



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:10 AM GMT

PDB ID : 3DLS  
Title : Crystal structure of human PAS kinase bound to ADP  
Authors : Antonysamy, S.; Bonanno, J.B.; Romero, R.; Russell, M.; Iizuka, M.; Gheyi, T.; Wasserman, S.R.; Rutter, J.; Sauder, J.M.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-06-29  
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

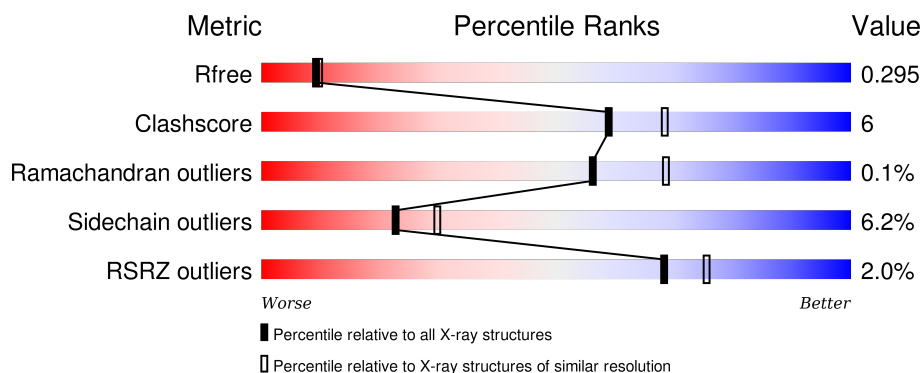
# 1 Overall quality at a glance

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.



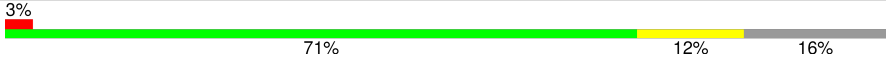
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	335	
1	B	335	
1	C	335	
1	D	335	
1	E	335	

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Mol	Chain	Length	Quality of chain
1	F	335	

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
2	MG	A	20	-	-	-	X
2	MG	A	25	-	-	-	X
2	MG	C	21	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13724 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 PAS domain-containing serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2236	1465	350	411	10			
1	B	280	Total	C	N	O	S	0	0	0
			2200	1435	353	403	9			
1	C	281	Total	C	N	O	S	0	0	0
			2217	1447	355	407	8			
1	D	284	Total	C	N	O	S	0	0	0
			2220	1453	351	406	10			
1	E	282	Total	C	N	O	S	0	0	0
			2216	1449	353	405	9			
1	F	281	Total	C	N	O	S	0	0	0
			2174	1420	345	400	9			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	974	MET	-	expression tag	UNP Q96RG2
A	975	ALA	-	expression tag	UNP Q96RG2
A	976	LEU	-	expression tag	UNP Q96RG2
A	1301	GLU	-	expression tag	UNP Q96RG2
A	1302	GLY	-	expression tag	UNP Q96RG2
A	1303	HIS	-	expression tag	UNP Q96RG2
A	1304	HIS	-	expression tag	UNP Q96RG2
A	1305	HIS	-	expression tag	UNP Q96RG2
A	1306	HIS	-	expression tag	UNP Q96RG2
A	1307	HIS	-	expression tag	UNP Q96RG2
A	1308	HIS	-	expression tag	UNP Q96RG2
B	974	MET	-	expression tag	UNP Q96RG2
B	975	ALA	-	expression tag	UNP Q96RG2
B	976	LEU	-	expression tag	UNP Q96RG2
B	1301	GLU	-	expression tag	UNP Q96RG2
B	1302	GLY	-	expression tag	UNP Q96RG2
B	1303	HIS	-	expression tag	UNP Q96RG2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1304	HIS	-	expression tag	UNP Q96RG2
B	1305	HIS	-	expression tag	UNP Q96RG2
B	1306	HIS	-	expression tag	UNP Q96RG2
B	1307	HIS	-	expression tag	UNP Q96RG2
B	1308	HIS	-	expression tag	UNP Q96RG2
C	974	MET	-	expression tag	UNP Q96RG2
C	975	ALA	-	expression tag	UNP Q96RG2
C	976	LEU	-	expression tag	UNP Q96RG2
C	1301	GLU	-	expression tag	UNP Q96RG2
C	1302	GLY	-	expression tag	UNP Q96RG2
C	1303	HIS	-	expression tag	UNP Q96RG2
C	1304	HIS	-	expression tag	UNP Q96RG2
C	1305	HIS	-	expression tag	UNP Q96RG2
C	1306	HIS	-	expression tag	UNP Q96RG2
C	1307	HIS	-	expression tag	UNP Q96RG2
C	1308	HIS	-	expression tag	UNP Q96RG2
D	974	MET	-	expression tag	UNP Q96RG2
D	975	ALA	-	expression tag	UNP Q96RG2
D	976	LEU	-	expression tag	UNP Q96RG2
D	1301	GLU	-	expression tag	UNP Q96RG2
D	1302	GLY	-	expression tag	UNP Q96RG2
D	1303	HIS	-	expression tag	UNP Q96RG2
D	1304	HIS	-	expression tag	UNP Q96RG2
D	1305	HIS	-	expression tag	UNP Q96RG2
D	1306	HIS	-	expression tag	UNP Q96RG2
D	1307	HIS	-	expression tag	UNP Q96RG2
D	1308	HIS	-	expression tag	UNP Q96RG2
E	974	MET	-	expression tag	UNP Q96RG2
E	975	ALA	-	expression tag	UNP Q96RG2
E	976	LEU	-	expression tag	UNP Q96RG2
E	1301	GLU	-	expression tag	UNP Q96RG2
E	1302	GLY	-	expression tag	UNP Q96RG2
E	1303	HIS	-	expression tag	UNP Q96RG2
E	1304	HIS	-	expression tag	UNP Q96RG2
E	1305	HIS	-	expression tag	UNP Q96RG2
E	1306	HIS	-	expression tag	UNP Q96RG2
E	1307	HIS	-	expression tag	UNP Q96RG2
E	1308	HIS	-	expression tag	UNP Q96RG2
F	974	MET	-	expression tag	UNP Q96RG2
F	975	ALA	-	expression tag	UNP Q96RG2
F	976	LEU	-	expression tag	UNP Q96RG2
F	1301	GLU	-	expression tag	UNP Q96RG2

