



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:34 PM UTC

PDB ID : 5VYZ / pdb_00005vyz
Title : Crystal structure of Lactococcus lactis pyruvate carboxylase in complex with cyclic-di-AMP
Authors : Choi, P.H.; Tong, L.
Deposited on : 2017-05-26
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

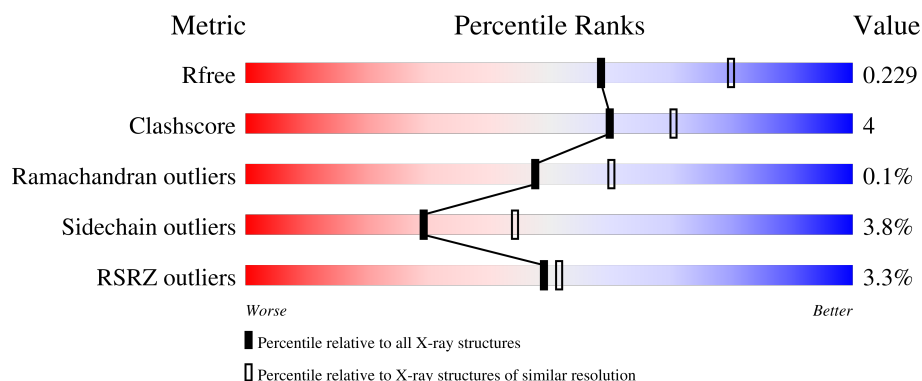
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

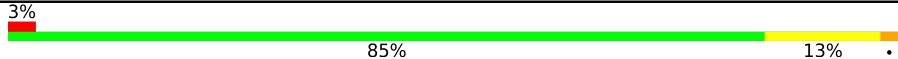
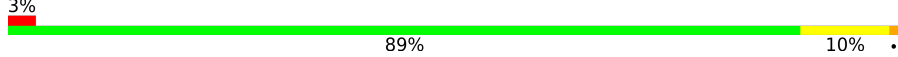
The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1145	
1	B	1145	
1	C	1145	
1	D	1145	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36479 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1144	Total	C	N	O	S	0	0	0
			8956	5677	1547	1697	35			
1	B	1142	Total	C	N	O	S	0	0	0
			8934	5665	1539	1695	35			
1	C	1083	Total	C	N	O	S	0	0	0
			8520	5406	1470	1612	32			
1	D	1144	Total	C	N	O	S	0	0	0
			8946	5670	1544	1697	35			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A089XIW4
A	-6	LEU	-	expression tag	UNP A0A089XIW4
A	-5	VAL	-	expression tag	UNP A0A089XIW4
A	-4	PRO	-	expression tag	UNP A0A089XIW4
A	-3	ARG	-	expression tag	UNP A0A089XIW4
A	-2	GLY	-	expression tag	UNP A0A089XIW4
A	-1	SER	-	expression tag	UNP A0A089XIW4
A	0	HIS	-	expression tag	UNP A0A089XIW4
A	1055	ALA	THR	conflict	UNP A0A089XIW4
B	-7	GLY	-	expression tag	UNP A0A089XIW4
B	-6	LEU	-	expression tag	UNP A0A089XIW4
B	-5	VAL	-	expression tag	UNP A0A089XIW4
B	-4	PRO	-	expression tag	UNP A0A089XIW4
B	-3	ARG	-	expression tag	UNP A0A089XIW4
B	-2	GLY	-	expression tag	UNP A0A089XIW4
B	-1	SER	-	expression tag	UNP A0A089XIW4
B	0	HIS	-	expression tag	UNP A0A089XIW4
B	1055	ALA	THR	conflict	UNP A0A089XIW4
C	-7	GLY	-	expression tag	UNP A0A089XIW4
C	-6	LEU	-	expression tag	UNP A0A089XIW4
C	-5	VAL	-	expression tag	UNP A0A089XIW4

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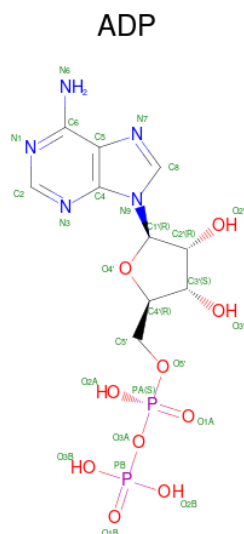
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A089XIW4
C	-3	ARG	-	expression tag	UNP A0A089XIW4
C	-2	GLY	-	expression tag	UNP A0A089XIW4
C	-1	SER	-	expression tag	UNP A0A089XIW4
C	0	HIS	-	expression tag	UNP A0A089XIW4
C	1055	ALA	THR	conflict	UNP A0A089XIW4
D	-7	GLY	-	expression tag	UNP A0A089XIW4
D	-6	LEU	-	expression tag	UNP A0A089XIW4
D	-5	VAL	-	expression tag	UNP A0A089XIW4
D	-4	PRO	-	expression tag	UNP A0A089XIW4
D	-3	ARG	-	expression tag	UNP A0A089XIW4
D	-2	GLY	-	expression tag	UNP A0A089XIW4
D	-1	SER	-	expression tag	UNP A0A089XIW4
D	0	HIS	-	expression tag	UNP A0A089XIW4
D	1055	ALA	THR	conflict	UNP A0A089XIW4

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

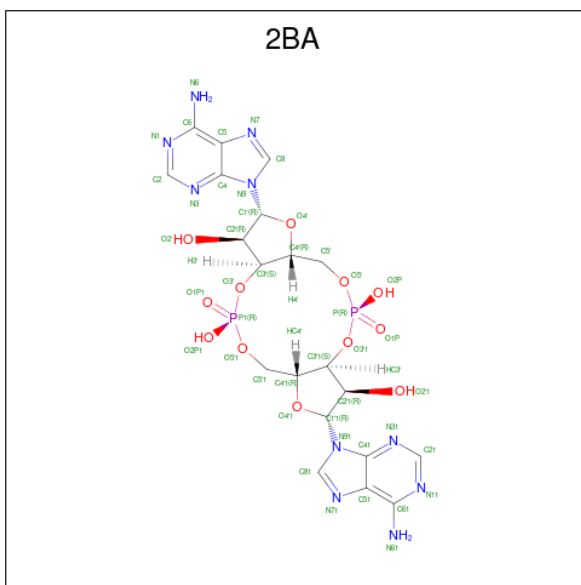


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is (2R,3R,3aS,5R,7aR,9R,10R,10aS,12R,14aR)-2,9-bis(6-amino-9H-purin-9-yl)octahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-3,5,10,12-tetrol 5,12-dioxide (CCD ID: 2BA) (formula: $C_{20}H_{24}N_{10}O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 20	N 10	O 12	P 2	0	0
5	D	1	Total 44	C 20	N 10	O 12	P 2	0	0

