



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:45 am GMT

PDB ID : 5SUP  
Title : Structure of mRNA export factors  
Authors : Ren, Y.; Schmiede, P.; Blobel, G.  
Deposited on : 2016-08-03  
Resolution : 2.60 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:

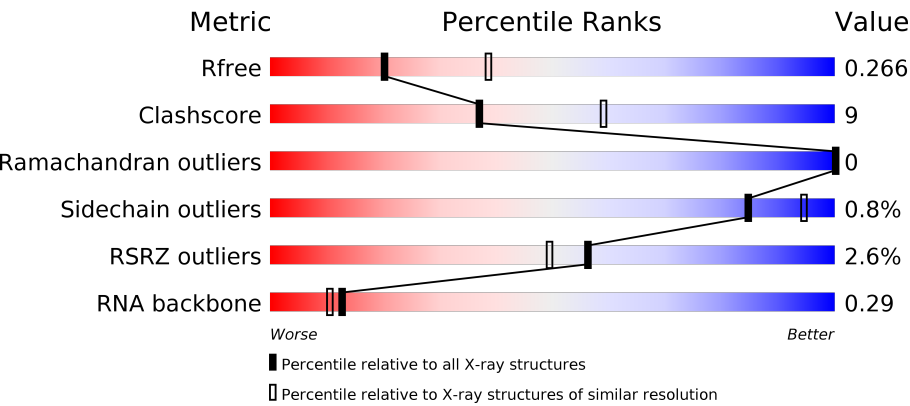
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : recalc28906  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28906

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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 <sub>free</sub>	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

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	390	<div><div>3%</div><div><div></div><div>82%</div><div>15%</div><div>..</div></div></div>
1	B	390	<div><div>%</div><div><div></div><div>81%</div><div>17%</div><div>.</div></div></div>
1	C	390	<div><div>%</div><div><div></div><div>73%</div><div>25%</div><div>..</div></div></div>
2	G	32	<div><div>6%</div><div><div></div><div>44%</div><div>9%</div><div>47%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	H	32	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%38%13%47%</div></div>
2	I	32	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>22%16%22%6%53%</div></div>
3	D	15	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%13%13%60%</div></div>
3	E	15	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>20%13%7%60%</div></div>
3	F	15	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%7%20%13%60%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10127 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 ATP-dependent RNA helicase SUB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3082	1960	535	576	11			
1	B	383	Total	C	N	O	S	0	0	0
			3082	1960	535	576	11			
1	C	381	Total	C	N	O	S	0	0	0
			3071	1954	533	573	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLY	-	expression tag	UNP Q07478
A	58	ALA	-	expression tag	UNP Q07478
A	59	MET	-	expression tag	UNP Q07478
A	60	GLY	-	expression tag	UNP Q07478
B	57	GLY	-	expression tag	UNP Q07478
B	58	ALA	-	expression tag	UNP Q07478
B	59	MET	-	expression tag	UNP Q07478
B	60	GLY	-	expression tag	UNP Q07478
C	57	GLY	-	expression tag	UNP Q07478
C	58	ALA	-	expression tag	UNP Q07478
C	59	MET	-	expression tag	UNP Q07478
C	60	GLY	-	expression tag	UNP Q07478

- Molecule 2 is a protein called RNA annealing protein YRA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	17	Total	C	N	O	S	0	0	0
			141	89	20	31	1			
2	H	17	Total	C	N	O	S	0	0	0
			141	89	20	31	1			
2	I	15	Total	C	N	O	S	0	0	0
			127	80	17	29	1			

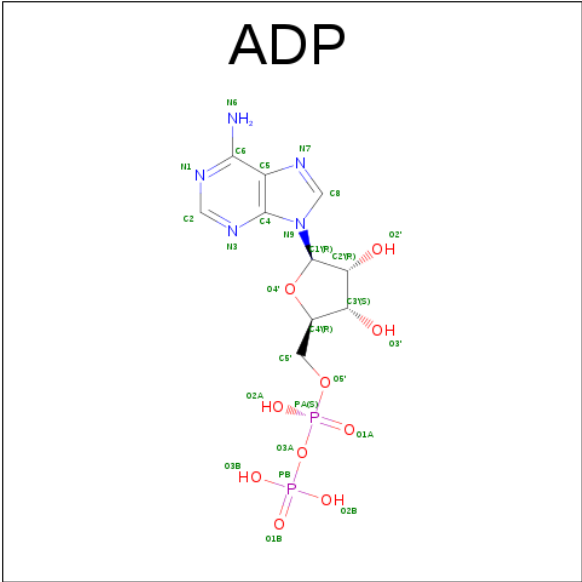
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	195	GLY	-	expression tag	UNP Q12159
G	196	ALA	-	expression tag	UNP Q12159
G	197	MET	-	expression tag	UNP Q12159
G	198	GLY	-	expression tag	UNP Q12159
G	199	SER	-	expression tag	UNP Q12159
H	195	GLY	-	expression tag	UNP Q12159
H	196	ALA	-	expression tag	UNP Q12159
H	197	MET	-	expression tag	UNP Q12159
H	198	GLY	-	expression tag	UNP Q12159
H	199	SER	-	expression tag	UNP Q12159
I	195	GLY	-	expression tag	UNP Q12159
I	196	ALA	-	expression tag	UNP Q12159
I	197	MET	-	expression tag	UNP Q12159
I	198	GLY	-	expression tag	UNP Q12159
I	199	SER	-	expression tag	UNP Q12159

