



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:06 pm BST

PDB ID : 3EX7
Title : The crystal structure of EJC in its transition state
Authors : Andersen, G.R.; Nielsen, K.H.
Deposited on : 2008-10-16
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

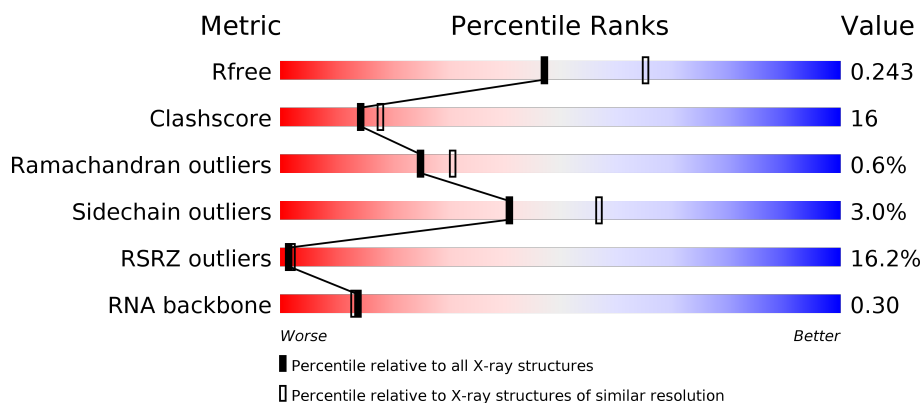
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	146	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	E	146	<div> <div>38%</div> <div>51%</div> <div>45%</div> <div>..</div> </div>
2	B	126	<div> <div>10%</div> <div>51%</div> <div>22%</div> <div>25%</div> </div>
2	G	126	<div> <div>44%</div> <div>39%</div> <div>33%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	413	<div><div></div><div>4%</div><div>76%</div><div>17%</div><div>• 5%</div></div>
3	H	413	<div><div></div><div>14%</div><div>65%</div><div>27%</div><div>• 5%</div></div>
4	D	146	<div><div></div><div>6%</div><div>23%</div><div>14%</div><div>• 61%</div></div>
4	I	146	<div><div></div><div>9%</div><div>24%</div><div>18%</div><div>• 58%</div></div>
5	F	6	<div><div></div><div>50%</div><div>17%</div><div>17%</div><div>17%</div></div>
5	J	6	<div><div></div><div>33%</div><div>17%</div><div>33%</div><div>17%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11856 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 Protein mago nashi homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1196	772	200	221	3			
1	E	142	Total	C	N	O	S	0	0	0
			1182	765	198	216	3			

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	0	0	0
			750	476	126	145	3			
2	G	91	Total	C	N	O	S	0	0	0
			730	463	122	142	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	LEU	-	EXPRESSION TAG	UNP Q9Y5S9
B	176	GLU	-	EXPRESSION TAG	UNP Q9Y5S9
G	175	LEU	-	EXPRESSION TAG	UNP Q9Y5S9
G	176	GLU	-	EXPRESSION TAG	UNP Q9Y5S9

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	392	Total	C	N	O	S	0	0	0
			3148	1987	548	594	19			
3	H	392	Total	C	N	O	S	0	0	0
			3148	1987	548	594	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	412	LEU	-	EXPRESSION TAG	UNP P38919
C	413	GLU	-	EXPRESSION TAG	UNP P38919
H	412	LEU	-	EXPRESSION TAG	UNP P38919
H	413	GLU	-	EXPRESSION TAG	UNP P38919

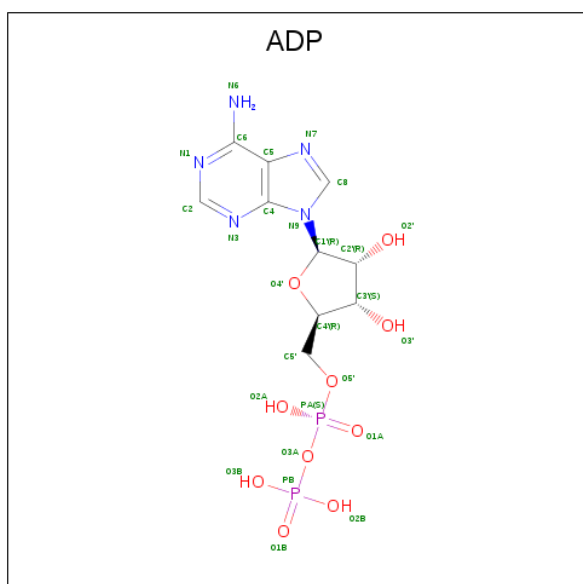
- Molecule 4 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	57	Total	C	N	O	0	0	0
			491	306	93	92			
4	I	62	Total	C	N	O	0	0	0
			533	333	101	99			

- Molecule 5 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			
5	J	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



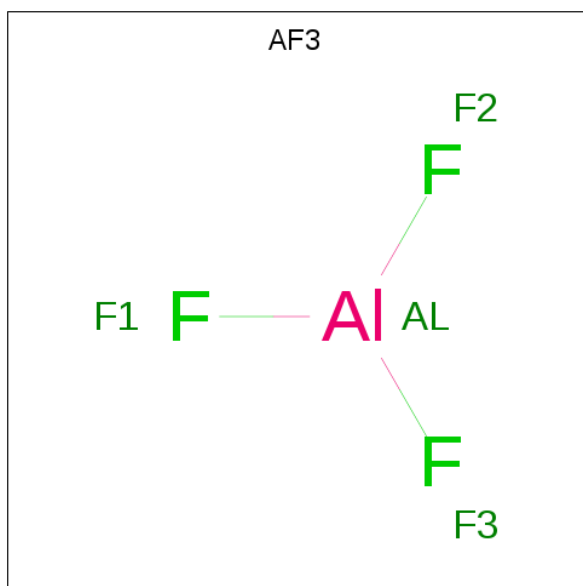
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Al	F	0	0
			4	1	3		
7	H	1	Total	Al	F	0	0
			4	1	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	72	Total	O	0	0
			72	72		
9	B	15	Total	O	0	0
			15	15		

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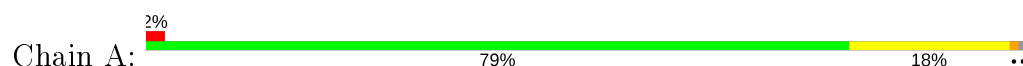
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	158	Total 158	O 158	0	0
9	D	25	Total 25	O 25	0	0
9	E	3	Total 3	O 3	0	0
9	G	2	Total 2	O 2	0	0
9	H	76	Total 76	O 76	0	0
9	I	18	Total 18	O 18	0	0
9	F	6	Total 6	O 6	0	0
9	J	5	Total 5	O 5	0	0

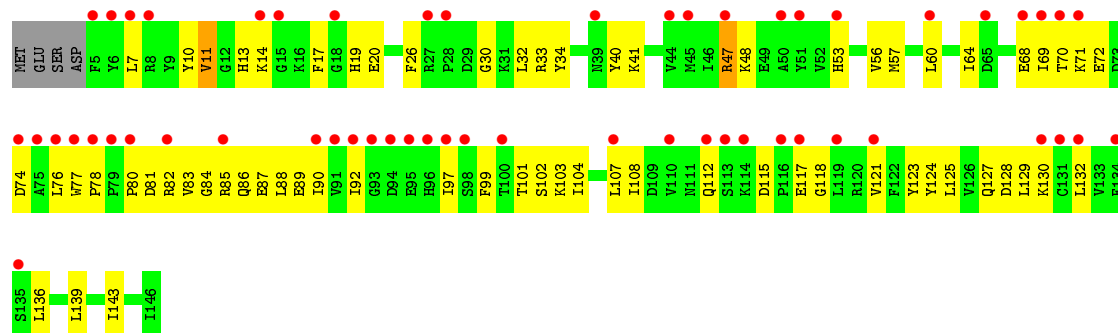
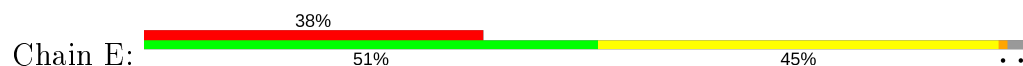
3 Residue-property plots [i](#)

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

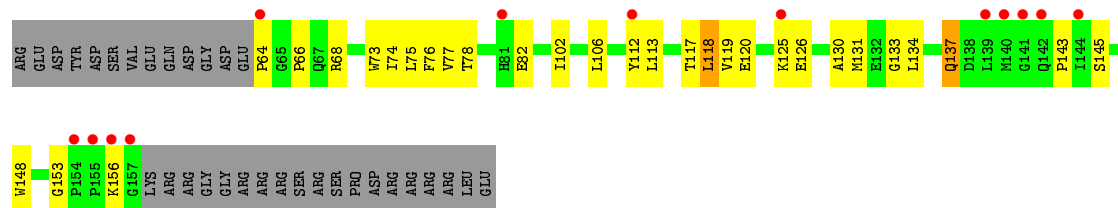
- Molecule 1: Protein mago nashi homolog