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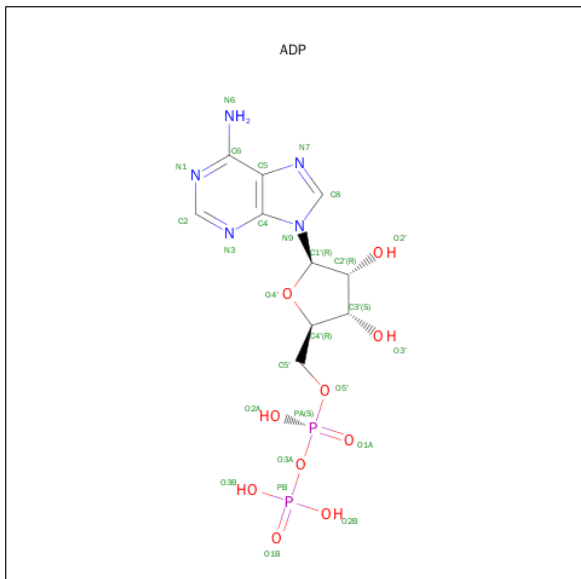
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1302	GLY	-	expression tag	UNP Q96RG2
F	1303	HIS	-	expression tag	UNP Q96RG2
F	1304	HIS	-	expression tag	UNP Q96RG2
F	1305	HIS	-	expression tag	UNP Q96RG2
F	1306	HIS	-	expression tag	UNP Q96RG2
F	1307	HIS	-	expression tag	UNP Q96RG2
F	1308	HIS	-	expression tag	UNP Q96RG2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	A	4	Total Mg 4 4	0	0
2	F	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

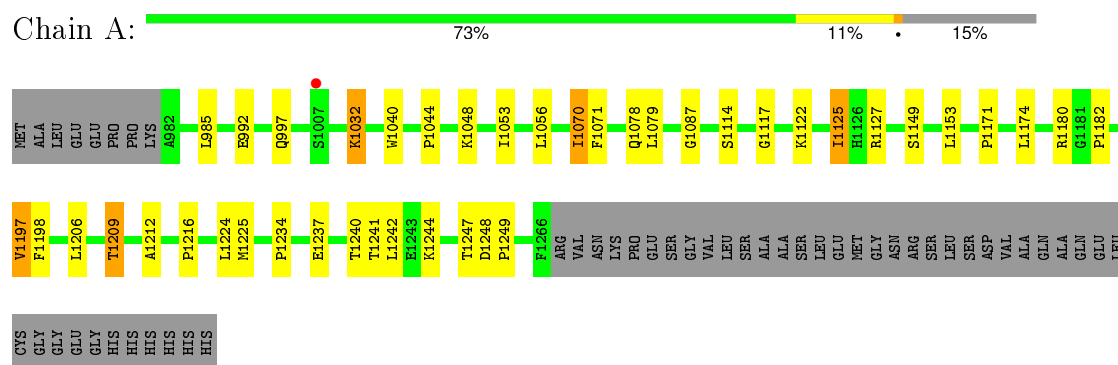
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	57	Total	O	0	0
			57	57		
4	C	47	Total	O	0	0
			47	47		
4	D	48	Total	O	0	0
			48	48		
4	E	39	Total	O	0	0
			39	39		
4	F	34	Total	O	0	0
			34	34		

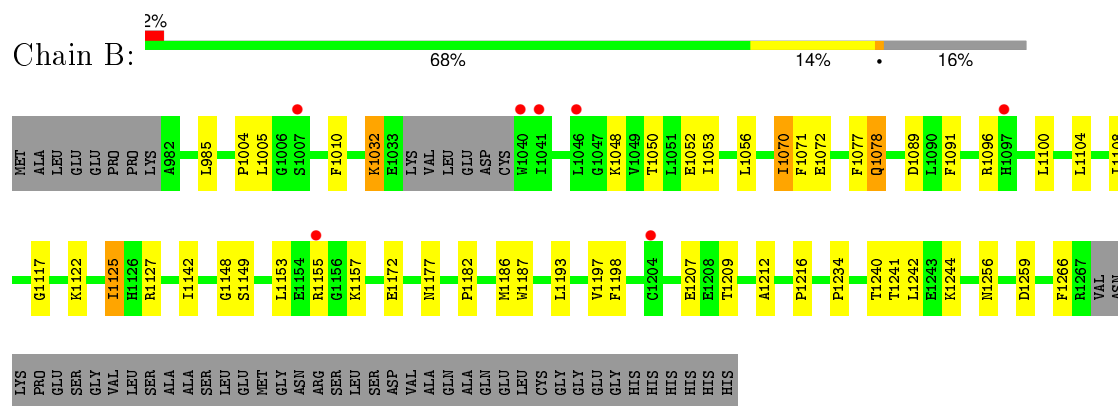
### 3 Residue-property plots

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.

