



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:57 AM UTC

PDB ID : 6PLM / pdb_00006plm
Title : Legionella pneumophila SidJ/ Calmodulin 2 complex
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Deposited on : 2019-07-01
Resolution : 2.59 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

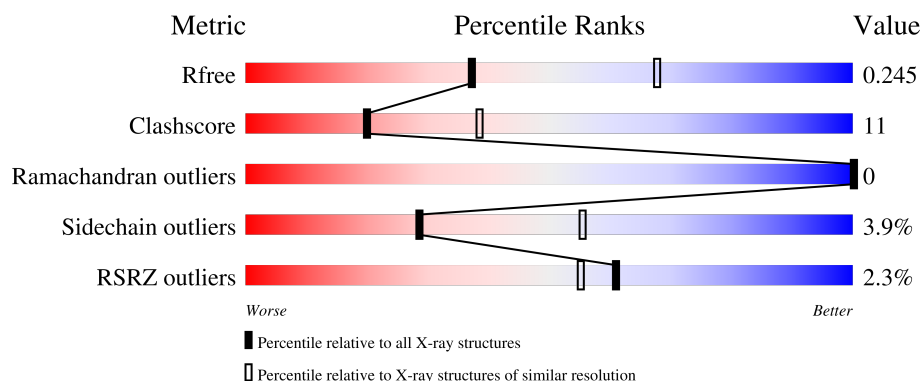
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	757	78% 20% ..
1	B	757	81% 17% ..
2	C	147	12% 53% 35% 9%
2	D	147	5% 63% 33% ...

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14660 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 SidJ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	0	0
			6105	3908	1036	1146	15			
1	B	752	Total	C	N	O	S	0	0	0
			6131	3923	1041	1152	15			

- Molecule 2 is a protein called Calmodulin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	134	Total	C	N	O	S	0	0	0
			1064	658	169	228	9			
2	D	145	Total	C	N	O	S	0	0	0
			1134	695	181	249	9			

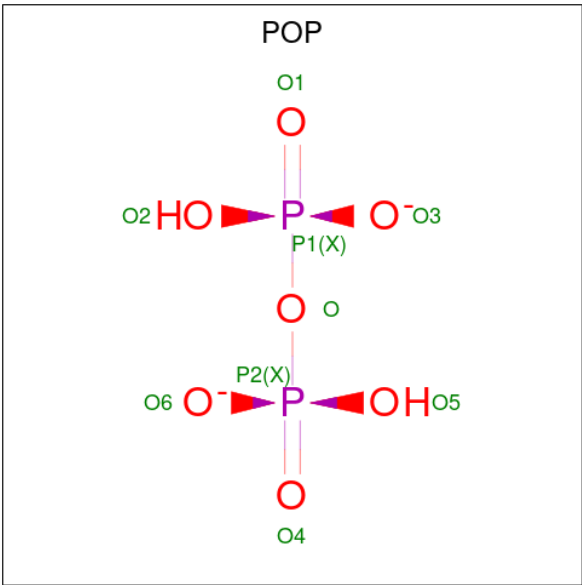
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	86	ALA	ARG	conflict	UNP P0DP24
D	86	ALA	ARG	conflict	UNP P0DP24

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

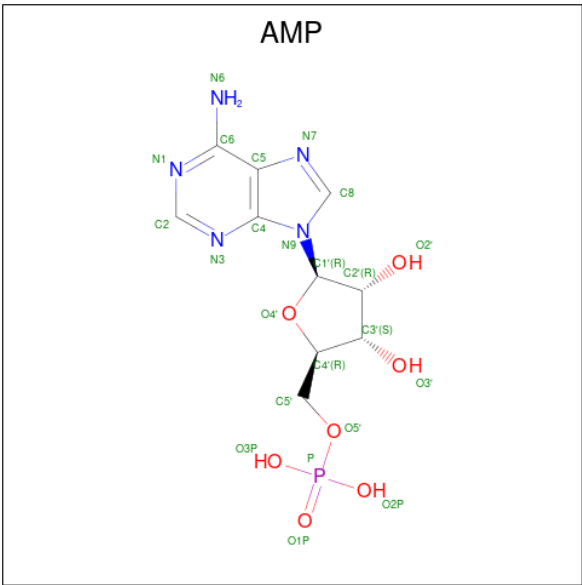
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
5	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

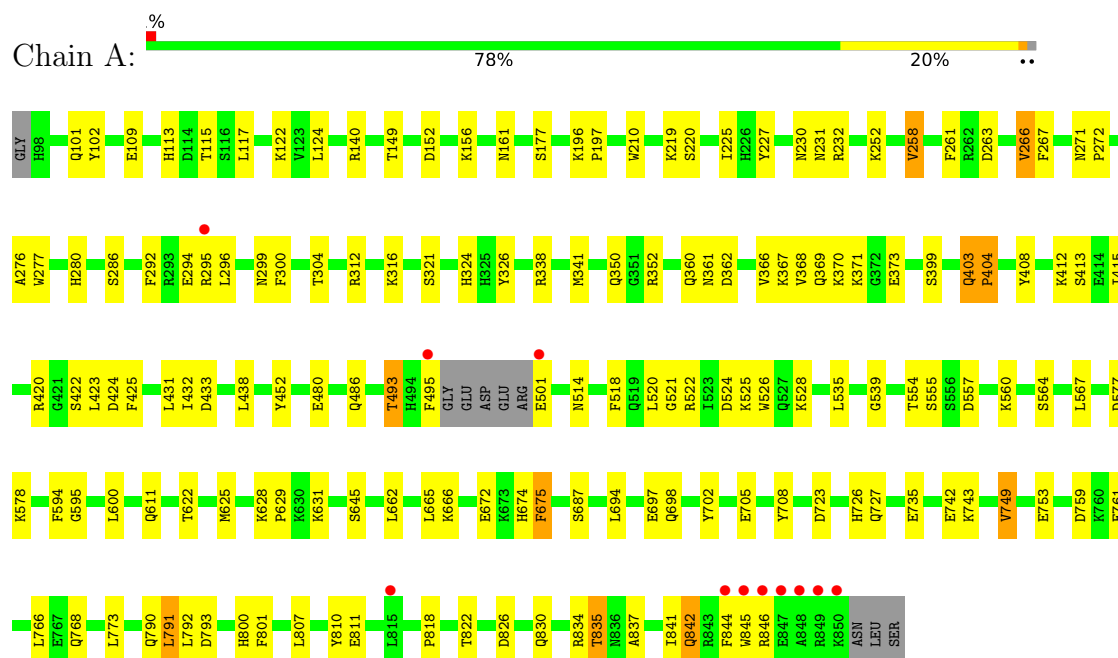
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total 80	O 80	0	0
6	B	67	Total 67	O 67	0	0
6	C	3	Total 3	O 3	0	0
6	D	6	Total 6	O 6	0	0

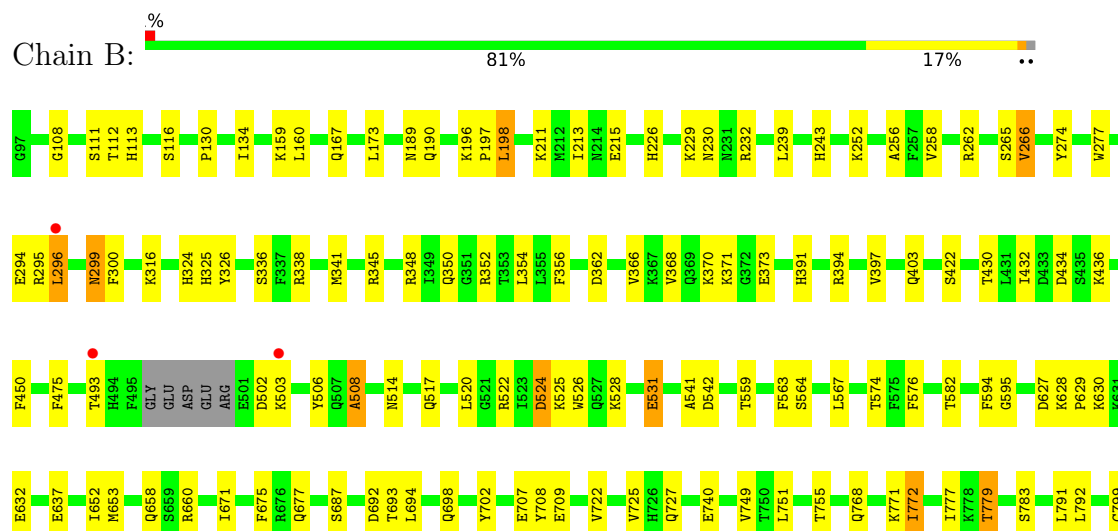
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SidJ protein

