



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2016 – 02:32 PM EST

PDB ID : 5JJL  
Title : Rho transcription termination factor bound to rU8 and 5 ADP-BeF3 molecules  
Authors : Thomsen, N.D.; Lawson, M.R.; Witkowsky, L.B.; Qu, S.; Berger, J.M.  
Deposited on : 2016-04-24  
Resolution : 3.20 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

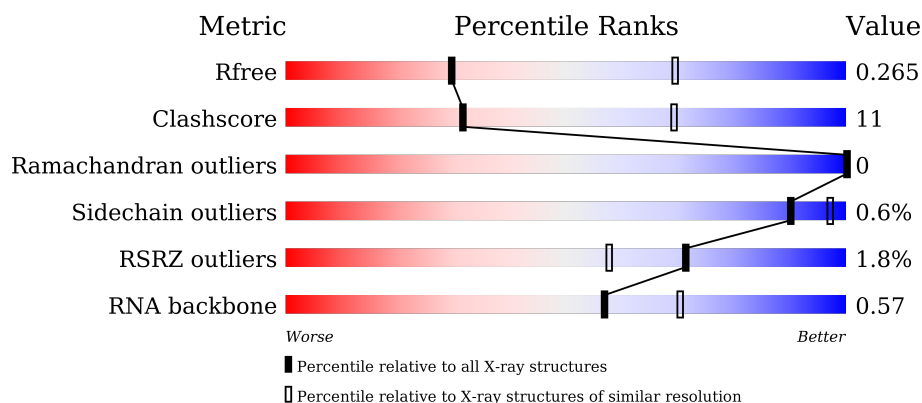
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 24%, green 70%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>70%</span> <span>24%</span> <span>6%</span> </div> </div>
1	B	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 77%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>77%</span> <span>20%</span> <span>.</span> </div> </div>
1	C	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 26%, green 73%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>73%</span> <span>26%</span> <span>.</span> </div> </div>
1	D	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 76%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>76%</span> <span>20%</span> <span>.</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	420	
1	F	420	
2	G	12	

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
5	BEF	B	1002	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19229 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	Se	0	0	0
			3108	1964	546	583	1	14			
1	B	409	Total	C	N	O	S	Se	0	0	0
			3219	2028	569	606	1	15			
1	C	415	Total	C	N	O	S	Se	0	0	0
			3264	2056	576	615	1	16			
1	D	406	Total	C	N	O	S	Se	0	0	0
			3192	2011	564	601	1	15			
1	E	381	Total	C	N	O	S	Se	0	0	0
			2944	1855	526	552	1	10			
1	F	402	Total	C	N	O	S	Se	0	0	0
			3161	1994	558	592	1	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	initiating methionine	UNP P0AG32
A	-1	GLY	-	expression tag	UNP P0AG32
A	0	HIS	-	expression tag	UNP P0AG32
A	1	MSE	-	expression tag	UNP P0AG32
B	-2	MSE	-	initiating methionine	UNP P0AG32
B	-1	GLY	-	expression tag	UNP P0AG32
B	0	HIS	-	expression tag	UNP P0AG32
B	1	MSE	-	expression tag	UNP P0AG32
C	-2	MSE	-	initiating methionine	UNP P0AG32
C	-1	GLY	-	expression tag	UNP P0AG32
C	0	HIS	-	expression tag	UNP P0AG32
C	1	MSE	-	expression tag	UNP P0AG32
D	-2	MSE	-	initiating methionine	UNP P0AG32
D	-1	GLY	-	expression tag	UNP P0AG32
D	0	HIS	-	expression tag	UNP P0AG32
D	1	MSE	-	expression tag	UNP P0AG32
E	-2	MSE	-	initiating methionine	UNP P0AG32

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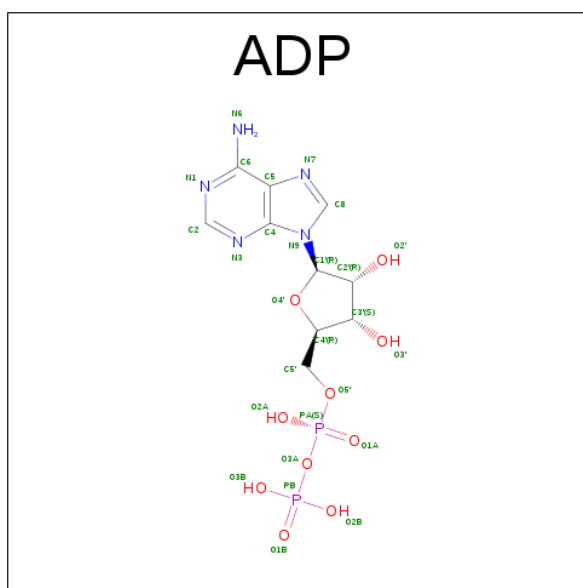
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP P0AG32
E	0	HIS	-	expression tag	UNP P0AG32
E	1	MSE	-	expression tag	UNP P0AG32
F	-2	MSE	-	initiating methionine	UNP P0AG32
F	-1	GLY	-	expression tag	UNP P0AG32
F	0	HIS	-	expression tag	UNP P0AG32
F	1	MSE	-	expression tag	UNP P0AG32

- Molecule 2 is a RNA chain called rU12: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	P	0	0	0
			165	72	16	68	9			

- Molecule 3 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
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

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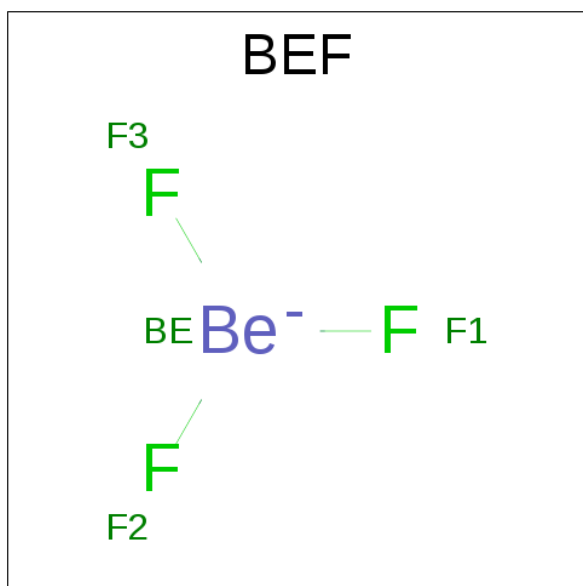
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		
5	B	1	Total	Be	F	0	0
			4	1	3		
5	C	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 4	Be 1	F 3	0	0
5	F	1	Total 4	Be 1	F 3	0	0

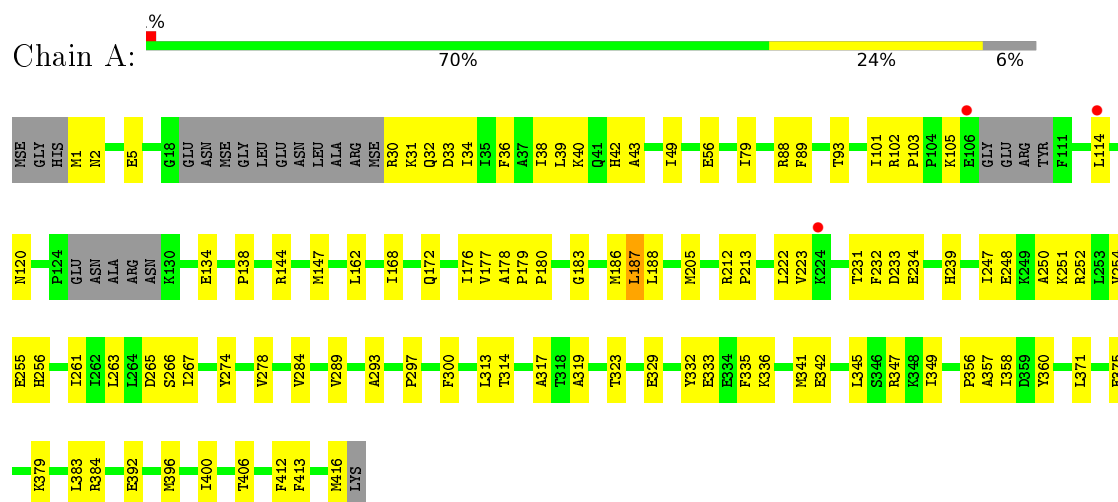
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	3	Total 3	O 3	0	0
6	C	4	Total 4	O 4	0	0
6	D	3	Total 3	O 3	0	0
6	F	3	Total 3	O 3	0	0