- Molecule 1: Protein mago nashi homolog

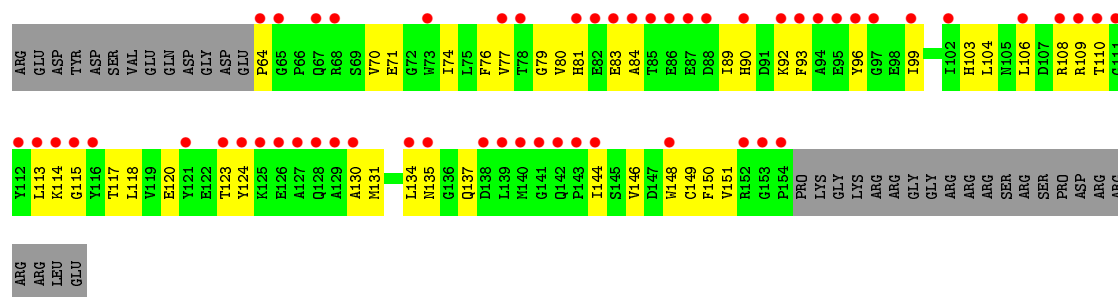


- Molecule 2: RNA-binding protein 8A

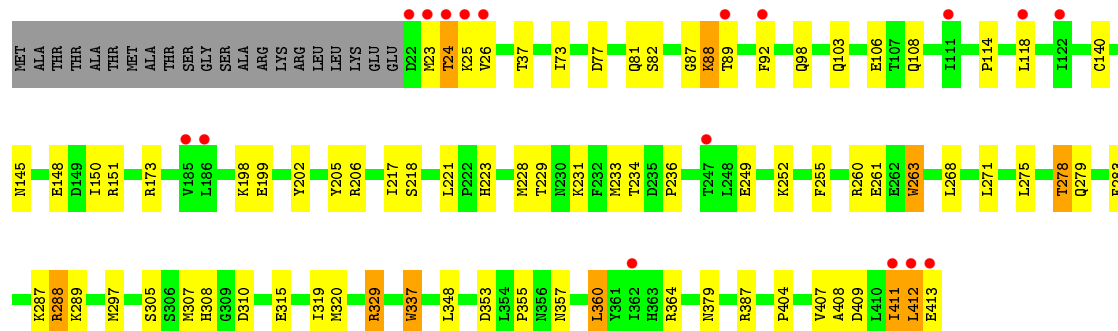
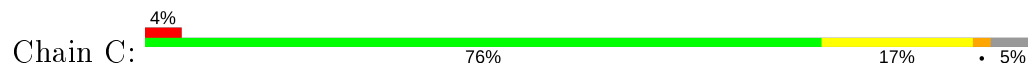


- Molecule 2: RNA-binding protein 8A

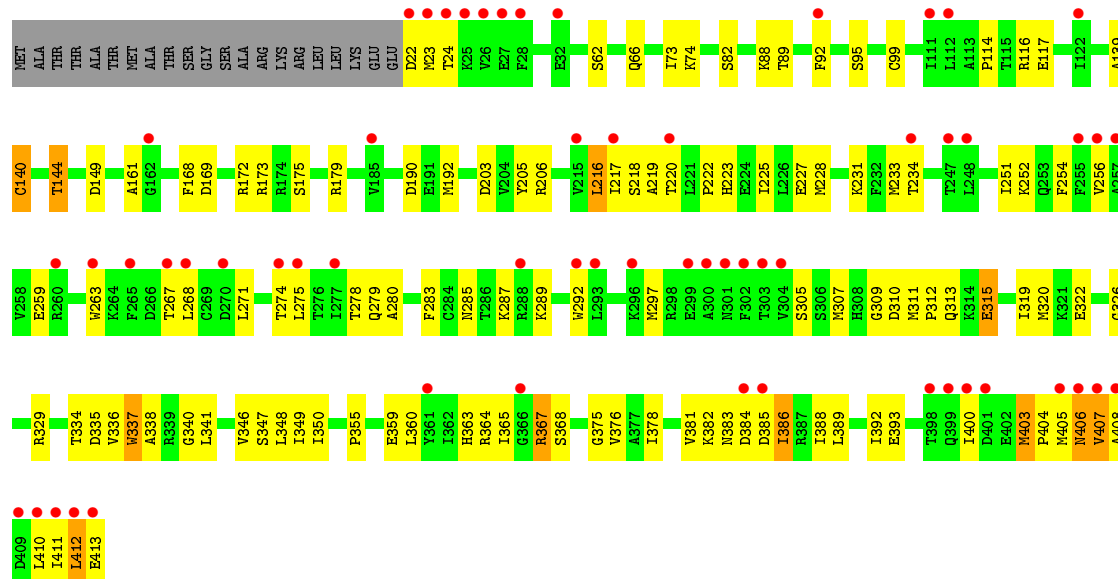




• Molecule 3: Eukaryotic initiation factor 4A-III

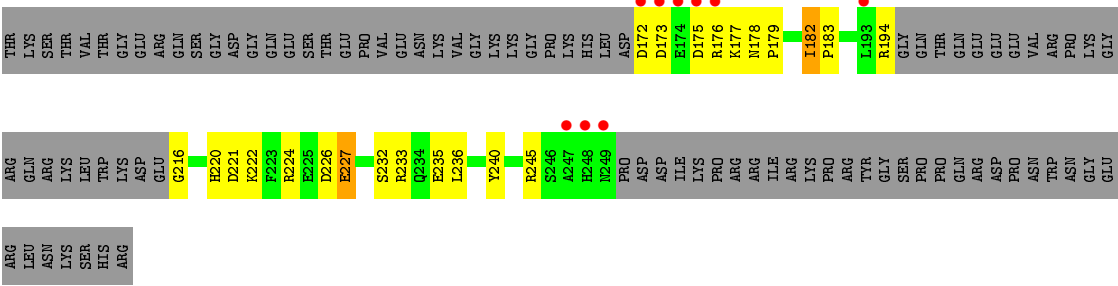


• Molecule 3: Eukaryotic initiation factor 4A-III

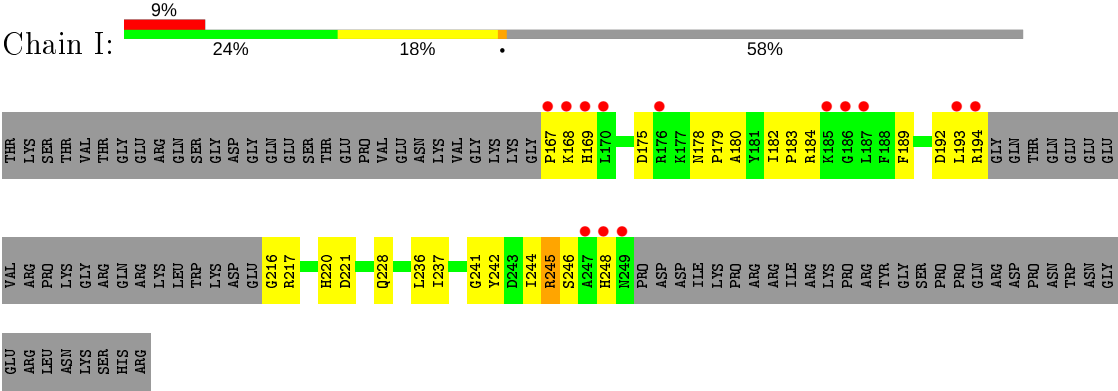


• Molecule 4: Protein CASC3





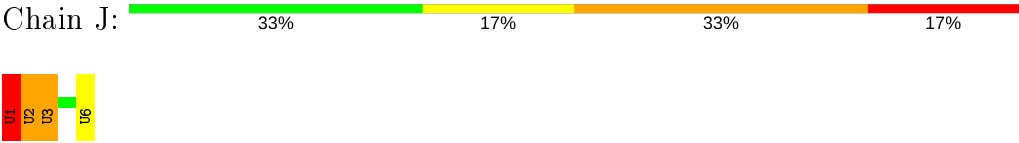
• Molecule 4: Protein CASC3



• Molecule 5: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')



• Molecule 5: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.04Å 100.75Å 145.88Å 90.00° 112.08° 90.00°	Depositor
Resolution (Å)	39.06 – 2.30 39.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.06-2.30) 99.3 (39.06-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, R_{free}	0.206 , 0.251 0.200 , 0.243	Depositor DCC
R_{free} test set	2144 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.017 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11856	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AF3