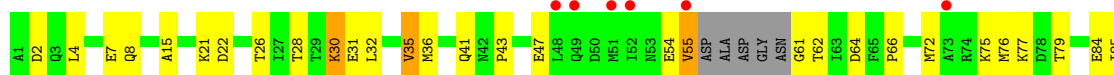


• Molecule 1: SidJ protein

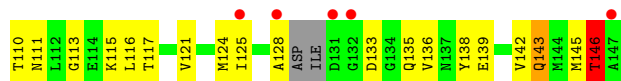
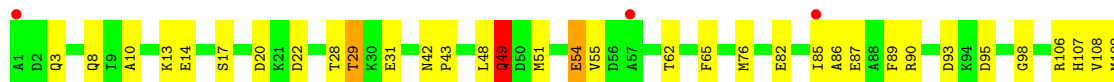




● Molecule 2: Calmodulin-2



● Molecule 2: Calmodulin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.35Å 103.79Å 110.19Å 90.00° 104.69° 90.00°	Depositor
Resolution (Å)	29.33 – 2.59 29.33 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.33-2.59) 97.7 (29.33-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.176 , 0.241 0.192 , 0.245	Depositor DCC
R_{free} test set	3457 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14660	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, POP, AMP

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	1.08	15/6246 (0.2%)	1.27	23/8443 (0.3%)
1	B	1.16	28/6272 (0.4%)	1.25	10/8478 (0.1%)
2	C	0.96	2/1074 (0.2%)	1.25	1/1438 (0.1%)
2	D	1.02	3/1145 (0.3%)	1.40	8/1537 (0.5%)
All	All	1.10	48/14737 (0.3%)	1.27	42/19896 (0.2%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	ILE	N-CA	-7.40	1.40	1.46
1	B	506	TYR	C-O	-6.97	1.15	1.23
1	B	524	ASP	C-O	-6.81	1.15	1.24
1	B	823	ASP	C-O	-6.63	1.16	1.24
1	A	818	PRO	C-O	6.44	1.32	1.24
1	B	541	ALA	C-O	-6.39	1.15	1.23
1	A	109	GLU	C-O	-6.33	1.16	1.23
1	A	300	PHE	C-O	-6.28	1.16	1.24
1	A	768	GLN	C-O	-6.28	1.16	1.24
1	B	112	THR	C-O	-6.28	1.16	1.23
1	B	299	ASN	C-O	-6.26	1.16	1.24
1	B	576	PHE	C-O	-6.06	1.17	1.24
1	B	852	LEU	N-CA	6.05	1.54	1.46
1	B	256	ALA	C-O	-6.04	1.17	1.24
2	D	17	SER	C-O	6.03	1.31	1.24
1	A	286	SER	N-CA	6.00	1.53	1.46
1	B	707	GLU	C-O	-5.98	1.16	1.23
2	C	21	LYS	C-O	-5.84	1.16	1.24
2	D	49	GLN	C-O	5.82	1.30	1.24
1	B	559	THR	C-O	-5.68	1.17	1.24
1	B	751	LEU	N-CA	-5.68	1.39	1.46
1	A	811	GLU	N-CA	-5.67	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	ASP	N-CA	5.67	1.52	1.45
1	A	369	GLN	C-O	5.64	1.30	1.23
1	A	404	PRO	C-O	-5.51	1.17	1.23
1	B	725	VAL	N-CA	5.50	1.51	1.46
1	A	276	ALA	N-CA	-5.45	1.39	1.46
1	B	755	THR	C-O	-5.44	1.17	1.24
2	D	22	ASP	N-CA	5.40	1.53	1.46
1	B	849	ARG	N-CA	5.35	1.53	1.46
1	B	243	HIS	C-O	-5.35	1.17	1.24
1	A	687	SER	C-O	-5.33	1.17	1.24
1	B	508	ALA	C-O	-5.33	1.17	1.24
1	A	792	LEU	C-O	-5.25	1.18	1.24
1	B	671	ILE	C-O	-5.24	1.17	1.24
2	C	136	VAL	N-CA	5.22	1.52	1.46
1	B	252	LYS	C-O	-5.20	1.18	1.24
1	A	665	LEU	C-O	-5.20	1.18	1.24
1	A	535	LEU	N-CA	-5.16	1.40	1.46
1	A	493	THR	C-O	5.14	1.29	1.23
1	A	645	SER	C-O	-5.14	1.18	1.24
1	B	531	GLU	N-CA	-5.10	1.40	1.46
1	B	632	GLU	C-O	-5.10	1.18	1.24
1	B	687	SER	N-CA	5.10	1.52	1.46
1	B	108	GLY	N-CA	-5.10	1.41	1.45
1	B	111	SER	CA-CB	-5.07	1.45	1.53
1	B	300	PHE	C-O	-5.03	1.18	1.24
1	B	397	VAL	C-O	-5.01	1.18	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	HIS	CA-CB-CG	-8.30	105.50	113.80
1	B	692	ASP	CA-CB-CG	-6.79	105.81	112.60
2	C	22	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	403	GLN	CB-CA-C	6.42	117.30	110.17
1	A	554	THR	CA-CB-OG1	-6.42	99.98	109.60
1	B	574	THR	CA-CB-OG1	-6.33	100.10	109.60
1	B	542	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	759	ASP	CA-CB-CG	6.07	118.67	112.60
2	D	146	THR	CB-CA-C	6.00	120.75	110.79
1	A	518	PHE	CB-CA-C	5.99	118.74	109.03
1	B	693	THR	CB-CA-C	5.99	120.73	110.79
1	A	735	GLU	CB-CG-CD	5.98	122.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	PHE	CA-CB-CG	-5.80	108.00	113.80
2	D	20	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	493	THR	CB-CA-C	5.67	118.51	110.24
1	B	265	SER	CA-C-N	5.66	128.21	120.46
1	B	265	SER	C-N-CA	5.66	128.21	120.46
1	B	502	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	761	GLU	CB-CG-CD	5.60	122.12	112.60
1	A	577	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	557	ASP	CA-C-N	5.50	127.90	120.65
1	A	557	ASP	C-N-CA	5.50	127.90	120.65
1	A	514	ASN	CA-C-N	5.44	129.17	121.66
1	A	514	ASN	C-N-CA	5.44	129.17	121.66
1	A	266	VAL	N-CA-CB	-5.42	102.30	111.23
1	A	811	GLU	N-CA-C	-5.40	105.29	111.07
1	B	637	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	766	LEU	CA-C-N	5.38	127.74	120.38
1	A	766	LEU	C-N-CA	5.38	127.74	120.38
1	B	403	GLN	CB-CA-C	5.36	115.48	110.17
2	D	93	ASP	CA-C-N	5.36	127.73	120.44
2	D	93	ASP	C-N-CA	5.36	127.73	120.44
1	A	304	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	210	TRP	CA-C-N	5.28	127.35	120.28
1	A	210	TRP	C-N-CA	5.28	127.35	120.28
1	A	362	ASP	CA-CB-CG	5.28	117.88	112.60
2	D	29	THR	CA-C-N	5.21	127.58	120.54
2	D	29	THR	C-N-CA	5.21	127.58	120.54
2	D	10	ALA	CA-C-N	5.05	127.47	120.29
2	D	10	ALA	C-N-CA	5.05	127.47	120.29
1	A	230	ASN	CA-C-N	5.00	128.61	120.60
1	A	230	ASN	C-N-CA	5.00	128.61	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6105	0	6076	164	0
1	B	6131	0	6101	101	0
2	C	1064	0	1008	94	0
2	D	1134	0	1059	39	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	23	0	12	2	0
5	B	23	0	12	1	0
6	A	80	0	0	1	0
6	B	67	0	0	1	0
6	C	3	0	0	0	0
6	D	6	0	0	0	0
All	All	14660	0	14268	329	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:TRP:CH2	2:C:120:GLU:HG2	1.38	1.52
1:A:844:PHE:CE2	2:C:85:ILE:HD13	1.64	1.32
1:A:845:TRP:CZ3	2:C:120:GLU:HG2	1.73	1.23
1:A:845:TRP:CH2	2:C:120:GLU:CG	2.26	1.17
1:A:295:ARG:HD2	1:B:294:GLU:OE2	1.44	1.14
1:A:846:ARG:HH22	2:C:114:GLU:HB3	0.99	1.13
1:A:846:ARG:HH12	2:C:7:GLU:HG2	1.14	1.13
2:C:127:GLU:C	2:C:141:PHE:HE1	1.58	1.10
1:A:844:PHE:CD2	2:C:85:ILE:HD13	1.84	1.10
1:A:845:TRP:CZ3	2:C:120:GLU:CG	2.44	1.00
1:A:846:ARG:NH2	2:C:114:GLU:HB3	1.76	1.00
1:A:625:MET:HE1	1:A:631:LYS:HA	1.42	1.00
2:C:72:MET:O	2:C:76:MET:HG3	1.62	1.00
2:C:127:GLU:C	2:C:141:PHE:CE1	2.41	0.99
1:A:352:ARG:HD2	1:A:368:VAL:O	1.65	0.96
1:A:296:LEU:HD21	1:B:258:VAL:HG12	1.45	0.95
1:A:526:TRP:HE1	1:A:727:GLN:HE21	1.14	0.95
1:A:844:PHE:CE2	2:C:85:ILE:CD1	2.50	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:ARG:HH22	2:C:114:GLU:CB	1.81	0.93
1:A:625:MET:CE	1:A:631:LYS:HA	1.99	0.92
1:A:844:PHE:CD2	2:C:85:ILE:CD1	2.53	0.91
1:A:295:ARG:HD2	1:B:294:GLU:CD	1.97	0.89
1:B:526:TRP:HE1	1:B:727:GLN:HE21	1.19	0.88
2:D:107:HIS:CD2	2:D:111:ASN:HD22	1.92	0.88
1:A:271:ASN:HD22	1:A:312:ARG:HH11	1.18	0.87
1:A:846:ARG:NH1	2:C:7:GLU:HG2	1.90	0.86
1:A:845:TRP:HH2	2:C:120:GLU:HG2	1.04	0.86
2:D:106:ARG:NH1	2:D:125:ILE:HD12	1.91	0.85
1:A:846:ARG:NH2	2:C:114:GLU:CB	2.39	0.84
2:C:77:LYS:HD2	2:C:77:LYS:O	1.78	0.83
1:A:296:LEU:HD11	1:B:262:ARG:CB	2.08	0.83
2:D:8:GLN:NE2	2:D:76:MET:CE	2.42	0.81
1:A:625:MET:HE1	1:A:631:LYS:CA	2.10	0.81
2:C:99:TYR:HB3	2:C:135:GLN:HE21	1.44	0.80
1:A:841:ILE:HG22	2:C:109:MET:HE1	1.63	0.80
1:A:295:ARG:CD	1:B:294:GLU:OE2	2.30	0.80
1:A:296:LEU:CD1	1:B:262:ARG:CB	2.61	0.79
1:B:677:GLN:HE22	1:B:740:GLU:H	1.30	0.79
2:C:110:THR:CG2	2:C:121:VAL:HG21	2.12	0.79