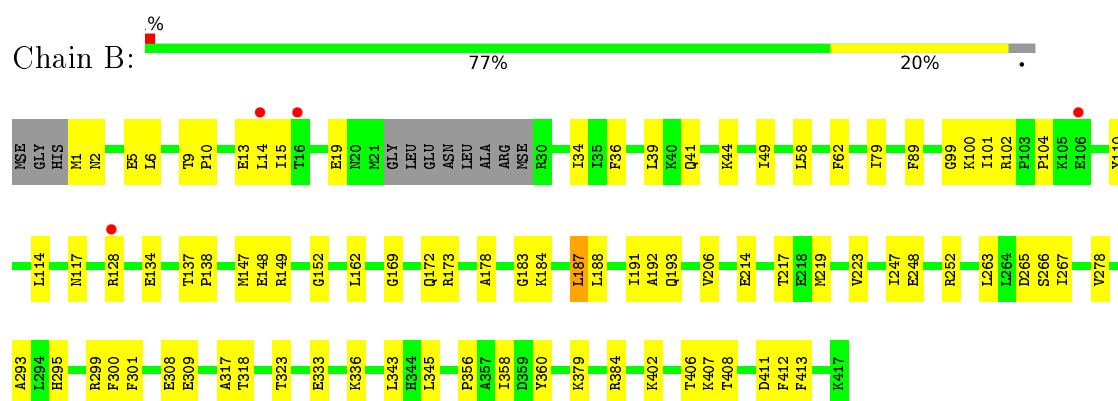
### 3 Residue-property plots

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.

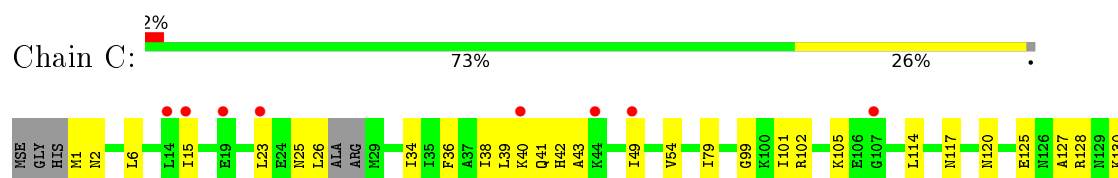
#### • Molecule 1: Transcription termination factor Rho



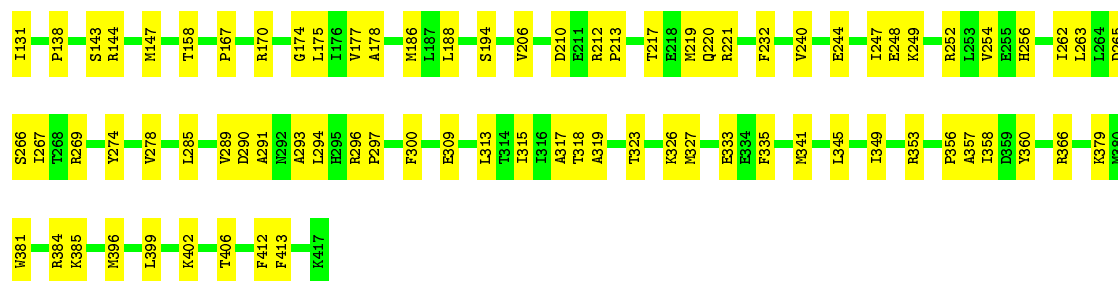
#### • Molecule 1: Transcription termination factor Rho



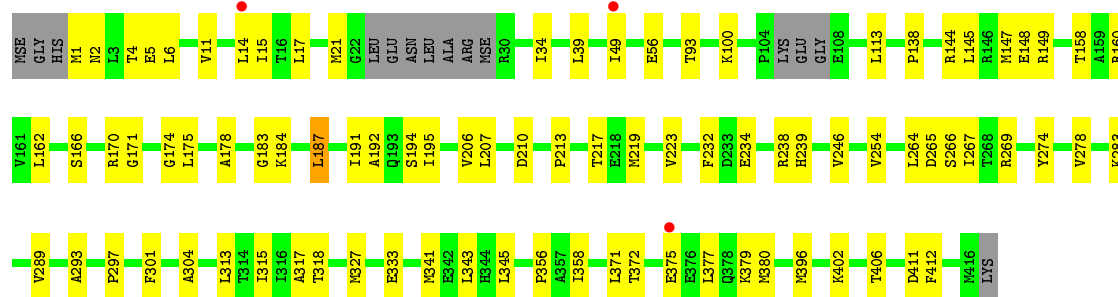
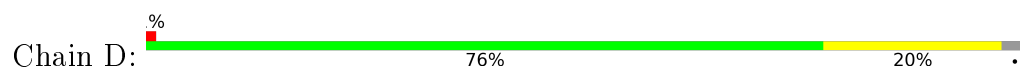
#### • Molecule 1: Transcription termination factor Rho



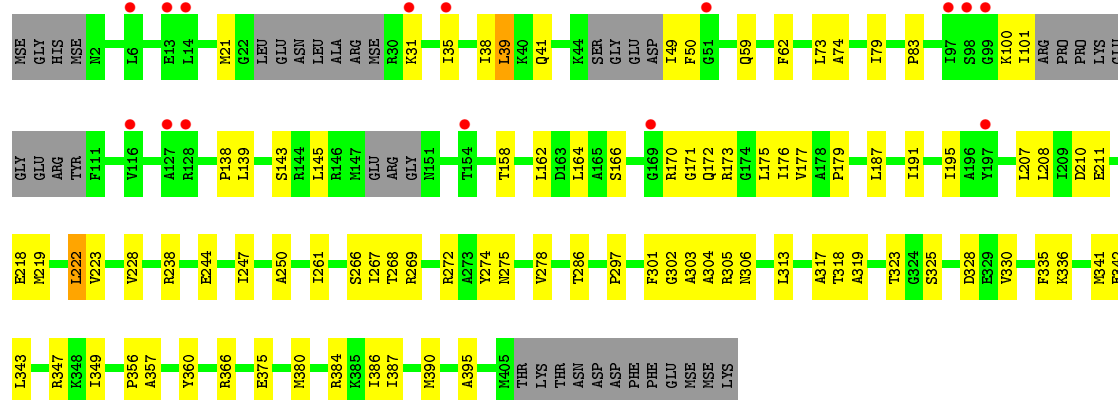




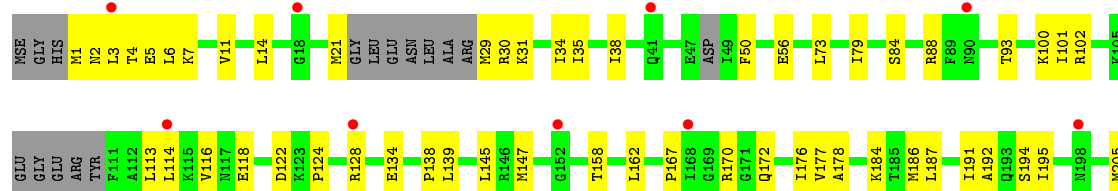
• Molecule 1: Transcription termination factor Rho