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

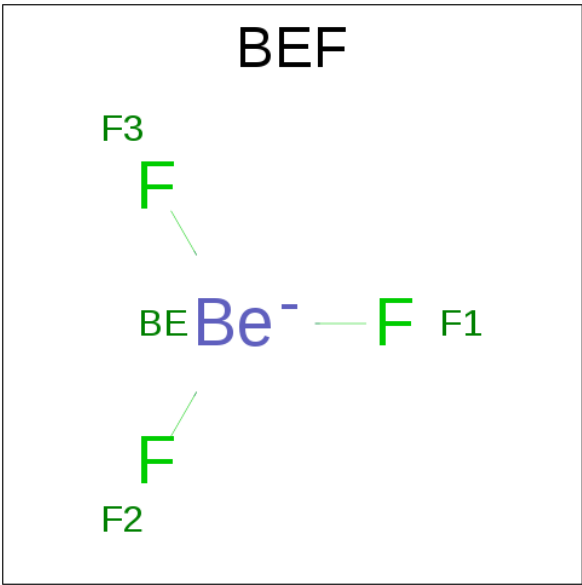
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
3	E	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
3	F	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- 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		

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Mg 1	0	0
6	A	1	Total 1	Mg 1	0	0
6	C	1	Total 1	Mg 1	0	0

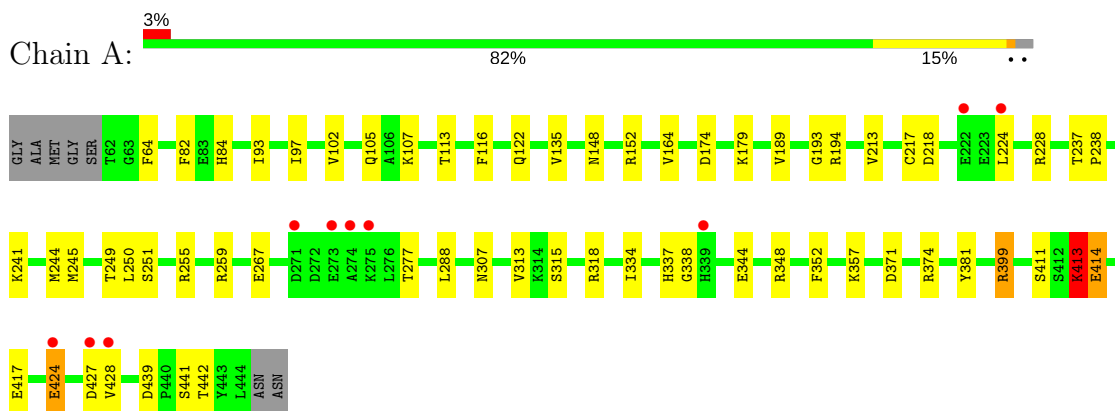
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total 13	O 13	0	0
7	B	9	Total 9	O 9	0	0
7	C	5	Total 5	O 5	0	0