1:A:295:ARG:HG3	1:B:294:GLU:OE1	1.83	0.78
1:A:324:HIS:HE1	1:A:480:GLU:O	1.67	0.78
1:A:296:LEU:HD11	1:B:262:ARG:HB3	1.64	0.77
2:C:47:GLU:OE1	2:C:75:LYS:HE2	1.84	0.77
1:A:113:HIS:HE1	1:A:316:LYS:O	1.68	0.76
2:C:97:ASN:ND2	2:C:99:TYR:HB2	2.01	0.76
1:A:846:ARG:HH12	2:C:7:GLU:CG	1.95	0.76
2:C:109:MET:HE2	2:C:116:LEU:HD11	1.66	0.76
2:C:110:THR:HG23	2:C:121:VAL:HG21	1.68	0.76
2:D:106:ARG:HG2	2:D:125:ILE:HD11	1.68	0.76
1:B:352:ARG:HH12	1:B:373:GLU:CD	1.94	0.75
1:A:625:MET:HE3	1:A:631:LYS:HG3	1.67	0.74
1:B:846:ARG:NH1	2:D:116:LEU:HD23	2.01	0.74
1:A:296:LEU:CD1	1:B:262:ARG:HB2	2.16	0.74
1:A:625:MET:HE3	1:A:631:LYS:CG	2.17	0.74
1:B:652:ILE:HG22	1:B:653:MET:HE2	1.68	0.74
1:A:341:MET:HE3	1:A:366:VAL:HG21	1.68	0.73
2:C:99:TYR:HB3	2:C:135:GLN:NE2	2.03	0.73
1:A:625:MET:CE	1:A:631:LYS:CA	2.65	0.73
1:B:846:ARG:HH11	2:D:116:LEU:HD23	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:TRP:CH2	2:C:120:GLU:CB	2.73	0.72
1:A:341:MET:HE3	1:A:366:VAL:HG11	1.71	0.71
1:B:230:ASN:OD1	1:B:232:ARG:HG3	1.90	0.70
1:A:846:ARG:NH1	2:C:7:GLU:CG	2.52	0.70
1:A:625:MET:CE	1:A:631:LYS:CG	2.68	0.70
1:B:779:THR:OG1	1:B:783:SER:HB2	1.92	0.69
1:A:296:LEU:CD1	1:B:262:ARG:HB3	2.22	0.69
1:A:845:TRP:HH2	2:C:120:GLU:CG	1.87	0.69
1:A:280:HIS:ND1	6:A:1101:HOH:O	2.26	0.69
1:A:113:HIS:HD2	1:A:595:GLY:H	1.41	0.69
1:A:271:ASN:ND2	1:A:312:ARG:HH11	1.90	0.69
2:D:86:ALA:O	2:D:90:ARG:HG3	1.92	0.68
1:B:493:THR:HB	1:B:522:ARG:NH1	2.09	0.68
1:B:526:TRP:HE1	1:B:727:GLN:NE2	1.90	0.68
1:A:341:MET:CE	1:A:366:VAL:HG11	2.23	0.68
1:B:352:ARG:NH1	1:B:370:LYS:HD3	2.09	0.67
1:A:295:ARG:CD	1:B:294:GLU:OE1	2.41	0.67
2:D:49:GLN:OE1	2:D:49:GLN:HA	1.94	0.67
2:C:77:LYS:HD2	2:C:77:LYS:C	2.20	0.67
1:A:295:ARG:CD	1:B:294:GLU:CD	2.66	0.67
1:A:625:MET:HE2	1:A:631:LYS:HG2	1.76	0.67
1:A:841:ILE:HG22	2:C:109:MET:CE	2.25	0.66
1:A:352:ARG:NH2	1:A:370:LYS:HD2	2.10	0.66
2:C:104:GLU:O	2:C:107:HIS:N	2.28	0.66
1:A:846:ARG:NH1	2:C:7:GLU:CD	2.54	0.66
2:C:31:GLU:O	2:C:35:VAL:HG12	1.96	0.66
2:C:95:ASP:OD2	2:C:97:ASN:CG	2.39	0.66
2:C:79:THR:HG21	2:C:84:GLU:OE1	1.96	0.66
1:A:296:LEU:CD2	1:B:258:VAL:HG12	2.23	0.65
1:A:625:MET:CE	1:A:631:LYS:HG2	2.25	0.65
1:A:845:TRP:CZ3	2:C:120:GLU:CD	2.74	0.65
1:A:844:PHE:HE2	2:C:85:ILE:HD13	1.52	0.65
2:C:55:VAL:HG13	2:C:61:GLY:N	2.12	0.65
1:A:835:THR:OG1	2:C:112:LEU:HD22	1.96	0.64
1:A:830:GLN:O	1:A:834:ARG:HG3	1.98	0.64
1:A:698:GLN:HE22	1:A:708:TYR:H	1.46	0.64
1:A:292:PHE:CZ	1:B:295:ARG:HD3	2.33	0.64
1:B:528:LYS:HE2	1:B:531:GLU:OE2	1.99	0.63
1:A:113:HIS:CD2	1:A:595:GLY:H	2.15	0.63
2:D:106:ARG:CG	2:D:125:ILE:HD11	2.28	0.63
1:A:845:TRP:HZ3	2:C:120:GLU:OE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:HE	1:B:262:ARG:HD2	1.64	0.62
1:A:611:GLN:OE1	1:A:674:HIS:CE1	2.52	0.62
1:A:294:GLU:O	1:A:294:GLU:HG3	1.98	0.62
2:D:143:GLN:HA	2:D:146:THR:HG22	1.81	0.62
1:A:842:GLN:HG3	2:C:109:MET:HE3	1.82	0.62
1:B:226:HIS:ND1	1:B:229:LYS:HE3	2.15	0.61
2:D:107:HIS:CD2	2:D:111:ASN:ND2	2.66	0.61
1:A:845:TRP:HZ3	2:C:120:GLU:CD	2.08	0.61
1:A:295:ARG:CG	1:B:294:GLU:OE1	2.49	0.61
1:A:296:LEU:HD11	1:B:262:ARG:HB2	1.76	0.61
2:D:128:ALA:HB1	2:D:136:VAL:HG13	1.83	0.61
1:A:292:PHE:HZ	1:B:295:ARG:HD3	1.65	0.61
2:C:95:ASP:OD2	2:C:97:ASN:ND2	2.34	0.60
1:B:324:HIS:HD2	1:B:326:TYR:H	1.49	0.59
1:A:844:PHE:HE2	2:C:85:ILE:CD1	2.12	0.59
2:D:8:GLN:NE2	2:D:76:MET:HE1	2.18	0.59
1:A:480:GLU:O	1:A:480:GLU:HG3	2.02	0.58
1:B:113:HIS:HE1	1:B:316:LYS:O	1.86	0.57
1:A:600:LEU:HD13	1:A:749:VAL:HG13	1.85	0.57
2:C:2:ASP:HB2	2:C:4:LEU:HG	1.85	0.57
1:A:495:PHE:HD2	1:A:501:GLU:HG2	1.68	0.57
1:B:352:ARG:NH1	1:B:373:GLU:OE2	2.38	0.57
1:A:495:PHE:CD2	1:A:501:GLU:HG2	2.40	0.57
2:D:13:LYS:HD2	2:D:65:PHE:CE2	2.39	0.56
1:A:352:ARG:HH22	1:A:373:GLU:CD	2.14	0.56
1:A:841:ILE:HG21	2:C:109:MET:SD	2.45	0.56
2:D:55:VAL:HG12	2:D:55:VAL:O	2.05	0.56
1:A:705:GLU:OE2	1:A:743:LYS:NZ	2.38	0.56
2:C:109:MET:CE	2:C:116:LEU:HD11	2.35	0.56
1:A:324:HIS:CE1	1:A:480:GLU:O	2.55	0.56
2:C:32:LEU:O	2:C:35:VAL:HG13	2.06	0.56
1:A:352:ARG:HH11	1:A:367:LYS:HE2	1.70	0.56
1:B:804:ARG:HE	1:B:836:ASN:HD21	1.53	0.56
2:D:8:GLN:HE21	2:D:76:MET:HE1	1.70	0.56
1:B:113:HIS:HD2	1:B:595:GLY:H	1.54	0.55
1:A:841:ILE:CG2	2:C:109:MET:SD	2.95	0.55
1:A:117:LEU:HD23	1:A:555:SER:HB3	1.88	0.55
1:A:801:PHE:CZ	2:C:15:ALA:HA	2.41	0.55
1:B:352:ARG:NH1	1:B:373:GLU:CD	2.62	0.55
1:B:352:ARG:NH1	1:B:373:GLU:OE1	2.39	0.55
1:B:475:PHE:HB3	1:B:653:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:MET:HE1	2:C:75:LYS:HD3	1.89	0.55
2:C:110:THR:HG23	2:C:121:VAL:CG2	2.35	0.55
1:A:258:VAL:HG12	1:B:296:LEU:HD11	1.89	0.55
2:C:43:PRO:HB3	2:C:75:LYS:HE3	1.87	0.54
2:C:98:GLY:HA2	2:C:138:TYR:CE2	2.43	0.54
2:C:109:MET:HB3	2:C:116:LEU:HD12	1.89	0.54
1:A:625:MET:HE1	1:A:631:LYS:N	2.22	0.54
1:A:423:LEU:O	1:A:424:ASP:HB2	2.07	0.54
1:B:677:GLN:NE2	1:B:740:GLU:H	2.00	0.54
2:C:26:THR:HB	2:C:62:THR:HB	1.89	0.54
2:C:127:GLU:CG	2:C:144:MET:HE1	2.38	0.54
1:A:520:LEU:HG	1:A:742:GLU:HG3	1.90	0.53
1:A:338:ARG:HD3	1:A:408:TYR:CE1	2.43	0.53
1:A:295:ARG:HB3	1:B:262:ARG:HD3	1.89	0.53
2:D:13:LYS:HA	2:D:65:PHE:CE1	2.43	0.53
1:B:341:MET:CE	1:B:354:LEU:HD12	2.38	0.53
1:A:261:PHE:HB3	1:A:267:PHE:CD2	2.43	0.53
1:A:493:THR:HB	1:A:522:ARG:NH1	2.24	0.53
1:A:846:ARG:NH2	2:C:114:GLU:HB2	2.21	0.52
1:B:852:LEU:O	1:B:853:SER:C	2.53	0.52
1:A:628:LYS:N	1:A:629:PRO:HD2	2.25	0.51
1:B:804:ARG:NE	1:B:836:ASN:HD21	2.08	0.51
2:C:127:GLU:HG2	2:C:144:MET:HE1	1.92	0.51
1:B:791:LEU:HD23	1:B:806:VAL:HG22	1.91	0.51
1:A:371:LYS:HA	1:A:433:ASP:OD1	2.11	0.51
2:C:28:THR:OG1	2:C:30:LYS:HB2	2.11	0.51
2:D:139:GLU:OE1	2:D:143:GLN:NE2	2.44	0.51
1:A:352:ARG:NH2	1:A:373:GLU:OE2	2.44	0.51
1:A:844:PHE:HD2	2:C:85:ILE:CD1	2.19	0.50
1:A:845:TRP:CH2	2:C:120:GLU:HA	2.45	0.50
2:C:104:GLU:O	2:C:106:ARG:N	2.45	0.50
1:B:266:VAL:HG11	1:B:277:TRP:CZ3	2.47	0.49
1:B:348:ARG:NH2	1:B:350:GLN:OE1	2.34	0.49
1:B:341:MET:HG2	1:B:356:PHE:CZ	2.47	0.49
1:B:324:HIS:CD2	1:B:325:HIS:N	2.80	0.49
2:D:28:THR:OG1	2:D:31:GLU:HG2	2.13	0.49
1:A:842:GLN:HG3	2:C:109:MET:CE	2.42	0.49
1:B:341:MET:HE3	1:B:366:VAL:HG11	1.94	0.49
2:C:32:LEU:O	2:C:35:VAL:CG1	2.61	0.49
2:C:55:VAL:CG1	2:C:61:GLY:N	2.75	0.49
1:B:113:HIS:CD2	1:B:595:GLY:H	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:GLN:HE21	2:C:76:MET:HE1	1.76	0.48
1:A:316:LYS:NZ	1:A:753:GLU:OE1	2.36	0.48
1:A:698:GLN:NE2	1:A:708:TYR:H	2.11	0.48
2:D:109:MET:HE2	2:D:124:MET:SD	2.53	0.48
1:A:622:THR:HA	1:A:625:MET:HG3	1.94	0.48
2:D:85:ILE:O	2:D:89:PHE:HD2	1.96	0.48
1:B:628:LYS:N	1:B:629:PRO:CD	2.77	0.48
1:B:189:ASN:OD1	6:B:1101:HOH:O	2.20	0.48
1:A:845:TRP:CZ2	2:C:120:GLU:HA	2.49	0.48
