



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:31 am GMT

PDB ID : 3WQT  
Title : Staphylococcus aureus FtsA complexed with AMPPNP  
Authors : Fujita, J.; Maeda, Y.; Miyazaki, Y.; Inoue, T.; Matsumura, H.  
Deposited on : 2014-02-01  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

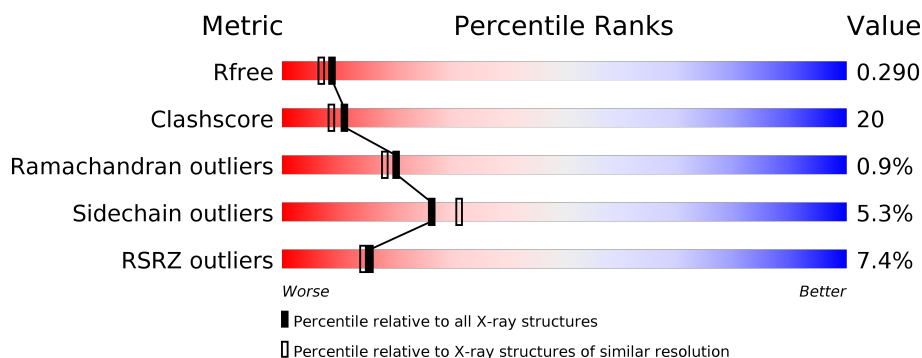
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	484	<div> <div> <div></div> <div>57%</div> <div>18%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	484	<div> <div>12%</div> <div>36%</div> <div>31%</div> <div>•</div> <div>31%</div> </div>
1	C	484	<div> <div> <div></div> <div>52%</div> <div>21%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	484	<div> <div>7%</div> <div>42%</div> <div>28%</div> <div>•</div> <div>27%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11614 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 Cell division protein FtsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2871	1811	458	595	7			
1	B	334	Total	C	N	O	S	0	0	0
			2590	1640	412	532	6			
1	C	368	Total	C	N	O	S	0	0	0
			2853	1801	453	592	7			
1	D	352	Total	C	N	O	S	0	0	0
			2733	1729	434	563	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
A	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
A	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0
A	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
A	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
A	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
A	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
A	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0
A	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
B	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
B	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
B	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
B	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
B	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
B	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0
B	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
C	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
C	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0
C	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
C	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
C	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
C	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
C	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0
C	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-15	MET	-	EXPRESSION TAG	UNP Q6GHQ0
D	-14	ASN	-	EXPRESSION TAG	UNP Q6GHQ0
D	-13	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-12	LYS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-11	VAL	-	EXPRESSION TAG	UNP Q6GHQ0
D	-10	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-9	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-8	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-7	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-6	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-5	HIS	-	EXPRESSION TAG	UNP Q6GHQ0
D	-4	ILE	-	EXPRESSION TAG	UNP Q6GHQ0
D	-3	GLU	-	EXPRESSION TAG	UNP Q6GHQ0
D	-2	GLY	-	EXPRESSION TAG	UNP Q6GHQ0
D	-1	ARG	-	EXPRESSION TAG	UNP Q6GHQ0

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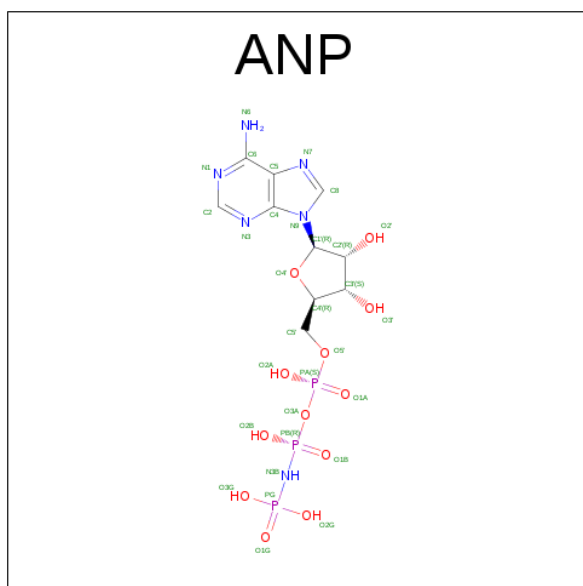
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP Q6GHQ0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

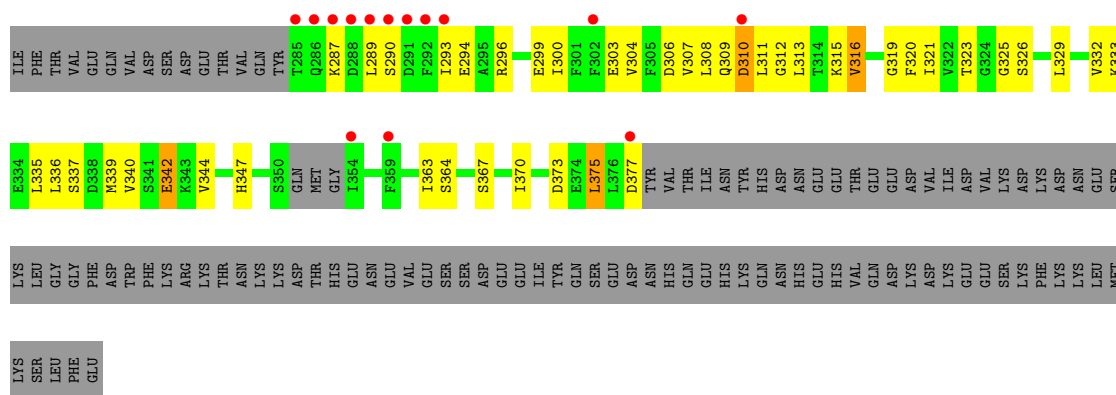
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	A	2	Total 2	Cl 2	0	0
4	D	2	Total 2	Cl 2	0	0
4	C	4	Total 4	Cl 4	0	0

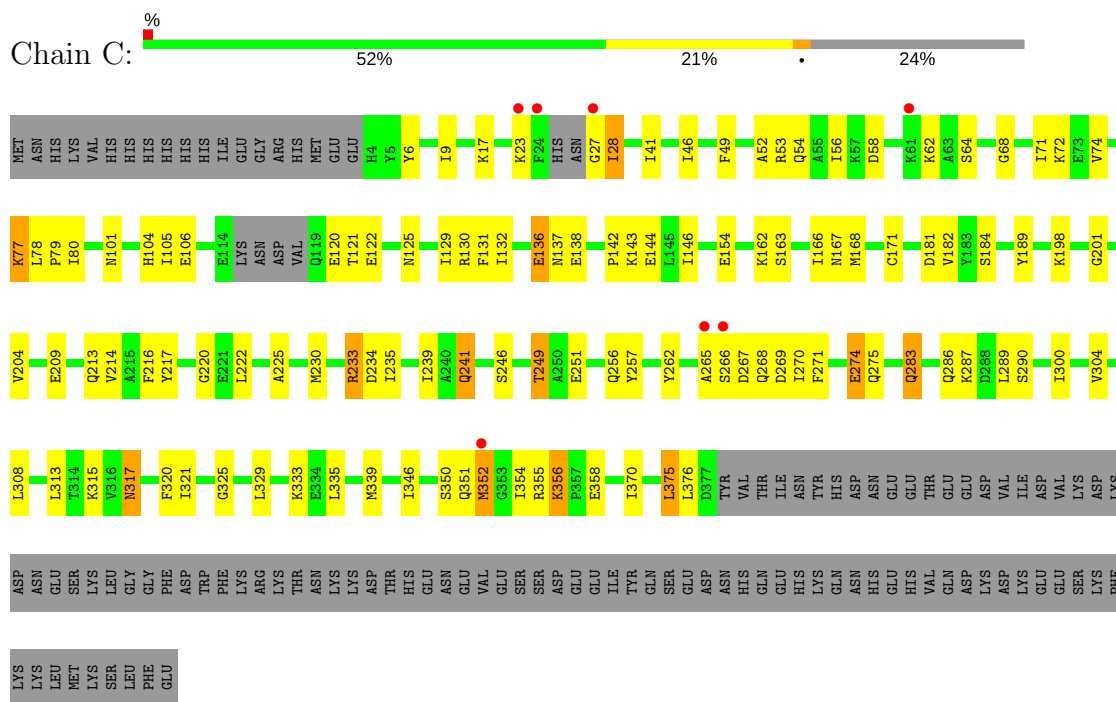
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0
5	B	49	Total 49	O 49	0	0
5	C	158	Total 158	O 158	0	0
5	D	85	Total 85	O 85	0	0