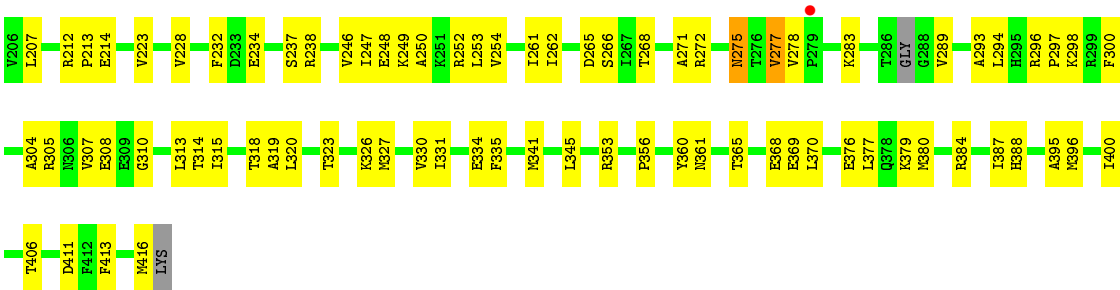


• Molecule 1: Transcription termination factor Rho

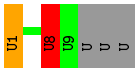


• Molecule 1: Transcription termination factor Rho





• Molecule 2: rU12: RNA (5'-R(P\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.09Å 199.07Å 111.67Å 90.00° 105.02° 90.00°	Depositor
Resolution (Å)	49.52 – 3.20 49.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.52-3.20) 96.1 (49.52-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.10.1_2155)	Depositor
R, $R_{free}$	0.232 , 0.266 0.229 , 0.265	Depositor DCC
$R_{free}$ test set	2305 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.24	0/3140	0.40	0/4206
1	B	0.25	0/3253	0.41	0/4357
1	C	0.24	0/3298	0.41	0/4417
1	D	0.24	0/3225	0.41	0/4320
1	E	0.25	0/2971	0.41	0/3985
1	F	0.25	0/3191	0.41	0/4270
2	G	0.37	0/180	1.37	5/275 (1.8%)
All	All	0.25	0/19258	0.43	5/25830 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	8	U	N3-C2-O2	-8.59	116.19	122.20
2	G	8	U	N1-C2-O2	8.56	128.79	122.80
2	G	1	U	N3-C2-O2	-7.31	117.08	122.20
2	G	1	U	N1-C2-O2	6.07	127.05	122.80
2	G	8	U	C2-N1-C1'	6.03	124.93	117.70

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	3108	0	3190	75	0
1	B	3219	0	3293	59	0
1	C	3264	0	3339	71	0
1	D	3192	0	3260	65	0
1	E	2944	0	2991	65	0
1	F	3161	0	3242	93	0
2	G	165	0	80	4	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	F	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	F	4	0	0	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	C	4	0	0	0	0
6	D	3	0	0	0	0
6	F	3	0	0	1	0
All	All	19229	0	19455	415	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 11.

