



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2016 – 12:34 PM EDT

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

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 : 1.7.1 (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

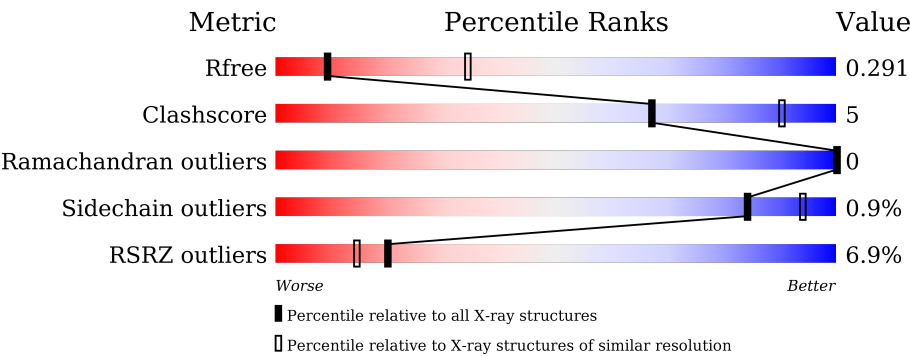
1 Overall quality at a glance i

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}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	305	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%81%15%. .</div>
1	E	305	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%84%11%. . .</div>
1	I	305	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%80%15%. . .</div>
2	B	113	<div><div></div><div></div><div></div><div></div><div></div></div> <div>12%61%9%30%</div>
2	F	113	<div><div></div><div></div><div></div><div></div><div></div></div> <div>15%59%7%34%</div>
2	J	113	<div><div></div><div></div><div></div><div></div><div></div></div> <div>8%55%12%33%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	351	
3	G	351	
3	N	351	
4	D	120	
4	H	120	
4	K	120	
5	L	10	
5	M	10	
5	O	10	

2 Entry composition

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
1	E	293	Total	C	N	O	S	0	0	0
			2479	1601	420	447	11			
1	A	292	Total	C	N	O	S	0	0	0
			2470	1596	419	445	10			
1	I	292	Total	C	N	O	S	0	0	0
			2470	1596	419	445	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	75	Total	C	N	O	S	0	0	0
			622	389	99	133	1			
2	B	79	Total	C	N	O	S	0	0	0
			660	413	108	138	1			
2	J	76	Total	C	N	O	S	0	0	0
			627	392	100	134	1			

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

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

Continued on next page...

Continued from previous page...

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			

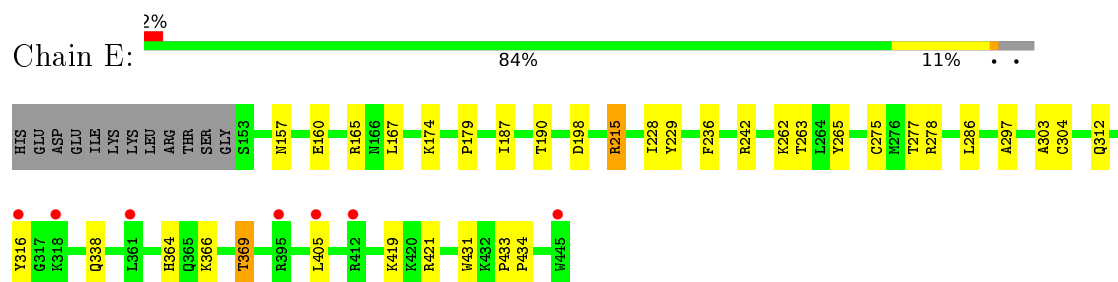
- Molecule 5 is a protein called Htz1.

