Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:21 PM EDT

PDB ID	:	5J9T
Title	:	Crystal structure of the NuA4 core complex
Authors	:	Chen, Z.C.; Xu, P.
Deposited on	:	2016-04-11
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

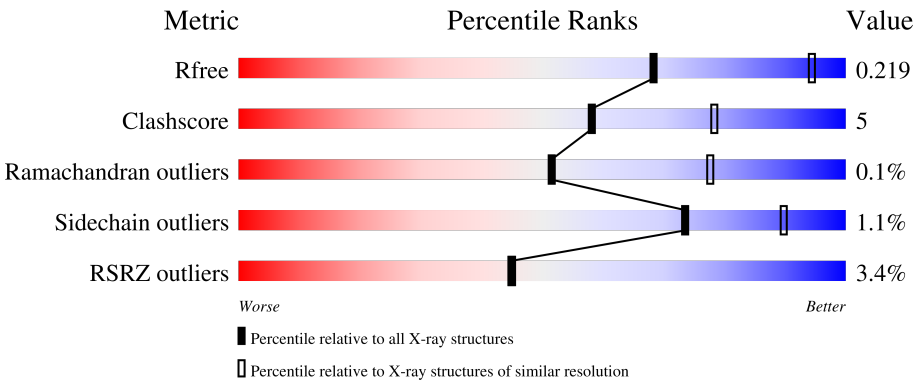
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	2%, 81%, 10%, 9%
1	E	305	3%, 82%, 9%, •, 9%
1	I	305	%, 81%, 10%, •, 9%
2	B	113	5%, 58%, 10%, 32%
2	F	113	4%, 51%, 9%, 40%

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Mol	Chain	Length	Quality of chain
2	J	113	7% 55% 12% 34%
3	C	280	2% 81% 13%
3	G	280	5% 81% 16%
3	K	280	3% 84% 11%
4	D	120	2% 89% 10%
4	H	120	4% 90% 9%
4	L	120	4% 91% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18881 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	278	2355	1523	396	426	10	0	0	0
1	A	278	2355	1523	396	426	10	0	0	0
1	I	277	2346	1518	395	423	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				
2	F	68	570	355	96	119		0	0	0
2	B	77	Total	C	N	O	S	0	0	0
			637	395	107	134	1			
2	J	75	Total	C	N	O	S	0	0	0
			625	391	102	131	1			

- 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	273	2294	1442	406	437	9	0	0	0
3	C	268	Total	C	N	O	S	0	0	0
			2252	1418	400	425	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	K	269	2261	1422	398	432	9	0	0	0

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

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

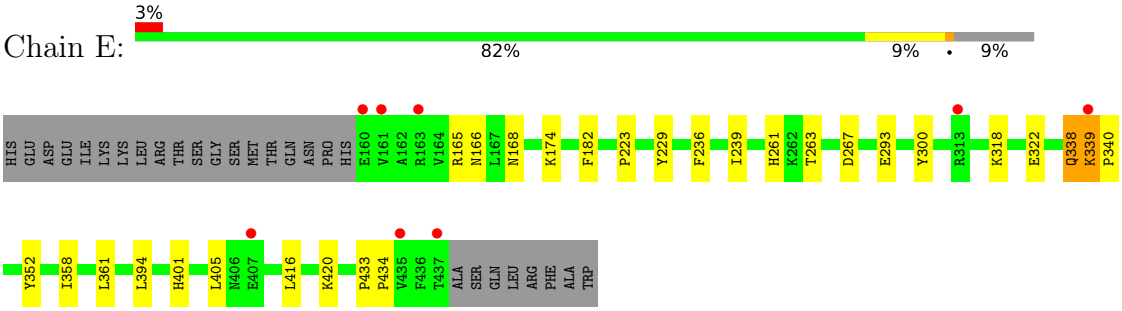
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	29	29	29	0	0
5	F	2	2	2	0	0
5	G	27	27	27	0	0
5	H	14	14	14	0	0
5	A	42	42	42	0	0
5	B	9	9	9	0	0
5	C	40	40	40	0	0
5	D	13	13	13	0	0
5	I	69	69	69	0	0
5	J	5	5	5	0	0
5	K	40	40	40	0	0
5	L	10	10	10	0	0