2:C:32:LEU:HA	2:C:35:VAL:CG1	2.44	0.48
1:A:324:HIS:HD2	1:A:326:TYR:H	1.60	0.48
1:A:567:LEU:HD21	1:A:594:PHE:CD1	2.50	0.47
2:D:8:GLN:NE2	2:D:76:MET:HE2	2.26	0.47
1:B:371:LYS:HE2	1:B:434:ASP:HB2	1.97	0.47
2:C:36:MET:HE3	2:C:36:MET:HB3	1.75	0.47
1:B:211:LYS:O	1:B:215:GLU:HG3	2.15	0.47
1:B:698:GLN:HE21	1:B:702:TYR:HE2	1.62	0.47
1:A:352:ARG:CD	1:A:368:VAL:O	2.50	0.47
1:B:198:LEU:HD23	1:B:198:LEU:N	2.30	0.47
1:A:296:LEU:HD21	1:B:258:VAL:CG1	2.31	0.47
1:B:526:TRP:NE1	1:B:727:GLN:HE21	2.00	0.47
1:B:345:ARG:O	1:B:356:PHE:HA	2.15	0.47
1:B:772:ILE:HG23	1:B:779:THR:CG2	2.45	0.47
1:A:694:LEU:HD23	1:A:698:GLN:HG3	1.96	0.47
1:B:524:ASP:O	1:B:525:LYS:C	2.57	0.47
1:A:521:GLY:CA	5:A:1004:AMP:O4'	2.63	0.47
1:A:296:LEU:HD13	1:B:262:ARG:CD	2.45	0.46
1:B:352:ARG:HD2	1:B:368:VAL:O	2.16	0.46
1:A:698:GLN:HE22	1:A:708:TYR:N	2.13	0.46
1:A:227:TYR:O	1:A:232:ARG:NH2	2.48	0.46
1:B:266:VAL:HG13	1:B:274:TYR:CD1	2.51	0.46
2:C:36:MET:CE	2:C:41:GLN:O	2.64	0.46
2:D:42:ASN:OD1	2:D:43:PRO:HD2	2.16	0.46
2:D:51:MET:O	2:D:55:VAL:HG23	2.16	0.46
1:A:846:ARG:HH11	2:C:7:GLU:CD	2.23	0.45
1:B:493:THR:HB	1:B:522:ARG:HH11	1.77	0.45
1:B:517:GLN:OE1	5:B:1004:AMP:H2'	2.16	0.45
2:C:144:MET:HG2	2:C:145:MET:HE2	1.97	0.45
2:D:145:MET:SD	2:D:145:MET:N	2.89	0.45
1:A:220:SER:OG	1:A:793:ASP:OD1	2.25	0.45
1:A:352:ARG:NH2	1:A:373:GLU:CD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:HB2	1:B:582:THR:HG22	1.98	0.45
2:D:98:GLY:HA2	2:D:138:TYR:CE2	2.52	0.45
1:A:338:ARG:HH11	1:A:338:ARG:HG2	1.80	0.45
1:B:844:PHE:CD1	2:D:85:ILE:HD13	2.52	0.45
1:A:101:GLN:O	1:A:102:TYR:HB3	2.16	0.45
1:A:567:LEU:CD2	1:A:594:PHE:CD1	3.00	0.45
1:B:113:HIS:CE1	1:B:316:LYS:O	2.69	0.45
1:A:296:LEU:HD13	1:B:262:ARG:CB	2.45	0.45
1:B:324:HIS:CD2	1:B:326:TYR:H	2.32	0.44
2:D:82:GLU:OE2	2:D:146:THR:HG21	2.17	0.44
1:A:225:ILE:HB	1:A:277:TRP:HA	2.00	0.44
1:A:420:ARG:HG3	1:A:420:ARG:HH21	1.82	0.44
1:A:152:ASP:OD1	1:A:156:LYS:HE3	2.18	0.44
1:B:391:HIS:CG	1:B:394:ARG:HH21	2.35	0.44
2:D:109:MET:HE3	2:D:116:LEU:CD1	2.48	0.44
1:A:341:MET:HE3	1:A:366:VAL:CG1	2.46	0.44
1:B:658:GLN:HE21	1:B:658:GLN:HB2	1.57	0.44
1:A:844:PHE:CZ	2:C:145:MET:HB2	2.53	0.44
1:B:698:GLN:HE22	1:B:708:TYR:HB3	1.82	0.44
1:A:271:ASN:N	1:A:272:PRO:HD2	2.33	0.43
1:A:841:ILE:HG22	2:C:109:MET:SD	2.57	0.43
1:A:625:MET:HE2	1:A:631:LYS:HA	1.95	0.43
1:B:627:ASP:HB2	1:B:630:LYS:HE2	2.00	0.43
2:C:106:ARG:HG2	2:C:125:ILE:HD11	2.00	0.43
2:C:110:THR:CG2	2:C:121:VAL:CG2	2.88	0.43
2:D:85:ILE:HG22	2:D:89:PHE:CE2	2.53	0.43
2:D:106:ARG:CZ	2:D:125:ILE:HD12	2.47	0.43
1:A:524:ASP:O	1:A:525:LYS:C	2.60	0.43
2:C:95:ASP:OD1	2:C:97:ASN:OD1	2.37	0.43
2:D:55:VAL:O	2:D:55:VAL:CG1	2.67	0.43
1:A:122:LYS:HE2	1:A:124:LEU:HD21	2.01	0.43
1:A:350:GLN:NE2	1:A:452:TYR:CE2	2.86	0.43
2:D:135:GLN:HA	2:D:135:GLN:NE2	2.33	0.43
1:A:560:LYS:O	1:A:564:SER:HB3	2.18	0.43
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.93	0.43
2:C:93:ASP:OD1	2:C:99:TYR:O	2.36	0.43
2:D:113:GLY:O	2:D:115:LYS:N	2.52	0.43
1:B:567:LEU:HD22	1:B:594:PHE:CD1	2.54	0.43
1:B:652:ILE:HG22	1:B:653:MET:CE	2.45	0.43
1:A:845:TRP:CH2	2:C:120:GLU:CA	3.02	0.43
1:B:196:LYS:HB3	1:B:197:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ARG:HG2	1:B:338:ARG:HH11	1.84	0.43
1:B:801:PHE:CD1	1:B:801:PHE:C	2.97	0.43
2:C:64:ASP:OD1	2:C:66:PRO:HD2	2.18	0.43
2:C:36:MET:CE	2:C:75:LYS:HD3	2.49	0.42
2:D:110:THR:HG22	2:D:121:VAL:HG21	2.02	0.42
1:A:341:MET:HE1	1:A:366:VAL:HG11	2.00	0.42
1:A:360:GLN:O	1:A:361:ASN:HB3	2.20	0.42
1:A:403:GLN:HA	1:A:404:PRO:HD2	1.94	0.42
2:C:64:ASP:OD1	2:C:64:ASP:C	2.62	0.42
1:A:149:THR:O	1:A:152:ASP:HB3	2.19	0.42
1:A:296:LEU:HD13	1:B:262:ARG:HD3	2.00	0.42
2:C:36:MET:HE3	2:C:41:GLN:O	2.20	0.42
2:D:54:GLU:O	2:D:54:GLU:HG2	2.19	0.42
1:A:837:ALA:O	1:A:841:ILE:HD13	2.19	0.42
1:B:528:LYS:CE	1:B:531:GLU:OE2	2.68	0.42
1:B:771:LYS:HB3	1:B:777:ILE:HG13	2.01	0.42
1:A:521:GLY:HA3	5:A:1004:AMP:O4'	2.20	0.42
1:B:352:ARG:HD3	1:B:370:LYS:HD3	2.02	0.42
1:B:508:ALA:O	1:B:520:LEU:HD21	2.20	0.42
1:A:271:ASN:HD21	1:A:312:ARG:HG2	1.85	0.41
1:B:627:ASP:HB3	1:B:630:LYS:HG3	2.02	0.41
1:B:660:ARG:NH1	2:D:14:GLU:OE2	2.49	0.41
2:D:117:THR:O	2:D:121:VAL:HG23	2.19	0.41
1:A:140:ARG:NH1	1:A:140:ARG:HG2	2.34	0.41
1:A:622:THR:HG22	1:A:625:MET:HE2	2.01	0.41
1:A:662:LEU:O	1:A:666:LYS:HG3	2.20	0.41
2:C:144:MET:HE2	2:C:145:MET:HE1	2.01	0.41
1:A:196:LYS:HB3	1:A:197:PRO:HD3	2.03	0.41
1:B:341:MET:HE2	1:B:354:LEU:HD12	2.01	0.41
2:C:43:PRO:HA	2:C:75:LYS:HE3	2.02	0.41
2:C:43:PRO:CB	2:C:75:LYS:HE3	2.50	0.41
1:B:173:LEU:HD21	1:B:213:ILE:HG23	2.01	0.41
1:B:792:LEU:HD23	1:B:792:LEU:HA	1.87	0.41
1:A:415:ILE:CD1	1:A:438:LEU:HD12	2.51	0.41
1:A:628:LYS:N	1:A:629:PRO:CD	2.83	0.41
1:A:822:THR:O	1:A:826:ASP:OD2	2.38	0.41
1:B:514:ASN:HB2	1:B:517:GLN:HG3	2.02	0.41
1:A:341:MET:HE3	1:A:366:VAL:CG2	2.44	0.41
1:A:424:ASP:O	1:A:425:PHE:C	2.63	0.41
1:A:675:PHE:CD1	1:A:675:PHE:C	2.98	0.41
1:A:807:LEU:O	1:A:810:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:PRO:CA	2:C:75:LYS:HE3	2.50	0.41
2:C:109:MET:HE2	2:C:116:LEU:CD1	2.45	0.41
1:A:350:GLN:NE2	1:A:452:TYR:CZ	2.88	0.41
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.89	0.41
1:A:611:GLN:OE1	1:A:674:HIS:HE1	1.99	0.41
1:A:773:LEU:HD23	1:A:773:LEU:HA	1.88	0.41
1:B:352:ARG:CZ	1:B:370:LYS:HD3	2.51	0.41
1:B:768:GLN:O	1:B:772:ILE:HG12	2.21	0.41
2:D:48:LEU:O	2:D:49:GLN:C	2.63	0.41
1:A:698:GLN:HE21	1:A:702:TYR:HE2	1.69	0.41
1:B:627:ASP:CG	1:B:629:PRO:HD2	2.46	0.41
1:A:152:ASP:OD1	1:A:156:LYS:CE	2.69	0.40
1:A:412:LYS:O	1:A:413:SER:C	2.62	0.40
1:B:799:CYS:SG	1:B:801:PHE:CE2	3.14	0.40
2:C:100:ILE:HG22	2:C:101:SER:H	1.86	0.40
1:B:160:LEU:HD11	1:B:198:LEU:HD22	2.02	0.40
1:B:213:ILE:HD13	1:B:213:ILE:HG21	1.82	0.40
1:A:526:TRP:HE1	1:A:727:GLN:NE2	1.97	0.40
1:B:436:LYS:HA	1:B:436:LYS:HD3	1.91	0.40
1:B:563:PHE:O	1:B:567:LEU:HG	2.21	0.40
2:C:100:ILE:O	2:C:135:GLN:HG3	2.21	0.40
1:A:263:ASP:OD1	1:A:299:ASN:ND2	2.48	0.40
1:A:399:SER:OG	1:A:539:GLY:HA3	2.22	0.40
1:A:723:ASP:OD2	1:A:726:HIS:HD2	2.04	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	744/757 (98%)	710 (95%)	34 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	748/757 (99%)	723 (97%)	25 (3%)	0	100	100
2	C	128/147 (87%)	119 (93%)	9 (7%)	0	100	100
2	D	141/147 (96%)	131 (93%)	10 (7%)	0	100	100
All	All	1761/1808 (97%)	1683 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	678/685 (99%)	656 (97%)	22 (3%)	34	62
1	B	681/685 (99%)	658 (97%)	23 (3%)	32	60
2	C	116/124 (94%)	110 (95%)	6 (5%)	21	44
2	D	122/124 (98%)	110 (90%)	12 (10%)	7	17
All	All	1597/1618 (99%)	1534 (96%)	63 (4%)	28	55

