



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:00 AM UTC

PDB ID : 5J9Q / pdb_00005j9q
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

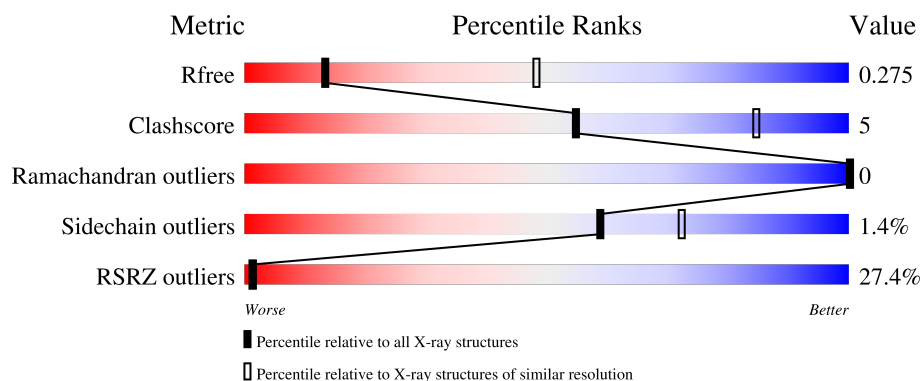
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 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 $\leq 5\%$. 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	21% 81%14%.
1	E	305	28% 83%12%..
1	I	305	20% 80%14%..
2	B	113	20% 62%8%30%
2	F	113	23% 59%7%34%

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Mol	Chain	Length	Quality of chain
2	J	113	
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			

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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			

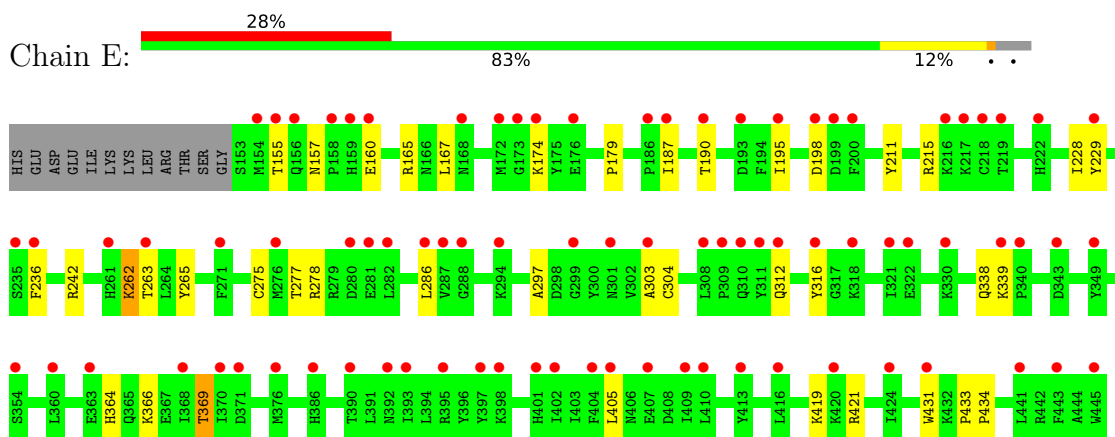
- Molecule 5 is a protein called Htz1.

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			

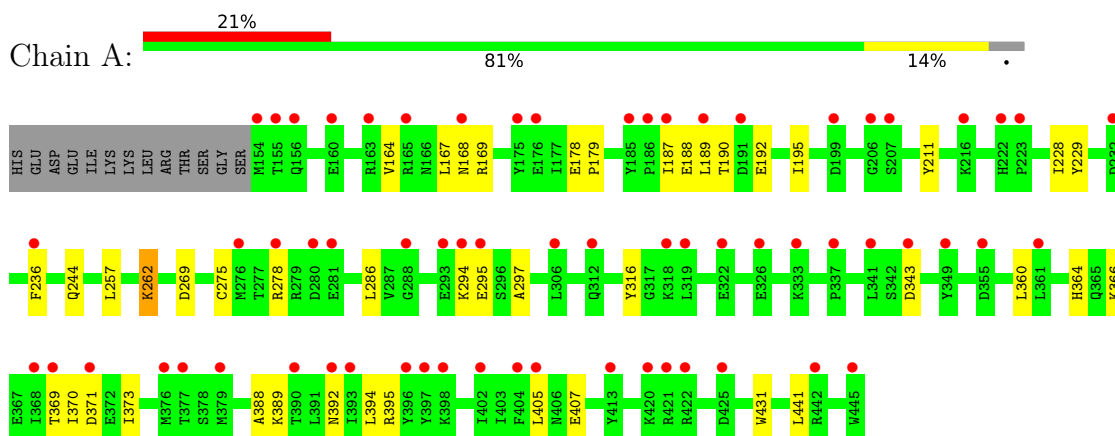
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

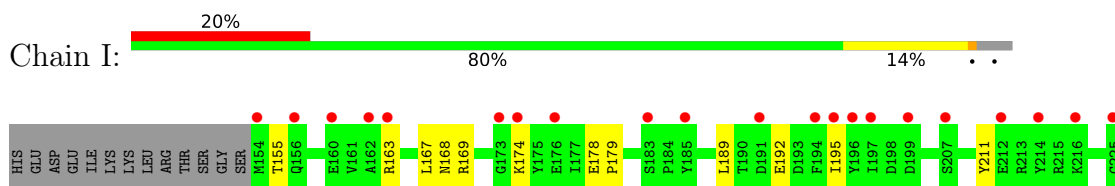
- Molecule 1: Histone acetyltransferase ESA1