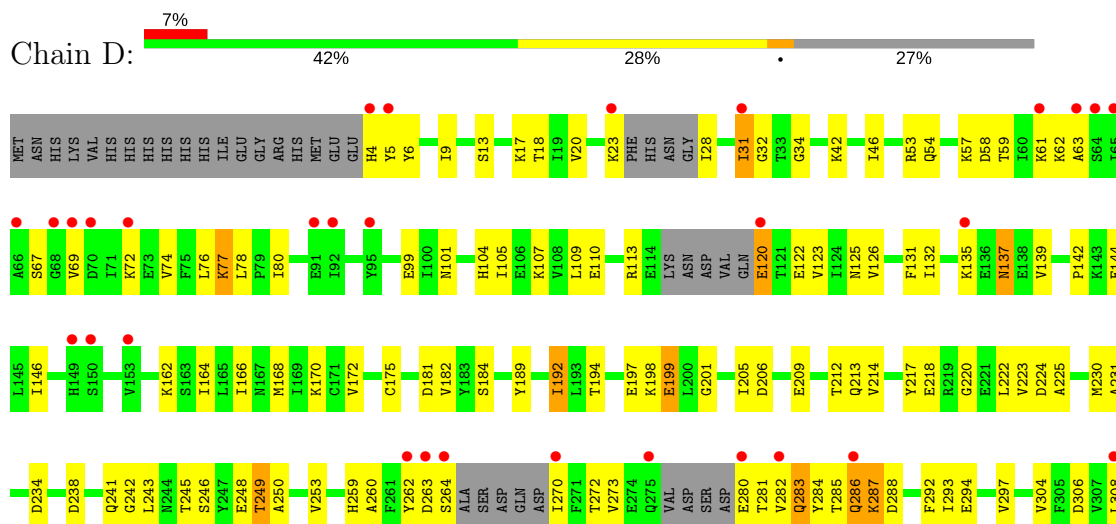




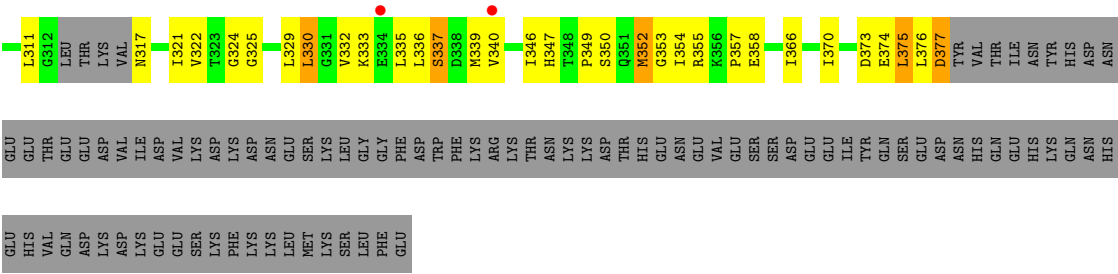
• Molecule 1: Cell division protein FtsA



• Molecule 1: Cell division protein FtsA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.26Å 102.74Å 105.86Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	37.98 – 2.20 37.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (37.98-2.20) 92.4 (37.98-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.234 , 0.289 0.234 , 0.290	Depositor DCC
$R_{free}$ test set	3818 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.39	0/2910	0.64	0/3935
1	B	0.31	0/2619	0.55	0/3535
1	C	0.39	0/2890	0.63	0/3906
1	D	0.34	0/2766	0.62	0/3733
All	All	0.36	0/11185	0.61	0/15109

There are no bond length outliers.

There are no bond angle outliers.

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	2871	0	2813	70	0
1	B	2590	0	2567	152	0
1	C	2853	0	2799	99	0
1	D	2733	0	2688	133	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	6	0
3	C	31	0	13	2	0
3	D	31	0	13	3	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0
4	C	4	0	0	1	0
4	D	2	0	0	1	0
5	A	136	0	0	2	0
5	B	49	0	0	7	0
5	C	158	0	0	7	0
5	D	85	0	0	7	0
All	All	11614	0	10919	444	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 20.

