEU:O	1:I:195:ILE:HD11	2.18	0.43
3:N:354:ARG:NH2	2:J:98:SER:OG	2.32	0.43
4:H:114:ASP:HB2	4:H:116:VAL:CG2	2.49	0.43
3:N:307:ASP:HB3	3:N:310:VAL:HG23	2.01	0.43
2:B:45:SER:HB3	2:B:88:PHE:CD2	2.53	0.43
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.92	0.43
2:F:69:ILE:HG21	4:H:21:PHE:CD1	2.53	0.43
3:G:251:THR:HB	4:H:92:THR:HG22	2.01	0.43
1:I:308:LEU:HB2	1:I:311:TYR:HD1	1.83	0.43
3:C:66:LEU:HD12	3:C:67:LYS:H	1.84	0.43
1:A:360:LEU:HD23	1:A:373:ILE:HG23	2.01	0.43
1:A:295:GLU:HG3	1:A:441:LEU:HD11	2.00	0.43
2:J:69:ILE:O	4:K:18:PRO:HB3	2.19	0.43
3:C:255:PRO:HG2	3:C:258:GLN:HG2	2.00	0.42
3:G:307:ASP:HB3	3:G:310:VAL:HG23	2.00	0.42
1:E:262:ALY:HH31	1:E:262:ALY:HE2	1.60	0.42
1:I:163:ARG:O	3:N:309:TYR:OH	2.18	0.42
3:N:234:LEU:HD13	4:K:102:ASN:ND2	2.35	0.42
1:E:167:LEU:HB2	1:E:179:PRO:HG3	2.01	0.42
4:H:2:ASP:HB3	4:H:5:LEU:HG	2.01	0.42
1:I:433:PRO:HA	1:I:434:PRO:HD3	1.90	0.42
1:I:339:LYS:O	1:I:341:LEU:N	2.52	0.41
1:A:169:ARG:NH1	1:A:178:GLU:HB2	2.34	0.41
1:I:410:LEU:HD22	3:C:63:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:PRO:HB3	3:C:306:ILE:HG12	2.02	0.41
2:B:8:TYR:CZ	2:B:12:LYS:HD3	2.56	0.41
1:I:230:ARG:HD2	3:N:143:GLU:OE2	2.21	0.41
1:E:275:CYS:HB3	1:E:286:LEU:HD13	2.02	0.41
2:F:8:TYR:CZ	2:F:12:LYS:HD3	2.56	0.41
4:H:117:LEU:HA	4:H:117:LEU:HD12	1.94	0.41
3:G:321:ARG:HH12	1:I:155:THR:HG21	1.84	0.41
4:K:103:LYS:HE3	4:K:103:LYS:HB2	1.96	0.41
1:I:344:LEU:HD12	1:I:344:LEU:H	1.85	0.41
1:A:187:ILE:O	1:A:190:THR:HG22	2.20	0.41
1:A:167:LEU:HD13	1:A:195:ILE:HD12	2.03	0.41
1:E:297:ALA:HB2	3:N:308:PRO:HB3	2.03	0.41
1:A:392:ASN:OD1	1:A:395:ARG:HD3	2.20	0.41
1:A:343:ASP:HB3	3:C:121:ILE:HG12	2.03	0.41
3:G:235:ARG:HG3	3:G:249:PHE:HB3	2.03	0.41
1:I:419:LYS:HE2	1:I:421:ARG:HH11	1.86	0.40
3:G:66:LEU:HD12	3:G:67:LYS:N	2.35	0.40
3:N:329:LEU:O	3:N:333:ARG:HG2	2.22	0.40
3:C:262:ARG:HH22	3:C:271:PHE:HE2	1.69	0.40
1:E:242:ARG:NH2	4:H:8:GLU:OE2	2.46	0.40
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.56	0.40
2:J:3:ASP:OD1	2:J:3:ASP:N	2.54	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	289/305 (95%)	273 (94%)	16 (6%)	0	100	100
1	E	290/305 (95%)	275 (95%)	15 (5%)	0	100	100
1	I	289/305 (95%)	274 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	73/113 (65%)	70 (96%)	3 (4%)	0	100	100
2	F	69/113 (61%)	67 (97%)	2 (3%)	0	100	100
2	J	70/113 (62%)	66 (94%)	4 (6%)	0	100	100
3	C	287/351 (82%)	273 (95%)	14 (5%)	0	100	100
3	G	289/351 (82%)	278 (96%)	11 (4%)	0	100	100
3	N	283/351 (81%)	275 (97%)	8 (3%)	0	100	100
4	D	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
4	H	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
4	K	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
5	L	3/10 (30%)	3 (100%)	0	0	100	100
5	M	2/10 (20%)	2 (100%)	0	0	100	100
5	O	1/10 (10%)	0	1 (100%)	0	100	100
All	All	2299/2697 (85%)	2206 (96%)	93 (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	270/283 (95%)	270 (100%)	0	100	100
1	E	272/283 (96%)	270 (99%)	2 (1%)	84	90
1	I	270/283 (95%)	269 (100%)	1 (0%)	91	94
2	B	73/100 (73%)	71 (97%)	2 (3%)	44	70
2	F	69/100 (69%)	69 (100%)	0	100	100
2	J	69/100 (69%)	68 (99%)	1 (1%)	67	81
3	C	279/333 (84%)	277 (99%)	2 (1%)	84	90
3	G	280/333 (84%)	275 (98%)	5 (2%)	59	77
3	N	274/333 (82%)	272 (99%)	2 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	111/111 (100%)	111 (100%)	0	100	100
4	H	111/111 (100%)	109 (98%)	2 (2%)	59	77
4	K	111/111 (100%)	110 (99%)	1 (1%)	78	87
5	L	3/7 (43%)	2 (67%)	1 (33%)	0	0
5	M	2/7 (29%)	1 (50%)	1 (50%)	0	0
5	O	1/7 (14%)	1 (100%)	0	100	100
All	All	2195/2502 (88%)	2175 (99%)	20 (1%)	78	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	215	ARG
1	E	369	THR
3	G	62	VAL
3	G	65	HIS
3	G	161	ASN
3	G	183	ILE
3	G	314	ARG
1	I	369	THR
3	N	183	ILE
3	N	250	ILE
3	C	65	HIS
3	C	314	ARG
2	B	27	ASP
2	B	106	GLN
2	J	27	ASP
4	H	42	TYR
4	H	116	VAL
4	K	42	TYR
5	L	5	ASP
5	M	5	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	I	338	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	10,11,12	0.79	0	7,12,14	1.17	1 (14%)
1	ALY	E	262	1	10,11,12	1.00	1 (10%)	7,12,14	1.02	0
1	ALY	I	262	1	10,11,12	0.83	0	7,12,14	0.89	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	A	262	1	-	3/9/10/12	-
1	ALY	E	262	1	-	4/9/10/12	-
1	ALY	I	262	1	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	262	ALY	CH-NZ	2.04	1.40	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ALY	CE-NZ-CH	2.40	126.24	122.56

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	262	ALY	O-C-CA-CB
1	I	262	ALY	CG-CD-CE-NZ
1	A	262	ALY	OH-CH-NZ-CE
1	A	262	ALY	CH3-CH-NZ-CE
1	E	262	ALY	OH-CH-NZ-CE
1	E	262	ALY	CH3-CH-NZ-CE
1	I	262	ALY	OH-CH-NZ-CE
1	I	262	ALY	CH3-CH-NZ-CE
1	A	262	ALY	CG-CD-CE-NZ
1	E	262	ALY	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	262	ALY	1	0
1	E	262	ALY	1	0
1	I	262	ALY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.