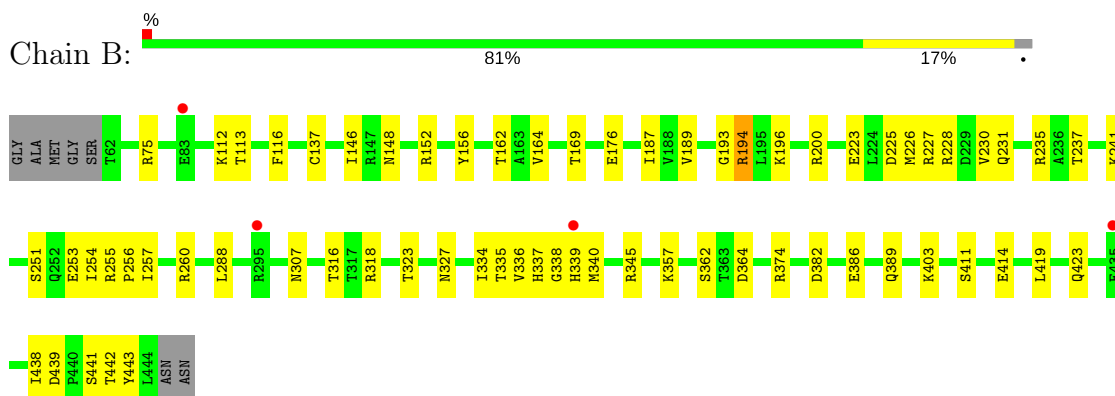
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

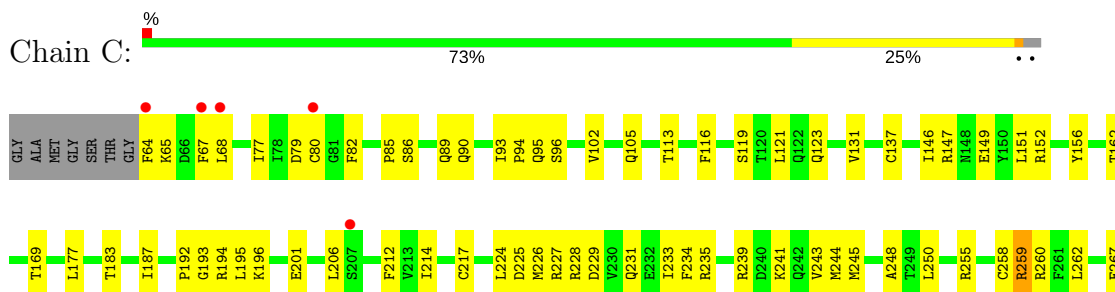
#### • Molecule 1: ATP-dependent RNA helicase SUB2



#### • Molecule 1: ATP-dependent RNA helicase SUB2



#### • Molecule 1: ATP-dependent RNA helicase SUB2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.35Å 99.35Å 247.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.67 – 2.60 49.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.67-2.60) 95.1 (49.67-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.219 , 0.268 0.215 , 0.266	Depositor DCC
$R_{free}$ test set	2233 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	1/3137 (0.0%)	0.66	9/4233 (0.2%)
1	B	0.38	2/3137 (0.1%)	0.57	1/4233 (0.0%)
1	C	0.36	1/3126 (0.0%)	0.56	3/4218 (0.1%)
2	G	0.25	0/142	0.41	0/187
2	H	1.24	3/142 (2.1%)	1.02	2/187 (1.1%)
2	I	1.40	2/128 (1.6%)	1.51	6/169 (3.6%)
3	D	0.13	0/131	0.72	0/200
3	E	0.13	0/131	0.72	0/200
3	F	0.19	0/131	0.87	0/200
All	All	0.43	9/10205 (0.1%)	0.63	21/13827 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	213	GLU	CD-OE1	-9.91	1.14	1.25
1	C	201	GLU	CD-OE1	-8.73	1.16	1.25
2	H	213	GLU	CD-OE2	-8.59	1.16	1.25
2	H	213	GLU	CD-OE1	-7.84	1.17	1.25
1	B	386	GLU	CD-OE1	-7.54	1.17	1.25
1	B	386	GLU	CD-OE2	-7.12	1.17	1.25
1	A	414	GLU	CD-OE1	-5.22	1.20	1.25
2	H	213	GLU	CG-CD	-5.22	1.44	1.51
2	I	213	GLU	CD-OE2	-5.16	1.20	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ASP	CB-CA-C	-8.71	92.98	110.40
1	A	427	ASP	CB-CG-OD2	8.37	125.83	118.30
1	A	427	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	B	438	ILE	CG1-CB-CG2	-7.14	95.70	111.40
1	A	417	GLU	CG-CD-OE2	6.74	131.78	118.30
1	A	414	GLU	CB-CA-C	-6.68	97.05	110.40
2	I	213	GLU	CG-CD-OE2	6.67	131.64	118.30
1	A	424	GLU	CG-CD-OE1	6.46	131.23	118.30
2	I	213	GLU	CG-CD-OE1	-6.45	105.40	118.30
2	H	213	GLU	CB-CA-C	-6.28	97.84	110.40
1	C	259	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	I	215	LEU	CA-CB-CG	6.14	129.42	115.30
1	C	65	LYS	CB-CG-CD	-6.13	95.66	111.60
1	A	427	ASP	N-CA-CB	6.04	121.47	110.60
1	A	417	GLU	CA-CB-CG	5.89	126.36	113.40
2	I	213	GLU	CB-CG-CD	-5.87	98.34	114.20
1	C	201	GLU	CA-CB-CG	5.86	126.29	113.40
2	I	215	LEU	CB-CG-CD1	-5.86	101.05	111.00
1	A	413	LYS	CD-CE-NZ	5.44	124.21	111.70
2	H	213	GLU	CA-CB-CG	5.28	125.01	113.40
2	I	210	LYS	CG-CD-CE	-5.21	96.26	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	95	GLN	Sidechain