All (444) 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:317:ASN:HD22	1:C:317:ASN:H	1.05	1.01
1:C:101:ASN:H	1:C:104:HIS:HD2	1.13	0.95
1:D:101:ASN:H	1:D:104:HIS:HD2	1.15	0.93
1:A:329:LEU:HD13	3:A:503:ANP:H2	1.54	0.89
1:B:213:GLN:HB2	5:B:649:HOH:O	1.73	0.87
1:D:17:LYS:HE2	1:D:358:GLU:HB2	1.56	0.87
4:C:504:CL:CL	5:C:680:HOH:O	2.30	0.85
1:C:265:ALA:HB3	1:C:287:LYS:HG2	1.57	0.84
1:B:167:ASN:HB3	5:B:647:HOH:O	1.78	0.83
1:A:80:ILE:H	1:A:213:GLN:NE2	1.77	0.83
1:D:58:ASP:O	1:D:62:LYS:HG2	1.79	0.83
1:A:142:PRO:O	1:A:145:LEU:HD22	1.81	0.81
1:D:352:MET:HA	1:D:355:ARG:HG3	1.63	0.81
1:B:61:LYS:O	1:B:65:ILE:HG13	1.81	0.81
1:A:314:THR:HG23	5:A:706:HOH:O	1.79	0.81
1:C:130:ARG:HD2	1:C:138:GLU:OE1	1.81	0.80
1:C:317:ASN:H	1:C:317:ASN:ND2	1.80	0.80
1:A:246:SER:OG	1:A:249:THR:HG22	1.82	0.79
1:D:101:ASN:H	1:D:104:HIS:CD2	1.98	0.79
1:A:125:ASN:HD21	1:A:184:SER:H	1.31	0.78
4:D:504:CL:CL	5:D:673:HOH:O	2.37	0.78
1:C:80:ILE:H	1:C:213:GLN:NE2	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LEU:HD13	3:D:503:ANP:H2	1.66	0.77
1:C:246:SER:OG	1:C:249:THR:HG23	1.85	0.76
1:D:32:GLY:HA3	1:D:67:SER:HB3	1.67	0.76
1:C:130:ARG:NH2	1:C:130:ARG:HB2	2.01	0.75
1:C:198:LYS:HB3	1:C:220:GLY:HA2	1.69	0.75
1:B:88:GLU:HG2	1:B:112:ILE:HG23	1.70	0.74
1:D:101:ASN:N	1:D:104:HIS:HD2	1.86	0.73
1:B:101:ASN:H	1:B:104:HIS:HD2	1.37	0.73
1:B:309:GLN:HG3	1:C:27:GLY:HA2	1.70	0.72
1:D:53:ARG:NH2	1:D:54:GLN:HE21	1.87	0.72
1:B:7:VAL:HG22	1:B:20:VAL:HG22	1.70	0.72
1:D:352:MET:SD	1:D:353:GLY:N	2.62	0.72
1:A:352:MET:HA	1:A:355:ARG:HE	1.55	0.71
1:D:242:GLY:HA3	1:D:292:PHE:CZ	2.26	0.71
1:D:246:SER:OG	1:D:249:THR:HG22	1.90	0.71
1:B:80:ILE:H	1:B:213:GLN:NE2	1.88	0.70
1:C:17:LYS:HE2	1:C:358:GLU:HB2	1.74	0.70
1:D:336:LEU:O	1:D:340:VAL:HG22	1.91	0.70
1:D:4:HIS:CG	1:D:5:TYR:H	2.08	0.70
1:A:245:THR:OG1	1:A:249:THR:HG21	1.93	0.69
1:D:270:ILE:HD12	1:D:270:ILE:N	2.07	0.69
1:C:335:LEU:HG	1:C:339:MET:CE	2.22	0.69
1:C:125:ASN:HD21	1:C:184:SER:H	1.39	0.69
1:B:80:ILE:H	1:B:213:GLN:HE22	1.39	0.69
1:D:241:GLN:HG3	5:D:676:HOH:O	1.92	0.69
1:C:335:LEU:HG	1:C:339:MET:HE2	1.75	0.68
1:C:41:ILE:HD13	1:C:46:ILE:HA	1.73	0.68
1:A:335:LEU:HG	1:A:339:MET:CE	2.23	0.68
1:A:101:ASN:H	1:A:104:HIS:HD2	1.41	0.68
1:D:168:MET:O	1:D:172:VAL:HG23	1.95	0.67
1:B:52:ALA:O	1:B:56:ILE:HG13	1.95	0.67
1:A:77:LYS:HD2	1:A:77:LYS:C	2.15	0.66
1:A:23:LYS:HD3	1:A:370:ILE:HG23	1.78	0.65
1:B:43:ASN:N	1:B:43:ASN:HD22	1.93	0.65
1:D:6:TYR:CE2	1:D:370:ILE:HG12	2.32	0.65
1:A:335:LEU:HG	1:A:339:MET:HE3	1.79	0.65
1:B:49:PHE:CE2	1:B:170:LYS:HE3	2.32	0.64
1:B:183:TYR:HB3	1:B:188:ASN:HD21	1.63	0.64
1:B:46:ILE:HD11	1:B:168:MET:HG3	1.80	0.64
1:C:120:GLU:HG3	1:C:121:THR:HG23	1.78	0.64
1:D:120:GLU:O	1:D:162:LYS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:HE2	1:D:61:LYS:NZ	2.12	0.63
1:C:267:ASP:HB2	1:C:287:LYS:HE2	1.80	0.63
1:C:71:ILE:O	1:C:72:LYS:HD2	1.98	0.63
1:D:352:MET:HB2	1:D:355:ARG:CZ	2.29	0.63
1:D:53:ARG:NH2	1:D:54:GLN:HG2	2.14	0.63
1:B:210:ASP:OD1	1:B:233:ARG:HD3	1.98	0.63
1:D:262:TYR:HB2	1:D:294:GLU:OE2	1.99	0.63
1:B:307:VAL:HA	1:B:310:ASP:OD2	1.99	0.62
1:B:73:GLU:HB3	1:B:180:LEU:HD21	1.82	0.62
1:A:244:ASN:HD22	1:A:275:GLN:NE2	1.98	0.61
1:D:125:ASN:HD21	1:D:184:SER:H	1.47	0.61
1:D:270:ILE:HA	1:D:285:THR:HA	1.82	0.61
1:D:105:ILE:HG21	1:D:375:LEU:CD2	2.30	0.61
1:B:189:TYR:HB2	1:B:217:TYR:OH	2.00	0.61
1:B:196:THR:HG22	1:B:200:LEU:HD12	1.82	0.61
1:B:293:ILE:CG2	1:B:329:LEU:HD21	2.31	0.61
1:C:274:GLU:HG2	1:C:275:GLN:N	2.14	0.61
1:D:262:TYR:O	1:D:287:LYS:HE3	1.99	0.61
1:D:373:ASP:O	1:D:377:ASP:HB2	2.00	0.61
1:B:234:ASP:HB3	1:B:296:ARG:HH21	1.65	0.61
1:D:18:THR:HB	1:D:59:THR:HG22	1.81	0.61
1:C:266:SER:OG	1:C:286:GLN:HB3	2.02	0.60
1:C:315:LYS:HE3	1:C:317:ASN:HD21	1.65	0.60
1:D:125:ASN:ND2	1:D:184:SER:H	2.00	0.60
1:B:92:ILE:HG22	1:B:151:LEU:HB3	1.81	0.60
1:B:333:LYS:HE3	1:B:344:VAL:O	2.01	0.60
1:B:64:SER:HB2	1:B:71:ILE:HD13	1.83	0.60
1:C:46:ILE:HG13	5:C:680:HOH:O	2.02	0.60
1:B:6:TYR:CZ	1:B:370:ILE:HG12	2.37	0.60
1:A:189:TYR:HB2	1:A:217:TYR:OH	2.02	0.60
1:D:262:TYR:C	1:D:264:SER:H	2.05	0.60
1:B:216:PHE:HB3	1:B:313:LEU:HD13	1.83	0.60
1:D:6:TYR:CZ	1:D:370:ILE:HG12	2.37	0.59
1:B:13:SER:N	3:B:502:ANP:HNB1	1.99	0.59
1:D:285:THR:OG1	1:D:288:ASP:HB2	2.02	0.59
1:B:320:PHE:CE2	1:B:340:VAL:HG21	2.36	0.59
1:B:197:GLU:HB3	1:B:202:ALA:HB2	1.83	0.59
1:C:235:ILE:O	1:C:239:ILE:HG13	2.01	0.59
1:A:112:ILE:C	1:A:114:GLU:H	2.05	0.59
1:A:352:MET:O	1:A:352:MET:SD	2.61	0.59
1:C:329:LEU:HD13	3:C:502:ANP:H2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LYS:HD3	5:D:640:HOH:O	2.02	0.59
1:B:122:GLU:HB2	1:B:162:LYS:HG2	1.83	0.59
1:C:241:GLN:HG2	5:C:685:HOH:O	2.02	0.59
1:B:194:THR:OG1	1:B:197:GLU:HG3	2.03	0.59
1:C:317:ASN:HD22	1:C:317:ASN:N	1.87	0.59
1:B:312:GLY:HA3	1:C:350:SER:HB2	1.83	0.59
1:D:280:GLU:HG2	1:D:281:THR:H	1.68	0.59
1:B:309:GLN:CG	1:C:27:GLY:HA2	2.33	0.58