All (415) 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:A:1:MSE:HE1	1:A:38:ILE:HG22	1.56	0.88
1:A:1:MSE:HE3	1:A:39:LEU:HD23	1.61	0.81
1:A:278:VAL:HG21	1:A:293:ALA:HB2	1.63	0.81
1:E:158:THR:HG22	1:E:356:PRO:HB3	1.63	0.79
1:E:162:LEU:HD13	1:E:343:LEU:HD22	1.66	0.76
1:D:213:PRO:HG2	1:E:305:ARG:HH21	1.52	0.74
5:F:1002:BEF:F3	6:F:1102:HOH:O	1.96	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD12	1:A:223:VAL:HG23	1.70	0.73
1:B:323:THR:HA	1:C:333:GLU:HG2	1.69	0.73
1:D:160:ARG:HH22	1:D:406:THR:HG23	1.54	0.72
1:F:6:LEU:HD23	1:F:35:ILE:HG13	1.72	0.72
1:F:113:LEU:HD21	1:F:116:VAL:HG12	1.71	0.71
1:C:188:LEU:HD11	1:C:263:LEU:HB3	1.72	0.71
1:A:323:THR:HA	1:B:333:GLU:HG2	1.73	0.70
1:A:138:PRO:HG3	1:F:213:PRO:HB2	1.73	0.70
1:B:162:LEU:HD13	1:B:343:LEU:HD22	1.74	0.69
1:D:372:THR:HG21	1:D:380:MSE:HE1	1.73	0.69
1:D:192:ALA:HB1	1:D:223:VAL:HG23	1.75	0.69
1:F:192:ALA:HB1	1:F:223:VAL:HG21	1.76	0.68
1:C:125:GLU:HA	1:C:128:ARG:HD3	1.75	0.68
1:C:147:MSE:HE3	1:C:194:SER:HB2	1.74	0.68
1:B:188:LEU:HD11	1:B:263:LEU:HB3	1.76	0.68
1:C:323:THR:HA	1:D:333:GLU:HG2	1.76	0.68
1:F:29:MSE:HE3	1:F:34:ILE:HG12	1.76	0.68
1:A:43:ALA:HB2	1:A:49:ILE:HD11	1.76	0.66
1:F:278:VAL:HG21	1:F:293:ALA:HB2	1.76	0.66
1:E:79:ILE:HD13	1:E:101:ILE:HG21	1.78	0.66
1:E:175:LEU:HD23	1:E:319:ALA:HB2	1.77	0.66
1:A:375:GLU:HG2	1:A:379:LYS:HE3	1.78	0.65
1:E:360:TYR:HE2	1:E:384:ARG:HG2	1.61	0.65
1:F:369:GLU:HG2	1:F:370:LEU:HD12	1.78	0.65
1:F:377:LEU:HA	1:F:380:MSE:HE2	1.78	0.65
1:D:17:LEU:HD22	1:D:21:MSE:HE3	1.78	0.64
1:C:1:MSE:HE1	1:C:38:ILE:HG22	1.80	0.64
1:C:43:ALA:HB2	1:C:49:ILE:HD11	1.78	0.64
1:C:79:ILE:HD13	1:C:101:ILE:HG21	1.80	0.64
1:F:234:GLU:HB3	1:F:238:ARG:HD3	1.78	0.64
1:F:272:ARG:HH21	1:F:327:MSE:HB3	1.62	0.64
1:A:79:ILE:HD13	1:A:101:ILE:HG21	1.79	0.63
1:E:39:LEU:HD13	1:E:49:ILE:HD11	1.80	0.62
1:A:177:VAL:HG22	1:A:319:ALA:HB3	1.82	0.62
1:F:73:LEU:HD11	1:F:238:ARG:HG3	1.80	0.62
1:A:297:PRO:HB2	1:A:335:PHE:HZ	1.66	0.61
1:C:206:VAL:HG11	1:C:219:MSE:HG2	1.82	0.61
1:E:145:LEU:HD21	1:E:170:ARG:HG2	1.83	0.61
1:B:217:THR:HG21	1:C:138:PRO:O	2.02	0.60
1:F:176:ILE:HB	1:F:318:THR:HG22	1.82	0.60
1:C:210:ASP:HB3	1:C:269:ARG:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB2	1:A:347:ARG:HD2	1.83	0.60
1:F:50:PHE:HA	1:F:100:LYS:HA	1.82	0.60
1:D:178:ALA:HB2	1:D:345:LEU:HB2	1.84	0.60
1:F:147:MSE:HE3	1:F:194:SER:HB2	1.84	0.60
1:A:172:GLN:HE21	1:A:341:MSE:HB2	1.67	0.59
1:B:137:THR:HG23	1:B:308:GLU:HB3	1.84	0.59
1:C:267:ILE:HB	1:C:317:ALA:HB1	1.83	0.59
1:F:341:MSE:HG2	1:F:365:THR:HG22	1.83	0.59
1:B:41:GLN:HG3	1:B:44:LYS:HD2	1.83	0.59
1:A:213:PRO:HG3	1:A:231:THR:HG21	1.85	0.59
1:C:290:ASP:HB3	1:C:293:ALA:HB2	1.84	0.59
1:D:278:VAL:HG11	1:D:293:ALA:HA	1.85	0.59
1:F:4:THR:HA	1:F:7:LYS:HE2	1.83	0.59
1:F:205:MSE:HE1	1:F:250:ALA:HB2	1.84	0.58
1:F:158:THR:HA	1:F:356:PRO:HG3	1.84	0.58
1:C:178:ALA:HB2	1:C:345:LEU:HB2	1.85	0.58
1:A:39:LEU:HD22	1:A:49:ILE:HG23	1.85	0.58
1:B:379:LYS:HD3	1:B:413:PHE:HB3	1.85	0.58
1:A:406:THR:HG21	1:A:412:PHE:N	2.18	0.58
1:E:50:PHE:HA	1:E:100:LYS:HA	1.86	0.58
1:E:179:PRO:HG2	1:E:347:ARG:HB2	1.85	0.58
1:B:102:ARG:CB	1:B:114:LEU:HD11	2.34	0.58
1:C:120:ASN:HD22	1:C:256:HIS:CE1	2.20	0.58
1:B:89:PHE:HA	1:B:128:ARG:HG2	1.86	0.58
1:C:217:THR:HG21	1:D:138:PRO:O	2.02	0.57
1:A:247:ILE:HB	1:A:300:PHE:CE1	2.40	0.57
1:A:88:ARG:HD2	1:A:89:PHE:CE2	2.39	0.57
1:C:26:LEU:HD23	1:C:34:ILE:HG13	1.87	0.57
1:F:172:GLN:HE21	1:F:341:MSE:HB2	1.70	0.57
1:D:406:THR:HG21	1:D:412:PHE:HB2	1.85	0.56
1:D:356:PRO:HB2	1:D:358:ILE:HG13	1.88	0.56
1:D:1:MSE:HB3	1:D:49:ILE:HD12	1.87	0.56
1:F:413:PHE:HA	1:F:416:MSE:HE2	1.88	0.56
1:E:244:GLU:HA	1:E:247:ILE:HG22	1.87	0.56
1:F:186:MSE:HG3	3:F:1000:ADP:C8	2.39	0.56
1:F:360:TYR:CE2	1:F:384:ARG:HG2	2.41	0.56
1:A:233:ASP:HA	1:B:299:ARG:HE	1.71	0.56
1:D:402:LYS:HD3	1:D:412:PHE:HE1	1.71	0.56
1:A:36:PHE:HZ	1:A:40:LYS:HZ2	1.54	0.56
1:C:217:THR:O	1:C:221:ARG:HD3	2.06	0.55
3:D:1000:ADP:O2A	1:E:366:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:THR:HA	1:D:356:PRO:HG3	1.89	0.55
1:D:396:MSE:HA	1:D:396:MSE:HE2	1.89	0.55
1:E:73:LEU:HB2	1:E:238:ARG:NH2	2.21	0.55
1:E:278:VAL:O	1:F:283:LYS:HD2	2.07	0.55
1:D:2:ASN:HB3	1:D:5:GLU:HG3	1.89	0.55
1:A:297:PRO:HB2	1:A:335:PHE:CZ	2.42	0.55
1:E:187:LEU:HD21	1:E:343:LEU:HD23	1.87	0.55
1:F:147:MSE:HG3	1:F:162:LEU:HD22	1.90	0.54
1:B:1:MSE:HE2	1:B:6:LEU:HD21	1.88	0.54
1:B:79:ILE:HD13	1:B:101:ILE:HG21	1.89	0.54
1:C:360:TYR:HE2	1:C:384:ARG:HG2	1.73	0.54
1:A:254:VAL:HG21	1:A:313:LEU:HB2	1.89	0.54
1:A:329:GLU:O	1:A:333:GLU:HG2	2.07	0.54
1:A:1:MSE:HG2	1:A:42:HIS:CD2	2.42	0.54
1:F:3:LEU:HD12	1:F:35:ILE:HD11	1.89	0.54
1:B:14:LEU:HB3	1:B:34:ILE:HG21	1.89	0.54
