



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:51 PM GMT

PDB ID : 4JHD  
Title : Crystal Structure of an Actin Dimer in Complex with the Actin Nucleator  
Cordon-Bleu  
Authors : Chen, X.; Ni, F.; Wang, Q.  
Deposited on : 2013-03-04  
Resolution : 2.91 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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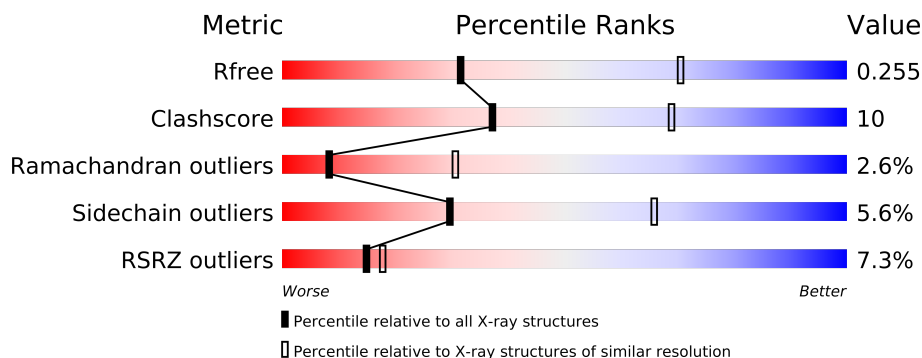
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.91 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))
$R_{free}$	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	384	
1	D	384	
2	B	384	
2	E	384	
3	C	171	
3	F	171	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	MG	A	402	-	X
5	MG	B	402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	MG	D	402	-	X
5	MG	E	402	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13002 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Actin-5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2890	1829	488	552	21			
1	D	371	Total	C	N	O	S	0	0	0
			2880	1821	488	552	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP P10987
A	-7	ALA	-	EXPRESSION TAG	UNP P10987
A	-6	HIS	-	EXPRESSION TAG	UNP P10987
A	-5	HIS	-	EXPRESSION TAG	UNP P10987
A	-4	HIS	-	EXPRESSION TAG	UNP P10987
A	-3	HIS	-	EXPRESSION TAG	UNP P10987
A	-2	HIS	-	EXPRESSION TAG	UNP P10987
A	-1	HIS	-	EXPRESSION TAG	UNP P10987
A	204	GLU	ALA	ENGINEERED MUTATION	UNP P10987
A	243	LYS	PRO	ENGINEERED MUTATION	UNP P10987
D	-8	MET	-	EXPRESSION TAG	UNP P10987
D	-7	ALA	-	EXPRESSION TAG	UNP P10987
D	-6	HIS	-	EXPRESSION TAG	UNP P10987
D	-5	HIS	-	EXPRESSION TAG	UNP P10987
D	-4	HIS	-	EXPRESSION TAG	UNP P10987
D	-3	HIS	-	EXPRESSION TAG	UNP P10987
D	-2	HIS	-	EXPRESSION TAG	UNP P10987
D	-1	HIS	-	EXPRESSION TAG	UNP P10987
D	204	GLU	ALA	ENGINEERED MUTATION	UNP P10987
D	243	LYS	PRO	ENGINEERED MUTATION	UNP P10987

- Molecule 2 is a protein called Actin-5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	371	Total 2886	C 1826	N 487	O 552	S 21	0	0	0
2	E	371	Total 2886	C 1826	N 487	O 552	S 21	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	EXPRESSION TAG	UNP P10987
B	-7	ALA	-	EXPRESSION TAG	UNP P10987
B	-6	HIS	-	EXPRESSION TAG	UNP P10987
B	-5	HIS	-	EXPRESSION TAG	UNP P10987
B	-4	HIS	-	EXPRESSION TAG	UNP P10987
B	-3	HIS	-	EXPRESSION TAG	UNP P10987
B	-2	HIS	-	EXPRESSION TAG	UNP P10987
B	-1	HIS	-	EXPRESSION TAG	UNP P10987
B	291	GLU	LYS	ENGINEERED MUTATION	UNP P10987
B	322	LYS	PRO	ENGINEERED MUTATION	UNP P10987
E	-8	MET	-	EXPRESSION TAG	UNP P10987
E	-7	ALA	-	EXPRESSION TAG	UNP P10987
E	-6	HIS	-	EXPRESSION TAG	UNP P10987
E	-5	HIS	-	EXPRESSION TAG	UNP P10987
E	-4	HIS	-	EXPRESSION TAG	UNP P10987
E	-3	HIS	-	EXPRESSION TAG	UNP P10987
E	-2	HIS	-	EXPRESSION TAG	UNP P10987
E	-1	HIS	-	EXPRESSION TAG	UNP P10987
E	291	GLU	LYS	ENGINEERED MUTATION	UNP P10987
E	322	LYS	PRO	ENGINEERED MUTATION	UNP P10987

- Molecule 3 is a protein called Protein cordon-bleu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total 603	C 368	N 116	O 118	S 1	0	0	0
3	F	75	Total 571	C 347	N 110	O 113	S 1	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

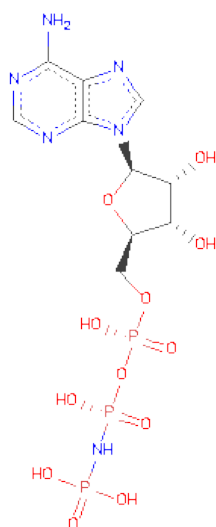
Chain	Residue	Modelled	Actual	Comment	Reference
C	49	MET	-	EXPRESSION TAG	UNP Q5NBX1
C	50	ALA	-	EXPRESSION TAG	UNP Q5NBX1
C	51	HIS	-	EXPRESSION TAG	UNP Q5NBX1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	52	HIS	-	EXPRESSION TAG	UNP Q5NBX1
C	53	HIS	-	EXPRESSION TAG	UNP Q5NBX1
C	54	HIS	-	EXPRESSION TAG	UNP Q5NBX1
C	55	HIS	-	EXPRESSION TAG	UNP Q5NBX1
C	56	HIS	-	EXPRESSION TAG	UNP Q5NBX1
C	57	VAL	-	EXPRESSION TAG	UNP Q5NBX1
C	87	VAL	THR	SEE REMARK 999	UNP Q5NBX1
C	167	THR	PRO	SEE REMARK 999	UNP Q5NBX1
F	49	MET	-	EXPRESSION TAG	UNP Q5NBX1
F	50	ALA	-	EXPRESSION TAG	UNP Q5NBX1
F	51	HIS	-	EXPRESSION TAG	UNP Q5NBX1
F	52	HIS	-	EXPRESSION TAG	UNP Q5NBX1
F	53	HIS	-	EXPRESSION TAG	UNP Q5NBX1
F	54	HIS	-	EXPRESSION TAG	UNP Q5NBX1
F	55	HIS	-	EXPRESSION TAG	UNP Q5NBX1
F	56	HIS	-	EXPRESSION TAG	UNP Q5NBX1
F	57	VAL	-	EXPRESSION TAG	UNP Q5NBX1
F	87	VAL	THR	SEE REMARK 999	UNP Q5NBX1
F	167	THR	PRO	SEE REMARK 999	UNP Q5NBX1