1:B:335:LEU:HG	1:B:339:MET:CE	2.33	0.58
1:B:206:ASP:HB3	5:B:649:HOH:O	2.03	0.58
1:D:31:ILE:HD13	1:D:31:ILE:H	1.69	0.58
1:D:57:LYS:HE2	1:D:61:LYS:HZ3	1.69	0.58
1:B:188:ASN:HB3	1:B:364:SER:OG	2.03	0.58
1:D:72:LYS:NZ	1:D:72:LYS:HB2	2.18	0.58
1:B:179:VAL:HG23	1:B:179:VAL:O	2.04	0.58
1:D:242:GLY:O	1:D:243:LEU:HD23	2.04	0.58
1:D:245:THR:HG21	1:D:273:VAL:HG21	1.86	0.58
1:D:280:GLU:HG2	1:D:281:THR:N	2.19	0.58
1:A:352:MET:HB3	1:A:355:ARG:HH21	1.69	0.57
1:B:207:ILE:HB	1:B:326:SER:HB2	1.85	0.57
1:D:250:ALA:O	1:D:253:VAL:HG22	2.03	0.57
1:B:46:ILE:HD12	5:B:647:HOH:O	2.02	0.57
1:C:125:ASN:ND2	1:C:184:SER:H	2.01	0.57
1:A:60:ILE:HD13	1:A:177:VAL:HG11	1.85	0.57
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.69	0.57
1:D:109:LEU:HD22	1:D:126:VAL:HG12	1.87	0.57
1:B:168:MET:O	1:B:172:VAL:HG23	2.04	0.57
1:A:125:ASN:ND2	1:A:184:SER:H	2.01	0.57
1:D:105:ILE:HD11	1:D:142:PRO:HG2	1.87	0.57
1:B:172:VAL:O	1:B:177:VAL:HG12	2.05	0.56
1:D:282:VAL:HG12	1:D:283:GLN:N	2.21	0.56
1:D:321:ILE:N	1:D:321:ILE:HD12	2.21	0.56
1:B:127:PHE:CE2	1:B:129:ILE:HD11	2.40	0.56
1:C:49:PHE:CZ	1:C:171:CYS:HA	2.41	0.56
1:D:53:ARG:HG2	1:D:175:CYS:SG	2.46	0.56
1:A:326:SER:O	1:A:329:LEU:HB2	2.05	0.56
1:A:17:LYS:HE3	1:A:358:GLU:O	2.06	0.56
1:C:130:ARG:HH21	1:C:130:ARG:HB2	1.70	0.56
1:A:316:VAL:HB	1:A:342:GLU:OE1	2.05	0.55
1:A:320:PHE:CE2	1:A:340:VAL:HG21	2.41	0.55
1:D:201:GLY:HA2	1:D:218:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:PHE:CD1	1:B:313:LEU:HD13	2.42	0.55
1:A:324:GLY:O	1:A:357:PRO:HB2	2.05	0.55
1:B:122:GLU:OE2	1:B:162:LYS:HE3	2.07	0.55
1:C:266:SER:O	1:C:267:ASP:HB3	2.07	0.55
1:D:370:ILE:O	1:D:374:GLU:HG3	2.05	0.55
1:D:4:HIS:CD2	1:D:5:TYR:H	2.24	0.55
1:B:167:ASN:N	1:B:167:ASN:HD22	2.04	0.55
1:B:70:ASP:O	1:B:72:LYS:HE2	2.07	0.55
1:D:166:ILE:O	1:D:170:LYS:HB2	2.07	0.55
1:D:105:ILE:HG21	1:D:375:LEU:HD22	1.88	0.55
1:B:194:THR:O	1:B:198:LYS:HG3	2.07	0.54
1:B:129:ILE:HB	1:B:154:GLU:O	2.08	0.54
1:B:209:GLU:CG	1:B:233:ARG:HB2	2.37	0.54
1:D:262:TYR:O	1:D:264:SER:N	2.37	0.54
1:D:325:GLY:HA3	3:D:503:ANP:O5'	2.07	0.54
1:C:189:TYR:HB2	1:C:217:TYR:OH	2.08	0.54
1:A:133:VAL:HG21	1:A:145:LEU:HD21	1.89	0.54
1:B:321:ILE:N	1:B:321:ILE:HD12	2.23	0.54
1:B:77:LYS:HD3	1:B:77:LYS:O	2.08	0.54
1:D:214:VAL:HG21	1:D:304:VAL:HG13	1.90	0.54
1:B:78:LEU:HG	1:B:182:VAL:CG2	2.37	0.54
1:B:196:THR:HG22	1:B:200:LEU:CD1	2.38	0.54
1:C:101:ASN:H	1:C:104:HIS:CD2	2.06	0.54
1:C:131:PHE:CD2	1:C:142:PRO:HD3	2.43	0.54
1:A:78:LEU:HD12	1:A:182:VAL:CG1	2.38	0.54
1:D:260:ALA:O	1:D:294:GLU:HB2	2.08	0.54
1:C:230:MET:HA	1:C:234:ASP:OD2	2.08	0.53
1:B:92:ILE:HD13	1:B:93:ASP:N	2.23	0.53
1:D:222:LEU:HD23	1:D:223:VAL:N	2.24	0.53
1:C:122:GLU:HB2	1:C:162:LYS:HD3	1.91	0.53
1:D:375:LEU:HD13	1:D:376:LEU:CD1	2.39	0.53
1:B:315:LYS:CB	1:C:352:MET:HG2	2.39	0.53
1:B:335:LEU:HG	1:B:339:MET:HE2	1.91	0.53
1:A:170:LYS:NZ	1:B:99:GLU:OE2	2.33	0.53
1:D:249:THR:O	1:D:253:VAL:HG13	2.07	0.53
1:D:99:GLU:CG	1:D:144:GLU:HA	2.38	0.53
1:B:315:LYS:HB2	1:C:352:MET:HG2	1.90	0.53
1:D:201:GLY:HA2	1:D:217:TYR:O	2.08	0.53
1:A:146:ILE:N	1:A:146:ILE:HD12	2.23	0.53
1:B:201:GLY:HA2	1:B:217:TYR:O	2.09	0.53
1:B:90:ASN:HB2	1:B:112:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HE3	1:B:61:LYS:HE3	1.91	0.52
1:B:101:ASN:N	1:B:104:HIS:HD2	2.07	0.52
1:D:248:GLU:H	1:D:248:GLU:CD	2.11	0.52
1:D:346:ILE:N	1:D:346:ILE:HD12	2.25	0.52
1:B:76:LEU:HD22	1:B:172:VAL:HG21	1.90	0.52
1:B:10:ASP:O	1:B:16:VAL:HA	2.09	0.52
1:D:350:SER:O	1:D:355:ARG:NH1	2.42	0.52
1:B:335:LEU:O	1:B:339:MET:HE2	2.09	0.52
1:C:49:PHE:CD1	1:D:144:GLU:HG3	2.45	0.52
1:B:112:ILE:C	1:B:114:GLU:H	2.12	0.52
1:B:150:SER:HB3	5:B:645:HOH:O	2.10	0.52
1:B:308:LEU:HB3	1:B:313:LEU:O	2.09	0.51
1:B:57:LYS:HE3	1:B:61:LYS:CE	2.39	0.51
1:D:304:VAL:O	1:D:308:LEU:HG	2.09	0.51
1:A:242:GLY:HA3	1:A:292:PHE:CZ	2.45	0.51
1:B:46:ILE:CD1	1:B:168:MET:HG3	2.41	0.51
1:A:333:LYS:HB2	1:A:346:ILE:CD1	2.40	0.51
1:A:242:GLY:HA3	1:A:292:PHE:CE1	2.45	0.51
1:B:13:SER:N	3:B:502:ANP:N3B	2.58	0.51
1:B:209:GLU:HG3	1:B:233:ARG:HB2	1.93	0.51
1:C:168:MET:HE3	5:C:754:HOH:O	2.09	0.51
1:D:107:LYS:O	1:D:110:GLU:HG2	2.10	0.51
1:C:9:ILE:HD12	1:C:74:VAL:HG21	1.93	0.51
1:B:240:ALA:HA	1:B:245:THR:HG23	1.93	0.51
1:B:261:PHE:HA	1:B:294:GLU:OE2	2.11	0.51
1:B:71:ILE:HD12	1:B:71:ILE:N	2.26	0.51
1:C:143:LYS:O	1:C:144:GLU:HB2	2.09	0.51
1:A:78:LEU:HD12	1:A:182:VAL:HG11	1.92	0.51
1:B:153:VAL:HG13	1:B:153:VAL:O	2.10	0.51
1:B:125:ASN:HB2	1:B:158:ILE:HB	1.93	0.51
1:D:20:VAL:HG11	1:D:69:VAL:HG21	1.92	0.51
1:C:333:LYS:HB2	1:C:346:ILE:CD1	2.41	0.51
1:D:352:MET:HB2	1:D:355:ARG:NH2	2.25	0.51
1:B:342:GLU:H	1:B:342:GLU:CD	2.13	0.51
1:C:189:TYR:HB3	1:C:204:VAL:HG21	1.92	0.51
1:D:192:ILE:HG13	1:D:347:HIS:CD2	2.45	0.51
1:D:335:LEU:HG	1:D:339:MET:HE3	1.92	0.51
1:B:15:SER:HB2	1:B:36:THR:O	2.11	0.51
1:D:286:GLN:HG3	1:D:287:LYS:N	2.26	0.51
1:D:67:SER:C	1:D:69:VAL:H	2.14	0.51