1:B:178:ALA:HB2	1:B:345:LEU:HB2	1.90	0.54
1:C:177:VAL:HG22	1:C:319:ALA:HB3	1.88	0.54
1:C:175:LEU:HD11	1:C:335:PHE:HB3	1.89	0.54
1:D:147:MSE:HE3	1:D:194:SER:HB2	1.90	0.54
1:F:178:ALA:HB2	1:F:345:LEU:HB2	1.89	0.54
1:E:349:ILE:HG21	1:E:357:ALA:HA	1.90	0.54
1:D:206:VAL:HG11	1:D:219:MSE:HG2	1.90	0.53
1:F:294:LEU:HD13	1:F:334:GLU:HG3	1.90	0.53
2:G:1:U:O2	2:G:1:U:H2'	2.07	0.53
1:A:278:VAL:CG2	1:A:293:ALA:HB2	2.37	0.53
1:E:35:ILE:O	1:E:39:LEU:HD23	2.07	0.53
1:A:284:VAL:HB	2:G:1:U:O2	2.09	0.53
1:C:266:SER:HB3	1:C:269:ARG:HG2	1.91	0.53
1:F:2:ASN:HB3	1:F:5:GLU:HB3	1.90	0.53
1:F:297:PRO:HB2	1:F:335:PHE:HZ	1.74	0.53
1:B:149:ARG:HH21	1:B:193:GLN:HB2	1.73	0.52
1:F:167:PRO:O	1:F:365:THR:HG21	2.09	0.52
1:B:15:ILE:O	1:B:19:GLU:HG2	2.10	0.52
1:E:143:SER:HB3	1:E:170:ARG:HG3	1.92	0.52
1:A:180:PRO:HB2	1:B:336:LYS:HG2	1.92	0.52
1:C:23:LEU:HD11	1:C:41:GLN:HG2	1.92	0.52
1:C:102:ARG:HB3	1:C:114:LEU:HD21	1.92	0.52
1:E:210:ASP:HB3	1:E:269:ARG:HD2	1.93	0.52
1:F:145:LEU:HD11	1:F:170:ARG:HG3	1.92	0.51
1:A:274:TYR:CD2	1:A:297:PRO:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:THR:HG23	1:E:325:SER:H	1.74	0.51
1:B:10:PRO:HG2	1:B:13:GLU:HG2	1.93	0.51
1:D:148:GLU:HG3	1:D:160:ARG:HG2	1.92	0.51
1:F:138:PRO:C	1:F:139:LEU:HD22	2.31	0.51
1:E:323:THR:HG21	1:E:328:ASP:OD2	2.11	0.51
1:B:219:MSE:O	1:B:223:VAL:HG12	2.11	0.51
1:A:147:MSE:HG3	1:A:162:LEU:HD22	1.91	0.51
1:A:356:PRO:HB2	1:A:358:ILE:HG13	1.91	0.51
1:E:173:ARG:HG2	1:E:301:PHE:CZ	2.46	0.51
1:D:219:MSE:O	1:D:223:VAL:HG12	2.10	0.50
1:F:138:PRO:HB3	1:F:305:ARG:HH21	1.75	0.50
1:A:188:LEU:HD11	1:A:263:LEU:HB3	1.93	0.50
1:F:268:THR:O	1:F:272:ARG:HG3	2.12	0.50
1:E:176:ILE:HB	1:E:318:THR:HG22	1.94	0.50
1:D:210:ASP:HB3	1:D:269:ARG:HB3	1.94	0.50
1:F:21:MSE:SE	1:F:38:ILE:HG23	2.62	0.50
1:F:79:ILE:HG12	1:F:101:ILE:HG21	1.92	0.50
1:D:14:LEU:HD12	1:D:34:ILE:HD12	1.93	0.50
1:A:176:ILE:HD13	1:A:187:LEU:HD12	1.93	0.50
1:C:127:ALA:O	1:C:130:LYS:HD2	2.12	0.50
1:E:274:TYR:CD2	1:E:297:PRO:HG3	2.47	0.50
1:B:267:ILE:HB	1:B:317:ALA:HB1	1.92	0.50
1:A:213:PRO:HD3	1:A:232:PHE:CE2	2.47	0.49
1:A:213:PRO:HB2	1:B:138:PRO:HG2	1.93	0.49
1:A:120:ASN:HD22	1:A:256:HIS:CD2	2.30	0.49
1:B:406:THR:CG2	1:B:411:ASP:HB2	2.42	0.49
1:C:402:LYS:HB3	1:C:412:PHE:HE1	1.77	0.49
1:F:139:LEU:CD2	1:F:308:GLU:HB2	2.43	0.49
1:F:178:ALA:CB	1:F:345:LEU:HB2	2.41	0.49
1:A:267:ILE:HB	1:A:317:ALA:HB1	1.95	0.49
1:F:247:ILE:HB	1:F:300:PHE:CE1	2.47	0.49
1:B:247:ILE:HB	1:B:300:PHE:CE1	2.48	0.49
1:D:183:GLY:O	1:D:187:LEU:HB2	2.13	0.49
1:F:207:LEU:HA	1:F:228:VAL:O	2.13	0.49
1:D:187:LEU:O	1:D:191:ILE:HG12	2.13	0.49
1:F:118:GLU:HG3	1:F:122:ASP:O	2.13	0.49
1:A:56:GLU:HA	1:A:93:THR:HG23	1.95	0.48
1:C:144:ARG:CZ	1:C:167:PRO:HB3	2.43	0.48
1:F:30:ARG:O	1:F:34:ILE:HG13	2.13	0.48
1:C:15:ILE:HA	1:C:26:LEU:HD22	1.95	0.48
1:C:274:TYR:CD2	1:C:297:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MSE:HE3	1:D:21:MSE:HE1	1.96	0.48
1:A:168:ILE:HD11	1:A:341:MSE:HE3	1.95	0.48
1:C:356:PRO:HB2	1:C:358:ILE:HG13	1.95	0.48
1:E:386:ILE:HG22	1:E:390:MSE:HE3	1.94	0.48
1:A:384:ARG:HG2	1:F:353:ARG:HG2	1.94	0.48
1:A:102:ARG:HG2	1:A:114:LEU:HD21	1.96	0.48
1:D:213:PRO:CG	1:E:305:ARG:HH21	2.24	0.48
1:E:172:GLN:HE21	1:E:341:MSE:HB2	1.79	0.48
1:E:208:LEU:HD13	1:E:211:GLU:HG2	1.95	0.48
1:E:336:LYS:HG3	1:E:342:GLU:OE1	2.13	0.48
1:E:73:LEU:HD22	1:E:74:ALA:H	1.79	0.48
1:A:379:LYS:NZ	1:A:413:PHE:HB3	2.28	0.48
1:B:148:GLU:OE1	1:B:408:THR:HA	2.14	0.48
1:C:158:THR:HA	1:C:356:PRO:HG3	1.96	0.48
1:B:356:PRO:HB2	1:B:358:ILE:HG13	1.96	0.48
1:E:219:MSE:O	1:E:223:VAL:HG12	2.14	0.48
1:F:6:LEU:HG	1:F:14:LEU:HD11	1.94	0.48
1:A:234:GLU:HB2	1:A:239:HIS:HE1	1.79	0.47
1:D:100:LYS:O	1:D:113:LEU:HD22	2.13	0.47
1:E:62:PHE:CD2	1:E:83:PRO:HG3	2.49	0.47
1:A:349:ILE:HD11	1:A:392:GLU:HB2	1.95	0.47
1:E:177:VAL:HA	1:E:319:ALA:O	2.13	0.47
1:F:261:ILE:HG12	1:F:314:THR:HB	1.97	0.47
1:B:102:ARG:HB3	1:B:114:LEU:HD11	1.96	0.47
1:A:40:LYS:HE3	1:A:103:PRO:CB	2.44	0.47
1:B:58:LEU:HD12	1:B:62:PHE:CE1	2.49	0.47
1:A:248:GLU:O	1:A:252:ARG:HG2	2.15	0.47
2:G:8:U:O2	2:G:8:U:H2'	2.13	0.47
1:B:39:LEU:HD22	1:B:49:ILE:HG23	1.96	0.47
1:C:212:ARG:HA	1:C:232:PHE:CE2	2.50	0.47
1:C:248:GLU:O	1:C:252:ARG:HG2	2.13	0.47
1:D:375:GLU:O	1:D:379:LYS:HG2	2.15	0.47
1:E:171:GLY:HA2	1:E:313:LEU:O	2.14	0.47
1:A:2:ASN:HB3	1:A:5:GLU:HB3	1.97	0.47
1:C:1:MSE:HE3	1:C:39:LEU:HD23	1.97	0.47
1:D:191:ILE:O	1:D:195:ILE:HG12	2.15	0.47
1:E:380:MSE:O	1:E:384:ARG:HG3	2.15	0.47
1:C:36:PHE:CZ	1:C:40:LYS:HD2	2.50	0.47
1:F:177:VAL:HG22	1:F:319:ALA:HB3	1.97	0.47
1:B:102:ARG:HB2	1:B:114:LEU:HD11	1.97	0.46
1:C:178:ALA:CB	1:C:345:LEU:HB2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ARG:NH1	1:D:372:THR:HG22	2.29	0.46
1:D:2:ASN:OD1	1:D:4:THR:HG22	2.16	0.46