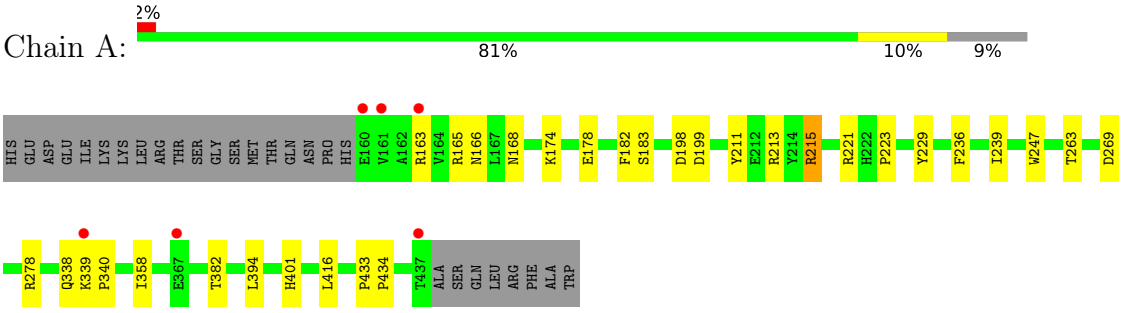
3 Residue-property plots (i)

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

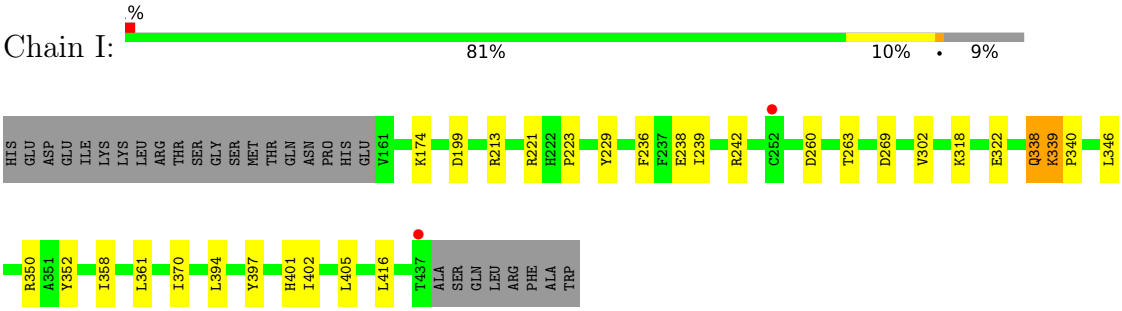
• Molecule 1: Histone acetyltransferase ESA1



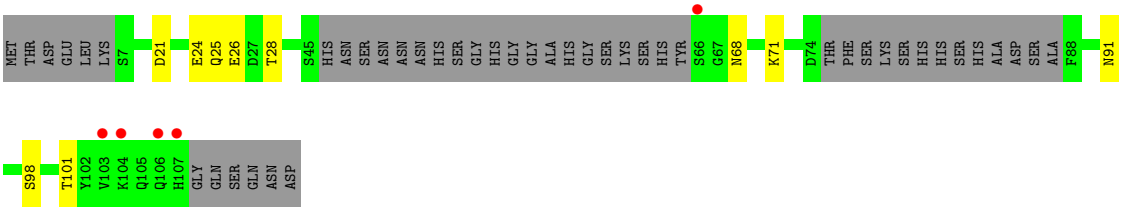
• Molecule 1: Histone acetyltransferase ESA1



• Molecule 1: Histone acetyltransferase ESA1

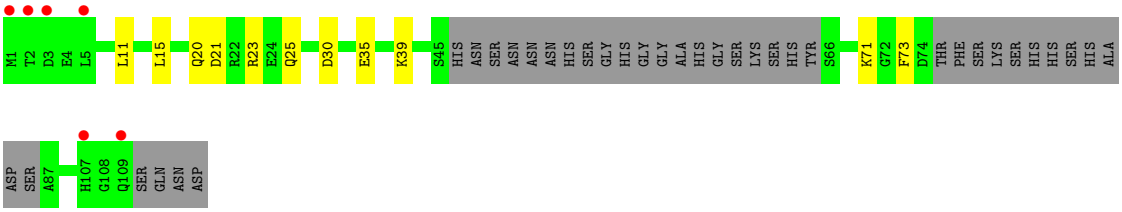


• Molecule 2: Chromatin modification-related protein EAF6



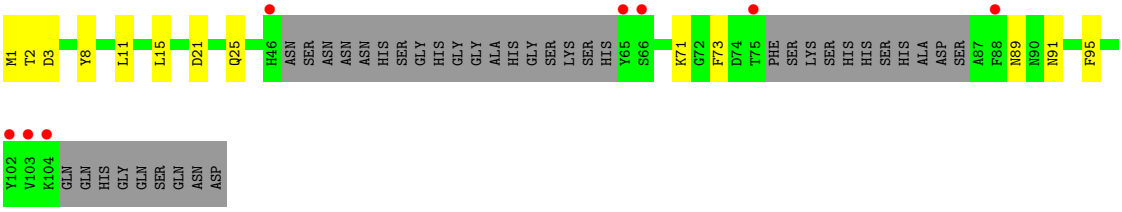
• Molecule 2: Chromatin modification-related protein EAF6