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	
			31	10	6	12	3	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

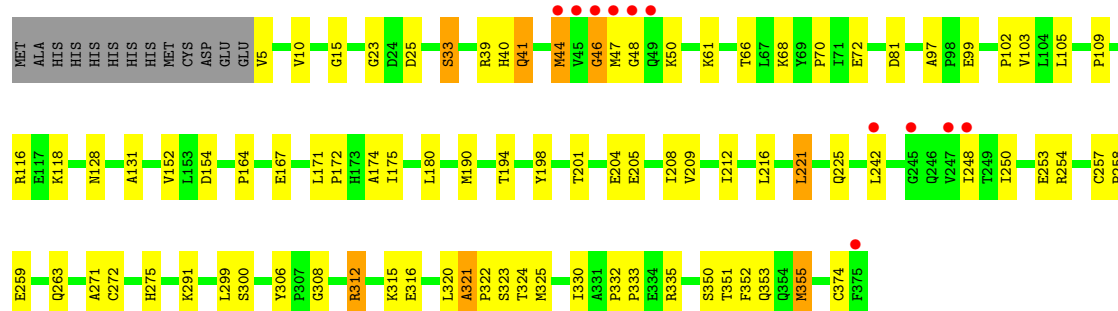
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	43	Total	O	0	0
			43	43		
6	C	10	Total	O	0	0
			10	10		
6	D	31	Total	O	0	0
			31	31		
6	E	22	Total	O	0	0
			22	22		
6	F	6	Total	O	0	0
			6	6		

### 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.

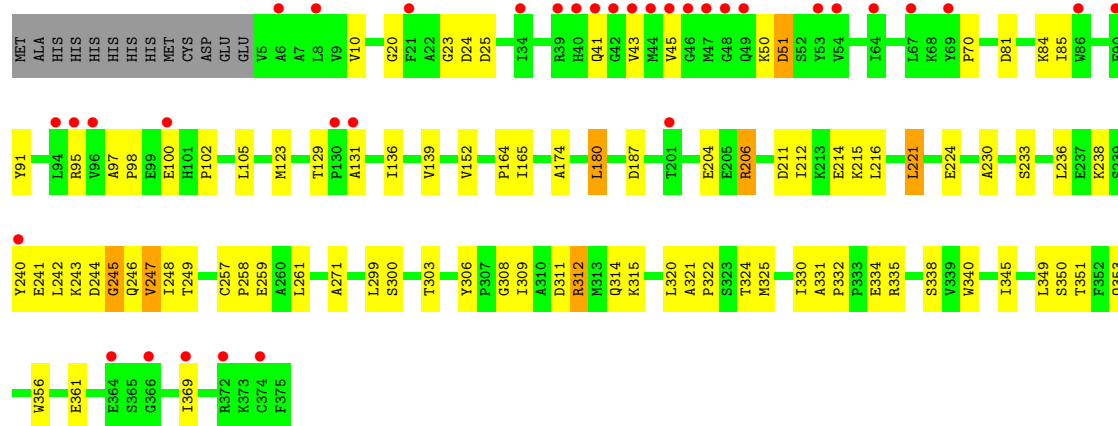
#### • Molecule 1: Actin-5C

Chain A: 



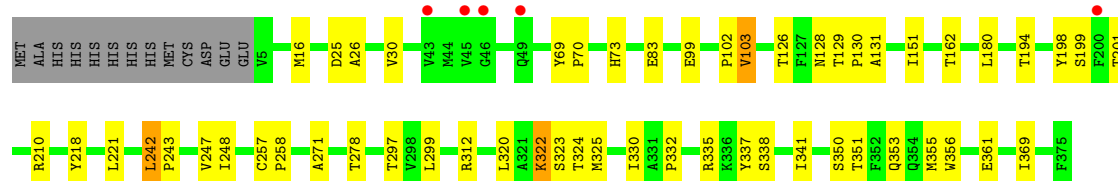
#### • Molecule 1: Actin-5C

Chain D: 



#### • Molecule 2: Actin-5C

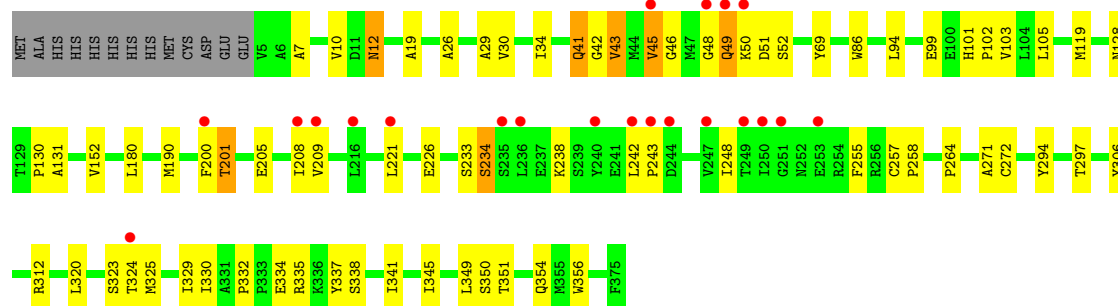
Chain B: 





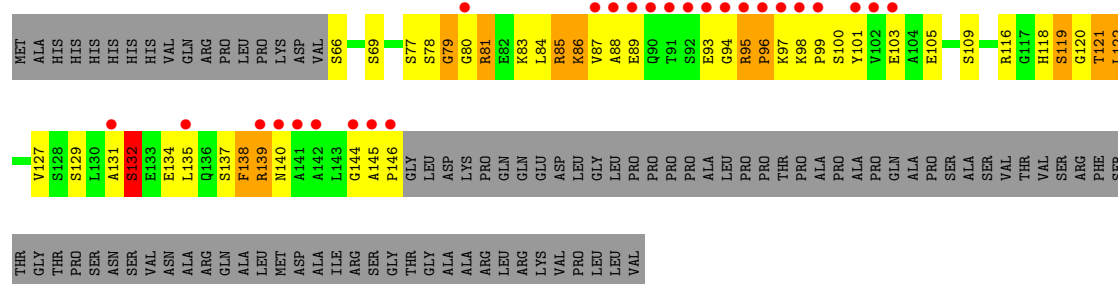
- Molecule 2: Actin-5C

Chain E:



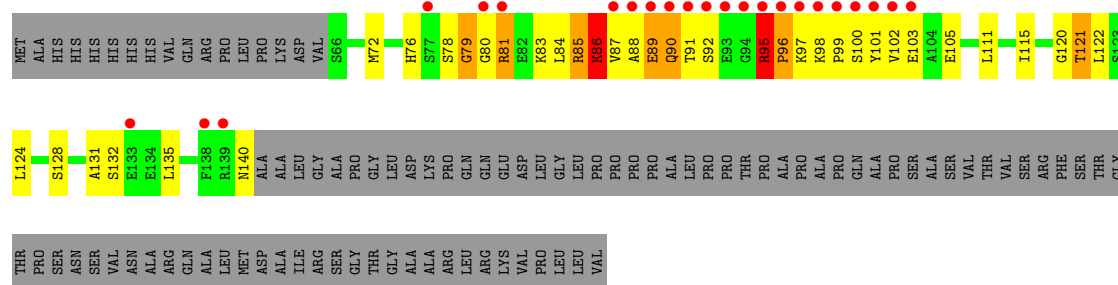
- Molecule 3: Protein cordon-bleu

Chain C:



- Molecule 3: Protein cordon-bleu

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.45Å 99.80Å 118.27Å 65.41° 90.03° 77.77°	Depositor
Resolution (Å)	45.02 – 2.91 45.02 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.02-2.91) 97.7 (45.02-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.255 0.200 , 0.255	Depositor DCC
$R_{free}$ test set	2341 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46313 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.42	0/2951	0.55	0/3996
1	D	0.45	1/2941 (0.0%)	0.53	0/3984
2	B	0.38	0/2947	0.52	0/3992
2	E	0.38	0/2947	0.53	0/3992
3	C	0.60	1/610 (0.2%)	0.64	0/816
3	F	0.83	4/577 (0.7%)	0.68	0/770
All	All	0.44	6/12973 (0.0%)	0.55	0/17550