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	0.54	1/1225 (0.1%)	0.65	0/1648
1	E	0.27	0/1211	0.44	0/1629
2	B	0.36	0/769	0.53	0/1040
2	G	0.26	0/748	0.42	0/1012
3	C	0.50	1/3197 (0.0%)	0.66	0/4314
3	H	0.40	1/3197 (0.0%)	0.57	0/4314
4	D	0.42	0/503	0.55	0/673
4	I	0.33	0/547	0.50	0/732
5	F	0.88	0/128	2.89	7/196 (3.6%)
5	J	0.84	0/128	1.49	2/196 (1.0%)
All	All	0.44	3/11653 (0.0%)	0.68	9/15754 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	140	CYS	CB-SG	-5.69	1.72	1.81
1	A	131	CYS	CB-SG	-5.13	1.73	1.81
3	C	140	CYS	CB-SG	-5.05	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6	U	C1'-O4'-C4'	-30.07	85.84	109.90
5	J	1	U	P-O3'-C3'	9.53	131.14	119.70
5	F	6	U	N1-C1'-C2'	9.41	126.23	114.00
5	F	6	U	C5'-C4'-C3'	7.93	128.70	116.00
5	J	1	U	C1'-O4'-C4'	-7.46	103.93	109.90
5	F	6	U	C3'-C2'-C1'	-6.37	96.41	101.50
5	F	1	U	C4'-C3'-C2'	6.30	108.90	102.60
5	F	6	U	O5'-C5'-C4'	-5.99	100.33	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	F	1	U	O5'-C5'-C4'	5.18	121.54	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1196	0	1182	17	0
1	E	1182	0	1173	63	0
2	B	750	0	713	18	0
2	G	730	0	690	36	0
3	C	3148	0	3189	76	0
3	H	3148	0	3189	115	0
4	D	491	0	455	24	0
4	I	533	0	498	34	0
5	F	117	0	62	7	0
5	J	117	0	62	7	0
6	C	27	0	12	1	0
6	H	27	0	12	0	0
7	C	4	0	0	0	0
7	H	4	0	0	1	0
8	C	1	0	0	0	0
8	H	1	0	0	0	0
9	A	72	0	0	1	0
9	B	15	0	0	2	0
9	C	158	0	0	6	0
9	D	25	0	0	2	0
9	E	3	0	0	1	0
9	F	6	0	0	0	0
9	G	2	0	0	0	0
9	H	76	0	0	3	0
9	I	18	0	0	1	0
9	J	5	0	0	0	0
All	All	11856	0	11237	352	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 16.