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	161	ASN
1	A	177	SER
1	A	219	LYS
1	A	231	ASN
1	A	252	LYS
1	A	258	VAL
1	A	266	VAL
1	A	321	SER
1	A	422	SER
1	A	432	ILE
1	A	486	GLN
1	A	528	LYS

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Mol	Chain	Res	Type
1	A	578	LYS
1	A	672	GLU
1	A	675	PHE
1	A	697	GLU
1	A	749	VAL
1	A	790	GLN
1	A	791	LEU
1	A	835	THR
1	A	842	GLN
1	B	116	SER
1	B	159	LYS
1	B	167	GLN
1	B	190	GLN
1	B	198	LEU
1	B	239	LEU
1	B	266	VAL
1	B	296	LEU
1	B	299	ASN
1	B	336	SER
1	B	422	SER
1	B	430	THR
1	B	432	ILE
1	B	503	LYS
1	B	564	SER
1	B	675	PHE
1	B	694	LEU
1	B	709	GLU
1	B	722	VAL
1	B	749	VAL
1	B	772	ILE
1	B	779	THR
1	B	852	LEU
2	C	30	LYS
2	C	35	VAL
2	C	54	GLU
2	C	55	VAL
2	C	119	GLU
2	C	121	VAL
2	D	3	GLN
2	D	29	THR
2	D	49	GLN
2	D	54	GLU