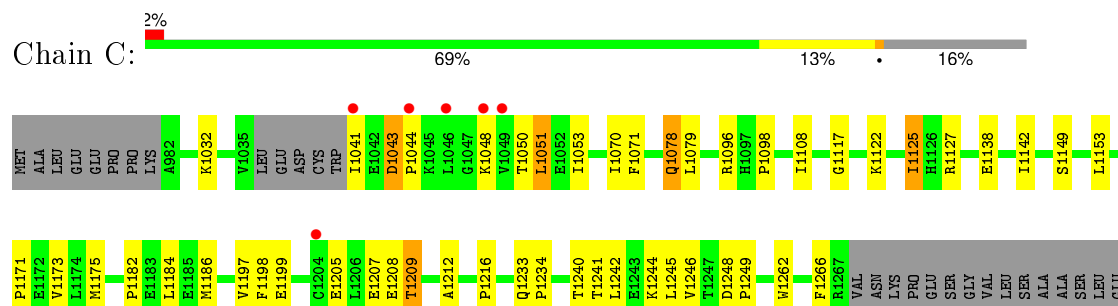
- Molecule 1: PAS domain-containing serine/threonine-protein kinase



- Molecule 1: PAS domain-containing serine/threonine-protein kinase



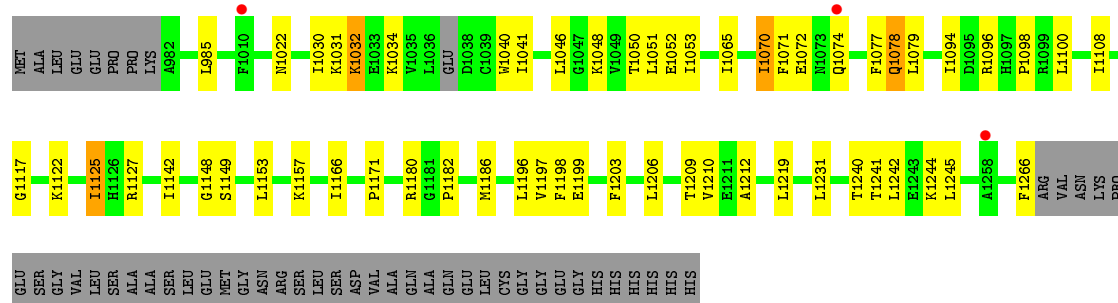
- Molecule 1: PAS domain-containing serine/threonine-protein kinase



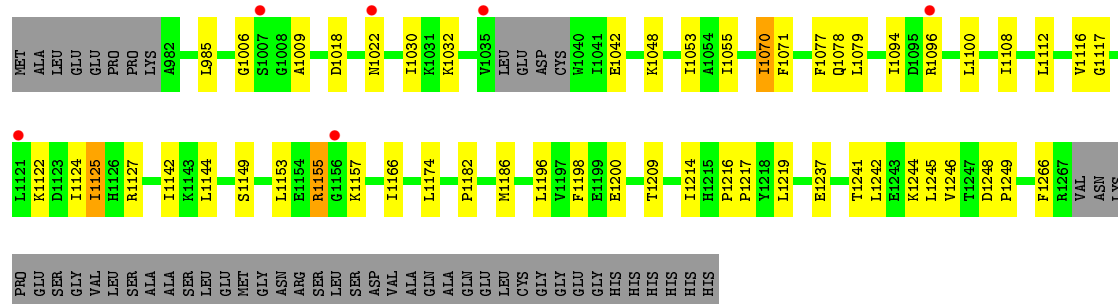


MET  
GLY  
ASN  
ARG  
SER  
LEU  
SER  
ASP  
VAL  
ALA  
GLN  
ALA  
GLN  
GLU  
LEU  
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GLU  
GLY  
HIS  
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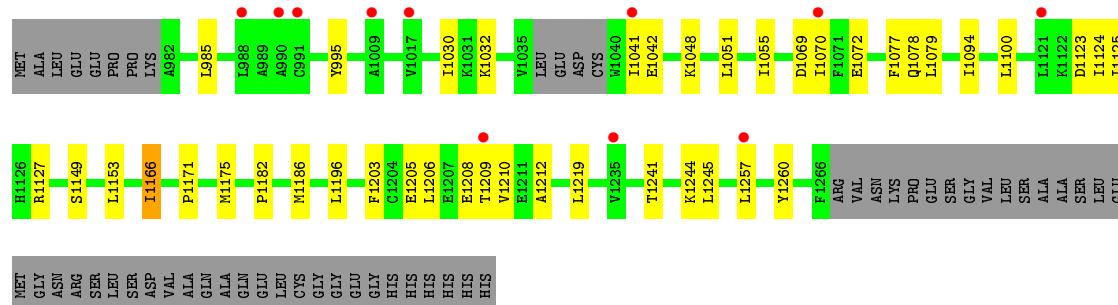
- Molecule 1: PAS domain-containing serine/threonine-protein kinase