1:E:218:GLU:O	1:E:222:LEU:HD12	2.15	0.46
1:C:1:MSE:HG2	1:C:42:HIS:CD2	2.50	0.46
1:B:406:THR:HG22	1:B:408:THR:H	1.80	0.46
1:C:262:ILE:HB	1:C:315:ILE:HG12	1.96	0.46
1:D:274:TYR:CD2	1:D:297:PRO:HG3	2.50	0.46
1:F:380:MSE:O	1:F:384:ARG:HG3	2.16	0.46
1:C:267:ILE:HG22	1:C:318:THR:O	2.16	0.46
1:D:377:LEU:HA	1:D:380:MSE:HE2	1.96	0.46
1:E:21:MSE:SE	1:E:38:ILE:HG23	2.65	0.46
1:F:265:ASP:HA	1:F:266:SER:HA	1.57	0.46
1:A:186:MSE:SE	3:A:1000:ADP:H2'	2.66	0.46
1:C:379:LYS:HD3	1:C:413:PHE:HB3	1.97	0.46
1:E:247:ILE:HD11	1:E:303:ALA:HB3	1.98	0.46
1:A:177:VAL:HG21	1:A:332:TYR:HE1	1.81	0.46
1:A:336:LYS:HG3	1:A:342:GLU:OE2	2.15	0.46
1:C:2:ASN:O	1:C:6:LEU:HD13	2.16	0.46
1:F:237:SER:HA	1:F:277:VAL:HG21	1.98	0.46
1:F:248:GLU:O	1:F:252:ARG:HG2	2.16	0.46
1:B:178:ALA:CB	1:B:345:LEU:HB2	2.46	0.46
1:C:174:GLY:HA2	1:C:341:MSE:O	2.16	0.46
1:D:234:GLU:HB3	1:D:238:ARG:HD3	1.97	0.46
1:A:265:ASP:HA	1:A:266:SER:HA	1.55	0.45
1:A:347:ARG:HH11	1:B:336:LYS:NZ	2.14	0.45
1:A:30:ARG:HE	1:A:32:GLN:HB3	1.81	0.45
1:F:207:LEU:HD13	1:F:246:VAL:HG21	1.99	0.45
1:F:275:ASN:OD1	1:F:289:VAL:HA	2.17	0.45
1:A:30:ARG:HG3	1:A:33:ASP:H	1.82	0.45
1:E:375:GLU:CD	1:E:375:GLU:H	2.19	0.45
1:A:102:ARG:NH1	1:A:105:LYS:HG3	2.32	0.45
1:D:178:ALA:CB	1:D:345:LEU:HB2	2.46	0.45
1:A:349:ILE:HB	1:A:357:ALA:HB1	1.98	0.45
1:E:275:ASN:O	1:F:283:LYS:HE2	2.17	0.45
1:A:1:MSE:HE2	1:A:42:HIS:HB2	1.99	0.45
1:B:147:MSE:HE1	1:B:191:ILE:HA	1.98	0.45
1:D:406:THR:OG1	1:D:411:ASP:HB2	2.17	0.45
1:A:396:MSE:HE2	1:A:396:MSE:HA	1.99	0.45
1:F:387:ILE:HG23	1:F:395:ALA:HB1	1.98	0.45
1:C:360:TYR:CE2	1:C:384:ARG:HG2	2.50	0.45
1:D:217:THR:HG21	1:E:138:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:VAL:HG23	1:F:31:LYS:HD2	1.99	0.45
1:A:179:PRO:CB	1:A:347:ARG:HD2	2.47	0.45
1:C:296:ARG:HB2	1:C:297:PRO:HD3	1.98	0.45
1:D:265:ASP:HA	1:D:266:SER:HA	1.50	0.45
1:F:268:THR:HG21	1:F:320:LEU:H	1.82	0.44
1:D:178:ALA:HB3	1:D:184:LYS:CG	2.47	0.44
1:D:267:ILE:HB	1:D:317:ALA:HB1	2.00	0.44
1:A:356:PRO:HD2	1:A:400:ILE:HD11	1.99	0.44
1:C:102:ARG:NH1	1:C:105:LYS:HG3	2.32	0.44
1:C:175:LEU:HA	1:C:317:ALA:O	2.17	0.44
1:D:56:GLU:HA	1:D:93:THR:HG23	2.00	0.44
1:C:254:VAL:HG21	1:C:313:LEU:HB2	1.99	0.44
1:D:264:LEU:HB3	1:D:317:ALA:HB2	2.00	0.44
1:F:298:LYS:HG2	1:F:335:PHE:CE2	2.52	0.44
1:C:240:VAL:O	1:C:244:GLU:HG2	2.18	0.44
1:E:164:LEU:HD23	1:E:380:MSE:HE2	2.00	0.44
1:E:21:MSE:HB3	1:E:41:GLN:HE22	1.83	0.44
1:B:147:MSE:CE	1:B:191:ILE:HA	2.48	0.44
1:C:349:ILE:HB	1:C:357:ALA:HB1	2.00	0.44
1:D:267:ILE:HD11	1:D:301:PHE:HB2	1.99	0.44
1:D:402:LYS:HD3	1:D:412:PHE:CE1	2.51	0.44
1:F:365:THR:OG1	1:F:368:GLU:HB3	2.16	0.44
1:B:49:ILE:O	1:B:100:LYS:HA	2.18	0.44
1:D:289:VAL:HG22	1:D:327:MSE:HE2	2.00	0.44
1:E:139:LEU:HB2	1:E:306:ASN:HD22	1.82	0.44
1:B:2:ASN:O	1:B:6:LEU:HD13	2.18	0.44
1:E:286:THR:O	1:E:330:VAL:HG21	2.18	0.44
1:C:213:PRO:HD3	1:C:232:PHE:CE2	2.53	0.43
1:C:247:ILE:HB	1:C:300:PHE:CE1	2.53	0.43
1:B:134:GLU:CD	1:B:134:GLU:H	2.22	0.43
1:B:137:THR:HG22	1:B:309:GLU:OE2	2.18	0.43
1:B:206:VAL:HG11	1:B:219:MSE:HG2	2.01	0.43
3:B:1000:ADP:O2A	1:C:366:ARG:NH2	2.50	0.43
1:C:396:MSE:HA	1:C:396:MSE:HE2	2.00	0.43
1:C:289:VAL:HG22	1:C:327:MSE:HE2	2.00	0.43
1:C:278:VAL:HG11	1:C:293:ALA:HB2	2.01	0.43
1:E:250:ALA:HB1	1:E:313:LEU:HD13	2.00	0.43
1:E:304:ALA:HA	1:E:313:LEU:HG	2.00	0.43
1:F:124:PRO:O	1:F:128:ARG:HG3	2.18	0.43
1:F:212:ARG:HA	1:F:232:PHE:CE2	2.54	0.43
1:F:271:ALA:HB3	1:F:331:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:LYS:O	1:F:35:ILE:HG22	2.18	0.43
1:A:183:GLY:O	1:A:187:LEU:HB2	2.18	0.43
1:C:130:LYS:NZ	1:C:256:HIS:HE1	2.17	0.43
1:D:234:GLU:HB2	1:D:239:HIS:CE1	2.53	0.43
1:E:387:ILE:HG23	1:E:395:ALA:HB1	2.01	0.43
1:F:102:ARG:HG2	1:F:114:LEU:HD11	2.01	0.43
1:C:36:PHE:CE1	1:C:40:LYS:HD2	2.53	0.43
1:F:361:ASN:OD1	1:F:388:HIS:HA	2.19	0.43
1:B:173:ARG:HG2	1:B:301:PHE:CE2	2.54	0.43
1:E:166:SER:OG	1:E:341:MSE:HE2	2.18	0.43
1:F:376:GLU:O	1:F:380:MSE:HG3	2.18	0.43
1:D:267:ILE:HG22	1:D:318:THR:O	2.19	0.43
1:D:264:LEU:O	1:D:317:ALA:HA	2.19	0.43
1:E:62:PHE:N	1:E:62:PHE:CD2	2.85	0.43
1:B:99:GLY:HA2	1:B:117:ASN:OD1	2.18	0.42
1:B:248:GLU:O	1:B:252:ARG:HG2	2.19	0.42
1:C:265:ASP:HA	1:C:266:SER:HA	1.51	0.42
1:E:173:ARG:HG2	1:E:301:PHE:CE2	2.53	0.42
1:F:205:MSE:HE3	1:F:262:ILE:HG12	2.00	0.42
1:F:296:ARG:HB2	1:F:297:PRO:HD3	2.01	0.42
1:A:360:TYR:HB2	1:A:396:MSE:HE3	2.01	0.42
1:B:183:GLY:O	1:B:187:LEU:HB2	2.19	0.42
1:D:304:ALA:HB2	1:D:315:ILE:HG13	2.01	0.42
1:E:173:ARG:HD2	1:E:302:GLY:HA2	2.01	0.42
1:F:1:MSE:HE1	1:F:38:ILE:HG22	2.01	0.42
1:A:267:ILE:HG13	1:A:335:PHE:CE1	2.55	0.42
1:B:360:TYR:CE2	1:B:384:ARG:HD2	2.55	0.42
1:F:320:LEU:HG	1:F:323:THR:HG21	1.99	0.42
1:C:54:VAL:HG21	1:C:249:LYS:HD2	2.02	0.42