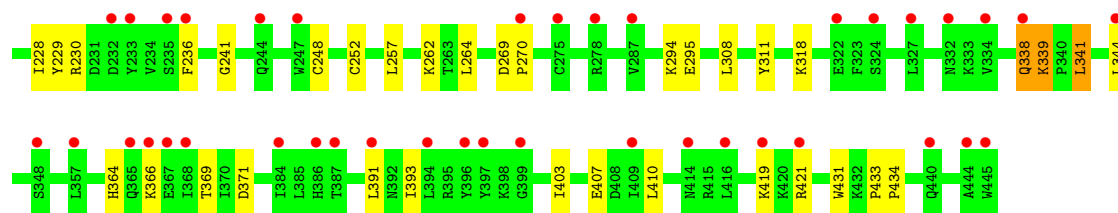


- Molecule 1: Histone acetyltransferase ESA1

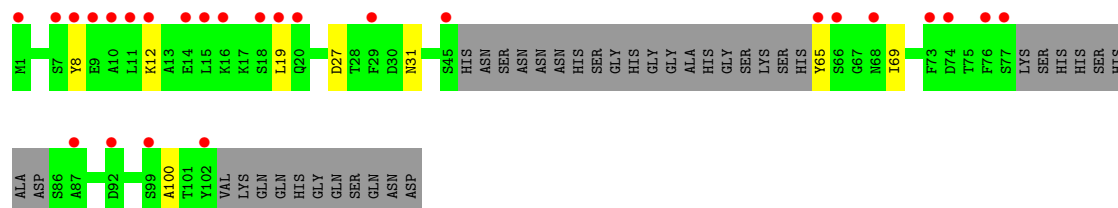


- Molecule 1: Histone acetyltransferase ESA1

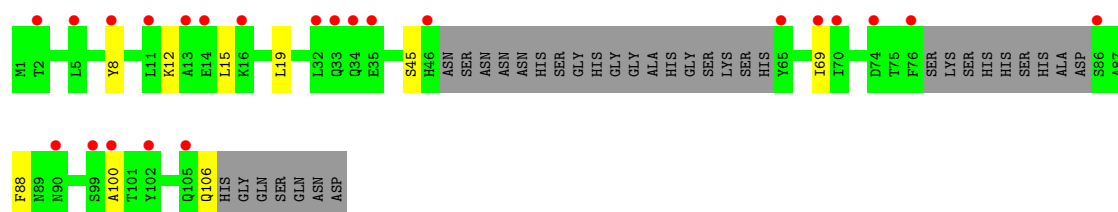




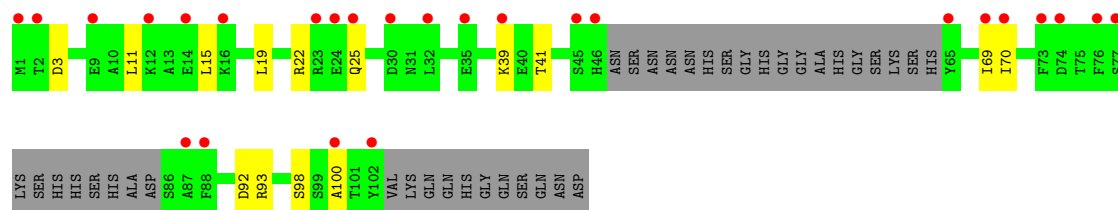
• Molecule 2: Chromatin modification-related protein EAF6



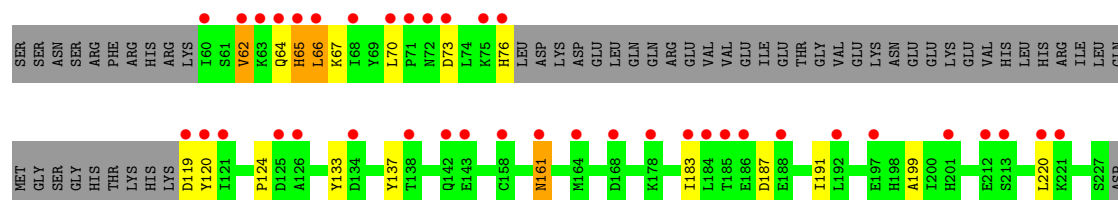
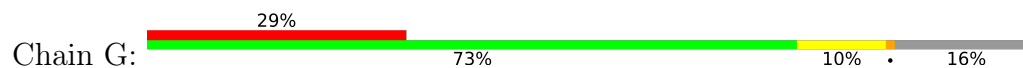
• Molecule 2: Chromatin modification-related protein EAF6

