



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 AM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

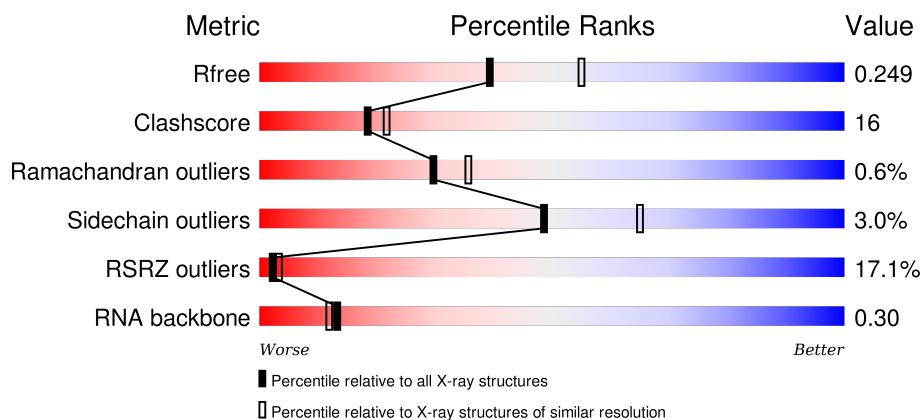
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)
RNA backbone	2183	1011 (2.84-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	146	<div> <div>3%</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>•</div> <div>25%</div> </div>
2	G	126	<div> <div>45%</div> <div>39%</div> <div>33%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	413	
3	H	413	
4	D	146	
4	I	146	
5	F	6	
5	J	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	AF3	H	415	-	-	-	X

## 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

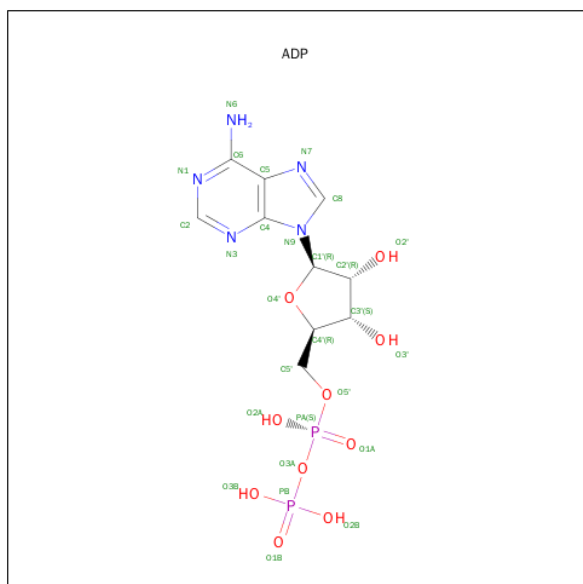
- Molecule 4 is a protein called Protein CASC3.

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: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



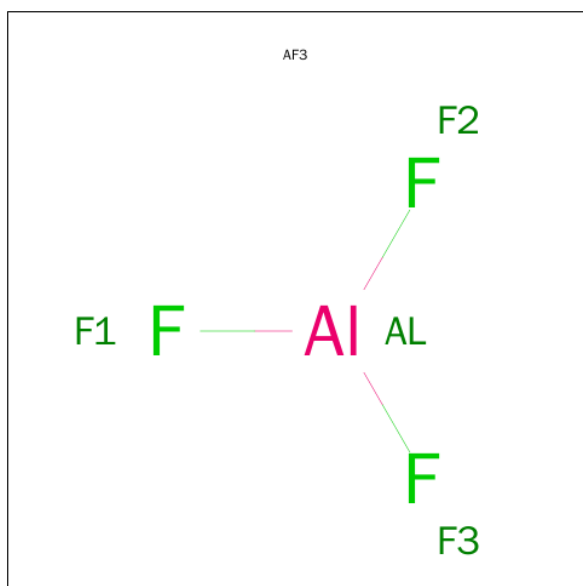
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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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:  $\text{AlF}_3$ ).



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:  $\text{Mg}$ ).

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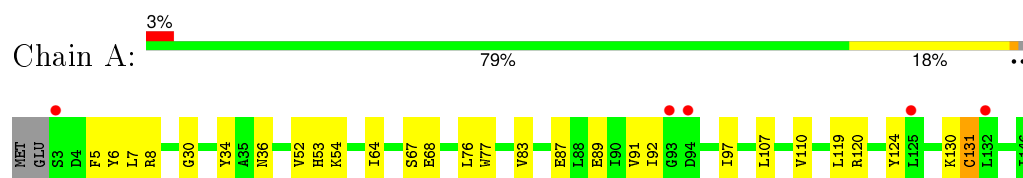
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	158	Total 158	O 158	0	0
9	D	25	Total 25	O 25	0	0
9	E	3	Total 3	O 3	0	0
9	G	2	Total 2	O 2	0	0
9	H	76	Total 76	O 76	0	0
9	I	18	Total 18	O 18	0	0
9	F	6	Total 6	O 6	0	0
9	J	5	Total 5	O 5	0	0