- Molecule 1: PAS domain-containing serine/threonine-protein kinase



- Molecule 1: PAS domain-containing serine/threonine-protein kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.78Å 85.84Å 94.15Å 77.28° 77.50° 60.09°	Depositor
Resolution (Å)	(Not available) – 2.30 31.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 91.7 (31.20-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.29Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, $R_{free}$	0.241 , 0.297 0.240 , 0.295	Depositor DCC
$R_{free}$ test set	4846 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.216 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 96810 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.47	0/2291	0.61	0/3118
1	B	0.46	0/2252	0.61	2/3062 (0.1%)
1	C	0.46	0/2269	0.58	0/3083
1	D	0.43	0/2274	0.59	0/3094
1	E	0.42	0/2270	0.57	0/3088
1	F	0.42	0/2226	0.55	0/3033
All	All	0.44	0/13582	0.59	2/18478 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005	LEU	O-C-N	6.14	133.64	123.20
1	B	1005	LEU	CA-C-N	-5.30	105.60	116.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2236	0	2198	21	0
1	B	2200	0	2168	27	0
1	C	2217	0	2190	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2220	0	2178	31	0
1	E	2216	0	2178	28	0
1	F	2174	0	2109	18	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
3	E	27	0	12	2	0
3	F	27	0	12	0	0
4	A	55	0	0	1	0
4	B	57	0	0	0	0
4	C	47	0	0	2	0
4	D	48	0	0	0	0
4	E	39	0	0	2	0
4	F	34	0	0	0	0
All	All	13724	0	13093	153	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 6.