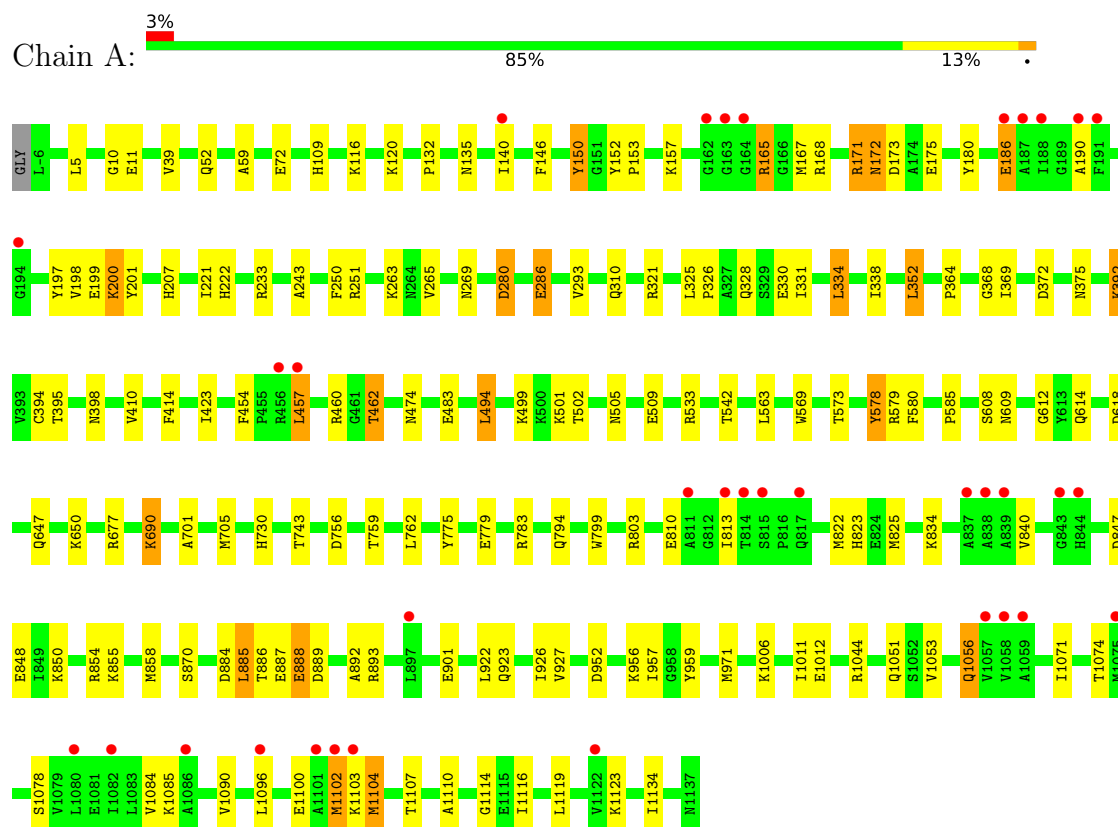
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O 210 210	0	0
6	B	243	Total O 243 243	0	0
6	C	220	Total O 220 220	0	0
6	D	246	Total O 246 246	0	0

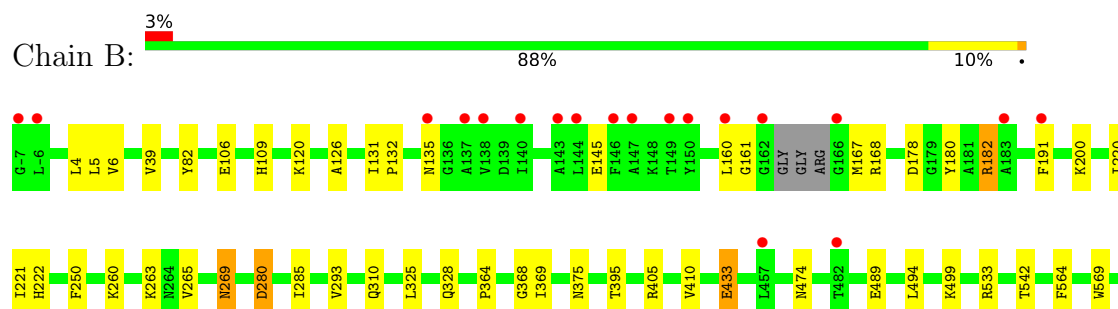
3 Residue-property plots [i](#)

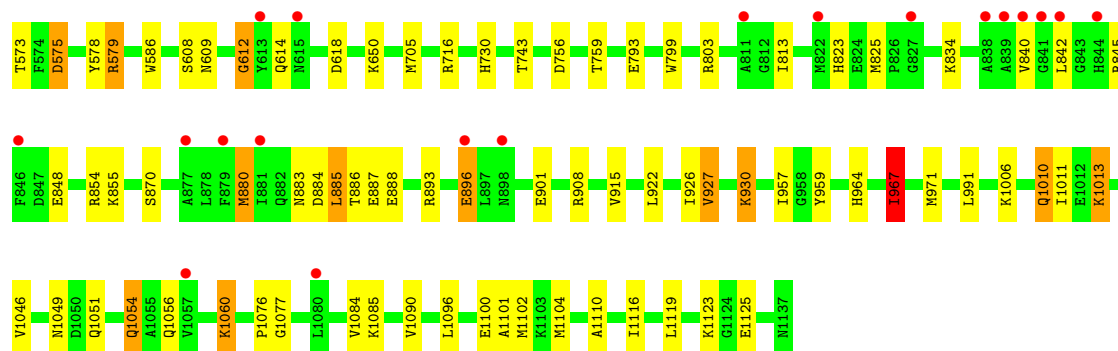
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyruvate carboxylase

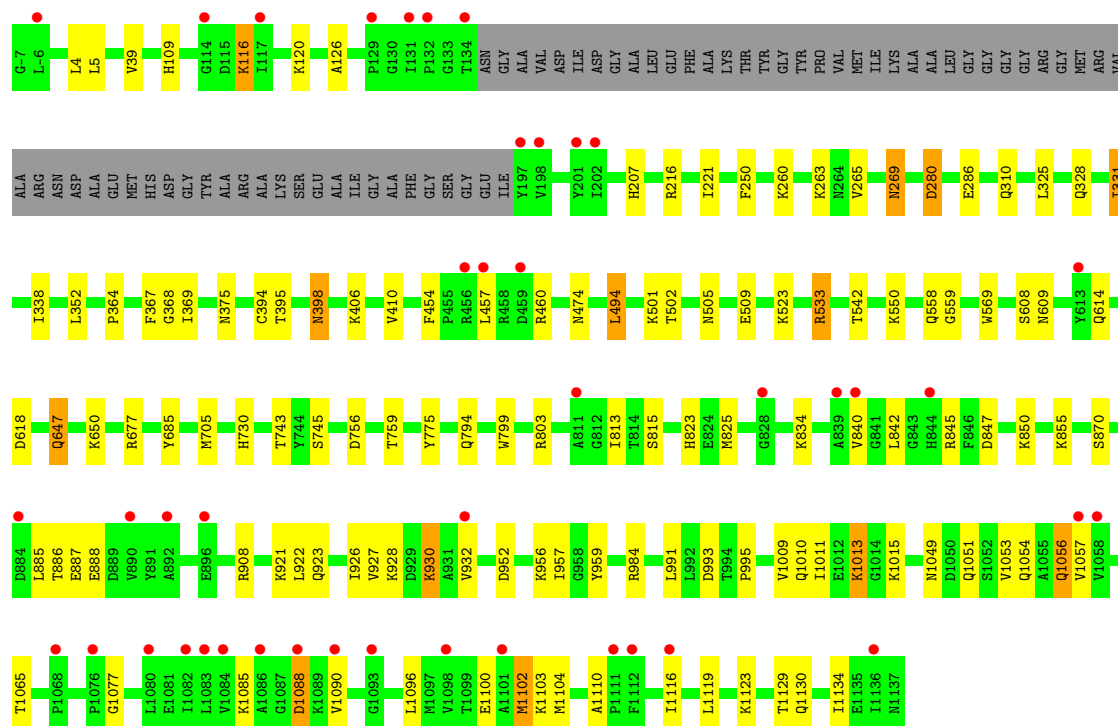
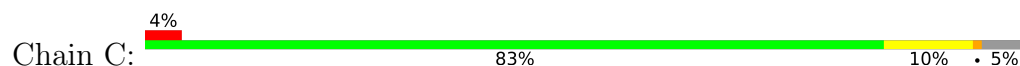


• Molecule 1: Pyruvate carboxylase

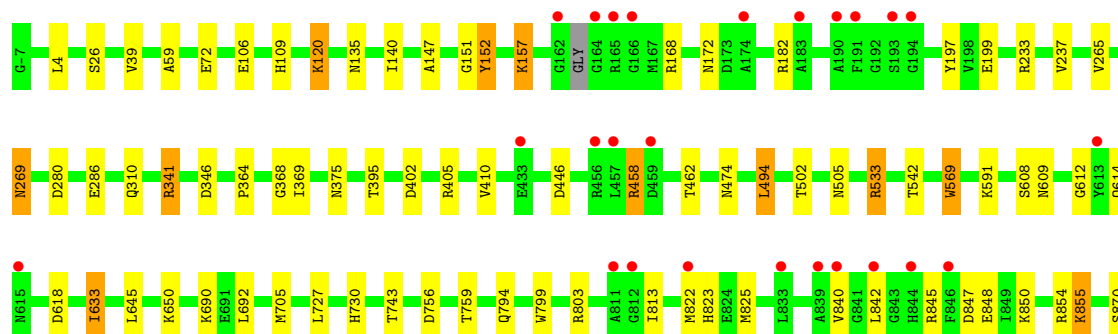
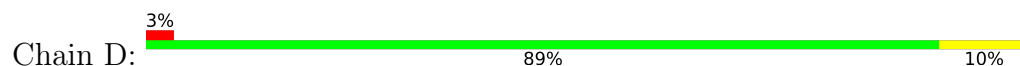