All (352) 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:C:268:LEU:HD23	3:C:297:MET:HE3	1.36	1.02
4:I:169:HIS:HD2	5:F:5:U:H3	1.02	0.99
4:I:183:PRO:HG2	5:J:1:U:H5"	1.44	0.97
1:E:69:ILE:HG13	1:E:125:LEU:HD22	1.51	0.92
3:H:88:LYS:HG2	3:H:217:ILE:HG23	1.52	0.89
3:H:73:ILE:HD11	3:H:95:SER:HA	1.57	0.87
3:H:382:LYS:HG2	3:H:383:ASN:H	1.39	0.86
4:I:169:HIS:CD2	5:F:5:U:H3	1.93	0.84
3:H:252:LYS:HB2	3:H:376:VAL:HG22	1.57	0.84
3:H:381:VAL:HG13	3:H:385:ASP:HB3	1.60	0.83
3:H:405:MET:HG2	3:H:406:ASN:H	1.43	0.82
3:H:222:PRO:HB2	3:H:225:ILE:HD13	1.60	0.81
3:C:88:LYS:HE2	3:C:218:SER:C	2.02	0.80
3:H:279:GLN:NE2	3:H:326:GLY:HA2	1.97	0.79
4:I:183:PRO:CG	5:J:1:U:H5"	2.12	0.79
3:H:206:ARG:HD2	4:I:221:ASP:OD1	1.82	0.79
1:E:10:TYR:OH	1:E:19:HIS:HE1	1.66	0.78
3:H:82:SER:OG	3:H:88:LYS:HD3	1.84	0.78
3:H:289:LYS:NZ	4:I:182:ILE:HD11	1.98	0.77
3:H:278:THR:HG23	3:H:279:GLN:H	1.48	0.77
1:E:108:ILE:O	1:E:112:GLN:HG2	1.86	0.76
3:H:88:LYS:HG2	3:H:217:ILE:CG2	2.15	0.76
1:E:70:THR:HG21	1:E:92:ILE:HD11	1.68	0.76
3:C:88:LYS:HD2	3:C:217:ILE:HG23	1.68	0.75
3:C:206:ARG:HD2	4:D:221:ASP:OD1	1.87	0.74
3:H:388:ILE:HD11	4:I:193:LEU:HD21	1.70	0.73
3:C:82:SER:OG	3:C:88:LYS:HG3	1.89	0.72
3:H:312:PRO:HG2	3:H:315:GLU:HB3	1.71	0.72
3:H:275:LEU:HG	3:H:348:LEU:HD23	1.71	0.71
3:C:198:LYS:HD2	3:C:228:MET:HE1	1.72	0.71
3:H:307:MET:HA	3:H:311:MET:SD	2.31	0.71
3:H:349:ILE:HG13	3:H:365:ILE:HA	1.72	0.71
4:D:224:ARG:HB3	4:D:227:GLU:HG3	1.72	0.71
3:C:231:LYS:HE3	4:D:216:GLY:N	2.06	0.70
3:C:24:THR:HG22	3:C:25:LYS:HG2	1.72	0.70
4:D:233:ARG:HB3	4:D:233:ARG:NH1	2.07	0.70
3:C:261:GLU:HB3	4:D:172:ASP:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:GLN:HB2	3:C:221:LEU:HD12	1.72	0.69
3:H:223:HIS:O	3:H:227:GLU:HG3	1.92	0.69
3:C:408:ALA:O	3:C:412:LEU:HB2	1.92	0.69
2:B:82:GLU:HG3	2:B:112:TYR:HB3	1.74	0.69
2:B:77:VAL:HB	2:B:117:THR:HG22	1.75	0.69
3:C:106:GLU:O	3:C:108:GLN:HG3	1.92	0.69
1:E:17:PHE:CE2	4:I:192:ASP:HB2	2.27	0.69
3:H:382:LYS:HG2	3:H:383:ASN:N	2.09	0.68
1:E:30:GLY:HA2	1:E:57:MET:HE2	1.76	0.67
3:H:285:ASN:O	5:J:1:U:H4'	1.95	0.67
3:H:62:SER:O	3:H:66:GLN:HG3	1.94	0.67
4:D:173:ASP:OD2	4:D:182:ILE:HB	1.95	0.66
3:C:268:LEU:CD2	3:C:297:MET:HE3	2.19	0.66
4:I:168:LYS:HG2	5:F:6:U:O4	1.95	0.66
4:D:233:ARG:HB3	4:D:233:ARG:HH11	1.61	0.66
3:H:220:THR:OG1	3:H:359:GLU:HG3	1.94	0.66
1:E:30:GLY:HA2	1:E:57:MET:CE	2.27	0.65
3:H:139:ALA:HA	3:H:161:ALA:O	1.97	0.65
3:C:88:LYS:HE2	3:C:218:SER:CA	2.27	0.64
3:H:220:THR:HG22	3:H:363:HIS:NE2	2.11	0.64
4:D:224:ARG:HB3	4:D:227:GLU:CG	2.26	0.64
3:C:411:ILE:C	3:C:413:GLU:H	1.98	0.64
3:C:315:GLU:O	3:C:319:ILE:HG12	1.98	0.63
3:H:278:THR:HG21	3:H:347:SER:OG	1.98	0.63
3:C:199:GLU:HG3	9:C:468:HOH:O	1.99	0.62
3:H:220:THR:CG2	3:H:363:HIS:NE2	2.62	0.62
1:E:128:ASP:OD1	2:G:108:ARG:HG2	1.99	0.62
1:E:10:TYR:OH	1:E:19:HIS:CE1	2.50	0.62
3:H:190:ASP:OD2	3:H:220:THR:HG23	2.00	0.62
3:H:307:MET:HE3	3:H:337:TRP:HE1	1.64	0.61
2:G:131:MET:O	2:G:135:ASN:HB2	2.01	0.61
3:H:256:VAL:HG11	3:H:267:THR:HG21	1.83	0.61
3:H:116:ARG:HD2	3:H:313:GLN:OE1	2.01	0.61
3:C:283:PHE:CD1	3:C:364:ARG:HG2	2.36	0.60
1:A:6:TYR:HB3	1:A:91:VAL:HB	1.83	0.60
1:A:8:ARG:NH2	1:A:87:GLU:OE1	2.35	0.60
3:H:289:LYS:HZ2	4:I:182:ILE:HD11	1.64	0.60
1:E:101:THR:HG22	1:E:102:SER:H	1.67	0.59
1:E:127:GLN:HB3	2:G:108:ARG:HG3	1.84	0.59
3:H:393:GLU:HB2	3:H:400:ILE:HD12	1.84	0.59
2:G:90:HIS:CD2	2:G:99:ILE:HD12	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:387:ARG:NH1	4:D:194:ARG:H	2.01	0.59
1:E:101:THR:HG22	1:E:102:SER:N	2.17	0.59
1:E:83:VAL:HA	4:I:194:ARG:HE	1.68	0.59
3:H:169:ASP:O	3:H:173:ARG:HB2	2.01	0.59
3:H:225:ILE:H	3:H:225:ILE:HD12	1.67	0.59
4:I:244:ILE:C	4:I:246:SER:H	2.06	0.59
1:A:53:HIS:CE1	1:A:54:LYS:HG2	2.38	0.58
3:C:308:HIS:CE1	3:C:310:ASP:HB2	2.38	0.58
1:E:143:ILE:HG23	2:G:71:GLU:OE2	2.03	0.58
1:E:70:THR:HG22	1:E:97:ILE:HD13	1.85	0.58
3:H:309:GLY:N	5:J:3:U:OP1	2.32	0.58
1:E:34:TYR:HB3	1:E:48:LYS:O	2.03	0.58
3:H:89:THR:HA	3:H:92:PHE:CE2	2.38	0.58
2:G:81:HIS:CE1	2:G:83:GLU:H	2.21	0.58
3:H:279:GLN:HG2	3:H:329:ARG:HA	1.84	0.58
3:H:279:GLN:HE21	3:H:326:GLY:HA2	1.68	0.58
3:H:88:LYS:HE3	3:H:218:SER:C	2.24	0.58
3:H:404:PRO:O	3:H:407:VAL:HG22	2.04	0.58
3:H:179:ARG:HB2	4:I:228:GLN:O	2.04	0.58
1:A:5:PHE:CZ	1:A:64:ILE:HD12	2.39	0.57
3:C:150:ILE:HD11	3:C:173:ARG:HD2	1.87	0.57
3:C:252:LYS:HE2	9:C:531:HOH:O	2.04	0.57
2:B:125:LYS:HG3	2:B:126:GLU:N	2.20	0.57
1:E:84:GLY:HA3	1:E:103:LYS:HE3	1.86	0.57
3:H:254:PHE:HB3	3:H:403:MET:HA	1.85	0.57
3:C:88:LYS:HD2	3:C:217:ILE:CG2	2.35	0.57
4:I:175:ASP:HB3	4:I:178:ASN:HB2	1.86	0.57
3:C:307:MET:HE3	3:C:320:MET:SD	2.45	0.56
3:H:292:TRP:CD1	4:I:179:PRO:HB2	2.41	0.56
3:C:275:LEU:HA	3:C:348:LEU:HD23	1.88	0.56
3:C:278:THR:O	3:C:329:ARG:HD2	2.05	0.56
3:H:256:VAL:HG23	3:H:403:MET:HG3	1.87	0.56
2:B:106:LEU:HD23	2:B:113:LEU:HD12	1.87	0.56
3:C:23:MET:O	3:C:26:VAL:HG12	2.06	0.56
3:H:216:LEU:HD22	3:H:233:MET:SD	2.46	0.56
3:C:23:MET:O	3:C:223:HIS:HE1	1.89	0.56
2:G:131:MET:HG3	2:G:146:VAL:O	2.06	0.56
4:D:232:SER:OG	4:D:235:GLU:HG3	2.07	0.55
1:E:10:TYR:HB3	1:E:87:GLU:HB2	1.88	0.55
4:D:224:ARG:HG3	4:D:226:ASP:OD1	2.07	0.55
2:G:89:ILE:O	2:G:93:PHE:HD1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:242:TYR:CE2	4:I:244:ILE:HA	2.41	0.55
3:C:279:GLN:HG2	3:C:329:ARG:HA	1.89	0.55
3:H:307:MET:HB3	3:H:319:ILE:HG21	1.89	0.55
3:C:387:ARG:NH1	4:D:194:ARG:N	2.56	0.54
2:G:81:HIS:HB3	2:G:84:ALA:HB2	1.88	0.54
3:H:99:CYS:HB2	9:H:442:HOH:O	2.06	0.54
2:G:118:LEU:N	2:G:118:LEU:HD22	2.23	0.54
1:A:5:PHE:HZ	1:A:64:ILE:HD12	1.72	0.54
4:D:224:ARG:CG	4:D:226:ASP:OD1	2.56	0.54
1:E:80:PRO:HB3	1:E:85:ARG:HG3	1.89	0.53
2:G:79:GLY:O	2:G:144:ILE:HG22	2.08	0.53
1:E:86:GLN:NE2	1:E:104:ILE:HG13	2.23	0.53
5:F:1:U:H5''	5:F:1:U:C6	2.44	0.53
4:D:236:LEU:CD1	4:D:245:ARG:HG3	2.39	0.53
1:E:123:TYR:O	1:E:127:GLN:HG3	2.09	0.53
3:C:173:ARG:NH2	5:F:6:U:O3'	2.41	0.53
2:G:96:TYR:CD2	2:G:130:ALA:HA	2.44	0.53
3:H:225:ILE:N	3:H:225:ILE:HD12	2.23	0.53
1:A:7:LEU:CD1	1:A:64:ILE:HD11	2.39	0.53
3:H:278:THR:HG23	3:H:279:GLN:N	2.21	0.53
3:H:231:LYS:HE2	4:I:216:GLY:N	2.23	0.53
3:H:222:PRO:HB2	3:H:225:ILE:CD1	2.35	0.52
4:I:242:TYR:OH	4:I:244:ILE:HD12	2.09	0.52
1:A:8:ARG:NH1	1:A:89:GLU:OE2	2.42	0.52
1:E:127:GLN:HB3	2:G:108:ARG:CG	2.39	0.52
2:G:80:VAL:HG21	2:G:117:THR:HG22	1.92	0.52
3:C:81:GLN:HA	3:C:218:SER:O	2.09	0.52
1:E:69:ILE:CG1	1:E:125:LEU:HD22	2.30	0.52
3:C:82:SER:OG	3:C:88:LYS:CG	2.56	0.52
3:C:89:THR:HA	3:C:92:PHE:CE2	2.44	0.52
1:E:60:LEU:O	1:E:64:ILE:HG13	2.10	0.52
1:E:68:GLU:HB3	1:E:71:LYS:CG	2.39	0.52
3:C:411:ILE:C	3:C:413:GLU:N	2.63	0.52
3:H:259:GLU:HA	3:H:383:ASN:HD21	1.74	0.52
3:C:198:LYS:CD	3:C:228:MET:HE1	2.40	0.51
3:C:409:ASP:HA	3:C:412:LEU:HB2	1.93	0.51
2:G:130:ALA:O	2:G:134:LEU:HB2	2.11	0.51
1:E:82:ARG:HG3	9:E:149:HOH:O	2.10	0.51
3:C:387:ARG:HG2	9:D:288:HOH:O	2.10	0.51
1:E:82:ARG:O	4:I:194:ARG:HD2	2.10	0.51
2:B:76:PHE:HD1	2:B:118:LEU:HD13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:LEU:HB2	1:E:115:ASP:HB2	1.92	0.51
3:H:289:LYS:HZ3	4:I:182:ILE:HD11	1.74	0.51
4:I:175:ASP:HB3	4:I:178:ASN:CB	2.41	0.51
1:E:117:GLU:O	1:E:121:VAL:HG23	2.10	0.51
4:D:233:ARG:HD2	9:D:296:HOH:O	2.11	0.50
2:G:76:PHE:HD1	2:G:118:LEU:HD13	1.76	0.50
3:C:260:ARG:HD2	3:C:263:TRP:CZ2	2.46	0.50
1:E:74:ASP:HA	1:E:77:TRP:CD2	2.46	0.50
1:E:70:THR:CG2	1:E:92:ILE:HD11	2.40	0.50
3:H:408:ALA:O	3:H:412:LEU:HD13	2.11	0.50
4:I:236:LEU:HD13	4:I:244:ILE:HG22	1.93	0.50
1:E:14:LYS:HD3	1:E:19:HIS:HB2	1.93	0.50
3:H:389:LEU:O	3:H:392:ILE:HB	2.11	0.50
3:H:279:GLN:HE22	3:H:326:GLY:HA2	1.77	0.50
2:B:137:GLN:O	2:B:143:PRO:HA	2.12	0.50
1:E:86:GLN:HE22	1:E:104:ILE:HG13	1.75	0.50
3:C:275:LEU:HD23	3:C:348:LEU:CD2	2.41	0.49
3:H:144:THR:HG21	9:H:420:HOH:O	2.12	0.49
1:E:72:GLU:HG2	1:E:118:GLY:HA2	1.94	0.49
1:A:7:LEU:HD12	1:A:64:ILE:HD11	1.94	0.49
1:E:125:LEU:O	1:E:129:LEU:HG	2.13	0.49
2:B:77:VAL:HB	2:B:117:THR:CG2	2.41	0.48