1:F:396:MSE:O	1:F:400:ILE:HG12	2.19	0.42
1:F:406:THR:CG2	1:F:411:ASP:HB2	2.50	0.42
1:C:143:SER:HB3	1:C:170:ARG:HD2	2.02	0.42
1:C:213:PRO:HD3	1:C:232:PHE:CZ	2.55	0.42
1:E:267:ILE:HB	1:E:317:ALA:HB1	2.01	0.42
1:F:307:VAL:HG12	1:F:310:GLY:H	1.85	0.42
1:A:261:ILE:HG12	1:A:314:THR:HB	2.01	0.42
1:B:192:ALA:HB1	1:B:223:VAL:HG23	2.01	0.42
1:B:36:PHE:HE1	1:B:104:PRO:HD2	1.85	0.42
1:F:254:VAL:HG21	1:F:313:LEU:HB2	2.01	0.42
1:F:3:LEU:HD23	1:F:79:ILE:HD11	2.01	0.42
1:E:268:THR:O	1:E:272:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ALA:HB2	1:A:345:LEU:HB2	2.01	0.42
1:D:178:ALA:HB3	1:D:184:LYS:HG3	2.02	0.42
1:A:144:ARG:HD3	1:A:371:LEU:HB3	2.02	0.42
1:A:396:MSE:O	1:A:400:ILE:HG12	2.19	0.42
1:B:267:ILE:HG22	1:B:318:THR:O	2.19	0.42
1:C:285:LEU:HD13	1:C:291:ALA:HA	2.01	0.42
1:C:131:ILE:HD12	1:C:309:GLU:HG2	2.02	0.42
1:F:249:LYS:O	1:F:253:LEU:HD13	2.20	0.42
1:F:289:VAL:HG21	1:F:294:LEU:HD21	2.01	0.42
1:B:402:LYS:HB3	1:B:412:PHE:HE1	1.85	0.42
1:E:139:LEU:O	1:E:306:ASN:HB3	2.19	0.42
1:A:274:TYR:O	1:A:278:VAL:HG13	2.19	0.41
1:B:104:PRO:HB3	1:B:110:TYR:O	2.20	0.41
1:A:212:ARG:HA	1:A:232:PHE:HE2	1.84	0.41
1:B:169:GLY:O	1:B:172:GLN:HB2	2.19	0.41
1:B:152:GLY:HA3	1:B:407:LYS:HE2	2.02	0.41
1:C:1:MSE:HE2	1:C:42:HIS:HB2	2.02	0.41
1:D:171:GLY:HA2	1:D:313:LEU:O	2.20	0.41
1:E:297:PRO:HB2	1:E:335:PHE:HZ	1.84	0.41
1:F:100:LYS:O	1:F:113:LEU:HD12	2.20	0.41
1:F:212:ARG:HB3	1:F:214:GLU:OE1	2.20	0.41
1:A:231:THR:HG22	1:A:232:PHE:N	2.35	0.41
1:C:294:LEU:C	1:C:297:PRO:HD2	2.40	0.41
1:D:213:PRO:HD3	1:D:232:PHE:CZ	2.55	0.41
1:E:172:GLN:NE2	1:E:341:MSE:HB2	2.34	0.41
1:A:205:MSE:HE1	1:A:250:ALA:HB2	2.02	0.41
1:B:214:GLU:H	1:B:214:GLU:CD	2.23	0.41
1:B:295:HIS:CE1	1:B:299:ARG:HD2	2.56	0.41
1:C:217:THR:HA	1:C:220:GLN:HG2	2.01	0.41
1:D:11:VAL:O	1:D:15:ILE:HG13	2.20	0.41
1:F:147:MSE:HE2	1:F:191:ILE:HG12	2.01	0.41
1:F:294:LEU:C	1:F:297:PRO:HD2	2.41	0.41
1:F:56:GLU:HA	1:F:93:THR:HG23	2.01	0.41
1:E:195:ILE:HD13	1:E:261:ILE:HG21	2.03	0.41
1:E:62:PHE:N	1:E:62:PHE:HD2	2.19	0.41
1:B:178:ALA:HB3	1:B:184:LYS:CG	2.50	0.41
1:B:278:VAL:HG11	1:B:293:ALA:HB2	2.03	0.41
1:D:147:MSE:HG3	1:D:162:LEU:HD22	2.03	0.41
1:E:360:TYR:CE2	1:E:384:ARG:HG2	2.49	0.41
1:A:383:LEU:HB2	1:A:416:MSE:HE1	2.02	0.41
1:D:145:LEU:HD11	1:D:170:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:LYS:HB3	1:E:31:LYS:HE2	1.88	0.41
1:A:134:GLU:H	1:A:134:GLU:CD	2.24	0.41
1:C:326:LYS:HE3	2:G:8:U:OP2	2.20	0.41
1:D:207:LEU:HD13	1:D:246:VAL:HG21	2.03	0.41
1:D:274:TYR:O	1:D:278:VAL:HG13	2.21	0.41
1:D:166:SER:OG	1:D:341:MSE:HE2	2.21	0.41
1:F:178:ALA:HB3	1:F:184:LYS:HD3	2.02	0.41
1:F:304:ALA:HB2	1:F:315:ILE:HB	2.02	0.41
1:B:2:ASN:HB3	1:B:5:GLU:HG2	2.03	0.41
1:F:191:ILE:O	1:F:195:ILE:HG12	2.21	0.41
1:D:6:LEU:CD1	1:D:39:LEU:HD21	2.50	0.41
1:F:297:PRO:HB2	1:F:335:PHE:CZ	2.55	0.41
1:D:254:VAL:HG21	1:D:313:LEU:HB2	2.02	0.41
1:E:266:SER:OG	1:E:269:ARG:HG3	2.21	0.41
1:B:6:LEU:O	1:B:9:THR:HG22	2.22	0.40
1:C:396:MSE:HE1	1:C:399:LEU:HD23	2.04	0.40
1:D:174:GLY:HA3	1:D:341:MSE:SE	2.71	0.40
1:F:84:SER:O	1:F:88:ARG:HG3	2.21	0.40
1:C:186:MSE:SE	3:C:1000:ADP:H2'	2.71	0.40
1:C:381:TRP:CZ2	1:C:385:LYS:HE3	2.55	0.40
1:D:144:ARG:HD2	1:D:371:LEU:O	2.21	0.40
1:E:207:LEU:HA	1:E:228:VAL:O	2.20	0.40
1:F:139:LEU:HD21	1:F:308:GLU:HB2	2.02	0.40
1:A:31:LYS:HA	1:A:34:ILE:HG22	2.02	0.40
1:D:175:LEU:HA	1:D:317:ALA:O	2.22	0.40
1:D:343:LEU:HD11	1:D:358:ILE:HD13	2.04	0.40
1:F:176:ILE:HG13	1:F:187:LEU:HD12	2.02	0.40
1:A:251:LYS:O	1:A:255:GLU:HG3	2.22	0.40
1:B:265:ASP:HA	1:B:266:SER:HA	1.53	0.40
1:C:99:GLY:HA2	1:C:117:ASN:ND2	2.37	0.40
1:D:283:LYS:HE2	1:D:283:LYS:HB2	1.96	0.40
1:E:267:ILE:HG22	1:E:318:THR:O	2.20	0.40
1:F:50:PHE:CD1	1:F:100:LYS:HB3	2.57	0.40
1:F:134:GLU:CD	1:F:134:GLU:H	2.25	0.40
1:F:326:LYS:O	1:F:330:VAL:HG23	2.21	0.40
1:A:231:THR:HG22	1:A:233:ASP:H	1.87	0.40
1:E:191:ILE:O	1:E:195:ILE:HG13	2.21	0.40
1:F:266:SER:HB2	1:F:318:THR:O	2.22	0.40
1:F:379:LYS:HD3	1:F:416:MSE:HE3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	388/420 (92%)	380 (98%)	8 (2%)	0	100	100
1	B	405/420 (96%)	392 (97%)	13 (3%)	0	100	100
1	C	411/420 (98%)	403 (98%)	8 (2%)	0	100	100
1	D	400/420 (95%)	388 (97%)	12 (3%)	0	100	100
1	E	371/420 (88%)	361 (97%)	10 (3%)	0	100	100
1	F	392/420 (93%)	388 (99%)	4 (1%)	0	100	100
All	All	2367/2520 (94%)	2312 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/342 (99%)	338 (99%)	2 (1%)	90	97
1	B	351/342 (103%)	350 (100%)	1 (0%)	94	98
1	C	356/342 (104%)	353 (99%)	3 (1%)	86	96
1	D	348/342 (102%)	346 (99%)	2 (1%)	90	97
1	E	314/342 (92%)	311 (99%)	3 (1%)	82	95
1	F	346/342 (101%)	344 (99%)	2 (1%)	90	97
All	All	2055/2052 (100%)	2042 (99%)	13 (1%)	90	97