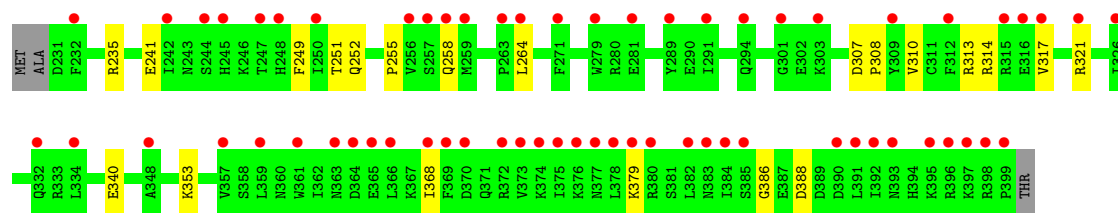


• Molecule 2: Chromatin modification-related protein EAF6

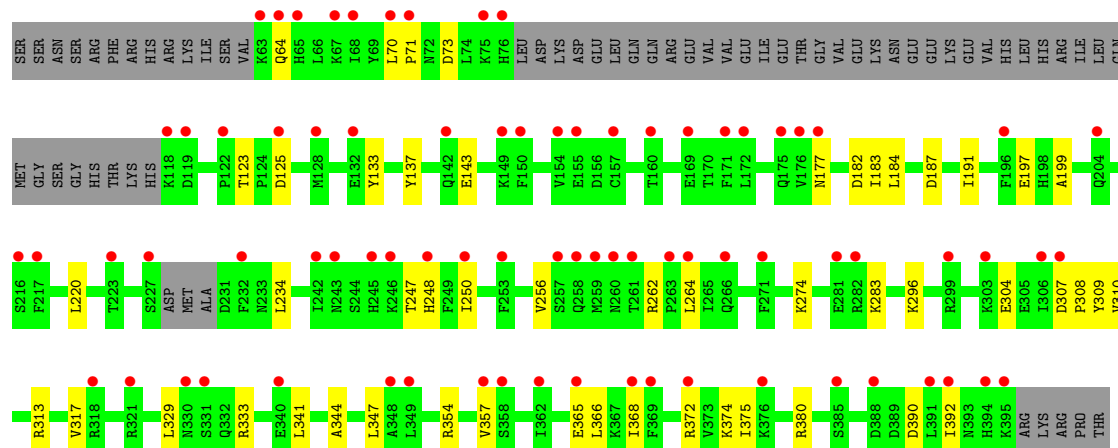


• Molecule 3: Enhancer of polycomb-like protein 1

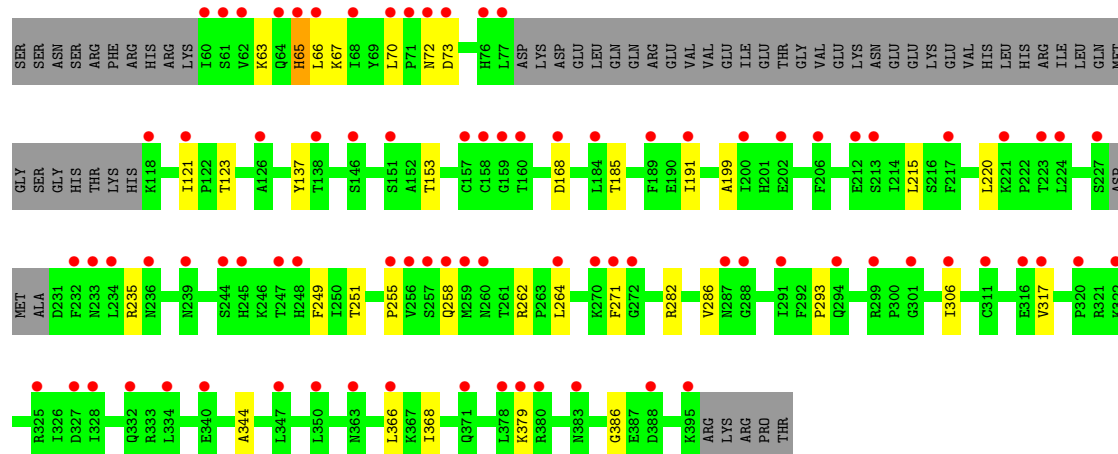
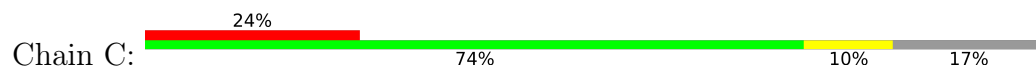




• Molecule 3: Enhancer of polycomb-like protein 1



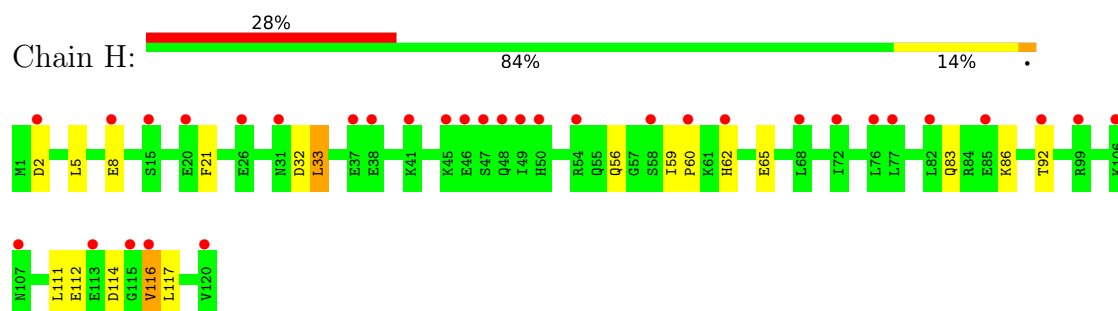
• Molecule 3: Enhancer of polycomb-like protein 1



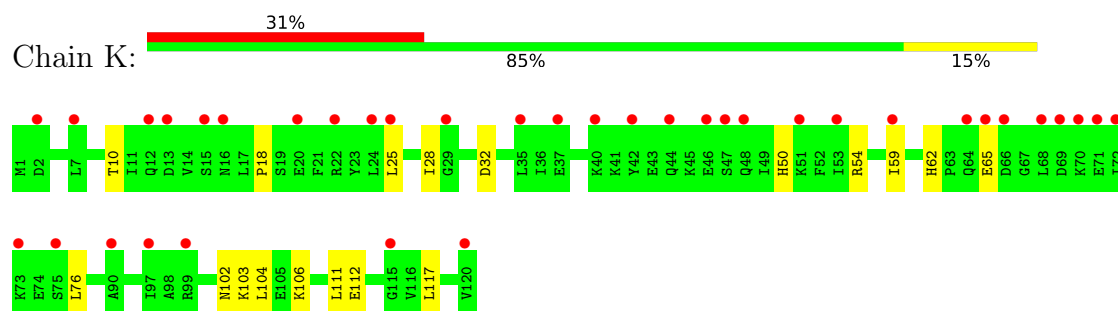
• Molecule 4: Chromatin modification-related protein YNG2



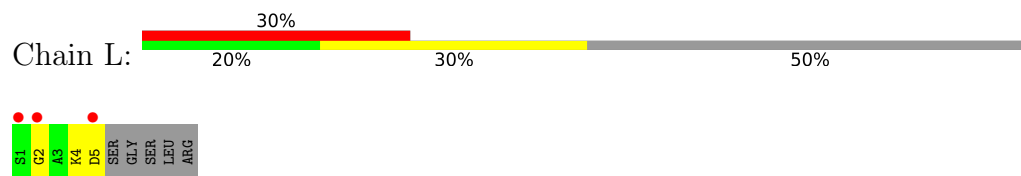
- Molecule 4: Chromatin modification-related protein YNG2



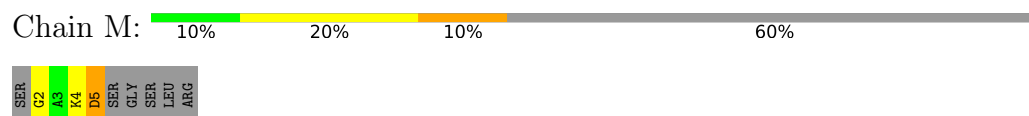
- Molecule 4: Chromatin modification-related protein YNG2