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Mol	Chain	Res	Type
2	D	62	THR
2	D	87	GLU
2	D	95	ASP
2	D	108	VAL
2	D	133	ASP
2	D	142	VAL
2	D	143	GLN
2	D	146	THR

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

Mol	Chain	Res	Type
1	A	113	HIS
1	A	180	ASN
1	A	231	ASN
1	A	271	ASN
1	A	324	HIS
1	A	340	GLN
1	A	360	GLN
1	A	392	GLN
1	A	457	ASN
1	A	494	HIS
1	A	507	GLN
1	A	527	GLN
1	A	674	HIS
1	A	698	GLN
1	A	726	HIS
1	A	727	GLN
1	A	733	ASN
1	A	757	GLN
1	B	113	HIS
1	B	180	ASN
1	B	190	GLN
1	B	243	HIS
1	B	254	GLN
1	B	299	ASN
1	B	324	HIS
1	B	392	GLN
1	B	584	ASN
1	B	658	GLN
1	B	674	HIS
1	B	677	GLN

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Mol	Chain	Res	Type
1	B	698	GLN
1	B	727	GLN
1	B	765	GLN
1	B	768	GLN
1	B	782	ASN
1	B	836	ASN
2	C	3	GLN
2	C	111	ASN
2	C	135	GLN
2	D	60	ASN
2	D	107	HIS
2	D	135	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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	$\# Z > 2$
5	AMP	B	1004	-	25,25,25	2.69	8 (32%)	37,38,38	3.01	12 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AMP	A	1004	-	25,25,25	2.14	7 (28%)	37,38,38	2.20	11 (29%)
4	POP	B	1003	3	6,8,8	1.18	0	12,13,13	1.29	1 (8%)
4	POP	A	1003	3	6,8,8	0.79	0	12,13,13	2.15	5 (41%)