9:B:183:HOH:O	3:C:249:GLU:HG2	2.12	0.48
3:C:307:MET:HE3	3:C:337:TRP:HE1	1.78	0.48
3:H:256:VAL:CG2	3:H:403:MET:HG3	2.43	0.48
1:E:53:HIS:O	1:E:56:VAL:HB	2.12	0.48
3:H:225:ILE:HA	3:H:228:MET:CE	2.44	0.48
3:H:283:PHE:HB2	3:H:364:ARG:HH21	1.78	0.48
3:H:311:MET:HB3	3:H:315:GLU:HG2	1.94	0.48
2:B:75:LEU:HD22	2:B:131:MET:HE2	1.95	0.48
3:C:114:PRO:HD2	3:C:118:LEU:HD23	1.95	0.48
1:E:74:ASP:HA	1:E:77:TRP:CG	2.49	0.48
3:H:117:GLU:HG2	3:H:320:MET:HG3	1.96	0.48
2:G:134:LEU:HA	2:G:137:GLN:HG3	1.95	0.48
1:E:127:GLN:HA	1:E:130:LYS:HE2	1.96	0.48
3:H:381:VAL:HG11	3:H:386:ILE:HD13	1.95	0.48
1:E:78:PRO:O	1:E:101:THR:HG23	2.13	0.47
2:G:114:LYS:HG3	2:G:115:GLY:H	1.79	0.47
2:G:123:THR:HG22	2:G:124:TYR:H	1.80	0.47
3:H:322:GLU:OE2	3:H:322:GLU:HA	2.13	0.47
1:E:83:VAL:HA	4:I:194:ARG:NE	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:LEU:HD23	3:C:348:LEU:HD23	1.97	0.47
1:A:110:VAL:HG11	1:A:120:ARG:HG2	1.95	0.47
1:A:30:GLY:O	1:A:52:VAL:HG22	2.15	0.47
1:E:124:TYR:CD2	2:G:109:ARG:HB3	2.50	0.47
3:C:206:ARG:CZ	4:D:222:LYS:HE3	2.45	0.47
4:I:237:ILE:O	4:I:241:GLY:N	2.47	0.47
1:E:107:LEU:HD12	1:E:108:ILE:N	2.30	0.47
3:C:202:TYR:CZ	3:C:206:ARG:HD3	2.50	0.46
3:C:23:MET:HA	3:C:26:VAL:HG12	1.97	0.46
3:C:77:ASP:HB3	3:C:233:MET:HE2	1.97	0.46
2:B:78:THR:HG22	2:B:145:SER:HB2	1.96	0.46
3:C:205:TYR:O	4:D:220:HIS:HD2	1.99	0.46
3:C:87:GLY:HA2	6:C:414:ADP:O1A	2.15	0.46
4:I:167:PRO:C	5:F:6:U:H3	2.18	0.46
1:E:127:GLN:CB	2:G:108:ARG:HG3	2.46	0.46
3:C:353:ASP:O	3:C:364:ARG:NH2	2.49	0.46
1:E:81:ASP:OD1	1:E:83:VAL:HB	2.15	0.46
1:E:11:VAL:HG13	1:E:11:VAL:O	2.16	0.46
3:H:334:THR:C	3:H:336:VAL:H	2.20	0.46
1:A:77:TRP:CD2	1:A:119:LEU:HD13	2.50	0.46
3:H:263:TRP:CE3	3:H:263:TRP:HA	2.52	0.45
2:B:74:ILE:HD13	2:B:120:GLU:HB2	1.98	0.45
1:E:132:LEU:O	1:E:136:LEU:HG	2.17	0.45
1:E:139:LEU:HD11	2:G:103:HIS:ND1	2.31	0.45
1:E:7:LEU:HD11	1:E:88:LEU:HD11	1.98	0.45
2:G:70:VAL:HG22	2:G:71:GLU:HG3	1.98	0.45
1:E:68:GLU:HB3	1:E:71:LYS:HG3	1.98	0.45
3:H:23:MET:O	3:H:223:HIS:HE1	2.00	0.45
4:I:244:ILE:O	4:I:246:SER:N	2.46	0.45
2:G:77:VAL:HB	2:G:117:THR:HG22	1.99	0.45
3:H:168:PHE:CE1	3:H:203:ASP:HB3	2.52	0.45
3:H:278:THR:O	3:H:279:GLN:HG3	2.17	0.45
2:G:109:ARG:HG3	2:G:110:THR:N	2.32	0.45
2:G:64:PRO:HG2	2:G:151:VAL:HB	1.98	0.45
2:G:76:PHE:HD1	2:G:118:LEU:CD1	2.29	0.45
1:E:68:GLU:HB3	1:E:71:LYS:HG2	1.98	0.45
1:A:83:VAL:HG22	3:C:387:ARG:HD3	1.98	0.45
3:H:259:GLU:HA	3:H:383:ASN:ND2	2.30	0.45
3:H:219:ALA:HB2	7:H:415:AF3:F2	2.07	0.45
3:C:88:LYS:CE	3:C:218:SER:C	2.79	0.45
3:H:338:ALA:O	3:H:363:HIS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:73:ILE:HD13	3:H:73:ILE:N	2.32	0.45
1:E:74:ASP:OD2	1:E:99:PHE:HA	2.17	0.44
2:G:106:LEU:HD23	2:G:113:LEU:HD23	1.99	0.44
3:H:263:TRP:HA	3:H:263:TRP:HE3	1.82	0.44
3:H:349:ILE:HD11	3:H:367:ARG:HB2	1.98	0.44
1:E:26:PHE:CE2	1:E:32:LEU:HD22	2.52	0.44
3:H:355:PRO:HA	3:H:364:ARG:NH1	2.32	0.44
5:F:5:U:H2'	5:F:6:U:H4'	1.98	0.44
2:G:131:MET:HE1	2:G:148:TRP:N	2.32	0.44
4:I:169:HIS:HB3	9:I:296:HOH:O	2.18	0.44
1:A:36:ASN:C	1:A:36:ASN:OD1	2.55	0.44
2:B:68:ARG:HB2	2:B:73:TRP:CZ2	2.52	0.44
3:C:103:GLN:HG2	9:C:519:HOH:O	2.18	0.44
3:C:387:ARG:HG3	9:C:537:HOH:O	2.18	0.44
2:G:149:CYS:HB3	2:G:150:PHE:CD1	2.53	0.44
1:E:33:ARG:HE	1:E:47:ARG:NH2	2.15	0.44
4:I:244:ILE:C	4:I:246:SER:N	2.71	0.44
1:E:13:HIS:CE1	1:E:20:GLU:HB2	2.52	0.44
1:E:76:LEU:HD12	1:E:76:LEU:N	2.33	0.44
3:C:278:THR:HB	3:C:279:GLN:H	1.42	0.43
3:C:355:PRO:HB2	3:C:360:LEU:HB3	2.00	0.43
2:B:78:THR:CG2	2:B:145:SER:HB2	2.48	0.43
3:H:289:LYS:HE3	4:I:180:ALA:HB1	2.00	0.43
3:H:252:LYS:HG3	3:H:410:LEU:HD21	1.99	0.43
3:C:404:PRO:O	3:C:407:VAL:HG22	2.18	0.43
1:A:130:LYS:NZ	9:A:210:HOH:O	2.48	0.43
3:C:151:ARG:HG3	4:D:240:TYR:CE1	2.53	0.43
3:H:89:THR:HG23	3:H:92:PHE:CZ	2.52	0.43
1:A:67:SER:O	1:A:68:GLU:HB2	2.18	0.43
3:H:283:PHE:HB3	3:H:364:ARG:NH2	2.34	0.43
3:H:405:MET:HG2	3:H:406:ASN:N	2.22	0.43
2:B:130:ALA:O	2:B:134:LEU:HB2	2.18	0.43
4:D:175:ASP:OD2	4:D:177:LYS:HB2	2.19	0.43
3:H:222:PRO:CB	3:H:225:ILE:HD13	2.41	0.43
3:H:225:ILE:CD1	3:H:225:ILE:H	2.31	0.43
4:D:182:ILE:HA	4:D:183:PRO:HD3	1.87	0.43
3:H:220:THR:HG23	3:H:220:THR:O	2.19	0.43
3:H:231:LYS:O	4:I:217:ARG:HD2	2.19	0.43
2:G:123:THR:HG22	2:G:124:TYR:N	2.34	0.43
3:C:233:MET:HE1	3:C:236:PRO:HB3	2.01	0.43
3:H:287:LYS:HD2	3:H:310:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:346:VAL:O	3:H:368:SER:HA	2.18	0.43
3:C:145:ASN:OD1	3:C:148:GLU:HG3	2.18	0.42
1:A:107:LEU:HD11	1:A:124:TYR:OH	2.20	0.42
2:B:66:PRO:HB3	2:B:148:TRP:CD2	2.54	0.42
2:G:104:LEU:HA	2:G:104:LEU:HD23	1.84	0.42
3:C:288:ARG:NH2	4:D:176:ARG:O	2.53	0.42
3:H:173:ARG:HD3	3:H:175:SER:OG	2.20	0.42
2:B:133:GLY:O	2:B:137:GLN:HG3	2.19	0.42
3:C:357:ASN:OD1	3:C:360:LEU:HB2	2.19	0.42
3:C:37:THR:HG23	9:C:424:HOH:O	2.18	0.42
3:C:81:GLN:HB2	3:C:221:LEU:CD1	2.47	0.42
3:H:88:LYS:HE2	3:H:218:SER:N	2.34	0.42
4:D:224:ARG:HG2	4:D:226:ASP:OD1	2.20	0.42
2:G:70:VAL:HG13	2:G:71:GLU:N	2.35	0.42
2:G:74:ILE:HD13	2:G:120:GLU:HB2	2.02	0.42
2:B:102:ILE:HD13	2:B:119:VAL:HG13	2.01	0.42
3:H:337:TRP:CD2	3:H:341:LEU:HD12	2.54	0.42
2:B:64:PRO:HG3	2:B:153:GLY:O	2.20	0.42
1:E:77:TRP:CD1	1:E:77:TRP:N	2.87	0.42
3:H:220:THR:HG21	3:H:363:HIS:NE2	2.34	0.42
3:H:393:GLU:HB2	3:H:400:ILE:CD1	2.48	0.42
2:G:134:LEU:HA	2:G:137:GLN:CG	2.50	0.42
1:A:92:ILE:HG22	1:A:92:ILE:O	2.19	0.42
4:D:178:ASN:HA	4:D:179:PRO:HD3	1.94	0.42
1:E:7:LEU:HD13	1:E:90:ILE:HG12	2.02	0.42
3:H:82:SER:O	3:H:219:ALA:HA	2.20	0.42
3:H:231:LYS:HA	4:I:217:ARG:HD2	2.02	0.42
3:H:350:ILE:CD1	3:H:378:ILE:HB	2.50	0.42
3:C:263:TRP:HE3	3:C:263:TRP:HA	1.85	0.42
3:H:114:PRO:HD3	3:H:192:MET:SD	2.60	0.42
3:H:22:ASP:OD1	3:H:24:THR:HB	2.20	0.42
3:H:411:ILE:C	3:H:413:GLU:H	2.22	0.42
3:H:205:TYR:O	4:I:220:HIS:HD2	2.03	0.41
5:J:6:U:H6	5:J:6:U:O5'	2.03	0.41
3:C:73:ILE:HD13	3:C:98:GLN:HG2	2.02	0.41
4:I:184:ARG:HG2	4:I:189:PHE:CE1	2.55	0.41
1:E:83:VAL:HA	4:I:194:ARG:HD2	2.02	0.41
1:E:40:TYR:CE2	1:E:41:LYS:HG3	2.54	0.41
1:E:7:LEU:HA	1:E:89:GLU:O	2.19	0.41
2:G:92:LYS:O	2:G:134:LEU:HD11	2.20	0.41
3:H:393:GLU:HG3	3:H:400:ILE:HG13	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:411:ILE:O	3:C:413:GLU:N	2.53	0.41
3:H:225:ILE:HA	3:H:228:MET:HE2	2.02	0.41
3:H:307:MET:HE2	3:H:319:ILE:CG2	2.50	0.41
3:C:307:MET:HE2	3:C:319:ILE:HG22	2.02	0.41
3:H:251:ILE:HA	3:H:375:GLY:O	2.21	0.41
3:H:312:PRO:HG2	3:H:315:GLU:CB	2.48	0.41
3:C:411:ILE:HG12	3:C:411:ILE:O	2.20	0.41
3:H:168:PHE:O	3:H:172:ARG:HG2	2.21	0.41
3:H:410:LEU:HB2	9:H:469:HOH:O	2.21	0.41
2:B:156:LYS:HB3	9:B:187:HOH:O	2.21	0.41
3:C:255:PHE:HA	3:C:379:ASN:O	2.20	0.41
3:C:287:LYS:HG2	3:C:308:HIS:HB2	2.02	0.40
3:C:289:LYS:HD3	4:D:182:ILE:HD11	2.03	0.40
1:E:130:LYS:HE3	1:E:130:LYS:HB2	1.84	0.40
1:E:69:ILE:CD1	1:E:121:VAL:HG12	2.51	0.40
3:H:271:LEU:O	3:H:274:THR:HG22	2.21	0.40
3:H:382:LYS:CG	3:H:383:ASN:H	2.22	0.40
5:J:2:U:H2'	5:J:3:U:O4'	2.21	0.40
3:C:23:MET:HA	3:C:26:VAL:CG1	2.51	0.40
3:H:268:LEU:HG	3:H:297:MET:HE3	2.02	0.40
3:H:74:LYS:HB3	3:H:74:LYS:HE2	1.64	0.40
3:C:268:LEU:HD23	3:C:297:MET:CE	2.27	0.40
3:C:387:ARG:NH2	9:C:536:HOH:O	2.54	0.40
3:H:410:LEU:HA	3:H:410:LEU:HD12	1.91	0.40
3:H:73:ILE:CD1	3:H:95:SER:HA	2.41	0.40
1:E:84:GLY:HA3	1:E:103:LYS:HG3	2.03	0.40
3:H:275:LEU:HD21	3:H:280:ALA:HB3	2.03	0.40
3:H:287:LYS:HD3	5:J:3:U:OP2	2.22	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	142/146 (97%)	137 (96%)	5 (4%)	0	100	100
1	E	140/146 (96%)	127 (91%)	12 (9%)	1 (1%)	22	26
2	B	92/126 (73%)	90 (98%)	1 (1%)	1 (1%)	14	15
2	G	89/126 (71%)	81 (91%)	8 (9%)	0	100	100
3	C	390/413 (94%)	380 (97%)	9 (2%)	1 (0%)	41	50
3	H	390/413 (94%)	371 (95%)	15 (4%)	4 (1%)	15	17
4	D	53/146 (36%)	51 (96%)	2 (4%)	0	100	100
4	I	58/146 (40%)	54 (93%)	3 (5%)	1 (2%)	9	8
All	All	1354/1662 (82%)	1291 (95%)	55 (4%)	8 (1%)	25	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	245	ARG
3	H	335	ASP
3	H	406	ASN
2	B	137	GLN
3	C	412	LEU
1	E	11	VAL
3	H	384	ASP
3	H	340	GLY