- 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 30.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	78.9 (30.00-3.25) 78.8 (30.00-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.250 , 0.273 0.253 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 17.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	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 3.45% 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	0.18	0/2523	0.39	0/3411
1	E	0.16	0/2532	0.37	0/3422
1	I	0.21	1/2523 (0.0%)	0.41	2/3411 (0.1%)
2	B	0.15	0/669	0.40	0/893
2	F	0.13	0/630	0.36	0/841
2	J	0.16	0/635	0.39	0/848
3	C	0.17	0/2509	0.41	0/3379
3	G	0.17	0/2528	0.43	0/3404
3	N	0.16	0/2477	0.40	0/3335
4	D	0.19	0/981	0.35	0/1317
4	H	0.24	1/981 (0.1%)	0.38	0/1317
4	K	0.18	0/981	0.35	0/1317
5	L	0.31	0/31	0.89	0/39
5	M	0.28	0/25	0.96	0/31
5	O	0.17	0/17	0.56	0/20
All	All	0.18	2/20042 (0.0%)	0.40	2/26985 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	339	LYS	C-N	5.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	59	ILE	CA-CB	-5.06	1.51	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	339	LYS	CA-C-N	-5.37	113.13	119.84
1	I	339	LYS	C-N-CA	-5.37	113.13	119.84

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	29	0
1	E	2479	0	2458	26	0
1	I	2470	0	2446	34	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	27	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	19429	187	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 (187) 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)
3:G:379:LYS:NZ	3:G:386:GLY:O	2.18	0.76
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
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:269:ASP:O	1:I:294:LYS:NZ	2.30	0.64
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:65:HIS:ND1	3:G:65:HIS:C	2.58	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:I:163:ARG:O	3:N:309:TYR:OH	2.18	0.60
4:K:103:LYS:HD3	4:K:106:LYS:HE3	1.84	0.59
1:E:211:TYR:OH	3:G:137:TYR:OH	2.20	0.59
1:A:211:TYR:HH	3:C:137:TYR:HH	1.50	0.59
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.84	0.59
3:C:235:ARG:HG3	3:C:249:PHE:HB3	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
3:N:191:ILE:HG22	3:N:264:LEU:HD13	1.84	0.58
1:E:312:GLN:NE2	3:G:124:PRO:O	2.36	0.57
3:C:366:LEU:HD12	4:D:76:LEU:HG	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:197:GLU:OE2	3:N:283:LYS:NZ	2.41	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
1:I:211:TYR:HH	3:N:137:TYR:HH	1.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:ALA:HB1	3:C:220:LEU:HD11	1.93	0.49
3:C:168:ASP:OD1	3:C:282:ARG:NH1	2.44	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
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
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
1:A:364:HIS:O	1:A:366:LYS:N	2.45	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
1:E:265:TYR:HA	3:G:313:ARG:HH21	1.79	0.47
3:C:379:LYS:HE3	3:C:386:GLY:H	1.80	0.47
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:83:GLN:HA	4:H:86:LYS:HZ3	1.83	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
1:I:169:ARG:NH1	1:I:178:GLU:HB2	2.33	0.43
4:D:112:GLU:HG3	4:D:117:LEU:HD23	1.99	0.43
2:J:70:ILE:HG21	2:J:92:ASP:HB3	2.00	0.43
1:E:277:THR:HG22	1:E:286:LEU:HA	1.99	0.43
1:A:407:GLU:H	1:A:407:GLU:CD	2.26	0.43
1:I:189:LEU:O	1:I:195:ILE:HD11	2.18	0.43
4:D:10:THR:O	4:D:14:VAL:HG23	2.18	0.43
3:N:354:ARG:NH2	2:J:98:SER:OG	2.32	0.43
3:N:307:ASP:HB3	3:N:310:VAL:HG23	2.01	0.43
4:H:114:ASP:HB2	4:H:116:VAL:CG2	2.49	0.43
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.92	0.43
2:B:45:SER:HB3	2:B:88:PHE:CD2	2.53	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:295:GLU:HG3	1:A:441:LEU:HD11	2.00	0.43
1:A:360:LEU:HD23	1:A:373:ILE:HG23	2.01	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
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
1:I:433:PRO:HA	1:I:434:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:2:ASP:HB3	4:H:5:LEU:HG	2.01	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
1:I:270:PRO:HB3	3:C:306:ILE:HG12	2.02	0.41
1:I:230:ARG:HD2	3:N:143:GLU:OE2	2.21	0.41
2:B:8:TYR:CZ	2:B:12:LYS:HD3	2.56	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
3:G:321:ARG:HH12	1:I:155:THR:HG21	1.84	0.41
4:H:117:LEU:HD12	4:H:117:LEU:HA	1.94	0.41
4:K:103:LYS:HE3	4:K:103:LYS:HB2	1.96	0.41
1:I:344:LEU:H	1:I:344:LEU:HD12	1.85	0.41
1:E:297:ALA:HB2	3:N:308:PRO:HB3	2.03	0.41
3:G:235:ARG:HG3	3:G:249:PHE:HB3	2.03	0.41
1:A:167:LEU:HD13	1:A:195:ILE:HD12	2.03	0.41
1:A:187:ILE:O	1:A:190:THR:HG22	2.20	0.41
1:A:343:ASP:HB3	3:C:121:ILE:HG12	2.03	0.41
1:A:392:ASN:OD1	1:A:395:ARG:HD3	2.20	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
1:E:242:ARG:NH2	4:H:8:GLU:OE2	2.46	0.40
3:C:262:ARG:HH22	3:C:271:PHE:HE2	1.69	0.40
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.56	0.40
2:J:3:ASP:N	2:J:3:ASP:OD1	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
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%)	268 (98%)	4 (2%)	57	71
1	I	270/283 (95%)	268 (99%)	2 (1%)	76	79
2	B	73/100 (73%)	72 (99%)	1 (1%)	59	72
2	F	69/100 (69%)	69 (100%)	0	100	100
2	J	69/100 (69%)	68 (99%)	1 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	279/333 (84%)	274 (98%)	5 (2%)	51	69
3	G	280/333 (84%)	273 (98%)	7 (2%)	42	63
3	N	274/333 (82%)	267 (97%)	7 (3%)	40	62
4	D	111/111 (100%)	111 (100%)	0	100	100
4	H	111/111 (100%)	109 (98%)	2 (2%)	51	69
4	K	111/111 (100%)	111 (100%)	0	100	100
5	L	3/7 (43%)	3 (100%)	0	100	100
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%)	2165 (99%)	30 (1%)	59	72

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	155	THR
1	E	195	ILE
1	E	339	LYS
1	E	369	THR
3	G	62	VAL
3	G	65	HIS
3	G	66	LEU
3	G	161	ASN
3	G	183	ILE
3	G	314	ARG
3	G	317	VAL
1	I	341	LEU
1	I	369	THR
3	N	183	ILE
3	N	250	ILE
3	N	256	VAL
3	N	274	LYS
3	N	317	VAL
3	N	341	LEU
3	N	357	VAL
3	C	65	HIS
3	C	185	THR
3	C	215	LEU
3	C	286	VAL
3	C	317	VAL