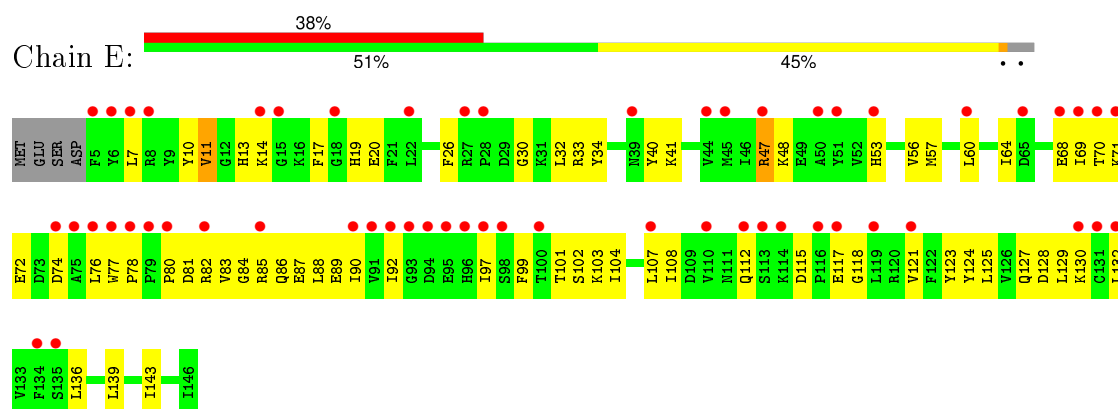
### 3 Residue-property plots [i](#)

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

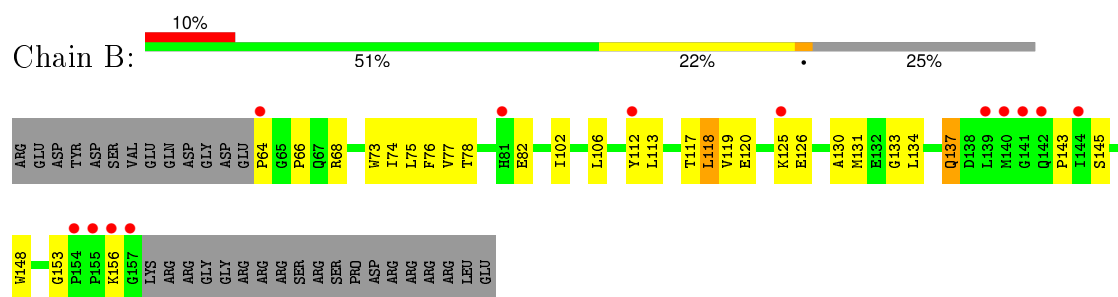
- Molecule 1: Protein mago nashi homolog



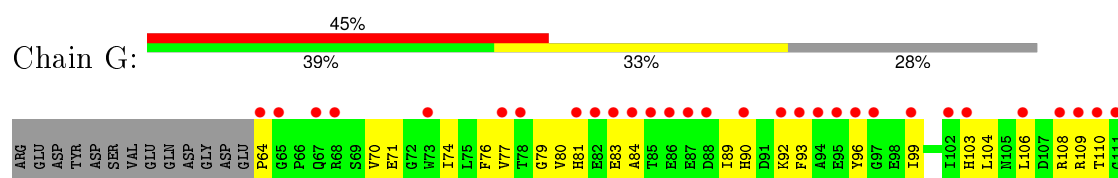
- Molecule 1: Protein mago nashi homolog