1:B:131:PHE:CD2	1:B:142:PRO:HD3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:SER:O	1:C:68:GLY:N	2.44	0.50
1:D:53:ARG:HH22	1:D:54:GLN:HE21	1.57	0.50
1:D:105:ILE:HD11	1:D:142:PRO:CG	2.42	0.50
1:B:259:HIS:HB3	1:B:290:SER:OG	2.11	0.50
1:C:77:LYS:C	1:C:77:LYS:HD2	2.32	0.50
1:A:145:LEU:O	1:A:145:LEU:HD23	2.12	0.50
1:D:375:LEU:HD22	1:D:376:LEU:HD12	1.94	0.50
1:D:78:LEU:HG	1:D:182:VAL:HG13	1.93	0.50
1:B:300:ILE:O	1:B:304:VAL:HG23	2.12	0.50
1:B:316:VAL:HG12	1:B:319:GLY:O	2.12	0.50
1:C:249:THR:HG21	1:C:274:GLU:OE2	2.11	0.50
1:C:356:LYS:HB3	1:C:358:GLU:OE1	2.12	0.50
1:C:58:ASP:O	1:C:62:LYS:HG3	2.12	0.50
1:A:320:PHE:HE2	1:A:340:VAL:HG21	1.75	0.49
1:B:216:PHE:CB	1:B:313:LEU:HD13	2.41	0.49
1:C:78:LEU:CD1	1:C:182:VAL:HG11	2.42	0.49
1:A:131:PHE:CD2	1:A:142:PRO:HD3	2.47	0.49
1:B:135:LYS:HD3	1:C:269:ASP:CG	2.32	0.49
1:A:336:LEU:O	1:A:340:VAL:HG12	2.12	0.49
1:A:80:ILE:H	1:A:213:GLN:HE22	1.60	0.49
1:D:131:PHE:HB2	1:D:139:VAL:O	2.13	0.49
1:D:28:ILE:HD13	1:D:366:ILE:HG22	1.95	0.49
1:D:181:ASP:OD1	1:D:182:VAL:N	2.37	0.49
1:D:324:GLY:O	1:D:357:PRO:HB2	2.13	0.49
1:D:4:HIS:CG	1:D:5:TYR:N	2.77	0.49
1:A:321:ILE:HD12	1:A:321:ILE:N	2.28	0.49
1:C:129:ILE:HB	1:C:154:GLU:O	2.12	0.49
1:C:201:GLY:HA2	1:C:217:TYR:O	2.13	0.48
1:D:270:ILE:CD1	1:D:270:ILE:N	2.76	0.48
1:B:293:ILE:HG21	1:B:329:LEU:HD21	1.95	0.48
1:A:109:LEU:HD22	1:A:126:VAL:HG12	1.94	0.48
1:B:186:ALA:O	1:B:222:LEU:HD22	2.12	0.48
1:D:80:ILE:HD13	1:D:225:ALA:HB1	1.95	0.48
1:A:262:TYR:CE1	1:A:287:LYS:HG2	2.49	0.48
1:A:325:GLY:HA3	3:A:503:ANP:O5'	2.13	0.48
1:C:101:ASN:N	1:C:104:HIS:HD2	1.96	0.48
1:C:78:LEU:HD12	1:C:182:VAL:HG11	1.96	0.48
1:C:265:ALA:CB	1:C:287:LYS:HG2	2.37	0.48
1:D:243:LEU:HD22	1:D:284:TYR:CE1	2.48	0.48
1:C:333:LYS:HB2	1:C:346:ILE:HD13	1.94	0.48
1:D:99:GLU:HG3	1:D:144:GLU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LEU:O	1:D:332:VAL:HG23	2.13	0.48
1:B:13:SER:HB3	3:B:502:ANP:PG	2.53	0.48
1:B:206:ASP:CB	5:B:649:HOH:O	2.60	0.48
1:B:13:SER:HB3	3:B:502:ANP:N3B	2.29	0.48
1:B:105:ILE:HG21	1:B:375:LEU:HD22	1.95	0.48
1:D:80:ILE:H	1:D:213:GLN:NE2	2.12	0.48
1:B:88:GLU:CG	1:B:112:ILE:HG23	2.41	0.48
1:D:245:THR:HB	1:D:249:THR:CG2	2.44	0.48
1:D:333:LYS:O	1:D:337:SER:HB2	2.14	0.48
1:D:105:ILE:HG21	1:D:375:LEU:HD21	1.95	0.48
1:D:286:GLN:C	1:D:288:ASP:H	2.16	0.48
1:B:240:ALA:HA	1:B:245:THR:CG2	2.44	0.47
1:B:234:ASP:HB3	1:B:296:ARG:HE	1.79	0.47
1:B:46:ILE:HD11	1:B:168:MET:CG	2.44	0.47
1:C:52:ALA:O	1:C:56:ILE:HG13	2.15	0.47
1:B:236:THR:OG1	1:B:254:LYS:HE3	2.15	0.47
1:D:285:THR:O	1:D:288:ASP:HB3	2.14	0.47
1:A:5:TYR:CE1	1:A:31:ILE:HD13	2.50	0.47
1:C:335:LEU:HG	1:C:339:MET:HE1	1.97	0.47
1:D:230:MET:HA	1:D:234:ASP:OD2	2.14	0.47
1:A:106:GLU:HB2	1:A:376:LEU:HD22	1.96	0.47
1:D:135:LYS:NZ	1:D:135:LYS:HB3	2.30	0.47
1:A:127:PHE:CZ	1:A:156:GLY:HA3	2.50	0.47
1:B:53:ARG:HD2	1:B:174:ALA:HB1	1.96	0.47
1:B:260:ALA:O	1:B:294:GLU:HB2	2.14	0.47
1:C:130:ARG:HH21	1:C:130:ARG:CB	2.28	0.47
1:D:270:ILE:HG13	1:D:285:THR:HG22	1.96	0.47
1:B:49:PHE:HE2	1:B:170:LYS:HE3	1.77	0.47
1:C:320:PHE:C	1:C:321:ILE:HD12	2.36	0.47
1:A:77:LYS:HD2	1:A:78:LEU:N	2.30	0.46
1:D:107:LYS:HA	1:D:110:GLU:HG2	1.97	0.46
1:A:100:ILE:HD12	1:A:151:LEU:HD22	1.98	0.46
1:B:101:ASN:H	1:B:104:HIS:CD2	2.25	0.46
1:D:20:VAL:HG23	1:D:63:ALA:HB1	1.98	0.46
1:B:262:TYR:CE1	1:B:287:LYS:HB3	2.50	0.46
1:B:73:GLU:HB3	1:B:180:LEU:CD2	2.44	0.46
1:C:308:LEU:HB3	1:C:313:LEU:O	2.15	0.46
1:B:54:GLN:O	1:B:58:ASP:OD1	2.34	0.46
1:D:209:GLU:O	1:D:231:ALA:HB3	2.15	0.46
1:B:15:SER:HB3	1:B:37:TYR:CD1	2.50	0.46
1:B:77:LYS:HD3	1:B:77:LYS:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LEU:HD22	1:D:284:TYR:CD1	2.51	0.46
1:A:200:LEU:O	1:A:317:ASN:HB2	2.16	0.46
1:A:73:GLU:HB3	1:A:180:LEU:HG	1.98	0.46
1:B:242:GLY:O	1:B:243:LEU:HD23	2.15	0.46
1:B:188:ASN:O	1:B:364:SER:HB2	2.15	0.46
1:C:214:VAL:O	1:C:225:ALA:HB1	2.16	0.46
1:C:325:GLY:HA3	3:C:502:ANP:O5'	2.16	0.46
1:D:31:ILE:HD13	1:D:31:ILE:N	2.31	0.46
1:D:9:ILE:HD12	1:D:74:VAL:HG21	1.98	0.46
1:B:127:PHE:HE2	1:B:129:ILE:HD11	1.81	0.46
1:D:246:SER:H	1:D:249:THR:CG2	2.28	0.46
1:B:224:ASP:OD1	1:B:311:LEU:HD22	2.16	0.46
1:B:7:VAL:HG21	1:B:71:ILE:HG13	1.96	0.46
1:D:222:LEU:C	1:D:222:LEU:HD23	2.36	0.46
1:D:282:VAL:CG1	1:D:283:GLN:N	2.79	0.46
1:C:246:SER:HG	1:C:249:THR:HG23	1.81	0.45
1:D:280:GLU:N	5:D:670:HOH:O	2.48	0.45
1:D:317:ASN:N	5:D:666:HOH:O	2.49	0.45
1:D:132:ILE:N	1:D:132:ILE:HD12	2.31	0.45
1:C:239:ILE:HD13	1:C:289:LEU:HD11	1.99	0.45
1:D:224:ASP:OD1	1:D:311:LEU:HD22	2.17	0.45
1:D:164:ILE:O	1:D:168:MET:HG2	2.16	0.45
1:A:100:ILE:O	1:A:144:GLU:N	2.46	0.45
1:B:198:LYS:HB3	1:B:220:GLY:HA2	1.99	0.45
1:D:238:ASP:O	1:D:242:GLY:N	2.46	0.45
1:D:46:ILE:HG13	5:D:673:HOH:O	2.17	0.45
1:C:300:ILE:O	1:C:304:VAL:HG23	2.17	0.45
1:B:6:TYR:O	1:B:20:VAL:HA	2.16	0.45
1:C:132:ILE:HD13	1:C:138:GLU:HA	1.99	0.45
1:B:57:LYS:HG2	1:B:61:LYS:HE3	1.98	0.45