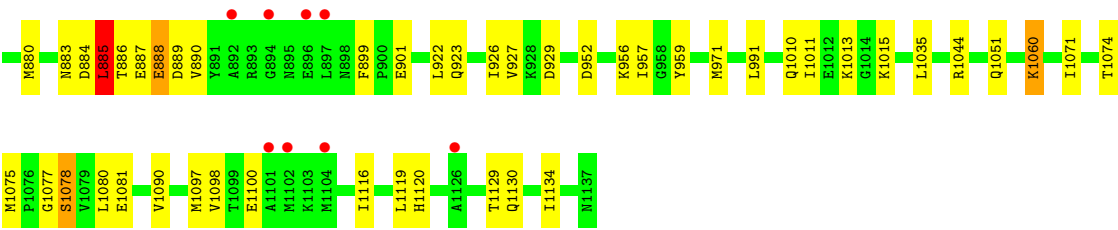


• Molecule 1: Pyruvate carboxylase



• Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.27Å 130.43Å 133.37Å 66.08° 89.05° 70.60°	Depositor
Resolution (Å)	48.60 – 2.30 48.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (48.60-2.30) 89.8 (48.60-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.221 0.193 , 0.229	Depositor DCC
R_{free} test set	11256 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36479	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: ADP, MG, MN, 2BA

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	1.13	13/9130 (0.1%)	1.03	17/12354 (0.1%)
1	B	1.09	6/9107 (0.1%)	1.01	10/12323 (0.1%)
1	C	1.09	4/8686 (0.0%)	1.01	8/11756 (0.1%)
1	D	1.09	3/9119 (0.0%)	1.02	10/12338 (0.1%)
All	All	1.10	26/36042 (0.1%)	1.02	45/48771 (0.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	573	THR	C-O	-6.62	1.16	1.24
1	A	690	LYS	C-O	-6.28	1.16	1.24
1	A	573	THR	C-O	-6.17	1.16	1.24
1	B	612	GLY	N-CA	6.16	1.49	1.44
1	C	647	GLN	C-O	-6.10	1.16	1.24
1	A	580	PHE	C-O	-6.04	1.16	1.23
1	D	533	ARG	N-CA	5.95	1.53	1.46
1	C	1009	VAL	C-O	-5.89	1.17	1.24
1	C	558	GLN	C-O	-5.88	1.17	1.24
1	A	579	ARG	C-O	-5.85	1.17	1.24
1	B	575	ASP	C-O	-5.70	1.17	1.24
1	A	578	TYR	C-O	-5.51	1.17	1.24
1	C	685	TYR	C-O	-5.49	1.17	1.24
1	A	372	ASP	C-O	5.47	1.30	1.24
1	A	462	THR	C-O	-5.44	1.17	1.24
1	A	779	GLU	N-CA	5.43	1.52	1.46
1	A	563	LEU	C-O	-5.36	1.17	1.23
1	D	59	ALA	C-O	-5.35	1.17	1.24
1	B	579	ARG	C-O	-5.32	1.18	1.24
1	B	967	ILE	CA-CB	5.30	1.61	1.54
1	A	762	LEU	N-CA	5.22	1.52	1.46
1	B	578	TYR	C-O	-5.18	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ALA	C-O	-5.17	1.18	1.24
1	D	402	ASP	CB-CG	5.07	1.64	1.52
1	A	423	ILE	CA-CB	5.05	1.57	1.53
1	A	647	GLN	C-O	-5.04	1.17	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1104	MET	N-CA-C	-9.51	95.68	110.42
1	D	633	ILE	CA-CB-CG1	-8.54	95.88	110.40
1	D	341	ARG	NE-CZ-NH2	8.46	126.81	119.20
1	D	633	ILE	CB-CG1-CD1	8.31	131.25	113.80
1	A	579	ARG	N-CA-C	8.15	120.24	111.36
1	D	341	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	C	1056	GLN	N-CA-C	7.83	121.54	110.50
1	A	172	ASN	CB-CA-C	-7.80	96.11	110.62
1	D	152	TYR	C-N-CD	7.28	136.61	120.60
1	A	152	TYR	C-N-CD	7.20	136.44	120.60
1	B	1056	GLN	N-CA-C	6.86	120.17	110.23
1	B	579	ARG	N-CA-C	6.80	118.48	111.14
1	A	150	TYR	N-CA-C	6.77	121.83	113.50
1	A	286	GLU	CB-CA-C	-6.51	98.25	110.16
1	C	550	LYS	CB-CA-C	-6.50	98.19	110.67
1	B	967	ILE	N-CA-CB	6.20	121.98	110.77
1	A	885	LEU	N-CA-C	6.16	119.28	109.24
1	D	885	LEU	N-CA-C	6.14	118.96	109.07
1	D	286	GLU	CB-CA-C	-6.13	99.22	110.62
1	A	810	GLU	CA-CB-CG	6.04	126.17	114.10
1	C	454	PHE	CA-C-N	-5.90	114.19	120.03
1	C	454	PHE	C-N-CA	-5.90	114.19	120.03
1	B	880	MET	N-CA-C	5.89	117.70	111.28
1	C	559	GLY	N-CA-C	5.82	120.21	112.77
1	A	334	LEU	N-CA-C	5.81	118.28	107.99
1	A	892	ALA	N-CA-C	5.74	117.34	111.14
1	D	1097	MET	N-CA-CB	-5.68	102.92	111.56
1	A	810	GLU	CB-CA-C	5.66	118.75	110.26
1	C	885	LEU	N-CA-C	5.63	118.13	109.07
1	A	454	PHE	CA-C-N	-5.59	114.50	120.03
1	A	454	PHE	C-N-CA	-5.59	114.50	120.03
1	D	237	VAL	N-CA-C	-5.49	107.28	111.62
1	D	405	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	564	PHE	N-CA-C	-5.34	105.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	716	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	285	ILE	N-CA-C	5.29	116.56	112.12
1	A	783	ARG	CG-CD-NE	-5.14	100.68	112.00
1	A	352	LEU	CA-C-N	-5.10	114.36	120.13
1	A	352	LEU	C-N-CA	-5.10	114.36	120.13
1	A	1056	GLN	N-CA-C	5.09	117.61	110.23
1	C	460	ARG	CA-C-N	5.07	125.71	120.03
1	C	460	ARG	C-N-CA	5.07	125.71	120.03
1	B	573	THR	N-CA-C	5.06	116.80	111.28
1	B	854	ARG	CG-CD-NE	-5.02	100.95	112.00
1	A	52	GLN	CB-CA-C	-5.00	102.75	109.71

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	8956	0	8931	88	0
1	B	8934	0	8899	79	0
1	C	8520	0	8510	75	0
1	D	8946	0	8906	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
3	C	27	0	12	3	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	44	0	23	0	0
5	D	44	0	23	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	210	0	0	3	0
6	B	243	0	0	6	0
6	C	220	0	0	6	0
6	D	246	0	0	4	0
All	All	36479	0	35340	303	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 4.