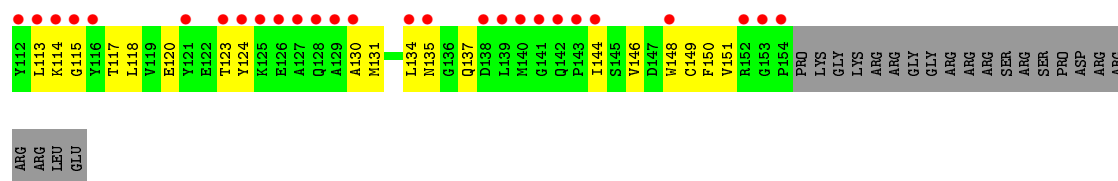
- Molecule 2: RNA-binding protein 8A



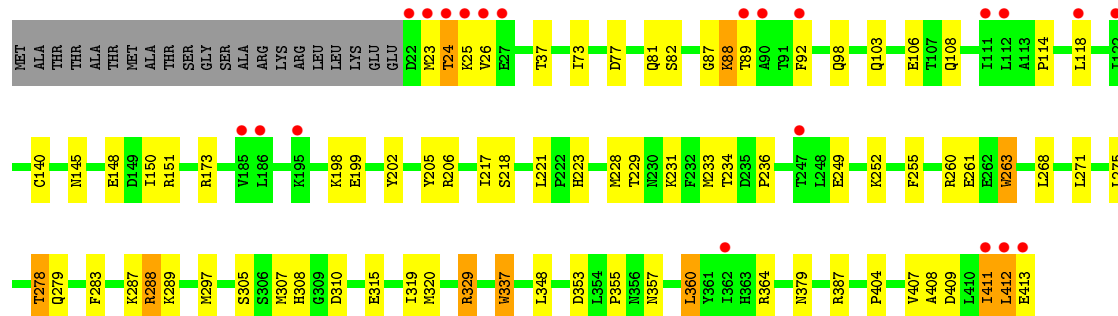
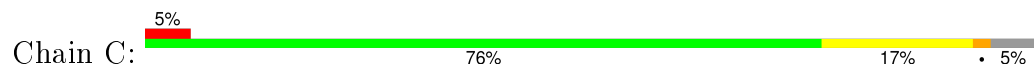
- Molecule 2: RNA-binding protein 8A



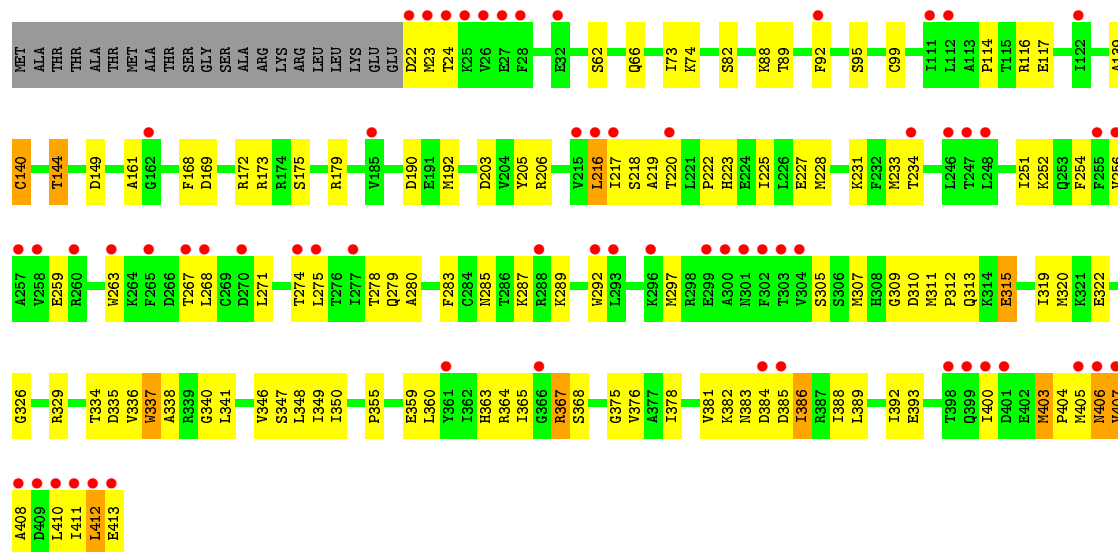




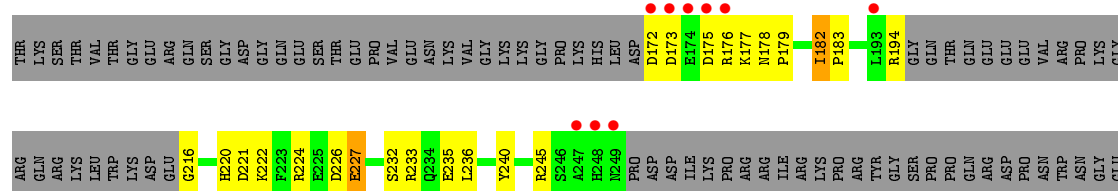
### • Molecule 3: Eukaryotic initiation factor 4A-III