1:C:270:ILE:HG22	1:C:271:PHE:N	2.32	0.45
1:C:321:ILE:HD12	1:C:321:ILE:N	2.31	0.45
1:C:71:ILE:C	1:C:72:LYS:HD2	2.37	0.45
1:D:322:VAL:O	1:D:346:ILE:HA	2.17	0.45
1:A:314:THR:O	1:A:315:LYS:HB3	2.16	0.44
1:B:336:LEU:O	1:B:340:VAL:HG12	2.17	0.44
1:D:272:THR:HG22	1:D:273:VAL:N	2.33	0.44
1:B:218:GLU:H	1:B:223:VAL:HG23	1.81	0.44
1:D:34:GLY:C	1:D:59:THR:HG23	2.37	0.44
1:D:349:PRO:HB2	1:D:354:ILE:O	2.16	0.44
1:C:266:SER:O	1:C:267:ASP:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLN:HG2	5:C:706:HOH:O	2.17	0.44
1:B:296:ARG:O	1:B:299:GLU:HB3	2.16	0.44
1:B:43:ASN:N	1:B:43:ASN:ND2	2.62	0.44
1:C:79:PRO:HA	1:C:213:GLN:HE22	1.81	0.44
1:B:198:LYS:HE2	1:B:220:GLY:O	2.17	0.44
1:B:218:GLU:OE1	1:C:355:ARG:NH2	2.44	0.44
1:D:199:GLU:HG2	1:D:220:GLY:N	2.33	0.44
1:B:73:GLU:OE1	1:B:178:ASP:HB2	2.17	0.44
1:B:13:SER:HB3	3:B:502:ANP:HNB1	1.83	0.43
1:B:165:LEU:O	1:B:169:ILE:HG13	2.18	0.43
1:B:234:ASP:HB3	1:B:296:ARG:NH2	2.31	0.43
1:B:216:PHE:CD1	1:B:313:LEU:HD22	2.53	0.43
1:B:168:MET:HE3	5:B:646:HOH:O	2.17	0.43
1:B:19:ILE:HG22	1:B:20:VAL:N	2.33	0.43
1:C:163:SER:O	1:C:167:ASN:ND2	2.51	0.43
1:C:317:ASN:ND2	1:C:317:ASN:N	2.52	0.43
1:A:58:ASP:O	1:A:62:LYS:HG3	2.17	0.43
1:B:56:ILE:O	1:B:60:ILE:HG13	2.19	0.43
1:D:198:LYS:HG2	1:D:220:GLY:HA2	2.00	0.43
1:C:53:ARG:NH1	1:C:54:GLN:NE2	2.66	0.43
1:D:13:SER:N	3:D:503:ANP:HNB1	2.17	0.43
1:B:303:GLU:O	1:B:307:VAL:HG23	2.19	0.43
1:B:120:GLU:H	1:B:120:GLU:CD	2.22	0.43
1:D:189:TYR:HB2	1:D:217:TYR:OH	2.19	0.43
1:A:275:GLN:NE2	5:A:619:HOH:O	2.43	0.42
1:D:262:TYR:C	1:D:264:SER:N	2.71	0.42
1:B:335:LEU:HG	1:B:339:MET:HE1	2.01	0.42
1:B:321:ILE:CG2	1:B:347:HIS:HB2	2.49	0.42
1:C:78:LEU:HD12	1:C:182:VAL:CG1	2.49	0.42
1:C:146:ILE:HD12	1:C:146:ILE:N	2.34	0.42
1:A:120:GLU:HG3	1:C:270:ILE:HB	2.01	0.42
1:A:48:ASP:OD1	1:A:51:ILE:HG13	2.19	0.42
1:C:256:GLN:HG2	1:C:257:TYR:CE2	2.55	0.42
1:C:216:PHE:CD1	1:C:313:LEU:HD13	2.54	0.42
1:D:206:ASP:O	1:D:212:THR:HA	2.20	0.42
1:A:152:LYS:HE3	4:A:505:CL:CL	2.57	0.42
1:B:364:SER:HA	1:B:367:SER:HB3	2.02	0.42
1:A:217:TYR:N	1:A:217:TYR:CD1	2.86	0.42
1:B:131:PHE:O	1:B:138:GLU:HA	2.20	0.42
1:A:186:ALA:O	1:A:217:TYR:OH	2.29	0.42
1:B:89:SER:HA	1:B:153:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLU:OE1	1:C:376:LEU:HD13	2.19	0.42
1:C:80:ILE:H	1:C:213:GLN:HE22	1.64	0.42
1:D:205:ILE:CD1	1:D:304:VAL:HG11	2.50	0.42
1:B:120:GLU:O	1:B:162:LYS:HG3	2.20	0.42
1:B:206:ASP:HA	1:B:323:THR:O	2.20	0.42
1:B:325:GLY:HA3	3:B:502:ANP:O5'	2.19	0.42
1:C:6:TYR:CE2	1:C:23:LYS:HG2	2.54	0.42
1:D:28:ILE:N	5:D:677:HOH:O	2.53	0.42
1:A:88:GLU:OE1	1:A:89:SER:N	2.40	0.41
1:B:129:ILE:HG22	1:B:130:ARG:NH1	2.34	0.41
1:B:209:GLU:HG2	1:B:233:ARG:HB2	2.01	0.41
1:D:31:ILE:O	1:D:67:SER:HA	2.20	0.41
1:A:228:ILE:HD13	1:A:303:GLU:HB3	2.03	0.41
1:B:228:ILE:HD13	1:B:303:GLU:HB3	2.02	0.41
1:B:92:ILE:HD13	1:B:93:ASP:H	1.84	0.41
1:C:28:ILE:HD11	1:C:370:ILE:HD12	2.03	0.41
1:D:293:ILE:O	1:D:297:VAL:HG23	2.21	0.41
1:A:99:GLU:HG2	1:A:144:GLU:HA	2.00	0.41
1:C:267:ASP:HB2	1:C:287:LYS:CE	2.47	0.41
1:C:6:TYR:HE1	5:C:694:HOH:O	2.03	0.41
1:D:34:GLY:O	1:D:59:THR:HG23	2.20	0.41
1:D:194:THR:OG1	1:D:197:GLU:HG3	2.20	0.41
1:D:259:HIS:CD2	1:D:330:LEU:HD22	2.55	0.41
1:A:78:LEU:CD1	1:A:182:VAL:HG11	2.50	0.41
1:B:329:LEU:O	1:B:332:VAL:HG23	2.20	0.41
1:B:373:ASP:O	1:B:377:ASP:OD2	2.39	0.41
1:D:113:ARG:HG2	1:D:123:VAL:HG11	2.03	0.41
1:A:320:PHE:C	1:A:321:ILE:HD12	2.41	0.41
1:B:192:ILE:HB	1:B:347:HIS:NE2	2.36	0.41
1:C:262:TYR:HA	1:C:290:SER:OG	2.21	0.41
1:C:53:ARG:HH12	1:C:54:GLN:HE22	1.68	0.41
1:A:106:GLU:O	1:A:110:GLU:HB2	2.21	0.41
1:B:257:TYR:O	1:B:289:LEU:HD23	2.21	0.41
1:C:105:ILE:HG21	1:C:375:LEU:CD2	2.51	0.41
1:A:77:LYS:CD	1:A:77:LYS:C	2.83	0.41
1:B:167:ASN:O	1:B:170:LYS:HB3	2.21	0.41
1:C:209:GLU:O	1:C:233:ARG:HB3	2.21	0.41
1:C:315:LYS:HE3	1:C:317:ASN:ND2	2.34	0.41
1:A:100:ILE:HB	1:A:142:PRO:O	2.21	0.40
1:A:266:SER:HB3	1:A:286:GLN:NE2	2.36	0.40
1:A:268:GLN:HA	1:A:268:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:C	1:B:114:GLU:N	2.75	0.40
1:C:351:GLN:HB2	1:C:354:ILE:HD11	2.02	0.40
1:A:112:ILE:C	1:A:114:GLU:N	2.73	0.40
1:B:73:GLU:HB3	1:B:180:LEU:CG	2.52	0.40
1:C:129:ILE:HD11	5:C:742:HOH:O	2.21	0.40
1:C:166:ILE:CG2	1:D:146:ILE:HD12	2.52	0.40
1:D:245:THR:HB	1:D:249:THR:HG21	2.04	0.40
1:A:146:ILE:CD1	1:A:146:ILE:N	2.85	0.40
1:B:262:TYR:N	1:B:294:GLU:OE2	2.51	0.40
1:B:149:HIS:HB3	1:C:268:GLN:HB3	2.04	0.40
1:D:57:LYS:HE2	1:D:61:LYS:HZ1	1.86	0.40
1:B:76:LEU:O	1:B:182:VAL:HA	2.22	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	366/484 (76%)	350 (96%)	14 (4%)	2 (0%)	32	34
1	B	322/484 (66%)	297 (92%)	21 (6%)	4 (1%)	15	12
1	C	362/484 (75%)	343 (95%)	17 (5%)	2 (1%)	28	29
1	D	340/484 (70%)	308 (91%)	28 (8%)	4 (1%)	15	12
All	All	1390/1936 (72%)	1298 (93%)	80 (6%)	12 (1%)	20	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
1	D	263	ASP
1	A	136	GLU