Chain B:



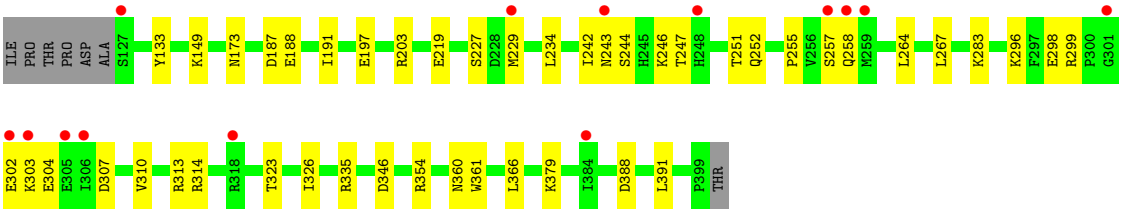
• Molecule 2: Chromatin modification-related protein EAF6

Chain J:



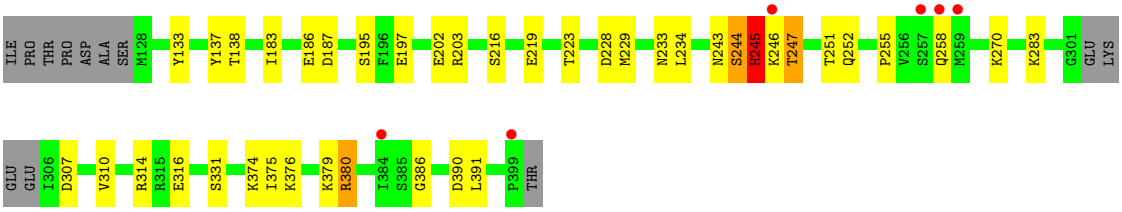
• Molecule 3: Enhancer of polycomb-like protein 1

Chain G:



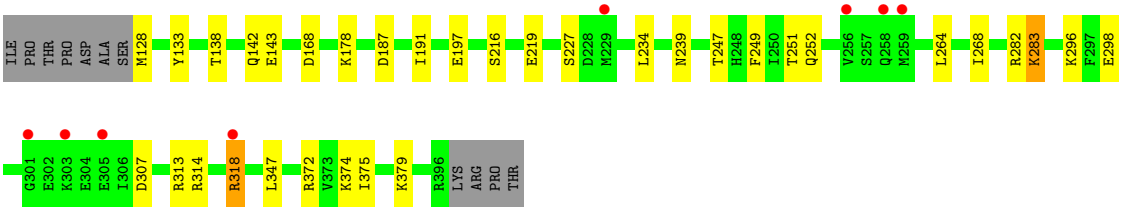
• Molecule 3: Enhancer of polycomb-like protein 1

Chain C:



• Molecule 3: Enhancer of polycomb-like protein 1

Chain K:

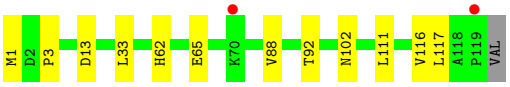


• Molecule 4: Chromatin modification-related protein YNG2

Chain H:

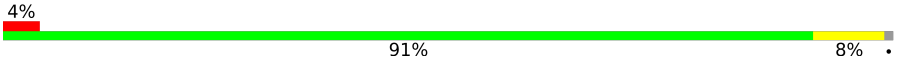
• Molecule 4: Chromatin modification-related protein YNG2

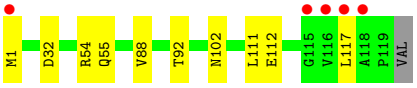
Chain D:



• Molecule 4: Chromatin modification-related protein YNG2

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.69Å 137.58Å 168.08Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	29.97 – 2.70 29.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.97-2.70) 91.4 (29.97-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.219 0.187 , 0.219	Depositor DCC
R_{free} test set	2000 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18881	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.28	0/2403	0.47	0/3246
1	E	0.28	0/2403	0.48	0/3246
1	I	0.29	0/2394	0.51	0/3234
2	B	0.28	0/644	0.46	0/858
2	F	0.38	0/577	0.51	0/769
2	J	0.27	0/633	0.39	0/845
3	C	0.27	0/2298	0.45	0/3092
3	G	0.29	0/2341	0.48	0/3150
3	K	0.29	0/2307	0.44	0/3105
4	D	0.27	0/974	0.39	0/1307
4	H	0.26	0/974	0.39	0/1307
4	L	0.27	0/974	0.42	0/1307
All	All	0.28	0/18922	0.46	0/25466