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			

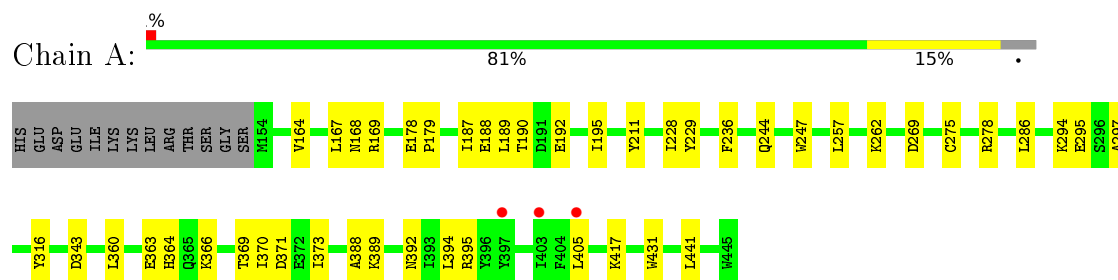
3 Residue-property plots [i](#)

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

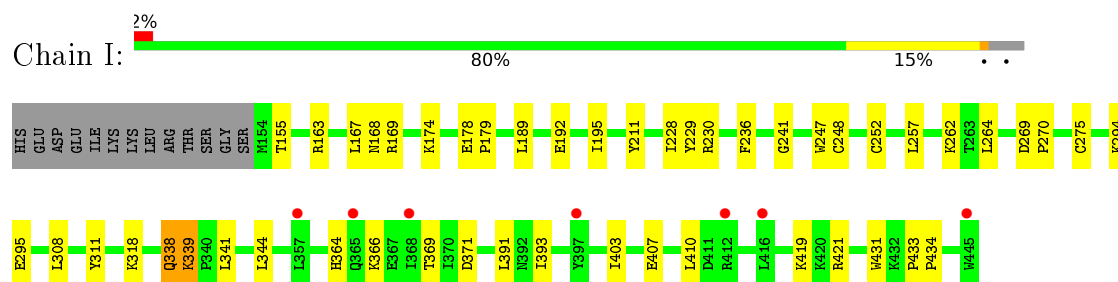
- Molecule 1: Histone acetyltransferase ESA1



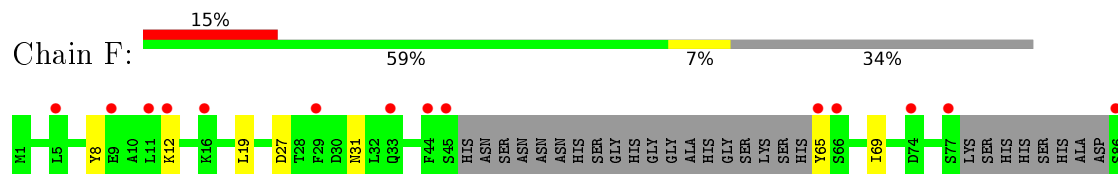
- Molecule 1: Histone acetyltransferase ESA1

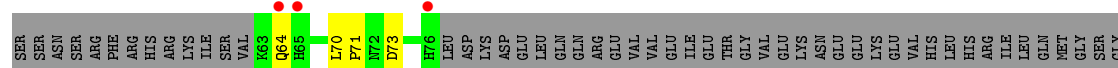


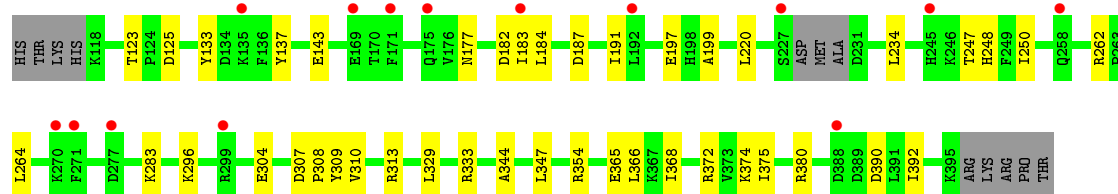
- Molecule 1: Histone acetyltransferase ESA1



