Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:29 PM EDT

PDB ID	:	5J9U
Title	:	Crystal structure of the NuA4 core complex
Authors	:	Chen, Z.C.; Xu, P.
Deposited on	:	2016-04-11
Resolution	:	2.95 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:

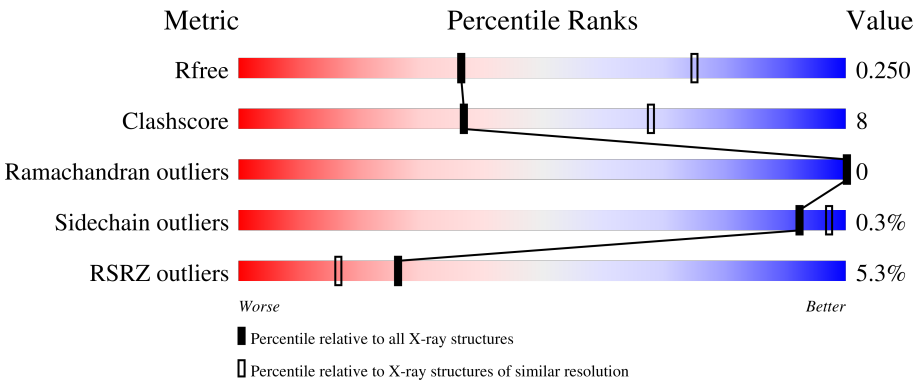
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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%, 76%, 19%, •
1	E	305	2%, 76%, 19%, •
1	I	305	3%, 80%, 16%, •
2	B	113	13%, 60%, 10%, 30%
2	F	113	7%, 54%, 12%, 34%

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Mol	Chain	Length	Quality of chain
2	J	113	6% 53% 14% 33%
3	C	351	6% 67% 16% 16%
3	G	351	9% 67% 17% 15%
3	N	351	5% 62% 22% • 16%
4	D	120	85% 15%
4	H	120	4% 84% 16%
4	K	120	% 84% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19676 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone acetyltransferase ESA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	293	2479	1601	419	448	11	0	0	0
1	A	292	2470	1596	418	446	10	0	0	0
1	I	292	2470	1596	418	446	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	75	622	389	99	133	1	0	0	0
2	B	79	660	413	108	138	1	0	0	0
2	J	76	627	392	100	134	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	297	2499	1577	443	471	8	0	0	0
3	N	295	2475	1565	434	468	8	0	0	0
3	C	294	2467	1560	431	468	8	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	D	120	969	613	165	188	3	0	0	0

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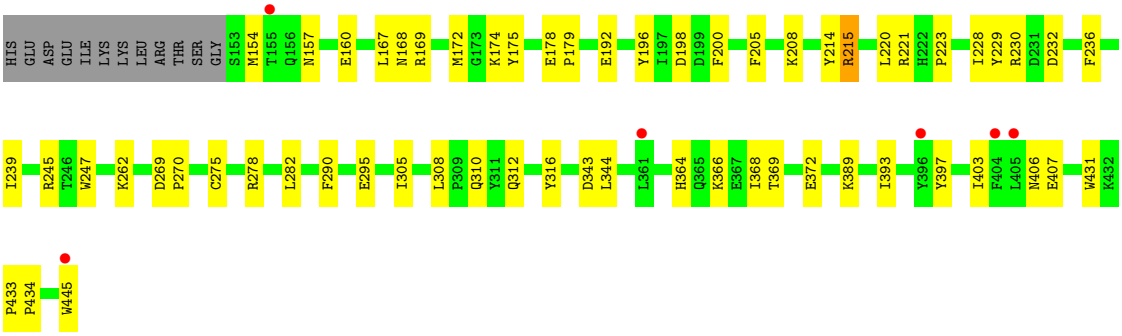
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	120	969	613	165	188	3	0	0	0
			Total	C	N	O	S			
4	K	120	969	613	165	188	3	0	0	0

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.

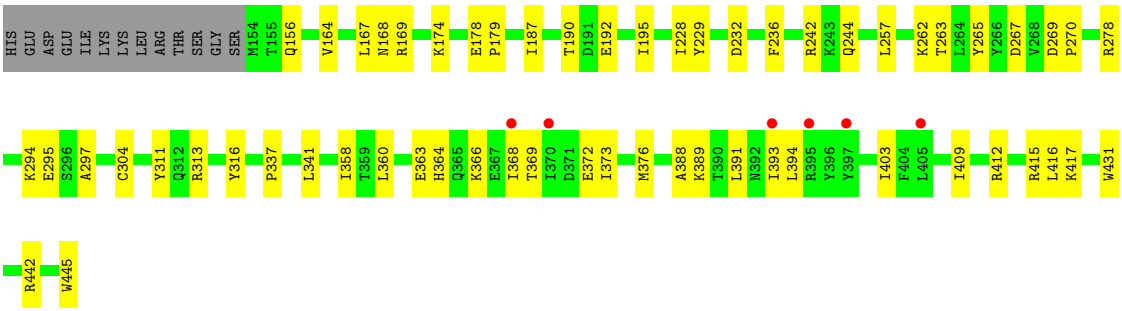
• Molecule 1: Histone acetyltransferase ESA1

Chain E:



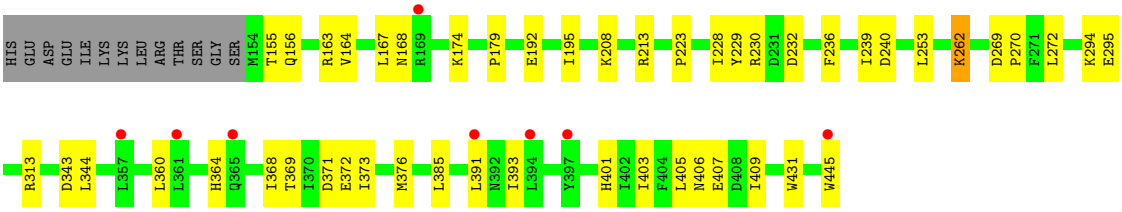
• Molecule 1: Histone acetyltransferase ESA1

Chain A:



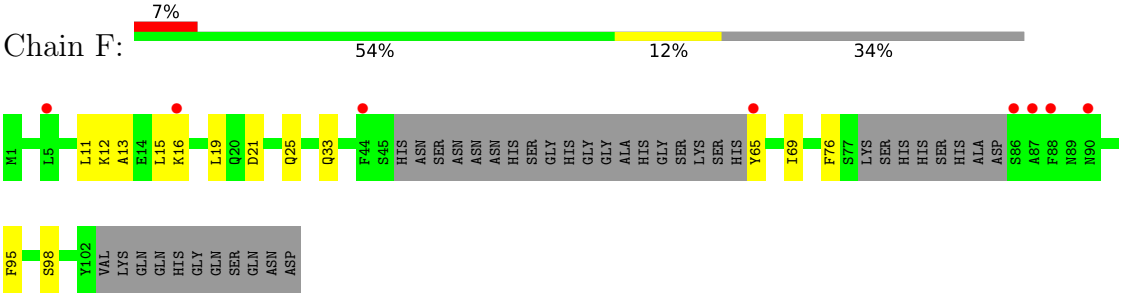
• Molecule 1: Histone acetyltransferase ESA1

Chain I:



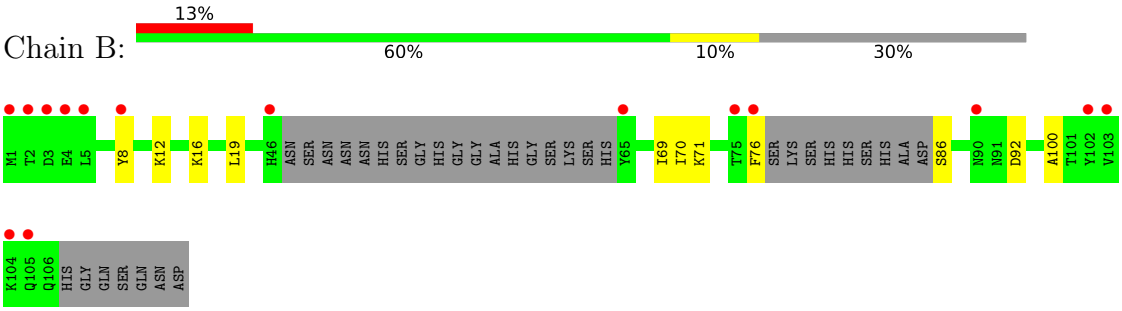
• Molecule 2: Chromatin modification-related protein EAF6

Chain F:



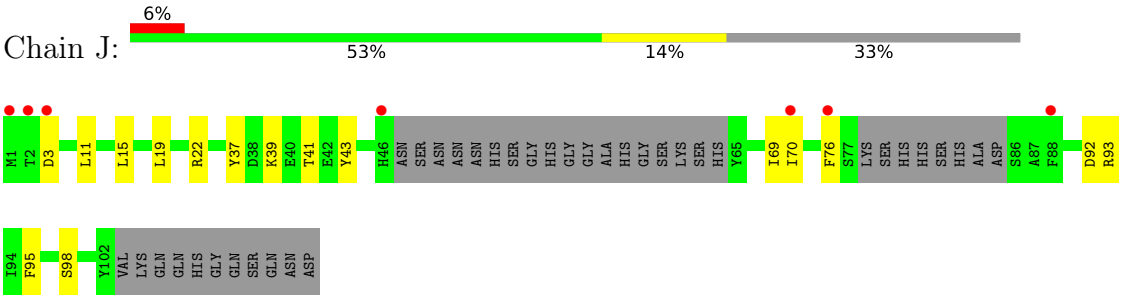
• Molecule 2: Chromatin modification-related protein EAF6

Chain B:



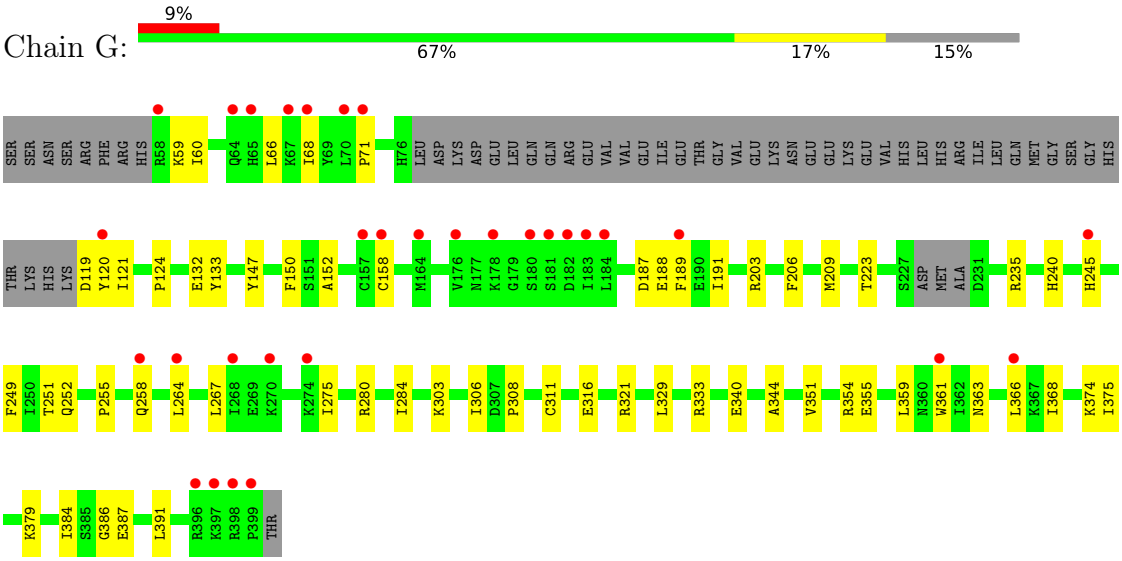
• Molecule 2: Chromatin modification-related protein EAF6

Chain J:



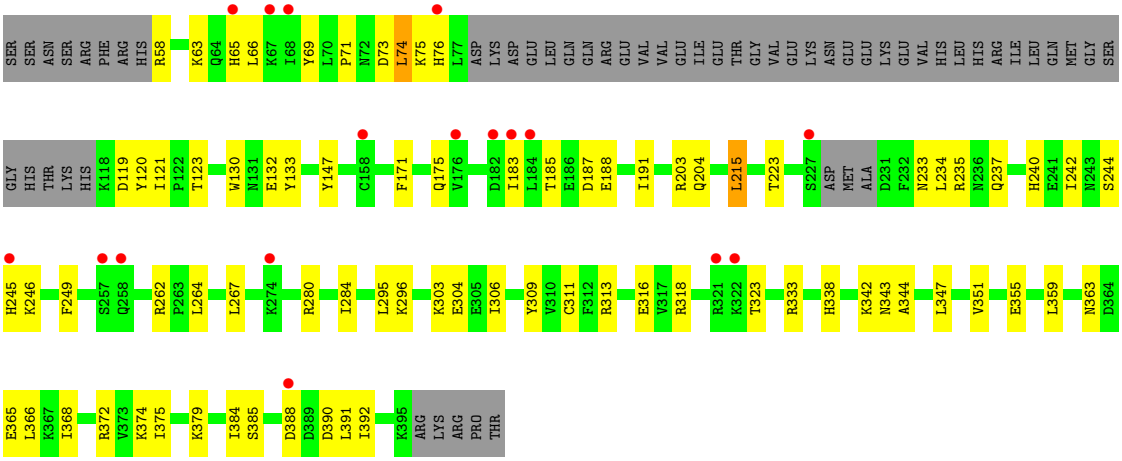
• Molecule 3: Enhancer of polycomb-like protein 1