### • Molecule 3: Eukaryotic initiation factor 4A-III

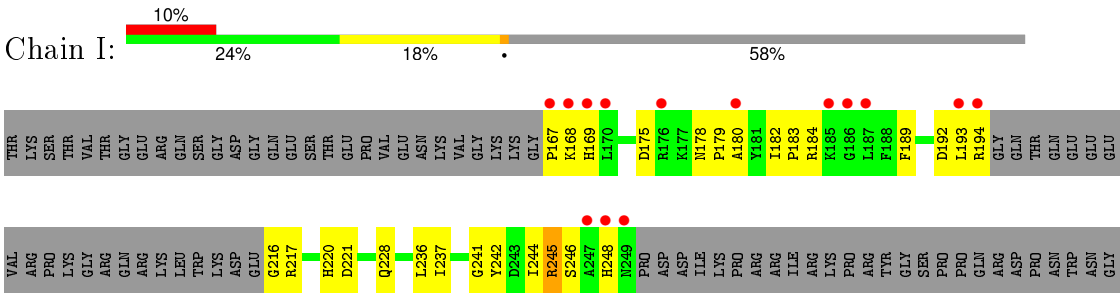


### • Molecule 4: Protein CASC3



ARG  
LEU  
ASN  
LYS  
SER  
HIS  
ARG

• Molecule 4: Protein CASC3

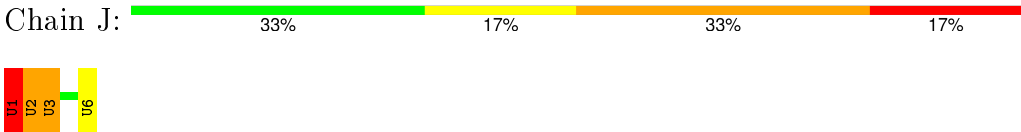


GLU  
ARG  
LEU  
ASN  
LYS  
SER  
HIS  
ARG

• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.206 , 0.251 0.205 , 0.249	Depositor DCC
$R_{free}$ test set	2144 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.7	EDS
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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 107634 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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:24:THR:HG22	3:C:25:LYS:HG2	1.72	0.70
3:C:231:LYS:HE3	4:D:216:GLY:N	2.06	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
1:E:17:PHE:CE2	4:I:192:ASP:HB2	2.27	0.69
3:C:106:GLU:O	3:C:108:GLN:HG3	1.92	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
3:H:289:LYS:HZ2	4:I:182:ILE:HD11	1.64	0.60
1:A:8:ARG:NH2	1:A:87:GLU:OE1	2.35	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)
1:E:101:THR:HG22	1:E:102:SER:N	2.17	0.59
3:C:387:ARG:NH1	4:D:194:ARG:H	2.01	0.59
1:E:83:VAL:HA	4:I:194:ARG:HE	1.68	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
3:H:169:ASP:O	3:H:173:ARG:HB2	2.01	0.59
1:E:70:THR:HG22	1:E:97:ILE:HD13	1.85	0.58
1:A:53:HIS:CE1	1:A:54:LYS:HG2	2.38	0.58
3:H:309:GLY:N	5:J:3:U:OP1	2.32	0.58
1:E:143:ILE:HG23	2:G:71:GLU:OE2	2.03	0.58
3:C:308:HIS:CE1	3:C:310:ASP:HB2	2.38	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
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
2:G:81:HIS:CE1	2:G:83:GLU:H	2.21	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
1:E:84:GLY:HA3	1:E:103:LYS:HE3	1.86	0.57
2:B:125:LYS:HG3	2:B:126:GLU:N	2.20	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:H:256:VAL:HG23	3:H:403:MET:HG3	1.87	0.56
3:C:278:THR:O	3:C:329:ARG:HD2	2.05	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
2:G:131:MET:HG3	2:G:146:VAL:O	2.06	0.56
3:C:23:MET:O	3:C:223:HIS:HE1	1.89	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:H:307:MET:HB3	3:H:319:ILE:HG21	1.89	0.55
3:C:279:GLN:HG2	3:C:329:ARG:HA	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
4:D:224:ARG:CG	4:D:226:ASP:OD1	2.56	0.54
1:A:5:PHE:HZ	1:A:64:ILE:HD12	1.72	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
3:C:173:ARG:NH2	5:F:6:U:O3'	2.41	0.53
1:E:123:TYR:O	1:E:127:GLN:HG3	2.09	0.53
4:D:236:LEU:CD1	4:D:245:ARG:HG3	2.39	0.53
3:H:225:ILE:HD12	3:H:225:ILE:N	2.23	0.53
2:G:96:TYR:CD2	2:G:130:ALA:HA	2.44	0.53
3:H:278:THR:HG23	3:H:279:GLN:N	2.21	0.53
1:A:7:LEU:CD1	1:A:64:ILE:HD11	2.39	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:E:127:GLN:HB3	2:G:108:ARG:CG	2.39	0.52
1:A:8:ARG:NH1	1:A:89:GLU:OE2	2.42	0.52
2:G:80:VAL:HG21	2:G:117:THR:HG22	1.92	0.52
1:E:69:ILE:CG1	1:E:125:LEU:HD22	2.30	0.52
3:C:81:GLN:HA	3:C:218:SER:O	2.09	0.52
3:C:82:SER:OG	3:C:88:LYS:CG	2.56	0.52
1:E:68:GLU:HB3	1:E:71:LYS:CG	2.39	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