## 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	3082	0	3117	41	0
1	B	3082	0	3118	49	0
1	C	3071	0	3108	78	0
2	G	141	0	132	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	141	0	132	3	0
2	I	127	0	114	22	0
3	D	120	0	61	2	0
3	E	120	0	61	2	0
3	F	120	0	61	2	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
5	A	4	0	0	0	0
5	B	4	0	0	1	0
5	C	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	13	0	0	0	0
7	B	9	0	0	0	0
7	C	5	0	0	0	0
All	All	10127	0	9940	179	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 9.

All (179) 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)
2:I:210:LYS:NZ	2:I:218:GLU:OE1	1.73	1.18
1:C:86:SER:O	1:C:89:GLN:NE2	1.79	1.15
1:A:413:LYS:HD2	1:A:414:GLU:H	1.19	1.02
1:C:228:ARG:HE	2:I:210:LYS:HG2	1.36	0.90
1:C:89:GLN:HE22	1:C:90:GLN:HG3	1.39	0.87
1:C:85:PRO:HB2	1:C:89:GLN:NE2	1.93	0.84
1:A:413:LYS:HD2	1:A:414:GLU:N	1.91	0.84
1:A:277:THR:HG21	1:A:428:VAL:HG11	1.60	0.82
2:I:210:LYS:HG3	2:I:215:LEU:HD11	1.62	0.79
1:C:194:ARG:NH1	3:E:5:U:O2'	2.17	0.78
1:C:259:ARG:NH1	1:C:267:GLU:OE2	2.16	0.76
1:C:228:ARG:HE	2:I:210:LYS:CG	1.98	0.75
1:B:227:ARG:HE	1:B:231:GLN:NE2	1.86	0.73
1:A:228:ARG:NH1	2:H:210:LYS:O	2.21	0.73
2:H:211:SER:OG	2:H:213:GLU:HB2	1.89	0.73
1:B:227:ARG:HE	1:B:231:GLN:HE21	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ARG:HH21	2:I:210:LYS:N	1.89	0.70
1:C:89:GLN:NE2	1:C:90:GLN:HG3	2.07	0.69
1:C:334:ILE:HG23	1:C:357:LYS:HD2	1.75	0.69
1:C:131:VAL:HG11	1:C:206:LEU:HD23	1.74	0.68
1:C:231:GLN:HA	1:C:234:PHE:HB3	1.75	0.68
1:B:337:HIS:ND1	1:B:338:GLY:O	2.27	0.68
1:B:334:ILE:HG23	1:B:357:LYS:HD2	1.75	0.67
1:C:229:ASP:O	1:C:233:ILE:HD12	1.94	0.67
1:A:337:HIS:ND1	1:A:338:GLY:O	2.29	0.65
1:A:174:ASP:OD1	1:A:194:ARG:NH1	2.30	0.64
1:C:227:ARG:HD3	2:I:215:LEU:HD23	1.78	0.64
1:A:224:LEU:O	1:A:228:ARG:HG3	1.99	0.63
1:B:223:GLU:HG2	1:B:226:MET:HG3	1.79	0.63
1:C:192:PRO:HG2	1:C:226:MET:HE3	1.80	0.62
2:I:210:LYS:HD3	2:I:215:LEU:CD1	2.30	0.62
1:C:79:ASP:OD2	1:C:156:TYR:HE2	1.83	0.62
2:H:211:SER:OG	2:H:214:ASP:OD2	2.12	0.61
1:C:259:ARG:HH12	1:C:267:GLU:CD	2.03	0.61
1:A:318:ARG:NH2	1:A:381:TYR:HE2	1.99	0.61
1:B:169:THR:O	1:B:194:ARG:NH2	2.24	0.61
2:I:212:LEU:O	2:I:215:LEU:HB2	2.01	0.61
1:B:237:THR:OG1	1:B:241:LYS:NZ	2.29	0.60
1:C:337:HIS:ND1	1:C:338:GLY:O	2.34	0.60
1:B:176:GLU:HG2	1:C:330:ASN:ND2	2.17	0.60
1:C:149:GLU:OE1	1:C:152:ARG:NH1	2.34	0.60