Chain G:



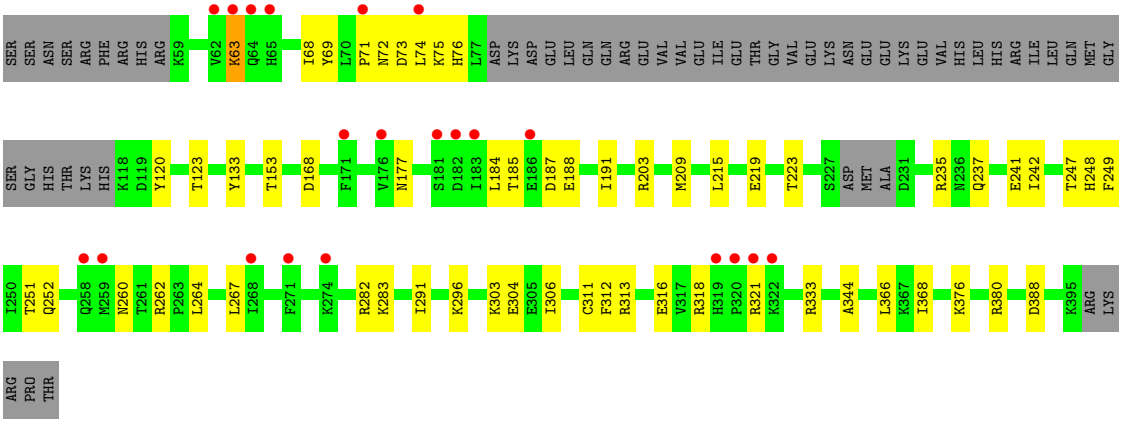
• Molecule 3: Enhancer of polycomb-like protein 1

Chain N:



• Molecule 3: Enhancer of polycomb-like protein 1

Chain C:

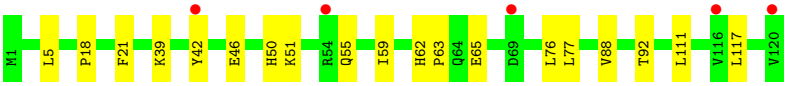


• Molecule 4: Chromatin modification-related protein YNG2

Chain D:

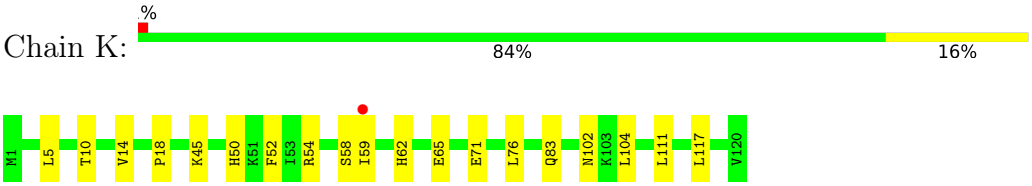
• Molecule 4: Chromatin modification-related protein YNG2

Chain H:



• Molecule 4: Chromatin modification-related protein YNG2

Chain K:


%
84%
16%
M1
L5
T10
V14
P18
K45
H50
K51
F52
I53
R54
S58
I59
H62
E65
E71
L76
Q83
N102
K103
L104
L111
L117
V120

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	217.91Å 189.89Å 173.56Å 90.00° 113.61° 90.00°	Depositor
Resolution (Å)	29.69 – 2.95 45.87 – 2.93	Depositor EDS
% Data completeness (in resolution range)	78.8 (29.69-2.95) 77.4 (45.87-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.216 , 0.246 0.218 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19676	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.25	0/2523	0.46	0/3411
1	E	0.25	0/2532	0.45	0/3422
1	I	0.26	0/2523	0.45	0/3411
2	B	0.25	0/669	0.41	0/893
2	F	0.25	0/630	0.44	0/841
2	J	0.26	0/635	0.41	0/848
3	C	0.29	0/2518	0.45	0/3390
3	G	0.25	0/2551	0.44	0/3433
3	N	0.26	0/2526	0.47	1/3400 (0.0%)
4	D	0.26	0/981	0.41	0/1317
4	H	0.25	0/981	0.41	0/1317
4	K	0.24	0/981	0.40	0/1317
All	All	0.26	0/20050	0.44	1/27000 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	74	LEU	CA-CB-CG	5.14	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2444	48	0
1	E	2479	0	2456	50	0
1	I	2470	0	2444	44	0
2	B	660	0	619	10	0
2	F	622	0	579	15	0
2	J	627	0	581	18	0
3	C	2467	0	2427	59	0
3	G	2499	0	2462	57	0
3	N	2475	0	2436	70	0
4	D	969	0	1003	16	0
4	H	969	0	1003	19	0
4	K	969	0	1003	15	0
All	All	19676	0	19457	305	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 8.