All (153) 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:C:1125:ILE:HG23	1:C:1127:ARG:HG3	1.67	0.74
1:D:1032:LYS:HZ1	1:D:1074:GLN:HA	1.51	0.74
1:A:1240:THR:HG23	1:A:1244:LYS:HD2	1.70	0.73
1:A:1125:ILE:HG23	1:A:1127:ARG:HG3	1.72	0.71
1:E:1094:ILE:HD11	1:E:1196:LEU:HA	1.71	0.71
1:C:1117:GLY:HA2	1:C:1242:LEU:HD21	1.72	0.71
1:E:1053:ILE:CG2	1:E:1070:ILE:HD12	2.23	0.68
1:F:1127:ARG:HD3	1:F:1149:SER:O	1.92	0.67
1:C:1071:PHE:HB2	1:C:1078:GLN:HE21	1.60	0.67
1:F:1041:ILE:HG13	1:F:1051:LEU:HD13	1.75	0.66
1:D:1125:ILE:HG23	1:D:1127:ARG:HG3	1.78	0.66
1:E:1174:LEU:HD12	1:E:1209:THR:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1182:PRO:O	1:B:1186:MET:HG2	1.96	0.66
1:B:1240:THR:HG23	1:B:1244:LYS:HD2	1.79	0.65
1:E:1053:ILE:HG21	1:E:1070:ILE:HD12	1.79	0.65
1:E:1241:THR:HG22	1:E:1244:LYS:HE2	1.79	0.65
1:D:1032:LYS:NZ	1:D:1074:GLN:HA	2.13	0.62
1:A:1117:GLY:HA2	1:A:1242:LEU:HD21	1.82	0.62
1:A:1053:ILE:HG21	1:A:1070:ILE:HD12	1.82	0.61
1:A:1127:ARG:HD3	1:A:1149:SER:O	2.00	0.61
1:C:1241:THR:HG23	1:C:1244:LYS:H	1.65	0.61
1:D:1166:ILE:HG22	1:D:1206:LEU:HD11	1.83	0.60
1:F:1094:ILE:HD11	1:F:1196:LEU:HA	1.83	0.60
1:D:1053:ILE:CG2	1:D:1070:ILE:HD12	2.32	0.60
1:E:1242:LEU:O	1:E:1246:VAL:HG23	2.03	0.59
1:D:1053:ILE:HG21	1:D:1070:ILE:HD12	1.85	0.59
1:B:1125:ILE:HG23	1:B:1127:ARG:HG3	1.85	0.59
1:C:1127:ARG:HD3	1:C:1149:SER:O	2.02	0.58
1:D:1041:ILE:HG13	1:D:1051:LEU:HD13	1.86	0.58
1:F:1030:ILE:HB	1:F:1077:PHE:HB2	1.84	0.58
1:F:1166:ILE:HG23	1:F:1206:LEU:HD21	1.86	0.57
1:D:1108:ILE:HG23	1:D:1142:ILE:HG21	1.87	0.56
1:A:1212:ALA:HB3	1:A:1234:PRO:HG3	1.88	0.56
1:E:1096:ARG:HG3	1:E:1266:PHE:CZ	2.42	0.55
1:E:1125:ILE:HG23	1:E:1127:ARG:HG3	1.89	0.55
1:E:1108:ILE:HG23	1:E:1142:ILE:HG21	1.88	0.54
1:B:1052:GLU:O	1:B:1056:LEU:HB2	2.08	0.54
1:D:1096:ARG:HG3	1:D:1266:PHE:CZ	2.43	0.54
1:A:1171:PRO:HB3	1:A:1209:THR:HG23	1.90	0.54
1:A:1174:LEU:HD12	1:A:1209:THR:HG21	1.90	0.53
1:E:1030:ILE:HB	1:E:1077:PHE:HB2	1.90	0.53
1:B:1117:GLY:HA2	1:B:1242:LEU:HD21	1.90	0.53
1:A:1125:ILE:HG23	1:A:1127:ARG:CG	2.37	0.53
1:C:1078:GLN:NE2	4:C:113:HOH:O	2.42	0.52
1:A:1053:ILE:CG2	1:A:1070:ILE:HD12	2.39	0.52
1:B:1052:GLU:HB2	1:B:1148:GLY:HA2	1.91	0.52
1:D:1032:LYS:HE3	1:D:1072:GLU:HG3	1.91	0.52
1:F:1205:GLU:O	1:F:1208:GLU:HG2	2.09	0.52
1:D:1030:ILE:HB	1:D:1077:PHE:HB2	1.91	0.52
1:F:1166:ILE:CG2	1:F:1206:LEU:HD21	2.40	0.52
1:D:1127:ARG:HD3	1:D:1149:SER:O	2.09	0.52
1:B:1050:THR:HG23	1:B:1053:ILE:H	1.75	0.52
1:C:1096:ARG:HB2	1:C:1266:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1144:LEU:HB2	4:E:270:HOH:O	2.11	0.51
1:D:1046:LEU:HD22	1:D:1070:ILE:HD13	1.92	0.51
1:C:1050:THR:HG22	1:C:1053:ILE:HD12	1.92	0.51
1:A:1197:VAL:HG21	1:A:1224:LEU:HD21	1.93	0.51
1:D:1050:THR:HG22	1:D:1053:ILE:HD12	1.93	0.51
1:E:1078:GLN:NE2	4:E:244:HOH:O	2.43	0.50
1:C:1182:PRO:O	1:C:1186:MET:HG2	2.12	0.50
1:A:1044:PRO:HB2	1:D:1072:GLU:HB3	1.94	0.50
1:E:1127:ARG:HD3	1:E:1149:SER:O	2.12	0.50
1:F:1055:ILE:HG23	1:F:1124:ILE:HD13	1.94	0.50
1:B:1071:PHE:HB2	1:B:1078:GLN:HE21	1.77	0.49
1:D:1182:PRO:O	1:D:1186:MET:HG2	2.12	0.49
1:A:1180:ARG:NH2	1:A:1182:PRO:HG2	2.28	0.49
1:C:1125:ILE:HG23	1:C:1127:ARG:CG	2.39	0.48
1:D:1197:VAL:HG23	1:D:1198:PHE:CD2	2.47	0.48
1:E:1117:GLY:HA2	1:E:1242:LEU:HD21	1.95	0.48
1:A:1071:PHE:HB2	1:A:1078:GLN:HE21	1.78	0.48
1:E:1071:PHE:HB2	1:E:1078:GLN:HE21	1.79	0.48
1:B:1212:ALA:HB3	1:B:1234:PRO:HG3	1.96	0.48
1:E:1200:GLU:CD	1:E:1217:PRO:HG3	2.34	0.48
1:D:1065:ILE:HG12	3:D:4:ADP:N6	2.29	0.48
1:A:1078:GLN:NE2	4:A:74:HOH:O	2.46	0.47
1:E:1155:ARG:H	1:E:1155:ARG:HD3	1.79	0.47
1:C:1041:ILE:HG13	1:C:1051:LEU:HD13	1.96	0.47
1:A:1087:GLY:HA2	3:A:1:ADP:N3	2.30	0.47
1:C:1240:THR:HG23	1:C:1244:LYS:HD2	1.97	0.47
1:D:1117:GLY:HA2	1:D:1242:LEU:HD21	1.96	0.47