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
5	AMP	B	1004	-	-	6/10/26/26	0/3/3/3
5	AMP	A	1004	-	-	1/10/26/26	0/3/3/3
4	POP	B	1003	3	-	3/6/6/6	-
4	POP	A	1003	3	-	2/6/6/6	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	AMP	C5-C4	7.53	1.52	1.39
5	A	1004	AMP	C5-C4	6.79	1.51	1.39
5	B	1004	AMP	C5-C6	5.68	1.56	1.41
5	B	1004	AMP	C4-N3	5.04	1.43	1.34
5	A	1004	AMP	C5-C6	4.64	1.53	1.41
5	B	1004	AMP	C1'-N9	4.10	1.57	1.46
5	B	1004	AMP	C8-N7	3.62	1.38	1.31
5	A	1004	AMP	C4-N3	2.93	1.39	1.34
5	B	1004	AMP	C2-N3	2.87	1.39	1.33
5	A	1004	AMP	C2-N3	2.74	1.38	1.33
5	A	1004	AMP	C8-N7	2.64	1.36	1.31
5	A	1004	AMP	C1'-N9	2.57	1.53	1.46
5	A	1004	AMP	C2-N1	2.55	1.38	1.33
5	B	1004	AMP	C4-N9	2.42	1.42	1.37
5	B	1004	AMP	C2-N1	2.08	1.37	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	AMP	C5-C4-N3	-9.02	114.30	126.72
5	B	1004	AMP	N3-C4-N9	6.45	138.13	127.17
5	A	1004	AMP	C5-C4-N3	-6.44	117.85	126.72
5	B	1004	AMP	O4'-C1'-N9	6.29	120.17	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	AMP	C2-N3-C4	5.77	125.93	111.83
5	B	1004	AMP	C3'-C2'-C1'	5.19	111.28	101.46
5	A	1004	AMP	N3-C4-N9	5.17	135.95	127.17
5	B	1004	AMP	C4-C5-N7	-4.75	105.15	110.58
5	A	1004	AMP	C2-N3-C4	4.35	122.45	111.83
5	B	1004	AMP	N3-C2-N1	-4.20	122.23	128.58
5	A	1004	AMP	N3-C2-N1	-3.79	122.84	128.58
5	A	1004	AMP	C4-C5-N7	-3.65	106.40	110.58
4	A	1003	POP	O-P1-O1	-3.57	92.25	111.04
5	B	1004	AMP	O4'-C1'-C2'	-3.44	99.25	106.62
4	A	1003	POP	O6-P2-O	-3.38	93.29	104.64
5	B	1004	AMP	C5-N7-C8	3.29	108.62	103.45
4	A	1003	POP	O5-P2-O	3.26	115.58	104.64
5	B	1004	AMP	C6-C5-N7	3.18	138.23	132.09
5	B	1004	AMP	O3'-C3'-C2'	2.79	120.77	111.82
5	A	1004	AMP	C6-C5-N7	2.77	137.44	132.09
5	A	1004	AMP	O2P-P-O5'	-2.65	99.76	106.67
4	A	1003	POP	O3-P1-O	2.65	113.52	104.64
4	A	1003	POP	O2-P1-O	2.49	112.99	104.64
5	A	1004	AMP	C5-N7-C8	2.44	107.28	103.45
5	B	1004	AMP	C4'-O4'-C1'	2.39	114.73	109.47
5	A	1004	AMP	C4-N9-C8	2.28	108.13	105.74
4	B	1003	POP	O6-P2-O5	2.22	116.11	107.80
5	A	1004	AMP	C4'-O4'-C1'	2.13	114.17	109.47
5	A	1004	AMP	C2'-C1'-N9	2.07	118.44	113.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

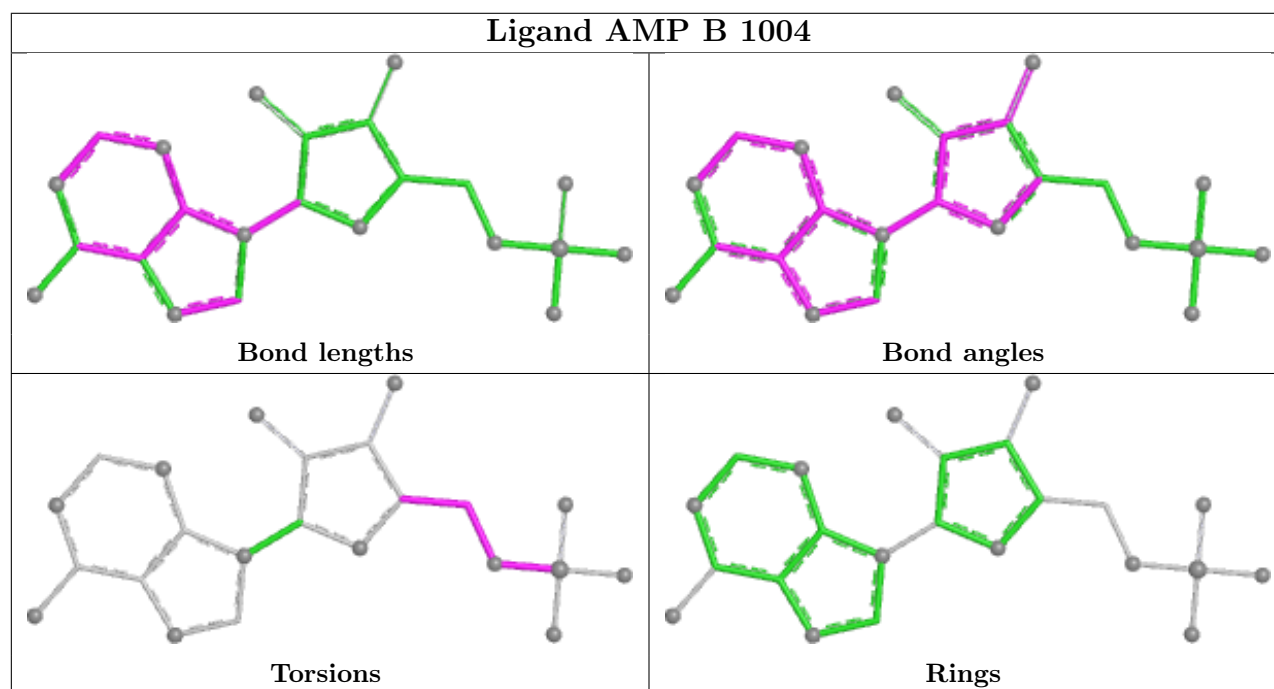
Mol	Chain	Res	Type	Atoms
4	A	1003	POP	P2-O-P1-O2
5	B	1004	AMP	C5'-O5'-P-O2P
5	B	1004	AMP	C5'-O5'-P-O3P
5	B	1004	AMP	C4'-C5'-O5'-P
5	B	1004	AMP	C5'-O5'-P-O1P
5	B	1004	AMP	O4'-C4'-C5'-O5'
4	B	1003	POP	P1-O-P2-O4
5	A	1004	AMP	C4'-C5'-O5'-P
5	B	1004	AMP	C3'-C4'-C5'-O5'
4	A	1003	POP	P2-O-P1-O3
4	B	1003	POP	P1-O-P2-O5
4	B	1003	POP	P1-O-P2-O6