All (305) 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:407:GLU:HG3	3:N:63:LYS:HD3	1.52	0.92
2:J:41:THR:HG22	2:J:93:ARG:HH22	1.42	0.83
1:A:388:ALA:HB1	1:A:394:LEU:HD23	1.60	0.81
3:N:76:HIS:CD2	3:N:120:TYR:HA	2.17	0.80
1:I:391:LEU:HB2	1:I:393:ILE:HG12	1.66	0.76
3:C:76:HIS:CD2	3:C:120:TYR:HA	2.20	0.76
3:N:392:ILE:HG23	4:K:50:HIS:HB3	1.70	0.73
1:I:406:ASN:HA	3:C:63:LYS:HD2	1.70	0.73
1:I:407:GLU:HG3	3:C:63:LYS:HD3	1.70	0.72
1:I:213:ARG:NH2	3:N:187:ASP:OD1	2.22	0.72
2:F:33:GLN:HE22	3:G:354:ARG:HH11	1.39	0.71
3:G:379:LYS:NZ	3:G:386:GLY:O	2.23	0.71
1:E:407:GLU:N	3:N:63:LYS:HD2	2.06	0.70
1:E:198:ASP:OD1	1:E:215:ARG:NH1	2.24	0.70
1:E:397:TYR:HH	3:N:58:ARG:N	1.89	0.69
3:N:344:ALA:HB1	2:J:69:ILE:HD11	1.73	0.69
4:K:111:LEU:HB3	4:K:117:LEU:HB2	1.73	0.69
2:F:69:ILE:HD11	3:G:344:ALA:HB1	1.75	0.68
4:H:111:LEU:HB3	4:H:117:LEU:HB2	1.75	0.68
3:G:321:ARG:NH1	1:I:155:THR:OG1	2.26	0.68
1:A:358:ILE:HD11	1:A:416:LEU:HD13	1.76	0.68
3:C:235:ARG:HG3	3:C:249:PHE:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:MET:HE1	3:C:321:ARG:HG2	1.77	0.66
3:N:372:ARG:HG3	2:J:15:LEU:HD11	1.78	0.66
3:N:76:HIS:NE2	3:N:119:ASP:O	2.31	0.65
1:A:242:ARG:HG2	4:D:12:GLN:HE22	1.62	0.64
1:E:312:GLN:NE2	3:G:124:PRO:O	2.20	0.64
3:N:183:ILE:O	3:N:262:ARG:NH2	2.29	0.64
3:N:347:LEU:HD21	2:J:39:LYS:HB3	1.77	0.64
2:J:69:ILE:HG23	4:K:18:PRO:HA	1.80	0.64
3:G:187:ASP:OD1	3:G:258:GLN:NE2	2.32	0.63
3:G:191:ILE:HG22	3:G:264:LEU:HD23	1.82	0.62
1:A:229:TYR:HB3	1:A:236:PHE:HB2	1.81	0.62
1:A:278:ARG:HD2	1:A:316:TYR:OH	2.00	0.61
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.83	0.61
1:I:155:THR:HG22	1:I:156:GLN:H	1.66	0.61
1:A:167:LEU:HB2	1:A:179:PRO:HG2	1.83	0.60
1:I:269:ASP:O	1:I:294:LYS:NZ	2.34	0.60
3:N:304:GLU:O	3:N:313:ARG:NH1	2.34	0.60
3:N:388:ASP:OD1	4:K:58:SER:OG	2.17	0.60
1:A:263:THR:HG22	1:A:265:TYR:H	1.66	0.59
1:A:179:PRO:HB3	1:A:257:LEU:HD22	1.84	0.59
1:E:406:ASN:HA	3:N:63:LYS:HD2	1.84	0.59
1:E:208:LYS:NZ	3:G:132:GLU:OE2	2.35	0.58
3:G:235:ARG:HG3	3:G:249:PHE:HB3	1.84	0.58
3:G:361:TRP:CZ3	4:H:39:LYS:HE2	2.39	0.58
3:N:374:LYS:HE2	2:J:11:LEU:HD11	1.86	0.58
1:E:389:LYS:HD2	3:N:119:ASP:HA	1.86	0.58
3:N:368:ILE:HD13	2:J:19:LEU:HD23	1.85	0.58
1:I:371:ASP:HB2	3:C:72:ASN:HB2	1.85	0.57
3:N:188:GLU:HG2	3:N:267:LEU:HD11	1.86	0.57
3:C:304:GLU:O	3:C:313:ARG:NH1	2.38	0.57
3:C:251:THR:HB	4:D:92:THR:HG22	1.87	0.57
3:C:388:ASP:OD1	4:D:58:SER:OG	2.19	0.57
3:N:392:ILE:HD13	4:K:54:ARG:HG3	1.87	0.56
3:N:69:TYR:CD1	3:N:71:PRO:HD3	2.41	0.56
3:C:368:ILE:HD13	2:B:19:LEU:HD23	1.87	0.56
1:I:174:LYS:HB3	3:N:133:TYR:CG	2.41	0.56
3:N:73:ASP:HB2	3:N:123:THR:HB	1.87	0.56
3:C:69:TYR:CD1	3:C:71:PRO:HD3	2.41	0.56
3:C:76:HIS:NE2	3:C:120:TYR:HA	2.19	0.56
1:I:270:PRO:HB3	3:C:306:ILE:HG12	1.88	0.56
1:A:168:ASN:ND2	1:A:192:GLU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:HIS:ND1	1:E:366:LYS:O	2.39	0.55
3:C:344:ALA:HB1	2:B:69:ILE:HD11	1.87	0.55
3:N:372:ARG:HG2	3:N:391:LEU:HD23	1.88	0.55
4:H:88:VAL:O	4:H:92:THR:HG23	2.06	0.55
1:I:223:PRO:HB3	1:I:239:ILE:HD11	1.87	0.55
3:C:252:GLN:H	4:D:92:THR:HG22	1.71	0.55
4:D:88:VAL:O	4:D:92:THR:HG23	2.07	0.55
2:F:69:ILE:HG23	4:H:18:PRO:HA	1.89	0.55
2:F:19:LEU:HD23	3:G:368:ILE:HD13	1.88	0.55
3:G:252:GLN:HG3	4:H:92:THR:HG21	1.89	0.55
1:E:278:ARG:HD2	1:E:316:TYR:OH	2.06	0.54
1:A:337:PRO:HB2	1:A:341:LEU:HD21	1.88	0.54
1:A:164:VAL:HG23	1:I:295:GLU:HB3	1.88	0.54
1:A:187:ILE:O	1:A:190:THR:HG22	2.08	0.54
1:E:445:TRP:HD1	4:H:5:LEU:HD21	1.71	0.54
2:F:33:GLN:HE22	3:G:354:ARG:NH1	2.04	0.54
1:E:407:GLU:H	3:N:63:LYS:HD2	1.72	0.54
3:C:344:ALA:CB	2:B:69:ILE:HD11	2.39	0.53
1:A:445:TRP:HB2	3:C:318:ARG:HH11	1.72	0.53