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	E	0	1
1	I	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	E	338	GLN	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	2355	0	2343	26	0
1	E	2355	0	2343	21	0
1	I	2346	0	2337	24	0
2	B	637	0	600	10	0
2	F	570	0	531	5	0
2	J	625	0	589	9	0
3	C	2252	0	2209	35	0
3	G	2294	0	2246	34	0
3	K	2261	0	2208	28	0
4	D	962	0	994	10	0
4	H	962	0	994	11	0
4	L	962	0	994	10	0
5	A	42	0	0	5	0
5	B	9	0	0	2	0
5	C	40	0	0	5	0
5	D	13	0	0	1	0
5	E	29	0	0	2	0
5	F	2	0	0	0	0
5	G	27	0	0	3	0
5	H	14	0	0	0	0
5	I	69	0	0	4	0
5	J	5	0	0	1	0
5	K	40	0	0	4	0
5	L	10	0	0	2	0
All	All	18881	0	18388	179	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 (179) 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:261:HIS:ND1	5:E:501:HOH:O	1.81	1.12
1:E:293:GLU:OE2	5:E:502:HOH:O	1.91	0.89
2:J:73:PHE:N	5:J:201:HOH:O	2.11	0.81
1:E:339:LYS:HB3	1:E:340:PRO:CD	2.13	0.79
1:A:215:ARG:NH2	5:A:501:HOH:O	2.04	0.78
1:I:358:ILE:HD11	1:I:416:LEU:HD21	1.64	0.77
1:I:338:GLN:HG2	1:I:339:LYS:HB2	1.63	0.77
1:I:339:LYS:HB3	1:I:340:PRO:CD	2.15	0.77
1:E:339:LYS:HB3	1:E:340:PRO:HD3	1.69	0.75
3:K:178:LYS:O	5:K:501:HOH:O	2.04	0.75
1:E:338:GLN:HG2	1:E:339:LYS:HB2	1.68	0.75
1:I:238:GLU:O	5:I:501:HOH:O	2.06	0.73
3:G:299:ARG:HB2	3:G:302:GLU:HG2	1.70	0.73
1:I:242:ARG:NH2	5:I:504:HOH:O	2.22	0.73
1:A:165:ARG:NH2	1:A:168:ASN:O	2.21	0.70
1:A:198:ASP:OD2	1:A:215:ARG:NH1	2.23	0.70
1:I:260:ASP:OD1	5:I:502:HOH:O	2.09	0.69
1:E:358:ILE:HD11	1:E:416:LEU:HD13	1.75	0.68
1:A:269:ASP:OD1	3:C:314:ARG:NH1	2.27	0.68
3:C:197:GLU:OE2	3:C:283:LYS:NZ	2.27	0.67
2:B:11:LEU:HD21	3:C:374:LYS:HE2	1.77	0.67
4:D:13:ASP:OD2	5:D:201:HOH:O	2.12	0.66
3:G:296:LYS:NZ	3:G:307:ASP:OD1	2.24	0.66
1:A:382:THR:OG1	5:A:502:HOH:O	2.14	0.66
3:C:244:SER:O	3:C:246:LYS:N	2.28	0.66
3:C:247:THR:O	5:C:501:HOH:O	2.13	0.66
3:C:252:GLN:H	4:D:92:THR:HG22	1.60	0.66
3:C:379:LYS:NZ	3:C:386:GLY:O	2.29	0.65
1:E:361:LEU:HB3	1:E:405:LEU:HD21	1.78	0.64
1:I:361:LEU:HB3	1:I:405:LEU:HD21	1.80	0.64
3:G:379:LYS:NZ	4:H:58:SER:OG	2.30	0.64
1:I:221:ARG:NH2	3:K:138:THR:O	2.29	0.64
1:E:420:LYS:NZ	1:A:178:GLU:OE1	2.31	0.64
2:F:98:SER:HB2	3:G:354:ARG:HH22	1.62	0.63
4:L:88:VAL:O	4:L:92:THR:HG23	1.98	0.63
3:C:251:THR:HB	4:D:92:THR:HG22	1.81	0.63
1:I:318:LYS:HE2	1:I:322:GLU:OE2	1.99	0.63
4:D:1:MET:HB3	4:D:111:LEU:HD23	1.80	0.63
3:C:202:GLU:OE1	5:C:502:HOH:O	2.15	0.62
1:A:278:ARG:NH1	5:A:507:HOH:O	2.33	0.62
4:H:1:MET:HB3	4:H:111:LEU:HD23	1.82	0.62
3:G:197:GLU:OE2	3:G:283:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:252:GLN:H	4:H:92:THR:HG22	1.66	0.60
3:K:252:GLN:H	4:L:92:THR:HG22	1.65	0.60
1:I:339:LYS:HB3	1:I:340:PRO:HD3	1.84	0.60
3:G:251:THR:HB	4:H:92:THR:HG22	1.83	0.60
1:I:174:LYS:HB3	3:K:133:TYR:CG	2.37	0.60
3:C:252:GLN:H	4:D:92:THR:CG2	2.14	0.60
2:J:15:LEU:HD11	3:K:372:ARG:HG3	1.84	0.59
3:G:246:LYS:NZ	3:G:360:ASN:OD1	2.36	0.59
4:D:3:PRO:HD3	4:D:116:VAL:HG11	1.85	0.59
1:E:318:LYS:HE2	1:E:322:GLU:OE2	2.03	0.59
3:C:270:LYS:NZ	5:C:509:HOH:O	2.36	0.59
3:C:307:ASP:HB3	3:C:310:VAL:HG23	1.84	0.58
4:L:54:ARG:NH1	5:L:203:HOH:O	2.36	0.58