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
3	F	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	140	ASN	C-O	8.89	1.40	1.23
3	C	89	GLU	CD-OE1	7.83	1.34	1.25
3	F	86	LYS	CD-CE	7.72	1.70	1.51
3	F	128	SER	CB-OG	5.94	1.50	1.42
3	F	89	GLU	CD-OE2	5.71	1.31	1.25
1	D	51	ASP	CG-OD1	5.13	1.37	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	95	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2890	0	2865	52	0
1	D	2880	0	2837	71	0
2	B	2886	0	2857	37	0
2	E	2886	0	2857	52	0
3	C	603	0	611	55	0
3	F	571	0	580	43	0
4	A	31	0	13	4	0
4	B	31	0	13	2	0
4	D	31	0	13	5	0
4	E	31	0	13	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	46	0	0	1	0
6	B	43	0	0	0	0
6	C	10	0	0	0	0
6	D	31	0	0	0	0
6	E	22	0	0	0	0
6	F	6	0	0	0	0
All	All	13002	0	12659	257	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (257) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:401:ANP:N6	3:F:101:TYR:CD1	2.13	1.17
1:D:70:PRO:HG2	1:D:85:ILE:HD11	1.52	0.91
3:C:122:LEU:HB3	1:D:41:GLN:HB3	1.50	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:26:ALA:CB	3:C:132:SER:HB2	2.03	0.88
2:B:210:ARG:HH12	3:C:144:GLY:H	1.23	0.86
1:D:240:TYR:O	1:D:247:VAL:HA	1.75	0.86
1:A:321:ALA:HB1	1:A:322:PRO:HD2	1.57	0.86
1:A:306:TYR:CZ	4:A:401:ANP:H2	2.10	0.85
3:C:95:ARG:HB3	3:C:96:PRO:HD3	1.59	0.84
2:B:242:LEU:HB3	2:B:243:PRO:HD2	1.60	0.83
3:C:134:GLU:HA	3:C:140:ASN:HD22	1.45	0.80
4:B:401:ANP:H3'	3:C:145:ALA:HB3	1.65	0.79
3:C:137:SER:HB3	3:C:140:ASN:HD21	1.47	0.78
1:D:240:TYR:CE1	1:D:242:LEU:HG	2.19	0.78
3:C:78:SER:O	3:C:80:GLY:N	2.19	0.76
1:A:25:ASP:OD2	3:C:88:ALA:HB2	1.85	0.76
4:D:401:ANP:N6	3:F:101:TYR:HD1	1.79	0.76
1:A:306:TYR:CE1	4:A:401:ANP:H2	2.22	0.75
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.69	0.74
3:F:95:ARG:HB3	3:F:96:PRO:HD3	1.69	0.73
1:D:238:LYS:HE2	3:F:105:GLU:CG	2.18	0.73
3:F:78:SER:O	3:F:80:GLY:N	2.21	0.72
3:C:79:GLY:HA2	3:C:81:ARG:HD2	1.69	0.72
1:D:240:TYR:HE1	1:D:242:LEU:CD1	2.04	0.71
2:E:42:GLY:CA	2:E:43:VAL:HB	2.21	0.70
3:C:122:LEU:HD12	1:D:41:GLN:HG2	1.74	0.70
1:D:187:ASP:OD1	1:D:206:ARG:NH2	2.25	0.69
2:B:26:ALA:HB1	3:C:132:SER:HB2	1.72	0.69
2:E:242:LEU:HB3	2:E:243:PRO:HD2	1.74	0.69
1:A:190:MET:HG3	1:A:209:VAL:HG21	1.74	0.69
2:E:43:VAL:O	2:E:43:VAL:HG13	1.92	0.68
2:E:48:GLY:O	2:E:49:GLN:HB2	1.93	0.67
1:D:306:TYR:CZ	4:D:401:ANP:H2	2.28	0.67
3:C:122:LEU:HB3	1:D:41:GLN:CB	2.22	0.67
2:E:337:TYR:HD2	3:F:135:LEU:HD13	1.60	0.66
3:F:121:THR:HA	3:F:124:LEU:HD12	1.78	0.65
2:E:242:LEU:HB3	2:E:243:PRO:CD	2.26	0.65
3:C:81:ARG:HG2	3:C:83:LYS:HG2	1.78	0.65
1:D:238:LYS:HE2	3:F:105:GLU:HG2	1.77	0.64
1:D:330:ILE:HA	3:F:97:LYS:HG3	1.79	0.64
2:B:210:ARG:HH12	3:C:144:GLY:N	1.95	0.63
1:A:335:ARG:HH22	3:C:100:SER:H	1.46	0.63
3:C:97:LYS:HD3	3:C:98:LYS:HD2	1.81	0.63
3:F:122:LEU:H	3:F:122:LEU:HD22	1.63	0.63
3:C:86:LYS:O	3:C:86:LYS:HG3	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:25:ASP:HB2	3:C:121:THR:HG22	1.81	0.62
2:E:42:GLY:HA2	2:E:43:VAL:HB	1.81	0.62
1:D:215:LYS:HD2	1:D:242:LEU:CD1	2.29	0.62
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.81	0.62
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.82	0.61
2:E:131:ALA:HB1	2:E:356:TRP:HB3	1.83	0.61
1:D:23:GLY:O	3:F:84:LEU:HB3	2.01	0.60
3:C:134:GLU:HB2	3:C:140:ASN:HB2	1.83	0.60
1:D:306:TYR:CE1	4:D:401:ANP:H2	2.37	0.60
1:A:44:MET:HB2	1:A:46:GLY:H	1.67	0.60
2:E:10:VAL:HB	2:E:105:LEU:HD23	1.83	0.60
3:C:137:SER:HB3	3:C:140:ASN:ND2	2.14	0.60
3:F:84:LEU:O	3:F:85:ARG:HB3	2.02	0.60
2:B:242:LEU:HB3	2:B:243:PRO:CD	2.31	0.60
3:F:81:ARG:H	3:F:81:ARG:HD2	1.67	0.60
1:A:321:ALA:HB1	1:A:322:PRO:CD	2.31	0.59
1:A:322:PRO:HG2	1:A:325:MET:HB2	1.85	0.59
3:F:97:LYS:HD3	3:F:98:LYS:HD2	1.83	0.59
2:E:257:CYS:HB3	2:E:258:PRO:HD3	1.85	0.59
2:E:330:ILE:HG22	2:E:332:PRO:HD3	1.84	0.59
1:D:238:LYS:HE2	3:F:105:GLU:HG3	1.84	0.58
1:A:97:ALA:HB1	1:A:99:GLU:OE2	2.03	0.58
1:A:323:SER:O	1:A:325:MET:N	2.32	0.58
1:D:244:ASP:O	1:D:246:GLN:N	2.36	0.57
4:D:401:ANP:N6	3:F:101:TYR:CE1	2.71	0.57
2:E:26:ALA:HB3	3:F:132:SER:HB2	1.86	0.57
2:E:205:GLU:HA	2:E:208:ILE:HD12	1.86	0.57
2:B:16:MET:CE	2:B:30:VAL:HG12	2.34	0.56
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.88	0.56
2:B:341:ILE:HD11	3:C:135:LEU:HD21	1.87	0.56
1:D:322:PRO:HG2	1:D:325:MET:HB2	1.88	0.55
2:E:233:SER:O	2:E:234:SER:CB	2.55	0.55
3:F:95:ARG:HB3	3:F:96:PRO:CD	2.35	0.55
2:E:42:GLY:N	2:E:43:VAL:HB	2.22	0.55
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.88	0.55
2:B:330:ILE:HG22	2:B:332:PRO:HD3	1.89	0.55
1:A:116:ARG:NH2	1:A:374:CYS:SG	2.80	0.54
2:B:257:CYS:HB3	2:B:258:PRO:HD3	1.89	0.54
1:D:230:ALA:HB2	1:D:236:LEU:HD12	1.88	0.54
1:D:321:ALA:HB1	1:D:322:PRO:HD2	1.90	0.54
3:F:79:GLY:HA3	3:F:83:LYS:HE2	1.89	0.54
1:D:240:TYR:HE1	1:D:242:LEU:HD12	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:240:TYR:CE1	1:D:242:LEU:CG	2.89	0.54
1:D:240:TYR:CE1	1:D:242:LEU:CD1	2.90	0.54
2:E:30:VAL:HG21	3:F:131:ALA:HB2	1.89	0.54
1:D:221:LEU:HD22	1:D:315:LYS:HD3	1.89	0.54
1:A:99:GLU:HA	1:A:128:ASN:O	2.08	0.53
3:F:86:LYS:HZ3	3:F:88:ALA:HB2	1.72	0.53
1:A:10:VAL:HB	1:A:105:LEU:HD23	1.91	0.53
2:E:335:ARG:HA	2:E:338:SER:OG	2.09	0.53
3:C:118:HIS:ND1	3:C:119:SER:O	2.32	0.53
1:A:15:GLY:H	4:A:401:ANP:HNB1	1.56	0.53
3:C:79:GLY:CA	3:C:81:ARG:HD2	2.37	0.53
3:C:122:LEU:H	3:C:122:LEU:HD22	1.74	0.53
1:A:23:GLY:O	3:C:85:ARG:HG2	2.08	0.53
1:D:334:GLU:HB2	3:F:89:GLU:OE2	2.09	0.53
2:E:50:LYS:O	2:E:52:SER:N	2.42	0.53
1:D:240:TYR:CE1	1:D:242:LEU:HD12	2.44	0.52
1:D:131:ALA:HB1	1:D:356:TRP:HB3	1.92	0.52
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.92	0.52
3:F:91:THR:HG22	3:F:92:SER:H	1.75	0.52
2:B:131:ALA:HB1	2:B:356:TRP:HB3	1.90	0.52
1:D:211:ASP:OD2	1:D:242:LEU:HD13	2.10	0.51
1:D:215:LYS:HD2	1:D:242:LEU:HD11	1.91	0.51
2:B:350:SER:HA	3:C:96:PRO:HG2	1.91	0.51
2:B:337:TYR:HD2	3:C:135:LEU:HD13	1.76	0.51
1:D:334:GLU:CB	3:F:89:GLU:OE2	2.59	0.51
2:E:12:ASN:H	2:E:12:ASN:ND2	2.09	0.51
1:D:139:VAL:HA	1:D:165:ILE:HD13	1.93	0.51
2:E:42:GLY:HA2	2:E:43:VAL:CB	2.41	0.50
2:B:26:ALA:HB3	3:C:132:SER:HB2	1.91	0.50
1:D:215:LYS:HD2	1:D:242:LEU:HD13	1.93	0.50
2:E:43:VAL:O	2:E:43:VAL:CG1	2.60	0.50
1:D:350:SER:HA	1:D:353:GLN:HG2	1.94	0.50
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.94	0.50
1:D:211:ASP:OD2	1:D:242:LEU:CD1	2.60	0.49