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Mol	Chain	Res	Type
2	B	106	GLN
2	J	25	GLN
4	H	33	LEU
4	H	116	VAL
5	M	5	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	168	ASN
3	G	201	HIS
1	I	338	GLN
3	N	177	ASN
3	N	236	ASN
3	N	237	GLN
3	N	252	GLN
3	C	72	ASN
3	C	76	HIS
3	C	236	ASN
3	C	343	ASN
2	B	25	GLN
2	J	25	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	E	262	1	10,11,12	1.05	1 (10%)	7,12,14	1.03	0
1	ALY	I	262	1	10,11,12	0.86	0	7,12,14	0.90	0
1	ALY	A	262	1	10,11,12	0.82	0	7,12,14	1.20	1 (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
1	ALY	E	262	1	-	4/9/10/12	-
1	ALY	I	262	1	-	3/9/10/12	-
1	ALY	A	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	2.21	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	2.50	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	E	262	ALY	OH-CH-NZ-CE
1	E	262	ALY	CH3-CH-NZ-CE
1	A	262	ALY	OH-CH-NZ-CE
1	A	262	ALY	CH3-CH-NZ-CE
1	I	262	ALY	OH-CH-NZ-CE
1	I	262	ALY	CH3-CH-NZ-CE
1	I	262	ALY	CG-CD-CE-NZ
1	E	262	ALY	CG-CD-CE-NZ
1	A	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	E	262	ALY	1	0
1	I	262	ALY	1	0
1	A	262	ALY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	1.38	65 (22%) 2 2	7, 38, 100, 144	0
1	E	292/305 (95%)	1.57	84 (28%) 1 1	18, 57, 108, 129	0
1	I	291/305 (95%)	1.37	60 (20%) 2 2	11, 42, 81, 111	0
2	B	79/113 (69%)	1.59	23 (29%) 1 1	20, 60, 111, 133	0
2	F	75/113 (66%)	1.74	26 (34%) 1 1	47, 81, 129, 135	0
2	J	76/113 (67%)	1.58	26 (34%) 1 1	24, 53, 102, 119	0
3	C	293/351 (83%)	1.61	85 (29%) 1 1	20, 56, 106, 142	0
3	G	295/351 (84%)	1.84	102 (34%) 1 1	17, 75, 135, 159	0
3	N	289/351 (82%)	1.53	78 (26%) 1 1	17, 50, 96, 130	0
4	D	120/120 (100%)	1.33	23 (19%) 3 3	20, 40, 69, 89	0
4	H	120/120 (100%)	1.62	33 (27%) 1 1	33, 69, 129, 140	0
4	K	120/120 (100%)	1.58	37 (30%) 1 1	19, 35, 59, 65	0
5	L	5/10 (50%)	1.85	3 (60%) 0 0	63, 65, 88, 95	0
5	M	4/10 (40%)	1.06	0 100 100	50, 58, 59, 70	0
5	O	3/10 (30%)	1.38	0 100 100	48, 48, 48, 50	0
All	All	2353/2697 (87%)	1.55	645 (27%) 1 1	7, 52, 113, 159	0

All (645) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	258	GLN	6.8
3	G	64	GLN	6.0
3	N	71	PRO	6.0
1	E	294	LYS	5.9
3	N	388	ASP	5.8
4	K	48	GLN	5.7
3	G	212	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	405	LEU	5.5
3	G	399	PRO	5.4
3	G	258	GLN	5.3
3	G	256	VAL	5.2
1	E	301	ASN	5.2
3	N	258	GLN	5.1
3	G	315	ARG	5.1
3	N	65	HIS	5.1
1	A	404	PHE	5.0
1	I	445	TRP	5.0
3	G	382	LEU	5.0
3	N	70	LEU	5.0
3	C	64	GLN	5.0
3	C	202	GLU	5.0
3	G	168	ASP	4.9
3	C	76	HIS	4.9
3	G	71	PRO	4.8
1	A	341	LEU	4.8
3	C	322	LYS	4.7
4	K	69	ASP	4.7
2	J	46	HIS	4.6
3	G	164	MET	4.6
3	G	183	ILE	4.5
3	C	70	LEU	4.5
3	G	158	CYS	4.5
2	F	77	SER	4.5
3	N	232	PHE	4.5
1	A	160	GLU	4.5
3	C	159	GLY	4.5
4	H	41	LYS	4.5
3	G	184	LEU	4.5
3	G	197	GLU	4.4
3	C	245	HIS	4.4
3	N	155	GLU	4.4
3	G	390	ASP	4.4
1	E	405	LEU	4.3
3	C	217	PHE	4.3
3	N	64	GLN	4.3
3	G	60	ILE	4.2
4	H	8	GLU	4.2
2	B	70	ILE	4.2
3	N	257	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	299	GLY	4.1
3	G	161	ASN	4.1
3	N	76	HIS	4.1
3	N	227	SER	4.1
3	C	325	ARG	4.1
3	C	363	ASN	4.1
4	H	120	VAL	4.1
4	H	116	VAL	4.0
3	G	250	ILE	4.0
1	A	420	LYS	4.0
4	K	71	GLU	4.0
4	D	115	GLY	3.9
4	D	97	ILE	3.9
2	J	77	SER	3.9
4	D	12	GLN	3.9
3	C	60	ILE	3.9
1	E	404	PHE	3.9
3	C	138	THR	3.9
1	I	344	LEU	3.8
3	G	185	THR	3.8
2	F	19	LEU	3.8
3	G	245	HIS	3.8
2	B	8	TYR	3.8
3	G	365	GLU	3.8
1	I	419	LYS	3.8
3	C	255	PRO	3.8
3	N	271	PHE	3.8
3	G	376	LYS	3.7
1	E	159	HIS	3.7
3	C	257	SER	3.7
2	J	87	ALA	3.7
3	G	385	SER	3.7
3	G	125	ASP	3.6
3	G	372	ARG	3.6
3	C	256	VAL	3.6
4	H	85	GLU	3.6
1	A	369	THR	3.6
2	F	20	GLN	3.6
4	H	45	LYS	3.6
2	F	65	TYR	3.6
1	E	321	ILE	3.6
2	B	2	THR	3.6