3:G:346:ASP:OD2	5:G:501:HOH:O	2.16	0.58
4:H:88:VAL:O	4:H:92:THR:HG23	2.04	0.58
1:A:174:LYS:HB3	3:C:133:TYR:CG	2.39	0.58
1:A:358:ILE:HD11	1:A:416:LEU:HD22	1.86	0.58
4:D:88:VAL:O	4:D:92:THR:HG23	2.05	0.57
1:A:163:ARG:NH2	5:A:509:HOH:O	2.36	0.57
1:A:211:TYR:HH	3:C:137:TYR:HH	1.51	0.56
1:E:223:PRO:HB3	1:E:239:ILE:HD11	1.88	0.55
1:I:213:ARG:NH2	3:K:187:ASP:OD2	2.33	0.55
1:E:165:ARG:NH2	1:E:168:ASN:O	2.24	0.55
2:B:15:LEU:HD22	3:C:390:ASP:HB3	1.88	0.55
3:C:195:SER:HA	3:C:229:MET:SD	2.47	0.55
1:I:223:PRO:HB3	1:I:239:ILE:HD11	1.89	0.55
2:B:73:PHE:N	5:B:201:HOH:O	2.39	0.54
3:C:331:SER:HB3	4:D:117:LEU:HD13	1.89	0.54
1:A:339:LYS:N	1:A:340:PRO:HD2	2.23	0.54
3:G:299:ARG:HB2	3:G:302:GLU:CG	2.36	0.54
1:A:229:TYR:HB3	1:A:236:PHE:HB2	1.89	0.54
1:E:394:LEU:HD11	1:E:401:HIS:HB3	1.89	0.54
3:G:244:SER:C	3:G:246:LYS:H	2.11	0.53
3:G:252:GLN:H	4:H:92:THR:CG2	2.21	0.53
3:G:149:LYS:HD2	4:H:19:SER:HB3	1.90	0.52
3:K:252:GLN:H	4:L:92:THR:CG2	2.22	0.52
1:I:394:LEU:HD11	1:I:401:HIS:HB3	1.91	0.52
1:A:213:ARG:NH2	3:C:187:ASP:OD1	2.37	0.52
1:I:199:ASP:OD2	5:I:503:HOH:O	2.18	0.52
2:J:1:MET:HG3	2:J:3:ASP:H	1.75	0.52
1:E:166:ASN:HB2	1:E:182:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:GLU:CD	5:C:502:HOH:O	2.48	0.51
3:G:303:LYS:O	3:G:304:GLU:HB3	2.10	0.51
3:C:203:ARG:HD2	3:C:223:THR:OG1	2.11	0.51
3:K:143:GLU:OE2	5:K:502:HOH:O	2.19	0.51
3:C:314:ARG:NH2	3:C:316:GLU:OE1	2.40	0.51
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.46	0.51
3:G:257:SER:OG	5:G:503:HOH:O	2.19	0.50
1:A:223:PRO:HB3	1:A:239:ILE:HD11	1.92	0.50
1:I:397:TYR:HB3	1:I:402:ILE:HD13	1.94	0.50
1:E:300:TYR:CD2	1:E:338:GLN:HG3	2.47	0.50
3:G:191:ILE:HG22	3:G:264:LEU:HD13	1.94	0.50
2:J:15:LEU:HD13	3:K:375:ILE:HD12	1.94	0.50
3:K:251:THR:HB	4:L:92:THR:HG22	1.93	0.50
1:A:199:ASP:OD2	5:A:503:HOH:O	2.19	0.49
1:I:269:ASP:OD2	3:K:314:ARG:NH2	2.45	0.49
3:K:142:GLN:HG3	5:K:522:HOH:O	2.10	0.49
3:G:173:ASN:OD1	5:G:502:HOH:O	2.19	0.49
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.95	0.49
3:K:128:MET:N	5:K:507:HOH:O	2.45	0.49
1:E:267:ASP:OD2	3:G:314:ARG:NH1	2.44	0.48
1:A:269:ASP:CG	3:C:314:ARG:HH11	2.16	0.48
3:C:376:LYS:O	3:C:380:ARG:HD3	2.13	0.48
3:K:239:ASN:HB2	3:K:249:PHE:HB2	1.95	0.48
1:A:394:LEU:HD11	1:A:401:HIS:HB3	1.95	0.47
1:I:229:TYR:HB3	1:I:236:PHE:HB2	1.96	0.47
3:K:191:ILE:HG22	3:K:264:LEU:HD23	1.96	0.47
3:K:197:GLU:OE2	3:K:283:LYS:NZ	2.47	0.47
3:G:203:ARG:NH1	3:G:219:GLU:O	2.48	0.47
3:G:323:THR:HG23	3:G:326:ILE:H	1.79	0.47
3:C:186:GLU:OE1	5:C:503:HOH:O	2.20	0.47
1:A:166:ASN:HB2	1:A:182:PHE:HA	1.96	0.47
3:K:168:ASP:OD1	3:K:282:ARG:NH1	2.48	0.46
1:A:166:ASN:ND2	1:A:183:SER:O	2.46	0.46
1:A:221:ARG:NH2	3:C:138:THR:O	2.47	0.46
1:A:338:GLN:HG2	1:A:340:PRO:HD2	1.98	0.46
4:L:32:ASP:OD2	5:L:201:HOH:O	2.20	0.46
2:B:30:ASP:OD2	5:B:202:HOH:O	2.21	0.46
2:B:71:LYS:HB2	2:B:71:LYS:NZ	2.31	0.45
3:G:298:GLU:CD	3:G:313:ARG:HG2	2.36	0.45
3:G:255:PRO:HG2	3:G:258:GLN:HG2	1.99	0.45
1:A:174:LYS:HB3	3:C:133:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:HIS:HB3	4:D:65:GLU:HB2	1.99	0.45
3:G:388:ASP:HA	3:G:391:LEU:HD23	1.98	0.45