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	132/134 (98%)	128 (97%)	4 (3%)	41	57
1	E	130/134 (97%)	129 (99%)	1 (1%)	81	91
2	B	78/107 (73%)	77 (99%)	1 (1%)	69	82
2	G	76/107 (71%)	76 (100%)	0	100	100
3	C	347/363 (96%)	334 (96%)	13 (4%)	34	48
3	H	347/363 (96%)	333 (96%)	14 (4%)	31	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	50/130 (38%)	48 (96%)	2 (4%)	31	44
4	I	55/130 (42%)	53 (96%)	2 (4%)	35	49
All	All	1215/1468 (83%)	1178 (97%)	37 (3%)	41	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	TYR
1	A	76	LEU
1	A	97	ILE
1	A	131	CYS
2	B	118	LEU
3	C	24	THR
3	C	88	LYS
3	C	229	THR
3	C	234	THR
3	C	263	TRP
3	C	271	LEU
3	C	278	THR
3	C	288	ARG
3	C	305	SER
3	C	329	ARG
3	C	337	TRP
3	C	360	LEU
3	C	411	ILE
4	D	182	ILE
4	D	227	GLU
1	E	47	ARG
3	H	140	CYS
3	H	144	THR
3	H	149	ASP
3	H	216	LEU
3	H	234	THR
3	H	305	SER
3	H	315	GLU
3	H	337	TRP
3	H	360	LEU
3	H	367	ARG
3	H	386	ILE
3	H	403	MET
3	H	407	VAL