All (303) 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:B:915:VAL:HG23	6:B:1317:HOH:O	1.48	1.14
1:A:886:THR:HG22	1:A:888:GLU:OE2	1.58	1.04
1:D:690:LYS:HE2	6:D:1443:HOH:O	1.65	0.94
1:D:1078:SER:OG	1:D:1100:GLU:OE2	1.87	0.93
1:B:1010:GLN:HG3	6:B:1309:HOH:O	1.68	0.92
1:C:618:ASP:OD2	1:C:650:LYS:HE2	1.69	0.92
1:A:222:HIS:H	1:A:328:GLN:HE22	1.19	0.91
1:C:501:LYS:NZ	1:C:509:GLU:OE1	2.03	0.91
1:B:1060:LYS:HE3	1:B:1125:GLU:OE2	1.69	0.91
1:D:1078:SER:OG	1:D:1100:GLU:CG	2.19	0.90
1:B:880:MET:HA	1:B:885:LEU:CD1	2.02	0.90
1:C:677:ARG:HD3	6:C:1379:HOH:O	1.72	0.89
1:D:1060:LYS:NZ	1:D:1120:HIS:O	2.05	0.89
1:D:1078:SER:OG	1:D:1100:GLU:CD	2.18	0.86
1:A:886:THR:CG2	1:A:888:GLU:CD	2.53	0.82
1:B:880:MET:HA	1:B:885:LEU:HD12	1.60	0.81
1:B:405:ARG:NH2	6:B:1301:HOH:O	2.13	0.81
1:B:1076:PRO:HG3	6:B:1486:HOH:O	1.80	0.81
1:A:1078:SER:HB3	1:A:1100:GLU:OE1	1.80	0.81
1:A:618:ASP:OD2	1:A:650:LYS:HE2	1.82	0.79
1:C:1119:LEU:HD13	1:C:1134:ILE:HG12	1.63	0.79
1:A:886:THR:CG2	1:A:888:GLU:OE2	2.31	0.79
1:B:1049:ASN:HD21	1:B:1054:GLN:CD	1.92	0.78
1:D:609:ASN:OD1	1:D:614:GLN:O	2.04	0.76
1:D:618:ASP:OD2	1:D:650:LYS:HE2	1.85	0.75
1:C:608:SER:HB3	1:C:647:GLN:OE1	1.86	0.75
1:A:886:THR:HG21	1:A:888:GLU:CD	2.12	0.74
1:D:1078:SER:OG	1:D:1100:GLU:HG3	1.85	0.74
1:C:1049:ASN:HD21	1:C:1054:GLN:HG3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:HIS:H	1:B:328:GLN:HE22	1.34	0.72
1:B:927:VAL:O	1:B:930:LYS:HG2	1.88	0.72
1:A:886:THR:HG22	1:A:888:GLU:CD	2.13	0.71
1:C:328:GLN:HA	1:C:331:ILE:HD12	1.73	0.71
1:C:984:ARG:HD2	6:C:1456:HOH:O	1.91	0.70
1:B:369:ILE:HD12	1:B:410:VAL:HG21	1.74	0.70
1:D:823:HIS:HD2	1:D:825:MET:H	1.39	0.70
1:C:369:ILE:HD12	1:C:410:VAL:HG21	1.73	0.69
1:C:608:SER:OG	1:C:609:ASN:OD1	2.09	0.69
1:A:369:ILE:HD12	1:A:410:VAL:HG21	1.74	0.69
1:C:618:ASP:OD2	1:C:650:LYS:CE	2.40	0.69
1:D:152:TYR:CE2	1:D:172:ASN:HA	2.28	0.68
1:B:823:HIS:HD2	1:B:825:MET:H	1.40	0.68
1:A:823:HIS:HD2	1:A:825:MET:H	1.40	0.67
1:D:369:ILE:HD12	1:D:410:VAL:HG21	1.75	0.67
1:B:908:ARG:HG2	1:B:927:VAL:HG23	1.78	0.66
1:C:908:ARG:HD3	1:C:930:LYS:HB3	1.76	0.66
1:B:608:SER:OG	1:B:609:ASN:OD1	2.13	0.65
1:A:886:THR:O	1:A:889:ASP:HB2	1.96	0.65
1:A:72:GLU:O	1:C:1013:LYS:NZ	2.30	0.64
1:A:326:PRO:HB2	1:A:330:GLU:HB2	1.80	0.64
1:C:823:HIS:HD2	1:C:825:MET:H	1.44	0.64
1:D:883:ASN:HB2	1:D:885:LEU:CD2	2.28	0.64
1:A:608:SER:OG	1:A:609:ASN:OD1	2.14	0.63
1:C:207:HIS:HD2	3:C:1202:ADP:O3'	1.82	0.63
1:A:168:ARG:NH1	1:A:186:GLU:OE2	2.32	0.62
1:D:885:LEU:HD23	1:D:885:LEU:H	1.63	0.62
1:B:893:ARG:HB2	1:B:896:GLU:OE1	2.00	0.61
1:C:1088:ASP:N	1:C:1088:ASP:OD1	2.33	0.61
1:A:120:LYS:HE2	1:A:199:GLU:OE2	2.01	0.60
1:C:952:ASP:OD1	1:C:956:LYS:HE2	2.01	0.60
1:C:1102:MET:O	1:C:1103:LYS:HG2	2.02	0.60
1:A:886:THR:HG22	1:A:887:GLU:N	2.16	0.60
1:C:847:ASP:OD1	1:C:850:LYS:NZ	2.32	0.60
1:C:286:GLU:OE1	3:C:1202:ADP:O1A	2.20	0.59
1:B:908:ARG:HG2	1:B:927:VAL:CG2	2.31	0.59
1:A:116:LYS:HE3	1:A:286:GLU:CG	2.33	0.59
1:C:1096:LEU:HD11	1:C:1110:ALA:HB2	1.85	0.59
1:A:952:ASP:OD1	1:A:956:LYS:HE2	2.03	0.58
1:B:293:VAL:HG23	6:B:1449:HOH:O	2.02	0.58
1:B:609:ASN:ND2	1:B:614:GLN:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:952:ASP:OD1	1:D:956:LYS:HE2	2.03	0.58
1:B:474:ASN:HD21	1:B:1051:GLN:H	1.50	0.58
1:A:474:ASN:HD21	1:A:1051:GLN:H	1.51	0.58
1:C:207:HIS:CD2	3:C:1202:ADP:O3'	2.57	0.58
1:A:167:MET:O	1:A:168:ARG:HD2	2.04	0.57
1:A:822:MET:HE1	1:B:793:GLU:OE1	2.04	0.57
1:A:847:ASP:OD1	1:A:850:LYS:NZ	2.32	0.57
1:D:645:LEU:HD12	1:D:692:LEU:HD23	1.87	0.57
1:A:116:LYS:HE3	1:A:286:GLU:HG2	1.86	0.57
1:C:815:SER:HB3	6:D:1336:HOH:O	2.05	0.56
1:C:398:ASN:ND2	6:C:1306:HOH:O	2.38	0.56
1:C:813:ILE:HG21	1:D:803:ARG:CZ	2.35	0.56
1:D:847:ASP:OD1	1:D:850:LYS:NZ	2.32	0.56
1:D:474:ASN:HD21	1:D:1051:GLN:H	1.51	0.56
1:B:1060:LYS:CE	1:B:1125:GLU:OE2	2.49	0.56
1:C:474:ASN:HD21	1:C:1051:GLN:H	1.52	0.56
1:C:364:PRO:HG2	1:C:410:VAL:HG13	1.88	0.56
1:A:11:GLU:CD	1:A:392:LYS:HE3	2.31	0.55
1:A:364:PRO:HG2	1:A:410:VAL:HG13	1.88	0.55
1:D:883:ASN:HB2	1:D:885:LEU:HD22	1.88	0.55
1:C:1057:VAL:HG12	1:C:1057:VAL:O	2.05	0.55
1:A:609:ASN:ND2	1:A:614:GLN:O	2.40	0.55
1:C:908:ARG:NH1	6:C:1307:HOH:O	2.40	0.54
1:B:586:TRP:CZ2	1:B:967:ILE:HD11	2.42	0.54
1:B:132:PRO:HG2	1:B:200:LYS:HD3	1.90	0.54
1:A:11:GLU:OE1	1:A:392:LYS:HE2	2.07	0.54
1:A:132:PRO:HG2	1:A:200:LYS:HD3	1.90	0.54
1:A:293:VAL:HG23	1:A:392:LYS:HE2	1.90	0.54
1:B:474:ASN:ND2	1:B:1051:GLN:H	2.05	0.54
1:C:474:ASN:ND2	1:C:1051:GLN:H	2.06	0.54
1:D:822:MET:HG2	1:D:854:ARG:HH21	1.73	0.54
1:B:364:PRO:HG2	1:B:410:VAL:HG13	1.89	0.53