4:L:112:GLU:HG3	4:L:117:LEU:HD23	1.98	0.45
1:A:339:LYS:N	1:A:340:PRO:CD	2.79	0.45
3:C:234:LEU:HD13	4:D:102:ASN:ND2	2.31	0.45
3:C:244:SER:C	3:C:246:LYS:H	2.20	0.45
1:I:338:GLN:HE21	1:I:339:LYS:HD2	1.81	0.44
2:B:11:LEU:HB3	3:C:375:ILE:HD11	1.99	0.44
2:F:24:GLU:O	2:F:28:THR:HG22	2.17	0.44
4:L:1:MET:HB3	4:L:111:LEU:HD23	1.99	0.44
3:G:188:GLU:HG2	3:G:267:LEU:HD11	1.99	0.44
1:E:338:GLN:HG2	1:E:339:LYS:CB	2.42	0.44
4:H:62:HIS:HB3	4:H:65:GLU:HB2	1.99	0.44
3:C:203:ARG:NH1	3:C:219:GLU:O	2.51	0.43
1:E:322:GLU:HG2	1:E:352:TYR:HE1	1.84	0.43
2:F:68:ASN:HB3	2:F:71:LYS:H	1.83	0.43
2:B:39:LYS:HA	2:B:39:LYS:HD2	1.91	0.43
1:I:338:GLN:HG2	1:I:339:LYS:CB	2.41	0.43
3:K:298:GLU:CD	3:K:313:ARG:HG2	2.38	0.43
2:J:21:ASP:O	2:J:25:GLN:HG2	2.19	0.43
1:A:433:PRO:HA	1:A:434:PRO:HD3	1.94	0.43
3:C:255:PRO:HG2	3:C:258:GLN:HG2	2.01	0.43
1:I:322:GLU:HG2	1:I:352:TYR:HE1	1.83	0.43
2:J:11:LEU:HD21	3:K:374:LYS:HE2	1.99	0.43
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.92	0.42
2:B:35:GLU:O	2:B:39:LYS:HG2	2.18	0.42
3:C:243:ASN:HA	3:C:245:HIS:CE1	2.54	0.42
2:B:20:GLN:OE1	2:B:23:ARG:NH1	2.49	0.42
3:K:234:LEU:HD13	4:L:102:ASN:ND2	2.35	0.42
3:G:335:ARG:HH22	4:H:119:PRO:HA	1.85	0.42
1:I:174:LYS:HB3	3:K:133:TYR:CD1	2.55	0.42
3:G:242:ILE:O	3:G:243:ASN:HB2	2.20	0.42
3:K:296:LYS:NZ	3:K:307:ASP:OD2	2.34	0.42
3:G:234:LEU:HD13	4:H:102:ASN:ND2	2.34	0.42
3:G:296:LYS:HG2	3:G:310:VAL:HG22	2.01	0.42
3:G:366:LEU:HD21	4:H:77:LEU:HD12	2.02	0.42
3:G:187:ASP:OD2	3:G:258:GLN:NE2	2.52	0.42
3:C:244:SER:C	3:C:246:LYS:N	2.73	0.42
1:E:174:LYS:HB3	3:G:133:TYR:CD1	2.55	0.41
2:F:21:ASP:O	2:F:25:GLN:HG2	2.19	0.41
3:G:227:SER:OG	3:G:229:MET:SD	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:LEU:O	1:I:350:ARG:HG2	2.20	0.41
2:J:8:TYR:CE1	3:K:379:LYS:HG3	2.54	0.41
3:C:228:ASP:OD2	3:C:233:ASN:HB2	2.20	0.41
1:A:239:ILE:HD12	1:A:247:TRP:CZ3	2.55	0.41
2:F:26:GLU:HG3	3:G:361:TRP:CD1	2.55	0.41
3:C:216:SER:OG	3:C:219:GLU:HG3	2.21	0.41
1:I:370:ILE:HG13	1:I:401:HIS:HB2	2.03	0.41
2:J:89:ASN:ND2	2:J:91:ASN:OD1	2.54	0.41
2:J:95:PHE:CE1	3:K:347:LEU:HB3	2.55	0.41
3:K:252:GLN:HG3	4:L:92:THR:HG21	2.02	0.41
3:K:216:SER:OG	3:K:219:GLU:HG3	2.21	0.41
2:B:21:ASP:O	2:B:25:GLN:HG2	2.21	0.40
3:K:264:LEU:O	3:K:268:ILE:HG12	2.22	0.40
3:K:318:ARG:H	3:K:318:ARG:HG3	1.26	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%)	269 (98%)	6 (2%)	0	100	100
1	E	275/305 (90%)	267 (97%)	7 (2%)	1 (0%)	34	60
1	I	274/305 (90%)	265 (97%)	8 (3%)	1 (0%)	34	60
2	B	71/113 (63%)	71 (100%)	0	0	100	100
2	F	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
2	J	69/113 (61%)	68 (99%)	1 (1%)	0	100	100
3	C	264/280 (94%)	255 (97%)	8 (3%)	1 (0%)	34	60
3	G	271/280 (97%)	257 (95%)	14 (5%)	0	100	100
3	K	267/280 (95%)	257 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	117/120 (98%)	117 (100%)	0	0	100	100
4	H	117/120 (98%)	117 (100%)	0	0	100	100
4	L	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
All	All	2179/2454 (89%)	2119 (97%)	57 (3%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	339	LYS
3	C	245	HIS
1	I	339	LYS