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
3:H:289:LYS:HZ3	4:I:182:ILE:HD11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:PHE:HD1	2:B:118:LEU:HD13	1.76	0.51
1:E:76:LEU:HB2	1:E:115:ASP:HB2	1.92	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
1:E:70:THR:CG2	1:E:92:ILE:HD11	2.40	0.50
1:E:74:ASP:HA	1:E:77:TRP:CD2	2.46	0.50
3:C:260:ARG:HD2	3:C:263:TRP:CZ2	2.46	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
1:E:86:GLN:HE22	1:E:104:ILE:HG13	1.75	0.50
2:B:137:GLN:O	2:B:143:PRO:HA	2.12	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:E:125:LEU:O	1:E:129:LEU:HG	2.13	0.49
1:A:7:LEU:HD12	1:A:64:ILE:HD11	1.94	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
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
1:E:53:HIS:O	1:E:56:VAL:HB	2.12	0.48
3:H:311:MET:HB3	3:H:315:GLU:HG2	1.94	0.48
1:E:74:ASP:HA	1:E:77:TRP:CG	2.49	0.48
3:C:114:PRO:HD2	3:C:118:LEU:HD23	1.95	0.48
2:B:75:LEU:HD22	2:B:131:MET:HE2	1.95	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
3:H:381:VAL:HG11	3:H:386:ILE:HD13	1.95	0.48
1:E:127:GLN:HA	1:E:130:LYS:HE2	1.96	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
3:H:322:GLU:OE2	3:H:322:GLU:HA	2.13	0.47
2:G:123:THR:HG22	2:G:124:TYR:H	1.80	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:30:GLY:O	1:A:52:VAL:HG22	2.15	0.47
1:A:110:VAL:HG11	1:A:120:ARG:HG2	1.95	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
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: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
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:G:70:VAL:HG22	2:G:71:GLU:HG3	1.98	0.45
1:E:7:LEU:HD11	1:E:88:LEU:HD11	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
2:B:74:ILE:HD13	2:B:120:GLU:HB2	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
1:E:68:GLU:HB3	1:E:71:LYS:HG3	1.98	0.45
3:H:278:THR:O	3:H:279:GLN:HG3	2.17	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
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
3:H:219:ALA:HB2	7:H:415:AF3:F2	2.07	0.45
3:H:259:GLU:HA	3:H:383:ASN:ND2	2.30	0.45
1:A:83:VAL:HG22	3:C:387:ARG:HD3	1.98	0.45
3:H:73:ILE:N	3:H:73:ILE:HD13	2.32	0.45
3:C:88:LYS:CE	3:C:218:SER:C	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:338:ALA:O	3:H:363:HIS:HB3	2.16	0.45
1:E:74:ASP:OD2	1:E:99:PHE:HA	2.17	0.44
3:H:349:ILE:HD11	3:H:367:ARG:HB2	1.98	0.44
3:H:263:TRP:HA	3:H:263:TRP:HE3	1.82	0.44
2:G:106:LEU:HD23	2:G:113:LEU:HD23	1.99	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
4:I:169:HIS:HB3	9:I:296:HOH:O	2.18	0.44
2:G:131:MET:HE1	2:G:148:TRP:N	2.32	0.44
3:C:387:ARG:HG3	9:C:537: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
2:G:149:CYS:HB3	2:G:150:PHE:CD1	2.53	0.44
4:I:244:ILE:C	4:I:246:SER:N	2.71	0.44
1:E:33:ARG:HE	1:E:47:ARG:NH2	2.15	0.44
1:E:76:LEU:HD12	1:E:76:LEU:N	2.33	0.44
1:E:13:HIS:CE1	1:E:20:GLU:HB2	2.52	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
3:H:252:LYS:HG3	3:H:410:LEU:HD21	1.99	0.43
3:H:289:LYS:HE3	4:I:180:ALA:HB1	2.00	0.43
2:B:78:THR:CG2	2:B:145:SER:HB2	2.48	0.43