1:D:1244:LYS:HB2	1:D:1244:LYS:HE3	1.77	0.46
1:E:1182:PRO:O	1:E:1186:MET:HG2	2.15	0.46
1:C:1053:ILE:HG23	1:C:1070:ILE:HD13	1.97	0.46
1:B:1187:TRP:CZ2	1:B:1209:THR:HG23	2.50	0.46
1:A:1241:THR:HG23	1:A:1244:LYS:H	1.81	0.46
1:E:1094:ILE:CD1	1:E:1196:LEU:HA	2.45	0.46
1:D:1203:PHE:CE1	1:D:1212:ALA:HA	2.50	0.46
1:F:1171:PRO:HB3	1:F:1210:VAL:HG12	1.98	0.46
1:F:1203:PHE:HB3	1:F:1208:GLU:HG3	1.98	0.45
1:A:1032:LYS:HG3	1:A:1040:TRP:HH2	1.82	0.45
1:C:1205:GLU:O	1:C:1208:GLU:HG2	2.16	0.45
1:B:1096:ARG:HB2	1:B:1266:PHE:CE1	2.51	0.45
1:B:1207:GLU:C	1:B:1209:THR:H	2.20	0.45
1:B:1108:ILE:HG23	1:B:1142:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1207:GLU:C	1:C:1209:THR:H	2.20	0.44
1:A:1248:ASP:HA	1:A:1249:PRO:HD3	1.90	0.44
1:D:1071:PHE:HB2	1:D:1078:GLN:HE21	1.82	0.44
1:A:1174:LEU:CD1	1:A:1209:THR:HG21	2.48	0.44
1:B:1100:LEU:HD23	1:B:1104:LEU:HD23	1.99	0.44
1:F:995:TYR:HB2	1:F:1078:GLN:HE21	1.82	0.44
1:D:1094:ILE:HD11	1:D:1196:LEU:HA	2.00	0.44
1:F:1182:PRO:O	1:F:1186:MET:HG2	2.18	0.44
1:B:1053:ILE:CG2	1:B:1070:ILE:HD12	2.48	0.43
1:B:1256:ASN:O	1:B:1259:ASP:HB2	2.18	0.43
1:F:1257:LEU:HA	1:F:1260:TYR:HD2	1.82	0.43
1:B:1172:GLU:O	1:B:1177:ASN:HB2	2.19	0.43
1:D:1052:GLU:HB2	1:D:1148:GLY:HA2	1.99	0.43
1:D:1098:PRO:HD2	1:D:1199:GLU:OE2	2.19	0.43
1:C:1212:ALA:HB3	1:C:1234:PRO:HG3	2.01	0.43
1:C:1096:ARG:HB2	1:C:1266:PHE:CE1	2.52	0.43
1:C:1043:ASP:HA	1:C:1044:PRO:HD3	1.91	0.43
1:F:1125:ILE:HG23	1:F:1127:ARG:HG3	2.00	0.42
1:E:1155:ARG:N	1:E:1155:ARG:HD3	2.33	0.42
1:E:1006:GLY:HA2	3:E:5:ADP:H4'	2.02	0.42
1:D:1031:LYS:HD3	1:D:1034:LYS:HD3	2.02	0.42
1:B:1241:THR:HG22	1:B:1244:LYS:HE3	2.01	0.42
1:B:1241:THR:HG22	1:B:1244:LYS:HB2	2.02	0.42
1:E:1006:GLY:CA	3:E:5:ADP:H4'	2.50	0.42
1:D:1171:PRO:HB3	1:D:1210:VAL:HG12	2.01	0.42
1:A:1198:PHE:CZ	1:A:1216:PRO:HB3	2.55	0.41
1:F:1203:PHE:CD2	1:F:1209:THR:HG22	2.55	0.41
1:D:1032:LYS:HG3	1:D:1040:TRP:HH2	1.85	0.41
1:E:1018:ASP:O	1:E:1022:ASN:HA	2.21	0.41
1:F:1166:ILE:HD13	1:F:1166:ILE:HA	1.96	0.41
1:D:1180:ARG:NH2	1:D:1182:PRO:HG2	2.36	0.41
1:E:1198:PHE:CD1	1:E:1217:PRO:HD2	2.56	0.41
1:F:1241:THR:H	1:F:1244:LYS:HZ2	1.69	0.41
1:B:1004:PRO:HG3	1:B:1010:PHE:CD1	2.55	0.41
1:B:1193:LEU:O	1:B:1197:VAL:HG22	2.21	0.41
1:E:1216:PRO:HA	1:E:1217:PRO:HD3	1.92	0.41
1:E:1248:ASP:HA	1:E:1249:PRO:HD3	1.90	0.41
1:B:1032:LYS:HD2	1:B:1032:LYS:H	1.85	0.41
1:C:1198:PHE:CE1	1:C:1216:PRO:HB3	2.55	0.41
1:B:1072:GLU:HG3	1:B:1077:PHE:CE2	2.56	0.41
1:B:1089:ASP:OD1	1:B:1091:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1171:PRO:O	1:C:1175:MET:HG3	2.21	0.41
1:E:1055:ILE:HG23	1:E:1124:ILE:HD13	2.03	0.41
1:D:1240:THR:HG23	1:D:1244:LYS:HD2	2.02	0.41
1:C:1173:VAL:HG21	1:C:1184:LEU:HD13	2.03	0.41
1:C:1242:LEU:O	1:C:1246:VAL:HG23	2.20	0.40
1:B:1198:PHE:CZ	1:B:1216:PRO:HB3	2.57	0.40
1:C:1098:PRO:HD2	1:C:1199:GLU:OE2	2.21	0.40
1:C:1108:ILE:HG23	1:C:1142:ILE:HG21	2.04	0.40
1:C:1248:ASP:HA	1:C:1249:PRO:HD3	1.91	0.40
1:D:1231:LEU:HD23	1:D:1240:THR:HB	2.03	0.40
1:C:1233:GLN:HA	1:C:1234:PRO:HD3	1.87	0.40
1:B:1197:VAL:HG23	1:B:1198:PHE:CD2	2.56	0.40
1:B:1127:ARG:HD3	1:B:1149:SER:O	2.21	0.40
1:F:1203:PHE:CE1	1:F:1212:ALA:HA	2.57	0.40
1:C:1197:VAL:HG23	1:C:1198:PHE:CD2	2.57	0.40
1:C:1044:PRO:HD3	4:C:193:HOH:O	2.21	0.40
1:E:1112:LEU:O	1:E:1116:VAL:HG23	2.21	0.40
1:C:1138:GLU:HG2	1:C:1262:TRP:CE2	2.56	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	283/335 (84%)	272 (96%)	11 (4%)	0	100	100
1	B	276/335 (82%)	264 (96%)	12 (4%)	0	100	100
1	C	277/335 (83%)	260 (94%)	17 (6%)	0	100	100
1	D	280/335 (84%)	271 (97%)	9 (3%)	0	100	100
1	E	278/335 (83%)	268 (96%)	9 (3%)	1 (0%)	39	48
1	F	277/335 (83%)	260 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1671/2010 (83%)	1595 (96%)	75 (4%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1009	ALA