2:E:48:GLY:O	2:E:49:GLN:CB	2.60	0.49
1:D:335:ARG:HH22	3:F:99:PRO:HA	1.78	0.49
2:E:30:VAL:CG2	3:F:131:ALA:HB2	2.42	0.49
3:C:129:SER:HB2	3:C:132:SER:HB3	1.93	0.49
1:D:308:GLY:N	3:F:99:PRO:HB2	2.28	0.49
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.95	0.49
3:C:79:GLY:C	3:C:81:ARG:H	2.16	0.48
1:A:225:GLN:HE22	3:C:116:ARG:HB3	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:200:PHE:O	2:E:201:THR:HG23	2.13	0.48
1:A:194:THR:HA	1:A:198:TYR:O	2.13	0.48
3:F:86:LYS:HZ3	3:F:88:ALA:CB	2.27	0.48
2:B:322:LYS:HG2	2:B:322:LYS:H	1.28	0.48
2:E:233:SER:O	2:E:234:SER:HB3	2.14	0.48
2:B:16:MET:HE3	2:B:30:VAL:HG12	1.96	0.47
2:B:361:GLU:HB3	2:B:369:ILE:CD1	2.44	0.47
1:A:335:ARG:HH22	3:C:99:PRO:HA	1.78	0.47
2:E:45:VAL:HG23	2:E:46:GLY:H	1.80	0.47
1:D:136:ILE:HB	1:D:139:VAL:HG23	1.95	0.47
2:E:101:HIS:O	2:E:130:PRO:HD2	2.13	0.47
3:C:95:ARG:HB3	3:C:96:PRO:CD	2.39	0.47
3:F:85:ARG:O	3:F:86:LYS:HG3	2.15	0.47
1:D:25:ASP:HB3	3:F:84:LEU:HB2	1.97	0.47
1:D:311:ASP:OD2	2:E:350:SER:OG	2.28	0.47
2:E:12:ASN:HD22	2:E:12:ASN:H	1.63	0.47
1:A:333:PRO:HD3	3:C:98:LYS:HD3	1.97	0.46
2:B:102:PRO:HB3	2:B:131:ALA:HB3	1.96	0.46
2:E:86:TRP:HH2	2:E:119:MET:HG2	1.81	0.46
3:C:131:ALA:O	3:C:134:GLU:HG2	2.15	0.46
3:C:66:SER:HB3	3:C:69:SER:HB3	1.97	0.46
2:B:151:ILE:HG23	2:B:297:THR:HG23	1.98	0.46
1:D:24:ASP:HB2	1:D:340:TRP:HH2	1.81	0.46
1:A:72:GLU:OE2	1:A:72:GLU:HA	2.16	0.46
2:B:103:VAL:HG11	2:B:129:THR:HG21	1.97	0.46
1:A:164:PRO:HG2	1:A:174:ALA:HB3	1.96	0.46
2:B:242:LEU:CB	2:B:243:PRO:HD2	2.38	0.46
1:A:350:SER:HA	1:A:353:GLN:HG2	1.98	0.45
1:D:81:ASP:O	1:D:84:LYS:HB2	2.16	0.45
1:D:241:GLU:HA	1:D:245:GLY:O	2.15	0.45
1:A:164:PRO:HG2	1:A:174:ALA:CB	2.47	0.45
2:B:162:THR:HG21	2:B:278:THR:HA	1.98	0.45
3:C:85:ARG:O	3:C:86:LYS:HB3	2.17	0.45
1:D:123:MET:O	1:D:129:THR:HG23	2.15	0.45
1:D:334:GLU:HA	3:F:89:GLU:OE2	2.15	0.45
2:E:19:ALA:HB1	2:E:94:LEU:HD11	1.99	0.45
1:D:345:ILE:O	1:D:349:LEU:HG	2.17	0.45
1:A:33:SER:HB3	6:A:504:HOH:O	2.16	0.45
1:A:330:ILE:HA	3:C:97:LYS:HG3	1.98	0.45
3:F:90:GLN:NE2	3:F:90:GLN:HA	2.32	0.45
1:D:102:PRO:HB3	1:D:131:ALA:HB3	1.99	0.45
1:A:291:LYS:HE2	1:A:291:LYS:HB3	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:401:ANP:N6	3:C:101:TYR:CD1	2.82	0.45
2:E:297:THR:HB	2:E:329:ILE:HD13	1.99	0.45
1:A:275:HIS:CD2	1:A:316:GLU:HB3	2.52	0.45
1:A:46:GLY:C	1:A:47:MET:HG3	2.37	0.44
1:A:259:GLU:OE2	1:A:263:GLN:NE2	2.41	0.44
2:B:83:GLU:OE2	2:B:126:THR:HG21	2.17	0.44
1:D:97:ALA:O	1:D:100:GLU:HG2	2.17	0.44
1:D:335:ARG:HH22	3:F:100:SER:H	1.65	0.44
2:B:16:MET:HE2	2:B:30:VAL:HG12	1.98	0.44
1:D:303:THR:HG22	1:D:303:THR:O	2.16	0.44
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.99	0.44
1:D:332:PRO:HG2	1:D:335:ARG:HB3	1.98	0.44
1:D:20:GLY:HA3	1:D:340:TRP:HZ2	1.82	0.44
1:D:70:PRO:HG2	1:D:85:ILE:CD1	2.35	0.44
2:B:353:GLN:HB2	3:C:98:LYS:HG3	2.00	0.44
2:B:335:ARG:HA	2:B:338:SER:OG	2.18	0.44
2:B:26:ALA:HB1	3:C:132:SER:CB	2.44	0.44
2:B:194:THR:HA	2:B:198:TYR:O	2.17	0.44
2:E:306:TYR:CE1	4:E:401:ANP:H2	2.53	0.44
3:C:137:SER:O	3:C:139:ARG:N	2.51	0.43
1:A:259:GLU:OE1	1:A:312:ARG:NH2	2.51	0.43
1:D:212:ILE:HG23	1:D:216:LEU:HD12	2.00	0.43
1:A:335:ARG:NH2	3:C:99:PRO:HA	2.34	0.43
1:D:221:LEU:CD2	1:D:315:LYS:HD3	2.48	0.43
1:A:250:ILE:HG13	1:A:253:GLU:HB2	2.00	0.43
1:D:361:GLU:HB3	1:D:369:ILE:HD13	2.00	0.43
1:D:214:GLU:O	3:F:101:TYR:CD2	2.72	0.43
2:E:10:VAL:HB	2:E:105:LEU:CD2	2.48	0.43
2:B:99:GLU:HA	2:B:128:ASN:O	2.19	0.43
2:E:341:ILE:HD11	3:F:135:LEU:HD21	2.00	0.43
1:A:308:GLY:H	3:C:99:PRO:HB2	1.83	0.43
1:A:323:SER:C	1:A:325:MET:H	2.20	0.43
3:C:137:SER:CB	3:C:140:ASN:HD21	2.26	0.43
4:B:401:ANP:H5'2	3:C:145:ALA:CB	2.49	0.43
2:E:190:MET:HG3	2:E:209:VAL:HG21	2.01	0.43
2:E:294:TYR:CD2	2:E:325:MET:HG2	2.54	0.43
3:F:89:GLU:HG3	3:F:90:GLN:H	1.84	0.42
2:E:354:GLN:OE1	3:F:92:SER:HB3	2.20	0.42
1:A:154:ASP:OD1	1:A:300:SER:OG	2.29	0.42
1:A:171:LEU:HA	1:A:172:PRO:HD2	1.88	0.42
1:D:259:GLU:OE1	1:D:312:ARG:NH2	2.52	0.42
1:D:308:GLY:H	3:F:99:PRO:HB2	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:352:PHE:O	1:A:355:MET:HB2	2.20	0.42
2:B:130:PRO:HB2	3:C:93:GLU:HG2	2.02	0.42
2:E:99:GLU:HA	2:E:128:ASN:O	2.20	0.42
1:D:164:PRO:HG2	1:D:174:ALA:CB	2.50	0.42
2:B:353:GLN:NE2	3:C:96:PRO:HD2	2.35	0.42
2:E:99:GLU:H	2:E:99:GLU:CD	2.23	0.42
2:E:264:PRO:CB	2:E:271:ALA:HB3	2.50	0.42
1:A:167:GLU:HA	1:A:167:GLU:OE2	2.20	0.41
2:E:34:ILE:HG12	2:E:69:TYR:CE1	2.55	0.41
1:A:47:MET:SD	1:A:61:LYS:NZ	2.85	0.41
1:D:97:ALA:HA	1:D:98:PRO:HD3	1.90	0.41
1:A:68:LYS:HD2	1:A:81:ASP:OD2	2.20	0.41
3:F:72:MET:O	3:F:76:HIS:CD2	2.73	0.41
2:B:353:GLN:OE1	3:C:94:GLY:HA2	2.20	0.41
1:D:25:ASP:OD1	3:F:86:LYS:NZ	2.51	0.41
2:E:19:ALA:HB3	2:E:29:ALA:HB3	2.03	0.41
3:F:111:LEU:O	3:F:115:ILE:HG13	2.21	0.41
2:B:218:TYR:O	2:B:258:PRO:HG2	2.20	0.41
1:A:221:LEU:HD22	1:A:315:LYS:HD3	2.02	0.41
2:E:233:SER:OG	2:E:234:SER:N	2.53	0.41
2:E:323:SER:OG	2:E:324:THR:N	2.53	0.41
2:E:7:ALA:HB2	2:E:102:PRO:HG2	2.02	0.41
1:D:240:TYR:HE1	1:D:242:LEU:HG	1.80	0.41
2:B:350:SER:CA	3:C:96:PRO:HG2	2.51	0.41
2:E:345:ILE:O	2:E:349:LEU:HG	2.21	0.41
2:B:323:SER:O	2:B:325:MET:N	2.54	0.41
1:D:335:ARG:HA	1:D:338:SER:OG	2.21	0.41
2:E:41:GLN:C	2:E:43:VAL:HB	2.41	0.40
1:D:243:LYS:C	1:D:245:GLY:H	2.25	0.40
2:E:334:GLU:OE1	2:E:334:GLU:N	2.52	0.40
2:B:69:TYR:HA	2:B:70:PRO:HD3	1.91	0.40
1:D:180:LEU:HD11	1:D:261:LEU:HD23	2.04	0.40
1:D:10:VAL:HB	1:D:105:LEU:HD23	2.02	0.40
2:E:226:GLU:HB3	2:E:255:PHE:CE1	2.57	0.40
3:C:96:PRO:HB2	3:C:97:LYS:H	1.78	0.40
2:E:337:TYR:CD2	3:F:135:LEU:HD13	2.47	0.40
1:D:309:ILE:HG22	3:F:99:PRO:HB3	2.02	0.40
1:A:23:GLY:O	3:C:84:LEU:HB3	2.20	0.40
1:D:224:GLU:HA	1:D:224:GLU:OE1	2.20	0.40
1:A:254:ARG:NH2	3:C:109:SER:OG	2.50	0.40
1:D:91:TYR:O	1:D:95:ARG:HA	2.21	0.40
3:C:145:ALA:HA	3:C:146:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:42:GLY:CA	2:E:43:VAL:CB	2.94	0.40
1:D:299:LEU:HD12	1:D:331:ALA:HB2	2.02	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	369/384 (96%)	338 (92%)	22 (6%)	9 (2%)	9	34
1	D	369/384 (96%)	339 (92%)	22 (6%)	8 (2%)	10	37
2	B	369/384 (96%)	338 (92%)	28 (8%)	3 (1%)	27	67
2	E	369/384 (96%)	342 (93%)	21 (6%)	6 (2%)	14	46
3	C	79/171 (46%)	52 (66%)	19 (24%)	8 (10%)	1	2
3	F	73/171 (43%)	52 (71%)	13 (18%)	8 (11%)	1	2
All	All	1628/1878 (87%)	1461 (90%)	125 (8%)	42 (3%)	8	31