1:A:888:GLU:OE2	1:A:888:GLU:N	2.32	0.53
1:C:5:LEU:C	1:C:5:LEU:HD23	2.33	0.53
1:D:364:PRO:HG2	1:D:410:VAL:HG13	1.89	0.53
1:C:842:LEU:HD22	1:C:845:ARG:HD3	1.91	0.53
1:D:474:ASN:ND2	1:D:1051:GLN:H	2.06	0.53
1:D:1071:ILE:HD12	1:D:1134:ILE:HG23	1.91	0.53
1:B:1049:ASN:HD21	1:B:1054:GLN:NE2	2.05	0.53
1:C:908:ARG:HG2	1:C:927:VAL:HG23	1.90	0.53
1:D:494:LEU:H	1:D:794:GLN:HE21	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HE2	1:A:197:TYR:OH	2.08	0.53
1:A:813:ILE:HG21	1:B:803:ARG:CZ	2.38	0.52
1:B:880:MET:CA	1:B:885:LEU:HD12	2.36	0.52
1:D:842:LEU:HD22	1:D:845:ARG:HD3	1.92	0.52
1:D:888:GLU:O	1:D:889:ASP:C	2.48	0.52
1:A:505:ASN:HA	6:A:1429:HOH:O	2.09	0.52
1:A:612:GLY:HA3	1:A:971:MET:CE	2.39	0.52
1:D:885:LEU:HD23	1:D:885:LEU:N	2.24	0.52
1:A:474:ASN:ND2	1:A:1051:GLN:H	2.08	0.51
1:D:880:MET:O	1:D:885:LEU:HD23	2.10	0.51
1:B:167:MET:O	1:B:168:ARG:HD2	2.10	0.51
1:A:501:LYS:NZ	1:A:509:GLU:OE1	2.44	0.51
1:A:1090:VAL:HG22	1:A:1114:GLY:O	2.10	0.51
1:B:433:GLU:H	1:B:433:GLU:CD	2.18	0.51
1:D:341:ARG:HD3	6:D:1307:HOH:O	2.10	0.51
1:C:927:VAL:HG21	1:C:932:VAL:HG22	1.93	0.50
1:D:458:ARG:HH21	1:D:458:ARG:HG2	1.76	0.50
1:D:1080:LEU:HB2	1:D:1098:VAL:HG13	1.92	0.50
1:C:609:ASN:ND2	1:C:614:GLN:O	2.43	0.50
1:A:885:LEU:CD2	1:A:889:ASP:HB3	2.42	0.50
1:D:612:GLY:HA3	1:D:971:MET:CE	2.42	0.50
1:D:1077:GLY:HA3	1:D:1100:GLU:O	2.11	0.50
1:A:1053:VAL:O	1:A:1056:GLN:HB2	2.12	0.50
1:B:612:GLY:HA3	1:B:971:MET:CE	2.42	0.50
1:B:759:THR:HG21	1:B:799:TRP:CD1	2.46	0.50
1:B:964:HIS:O	1:B:967:ILE:HD12	2.12	0.50
1:C:886:THR:CG2	1:C:888:GLU:HG2	2.42	0.50
1:C:803:ARG:CZ	1:D:813:ILE:HG21	2.42	0.50
1:C:908:ARG:CD	1:C:930:LYS:HB3	2.42	0.50
1:D:147:ALA:O	1:D:151:GLY:HA2	2.12	0.50
1:A:109:HIS:HE1	1:A:265:VAL:O	1.95	0.50
1:A:494:LEU:H	1:A:794:GLN:HE21	1.59	0.49
1:B:880:MET:HA	1:B:885:LEU:HD13	1.92	0.49
1:D:569:TRP:CE3	1:D:633:ILE:CD1	2.95	0.49
1:A:803:ARG:CZ	1:B:813:ILE:HG21	2.43	0.49
1:B:39:VAL:H	1:B:375:ASN:ND2	2.11	0.48
1:C:4:LEU:HD23	1:C:4:LEU:C	2.37	0.48
1:A:171:ARG:HG3	1:A:175:GLU:OE1	2.13	0.48
1:B:1049:ASN:ND2	1:B:1054:GLN:NE2	2.61	0.48
1:B:1101:ALA:O	1:B:1102:MET:HB2	2.12	0.48
1:D:855:LYS:HE3	1:D:855:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:HIS:HE1	1:D:265:VAL:O	1.96	0.48
1:B:880:MET:O	1:B:885:LEU:HD12	2.14	0.48
1:B:586:TRP:CZ2	1:B:967:ILE:CD1	2.97	0.48
1:D:120:LYS:HE2	1:D:199:GLU:OE2	2.14	0.47
1:D:4:LEU:C	1:D:4:LEU:HD23	2.39	0.47
1:C:126:ALA:O	1:C:260:LYS:HD3	2.14	0.47
1:C:908:ARG:HD3	1:C:930:LYS:CB	2.42	0.47
1:D:346:ASP:OD1	6:D:1301:HOH:O	2.20	0.47
1:C:109:HIS:HE1	1:C:265:VAL:O	1.97	0.47
1:B:1046:VAL:HG13	1:C:1065:THR:HB	1.97	0.47
1:A:10:GLY:HA2	6:A:1459:HOH:O	2.15	0.47
1:A:172:ASN:HB2	1:A:175:GLU:HB2	1.97	0.47
1:C:730:HIS:NE2	1:C:756:ASP:OD1	2.45	0.47
1:A:414:PHE:O	6:A:1301:HOH:O	2.21	0.47
1:B:109:HIS:HE1	1:B:265:VAL:O	1.98	0.47
1:B:886:THR:HG22	1:B:887:GLU:N	2.29	0.47
1:B:991:LEU:HD13	1:B:1011:ILE:HA	1.96	0.47
1:C:923:GLN:O	1:C:927:VAL:HG12	2.15	0.47
1:B:730:HIS:NE2	1:B:756:ASP:OD1	2.44	0.46
1:B:842:LEU:HD22	1:B:845:ARG:HD3	1.97	0.46
1:C:745:SER:OG	5:D:1201:2BA:O2P1	2.21	0.46
1:D:608:SER:OG	1:D:609:ASN:ND2	2.47	0.46
1:C:957:ILE:HD12	1:C:959:TYR:CZ	2.51	0.46
1:A:677:ARG:HD3	1:A:858:MET:HE1	1.97	0.46
1:B:4:LEU:C	1:B:4:LEU:HD23	2.41	0.46
1:C:991:LEU:HD13	1:C:1011:ILE:HA	1.96	0.46
1:D:1081:GLU:HB3	1:D:1098:VAL:HG12	1.98	0.46
1:D:886:THR:HG22	1:D:887:GLU:H	1.81	0.46
1:A:172:ASN:HB3	1:A:175:GLU:H	1.81	0.46
1:B:132:PRO:HG2	1:B:200:LYS:CD	2.46	0.46
1:C:494:LEU:H	1:C:794:GLN:HE21	1.64	0.46
1:C:886:THR:HG22	1:C:887:GLU:N	2.30	0.46
1:D:106:GLU:H	1:D:109:HIS:HD2	1.63	0.46
1:A:775:TYR:CD1	1:A:775:TYR:C	2.94	0.45
1:C:523:LYS:NZ	6:C:1304:HOH:O	2.35	0.45
1:D:533:ARG:HD2	1:D:533:ARG:C	2.41	0.45
1:D:923:GLN:O	1:D:927:VAL:HG22	2.17	0.45
1:B:126:ALA:O	1:B:260:LYS:HD3	2.16	0.45
1:C:369:ILE:HD12	1:C:410:VAL:CG2	2.44	0.45
1:D:368:GLY:O	1:D:395:THR:HA	2.15	0.45
1:D:446:ASP:OD1	1:D:446:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:OD1	1:A:310:GLN:HG2	2.17	0.45
1:B:618:ASP:OD2	1:B:650:LYS:HE3	2.17	0.45
1:B:842:LEU:CD2	1:B:845:ARG:HD3	2.46	0.45
1:C:221:ILE:HD11	1:C:325:LEU:HD13	1.98	0.45
1:A:886:THR:CG2	1:A:887:GLU:N	2.79	0.45
1:A:923:GLN:O	1:A:927:VAL:HG22	2.15	0.45
1:B:883:ASN:HB2	1:B:885:LEU:HD11	1.98	0.45
1:C:4:LEU:HD23	1:C:5:LEU:N	2.31	0.45
1:C:1085:LYS:O	1:C:1088:ASP:OD1	2.35	0.45
1:D:730:HIS:NE2	1:D:756:ASP:OD1	2.45	0.45
1:D:759:THR:HG21	1:D:799:TRP:CD1	2.52	0.45
1:A:462:THR:OG1	1:A:1044:ARG:NH1	2.50	0.45
1:A:922:LEU:HG	1:A:926:ILE:HD12	1.99	0.45
1:B:120:LYS:NZ	1:B:131:ILE:O	2.47	0.45