### 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	236/291 (81%)	218 (92%)	18 (8%)	16 20
1	B	233/291 (80%)	223 (96%)	10 (4%)	35 47
1	C	235/291 (81%)	224 (95%)	11 (5%)	32 43
1	D	234/291 (80%)	218 (93%)	16 (7%)	20 25
1	E	234/291 (80%)	217 (93%)	17 (7%)	17 22
1	F	226/291 (78%)	211 (93%)	15 (7%)	21 27
All	All	1398/1746 (80%)	1311 (94%)	87 (6%)	23 30

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	985	LEU
1	A	992	GLU
1	A	997	GLN
1	A	1032	LYS
1	A	1048	LYS
1	A	1056	LEU
1	A	1070	ILE
1	A	1079	LEU
1	A	1114	SER
1	A	1122	LYS
1	A	1125	ILE

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Mol	Chain	Res	Type
1	A	1153	LEU
1	A	1197	VAL
1	A	1206	LEU
1	A	1209	THR
1	A	1225	MET
1	A	1237	GLU
1	A	1247	THR
1	B	985	LEU
1	B	1032	LYS
1	B	1048	LYS
1	B	1070	ILE
1	B	1078	GLN
1	B	1122	LYS
1	B	1125	ILE
1	B	1153	LEU
1	B	1155	ARG
1	B	1157	LYS
1	C	1032	LYS
1	C	1043	ASP
1	C	1048	LYS
1	C	1051	LEU
1	C	1078	GLN
1	C	1079	LEU
1	C	1122	LYS
1	C	1125	ILE
1	C	1153	LEU
1	C	1209	THR
1	C	1245	LEU
1	D	985	LEU
1	D	1022	ASN
1	D	1032	LYS
1	D	1048	LYS
1	D	1070	ILE
1	D	1078	GLN
1	D	1079	LEU
1	D	1100	LEU
1	D	1122	LYS
1	D	1125	ILE
1	D	1153	LEU
1	D	1157	LYS
1	D	1209	THR
1	D	1219	LEU

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Mol	Chain	Res	Type
1	D	1241	THR
1	D	1245	LEU
1	E	985	LEU
1	E	1032	LYS
1	E	1042	GLU
1	E	1048	LYS
1	E	1070	ILE
1	E	1079	LEU
1	E	1100	LEU
1	E	1122	LYS
1	E	1125	ILE
1	E	1153	LEU
1	E	1155	ARG
1	E	1157	LYS
1	E	1166	ILE
1	E	1214	ILE
1	E	1219	LEU
1	E	1237	GLU
1	E	1245	LEU
1	F	985	LEU
1	F	1032	LYS
1	F	1042	GLU
1	F	1048	LYS
1	F	1069	ASP
1	F	1070	ILE
1	F	1072	GLU
1	F	1079	LEU
1	F	1100	LEU
1	F	1123	ASP
1	F	1153	LEU
1	F	1166	ILE
1	F	1175	MET
1	F	1219	LEU
1	F	1245	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	997	GLN
1	A	1078	GLN
1	B	997	GLN
1	B	1078	GLN

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Mol	Chain	Res	Type
1	C	997	GLN
1	C	1078	GLN
1	D	1078	GLN
1	E	1078	GLN
1	F	1253	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 25 ligands modelled in this entry, 19 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	$\# Z  > 2$
3	ADP	A	1	2	22,29,29	1.07	2 (9%)	27,45,45	1.84	3 (11%)
3	ADP	B	2	2	22,29,29	1.10	2 (9%)	27,45,45	1.83	4 (14%)
3	ADP	C	3	2	22,29,29	1.07	2 (9%)	27,45,45	1.77	2 (7%)
3	ADP	D	4	2	22,29,29	1.10	2 (9%)	27,45,45	1.63	2 (7%)
3	ADP	E	5	2	22,29,29	1.13	2 (9%)	27,45,45	1.74	3 (11%)
3	ADP	F	6	2	22,29,29	1.13	2 (9%)	27,45,45	1.62	2 (7%)