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	259/283 (92%)	257 (99%)	2 (1%)	81	93
1	E	259/283 (92%)	258 (100%)	1 (0%)	91	97
1	I	258/283 (91%)	256 (99%)	2 (1%)	81	93
2	B	70/100 (70%)	70 (100%)	0	100	100
2	F	63/100 (63%)	61 (97%)	2 (3%)	39	68
2	J	69/100 (69%)	67 (97%)	2 (3%)	42	71
3	C	254/265 (96%)	248 (98%)	6 (2%)	49	77
3	G	259/265 (98%)	258 (100%)	1 (0%)	91	97
3	K	255/265 (96%)	251 (98%)	4 (2%)	62	85
4	D	110/111 (99%)	109 (99%)	1 (1%)	78	92
4	H	110/111 (99%)	110 (100%)	0	100	100
4	L	110/111 (99%)	109 (99%)	1 (1%)	78	92
All	All	2076/2277 (91%)	2054 (99%)	22 (1%)	73	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	263	THR
2	F	91	ASN
2	F	101	THR
3	G	247	THR
1	A	215	ARG
1	A	263	THR
3	C	183	ILE
3	C	244	SER
3	C	245	HIS
3	C	247	THR
3	C	380	ARG
3	C	391	LEU
4	D	33	LEU
1	I	263	THR
1	I	302	VAL
2	J	2	THR
2	J	71	LYS
3	K	227	SER
3	K	247	THR
3	K	283	LYS
3	K	318	ARG
4	L	55	GLN