2:B:12:LYS:O	2:B:16:LYS:HG2	2.08	0.53
1:E:369:THR:OG1	3:N:71:PRO:HD2	2.09	0.53
1:E:393:ILE:HG23	1:E:403:ILE:HG23	1.91	0.53
1:E:403:ILE:HB	3:N:66:LEU:O	2.09	0.53
1:I:369:THR:HG23	1:I:372:GLU:H	1.74	0.53
3:N:379:LYS:HG2	3:N:384:ILE:O	2.09	0.53
4:H:42:TYR:CD2	4:H:76:LEU:HD21	2.44	0.53
3:N:76:HIS:HD2	3:N:120:TYR:HA	1.71	0.52
3:G:251:THR:HB	4:H:92:THR:HG22	1.90	0.52
3:G:209:MET:SD	3:C:321:ARG:NH1	2.83	0.52
3:G:366:LEU:HD11	4:H:77:LEU:HD12	1.92	0.52
3:N:233:ASN:O	3:N:237:GLN:HB2	2.09	0.52
3:G:119:ASP:OD1	3:G:120:TYR:N	2.43	0.52
3:C:188:GLU:HB3	3:C:267:LEU:HD21	1.92	0.51
2:B:71:LYS:HZ1	2:B:86:SER:N	2.08	0.51
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.46	0.51
1:A:174:LYS:HB3	3:C:133:TYR:CG	2.46	0.51
1:A:391:LEU:HB2	1:A:393:ILE:HG12	1.93	0.51
1:I:232:ASP:OD1	1:I:232:ASP:N	2.44	0.51
3:G:280:ARG:O	3:G:284:ILE:HG12	2.10	0.51
3:N:191:ILE:HG22	3:N:264:LEU:HD13	1.91	0.51
3:C:247:THR:OG1	3:C:248:HIS:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:ASN:HD21	3:C:184:LEU:H	1.59	0.51
3:C:366:LEU:HD11	4:D:77:LEU:HD12	1.91	0.51
1:E:270:PRO:HB3	3:N:306:ILE:HG12	1.91	0.50
1:A:445:TRP:HB2	3:C:318:ARG:NH1	2.26	0.50
4:D:39:LYS:HA	4:D:42:TYR:CE2	2.46	0.50
3:G:71:PRO:HD2	1:A:369:THR:OG1	2.11	0.50
1:I:230:ARG:HB3	3:N:147:TYR:CE2	2.46	0.50
1:E:232:ASP:OD1	1:E:232:ASP:N	2.45	0.50
1:A:232:ASP:N	1:A:232:ASP:OD1	2.44	0.50
1:I:229:TYR:HB3	1:I:236:PHE:HB2	1.93	0.50
3:N:366:LEU:HD13	4:K:76:LEU:HB3	1.93	0.50
3:G:316:GLU:HG2	3:N:303:LYS:O	2.12	0.49
3:C:191:ILE:HG22	3:C:264:LEU:HD13	1.94	0.49
1:E:364:HIS:CE1	1:E:368:ILE:HD13	2.47	0.49
3:C:168:ASP:OD1	3:C:282:ARG:NH1	2.45	0.49
4:H:62:HIS:HB3	4:H:65:GLU:HB2	1.95	0.49
1:E:172:MET:HE1	1:E:308:LEU:HD22	1.95	0.49
3:N:242:ILE:HD12	3:N:249:PHE:HE1	1.77	0.49
3:C:188:GLU:OE2	3:C:262:ARG:HD3	2.11	0.49
1:I:369:THR:CB	3:C:71:PRO:HD2	2.43	0.49
2:F:12:LYS:O	2:F:16:LYS:HG3	2.13	0.49
4:D:111:LEU:HB3	4:D:117:LEU:HB2	1.94	0.49
1:E:174:LYS:HB3	3:G:133:TYR:CD1	2.47	0.48
3:C:376:LYS:HD2	3:C:380:ARG:NH2	2.29	0.48
1:A:269:ASP:O	1:A:294:LYS:NZ	2.45	0.48
1:I:385:LEU:HB3	3:C:120:TYR:HB2	1.94	0.48
3:N:390:ASP:HB3	2:J:15:LEU:HD22	1.96	0.48
3:G:240:HIS:HA	3:G:245:HIS:CD2	2.49	0.48
3:N:365:GLU:OE2	2:J:22:ARG:NH1	2.47	0.48
1:E:196:TYR:HB2	1:E:205:PHE:HB2	1.95	0.48
2:F:65:TYR:HE2	3:G:340:GLU:HG3	1.79	0.48
1:A:363:GLU:OE2	1:A:417:LYS:NZ	2.40	0.48
4:K:62:HIS:HB3	4:K:65:GLU:HB2	1.96	0.48
3:N:316:GLU:HG2	3:C:303:LYS:O	2.14	0.47
3:C:252:GLN:HG3	4:D:92:THR:HG21	1.96	0.47
3:G:119:ASP:HA	1:A:389:LYS:HD2	1.97	0.47
3:C:75:LYS:O	3:C:76:HIS:CG	2.66	0.47
1:I:445:TRP:HD1	4:K:5:LEU:HD21	1.78	0.47
1:E:393:ILE:HG22	1:E:403:ILE:HD12	1.96	0.47
3:C:252:GLN:H	4:D:92:THR:CG2	2.28	0.47
1:I:360:LEU:HD23	1:I:373:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:187:ASP:O	3:N:191:ILE:HG12	2.15	0.47
3:C:242:ILE:HD12	3:C:249:PHE:HE1	1.79	0.47
1:E:344:LEU:HD12	1:E:344:LEU:H	1.78	0.47
3:N:240:HIS:HA	3:N:245:HIS:NE2	2.30	0.47
3:N:338:HIS:CE1	3:N:342:LYS:HD2	2.49	0.47
3:N:375:ILE:HD12	2:J:15:LEU:HD13	1.96	0.47
1:E:403:ILE:O	3:N:65:HIS:HB2	2.15	0.47
2:F:11:LEU:HD21	3:G:374:LYS:HE2	1.97	0.47
3:G:306:ILE:HG12	1:A:270:PRO:HB3	1.97	0.47
4:K:10:THR:HG21	4:K:104:LEU:HD13	1.97	0.47
3:G:188:GLU:HG2	3:G:267:LEU:HD11	1.97	0.47
3:G:203:ARG:HD2	3:G:223:THR:OG1	2.15	0.47
1:I:228:ILE:HB	1:I:431:TRP:HB2	1.97	0.47
3:N:185:THR:HG23	3:N:188:GLU:H	1.80	0.47
4:D:14:VAL:HG12	4:D:100:HIS:CD2	2.49	0.47
1:A:412:ARG:HA	1:A:415:ARG:HE	1.80	0.46
3:G:252:GLN:H	4:H:92:THR:HG22	1.80	0.46
1:E:262:ALY:HE2	1:E:262:ALY:HH31	1.60	0.46
1:I:344:LEU:HD12	1:I:344:LEU:H	1.80	0.46
2:J:70:ILE:HG21	2:J:92:ASP:HB3	1.97	0.46