2:I:213:GLU:HA	2:I:216:ASP:OD1	2.00	0.60
1:C:231:GLN:O	1:C:235:ARG:N	2.35	0.60
1:B:253:GLU:N	1:B:253:GLU:OE2	2.35	0.59
1:B:414:GLU:N	1:B:414:GLU:OE1	2.34	0.59
1:C:80:CYS:HB3	1:C:152:ARG:HH21	1.68	0.58
1:A:439:ASP:OD2	1:A:441:SER:OG	2.15	0.58
2:I:210:LYS:CG	2:I:215:LEU:HD11	2.34	0.57
1:A:313:VAL:HG12	1:A:315:SER:H	1.70	0.57
1:B:112:LYS:NZ	5:B:2001:BEF:F2	2.27	0.57
1:B:235:ARG:NE	2:G:218:GLU:OE2	2.38	0.56
1:A:334:ILE:HG23	1:A:357:LYS:HD2	1.87	0.56
1:B:364:ASP:OD1	1:B:389:GLN:NE2	2.36	0.56
1:C:420:ALA:O	1:C:424:GLU:HG3	2.04	0.56
2:I:210:LYS:HD3	2:I:215:LEU:HD12	1.88	0.56
1:B:225:ASP:OD1	1:B:228:ARG:NH1	2.39	0.56
1:C:255:ARG:O	1:C:259:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:PRO:HA	1:C:443:TYR:CE2	2.40	0.56
1:C:162:THR:HG22	1:C:187:ILE:HB	1.89	0.55
1:C:196:LYS:HB2	1:C:233:ILE:HD11	1.89	0.55
2:I:215:LEU:O	2:I:218:GLU:HB2	2.07	0.55
1:A:413:LYS:CD	1:A:414:GLU:N	2.69	0.54
1:C:67:PHE:CE1	1:C:94:PRO:HD3	2.43	0.54
1:C:225:ASP:OD1	1:C:228:ARG:NH1	2.41	0.54
2:I:210:LYS:CD	2:I:215:LEU:CD1	2.85	0.54
1:A:193:GLY:HA3	3:D:5:U:H5''	1.91	0.53
1:B:162:THR:HG22	1:B:187:ILE:HB	1.91	0.53
1:B:439:ASP:O	1:B:442:THR:HG22	2.09	0.53
1:A:237:THR:OG1	1:A:241:LYS:NZ	2.29	0.52
1:C:96:SER:O	1:C:123:GLN:NE2	2.41	0.52
1:B:137:CYS:SG	1:B:146:ILE:HD12	2.49	0.52
1:A:344:GLU:O	1:A:348:ARG:HG3	2.10	0.52
1:C:80:CYS:HB3	1:C:152:ARG:NH2	2.24	0.52
1:A:84:HIS:ND1	1:C:299:GLN:HB2	2.24	0.52
1:B:225:ASP:O	1:B:228:ARG:HG2	2.10	0.51
1:C:239:ARG:HH11	2:I:223:PHE:HA	1.74	0.51
1:A:255:ARG:O	1:A:259:ARG:HG3	2.10	0.51
1:B:254:ILE:O	1:B:257:ILE:HG22	2.11	0.51
1:C:177:LEU:HG	1:C:183:THR:HB	1.92	0.51
1:C:113:THR:HA	1:C:116:PHE:CE2	2.45	0.51
1:C:285:TYR:HD2	1:C:430:ILE:HG22	1.76	0.51
1:C:193:GLY:HA3	3:E:5:U:H5''	1.92	0.51
1:B:193:GLY:HA3	3:F:5:U:H5''	1.93	0.50
1:C:260:ARG:HH21	2:I:216:ASP:HB3	1.75	0.50
1:C:364:ASP:OD1	1:C:389:GLN:NE2	2.41	0.50
1:A:107:LYS:NZ	1:C:436:GLU:OE1	2.45	0.50
1:C:85:PRO:HB2	1:C:89:GLN:CD	2.32	0.50
1:A:288:LEU:O	1:A:411:SER:HA	2.12	0.50
1:C:255:ARG:HD3	1:C:269:PHE:CZ	2.47	0.50
1:B:318:ARG:NH2	1:B:382:ASP:OD2	2.45	0.49
1:B:403:LYS:HB3	1:B:443:TYR:HA	1.94	0.49
1:B:339:HIS:O	1:B:339:HIS:CG	2.66	0.49
1:B:231:GLN:HE22	2:G:215:LEU:HB3	1.77	0.49
1:C:231:GLN:HA	1:C:234:PHE:CB	2.40	0.49
1:B:307:ASN:HB3	1:B:374:ARG:O	2.13	0.49
1:C:224:LEU:O	1:C:228:ARG:HG3	2.13	0.48