3:C:404:PRO:O	3:C:407:VAL:HG22	2.18	0.43
3:H:89:THR:HG23	3:H:92:PHE:CZ	2.52	0.43
3:C:151:ARG:HG3	4:D:240:TYR:CE1	2.53	0.43
1:A:130:LYS:NZ	9:A:210:HOH:O	2.48	0.43
3:H:405:MET:HG2	3:H:406:ASN:N	2.22	0.43
3:H:283:PHE:HB3	3:H:364:ARG:NH2	2.34	0.43
1:A:67:SER:O	1:A:68:GLU:HB2	2.18	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:175:ASP:OD2	4:D:177:LYS:HB2	2.19	0.43
2:B:130:ALA:O	2:B:134:LEU:HB2	2.18	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:H:287:LYS:HD2	3:H:310:ASP:OD2	2.19	0.43
3:C:233:MET:HE1	3:C:236:PRO:HB3	2.01	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:H:173:ARG:HD3	3:H:175:SER:OG	2.20	0.42
3:C:288:ARG:NH2	4:D:176:ARG:O	2.53	0.42
3:H:88:LYS:HE2	3:H:218:SER:N	2.34	0.42
3:C:81:GLN:HB2	3:C:221:LEU:CD1	2.47	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
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
3:H:337:TRP:CD2	3:H:341:LEU:HD12	2.54	0.42
2:B:102:ILE:HD13	2:B:119:VAL:HG13	2.01	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
1:E:77:TRP:CD1	1:E:77:TRP:N	2.87	0.42
2:B:64:PRO:HG3	2:B:153:GLY:O	2.20	0.42
2:G:134:LEU:HA	2:G:137:GLN:CG	2.50	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
1:E:7:LEU:HD13	1:E:90:ILE:HG12	2.02	0.42
3:H:350:ILE:CD1	3:H:378:ILE:HB	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
3:C:263:TRP:HE3	3:C:263:TRP:HA	1.85	0.42
3:H:22:ASP:OD1	3:H:24:THR:HB	2.20	0.42
3:H:114:PRO:HD3	3:H:192:MET:SD	2.60	0.42
3:H:411:ILE:C	3:H:413:GLU:H	2.22	0.42
5:J:6:U:H6	5:J:6:U:O5'	2.03	0.41
3:H:205:TYR:O	4:I:220:HIS:HD2	2.03	0.41
1:E:83:VAL:HA	4:I:194:ARG:HD2	2.02	0.41
4:I:184:ARG:HG2	4:I:189:PHE:CE1	2.55	0.41
3:C:73:ILE:HD13	3:C:98:GLN:HG2	2.02	0.41
3:H:393:GLU:HG3	3:H:400:ILE:HG13	2.00	0.41
2:G:92:LYS:O	2:G:134:LEU:HD11	2.20	0.41
1:E:7:LEU:HA	1:E:89:GLU:O	2.19	0.41
1:E:40:TYR:CE2	1:E:41:LYS:HG3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:411:ILE:O	3:C:413:GLU:N	2.53	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:410:LEU:HB2	9:H:469:HOH: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:C:255:PHE:HA	3:C:379:ASN:O	2.20	0.41
2:B:156:LYS:HB3	9:B:187:HOH:O	2.21	0.41
1:E:69:ILE:CD1	1:E:121:VAL:HG12	2.51	0.40
3:H:382:LYS:CG	3:H:383:ASN:H	2.22	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
5:J:2:U:H2'	5:J:3:U:O4'	2.21	0.40
3:C:287:LYS:HG2	3:C:308:HIS:HB2	2.02	0.40
3:H:271:LEU:O	3:H:274:THR:HG22	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:H:73:ILE:CD1	3:H:95:SER:HA	2.41	0.40
3:H:410:LEU:HD12	3:H:410:LEU:HA	1.91	0.40
3:C:387:ARG:NH2	9:C:536:HOH:O	2.54	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
1:E:84:GLY:HA3	1:E:103:LYS:HG3	2.03	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%)	26	31
2	B	92/126 (73%)	90 (98%)	1 (1%)	1 (1%)	17	18
2	G	89/126 (71%)	81 (91%)	8 (9%)	0	100	100
3	C	390/413 (94%)	380 (97%)	9 (2%)	1 (0%)	46	57
3	H	390/413 (94%)	371 (95%)	15 (4%)	4 (1%)	19	21
4	D	53/146 (36%)	51 (96%)	2 (4%)	0	100	100
4	I	58/146 (40%)	54 (93%)	3 (5%)	1 (2%)	11	10
All	All	1354/1662 (82%)	1291 (95%)	55 (4%)	8 (1%)	30	36