1:A:369:ILE:HD12	1:A:410:VAL:CG2	2.45	0.45
1:D:922:LEU:HG	1:D:926:ILE:HD12	1.99	0.45
1:A:957:ILE:HD12	1:A:959:TYR:CZ	2.52	0.44
1:C:39:VAL:H	1:C:375:ASN:ND2	2.15	0.44
1:C:250:PHE:CZ	1:C:280:ASP:HA	2.53	0.44
1:D:39:VAL:H	1:D:375:ASN:ND2	2.15	0.44
1:A:5:LEU:C	1:A:5:LEU:HD23	2.43	0.44
1:A:1096:LEU:HD11	1:A:1110:ALA:HB2	2.00	0.44
1:D:957:ILE:HD12	1:D:959:TYR:CZ	2.53	0.44
1:A:207:HIS:ND1	3:A:1202:ADP:O3'	2.40	0.44
1:B:586:TRP:HZ2	1:B:967:ILE:CD1	2.31	0.44
1:A:885:LEU:HD22	1:A:889:ASP:HB3	1.98	0.44
1:B:82:TYR:CZ	1:B:293:VAL:HG22	2.53	0.44
1:B:369:ILE:HD12	1:B:410:VAL:CG2	2.46	0.44
1:D:886:THR:HG22	1:D:887:GLU:N	2.33	0.44
1:D:991:LEU:HD13	1:D:1011:ILE:HA	1.99	0.44
1:A:759:THR:HG21	1:A:799:TRP:CD1	2.53	0.44
1:D:152:TYR:CD2	1:D:172:ASN:HA	2.53	0.44
1:D:569:TRP:CE3	1:D:633:ILE:HD12	2.52	0.44
1:B:221:ILE:HD11	1:B:325:LEU:HD13	2.00	0.44
1:A:39:VAL:H	1:A:375:ASN:ND2	2.16	0.43
1:A:1084:VAL:HG12	1:A:1085:LYS:N	2.33	0.43
1:D:502:THR:H	1:D:505:ASN:HD22	1.66	0.43
1:A:146:PHE:CE1	1:A:150:TYR:CD2	3.05	0.43
1:C:368:GLY:O	1:C:395:THR:HA	2.19	0.43
1:B:586:TRP:HZ2	1:B:967:ILE:HD13	1.84	0.43
1:D:880:MET:HA	1:D:885:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:MET:H	1:A:1104:MET:HG2	1.63	0.43
1:B:180:TYR:C	1:B:180:TYR:CD2	2.96	0.43
1:B:161:GLY:HA2	1:B:191:PHE:CZ	2.54	0.43
1:B:368:GLY:O	1:B:395:THR:HA	2.18	0.43
1:A:578:TYR:CZ	1:A:585:PRO:HD2	2.54	0.43
1:B:533:ARG:HD2	1:B:533:ARG:C	2.43	0.43
1:C:116:LYS:HA	1:C:116:LYS:HD3	1.84	0.43
1:C:216:ARG:HD2	6:C:1345:HOH:O	2.18	0.43
1:B:1084:VAL:HG12	1:B:1085:LYS:N	2.34	0.43
1:A:221:ILE:HD11	1:A:325:LEU:HD13	2.01	0.43
1:B:269:ASN:OD1	1:B:310:GLN:HG2	2.19	0.43
1:A:701:ALA:HA	1:A:730:HIS:O	2.19	0.42
1:B:922:LEU:HG	1:B:926:ILE:HD12	2.01	0.42
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.85	0.42
1:A:368:GLY:O	1:A:395:THR:HA	2.19	0.42
1:C:269:ASN:OD1	1:C:310:GLN:HG2	2.18	0.42
1:D:612:GLY:N	1:D:971:MET:CE	2.83	0.42
1:A:250:PHE:CZ	1:A:280:ASP:HA	2.54	0.42
1:A:1011:ILE:O	1:A:1011:ILE:CG2	2.66	0.42
1:C:502:THR:H	1:C:505:ASN:HD22	1.68	0.42
1:C:608:SER:CB	1:C:647:GLN:OE1	2.64	0.42
1:D:840:VAL:HG12	1:D:840:VAL:O	2.19	0.42
1:D:890:VAL:HG13	1:D:899:PHE:CZ	2.54	0.42
1:A:730:HIS:NE2	1:A:756:ASP:OD1	2.45	0.42
1:B:1096:LEU:HD11	1:B:1110:ALA:HB2	2.00	0.42
1:C:922:LEU:HG	1:C:926:ILE:HD12	2.01	0.42
1:C:1119:LEU:CD1	1:C:1134:ILE:HG12	2.41	0.42
1:A:180:TYR:CD2	1:A:180:TYR:C	2.97	0.42
1:A:1011:ILE:O	1:A:1011:ILE:HG22	2.20	0.42
1:C:759:THR:HG21	1:C:799:TRP:CD1	2.55	0.42
1:A:840:VAL:HG12	1:A:840:VAL:O	2.19	0.42
1:B:106:GLU:H	1:B:109:HIS:HD2	1.68	0.42
1:B:132:PRO:HB2	1:B:200:LYS:HD2	2.02	0.42
1:B:840:VAL:HG12	1:B:840:VAL:O	2.20	0.42
1:D:269:ASN:OD1	1:D:310:GLN:HG2	2.19	0.42
1:A:198:VAL:HG12	1:A:199:GLU:N	2.34	0.42
1:A:165:ARG:NH1	1:A:190:ALA:HB1	2.35	0.41
1:C:840:VAL:O	1:C:840:VAL:HG12	2.19	0.41
1:A:1100:GLU:HA	1:A:1104:MET:O	2.20	0.41
1:C:338:ILE:O	1:C:394:CYS:HA	2.20	0.41
1:C:1129:THR:O	1:C:1130:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:O	1:A:251:ARG:HD2	2.21	0.41
1:D:880:MET:HA	1:D:885:LEU:HD21	2.02	0.41
1:A:502:THR:H	1:A:505:ASN:HD22	1.68	0.41
1:C:367:PHE:O	1:C:406:LYS:HE3	2.20	0.41
1:C:533:ARG:C	1:C:533:ARG:HD2	2.44	0.41
1:A:153:PRO:HG2	1:A:201:TYR:CD2	2.56	0.41
1:A:533:ARG:HD2	1:A:533:ARG:C	2.45	0.41
1:A:1102:MET:O	1:A:1103:LYS:HB2	2.21	0.41
1:B:575:ASP:CG	1:B:579:ARG:HH11	2.27	0.41
1:D:157:LYS:HE2	1:D:197:TYR:OH	2.21	0.41
1:A:338:ILE:O	1:A:394:CYS:HA	2.21	0.41
1:B:957:ILE:HD12	1:B:959:TYR:CZ	2.55	0.41
1:D:1129:THR:O	1:D:1130:GLN:HB2	2.21	0.41
1:A:1071:ILE:HD12	1:A:1134:ILE:HG23	2.02	0.41
1:B:178:ASP:OD1	1:B:182:ARG:NH1	2.54	0.41
1:B:1077:GLY:HA3	1:B:1100:GLU:O	2.21	0.41
1:C:775:TYR:CD1	1:C:775:TYR:C	2.98	0.41
1:B:220:ILE:HD12	1:B:263:LYS:HA	2.04	0.40
1:C:993:ASP:OD2	1:C:995:PRO:HD2	2.21	0.40
1:B:5:LEU:HD23	1:B:6:VAL:C	2.46	0.40
1:B:250:PHE:CZ	1:B:280:ASP:HA	2.56	0.40
1:B:1010:GLN:CG	6:B:1309:HOH:O	2.46	0.40
1:B:1013:LYS:NZ	1:D:72:GLU:O	2.55	0.40
1:C:1053:VAL:O	1:C:1056:GLN:HB2	2.20	0.40
1:D:462:THR:OG1	1:D:1044:ARG:NH1	2.54	0.40
1:B:964:HIS:HA	1:B:967:ILE:HD11	2.02	0.40
1:A:457:LEU:HD12	1:A:457:LEU:HA	1.83	0.40
1:C:1077:GLY:HA3	1:C:1100:GLU:O	2.21	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	1142/1145 (100%)	1114 (98%)	28 (2%)	0	100	100
1	B	1138/1145 (99%)	1110 (98%)	27 (2%)	1 (0%)	48	60
1	C	1079/1145 (94%)	1053 (98%)	25 (2%)	1 (0%)	48	60
1	D	1140/1145 (100%)	1114 (98%)	25 (2%)	1 (0%)	48	60
All	All	4499/4580 (98%)	4391 (98%)	105 (2%)	3 (0%)	48	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	269	ASN
1	D	269	ASN
1	B	269	ASN