1:C:102:VAL:HB	1:C:244:MET:HG2	1.95	0.48
1:C:316:THR:HG23	1:C:337:HIS:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:O	1:A:97:ILE:HG12	2.12	0.48
1:B:318:ARG:HH21	1:B:382:ASP:CG	2.16	0.48
1:B:323:THR:O	1:B:327:ASN:ND2	2.46	0.48
1:A:315:SER:HA	3:D:2:U:H5'	1.95	0.48
1:B:254:ILE:HD12	1:B:257:ILE:HG21	1.96	0.48
1:B:227:ARG:HD3	2:G:215:LEU:HD13	1.95	0.47
1:C:228:ARG:NE	2:I:210:LYS:HG2	2.17	0.47
1:B:75:ARG:HG2	1:B:156:TYR:CE2	2.49	0.47
1:C:214:ILE:HD12	1:C:245:MET:HE2	1.95	0.47
1:C:86:SER:N	1:C:89:GLN:HE21	2.12	0.47
1:A:277:THR:HG21	1:A:428:VAL:CG1	2.39	0.47
1:A:238:PRO:O	1:A:241:LYS:HD3	2.15	0.46
1:A:164:VAL:HA	1:A:189:VAL:O	2.14	0.46
1:C:239:ARG:HG2	2:I:222:TYR:CZ	2.50	0.46
1:A:439:ASP:HB3	1:A:442:THR:HG23	1.97	0.46
2:I:210:LYS:CG	2:I:215:LEU:CD1	2.94	0.46
1:A:371:ASP:OD2	1:A:399:ARG:HD3	2.15	0.46
1:C:64:PHE:CE1	1:C:85:PRO:HB3	2.50	0.46
2:I:210:LYS:HE2	2:I:210:LYS:HB3	1.67	0.46
1:A:251:SER:O	1:A:255:ARG:HG3	2.16	0.46
1:C:137:CYS:SG	1:C:146:ILE:HD12	2.56	0.46
1:C:228:ARG:NH2	2:I:210:LYS:N	2.60	0.46
1:C:89:GLN:HB2	1:C:93:ILE:HD12	1.96	0.46
1:C:260:ARG:CZ	2:I:216:ASP:OD2	2.64	0.46
1:B:196:LYS:O	1:B:200:ARG:HG3	2.16	0.45
2:I:220:ALA:O	2:I:224:GLU:OE2	2.34	0.45
1:A:307:ASN:HB3	1:A:374:ARG:O	2.15	0.45
1:C:105:GLN:HB2	1:C:250:LEU:HD12	1.98	0.45
1:C:258:CYS:O	1:C:262:LEU:HD12	2.17	0.45
1:A:179:LYS:HE3	1:A:179:LYS:HB2	1.57	0.45
1:C:86:SER:C	1:C:89:GLN:HE21	2.12	0.45
1:C:195:LEU:HG	1:C:233:ILE:HG12	1.99	0.45
1:B:260:ARG:NH1	2:G:216:ASP:HB3	2.32	0.45
1:A:64:PHE:CE2	1:A:82:PHE:HB3	2.51	0.45
1:B:227:ARG:NE	1:B:231:GLN:NE2	2.62	0.45
1:B:226:MET:O	1:B:230:VAL:HG13	2.18	0.44
1:B:288:LEU:O	1:B:411:SER:HA	2.17	0.44
1:B:176:GLU:HG2	1:C:330:ASN:HD21	1.81	0.44
1:B:419:LEU:O	1:B:423:GLN:HG3	2.18	0.44
1:A:334:ILE:HD11	1:A:352:PHE:HB2	2.00	0.43
1:B:316:THR:HG23	1:B:337:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:PHE:O	1:C:243:VAL:HA	2.18	0.43
1:C:344:GLU:O	1:C:348:ARG:HG3	2.17	0.43
1:C:267:GLU:HB3	1:C:269:PHE:CE2	2.53	0.43
1:B:164:VAL:HA	1:B:189:VAL:O	2.18	0.43
1:C:67:PHE:HZ	1:C:89:GLN:OE1	2.02	0.43
1:C:77:ILE:O	1:C:82:PHE:HB2	2.19	0.43
1:A:97:ILE:HD12	1:A:122:GLN:HG2	2.00	0.43
1:A:102:VAL:HB	1:A:244:MET:HG2	2.00	0.43
1:B:323:THR:OG1	1:B:335:THR:HB	2.19	0.43
1:C:119:SER:O	1:C:123:GLN:HG3	2.18	0.43
1:A:113:THR:HA	1:A:116:PHE:CE2	2.53	0.43
1:A:135:VAL:HG22	1:A:213:VAL:HB	2.01	0.43