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Mol	Chain	Res	Type
1	A	315	LYS
1	B	262	TYR
1	D	286	GLN
1	B	230	MET
1	C	28	ILE
1	C	136	GLU
1	B	113	ARG
1	D	287	LYS
1	B	316	VAL

### 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	321/432 (74%)	304 (95%)	17 (5%)	26	31
1	B	290/432 (67%)	274 (94%)	16 (6%)	25	29
1	C	319/432 (74%)	304 (95%)	15 (5%)	30	37
1	D	305/432 (71%)	287 (94%)	18 (6%)	23	26
All	All	1235/1728 (72%)	1169 (95%)	66 (5%)	26	31

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	77	LYS
1	A	136	GLU
1	A	137	ASN
1	A	145	LEU
1	A	181	ASP
1	A	182	VAL
1	A	252	LYS
1	A	268	GLN
1	A	269	ASP
1	A	283	GLN
1	A	314	THR

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Mol	Chain	Res	Type
1	A	334	GLU
1	A	342	GLU
1	A	352	MET
1	A	373	ASP
1	A	375	LEU
1	B	17	LYS
1	B	43	ASN
1	B	77	LYS
1	B	92	ILE
1	B	114	GLU
1	B	137	ASN
1	B	145	LEU
1	B	161	GLN
1	B	199	GLU
1	B	249	THR
1	B	306	ASP
1	B	310	ASP
1	B	337	SER
1	B	342	GLU
1	B	363	ILE
1	B	375	LEU
1	C	77	LYS
1	C	136	GLU
1	C	137	ASN
1	C	181	ASP
1	C	222	LEU
1	C	233	ARG
1	C	241	GLN
1	C	249	THR
1	C	251	GLU
1	C	274	GLU
1	C	283	GLN
1	C	317	ASN
1	C	352	MET
1	C	356	LYS
1	C	375	LEU
1	D	23	LYS
1	D	31	ILE
1	D	42	LYS
1	D	76	LEU
1	D	77	LYS
1	D	120	GLU

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Mol	Chain	Res	Type
1	D	122	GLU
1	D	137	ASN
1	D	192	ILE
1	D	199	GLU
1	D	249	THR
1	D	283	GLN
1	D	306	ASP
1	D	330	LEU
1	D	337	SER
1	D	352	MET
1	D	375	LEU
1	D	377	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	54	GLN
1	A	90	ASN
1	A	104	HIS
1	A	119	GLN
1	A	125	ASN
1	A	137	ASN
1	A	213	GLN
1	A	256	GLN
1	A	275	GLN
1	A	309	GLN
1	A	317	ASN
1	B	35	GLN
1	B	43	ASN
1	B	90	ASN
1	B	104	HIS
1	B	137	ASN
1	B	167	ASN
1	B	188	ASN
1	B	213	GLN
1	B	256	GLN
1	B	309	GLN
1	B	317	ASN
1	C	54	GLN
1	C	90	ASN
1	C	104	HIS

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Mol	Chain	Res	Type
1	C	119	GLN
1	C	125	ASN
1	C	137	ASN
1	C	161	GLN
1	C	213	GLN
1	C	241	GLN
1	C	317	ASN
1	D	4	HIS
1	D	29	ASN
1	D	35	GLN
1	D	54	GLN
1	D	90	ASN
1	D	104	HIS
1	D	125	ASN
1	D	167	ASN
1	D	213	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 19 ligands modelled in this entry, 15 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
3	ANP	A	503	2	29,33,33	3.76	8 (27%)	28,52,52	2.18	4 (14%)
3	ANP	B	502	2	29,33,33	4.07	9 (31%)	28,52,52	2.19	4 (14%)
3	ANP	C	502	2	29,33,33	2.82	8 (27%)	28,52,52	2.12	4 (14%)
3	ANP	D	503	2	29,33,33	3.05	8 (27%)	28,52,52	2.20	4 (14%)