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	955/956 (100%)	912 (96%)	43 (4%)	24	37
1	B	953/956 (100%)	919 (96%)	34 (4%)	31	47
1	C	917/956 (96%)	888 (97%)	29 (3%)	34	51
1	D	953/956 (100%)	917 (96%)	36 (4%)	29	44
All	All	3778/3824 (99%)	3636 (96%)	142 (4%)	29	44

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	140	ILE
1	A	165	ARG
1	A	171	ARG
1	A	173	ASP
1	A	186	GLU
1	A	200	LYS
1	A	233	ARG

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	280	ASP
1	A	331	ILE
1	A	334	LEU
1	A	352	LEU
1	A	392	LYS
1	A	398	ASN
1	A	457	LEU
1	A	460	ARG
1	A	483	GLU
1	A	494	LEU
1	A	499	LYS
1	A	542	THR
1	A	569	TRP
1	A	690	LYS
1	A	705	MET
1	A	743	THR
1	A	834	LYS
1	A	848	GLU
1	A	854	ARG
1	A	855	LYS
1	A	870	SER
1	A	884	ASP
1	A	888	GLU
1	A	893	ARG
1	A	901	GLU
1	A	1006	LYS
1	A	1012	GLU
1	A	1074	THR
1	A	1102	MET
1	A	1104	MET
1	A	1107	THR
1	A	1116	ILE
1	A	1119	LEU
1	A	1123	LYS
1	B	135	ASN
1	B	145	GLU
1	B	160	LEU
1	B	182	ARG
1	B	280	ASP
1	B	433	GLU
1	B	489	GLU

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Mol	Chain	Res	Type
1	B	494	LEU
1	B	499	LYS
1	B	542	THR
1	B	569	TRP
1	B	705	MET
1	B	743	THR
1	B	834	LYS
1	B	848	GLU
1	B	855	LYS
1	B	870	SER
1	B	884	ASP
1	B	885	LEU
1	B	888	GLU
1	B	896	GLU
1	B	901	GLU
1	B	927	VAL
1	B	930	LYS
1	B	967	ILE
1	B	1006	LYS
1	B	1010	GLN
1	B	1013	LYS
1	B	1054	GLN
1	B	1060	LYS
1	B	1090	VAL
1	B	1116	ILE
1	B	1119	LEU
1	B	1123	LYS
1	C	116	LYS
1	C	120	LYS
1	C	263	LYS
1	C	280	ASP
1	C	331	ILE
1	C	352	LEU
1	C	398	ASN
1	C	457	LEU
1	C	494	LEU
1	C	533	ARG
1	C	542	THR
1	C	569	TRP
1	C	705	MET
1	C	743	THR
1	C	834	LYS

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Mol	Chain	Res	Type
1	C	855	LYS
1	C	870	SER
1	C	921	LYS
1	C	928	LYS
1	C	930	LYS
1	C	1010	GLN
1	C	1013	LYS
1	C	1015	LYS
1	C	1088	ASP
1	C	1090	VAL
1	C	1102	MET
1	C	1104	MET
1	C	1116	ILE
1	C	1123	LYS
1	D	26	SER
1	D	120	LYS
1	D	135	ASN
1	D	140	ILE
1	D	157	LYS
1	D	168	ARG
1	D	182	ARG
1	D	233	ARG
1	D	280	ASP
1	D	458	ARG
1	D	494	LEU
1	D	542	THR
1	D	569	TRP
1	D	591	LYS
1	D	705	MET
1	D	727	LEU
1	D	743	THR
1	D	848	GLU
1	D	855	LYS
1	D	870	SER
1	D	884	ASP
1	D	885	LEU
1	D	888	GLU
1	D	901	GLU
1	D	929	ASP
1	D	1010	GLN
1	D	1013	LYS
1	D	1015	LYS

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Mol	Chain	Res	Type
1	D	1035	LEU
1	D	1060	LYS
1	D	1074	THR
1	D	1075	MET
1	D	1078	SER
1	D	1090	VAL
1	D	1116	ILE
1	D	1119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	109	HIS
1	A	177	HIS
1	A	219	ASN
1	A	308	GLN
1	A	328	GLN
1	A	375	ASN
1	A	412	HIS
1	A	439	GLN
1	A	474	ASN
1	A	492	GLN
1	A	505	ASN
1	A	510	GLN
1	A	739	ASN
1	A	794	GLN
1	A	823	HIS
1	A	832	ASN
1	A	1010	GLN
1	A	1049	ASN
1	A	1051	GLN
1	A	1094	GLN
1	B	109	HIS
1	B	204	ASN
1	B	308	GLN
1	B	328	GLN
1	B	375	ASN
1	B	412	HIS
1	B	439	GLN
1	B	474	ASN
1	B	481	ASN

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Mol	Chain	Res	Type
1	B	492	GLN
1	B	505	ASN
1	B	510	GLN
1	B	739	ASN
1	B	823	HIS
1	B	832	ASN
1	B	940	HIS
1	B	1010	GLN
1	B	1049	ASN
1	C	109	HIS
1	C	207	HIS
1	C	308	GLN
1	C	375	ASN
1	C	398	ASN
1	C	412	HIS
1	C	434	ASN
1	C	439	GLN
1	C	474	ASN
1	C	505	ASN
1	C	547	GLN
1	C	739	ASN
1	C	794	GLN
1	C	823	HIS
1	C	832	ASN
1	C	836	GLN
1	C	883	ASN
1	C	898	ASN
1	C	1010	GLN
1	C	1049	ASN
1	C	1137	ASN
1	D	109	HIS
1	D	177	HIS
1	D	219	ASN
1	D	234	ASN
1	D	308	GLN
1	D	375	ASN
1	D	412	HIS
1	D	434	ASN
1	D	439	GLN
1	D	474	ASN
1	D	481	ASN
1	D	492	GLN

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Mol	Chain	Res	Type
1	D	505	ASN
1	D	510	GLN
1	D	609	ASN
1	D	683	GLN
1	D	739	ASN
1	D	794	GLN
1	D	823	HIS
1	D	883	ASN
1	D	1010	GLN
1	D	1049	ASN
1	D	1054	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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	1202	4	28,29,29	1.63	7 (25%)	43,45,45	1.77	11 (25%)
3	ADP	D	1203	4	28,29,29	1.58	3 (10%)	43,45,45	1.59	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	2BA	A	1204	-	50,50,50	1.63	11 (22%)	74,78,78	2.10	20 (27%)
3	ADP	A	1202	4	28,29,29	1.40	4 (14%)	43,45,45	1.85	12 (27%)
3	ADP	C	1202	4	28,29,29	1.89	5 (17%)	43,45,45	1.92	13 (30%)
5	2BA	D	1201	-	50,50,50	1.48	10 (20%)	74,78,78	2.14	24 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	1202	4	-	2/16/32/32	0/3/3/3
3	ADP	D	1203	4	-	5/16/32/32	0/3/3/3
5	2BA	A	1204	-	-	0/30/62/62	0/6/7/7
3	ADP	A	1202	4	-	5/16/32/32	0/3/3/3
3	ADP	C	1202	4	-	6/16/32/32	0/3/3/3
5	2BA	D	1201	-	-	0/30/62/62	0/6/7/7