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Mol	Chain	Res	Type	RSRZ
4	H	48	GLN	3.6
1	E	390	THR	3.6
1	I	386	HIS	3.6
1	E	316	TYR	3.6
1	I	416	LEU	3.6
4	H	2	ASP	3.6
3	C	62	VAL	3.5
2	B	5	LEU	3.5
2	F	74	ASP	3.5
1	A	187	ILE	3.5
3	G	384	ILE	3.5
3	N	358	SER	3.5
3	G	263	PRO	3.5
1	I	232	ASP	3.5
1	A	445	TRP	3.5
3	G	361	TRP	3.5
4	H	58	SER	3.5
1	I	176	GLU	3.4
2	J	39	LYS	3.4
4	K	115	GLY	3.4
1	I	163	ARG	3.4
3	C	61	SER	3.4
3	G	73	ASP	3.4
1	E	154	MET	3.4
1	E	156	GLN	3.4
1	E	282	LEU	3.4
4	K	75	SER	3.4
3	G	391	LEU	3.4
3	N	223	THR	3.4
3	N	306	ILE	3.4
1	E	310	GLN	3.4
1	E	445	TRP	3.4
1	A	397	TYR	3.4
1	E	288	GLY	3.4
1	E	318	LYS	3.4
1	A	306	LEU	3.3
4	D	14	VAL	3.3
4	K	53	ILE	3.3
3	N	348	ALA	3.3
3	C	378	LEU	3.3
4	K	24	LEU	3.3
2	F	16	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	293	GLU	3.3
1	E	303	ALA	3.3
3	G	247	THR	3.3
4	K	12	GLN	3.3
1	I	154	MET	3.3
2	F	1	MET	3.3
4	K	65	GLU	3.3
2	B	65	TYR	3.3
1	I	394	LEU	3.3
3	C	223	THR	3.3
3	G	357	VAL	3.3
2	J	102	TYR	3.2
2	J	30	ASP	3.2
3	N	391	LEU	3.2
2	F	76	PHE	3.2
2	F	87	ALA	3.2
3	G	326	ILE	3.2
1	I	185	TYR	3.2
3	G	120	TYR	3.2
1	E	286	LEU	3.2
3	G	244	SER	3.2
2	J	76	PHE	3.2
3	C	271	PHE	3.2
3	N	125	ASP	3.2
4	K	66	ASP	3.2
3	G	126	ALA	3.2
3	C	212	GLU	3.2
3	N	171	PHE	3.2
3	C	151	SER	3.2
1	E	401	HIS	3.2
2	J	100	ALA	3.2
3	G	383	ASN	3.2
3	G	366	LEU	3.2
4	K	25	LEU	3.2
2	J	45	SER	3.2
3	G	392	ILE	3.2
1	A	413	TYR	3.2
1	A	207	SER	3.2
3	G	397	LYS	3.1
3	C	66	LEU	3.1
3	C	366	LEU	3.1
4	D	20	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	J	65	TYR	3.1
3	G	76	HIS	3.1
3	C	200	ILE	3.1
3	C	306	ILE	3.1
1	A	280	ASP	3.1
3	G	121	ILE	3.1
3	N	395	LYS	3.1
1	E	236	PHE	3.1
3	C	71	PRO	3.1
1	I	414	ASN	3.1
3	G	63	LYS	3.1
3	C	239	ASN	3.1
2	F	66	SER	3.1
3	N	157	CYS	3.1
3	C	383	ASN	3.1
2	F	99	SER	3.1
1	A	295	GLU	3.1
3	C	189	PHE	3.1
3	N	63	LYS	3.1
3	C	73	ASP	3.1
1	I	195	ILE	3.1
1	I	357	LEU	3.0
3	N	260	ASN	3.0
3	C	287	ASN	3.0
1	A	421	ARG	3.0
1	E	200	PHE	3.0
2	B	14	GLU	3.0
4	K	47	SER	3.0
4	K	72	ILE	3.0
1	A	189	LEU	3.0
3	G	264	LEU	3.0
3	N	303	LYS	3.0
3	C	395	LYS	3.0
2	F	8	TYR	3.0
2	B	46	HIS	3.0
3	N	248	HIS	3.0
1	I	156	GLN	3.0
1	I	365	GLN	3.0
1	E	287	VAL	3.0
3	G	257	SER	3.0
2	B	102	TYR	3.0
1	A	371	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	168	ASP	3.0
3	G	138	THR	3.0
1	A	154	MET	3.0
3	C	259	MET	3.0
3	C	334	LEU	3.0
1	A	422	ARG	3.0
3	N	385	SER	3.0
5	L	1	SER	3.0
1	E	339	LYS	3.0
3	G	379	LYS	2.9
2	B	34	GLN	2.9
1	I	368	ILE	2.9
3	N	357	VAL	2.9
1	E	222	HIS	2.9
3	G	332	GLN	2.9
4	K	35	LEU	2.9
3	N	169	GLU	2.9
3	G	375	ILE	2.9
3	G	294	GLN	2.9
2	F	68	ASN	2.9
1	E	349	TYR	2.9
1	E	199	ASP	2.9
1	A	206	GLY	2.9
1	I	278	ARG	2.9
2	B	76	PHE	2.9
1	E	187	ILE	2.9
1	A	318	LYS	2.9
1	I	409	ILE	2.9
3	G	374	LYS	2.9
3	G	395	LYS	2.9
3	C	234	LEU	2.9
4	H	76	LEU	2.9
4	K	97	ILE	2.9
3	N	245	HIS	2.8
2	B	105	GLN	2.8
4	K	90	ALA	2.8
1	E	219	THR	2.8
1	A	176	GLU	2.8
1	I	421	ARG	2.8
3	G	396	ARG	2.8
1	E	398	LYS	2.8
3	C	68	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
4	H	77	LEU	2.8
3	G	201	HIS	2.8
3	C	244	SER	2.8
4	K	64	GLN	2.8
2	J	2	THR	2.8
3	C	317	VAL	2.8
1	E	416	LEU	2.8
3	C	291	ILE	2.8
4	H	49	ILE	2.8
1	I	207	SER	2.8
1	I	235	SER	2.8
4	D	98	ALA	2.8
4	H	54	ARG	2.8
1	I	199	ASP	2.8
1	I	322	GLU	2.8
4	H	38	GLU	2.8
1	A	343	ASP	2.8
1	I	191	ASP	2.8
3	N	119	ASP	2.8