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Mol	Chain	Res	Type
3	H	412	LEU
4	I	245	ARG
4	I	248	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
3	C	134	ASN
3	C	230	ASN
3	C	345	GLN
4	D	220	HIS
1	E	19	HIS
1	E	86	GLN
2	G	90	HIS
2	G	128	GLN
3	H	103	GLN
3	H	383	ASN
3	H	399	GLN
4	I	169	HIS
4	I	220	HIS
4	I	248	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	F	5/6 (83%)	1 (20%)	0
5	J	6/6 (100%)	2 (33%)	1 (16%)
All	All	11/12 (91%)	3 (27%)	1 (9%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	F	6	U
5	J	2	U
5	J	3	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	J	1	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
6	ADP	H	414	-	24,29,29	1.11	2 (8%)	29,45,45	1.52	7 (24%)
7	AF3	H	415	-	0,3,3	0.00	-	-		
7	AF3	C	415	-	0,3,3	0.00	-	-		
6	ADP	C	414	-	24,29,29	1.05	2 (8%)	29,45,45	1.40	6 (20%)

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
6	ADP	H	414	-	-	1/12/32/32	0/3/3/3
6	ADP	C	414	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	414	ADP	C5-C4	2.77	1.48	1.40
6	C	414	ADP	C5-C4	2.35	1.47	1.40
6	C	414	ADP	C2-N3	2.05	1.35	1.32
6	H	414	ADP	O4'-C1'	2.03	1.43	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	414	ADP	N3-C2-N1	-3.52	123.18	128.68
6	H	414	ADP	N3-C2-N1	-3.10	123.83	128.68
6	C	414	ADP	C4-C5-N7	-2.61	106.68	109.40
6	H	414	ADP	PA-O3A-PB	-2.60	123.89	132.83
6	H	414	ADP	C4-C5-N7	-2.54	106.75	109.40
6	H	414	ADP	C2-N1-C6	2.39	122.84	118.75
6	C	414	ADP	O3B-PB-O2B	2.22	116.12	107.64
6	C	414	ADP	O2A-PA-O1A	2.19	123.07	112.24
6	H	414	ADP	O3B-PB-O2B	2.16	115.90	107.64
6	H	414	ADP	C1'-N9-C4	-2.12	122.91	126.64
6	C	414	ADP	O2B-PB-O3A	-2.10	97.60	104.64
6	H	414	ADP	O2A-PA-O1A	2.09	122.57	112.24
6	C	414	ADP	O3'-C3'-C4'	-2.08	105.03	111.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	414	ADP	PA-O3A-PB-O2B
6	C	414	ADP	PA-O3A-PB-O2B

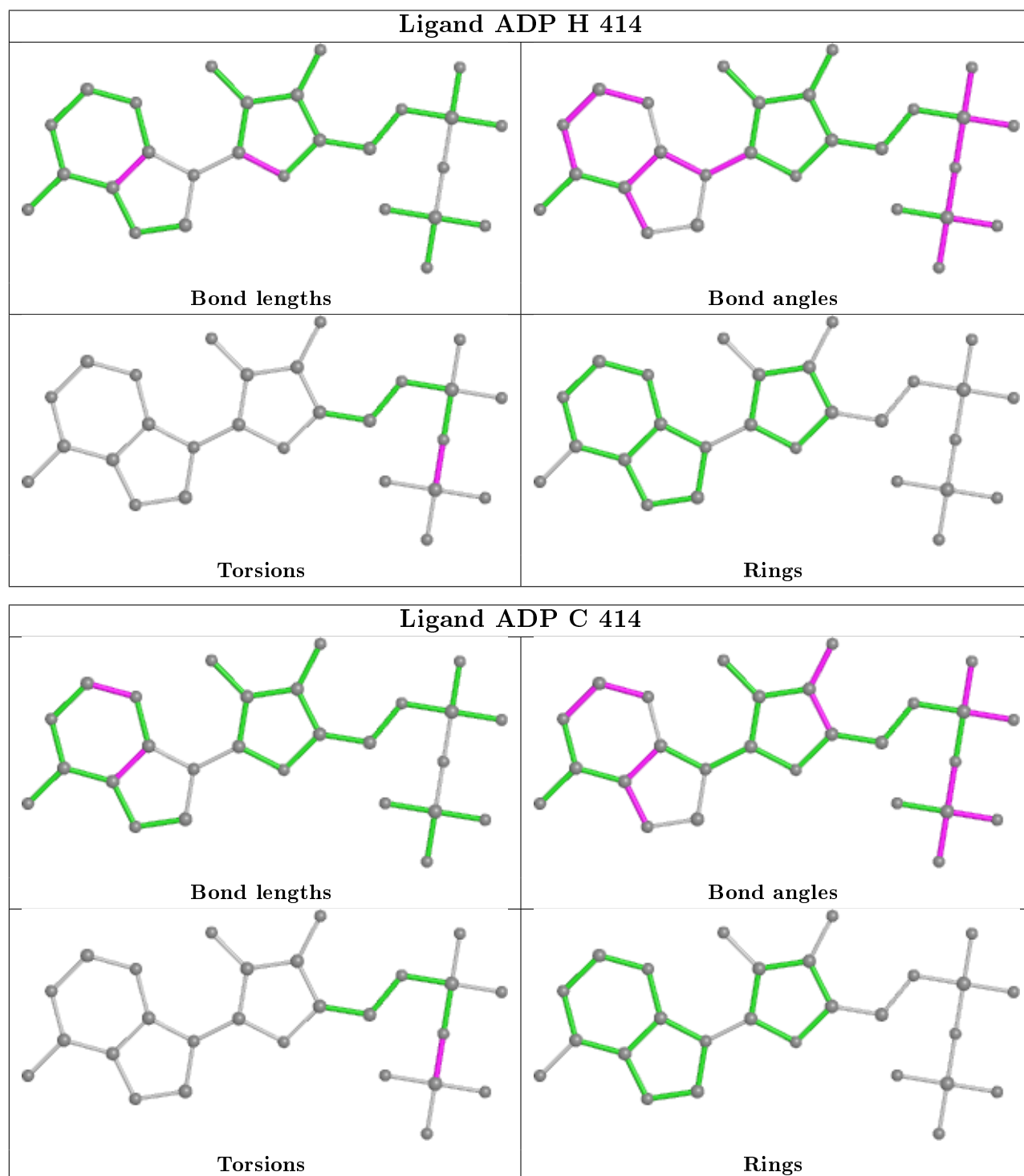
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	415	AF3	1	0
6	C	414	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	144/146 (98%)	-0.10	3 (2%) 63 70	24, 34, 65, 120	0
1	E	142/146 (97%)	1.92	55 (38%) 0 0	81, 119, 190, 266	0
2	B	94/126 (74%)	0.52	13 (13%) 2 4	35, 61, 98, 160	0
2	G	91/126 (72%)	3.01	56 (61%) 0 0	92, 128, 176, 192	0
3	C	392/413 (94%)	0.10	17 (4%) 35 42	23, 35, 63, 142	0
3	H	392/413 (94%)	0.66	59 (15%) 2 3	33, 61, 144, 267	0
4	D	57/146 (39%)	0.74	9 (15%) 2 2	29, 52, 148, 167	0
4	I	62/146 (42%)	0.97	13 (20%) 1 1	37, 73, 140, 185	0
5	F	6/6 (100%)	0.23	0 100 100	35, 39, 45, 74	0
5	J	6/6 (100%)	0.02	0 100 100	55, 63, 75, 104	0
All	All	1386/1674 (82%)	0.71	225 (16%) 1 2	23, 52, 155, 267	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	405	MET	11.4
2	G	139	LEU	11.0
4	D	172	ASP	10.2
4	D	174	GLU	10.0
2	G	84	ALA	9.4
1	E	110	VAL	9.3
2	G	115	GLY	8.8
1	E	96	HIS	8.3
3	H	413	GLU	8.3
2	G	140	MET	8.2
4	D	173	ASP	7.8
2	G	124	TYR	7.7
2	G	125	LYS	7.7