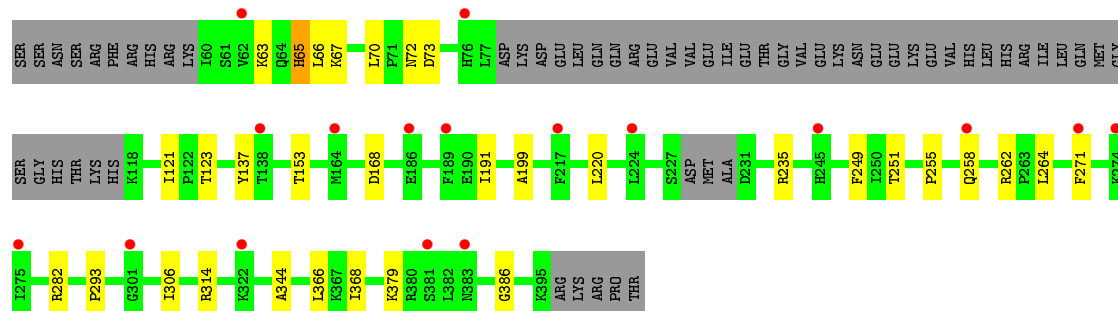
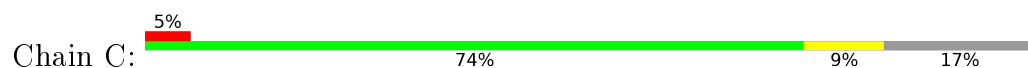
- Molecule 2: Chromatin modification-related protein EAF6







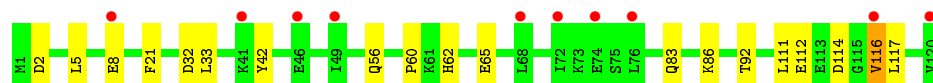
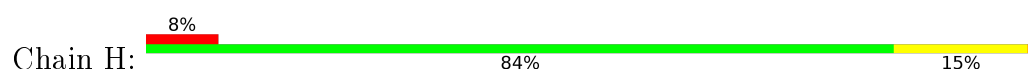
- Molecule 3: Enhancer of polycomb-like protein 1



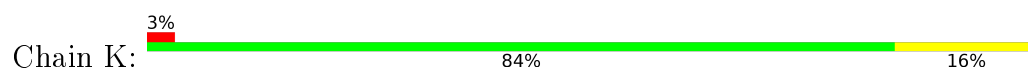
- Molecule 4: Chromatin modification-related protein YNG2



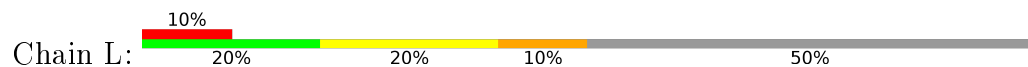
- Molecule 4: Chromatin modification-related protein YNG2



- Molecule 4: Chromatin modification-related protein YNG2



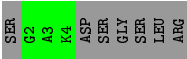
- Molecule 5: Htz1



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.250 , 0.273 0.262 , 0.291	Depositor DCC
R_{free} test set	1999 reflections (2.50%)	DCC
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	19671	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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 ⓘ

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
1:E:405:LEU:HB2	3:N:64:GLN:O	2.11	0.51
3:G:199:ALA:HB1	3:G:220:LEU:HD11	1.91	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

Continued on next page...

Continued from previous page...

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:263:THR:HG21	5:L:5:ASP:HB2	1.96	0.46
1:E:228:ILE:HB	1:E:431:TRP:HB2	1.97	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
1:I:403:ILE:O	3:C:65:HIS:HB2	2.17	0.45
2:F:100:ALA:HB2	4:H:33:LEU:HD22	1.97	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

Continued on next page...

Continued from previous page...

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
1:E:369:THR:HB	3:N:71:PRO:HD2	1.98	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
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:A:164:VAL:HG23	1:I:295:GLU:HB3	1.98	0.43
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
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
3:G:251:THR:HB	4:H:92:THR:HG22	2.01	0.43
2:F:69:ILE:HG21	4:H:21:PHE:CD1	2.53	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	88	96
1	I	270/283 (95%)	269 (100%)	1 (0%)	93	97
2	B	73/100 (73%)	71 (97%)	2 (3%)	52	83
2	F	69/100 (69%)	69 (100%)	0	100	100
2	J	69/100 (69%)	68 (99%)	1 (1%)	74	90
3	C	279/333 (84%)	277 (99%)	2 (1%)	88	96
3	G	280/333 (84%)	275 (98%)	5 (2%)	66	88
3	N	274/333 (82%)	272 (99%)	2 (1%)	88	96

Continued on next page...

Continued from previous page...