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%)	48	65
1	E	130/134 (97%)	129 (99%)	1 (1%)	86	94
2	B	78/107 (73%)	77 (99%)	1 (1%)	76	87
2	G	76/107 (71%)	76 (100%)	0	100	100
3	C	347/363 (96%)	334 (96%)	13 (4%)	41	55
3	H	347/363 (96%)	333 (96%)	14 (4%)	38	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	50/130 (38%)	48 (96%)	2 (4%)	38	52
4	I	55/130 (42%)	53 (96%)	2 (4%)	42	57
All	All	1215/1468 (83%)	1178 (97%)	37 (3%)	48	65

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	C	414	-	22,29,29	1.11	1 (4%)	27,45,45	1.96	5 (18%)
7	AF3	C	415	-	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	H	414	-	22,29,29	1.14	2 (9%)	27,45,45	1.93	6 (22%)
7	AF3	H	415	-	0,3,3	0.00	-	0,3,3	0.00	-

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	C	414	-	-	0/12/32/32	0/3/3/3
7	AF3	C	415	-	-	0/0/0/0	0/0/0/0
6	ADP	H	414	-	-	0/12/32/32	0/3/3/3
7	AF3	H	415	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	414	ADP	O4'-C1'	2.14	1.43	1.41
6	C	414	ADP	C5-C4	2.94	1.47	1.40
6	H	414	ADP	C5-C4	3.44	1.48	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	414	ADP	N3-C2-N1	-7.46	123.18	128.89
6	H	414	ADP	N3-C2-N1	-6.61	123.83	128.89
6	C	414	ADP	C4-C5-N7	-3.05	106.68	109.48
6	H	414	ADP	C4-C5-N7	-2.97	106.75	109.48
6	H	414	ADP	C1'-N9-C4	-2.67	122.91	126.94
6	H	414	ADP	PA-O3A-PB	-2.62	123.89	132.67
6	C	414	ADP	C1'-N9-C4	-2.23	123.57	126.94
6	C	414	ADP	O3'-C3'-C4'	-2.01	105.03	111.05
6	H	414	ADP	O3B-PB-O2B	2.24	115.90	107.38
6	H	414	ADP	C2-N1-C6	2.28	122.84	118.77
6	C	414	ADP	O3B-PB-O2B	2.30	116.12	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	144/146 (98%)	-0.05	5 (3%) 48 56	24, 34, 65, 120	0
1	E	142/146 (97%)	2.03	56 (39%) 0 0	81, 119, 190, 266	0
2	B	94/126 (74%)	0.59	13 (13%) 4 6	35, 61, 98, 160	0
2	G	91/126 (72%)	3.14	57 (62%) 0 0	92, 128, 176, 192	0
3	C	392/413 (94%)	0.16	21 (5%) 29 38	23, 35, 63, 142	0
3	H	392/413 (94%)	0.73	62 (15%) 3 4	33, 61, 144, 267	0
4	D	57/146 (39%)	0.81	9 (15%) 3 4	29, 52, 148, 167	0
4	I	62/146 (42%)	1.04	14 (22%) 1 1	37, 73, 140, 185	0
5	F	6/6 (100%)	0.27	0 100 100	35, 39, 45, 74	0
5	J	6/6 (100%)	0.05	0 100 100	55, 63, 75, 104	0
All	All	1386/1674 (82%)	0.78	237 (17%) 2 3	23, 52, 155, 267	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	405	MET	11.7
2	G	139	LEU	11.3
4	D	172	ASP	10.5
4	D	174	GLU	10.3
1	E	110	VAL	9.7
2	G	84	ALA	9.7
2	G	115	GLY	9.2
3	H	413	GLU	8.5
1	E	96	HIS	8.5
2	G	140	MET	8.4
4	D	173	ASP	8.1
2	G	124	TYR	7.9
2	G	125	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
2	B	156	LYS	7.8
3	H	411	ILE	7.8
4	I	249	ASN	7.6
3	H	277	ILE	7.3
3	C	23	MET	7.3
1	E	71	LYS	7.2
1	E	97	ILE	7.0
1	E	94	ASP	6.8
1	E	91	VAL	6.6
3	H	300	ALA	6.3
1	E	69	ILE	6.3
1	E	114	LYS	6.2
2	G	127	ALA	6.2
2	B	157	GLY	6.1
3	C	26	VAL	6.1
3	H	23	MET	6.1
1	E	77	TRP	6.0
2	G	81	HIS	6.0
1	E	119	LEU	5.6
1	E	14	LYS	5.5
2	G	121	TYR	5.4
2	G	143	PRO	5.4
3	H	263	TRP	5.4
2	G	112	TYR	5.4
2	G	86	GLU	5.3
2	G	154	PRO	5.3
3	H	275	LEU	5.3
2	G	82	GLU	5.2
3	H	257	ALA	5.2
1	E	113	SER	5.2
1	E	76	LEU	5.2
4	I	194	ARG	5.2
2	G	96	TYR	5.2
2	G	99	ILE	5.1
1	E	112	GLN	5.1
2	G	153	GLY	5.1
2	G	134	LEU	5.1
4	I	167	PRO	5.1
4	I	169	HIS	5.0
2	G	141	GLY	5.0
3	C	22	ASP	4.9
3	H	26	VAL	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	102	ILE	4.8
3	H	25	LYS	4.8
1	A	3	SER	4.8
1	E	70	THR	4.8
3	H	406	ASN	4.8
3	H	412	LEU	4.8
1	A	93	GLY	4.8
4	D	247	ALA	4.7
1	E	121	VAL	4.7
1	A	94	ASP	4.6
2	G	93	PHE	4.5
4	D	176	ARG	4.5
4	I	247	ALA	4.5
3	H	22	ASP	4.5
3	C	24	THR	4.5
2	B	141	GLY	4.4
2	G	68	ARG	4.3
2	G	90	HIS	4.3
2	G	142	GLN	4.2
2	G	73	TRP	4.2
1	E	28	PRO	4.2
2	B	155	PRO	4.2
2	G	64	PRO	4.2
2	G	123	THR	4.2
3	H	247	THR	4.2
3	C	412	LEU	4.2
3	C	413	GLU	4.2
2	B	64	PRO	4.0
4	I	193	LEU	4.0
1	E	50	ALA	4.0
1	E	18	GLY	4.0
2	G	129	ALA	3.9
3	H	270	ASP	3.9
1	E	74	ASP	3.9
2	G	114	LYS	3.8
2	G	148	TRP	3.8
1	E	68	GLU	3.8
2	G	138	ASP	3.8
2	G	113	LEU	3.8
1	E	93	GLY	3.8
3	C	122	ILE	3.8
2	G	78	THR	3.7