1:C:147:ARG:CZ	1:C:151:LEU:HD11	2.49	0.43
1:C:121:LEU:HD21	1:C:187:ILE:HD11	2.01	0.43
3:F:1:U:H2'	3:F:2:U:C6	2.53	0.43
1:B:148:ASN:O	1:B:152:ARG:HG3	2.19	0.43
1:C:85:PRO:HG2	1:C:90:GLN:HE21	1.84	0.42
1:B:113:THR:HA	1:B:116:PHE:CE2	2.55	0.42
1:B:340:MET:HG3	1:B:345:ARG:HG3	2.02	0.42
1:C:405:LEU:HD12	1:C:406:ALA:N	2.34	0.42
1:C:323:THR:O	1:C:327:ASN:ND2	2.47	0.42
1:A:105:GLN:HB2	1:A:250:LEU:HD12	2.02	0.42
1:C:419:LEU:O	1:C:423:GLN:HG3	2.20	0.42
1:C:248:ALA:HB3	1:C:392:HIS:CE1	2.54	0.42
1:A:148:ASN:O	1:A:152:ARG:HG3	2.20	0.41
1:A:259:ARG:NH1	1:A:267:GLU:OE1	2.53	0.41
1:B:336:VAL:O	1:B:362:SER:HB2	2.20	0.41
1:C:315:SER:OG	1:C:318:ARG:HG3	2.20	0.41
1:B:251:SER:O	1:B:255:ARG:HG3	2.20	0.41
1:C:217:CYS:SG	1:C:245:MET:HB3	2.60	0.41
1:A:217:CYS:SG	1:A:245:MET:HB3	2.61	0.40
1:A:218:ASP:OD2	1:A:249:THR:OG1	2.38	0.40
1:B:251:SER:O	1:B:254:ILE:HG22	2.21	0.40
1:C:323:THR:OG1	1:C:335:THR:HB	2.21	0.40
1:B:439:ASP:OD2	1:B:441:SER:HB3	2.22	0.40
1:A:313:VAL:CG1	1:A:318:ARG:HB2	2.51	0.40
1:B:152:ARG:HH11	1:B:152:ARG:HD2	1.78	0.40
1:B:255:ARG:N	1:B:256:PRO:HD2	2.36	0.40
1:C:67:PHE:CZ	1:C:89:GLN:OE1	2.74	0.40
1:C:169:THR:O	1:C:194:ARG:NH2	2.55	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	381/390 (98%)	370 (97%)	11 (3%)	0	100	100
1	B	381/390 (98%)	373 (98%)	8 (2%)	0	100	100
1	C	379/390 (97%)	371 (98%)	8 (2%)	0	100	100
2	G	15/32 (47%)	15 (100%)	0	0	100	100
2	H	15/32 (47%)	14 (93%)	1 (7%)	0	100	100
2	I	13/32 (41%)	13 (100%)	0	0	100	100
All	All	1184/1266 (94%)	1156 (98%)	28 (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	339/343 (99%)	336 (99%)	3 (1%)	82	93
1	B	339/343 (99%)	338 (100%)	1 (0%)	94	98
1	C	338/343 (98%)	335 (99%)	3 (1%)	82	93
2	G	15/27 (56%)	15 (100%)	0	100	100
2	H	15/27 (56%)	14 (93%)	1 (7%)	19	38
2	I	14/27 (52%)	13 (93%)	1 (7%)	17	34
All	All	1060/1110 (96%)	1051 (99%)	9 (1%)	85	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	413	LYS
1	A	424	GLU
1	B	194	ARG
1	C	68	LEU
1	C	241	LYS
1	C	405	LEU
2	H	209	LYS
2	I	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	299	GLN
1	B	231	GLN
1	C	89	GLN
1	C	123	GLN
1	C	330	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	5/15 (33%)	4 (80%)	0
3	E	5/15 (33%)	3 (60%)	0
3	F	5/15 (33%)	4 (80%)	0
All	All	15/45 (33%)	11 (73%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	2	U
3	D	4	U
3	D	5	U
3	D	6	U
3	E	4	U
3	E	5	U
3	E	6	U
3	F	2	U