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%)	66	88
4	K	111/111 (100%)	110 (99%)	1 (1%)	84	94
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%)	84	94

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 ⓘ

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	0.80	0	10,12,14	1.37	2 (20%)
1	ALY	E	262	1	9,11,12	1.04	1 (11%)	10,12,14	1.04	0
1	ALY	I	262	1	9,11,12	0.82	0	10,12,14	1.01	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	-	2/8/10/12	0/0/0/0
1	ALY	E	262	1	-	2/8/10/12	0/0/0/0
1	ALY	I	262	1	-	2/8/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	262	ALY	CH-NZ	2.39	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ALY	CE-NZ-CH	2.25	126.24	122.38
1	A	262	ALY	CB-CA-N	2.81	118.44	110.54

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	262	ALY	CH3-CH-NZ-CE
1	E	262	ALY	CH3-CH-NZ-CE
1	A	262	ALY	CH3-CH-NZ-CE
1	I	262	ALY	OH-CH-NZ-CE
1	A	262	ALY	OH-CH-NZ-CE
1	E	262	ALY	OH-CH-NZ-CE

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

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	291/305 (95%)	0.18	3 (1%) 84 78	7, 38, 100, 144	0
1	E	292/305 (95%)	0.37	7 (2%) 62 52	18, 57, 108, 129	0
1	I	291/305 (95%)	0.28	7 (2%) 62 52	11, 42, 81, 111	0
2	B	79/113 (69%)	0.77	13 (16%) 2 2	20, 60, 111, 133	0
2	F	75/113 (66%)	1.23	17 (22%) 1 1	47, 81, 129, 135	0
2	J	76/113 (67%)	0.71	9 (11%) 6 4	24, 53, 102, 119	0
3	C	293/351 (83%)	0.48	17 (5%) 26 19	20, 56, 106, 142	0
3	G	295/351 (84%)	0.90	53 (17%) 2 1	17, 75, 135, 159	0
3	N	289/351 (82%)	0.44	17 (5%) 26 18	17, 50, 96, 130	0
4	D	120/120 (100%)	0.16	4 (3%) 50 40	20, 40, 69, 89	0
4	H	120/120 (100%)	0.79	10 (8%) 14 9	33, 69, 129, 140	0
4	K	120/120 (100%)	0.27	4 (3%) 50 40	19, 35, 59, 65	0
5	L	5/10 (50%)	0.96	1 (20%) 1 1	63, 65, 88, 95	0
5	M	4/10 (40%)	0.63	0 100 100	50, 58, 59, 70	0
5	O	3/10 (30%)	0.41	0 100 100	48, 48, 48, 50	0
All	All	2353/2697 (87%)	0.48	162 (6%) 20 14	7, 52, 113, 159	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	385	SER	5.7
2	F	87	ALA	5.5
1	I	445	TRP	5.0
3	G	397	LYS	4.9
3	G	245	HIS	4.8
3	G	399	PRO	4.6
2	B	104	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	383	ASN	4.3
4	H	120	VAL	4.3
2	J	46	HIS	4.2
3	G	168	ASP	4.1
3	G	388	ASP	4.1
2	F	65	TYR	4.1
3	G	71	PRO	4.1
3	G	183	ILE	4.0
3	G	384	ILE	3.9
1	E	445	TRP	3.9
4	H	116	VAL	3.9
4	K	59	ILE	3.9
3	G	370	ASP	3.8
3	G	64	GLN	3.8
3	C	383	ASN	3.8
3	G	184	LEU	3.7
2	F	44	PHE	3.7
3	G	398	ARG	3.6
2	B	100	ALA	3.6
3	C	322	LYS	3.6
3	C	245	HIS	3.6
2	B	105	GLN	3.6
3	G	379	LYS	3.5
2	B	4	GLU	3.5
2	J	76	PHE	3.4