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Mol	Chain	Res	Type	RSRZ
2	B	156	LYS	7.6
3	H	411	ILE	7.5
4	I	249	ASN	7.2
3	H	277	ILE	7.1
1	E	71	LYS	7.1
3	C	23	MET	7.1
1	E	97	ILE	6.7
1	E	94	ASP	6.6
1	E	91	VAL	6.2
3	H	300	ALA	6.1
1	E	114	LYS	6.1
2	G	127	ALA	6.0
1	E	69	ILE	6.0
3	H	23	MET	5.9
2	B	157	GLY	5.9
3	C	26	VAL	5.8
1	E	77	TRP	5.8
2	G	81	HIS	5.7
1	E	14	LYS	5.4
1	E	119	LEU	5.4
2	G	121	TYR	5.3
3	H	263	TRP	5.3
2	G	112	TYR	5.2
2	G	143	PRO	5.2
2	G	86	GLU	5.2
2	G	154	PRO	5.1
3	H	257	ALA	5.1
1	E	113	SER	5.1
2	G	82	GLU	5.1
3	H	275	LEU	5.0
4	I	194	ARG	5.0
2	G	96	TYR	5.0
1	E	76	LEU	5.0
1	E	112	GLN	4.9
4	I	167	PRO	4.9
2	G	99	ILE	4.9
2	G	134	LEU	4.9
2	G	153	GLY	4.9
4	I	169	HIS	4.8
2	G	141	GLY	4.8
3	H	25	LYS	4.7
3	C	22	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	G	102	ILE	4.6
3	H	26	VAL	4.6
3	H	406	ASN	4.6
1	A	3	SER	4.6
1	E	70	THR	4.6
3	H	412	LEU	4.6
1	A	93	GLY	4.5
4	D	247	ALA	4.5
1	E	121	VAL	4.5
1	A	94	ASP	4.5
2	G	93	PHE	4.4
4	D	176	ARG	4.4
4	I	247	ALA	4.3
3	C	24	THR	4.3
3	H	22	ASP	4.3
2	B	141	GLY	4.2
2	G	68	ARG	4.2
2	G	64	PRO	4.1
2	G	90	HIS	4.1
2	G	142	GLN	4.1
2	G	73	TRP	4.1
1	E	28	PRO	4.0
3	C	412	LEU	4.0
3	C	413	GLU	4.0
2	G	123	THR	4.0
3	H	247	THR	4.0
2	B	155	PRO	4.0
2	B	64	PRO	3.9
4	I	193	LEU	3.8
1	E	50	ALA	3.8
1	E	18	GLY	3.8
2	G	129	ALA	3.8
3	H	270	ASP	3.7
1	E	74	ASP	3.7
2	G	114	LYS	3.7
1	E	68	GLU	3.7
2	G	113	LEU	3.7
2	G	148	TRP	3.7
2	G	138	ASP	3.6
1	E	47	ARG	3.6
1	E	107	LEU	3.6
4	I	187	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	G	78	THR	3.6
3	C	122	ILE	3.6
3	H	292	TRP	3.6
1	E	93	GLY	3.6
3	H	274	THR	3.6
2	G	97	GLY	3.6
2	G	130	ALA	3.5
4	D	248	HIS	3.5
1	E	98	SER	3.5
1	E	131	CYS	3.4
1	E	134	PHE	3.4
3	H	217	ILE	3.4
3	H	399	GLN	3.3
2	G	83	GLU	3.3
2	G	144	ILE	3.3
4	I	248	HIS	3.3
1	E	15	GLY	3.3
3	H	407	VAL	3.2
3	C	89	THR	3.2
1	E	75	ALA	3.2
2	G	94	ALA	3.2
1	E	95	GLU	3.2
3	H	398	THR	3.2
2	B	81	HIS	3.2
2	B	140	MET	3.2
3	H	296	LYS	3.2
2	G	85	THR	3.1
1	E	39	ASN	3.1
4	I	185	LYS	3.1
4	I	168	LYS	3.0
1	E	82	ARG	3.0
1	E	90	ILE	3.0
2	G	67	GLN	3.0
3	C	25	LYS	3.0
1	E	80	PRO	3.0
1	E	6	TYR	2.9
2	G	126	GLU	2.9
2	B	154	PRO	2.9
3	H	410	LEU	2.9
3	H	111	ILE	2.9
2	B	125	LYS	2.9
3	C	185	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	78	PRO	2.9
3	H	288	ARG	2.9
2	G	92	LYS	2.8
1	E	135	SER	2.8
3	H	361	TYR	2.8
3	H	32	GLU	2.8
2	G	116	TYR	2.8
1	E	44	VAL	2.7
1	E	92	ILE	2.7
1	E	79	PRO	2.7
3	C	92	PHE	2.7
3	H	268	LEU	2.7
3	H	302	PHE	2.7
4	I	176	ARG	2.7
3	H	303	THR	2.7
2	G	108	ARG	2.7
3	H	185	VAL	2.7
1	E	45	MET	2.7
3	H	27	GLU	2.7
3	H	400	ILE	2.7
3	H	234	THR	2.7
2	G	152	ARG	2.6
3	H	267	THR	2.6
3	H	408	ALA	2.6
1	E	7	LEU	2.6
3	H	256	VAL	2.6
1	E	53	HIS	2.6
3	H	385	ASP	2.6
3	H	409	ASP	2.6
3	H	384	ASP	2.6
1	E	27	ARG	2.5
1	E	85	ARG	2.5
1	E	60	LEU	2.5
1	E	100	THR	2.5
3	H	401	ASP	2.5
2	G	95	GLU	2.5
2	B	139	LEU	2.5
2	G	109	ARG	2.5
3	H	220	THR	2.5
3	H	299	GLU	2.5
2	B	142	GLN	2.5
3	C	411	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	215	VAL	2.4
4	D	193	LEU	2.4
1	E	116	PRO	2.4
3	C	118	LEU	2.4
3	H	112	LEU	2.4
2	G	135	ASN	2.4
1	E	51	TYR	2.4
3	H	248	LEU	2.4
3	H	260	ARG	2.3
2	G	111	GLY	2.3
1	E	5	PHE	2.3
3	H	122	ILE	2.3
2	G	128	GLN	2.3
3	C	111	ILE	2.3
2	G	110	THR	2.3
2	G	65	GLY	2.3
1	E	117	GLU	2.2
4	I	186	GLY	2.2
2	G	77	VAL	2.2
2	B	144	ILE	2.2
3	H	24	THR	2.2
3	H	304	VAL	2.2
3	H	293	LEU	2.2
1	E	130	LYS	2.1
3	H	255	PHE	2.1
1	E	132	LEU	2.1
2	G	106	LEU	2.1
4	I	170	LEU	2.1
2	G	87	GLU	2.1
2	B	112	TYR	2.1
3	H	28	PHE	2.1
3	H	92	PHE	2.1
3	H	366	GLY	2.1
2	G	88	ASP	2.1
4	D	175	ASP	2.1
3	H	301	ASN	2.1
3	H	162	GLY	2.1
3	H	265	PHE	2.1
3	C	186	LEU	2.0
3	C	362	ILE	2.0
4	D	249	ASN	2.0
1	E	65	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	8	ARG	2.0
3	C	247	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

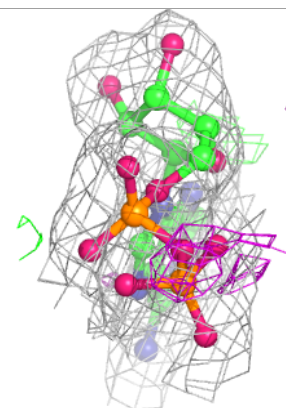
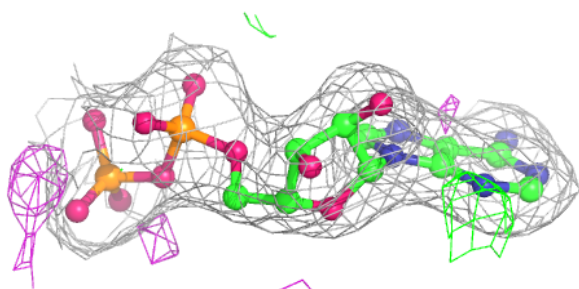
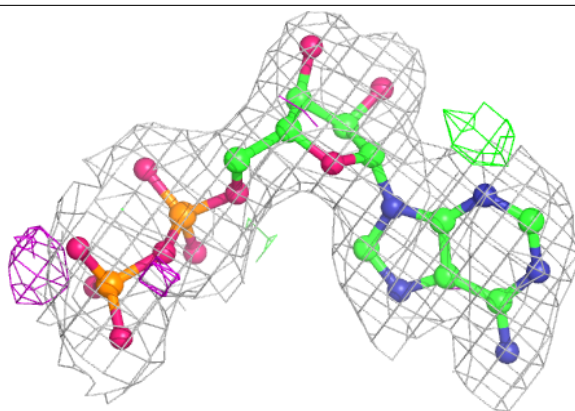
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	AF3	H	415	4/4	0.80	0.34	52,66,72,214	0
7	AF3	C	415	4/4	0.91	0.27	37,42,60,145	0
8	MG	H	416	1/1	0.92	0.18	40,40,40,40	0
6	ADP	H	414	27/27	0.94	0.13	35,44,54,61	0
8	MG	C	416	1/1	0.97	0.28	32,32,32,32	0
6	ADP	C	414	27/27	0.98	0.15	19,28,36,40	0

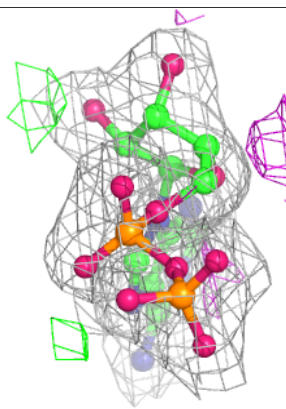
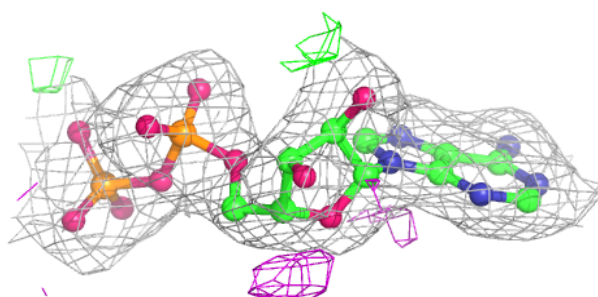
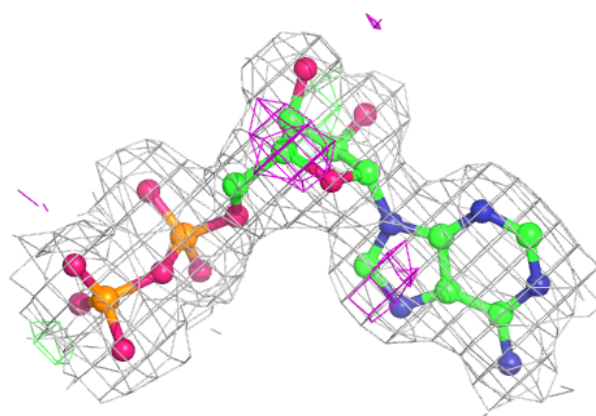
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP H 414:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP C 414:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.