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLY
1	A	324	THR
3	C	77	SER
3	C	79	GLY
3	C	138	PHE
1	D	50	LYS
1	D	245	GLY
1	D	247	VAL
2	E	43	VAL
2	E	49	GLN
2	E	51	ASP
2	E	234	SER
3	F	79	GLY

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Mol	Chain	Res	Type
1	A	41	GLN
1	A	46	GLY
1	A	50	LYS
2	B	271	ALA
3	C	120	GLY
1	D	45	VAL
1	D	271	ALA
1	D	324	THR
2	E	45	VAL
3	F	120	GLY
1	A	271	ALA
3	C	86	LYS
3	C	96	PRO
3	C	132	SER
1	D	51	ASP
3	C	87	VAL
3	F	85	ARG
3	F	96	PRO
1	A	44	MET
2	E	201	THR
3	F	86	LYS
3	F	87	VAL
1	A	40	HIS
2	B	247	VAL
2	B	324	THR
3	F	102	VAL
1	A	321	ALA
1	D	43	VAL
3	F	95	ARG

### 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	313/326 (96%)	293 (94%)	20 (6%)	25	58
1	D	309/326 (95%)	296 (96%)	13 (4%)	40	79
2	B	312/325 (96%)	298 (96%)	14 (4%)	38	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	312/325 (96%)	300 (96%)	12 (4%)	44	82
3	C	63/138 (46%)	51 (81%)	12 (19%)	2	6
3	F	62/138 (45%)	56 (90%)	6 (10%)	12	34
All	All	1371/1578 (87%)	1294 (94%)	77 (6%)	30	66