3	G	258	GLN	3.4
1	A	397	TYR	3.4
2	B	8	TYR	3.4
1	E	405	LEU	3.4
3	C	217	PHE	3.4
3	C	271	PHE	3.4
2	F	86	SER	3.3
3	G	395	LYS	3.3
2	B	76	PHE	3.2
2	J	86	SER	3.2
3	G	366	LEU	3.2
2	F	5	LEU	3.2
4	H	76	LEU	3.1
2	F	29	PHE	3.1
3	G	315	ARG	3.1
3	N	299	ARG	3.1
1	I	397	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	72	ILE	3.1
3	N	171	PHE	3.0
2	J	88	PHE	3.0
2	B	46	HIS	3.0
3	G	186	GLU	3.0
4	H	41	LYS	2.9
1	E	316	TYR	2.9
3	G	176	VAL	2.9
3	C	258	GLN	2.9
3	N	258	GLN	2.9
2	B	102	TYR	2.9
3	G	321	ARG	2.9
2	F	12	LYS	2.9
3	C	301	GLY	2.9
4	D	115	GLY	2.8
2	B	75	THR	2.8
3	G	189	PHE	2.8
3	C	189	PHE	2.8
2	J	65	TYR	2.8
2	B	86	SER	2.8
2	F	77	SER	2.8
1	A	403	ILE	2.7
2	F	9	GLU	2.7
2	B	1	MET	2.7
3	G	120	TYR	2.7
2	J	39	LYS	2.7
3	G	181	SER	2.7
3	C	62	VAL	2.7
4	D	58	SER	2.7
3	C	138	THR	2.7
3	C	76	HIS	2.7
1	E	318	LYS	2.7
3	G	389	ASP	2.7
3	N	64	GLN	2.6
3	N	175	GLN	2.6
2	F	74	ASP	2.6
3	G	164	MET	2.6
4	K	48	GLN	2.5
1	I	365	GLN	2.5
3	N	245	HIS	2.5
4	H	68	LEU	2.5
3	G	396	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	87	ALA	2.5
2	F	88	PHE	2.5
3	N	388	ASP	2.5
3	G	197	GLU	2.4
3	G	386	GLY	2.4
2	F	33	GLN	2.4
4	D	1	MET	2.4
3	G	320	PRO	2.4
3	G	180	SER	2.4
3	G	375	ILE	2.3
4	K	115	GLY	2.3
3	G	269	GLU	2.3
3	G	264	LEU	2.3
1	A	405	LEU	2.3
2	F	90	ASN	2.3
1	I	416	LEU	2.3
2	F	45	SER	2.3
3	G	357	VAL	2.3
3	G	394	HIS	2.3
3	N	271	PHE	2.3
3	N	270	LYS	2.2
4	H	46	GLU	2.2
2	J	45	SER	2.2
3	N	169	GLU	2.2
4	H	8	GLU	2.2
3	G	227	SER	2.2
3	N	76	HIS	2.2
3	G	182	ASP	2.2
3	G	279	TRP	2.2
3	N	65	HIS	2.2
2	F	11	LEU	2.2
3	G	207	LEU	2.2
3	C	186	GLU	2.2
3	G	391	LEU	2.2
3	G	185	THR	2.2
3	G	212	GLU	2.2
3	G	368	ILE	2.2
3	G	270	LYS	2.2
3	C	274	LYS	2.2
2	F	16	LYS	2.1
3	G	126	ALA	2.1
1	E	395	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	49	ILE	2.1
3	N	135	LYS	2.1
1	I	368	ILE	2.1
1	I	412	ARG	2.1
3	N	183	ILE	2.1
1	I	357	LEU	2.1
3	G	274	LYS	2.1
3	G	162	TYR	2.1
2	B	70	ILE	2.1
3	G	178	LYS	2.1
3	C	164	MET	2.1
3	G	248	HIS	2.1
2	B	66	SER	2.1
5	L	1	SER	2.1
1	E	361	LEU	2.1
3	C	224	LEU	2.1
4	D	120	VAL	2.1
4	K	69	ASP	2.1
4	H	74	GLU	2.0
1	E	412	ARG	2.0
3	N	227	SER	2.0
3	N	277	ASP	2.0
3	N	192	LEU	2.0
3	C	275	ILE	2.0
2	F	66	SER	2.0
3	G	220	LEU	2.0
3	C	381	SER	2.0
2	J	41	THR	2.0
3	G	259	MET	2.0

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

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	262	12/13	0.93	0.25	-	5,16,45,52	0
1	ALY	E	262	12/13	0.93	0.22	-	14,29,43,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	ALY	I	262	12/13	0.93	0.28	-	22,28,41,44	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.