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	1	2	-	0/12/32/32	0/3/3/3
3	ADP	B	2	2	-	0/12/32/32	0/3/3/3
3	ADP	C	3	2	-	0/12/32/32	0/3/3/3
3	ADP	D	4	2	-	0/12/32/32	0/3/3/3
3	ADP	E	5	2	-	0/12/32/32	0/3/3/3
3	ADP	F	6	2	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	ADP	O4'-C1'	2.08	1.43	1.41
3	E	5	ADP	O4'-C1'	2.13	1.43	1.41
3	D	4	ADP	O4'-C1'	2.40	1.44	1.41
3	A	1	ADP	O4'-C1'	2.40	1.44	1.41
3	B	2	ADP	O4'-C1'	2.51	1.44	1.41
3	C	3	ADP	O4'-C1'	2.52	1.44	1.41
3	B	2	ADP	C5-C4	2.79	1.46	1.40
3	A	1	ADP	C5-C4	3.12	1.47	1.40
3	D	4	ADP	C5-C4	3.15	1.47	1.40
3	C	3	ADP	C5-C4	3.17	1.47	1.40
3	E	5	ADP	C5-C4	3.39	1.48	1.40
3	F	6	ADP	C5-C4	3.50	1.48	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	ADP	N3-C2-N1	-7.80	122.92	128.89
3	A	1	ADP	N3-C2-N1	-7.65	123.03	128.89
3	B	2	ADP	N3-C2-N1	-7.54	123.12	128.89
3	E	5	ADP	N3-C2-N1	-7.17	123.41	128.89
3	D	4	ADP	N3-C2-N1	-6.71	123.76	128.89
3	F	6	ADP	N3-C2-N1	-6.55	123.88	128.89
3	A	1	ADP	C4-C5-N7	-3.20	106.53	109.48
3	B	2	ADP	C4-C5-N7	-3.10	106.63	109.48
3	F	6	ADP	C4-C5-N7	-2.83	106.87	109.48
3	D	4	ADP	C4-C5-N7	-2.83	106.88	109.48
3	C	3	ADP	C4-C5-N7	-2.30	107.36	109.48
3	E	5	ADP	C2'-C1'-N9	-2.29	110.80	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	ADP	C2'-C1'-N9	-2.22	110.90	114.29
3	E	5	ADP	C4-C5-N7	-2.20	107.45	109.48
3	A	1	ADP	C2'-C1'-N9	-2.05	111.16	114.29
3	B	2	ADP	O2B-PB-O1B	2.08	117.26	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	ADP	1	0
3	D	4	ADP	1	0
3	E	5	ADP	2	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	285/335 (85%)	-0.09	1 (0%) 93 95	14, 29, 46, 59	0
1	B	280/335 (83%)	0.07	7 (2%) 61 70	17, 33, 53, 72	0
1	C	281/335 (83%)	0.00	6 (2%) 67 74	17, 32, 54, 73	0
1	D	284/335 (84%)	0.05	3 (1%) 82 86	22, 38, 56, 70	0
1	E	282/335 (84%)	0.18	6 (2%) 67 74	22, 42, 58, 73	0
1	F	281/335 (83%)	0.29	11 (3%) 43 52	26, 46, 67, 76	0
All	All	1693/2010 (84%)	0.08	34 (2%) 68 75	14, 37, 59, 76	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1204	CYS	5.0
1	C	1046	LEU	4.7
1	F	1121	LEU	4.2
1	F	1041	ILE	3.7
1	B	1040	TRP	3.6
1	C	1048	LYS	3.6
1	B	1155	ARG	3.6
1	B	1007	SER	3.5
1	F	1257	LEU	3.3
1	B	1041	ILE	3.0
1	F	1017	VAL	3.0
1	F	1235	VAL	2.9
1	F	990	ALA	2.9
1	A	1007	SER	2.9
1	C	1041	ILE	2.8
1	E	1096	ARG	2.8
1	F	1070	ILE	2.7
1	E	1022	ASN	2.6
1	C	1044	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1097	HIS	2.5
1	E	1007	SER	2.4
1	B	1046	LEU	2.4
1	C	1049	VAL	2.4
1	F	1209	THR	2.4
1	B	1204	CYS	2.3
1	D	1074	GLN	2.3
1	F	1009	ALA	2.3
1	D	1010	PHE	2.3
1	F	991	CYS	2.2
1	E	1035	VAL	2.2
1	E	1156	GLY	2.1
1	E	1121	LEU	2.1
1	F	988	LEU	2.1
1	D	1258	ALA	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
2	MG	C	21	1/1	0.97	0.27	4.20	30,30,30,30	0
2	MG	A	20	1/1	0.89	0.18	3.11	24,24,24,24	0
2	MG	A	25	1/1	0.97	0.23	2.38	22,22,22,22	0
2	MG	B	19	1/1	0.90	0.20	1.07	33,33,33,33	0
2	MG	B	24	1/1	0.98	0.21	0.72	26,26,26,26	0
3	ADP	D	4	27/27	0.96	0.13	-0.27	22,32,37,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	B	2	27/27	0.97	0.13	-0.28	12,23,34,41	0
3	ADP	E	5	27/27	0.94	0.14	-0.36	27,36,52,53	0
3	ADP	C	3	27/27	0.98	0.12	-0.37	17,21,30,36	0
3	ADP	A	1	27/27	0.98	0.11	-0.52	13,20,33,36	0
2	MG	D	23	1/1	0.96	0.12	-0.89	31,31,31,31	0
2	MG	C	22	1/1	0.95	0.09	-1.18	35,35,35,35	0
3	ADP	F	6	27/27	0.96	0.10	-1.35	34,40,45,46	0
2	MG	B	10	1/1	0.96	0.18	-	23,23,23,23	0
2	MG	D	13	1/1	0.99	0.20	-	14,14,14,14	0
2	MG	A	7	1/1	0.96	0.14	-	10,10,10,10	0
2	MG	F	17	1/1	0.96	0.24	-	25,25,25,25	0
2	MG	C	12	1/1	0.93	0.30	-	35,35,35,35	0
2	MG	E	16	1/1	0.94	0.25	-	36,36,36,36	0
2	MG	C	11	1/1	0.99	0.20	-	13,13,13,13	0
2	MG	A	8	1/1	0.93	0.27	-	28,28,28,28	0
2	MG	D	14	1/1	0.95	0.29	-	33,33,33,33	0
2	MG	B	9	1/1	0.98	0.16	-	15,15,15,15	0
2	MG	E	15	1/1	0.95	0.21	-	24,24,24,24	0
2	MG	F	18	1/1	0.94	0.24	-	31,31,31,31	0

## 6.5 Other polymers

There are no such residues in this entry.