1	A	222	HIS	2.8
3	G	66	LEU	2.8
3	C	350	LEU	2.8
4	H	15	SER	2.8
4	D	27	GLU	2.8
1	A	393	ILE	2.8
2	J	70	ILE	2.8
3	N	321	ARG	2.7
1	I	174	LYS	2.7
3	C	320	PRO	2.7
4	D	111	LEU	2.7
2	F	14	GLU	2.7
2	J	9	GLU	2.7
3	G	279	TRP	2.7
1	A	186	PRO	2.7
3	G	378	LEU	2.7
1	E	195	ILE	2.7
3	G	188	GLU	2.7
3	C	301	GLY	2.7
1	E	343	ASP	2.7
1	I	338	GLN	2.7
1	E	393	ILE	2.7
1	E	409	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	N	250	ILE	2.7
3	N	362	ILE	2.7
1	A	288	GLY	2.7
1	I	173	GLY	2.7
3	G	186	GLU	2.7
3	G	316	GLU	2.7
3	G	398	ARG	2.7
1	I	366	LYS	2.7
2	J	12	LYS	2.7
2	B	74	ASP	2.7
3	G	119	ASP	2.7
1	E	441	LEU	2.7
3	G	393	ASN	2.7
1	A	312	GLN	2.7
2	J	69	ILE	2.7
2	J	35	GLU	2.7
3	C	347	LEU	2.7
4	K	13	ASP	2.7
3	G	363	ASN	2.7
3	G	232	PHE	2.6
4	D	1	MET	2.6
1	E	218	CYS	2.6
3	G	373	VAL	2.6
1	E	368	ILE	2.6
1	I	244	GLN	2.6
3	N	365	GLU	2.6
3	C	158	CYS	2.6
3	C	264	LEU	2.6
2	F	9	GLU	2.6
3	G	359	LEU	2.6
3	G	303	LYS	2.6
3	C	146	SER	2.6
3	G	259	MET	2.6
3	N	259	MET	2.6
1	A	319	LEU	2.6
2	B	32	LEU	2.6
3	C	224	LEU	2.6
1	A	390	THR	2.6
1	I	247	TRP	2.6
1	I	397	TYR	2.6
3	C	232	PHE	2.6
3	N	177	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	307	ASP	2.6
5	L	5	ASP	2.6
3	N	392	ILE	2.5
1	A	376	MET	2.5
1	I	214	TYR	2.5
1	E	173	GLY	2.5
1	E	312	GLN	2.5
1	E	168	ASN	2.5
1	E	395	ARG	2.5
3	G	321	ARG	2.5
3	C	72	ASN	2.5
1	E	160	GLU	2.5
2	B	100	ALA	2.5
1	E	190	THR	2.5
1	A	368	ILE	2.5
1	I	384	ILE	2.5
3	C	121	ILE	2.5
3	G	369	PHE	2.5
1	E	386	HIS	2.5
2	F	102	TYR	2.5
4	K	15	SER	2.5
3	N	118	LYS	2.5
3	C	270	LYS	2.5
1	E	308	LEU	2.5
2	J	32	LEU	2.5
3	C	184	LEU	2.5
3	N	266	GLN	2.5
1	I	387	THR	2.5
4	K	22	ARG	2.5
4	K	70	LYS	2.5
3	C	371	GLN	2.5
4	D	116	VAL	2.5
2	F	7	SER	2.5
3	C	316	GLU	2.5
4	K	59	ILE	2.5
3	N	150	PHE	2.5
4	D	114	ASP	2.5
1	A	294	LYS	2.5
3	G	221	LYS	2.5
3	C	118	LYS	2.5
1	E	309	PRO	2.5
1	I	391	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	261	HIS	2.5
3	C	248	HIS	2.5
4	K	42	TYR	2.5
3	G	317	VAL	2.5
2	B	99	SER	2.4
4	D	58	SER	2.4
1	E	172	MET	2.4
1	E	176	GLU	2.4
2	B	35	GLU	2.4
1	E	392	ASN	2.4
3	N	299	ARG	2.4
3	N	372	ARG	2.4
2	B	11	LEU	2.4
3	G	192	LEU	2.4
3	G	220	LEU	2.4
1	I	399	GLY	2.4
3	N	242	ILE	2.4
3	C	191	ILE	2.4
1	I	324	SER	2.4
3	C	311	CYS	2.4
4	K	46	GLU	2.4
1	E	174	LYS	2.4
2	F	12	LYS	2.4
4	D	107	ASN	2.4
4	D	60	PRO	2.4
3	N	176	VAL	2.4
4	K	29	GLY	2.4
1	E	402	ILE	2.4
1	I	160	GLU	2.4
1	A	361	LEU	2.4
1	E	155	THR	2.4
1	E	431	TRP	2.4
4	H	92	THR	2.4
1	I	440	GLN	2.4
3	G	178	LYS	2.4
1	I	194	PHE	2.4
2	F	73	PHE	2.4
3	N	264	LEU	2.4
4	H	37	GLU	2.4
1	A	223	PRO	2.4
1	A	168	ASN	2.4
4	H	62	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	229	TYR	2.4
1	A	396	TYR	2.4
1	A	402	ILE	2.4
1	I	444	ALA	2.4
3	C	126	ALA	2.4
1	E	216	LYS	2.4
1	E	217	LYS	2.4
1	A	216	LYS	2.4
1	A	379	MET	2.4
3	G	142	GLN	2.4
4	H	26	GLU	2.4
1	E	235	SER	2.4
1	A	377	THR	2.3
3	N	160	THR	2.3
3	N	261	THR	2.3
1	I	216	LYS	2.3
1	E	280	ASP	2.3
1	E	311	TYR	2.3
1	A	232	ASP	2.3
3	N	318	ARG	2.3
3	C	388	ASP	2.3
3	G	312	PHE	2.3
3	G	281	GLU	2.3
2	F	18	SER	2.3
3	N	216	SER	2.3
3	G	368	ILE	2.3
3	C	299	ARG	2.3
3	G	370	ASP	2.3
1	E	271	PHE	2.3
1	I	327	LEU	2.3
3	N	67	LYS	2.3
3	C	221	LYS	2.3
4	H	99	ARG	2.3
1	E	263	THR	2.3
1	A	155	THR	2.3
2	F	10	ALA	2.3
1	E	413	TYR	2.3
3	N	330	ASN	2.3
3	C	294	GLN	2.3
4	D	64	GLN	2.3
4	H	20	GLU	2.3