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	33	SER
1	A	39	ARG
1	A	41	GLN
1	A	66	THR
1	A	103	VAL
1	A	118	LYS
1	A	152	VAL
1	A	180	LEU
1	A	201	THR
1	A	204	GLU
1	A	221	LEU
1	A	242	LEU
1	A	248	ILE
1	A	272	CYS
1	A	299	LEU
1	A	312	ARG
1	A	320	LEU
1	A	351	THR
1	A	355	MET
2	B	73	HIS
2	B	103	VAL
2	B	180	LEU
2	B	199	SER
2	B	201	THR
2	B	221	LEU
2	B	242	LEU
2	B	248	ILE
2	B	299	LEU
2	B	312	ARG
2	B	320	LEU
2	B	322	LYS
2	B	351	THR

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Mol	Chain	Res	Type
2	B	355	MET
3	C	81	ARG
3	C	85	ARG
3	C	95	ARG
3	C	103	GLU
3	C	105	GLU
3	C	119	SER
3	C	121	THR
3	C	122	LEU
3	C	127	VAL
3	C	132	SER
3	C	138	PHE
3	C	139	ARG
1	D	152	VAL
1	D	180	LEU
1	D	204	GLU
1	D	206	ARG
1	D	221	LEU
1	D	233	SER
1	D	248	ILE
1	D	249	THR
1	D	300	SER
1	D	312	ARG
1	D	314	GLN
1	D	320	LEU
1	D	351	THR
2	E	12	ASN
2	E	41	GLN
2	E	103	VAL
2	E	152	VAL
2	E	180	LEU
2	E	221	LEU
2	E	238	LYS
2	E	248	ILE
2	E	272	CYS
2	E	312	ARG
2	E	320	LEU
2	E	351	THR
3	F	81	ARG
3	F	86	LYS
3	F	90	GLN
3	F	95	ARG

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Mol	Chain	Res	Type
3	F	103	GLU
3	F	121	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	140	ASN
3	F	90	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ANP	A	401	5	33,33,33	3.44	7 (21%)	51,52,52	1.96	11 (21%)
4	ANP	B	401	5	33,33,33	3.27	6 (18%)	51,52,52	2.28	13 (25%)
4	ANP	D	401	5	33,33,33	3.49	6 (18%)	51,52,52	2.06	10 (19%)
4	ANP	E	401	5	33,33,33	3.33	6 (18%)	51,52,52	2.08	12 (23%)