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Mol	Chain	Res	Type	RSRZ
3	H	292	TRP	3.7
1	E	107	LEU	3.7
3	H	274	THR	3.7
4	I	187	LEU	3.7
2	G	130	ALA	3.7
2	G	97	GLY	3.7
1	E	47	ARG	3.7
1	E	98	SER	3.7
4	D	248	HIS	3.6
1	E	131	CYS	3.6
1	E	134	PHE	3.6
3	H	217	ILE	3.5
4	I	248	HIS	3.5
2	G	144	ILE	3.5
2	G	83	GLU	3.4
3	H	399	GLN	3.4
3	H	407	VAL	3.4
1	E	15	GLY	3.4
2	G	94	ALA	3.4
1	E	75	ALA	3.4
3	C	89	THR	3.4
1	E	95	GLU	3.3
3	H	398	THR	3.3
2	B	81	HIS	3.3
2	B	140	MET	3.3
2	G	85	THR	3.2
3	H	296	LYS	3.2
1	E	39	ASN	3.2
1	E	90	ILE	3.2
1	E	82	ARG	3.1
4	I	185	LYS	3.1
2	G	67	GLN	3.1
4	I	168	LYS	3.1
3	H	410	LEU	3.1
1	E	80	PRO	3.1
2	B	154	PRO	3.1
1	E	6	TYR	3.1
3	C	25	LYS	3.1
3	H	111	ILE	3.0
3	C	185	VAL	3.0
2	G	126	GLU	3.0
1	E	78	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	125	LYS	3.0
1	E	135	SER	2.9
2	G	92	LYS	2.9
3	H	288	ARG	2.9
1	E	44	VAL	2.9
3	H	32	GLU	2.9
2	G	116	TYR	2.9
3	H	361	TYR	2.9
1	E	92	ILE	2.9
1	E	79	PRO	2.8
3	C	92	PHE	2.8
3	H	302	PHE	2.8
3	H	303	THR	2.8
3	H	268	LEU	2.8
3	H	185	VAL	2.8
2	G	108	ARG	2.8
3	H	400	ILE	2.8
3	H	267	THR	2.8
1	E	7	LEU	2.8
1	E	45	MET	2.8
3	H	27	GLU	2.8
4	I	176	ARG	2.8
3	H	234	THR	2.8
3	H	408	ALA	2.7
3	H	409	ASP	2.7
3	H	256	VAL	2.7
1	E	53	HIS	2.7
1	E	60	LEU	2.7
2	G	152	ARG	2.7
3	H	385	ASP	2.7
3	H	384	ASP	2.7
1	E	100	THR	2.6
3	H	401	ASP	2.6
1	E	27	ARG	2.6
2	B	139	LEU	2.6
3	H	220	THR	2.6
1	E	85	ARG	2.6
3	H	215	VAL	2.6
2	G	95	GLU	2.6
3	H	299	GLU	2.6
3	C	411	ILE	2.6
2	B	142	GLN	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	112	LEU	2.5
4	D	193	LEU	2.5
1	E	116	PRO	2.5
3	C	118	LEU	2.5
2	G	109	ARG	2.5
2	G	135	ASN	2.5
2	G	111	GLY	2.5
3	H	122	ILE	2.5
1	E	51	TYR	2.5
3	H	248	LEU	2.5
3	H	260	ARG	2.5
1	E	5	PHE	2.5
3	C	111	ILE	2.4
2	G	128	GLN	2.4
2	G	110	THR	2.4
2	G	65	GLY	2.4
2	B	144	ILE	2.4
2	G	77	VAL	2.4
4	I	186	GLY	2.3
1	E	117	GLU	2.3
3	H	304	VAL	2.3
3	H	24	THR	2.3
3	H	255	PHE	2.3
2	G	106	LEU	2.3
3	H	293	LEU	2.3
4	I	170	LEU	2.2
1	E	130	LYS	2.2
1	E	132	LEU	2.2
2	G	88	ASP	2.2
3	H	28	PHE	2.2
3	H	92	PHE	2.2
2	G	87	GLU	2.2
2	B	112	TYR	2.2
3	H	162	GLY	2.2
3	H	366	GLY	2.2
4	D	175	ASP	2.2
3	H	265	PHE	2.2
3	H	301	ASN	2.1
4	D	249	ASN	2.1
3	C	186	LEU	2.1
3	C	362	ILE	2.1
1	E	65	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	247	THR	2.1
3	H	258	VAL	2.1
1	A	125	LEU	2.1
3	H	216	LEU	2.1
4	I	180	ALA	2.1
1	E	8	ARG	2.1
3	C	112	LEU	2.0
2	G	103	HIS	2.0
1	E	22	LEU	2.0
3	C	195	LYS	2.0
3	C	27	GLU	2.0
1	A	132	LEU	2.0
3	C	90	ALA	2.0
3	H	246	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	AF3	H	415	4/4	0.80	0.34	3.73	52,66,72,214	0
7	AF3	C	415	4/4	0.91	0.27	1.58	37,42,60,145	0
6	ADP	C	414	27/27	0.98	0.15	-0.09	19,28,36,40	0
6	ADP	H	414	27/27	0.94	0.13	-0.67	35,44,54,61	0
8	MG	C	416	1/1	0.97	0.29	-	32,32,32,32	0
8	MG	H	416	1/1	0.92	0.18	-	40,40,40,40	0

## 6.5 Other polymers

There are no such residues in this entry.