1	E	330	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	288	GLY	2.3
1	E	276	MET	2.3
1	A	276	MET	2.3
3	G	248	HIS	2.3
4	H	47	SER	2.3
3	C	77	LEU	2.3
4	H	50	HIS	2.3
4	H	68	LEU	2.3
1	A	185	TYR	2.3
1	A	349	TYR	2.3
1	I	396	TYR	2.3
1	E	198	ASP	2.3
3	N	68	ILE	2.3
4	H	115	GLY	2.3
3	C	213	SER	2.3
1	I	332	ASN	2.3
3	G	377	ASN	2.3
1	E	371	ASP	2.3
3	G	364	ASP	2.3
4	K	2	ASP	2.3
4	H	113	GLU	2.2
1	E	424	ILE	2.2
1	E	376	MET	2.2
1	I	162	ALA	2.2
3	G	348	ALA	2.2
5	L	2	GLY	2.2
4	K	7	LEU	2.2
3	N	253	PHE	2.2
1	A	398	LYS	2.2
1	I	233	TYR	2.2
2	J	16	LYS	2.2
2	J	23	ARG	2.2
1	A	392	ASN	2.2
3	N	204	GLN	2.2
1	E	322	GLU	2.2
1	E	186	PRO	2.2
3	N	263	PRO	2.2
3	N	349	LEU	2.2
2	J	73	PHE	2.2
3	N	75	LYS	2.2
1	I	196	TYR	2.2
1	E	354	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLN	2.2
4	K	16	ASN	2.2
4	K	37	GLU	2.2
1	E	410	LEU	2.2
3	G	334	LEU	2.2
3	C	327	ASP	2.2
4	H	60	PRO	2.2
2	J	88	PHE	2.2
3	N	217	PHE	2.2
3	C	206	PHE	2.2
4	K	99	ARG	2.2
1	E	397	TYR	2.2
3	G	289	TYR	2.2
2	F	45	SER	2.2
3	N	331	SER	2.2
2	J	25	GLN	2.2
4	D	28	ILE	2.2
1	A	322	GLU	2.2
1	I	212	GLU	2.2
3	N	340	GLU	2.2
3	C	236	ASN	2.2
4	H	107	ASN	2.2
4	K	20	GLU	2.2
1	I	275	CYS	2.2
2	J	74	ASP	2.2
3	N	149	LYS	2.2
1	I	236	PHE	2.2
3	G	65	HIS	2.2
4	H	72	ILE	2.2
4	K	44	GLN	2.2
4	D	17	LEU	2.2
1	E	363	GLU	2.2
1	A	281	GLU	2.2
2	J	14	GLU	2.2
3	C	260	ASN	2.2
3	C	340	GLU	2.2
4	K	40	LYS	2.2
1	A	165	ARG	2.2
3	N	394	HIS	2.2
3	N	154	VAL	2.1
2	B	69	ILE	2.1
3	C	328	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	K	68	LEU	2.1
1	E	420	LYS	2.1
2	J	1	MET	2.1
3	N	128	MET	2.1
3	N	246	LYS	2.1
3	N	376	LYS	2.1
3	C	227	SER	2.1
1	A	163	ARG	2.1
1	A	442	ARG	2.1
3	G	301	GLY	2.1
3	G	380	ARG	2.1
3	N	281	GLU	2.1
3	N	282	ARG	2.1
4	D	57	GLY	2.1
3	G	271	PHE	2.1
4	D	95	PHE	2.1
1	A	191	ASP	2.1
3	C	157	CYS	2.1
4	K	73	LYS	2.1
1	A	326	GLU	2.1
1	I	348	SER	2.1
2	J	24	GLU	2.1
3	G	72	ASN	2.1
3	N	243	ASN	2.1
4	H	31	ASN	2.1
3	G	62	VAL	2.1
1	E	370	ILE	2.1
2	F	15	LEU	2.1
2	B	16	LYS	2.1
3	G	68	ILE	2.1
3	N	172	LEU	2.1
4	D	94	LEU	2.1
3	N	175	GLN	2.1
1	A	337	PRO	2.1
3	N	132	GLU	2.1
4	H	46	GLU	2.1
1	I	183	SER	2.1
1	A	333	LYS	2.1
1	A	425	ASP	2.1
2	F	92	ASP	2.1
3	C	65	HIS	2.1
4	D	13	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	309	TYR	2.1
1	E	443	PHE	2.1
2	F	29	PHE	2.1
3	N	122	PRO	2.1
1	I	287	VAL	2.1
2	B	90	ASN	2.1
3	C	233	ASN	2.1
4	H	106	LYS	2.1
1	E	360	LEU	2.1
1	A	278	ARG	2.1
1	I	197	ILE	2.1
3	G	291	ILE	2.1
4	D	53	ILE	2.1
1	E	193	ASP	2.1
1	A	175	TYR	2.1
3	C	160	THR	2.1
2	B	33	GLN	2.1
3	C	332	GLN	2.1
1	E	158	PRO	2.1
1	E	407	GLU	2.1
3	N	369	PHE	2.1
3	C	379	LYS	2.0
2	B	86	SER	2.0
3	G	213	SER	2.0
3	G	70	LEU	2.0
3	C	380	ARG	2.0
1	A	355	ASP	2.0
2	B	13	ALA	2.0
3	G	134	ASP	2.0
3	C	247	THR	2.0
1	A	236	PHE	2.0
3	N	142	GLN	2.0
1	I	367	GLU	2.0
3	G	75	LYS	2.0
3	G	143	GLU	2.0
4	K	51	LYS	2.0
1	I	334	VAL	2.0
2	F	11	LEU	2.0
3	G	242	ILE	2.0
4	D	92	THR	2.0
1	A	199	ASP	2.0
1	I	225	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	N	196	PHE	2.0
3	C	272	GLY	2.0
1	E	340	PRO	2.0
1	I	270	PRO	2.0
1	E	281	GLU	2.0
4	K	120	VAL	2.0
4	H	82	LEU	2.0
3	N	368	ILE	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	A	262	12/13	0.77	0.21	5,16,45,52	0
1	ALY	E	262	12/13	0.91	0.13	14,29,43,52	0
1	ALY	I	262	12/13	0.91	0.17	22,28,41,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.