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	ANP	A	401	5	-	0/18/38/38	0/1/3/3
4	ANP	B	401	5	-	0/18/38/38	0/1/3/3
4	ANP	D	401	5	-	0/18/38/38	0/1/3/3
4	ANP	E	401	5	-	0/18/38/38	0/1/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ANP	PG-N3B	12.84	1.75	1.64
4	A	401	ANP	PG-N3B	12.45	1.75	1.64
4	A	401	ANP	PB-N3B	12.31	1.75	1.64
4	D	401	ANP	PB-N3B	12.21	1.75	1.64
4	E	401	ANP	PG-N3B	11.99	1.74	1.64
4	B	401	ANP	PG-N3B	11.87	1.74	1.64
4	E	401	ANP	PB-N3B	11.79	1.74	1.64
4	B	401	ANP	PB-N3B	11.53	1.74	1.64
4	E	401	ANP	PG-O1G	5.17	1.52	1.46
4	D	401	ANP	PG-O1G	4.98	1.52	1.46
4	D	401	ANP	PB-O1B	4.59	1.51	1.46
4	E	401	ANP	PB-O1B	4.57	1.51	1.46
4	A	401	ANP	PB-O1B	4.48	1.51	1.46
4	B	401	ANP	PB-O1B	4.35	1.51	1.46
4	A	401	ANP	PG-O1G	4.26	1.51	1.46
4	B	401	ANP	PG-O1G	4.10	1.51	1.46
4	A	401	ANP	C5-C4	3.23	1.47	1.40
4	D	401	ANP	C5-C4	3.14	1.47	1.40
4	E	401	ANP	C4-N9	-3.13	1.33	1.37
4	B	401	ANP	C5-C4	3.11	1.47	1.40
4	B	401	ANP	C4-N9	-3.03	1.33	1.37
4	E	401	ANP	C5-C4	2.94	1.47	1.40
4	D	401	ANP	C4-N9	-2.84	1.33	1.37
4	A	401	ANP	C4-N9	-2.52	1.34	1.37
4	A	401	ANP	PB-O3A	2.52	1.62	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ANP	PB-N3B-PG	-8.37	115.99	130.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	401	ANP	N3-C2-N1	-6.36	123.39	128.71
4	B	401	ANP	N3-C2-N1	-6.25	123.48	128.71
4	E	401	ANP	PB-N3B-PG	-6.08	119.85	130.07
4	D	401	ANP	N3-C2-N1	-6.04	123.66	128.71
4	D	401	ANP	PB-N3B-PG	-6.04	119.91	130.07
4	B	401	ANP	O1G-PG-N3B	-5.97	102.81	111.83
4	D	401	ANP	O1G-PG-N3B	-5.77	103.11	111.83
4	D	401	ANP	N3-C4-N9	5.62	135.58	125.43
4	A	401	ANP	O1G-PG-N3B	-5.55	103.44	111.83
4	A	401	ANP	N3-C2-N1	-5.41	124.18	128.71
4	E	401	ANP	O1G-PG-N3B	-5.40	103.68	111.83
4	A	401	ANP	PB-N3B-PG	-5.29	121.17	130.07
4	E	401	ANP	N3-C4-N9	5.03	134.51	125.43
4	B	401	ANP	N3-C4-N9	4.93	134.33	125.43
4	A	401	ANP	N3-C4-N9	4.81	134.11	125.43
4	B	401	ANP	O2B-PB-O1B	4.11	119.38	109.89
4	A	401	ANP	C4-C5-N7	-3.94	106.15	109.52
4	D	401	ANP	O2B-PB-O1B	3.64	118.29	109.89
4	E	401	ANP	PA-O3A-PB	-3.63	119.41	131.81
4	E	401	ANP	O2B-PB-O1B	3.48	117.92	109.89
4	D	401	ANP	C8-N9-C4	3.34	109.45	106.90
4	B	401	ANP	C4-C5-N7	-3.30	106.69	109.52
4	A	401	ANP	C5-C4-N3	-3.00	119.16	125.70
4	E	401	ANP	C5-C4-N3	-2.98	119.20	125.70
4	D	401	ANP	C5-C4-N3	-2.95	119.28	125.70
4	A	401	ANP	O2B-PB-O1B	2.92	116.63	109.89
4	E	401	ANP	C4-C5-N7	-2.85	107.08	109.52
4	B	401	ANP	PA-O3A-PB	-2.82	122.17	131.81
4	B	401	ANP	C5-C4-N3	-2.80	119.60	125.70
4	B	401	ANP	C8-N9-C4	2.79	109.03	106.90
4	E	401	ANP	O4'-C1'-N9	2.70	110.95	108.44
4	A	401	ANP	C1'-N9-C4	-2.60	122.15	126.64
4	B	401	ANP	O4'-C1'-N9	2.51	110.77	108.44
4	A	401	ANP	O4'-C1'-N9	2.49	110.76	108.44
4	E	401	ANP	C2-N3-C4	2.37	120.76	114.01
4	D	401	ANP	PA-O3A-PB	-2.36	123.74	131.81
4	D	401	ANP	C2-N3-C4	2.34	120.68	114.01
4	A	401	ANP	C2-N3-C4	2.31	120.59	114.01
4	A	401	ANP	C8-N9-C4	2.26	108.63	106.90
4	B	401	ANP	O1B-PB-N3B	-2.18	108.53	111.83
4	B	401	ANP	C2-N3-C4	2.16	120.16	114.01
4	E	401	ANP	O3G-PG-O2G	2.09	113.67	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	401	ANP	C3'-C2'-C1'	2.08	104.16	100.91
4	B	401	ANP	C1'-N9-C4	-2.05	123.09	126.64
4	D	401	ANP	C4-C5-N7	-2.01	107.80	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	371/384 (96%)	-0.15	11 (2%)	48	57	34, 47, 85, 110	0
1	D	371/384 (96%)	0.30	35 (9%)	9	11	34, 62, 121, 130	0
2	B	371/384 (96%)	-0.12	5 (1%)	74	82	32, 55, 87, 119	0
2	E	371/384 (96%)	0.23	21 (5%)	23	28	40, 78, 118, 132	0
3	C	81/171 (47%)	1.43	26 (32%)	1	1	40, 76, 117, 142	0
3	F	75/171 (43%)	1.29	23 (30%)	1	1	41, 91, 124, 141	0
All	All	1640/1878 (87%)	0.19	121 (7%)	15	17	32, 61, 115, 142	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	GLY	11.3
1	D	46	GLY	10.0
1	D	43	VAL	9.2
3	C	92	SER	8.7
1	D	45	VAL	8.3
3	C	88	ALA	8.1
3	C	96	PRO	8.0
3	F	94	GLY	7.8
3	F	91	THR	7.6
1	D	47	MET	7.5
3	C	87	VAL	7.1
3	F	101	TYR	6.3
3	C	146	PRO	6.3
1	A	48	GLY	6.3
1	A	45	VAL	6.3
3	F	89	GLU	6.2
3	C	89	GLU	6.2
3	C	91	THR	6.0
3	F	102	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	46	GLY	5.9
1	D	44	MET	5.8
2	E	249	THR	5.7
1	A	49	GLN	5.7
3	C	94	GLY	5.6
3	C	101	TYR	5.5
2	E	251	GLY	5.4
2	E	250	ILE	5.3
3	F	96	PRO	5.2
1	D	53	TYR	5.2
3	F	88	ALA	5.1
2	B	45	VAL	5.0
1	D	67	LEU	5.0
1	D	41	GLN	4.8
3	F	87	VAL	4.7
1	D	40	HIS	4.6
2	E	244	ASP	4.6
2	E	48	GLY	4.4
1	A	47	MET	4.3
2	E	49	GLN	4.3
3	C	145	ALA	4.2
1	A	44	MET	4.1
2	B	49	GLN	3.9
3	F	98	LYS	3.9
3	F	92	SER	3.7
1	D	95	ARG	3.7
3	C	140	ASN	3.6
2	E	242	LEU	3.6
3	C	90	GLN	3.6
1	D	69	TYR	3.5
1	A	248	ILE	3.5
1	D	48	GLY	3.5
3	C	102	VAL	3.5
1	A	247	VAL	3.4
1	A	245	GLY	3.4
3	F	95	ARG	3.4
2	E	45	VAL	3.4
3	C	99	PRO	3.3
3	C	135	LEU	3.3
3	C	93	GLU	3.2
3	C	139	ARG	3.2
1	D	100	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	90	GLN	3.1
1	D	94	LEU	3.1
1	D	130	PRO	3.1
2	E	324	THR	3.1
1	D	240	TYR	3.1
3	F	97	LYS	3.0
2	E	240	TYR	3.0
2	E	216	LEU	3.0
3	F	138	PHE	3.0
1	D	6	ALA	2.9
3	C	144	GLY	2.9
3	F	99	PRO	2.9
1	D	364	GLU	2.9
3	C	142	ALA	2.9
1	D	21	PHE	2.9
2	E	243	PRO	2.9
1	D	366	GLY	2.9
1	D	369	ILE	2.8
3	F	80	GLY	2.7
1	A	242	LEU	2.7
3	C	97	LYS	2.7
1	D	86	TRP	2.7
3	F	93	GLU	2.7
2	E	236	LEU	2.7
1	A	46	GLY	2.7
2	E	200	PHE	2.6
1	A	375	PHE	2.5
3	C	103	GLU	2.5
3	C	141	ALA	2.5
1	D	96	VAL	2.5
1	D	131	ALA	2.5
2	E	209	VAL	2.5
3	C	131	ALA	2.4
3	F	139	ARG	2.4
1	D	201	THR	2.4
3	C	95	ARG	2.4
1	D	49	GLN	2.4
3	F	133	GLU	2.4
3	F	77	SER	2.4
1	D	34	ILE	2.4
1	D	64	ILE	2.4
3	F	103	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	39	ARG	2.3
1	D	8	LEU	2.3
2	E	50	LYS	2.3
3	F	100	SER	2.2
2	E	253	GLU	2.2
1	D	372	ARG	2.2
3	F	81	ARG	2.2
1	D	54	VAL	2.2
2	B	200	PHE	2.2
2	B	43	VAL	2.2
2	E	247	VAL	2.2
2	E	208	ILE	2.1
3	C	80	GLY	2.1
2	E	221	LEU	2.1
1	D	374	CYS	2.1
2	E	235	SER	2.1
3	C	98	LYS	2.0
1	D	90	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	D	402	1/1	0.46	15.63	69,69,69,69	0
5	MG	E	402	1/1	0.48	13.27	67,67,67,67	0
5	MG	A	402	1/1	0.37	11.53	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	402	1/1	0.40	8.92	53,53,53,53	0
4	ANP	E	401	31/31	0.20	-0.27	68,79,85,90	0
4	ANP	A	401	31/31	0.15	-0.36	56,65,76,77	0
4	ANP	B	401	31/31	0.14	-0.68	49,56,62,63	0
4	ANP	D	401	31/31	0.10	-0.92	54,63,85,103	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.