All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LEU
1	A	289	VAL
1	B	187	LEU
1	C	25	ASN
1	C	353	ARG
1	C	406	THR
1	D	149	ARG
1	D	187	LEU
1	E	39	LEU
1	E	59	GLN
1	E	222	LEU
1	F	275	ASN
1	F	277	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	172	GLN
1	A	256	HIS
1	A	340	ASN
1	B	59	GLN
1	B	189	GLN
1	B	401	ASN
1	C	32	GLN
1	C	41	GLN
1	C	42	HIS
1	C	117	ASN
1	C	241	GLN
1	C	256	HIS
1	D	388	HIS
1	E	41	GLN
1	E	198	ASN
1	E	239	HIS
1	E	306	ASN
1	E	388	HIS
1	F	172	GLN
1	F	189	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	7/12 (58%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	8	U

There are no RNA pucker outliers to report.

## 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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\# Z  > 2$
3	ADP	A	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.78	3 (13%)
5	BEF	A	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	B	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.79	3 (13%)
5	BEF	B	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	C	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.77	2 (8%)
5	BEF	C	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	D	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.78	2 (8%)
5	BEF	D	1002	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	F	1000	5,4	24,29,29	1.00	1 (4%)	23,45,45	1.77	2 (8%)
5	BEF	F	1002	3	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
3	ADP	A	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	A	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	B	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	B	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	C	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	C	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	D	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	D	1002	3	-	0/0/0/0	0/0/0/0
3	ADP	F	1000	5,4	-	0/12/32/32	0/3/3/3
5	BEF	F	1002	3	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1000	ADP	C5-C4	3.06	1.47	1.40
3	A	1000	ADP	C5-C4	3.06	1.47	1.40
3	F	1000	ADP	C5-C4	3.07	1.47	1.40
3	B	1000	ADP	C5-C4	3.08	1.47	1.40
3	D	1000	ADP	C5-C4	3.09	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	ADP	N3-C2-N1	-6.68	123.62	128.87
3	D	1000	ADP	N3-C2-N1	-6.66	123.64	128.87
3	A	1000	ADP	N3-C2-N1	-6.66	123.64	128.87
3	C	1000	ADP	N3-C2-N1	-6.62	123.67	128.87
3	F	1000	ADP	N3-C2-N1	-6.60	123.68	128.87
3	C	1000	ADP	C2'-C1'-N9	-2.68	106.30	113.47
3	B	1000	ADP	C2'-C1'-N9	-2.66	106.34	113.47
3	D	1000	ADP	C2'-C1'-N9	-2.66	106.34	113.47
3	F	1000	ADP	C2'-C1'-N9	-2.66	106.35	113.47
3	A	1000	ADP	C2'-C1'-N9	-2.64	106.39	113.47
3	A	1000	ADP	O3B-PB-O2B	2.01	114.83	107.44
3	B	1000	ADP	O3B-PB-O2B	2.02	114.85	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	ADP	1	0
3	B	1000	ADP	1	0
3	C	1000	ADP	1	0
3	D	1000	ADP	1	0
3	F	1000	ADP	1	0
5	F	1002	BEF	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	382/420 (90%)	-0.20	3 (0%) 87 80	29, 64, 124, 167	0
1	B	394/420 (93%)	-0.31	4 (1%) 84 75	17, 45, 122, 151	0
1	C	399/420 (95%)	-0.26	8 (2%) 68 54	14, 46, 116, 149	0
1	D	391/420 (93%)	-0.28	3 (0%) 87 80	15, 62, 111, 158	0
1	E	369/420 (87%)	0.25	15 (4%) 41 27	29, 90, 140, 177	0
1	F	386/420 (91%)	0.15	10 (2%) 59 45	63, 96, 137, 164	0
2	G	9/12 (75%)	0.06	0 100 100	48, 54, 138, 161	0
All	All	2330/2532 (92%)	-0.11	43 (1%) 71 58	14, 68, 130, 177	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	TYR	3.9
1	E	154	THR	3.7
1	F	90	ASN	3.6
1	E	169	GLY	3.6
1	E	6	LEU	3.5
1	C	49	ILE	3.2
1	B	14	LEU	3.2
1	E	99	GLY	3.2
1	E	127	ALA	3.1
1	F	152	GLY	3.0
1	E	128	ARG	2.9
1	E	13	GLU	2.9
1	C	15	ILE	2.9
1	F	128	ARG	2.8
1	F	198	ASN	2.8
1	F	18	GLY	2.8
1	C	19	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	51	GLY	2.8
1	E	14	LEU	2.7
1	E	98	SER	2.7
1	E	116	VAL	2.7
1	C	23	LEU	2.6
1	B	128	ARG	2.6
1	D	14	LEU	2.6
1	A	224	LYS	2.6
1	A	106	GLU	2.5
1	B	16	THR	2.5
1	D	375	GLU	2.5
1	C	14	LEU	2.4
1	B	106	GLU	2.4
1	C	40	LYS	2.3
1	C	44	LYS	2.3
1	A	114	LEU	2.3
1	F	114	LEU	2.3
1	F	3	LEU	2.2
1	E	31	LYS	2.2
1	F	41	GLN	2.2
1	F	168	ILE	2.2
1	E	97	ILE	2.1
1	D	49	ILE	2.1
1	F	279	PRO	2.1
1	C	107	GLY	2.0
1	E	35	ILE	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( $\text{\AA}^2$ )	Q<0.9
5	BEF	B	1002	4/4	0.93	0.26	2.41	45,46,46,46	0
5	BEF	C	1002	4/4	0.97	0.21	0.54	21,22,23,23	0
3	ADP	B	1000	27/27	0.95	0.20	0.33	27,32,36,37	0
3	ADP	C	1000	27/27	0.95	0.18	0.01	30,39,44,45	0
3	ADP	F	1000	27/27	0.91	0.19	-0.22	93,94,99,100	0
5	BEF	D	1002	4/4	0.94	0.21	-0.59	72,75,75,76	0
3	ADP	A	1000	27/27	0.95	0.15	-1.00	34,38,45,45	0
5	BEF	A	1002	4/4	0.96	0.16	-1.10	57,58,58,58	0
4	MG	D	1001	1/1	0.64	0.16	-1.14	80,80,80,80	0
5	BEF	F	1002	4/4	0.96	0.16	-1.19	67,67,68,68	0
3	ADP	D	1000	27/27	0.94	0.16	-1.27	51,66,74,76	0
4	MG	C	1001	1/1	0.98	0.13	-1.41	49,49,49,49	0
4	MG	F	1001	1/1	0.95	0.08	-2.42	64,64,64,64	0
4	MG	A	1001	1/1	0.96	0.10	-5.14	29,29,29,29	0
4	MG	B	1001	1/1	0.98	0.06	-6.75	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.