3:G:66:LEU:HB3	1:A:403:ILE:HB	1.96	0.46
1:A:262:ALY:HH31	1:A:262:ALY:HE2	1.59	0.46
1:I:313:ARG:NH2	3:N:75:LYS:HD2	2.30	0.46
1:A:187:ILE:HD12	1:A:187:ILE:H	1.81	0.46
1:I:343:ASP:HB3	3:N:121:ILE:HG12	1.97	0.46
3:N:333:ARG:HB2	2:J:76:PHE:CZ	2.51	0.46
3:N:244:SER:O	3:N:246:LYS:HD2	2.16	0.46
4:K:45:LYS:NZ	4:K:71:GLU:OE1	2.36	0.46
3:G:68:ILE:O	3:G:68:ILE:HG13	2.14	0.45
3:G:187:ASP:O	3:G:191:ILE:HG12	2.16	0.45
1:A:393:ILE:HG23	1:A:403:ILE:HG23	1.98	0.45
1:I:393:ILE:CG2	1:I:403:ILE:HG23	2.46	0.45
2:F:95:PHE:O	2:F:98:SER:OG	2.31	0.45
1:I:262:ALY:HH31	1:I:262:ALY:HE2	1.74	0.45
2:F:69:ILE:HD11	3:G:344:ALA:CB	2.45	0.45
3:G:308:PRO:HB3	1:A:297:ALA:HB2	1.98	0.45
1:I:167:LEU:HD13	1:I:195:ILE:HD12	1.99	0.45
1:E:295:GLU:HB3	1:I:164:VAL:HG23	1.99	0.45
3:C:68:ILE:HG13	3:C:68:ILE:O	2.17	0.45
4:D:21:PHE:CD1	2:B:69:ILE:HD13	2.51	0.45
2:F:21:ASP:O	2:F:25:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:HIS:NE2	1:A:368:ILE:HD13	2.31	0.45
3:C:203:ARG:HD2	3:C:223:THR:OG1	2.16	0.45
1:I:364:HIS:NE2	1:I:368:ILE:HD13	2.32	0.44
1:I:406:ASN:O	1:I:409:ILE:HB	2.17	0.44
3:C:185:THR:HG23	3:C:188:GLU:H	1.82	0.44
3:G:252:GLN:H	4:H:92:THR:CG2	2.29	0.44
3:G:308:PRO:HG3	1:A:295:GLU:O	2.17	0.44
3:C:75:LYS:O	3:C:76:HIS:CD2	2.71	0.44
1:I:369:THR:HB	3:C:71:PRO:HD2	1.98	0.44
1:I:393:ILE:HD12	1:I:405:LEU:HD23	1.99	0.44
3:N:234:LEU:HD23	4:K:102:ASN:ND2	2.32	0.44
3:C:333:ARG:HB3	2:B:76:PHE:CZ	2.53	0.44
1:E:168:ASN:ND2	1:E:192:GLU:O	2.49	0.44
1:A:369:THR:O	1:A:373:ILE:HG13	2.18	0.44
1:I:240:ASP:HA	1:I:272:LEU:HD23	1.99	0.44
1:I:372:GLU:O	1:I:376:MET:HG3	2.18	0.44
1:E:169:ARG:NH1	1:E:178:GLU:HB2	2.33	0.44
1:E:223:PRO:HB3	1:E:239:ILE:HD11	1.98	0.44
3:N:280:ARG:O	3:N:284:ILE:HG12	2.18	0.44
3:C:187:ASP:O	3:C:191:ILE:HG12	2.18	0.44
2:B:70:ILE:HG21	2:B:92:ASP:HB3	2.00	0.44
1:E:230:ARG:HB3	3:G:147:TYR:CE2	2.53	0.44
3:N:203:ARG:HD2	3:N:223:THR:OG1	2.17	0.44
1:E:393:ILE:CG2	1:E:403:ILE:HG23	2.48	0.44
4:D:62:HIS:HB3	4:D:65:GLU:HB2	1.99	0.44
1:E:343:ASP:HB3	3:G:121:ILE:HG12	2.00	0.43
3:N:76:HIS:HE2	3:N:121:ILE:HG13	1.83	0.43
1:I:208:LYS:NZ	3:N:132:GLU:OE2	2.46	0.43
1:E:366:LYS:O	3:N:66:LEU:HD21	2.17	0.43
3:G:329:LEU:O	3:G:333:ARG:HG2	2.18	0.43
3:G:387:GLU:O	3:G:391:LEU:HD13	2.18	0.43
1:I:401:HIS:CG	3:C:74:LEU:HD11	2.54	0.43
3:N:359:LEU:O	3:N:363:ASN:ND2	2.51	0.43
3:G:384:ILE:O	4:H:59:ILE:HD11	2.18	0.43
1:E:406:ASN:CA	3:N:63:LYS:HD2	2.48	0.43
1:I:174:LYS:O	3:N:130:TRP:N	2.50	0.43
4:H:51:LYS:HE3	4:H:55:GLN:NE2	2.34	0.43
1:E:157:ASN:HB3	1:E:160:GLU:HB2	1.99	0.43
1:E:175:TYR:CD1	1:E:310:GLN:HG3	2.54	0.43
1:A:360:LEU:HD23	1:A:373:ILE:HG23	2.00	0.43
3:C:73:ASP:HB2	3:C:123:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:ARG:CG	3:C:249:PHE:HB3	2.48	0.43
3:C:242:ILE:CD1	3:C:249:PHE:HE1	2.31	0.43
1:I:167:LEU:HB2	1:I:179:PRO:HG2	2.00	0.43
3:N:379:LYS:NZ	3:N:388:ASP:OD1	2.51	0.43
2:J:37:TYR:O	2:J:41:THR:HG23	2.18	0.43
4:D:32:ASP:OD2	2:B:100:ALA:N	2.49	0.43
1:A:393:ILE:HD13	1:A:409:ILE:HD13	2.01	0.42
1:I:168:ASN:ND2	1:I:192:GLU:O	2.49	0.42
4:H:46:GLU:HG2	4:H:50:HIS:CD2	2.54	0.42
1:E:247:TRP:HH2	1:E:275:CYS:HG	1.67	0.42
3:N:296:LYS:HB3	3:N:309:TYR:O	2.20	0.42
3:C:215:LEU:HD12	3:C:219:GLU:HB3	2.02	0.42
2:J:95:PHE:O	2:J:98:SER:OG	2.34	0.42
1:A:311:TYR:HB3	1:A:316:TYR:CE1	2.54	0.42
3:C:237:GLN:O	3:C:241:GLU:HG3	2.20	0.42
1:E:221:ARG:HD3	1:E:282:LEU:O	2.20	0.42
3:G:351:VAL:O	3:G:355:GLU:HG2	2.19	0.42
3:N:204:GLN:CD	3:N:215:LEU:HD13	2.40	0.42
1:E:214:TYR:HH	3:G:158:CYS:HG	1.66	0.42
1:A:394:LEU:HD13	1:A:394:LEU:HA	1.92	0.42
1:I:393:ILE:HG23	1:I:403:ILE:HG23	2.02	0.42
1:E:364:HIS:NE2	1:E:368:ILE:HD13	2.34	0.42
1:A:372:GLU:O	1:A:376:MET:HG3	2.20	0.42