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

Mol	Chain	Res	Type
3	C	360	ASN
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	E	262	1	10,11,12	0.58	0	7,12,14	0.79	0
1	ALY	A	262	1	10,11,12	0.60	0	7,12,14	0.52	0
1	ALY	I	262	1	10,11,12	0.65	0	7,12,14	0.56	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	E	262	1	-	1/9/10/12	-
1	ALY	A	262	1	-	1/9/10/12	-
1	ALY	I	262	1	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	262	ALY	CG-CD-CE-NZ
1	A	262	ALY	CG-CD-CE-NZ
1	I	262	ALY	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	277/305 (90%)	-0.20	6 (2%)	62	63	35, 55, 93, 125	0
1	E	277/305 (90%)	-0.05	8 (2%)	51	52	36, 63, 106, 132	0
1	I	276/305 (90%)	-0.24	2 (0%)	87	89	29, 49, 83, 118	0
2	B	77/113 (68%)	0.23	6 (7%)	13	11	43, 75, 123, 155	0
2	F	68/113 (60%)	0.19	5 (7%)	14	12	51, 79, 113, 127	0
2	J	75/113 (66%)	0.03	8 (10%)	6	4	44, 66, 113, 120	0
3	C	268/280 (95%)	-0.20	6 (2%)	62	63	40, 66, 108, 129	0
3	G	273/280 (97%)	-0.01	14 (5%)	28	26	39, 68, 114, 145	0
3	K	269/280 (96%)	-0.13	8 (2%)	50	51	34, 67, 109, 138	0
4	D	119/120 (99%)	-0.19	2 (1%)	70	72	38, 62, 107, 116	0
4	H	119/120 (99%)	0.04	5 (4%)	36	35	38, 66, 112, 123	0
4	L	119/120 (99%)	-0.17	5 (4%)	36	35	34, 54, 108, 141	0
All	All	2217/2454 (90%)	-0.11	75 (3%)	45	45	29, 62, 108, 155	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	258	GLN	5.4
3	K	301	GLY	5.4
3	K	258	GLN	5.2
3	G	303	LYS	4.7
3	G	127	SER	4.6
2	F	107	HIS	4.5
1	E	437	THR	4.5
3	G	306	ILE	4.4
4	L	118	ALA	4.4
3	G	259	MET	4.4
4	L	117	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
3	G	305	GLU	4.1
2	B	1	MET	3.8
3	G	257	SER	3.8
3	K	303	LYS	3.7
2	B	5	LEU	3.7
3	G	302	GLU	3.4
2	B	3	ASP	3.4
1	E	407	GLU	3.4
3	K	305	GLU	3.3
2	B	107	HIS	3.2
2	F	106	GLN	3.2
1	E	163	ARG	3.2
2	J	75	THR	3.2
3	G	258	GLN	3.2
4	H	119	PRO	3.2
1	E	161	VAL	3.2
3	K	259	MET	3.1
1	E	339	LYS	3.1
1	E	435	VAL	3.1
2	F	66	SER	3.0
1	A	163	ARG	2.9
1	A	437	THR	2.9
2	B	2	THR	2.9
2	F	103	VAL	2.9
3	C	384	ILE	2.9
3	K	318	ARG	2.9
4	D	119	PRO	2.8
3	C	259	MET	2.8
4	L	1	MET	2.7
2	F	104	LYS	2.7
2	J	66	SER	2.7
4	L	115	GLY	2.7
4	L	116	VAL	2.6
4	D	70	LYS	2.6
1	I	437	THR	2.6
2	J	103	VAL	2.6
3	G	318	ARG	2.5
3	K	256	VAL	2.5
3	G	301	GLY	2.5
2	J	102	TYR	2.5
3	G	248	HIS	2.5
3	K	229	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	104	LYS	2.4
4	H	59	ILE	2.4
3	G	384	ILE	2.4
3	G	229	MET	2.3
3	G	243	ASN	2.3
3	C	257	SER	2.3
2	J	65	TYR	2.3
2	J	46	HIS	2.3
1	I	252	CYS	2.2
1	A	339	LYS	2.2
4	H	54	ARG	2.2
4	H	118	ALA	2.2
2	J	88	PHE	2.2
4	H	56	GLN	2.2
1	A	367	GLU	2.1
2	B	109	GLN	2.1
1	A	161	VAL	2.1
1	A	160	GLU	2.1
1	E	313	ARG	2.1
1	E	160	GLU	2.1
3	C	399	PRO	2.1
3	C	246	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
1	ALY	E	262	12/13	0.97	0.14	35,45,58,58	0
1	ALY	A	262	12/13	0.98	0.13	34,39,51,52	0
1	ALY	I	262	12/13	0.98	0.14	24,35,47,53	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.