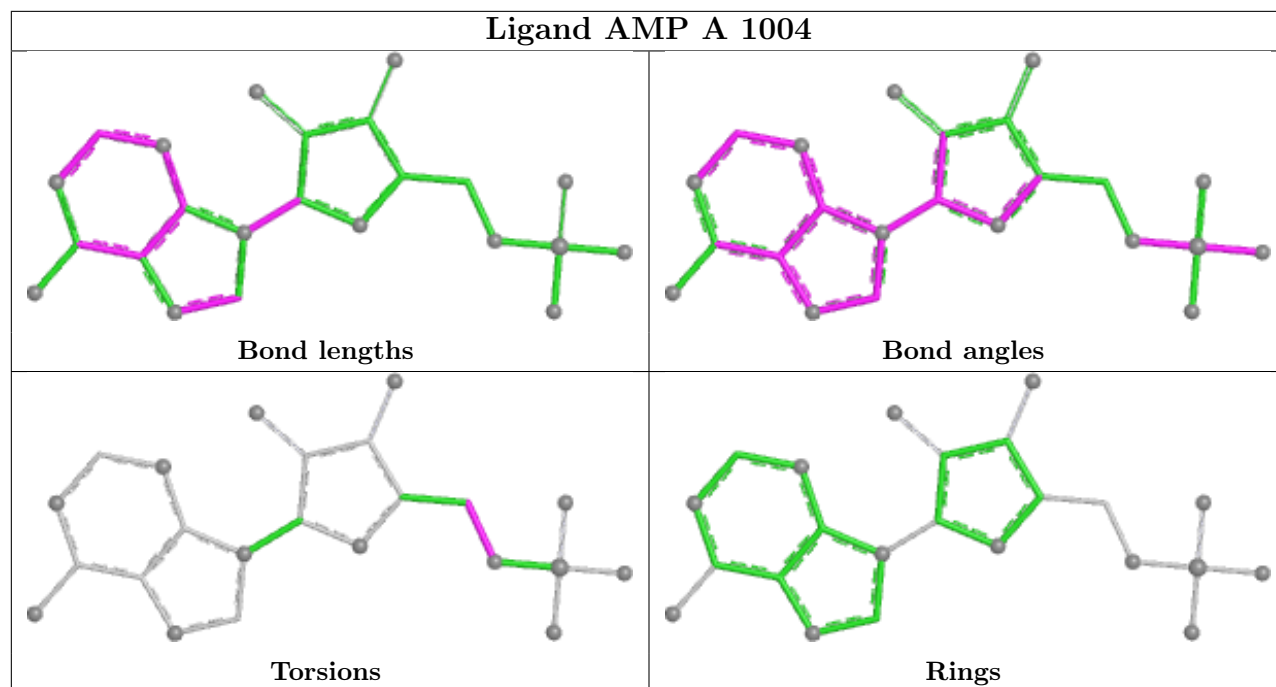
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	AMP	1	0
5	A	1004	AMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th 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 ²)	Q<0.9
1	A	748/757 (98%)	-0.18	11 (1%) 72 68	30, 56, 96, 147	0
1	B	752/757 (99%)	-0.36	5 (0%) 84 82	30, 50, 85, 132	0
2	C	134/147 (91%)	0.84	17 (12%) 8 6	62, 118, 152, 167	0
2	D	145/147 (98%)	0.36	8 (5%) 30 25	40, 94, 130, 156	0
All	All	1779/1808 (98%)	-0.13	41 (2%) 61 55	30, 56, 122, 167	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	846	ARG	7.2
1	A	501	GLU	6.8
1	A	849	ARG	6.7
1	A	847	GLU	5.5
1	A	850	LYS	5.3
2	C	55	VAL	4.9
1	A	848	ALA	4.8
1	A	845	TRP	4.2
2	D	128	ALA	3.9
2	C	136	VAL	3.8
2	D	131	ASP	3.6
2	C	134	GLY	3.5
1	B	852	LEU	3.5
2	C	51	MET	3.3
1	A	844	PHE	3.1
2	C	112	LEU	3.0
1	A	495	PHE	3.0
1	B	503	LYS	2.9
2	C	138	TYR	2.9
2	D	1	ALA	2.7
1	B	296	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	103	ALA	2.6
1	A	295	ARG	2.6
2	D	57	ALA	2.6
1	B	493	THR	2.5
2	C	102	ALA	2.5
2	C	73	ALA	2.4
2	C	92	PHE	2.4
2	C	52	ILE	2.4
2	C	141	PHE	2.4
2	C	145	MET	2.3
2	D	125	ILE	2.3
2	D	132	GLY	2.2
1	B	847	GLU	2.2
2	C	89	PHE	2.2
2	C	48	LEU	2.2
2	C	100	ILE	2.2
2	C	49	GLN	2.1
2	D	147	ALA	2.0
1	A	815	LEU	2.0
2	D	85	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
5	AMP	B	1004	23/23	0.68	0.18	73,103,168,177	0
5	AMP	A	1004	23/23	0.77	0.14	78,96,169,183	0
3	CA	C	201	1/1	0.94	0.09	102,102,102,102	0

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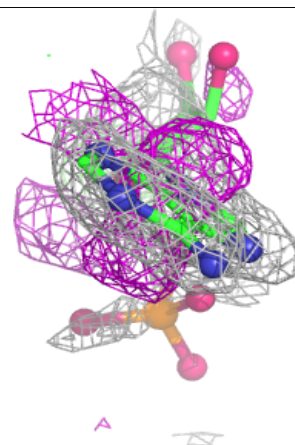
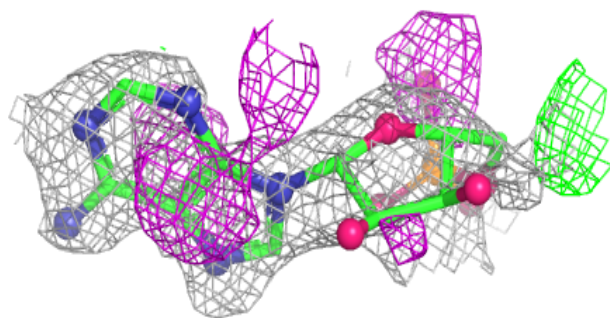
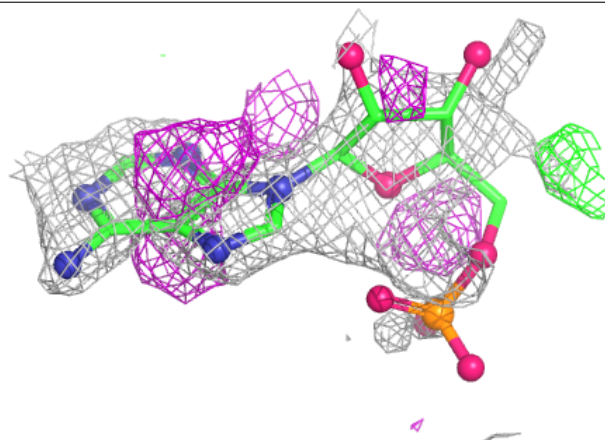
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	POP	A	1003	9/9	0.94	0.09	45,49,55,58	0
3	CA	B	1002	1/1	0.96	0.04	55,55,55,55	0
3	CA	B	1001	1/1	0.96	0.04	57,57,57,57	0
3	CA	D	201	1/1	0.96	0.06	79,79,79,79	0
3	CA	A	1001	1/1	0.97	0.05	57,57,57,57	0
4	POP	B	1003	9/9	0.97	0.09	50,51,55,56	0
3	CA	A	1002	1/1	0.98	0.03	53,53,53,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

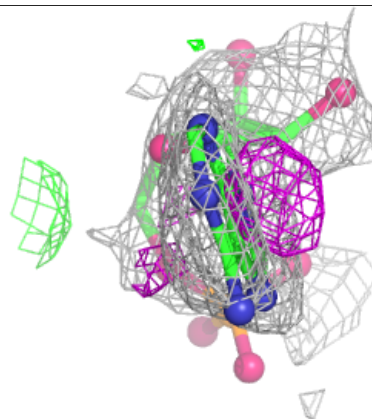
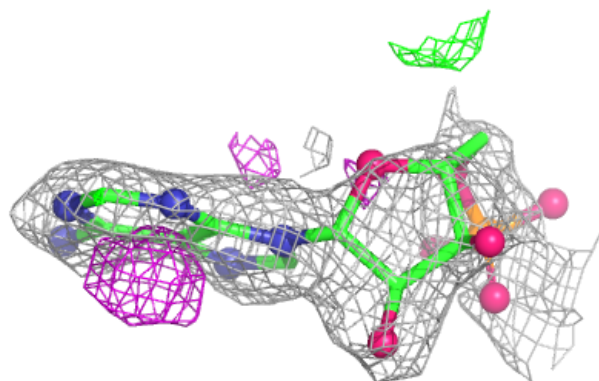
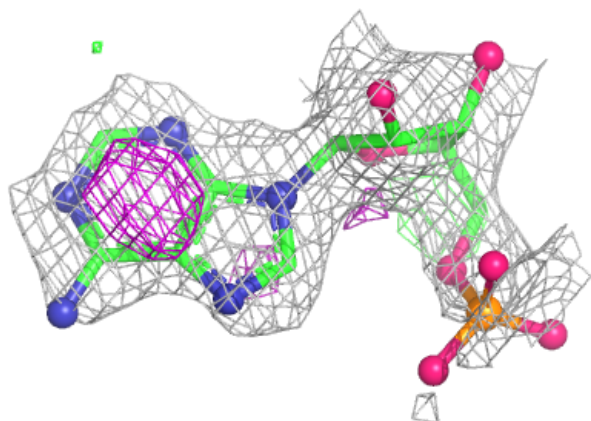
Electron density around AMP B 1004:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP A 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.