3:G:59:LYS:HD2	3:G:60:ILE:H	1.84	0.42
3:G:375:ILE:O	3:G:379:LYS:N	2.47	0.42
3:N:235:ARG:HG3	3:N:249:PHE:HB3	2.00	0.42
3:N:323:THR:HG21	3:C:209:MET:HE3	2.01	0.42
2:F:69:ILE:HD13	4:H:21:PHE:CD1	2.55	0.42
1:A:169:ARG:NH2	1:A:178:GLU:OE2	2.48	0.42
1:A:244:GLN:OE1	3:C:153:THR:HA	2.20	0.42
1:I:360:LEU:O	1:I:364:HIS:HB2	2.20	0.42
1:E:167:LEU:HB2	1:E:179:PRO:HG3	2.01	0.41
1:I:163:ARG:O	3:N:309:TYR:OH	2.27	0.41
2:F:76:PHE:CZ	3:G:333:ARG:HB2	2.54	0.41
3:G:303:LYS:O	3:C:316:GLU:HG2	2.20	0.41
2:J:3:ASP:OD1	2:J:3:ASP:N	2.53	0.41
3:G:255:PRO:HG2	3:G:258:GLN:HG2	2.02	0.41
3:N:171:PHE:O	3:N:175:GLN:HB2	2.20	0.41
2:J:39:LYS:HG3	2:J:43:TYR:CE2	2.56	0.41
1:E:369:THR:HG23	1:E:372:GLU:H	1.84	0.41
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:66:LEU:HD11	1:A:366:LYS:O	2.20	0.41
1:A:313:ARG:NH2	3:C:75:LYS:HD2	2.36	0.41
3:N:343:ASN:HB3	2:J:43:TYR:CD2	2.55	0.41
2:J:41:THR:HG22	2:J:93:ARG:NH2	2.23	0.41
4:K:52:PHE:HB2	4:K:62:HIS:HD2	1.85	0.41
4:D:10:THR:O	4:D:14:VAL:HG22	2.19	0.41
1:E:245:ARG:NH1	1:E:269:ASP:OD1	2.47	0.41
4:H:62:HIS:CG	4:H:63:PRO:HD2	2.56	0.41
4:K:10:THR:O	4:K:14:VAL:HG22	2.21	0.41
3:G:206:PHE:HB3	3:G:209:MET:HG3	2.03	0.41
1:A:156:GLN:HE22	3:C:296:LYS:HB2	1.86	0.41
1:A:228:ILE:HB	1:A:431:TRP:HB2	2.03	0.41
1:A:262:ALY:HG2	1:A:304:CYS:SG	2.61	0.41
1:A:442:ARG:HB2	3:C:318:ARG:HH22	1.86	0.41
4:D:17:LEU:N	4:D:18:PRO:HD2	2.35	0.41
1:E:228:ILE:HB	1:E:431:TRP:HB2	2.02	0.41
1:A:267:ASP:HA	3:C:312:PHE:HB3	2.02	0.41
3:N:359:LEU:HA	4:K:83:GLN:HG2	2.03	0.41
1:E:290:PHE:HB3	1:E:305:ILE:HG13	2.03	0.41
3:G:366:LEU:HD11	4:H:77:LEU:CD1	2.51	0.41
1:A:167:LEU:HD13	1:A:195:ILE:HD12	2.01	0.41
1:A:442:ARG:HB2	3:C:318:ARG:NH2	2.36	0.41
3:N:385:SER:HB3	4:K:59:ILE:HD11	2.02	0.41
3:G:361:TRP:HZ3	4:H:39:LYS:HE2	1.85	0.41
1:A:174:LYS:HB3	3:C:133:TYR:CD1	2.56	0.41
1:I:253:LEU:HD11	3:N:295:LEU:HD21	2.03	0.40
1:E:200:PHE:HB3	1:E:220:LEU:HD23	2.03	0.40
2:F:15:LEU:HD13	3:G:375:ILE:HD12	2.02	0.40
3:G:150:PHE:CZ	3:G:152:ALA:HB3	2.56	0.40
3:G:359:LEU:HG	3:G:363:ASN:ND2	2.36	0.40
3:N:351:VAL:O	3:N:355:GLU:HG2	2.21	0.40
2:F:13:ALA:HA	2:F:16:LYS:HD2	2.03	0.40
3:G:189:PHE:CE1	3:G:275:ILE:HD12	2.57	0.40
1:I:445:TRP:CG	3:N:318:ARG:HG3	2.57	0.40
3:C:283:LYS:HG2	3:C:291:ILE:HD11	2.03	0.40
2:B:8:TYR:CZ	2:B:12:LYS:HD3	2.56	0.40
3:C:260:ASN:OD1	3:C:260:ASN:N	2.49	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%)	278 (96%)	11 (4%)	0	100	100
1	E	290/305 (95%)	278 (96%)	12 (4%)	0	100	100
1	I	289/305 (95%)	278 (96%)	11 (4%)	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%)	67 (96%)	3 (4%)	0	100	100
3	C	288/351 (82%)	280 (97%)	8 (3%)	0	100	100
3	G	291/351 (83%)	282 (97%)	9 (3%)	0	100	100
3	N	289/351 (82%)	280 (97%)	9 (3%)	0	100	100
4	D	118/120 (98%)	118 (100%)	0	0	100	100
4	H	118/120 (98%)	118 (100%)	0	0	100	100
4	K	118/120 (98%)	118 (100%)	0	0	100	100
All	All	2302/2667 (86%)	2234 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/283 (95%)	270 (100%)	0	100	100
1	E	272/283 (96%)	271 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	270/283 (95%)	270 (100%)	0	100	100
2	B	73/100 (73%)	73 (100%)	0	100	100
2	F	69/100 (69%)	69 (100%)	0	100	100
2	J	69/100 (69%)	69 (100%)	0	100	100
3	C	280/333 (84%)	278 (99%)	2 (1%)	84	93
3	G	283/333 (85%)	282 (100%)	1 (0%)	91	96
3	N	280/333 (84%)	277 (99%)	3 (1%)	73	89
4	D	111/111 (100%)	111 (100%)	0	100	100
4	H	111/111 (100%)	111 (100%)	0	100	100
4	K	111/111 (100%)	111 (100%)	0	100	100
All	All	2199/2481 (89%)	2192 (100%)	7 (0%)	92	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	215	ARG
3	G	311	CYS
3	N	74	LEU
3	N	215	LEU
3	N	311	CYS
3	C	63	LYS
3	C	311	CYS