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	ANP	A	503	2	-	0/13/38/38	0/3/3/3
3	ANP	B	502	2	-	0/13/38/38	0/3/3/3
3	ANP	C	502	2	-	0/13/38/38	0/3/3/3
3	ANP	D	503	2	-	0/13/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PB-O2B	-3.07	1.48	1.56
3	A	503	ANP	PG-O3G	-2.98	1.48	1.56
3	D	503	ANP	PG-O2G	-2.92	1.48	1.56
3	B	502	ANP	PG-O3G	-2.74	1.49	1.56
3	A	503	ANP	PB-O2B	-2.73	1.49	1.56
3	C	502	ANP	PG-O2G	-2.50	1.49	1.56
3	A	503	ANP	C8-N7	-2.23	1.30	1.34
3	D	503	ANP	C8-N7	-2.12	1.30	1.34
3	B	502	ANP	C8-N7	-2.10	1.30	1.34
3	B	502	ANP	PB-N3B	2.03	1.68	1.63
3	C	502	ANP	PG-N3B	2.06	1.68	1.63
3	C	502	ANP	PB-O1B	2.07	1.48	1.46
3	C	502	ANP	PB-N3B	2.25	1.69	1.63
3	C	502	ANP	PA-O1A	2.35	1.59	1.50
3	B	502	ANP	O4'-C1'	2.38	1.44	1.41
3	A	503	ANP	O4'-C1'	2.42	1.44	1.41
3	D	503	ANP	PB-N3B	2.43	1.69	1.63
3	D	503	ANP	PA-O1A	2.46	1.60	1.50
3	D	503	ANP	O4'-C1'	2.51	1.44	1.41
3	A	503	ANP	PG-N3B	2.54	1.70	1.63
3	D	503	ANP	PB-O1B	2.66	1.49	1.46
3	C	502	ANP	O4'-C1'	2.78	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	ANP	PB-O3A	2.97	1.62	1.59
3	B	502	ANP	PG-N3B	2.99	1.71	1.63
3	C	502	ANP	PB-O3A	3.57	1.63	1.59
3	B	502	ANP	PB-O3A	4.01	1.64	1.59
3	A	503	ANP	PB-O3A	4.06	1.64	1.59
3	A	503	ANP	PB-O1B	12.87	1.60	1.46
3	C	502	ANP	PG-O1G	12.92	1.60	1.46
3	A	503	ANP	PG-O1G	13.39	1.61	1.46
3	D	503	ANP	PG-O1G	14.22	1.62	1.46
3	B	502	ANP	PB-O1B	14.31	1.62	1.46
3	B	502	ANP	PG-O1G	14.34	1.62	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	ANP	N3-C2-N1	-8.66	121.32	128.86
3	D	503	ANP	N3-C2-N1	-8.47	121.48	128.86
3	A	503	ANP	N3-C2-N1	-8.33	121.60	128.86
3	C	502	ANP	N3-C2-N1	-8.19	121.73	128.86
3	C	502	ANP	PA-O3A-PB	-5.58	112.69	132.38
3	A	503	ANP	PA-O3A-PB	-5.48	113.03	132.38
3	D	503	ANP	PA-O3A-PB	-5.29	113.70	132.38
3	B	502	ANP	PA-O3A-PB	-5.22	113.97	132.38
3	D	503	ANP	C4'-O4'-C1'	-3.57	105.97	109.77
3	A	503	ANP	O1B-PB-N3B	-3.32	106.83	111.79
3	B	502	ANP	C4'-O4'-C1'	-3.14	106.42	109.77
3	C	502	ANP	C4'-O4'-C1'	-2.52	107.08	109.77
3	D	503	ANP	C4-C5-N7	-2.38	107.11	109.41
3	C	502	ANP	C4-C5-N7	-2.35	107.14	109.41
3	A	503	ANP	C4-C5-N7	-2.30	107.19	109.41
3	B	502	ANP	C4-C5-N7	-2.18	107.30	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	ANP	2	0
3	B	502	ANP	6	0
3	C	502	ANP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	ANP	3	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	370/484 (76%)	0.13	7 (1%) 67 65	21, 37, 57, 73	0
1	B	334/484 (69%)	1.09	59 (17%) 2 1	37, 67, 88, 99	0
1	C	368/484 (76%)	0.07	7 (1%) 67 65	21, 37, 58, 72	0
1	D	352/484 (72%)	0.70	32 (9%) 10 9	28, 52, 77, 93	0
All	All	1424/1936 (73%)	0.48	105 (7%) 15 14	21, 45, 79, 99	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ALA	8.9
1	B	292	PHE	6.8
1	D	264	SER	6.1
1	B	31	ILE	6.0
1	B	70	ASP	5.7
1	C	24	PHE	5.2
1	B	257	TYR	5.2
1	D	5	TYR	5.1
1	B	262	TYR	5.0
1	B	302	PHE	4.8
1	B	40	GLY	4.6
1	B	71	ILE	4.5
1	B	30	VAL	4.4
1	B	288	ASP	4.3
1	B	256	GLN	4.2
1	B	20	VAL	4.1
1	D	262	TYR	4.1
1	B	6	TYR	4.0
1	B	247	TYR	3.9
1	B	28	ILE	3.9
1	B	285	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	49	PHE	3.7
1	D	65	ILE	3.7
1	D	4	HIS	3.6
1	B	243	LEU	3.6
1	B	377	ASP	3.6
1	B	64	SER	3.5
1	B	289	LEU	3.5
1	D	95	TYR	3.5
1	C	352	MET	3.4
1	B	61	LYS	3.4
1	B	293	ILE	3.4
1	B	241	GLN	3.2
1	B	286	GLN	3.2
1	B	354	ILE	3.0
1	D	263	ASP	3.0
1	D	64	SER	3.0
1	B	50	ASP	3.0
1	D	120	GLU	3.0
1	C	266	SER	2.9
1	B	166	ILE	2.9
1	B	177	VAL	2.9
1	B	73	GLU	2.9
1	D	23	LYS	2.8
1	B	29	ASN	2.8
1	B	291	ASP	2.8
1	A	262	TYR	2.8
1	B	32	GLY	2.7
1	C	265	ALA	2.7
1	D	31	ILE	2.7
1	B	248	GLU	2.7
1	D	61	LYS	2.7
1	B	19	ILE	2.7
1	B	179	VAL	2.7
1	D	70	ASP	2.6
1	D	66	ALA	2.6
1	A	283	GLN	2.6
1	C	61	LYS	2.6
1	D	334	GLU	2.6
1	D	153	VAL	2.6
1	B	41	ILE	2.6
1	B	65	ILE	2.6
1	D	72	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	119	GLN	2.6
1	B	178	ASP	2.5
1	B	287	LYS	2.5
1	B	239	ILE	2.5
1	D	286	GLN	2.5
1	B	244	ASN	2.5
1	D	149	HIS	2.5
1	D	91	GLU	2.5
1	D	135	LYS	2.5
1	A	139	VAL	2.5
1	B	310	ASP	2.5
1	B	112	ILE	2.4
1	D	150	SER	2.4
1	B	359	PHE	2.4
1	B	258	GLY	2.4
1	D	69	VAL	2.4
1	D	68	GLY	2.3
1	B	174	ALA	2.3
1	D	270	ILE	2.3
1	B	74	VAL	2.3
1	D	340	VAL	2.3
1	D	282	VAL	2.3
1	A	314	THR	2.2
1	B	33	THR	2.2
1	D	92	ILE	2.2
1	B	245	THR	2.1
1	B	240	ALA	2.1
1	C	27	GLY	2.1
1	B	290	SER	2.1
1	C	23	LYS	2.1
1	A	267	ASP	2.1
1	D	280	GLU	2.1
1	B	38	THR	2.1
1	D	308	LEU	2.0
1	D	275	GLN	2.0
1	B	109	LEU	2.0
1	B	242	GLY	2.0
1	A	4	HIS	2.0
1	B	253	VAL	2.0
1	A	136	GLU	2.0
1	B	60	ILE	2.0
1	D	63	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
4	CL	C	504	1/1	0.97	0.18	0.99	33,33,33,33	0
4	CL	D	504	1/1	0.99	0.19	0.85	43,43,43,43	0
3	ANP	C	502	31/31	0.98	0.15	0.51	21,27,29,30	0
3	ANP	A	503	31/31	0.98	0.16	0.26	20,31,36,37	0
3	ANP	D	503	31/31	0.98	0.14	-0.50	21,30,34,35	0
3	ANP	B	502	31/31	0.92	0.13	-1.41	46,56,58,58	0
2	MG	C	501	1/1	0.97	0.11	-1.88	23,23,23,23	0
2	MG	A	502	1/1	0.95	0.07	-4.67	45,45,45,45	0
4	CL	D	505	1/1	0.95	0.18	-	38,38,38,38	0
4	CL	C	505	1/1	0.94	0.19	-	48,48,48,48	0
4	CL	C	503	1/1	0.99	0.20	-	20,20,20,20	0
4	CL	A	504	1/1	0.99	0.18	-	34,34,34,34	0
4	CL	C	506	1/1	0.91	0.07	-	50,50,50,50	0
2	MG	D	502	1/1	0.94	0.05	-	46,46,46,46	0
2	MG	B	501	1/1	0.91	0.25	-	72,72,72,72	0
2	MG	D	501	1/1	0.90	0.19	-	33,33,33,33	0
2	MG	A	501	1/1	0.96	0.12	-	23,23,23,23	0
4	CL	A	505	1/1	0.95	0.06	-	45,45,45,45	0
4	CL	B	503	1/1	0.77	0.16	-	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.