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Mol	Chain	Res	Type
3	F	4	U
3	F	5	U
3	F	6	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z  > 2$
4	ADP	A	1000	5,6	25,29,29	0.97	1 (4%)	24,45,45	1.69	2 (8%)
5	BEF	A	1001	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	2000	5,6	25,29,29	0.94	1 (4%)	24,45,45	1.73	2 (8%)
5	BEF	B	2001	4	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	C	3000	5,6	25,29,29	0.98	1 (4%)	24,45,45	1.66	2 (8%)
5	BEF	C	3001	4	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
4	ADP	A	1000	5,6	-	0/12/32/32	0/3/3/3
5	BEF	A	1001	4	-	0/0/0/0	0/0/0/0
4	ADP	B	2000	5,6	-	0/12/32/32	0/3/3/3
5	BEF	B	2001	4	-	0/0/0/0	0/0/0/0
4	ADP	C	3000	5,6	-	0/12/32/32	0/3/3/3
5	BEF	C	3001	4	-	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)
4	B	2000	ADP	C5-C4	2.98	1.47	1.40
4	A	1000	ADP	C5-C4	3.02	1.47	1.40
4	C	3000	ADP	C5-C4	3.09	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2000	ADP	N3-C2-N1	-6.19	123.47	128.86
4	A	1000	ADP	N3-C2-N1	-6.15	123.50	128.86
4	C	3000	ADP	N3-C2-N1	-6.03	123.61	128.86
4	A	1000	ADP	C4-C5-N7	-2.95	106.56	109.41
4	C	3000	ADP	C4-C5-N7	-2.81	106.69	109.41
4	B	2000	ADP	C4-C5-N7	-2.76	106.74	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	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	383/390 (98%)	-0.06	10 (2%) 56 49	31, 50, 79, 99	0
1	B	383/390 (98%)	-0.15	4 (1%) 82 79	32, 51, 77, 104	0
1	C	381/390 (97%)	0.05	5 (1%) 77 73	34, 56, 85, 99	0
2	G	17/32 (53%)	0.63	2 (11%) 5 3	52, 66, 99, 100	0
2	H	17/32 (53%)	0.67	2 (11%) 5 3	58, 75, 93, 93	0
2	I	15/32 (46%)	1.73	7 (46%) 0 0	81, 98, 110, 113	0
3	D	6/15 (40%)	-0.30	0 100 100	56, 61, 80, 99	0
3	E	6/15 (40%)	0.11	0 100 100	48, 58, 90, 92	0
3	F	6/15 (40%)	0.26	1 (16%) 2 1	52, 57, 67, 110	0
All	All	1214/1311 (92%)	-0.01	31 (2%) 56 49	31, 53, 85, 113	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	213	GLU	4.6
1	C	67	PHE	4.4
2	I	210	LYS	3.8
2	G	208	ALA	3.7
1	C	80	CYS	3.5
1	A	271	ASP	3.3
2	H	208	ALA	3.1
2	I	211	SER	3.1
1	C	68	LEU	2.8
1	A	275	LYS	2.8
2	I	224	GLU	2.8
2	H	213	GLU	2.6
1	A	424	GLU	2.6
1	C	64	PHE	2.6
3	F	1	U	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	207	SER	2.5
2	G	209	LYS	2.5
1	A	274	ALA	2.4
1	A	224	LEU	2.4
1	B	83	GLU	2.4
1	A	273	GLU	2.3
1	B	435	GLU	2.3
1	A	339	HIS	2.3
2	I	215	LEU	2.3
1	B	295	ARG	2.1
1	A	427	ASP	2.1
1	A	222	GLU	2.1
2	I	218	GLU	2.1
1	A	428	VAL	2.0
2	I	223	PHE	2.0
1	B	339	HIS	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
5	BEF	A	1001	4/4	0.92	0.18	1.13	34,34,38,41	0
4	ADP	A	1000	27/27	0.98	0.17	0.03	28,36,44,48	0
5	BEF	C	3001	4/4	0.96	0.14	-0.32	47,47,51,53	0
4	ADP	B	2000	27/27	0.97	0.15	-0.46	36,46,53,55	0
6	MG	B	2002	1/1	0.97	0.12	-0.79	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	C	3000	27/27	0.95	0.14	-0.81	38,57,70,73	0
5	BEF	B	2001	4/4	0.94	0.12	-1.03	31,40,41,42	0
6	MG	C	3002	1/1	0.98	0.07	-	44,44,44,44	0
6	MG	A	1002	1/1	0.98	0.12	-	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.