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

Mol	Chain	Res	Type
2	F	33	GLN
4	D	12	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	I	262	1	10,11,12	0.83	0	7,12,14	1.18	1 (14%)
1	ALY	A	262	1	10,11,12	0.83	0	7,12,14	0.71	0
1	ALY	E	262	1	10,11,12	0.82	0	7,12,14	0.70	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	I	262	1	-	2/9/10/12	-
1	ALY	A	262	1	-	2/9/10/12	-
1	ALY	E	262	1	-	2/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	262	ALY	CE-NZ-CH	2.29	126.08	122.56

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	262	ALY	1	0
1	A	262	ALY	2	0
1	E	262	ALY	1	0

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	291/305 (95%)	0.11	6 (2%) 63 46	23, 54, 102, 144	0
1	E	292/305 (95%)	0.25	6 (2%) 63 46	30, 63, 115, 127	0
1	I	291/305 (95%)	0.08	8 (2%) 54 38	27, 55, 95, 113	0
2	B	79/113 (69%)	0.90	15 (18%) 1 0	42, 76, 125, 149	0
2	F	75/113 (66%)	0.59	8 (10%) 6 3	60, 84, 123, 136	0
2	J	76/113 (67%)	0.52	7 (9%) 9 5	46, 73, 113, 138	0
3	C	294/351 (83%)	0.39	21 (7%) 16 9	30, 67, 116, 158	0
3	G	297/351 (84%)	0.67	31 (10%) 6 4	37, 79, 125, 152	0
3	N	295/351 (84%)	0.30	17 (5%) 23 14	36, 69, 122, 145	0
4	D	120/120 (100%)	0.00	0 100 100	31, 56, 79, 91	0
4	H	120/120 (100%)	0.53	5 (4%) 36 23	41, 72, 116, 119	0
4	K	120/120 (100%)	0.01	1 (0%) 86 73	31, 55, 80, 92	0
All	All	2350/2667 (88%)	0.32	125 (5%) 26 16	23, 65, 114, 158	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	86	SER	6.4
1	A	397	TYR	5.9
3	G	64	GLN	4.9
3	C	62	VAL	4.9
3	G	398	ARG	4.7
3	G	396	ARG	4.6
3	G	181	SER	4.6
3	C	258	GLN	4.4
2	B	104	LYS	4.4
3	G	264	LEU	4.2
1	E	405	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	63	LYS	3.9
3	N	68	ILE	3.8
2	J	46	HIS	3.8
2	F	87	ALA	3.8
3	C	321	ARG	3.7
2	B	46	HIS	3.7
1	E	445	TRP	3.7
3	G	399	PRO	3.7
3	G	58	ARG	3.7
3	G	258	GLN	3.7
2	B	1	MET	3.6
2	B	4	GLU	3.6
3	G	397	LYS	3.6
3	C	259	MET	3.4
3	G	182	ASP	3.4
3	G	183	ILE	3.2
3	C	183	ILE	3.2
3	G	176	VAL	3.2
3	G	274	LYS	3.2
3	N	184	LEU	3.2
3	C	64	GLN	3.1
3	N	258	GLN	3.1
1	I	397	TYR	3.1
2	J	76	PHE	3.1
3	N	67	LYS	3.1
1	I	445	TRP	3.0
3	N	182	ASP	3.0
2	B	105	GLN	3.0
3	G	180	SER	3.0
2	B	76	PHE	2.9
3	C	271	PHE	2.9
3	G	245	HIS	2.8
4	H	120	VAL	2.8
1	I	394	LEU	2.8
2	B	2	THR	2.8
2	B	3	ASP	2.8
3	C	74	LEU	2.8
3	N	227	SER	2.8
3	N	65	HIS	2.7
3	G	178	LYS	2.7
3	C	182	ASP	2.7
3	G	270	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	65	HIS	2.7
3	C	181	SER	2.6
3	N	257	SER	2.6
3	G	65	HIS	2.6
3	G	158	CYS	2.6
3	G	67	LYS	2.6
3	C	322	LYS	2.6
3	N	321	ARG	2.6
1	A	370	ILE	2.6
3	G	120	TYR	2.6
2	B	5	LEU	2.5
3	C	320	PRO	2.5
3	C	274	LYS	2.5
3	G	189	PHE	2.5
1	E	404	PHE	2.5
3	G	68	ILE	2.5
3	G	70	LEU	2.5
3	N	183	ILE	2.5
1	A	395	ARG	2.5
1	I	169	ARG	2.5
3	N	76	HIS	2.5
2	J	3	ASP	2.4
4	H	116	VAL	2.4
1	E	361	LEU	2.4
2	B	8	TYR	2.4
1	I	361	LEU	2.4
3	C	71	PRO	2.4
3	G	184	LEU	2.4
1	A	405	LEU	2.4
2	J	88	PHE	2.3
4	H	69	ASP	2.3
2	J	2	THR	2.3
2	F	5	LEU	2.3
2	B	90	ASN	2.3
2	F	16	LYS	2.3
4	H	42	TYR	2.3
1	I	391	LEU	2.3
3	N	388	ASP	2.3
2	F	88	PHE	2.3
3	G	71	PRO	2.3
1	A	368	ILE	2.3
3	G	366	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	365	GLN	2.3
2	J	1	MET	2.2
2	B	102	TYR	2.2
3	G	268	ILE	2.2
3	N	158	CYS	2.2
2	B	75	THR	2.2
3	C	186	GLU	2.2
3	C	171	PHE	2.2
3	C	268	ILE	2.2
3	C	176	VAL	2.2
2	J	70	ILE	2.2
4	K	59	ILE	2.2
3	N	245	HIS	2.2
2	B	65	TYR	2.2
2	F	90	ASN	2.2
2	F	65	TYR	2.2
1	E	396	TYR	2.1
3	N	274	LYS	2.1
3	G	361	TRP	2.1
3	C	319	HIS	2.1
4	H	54	ARG	2.1
1	A	393	ILE	2.1
3	N	322	LYS	2.1
2	B	103	VAL	2.0
3	G	164	MET	2.0
3	N	176	VAL	2.0
1	E	155	THR	2.0
2	F	44	PHE	2.0
3	G	157	CYS	2.0
1	I	357	LEU	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	0.95	0.20	26,46,64,66	0
1	ALY	I	262	12/13	0.95	0.18	29,43,55,68	0
1	ALY	A	262	12/13	0.96	0.18	22,41,49,53	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.