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	ADP	PA-O3A	5.51	1.65	1.59
3	C	1202	ADP	C5-C4	5.09	1.48	1.39
5	A	1204	2BA	C51-C41	4.89	1.47	1.39
3	B	1202	ADP	C5-C4	4.59	1.47	1.39
3	D	1203	ADP	C5-C4	4.58	1.47	1.39
3	A	1202	ADP	C5-C4	3.95	1.46	1.39
5	A	1204	2BA	C51-N71	-3.83	1.32	1.39
5	D	1201	2BA	C51-N71	-3.64	1.32	1.39
5	D	1201	2BA	C81-N71	3.57	1.38	1.31
3	D	1203	ADP	C4-N9	-3.54	1.30	1.37
5	D	1201	2BA	C5-C4	3.47	1.45	1.39
3	D	1203	ADP	C5-N7	-3.45	1.32	1.39
3	A	1202	ADP	C5-C6	3.15	1.49	1.41
5	A	1204	2BA	C8-N7	3.13	1.37	1.31
3	A	1202	ADP	PA-O3A	3.11	1.62	1.59
3	B	1202	ADP	C5-N7	-3.10	1.33	1.39
3	C	1202	ADP	C5-C6	3.00	1.49	1.41
3	B	1202	ADP	C5-C6	2.77	1.48	1.41
3	B	1202	ADP	PA-O3A	2.69	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1204	2BA	C4-N3	2.62	1.39	1.34
3	B	1202	ADP	C8-N7	2.62	1.36	1.31
3	A	1202	ADP	C4-N9	-2.61	1.32	1.37
3	C	1202	ADP	C8-N7	2.55	1.36	1.31
5	A	1204	2BA	C5-C6	2.53	1.48	1.41
5	D	1201	2BA	C5-N7	-2.51	1.34	1.39
3	B	1202	ADP	C2-N1	2.48	1.38	1.33
5	A	1204	2BA	C5-C4	2.38	1.43	1.39
5	A	1204	2BA	C81-N71	2.35	1.36	1.31
5	A	1204	2BA	C81-N91	-2.31	1.33	1.37
5	A	1204	2BA	C8-N9	-2.27	1.33	1.37
5	D	1201	2BA	C2-N1	2.22	1.37	1.33
5	D	1201	2BA	C8-N7	2.22	1.35	1.31
3	B	1202	ADP	C4-N9	-2.21	1.33	1.37
5	D	1201	2BA	C8-N9	-2.19	1.33	1.37
5	A	1204	2BA	C21-N11	2.17	1.37	1.33
3	C	1202	ADP	C2-N1	2.13	1.37	1.33
5	A	1204	2BA	C51-C61	2.06	1.46	1.41
5	D	1201	2BA	P1-O5'1	2.06	1.67	1.59
5	D	1201	2BA	C5-C6	2.05	1.46	1.41
5	D	1201	2BA	O4'1-C1'1	-2.02	1.37	1.42

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1201	2BA	C51-C41-N31	-6.69	117.51	126.72
5	A	1204	2BA	C5-C4-N3	-6.25	118.11	126.72
5	A	1204	2BA	N3-C4-N9	5.72	136.90	127.17
5	D	1201	2BA	N31-C41-N91	5.24	136.09	127.17
3	A	1202	ADP	C5-C4-N3	-5.23	119.52	126.72
5	D	1201	2BA	C5-C4-N3	-4.99	119.85	126.72
3	B	1202	ADP	C5-C4-N3	-4.95	119.90	126.72
5	A	1204	2BA	C51-C41-N31	-4.77	120.15	126.72
5	D	1201	2BA	N3-C4-N9	4.63	135.04	127.17
5	D	1201	2BA	C21-N31-C41	4.63	123.13	111.83
5	D	1201	2BA	N31-C21-N11	-4.60	121.61	128.58
5	A	1204	2BA	C2-N3-C4	4.55	122.93	111.83
3	A	1202	ADP	N3-C4-N9	4.48	134.78	127.17
3	C	1202	ADP	C5-C4-N3	-4.39	120.67	126.72
5	A	1204	2BA	N3-C2-N1	-4.31	122.05	128.58
5	A	1204	2BA	N31-C41-N91	4.29	134.47	127.17
3	D	1203	ADP	C5-C4-N3	-4.16	120.99	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	ADP	C2-N3-C4	4.09	121.83	111.83
3	C	1202	ADP	N3-C4-N9	3.97	133.91	127.17
3	C	1202	ADP	C4-N9-C8	3.90	109.84	105.74
3	C	1202	ADP	N3-C2-N1	-3.90	122.69	128.58
5	D	1201	2BA	C51-C61-N61	-3.89	113.66	123.29
3	D	1203	ADP	N3-C4-N9	3.88	133.76	127.17
5	A	1204	2BA	N31-C21-N11	-3.83	122.79	128.58
3	B	1202	ADP	N3-C4-N9	3.82	133.66	127.17
3	A	1202	ADP	N3-C2-N1	-3.76	122.89	128.58
5	A	1204	2BA	C4-N9-C8	3.76	109.68	105.74
5	A	1204	2BA	C5-C6-N6	-3.76	113.98	123.29
5	A	1204	2BA	C21-N31-C41	3.45	120.27	111.83
3	C	1202	ADP	C2-N3-C4	3.42	120.19	111.83
5	D	1201	2BA	N3-C2-N1	-3.39	123.44	128.58
5	D	1201	2BA	C2-N3-C4	3.37	120.06	111.83
5	A	1204	2BA	O4'1-C1'1-N91	3.31	114.44	108.09
3	B	1202	ADP	C4-C5-N7	-3.29	106.82	110.58
5	D	1201	2BA	N6-C6-N1	3.24	125.59	118.38
5	D	1201	2BA	O5'1-P1-O1P1	-3.12	96.55	108.94
3	D	1203	ADP	N6-C6-N1	3.11	125.30	118.38
3	A	1202	ADP	C4-N9-C8	3.07	108.96	105.74
3	A	1202	ADP	C6-C5-N7	3.05	137.97	132.09
3	D	1203	ADP	O3B-PB-O1B	2.95	122.32	110.83
5	D	1201	2BA	C2'-C1'-N9	-2.94	106.00	113.30
3	C	1202	ADP	C4-C5-N7	-2.90	107.26	110.58
3	C	1202	ADP	N9-C8-N7	-2.85	109.89	113.94
5	A	1204	2BA	N61-C61-N11	2.77	124.54	118.38
5	D	1201	2BA	C2'1-C3'1-C4'1	-2.76	98.41	103.24
5	A	1204	2BA	C41-C51-N71	-2.75	107.44	110.58
5	D	1201	2BA	C4-N9-C8	2.72	108.59	105.74
5	D	1201	2BA	C5-C6-N6	-2.70	116.60	123.29
3	D	1203	ADP	C4-N9-C8	2.67	108.54	105.74
5	D	1201	2BA	N91-C81-N71	-2.67	110.15	113.94
5	A	1204	2BA	C5-C6-N1	2.66	124.28	117.51
3	D	1203	ADP	N3-C2-N1	-2.65	124.58	128.58
3	C	1202	ADP	C5-N7-C8	2.65	107.61	103.45
3	A	1202	ADP	C4-C5-N7	-2.61	107.60	110.58
3	B	1202	ADP	C5-N7-C8	2.57	107.49	103.45
3	B	1202	ADP	C4-N9-C8	2.56	108.43	105.74
5	A	1204	2BA	C41-N91-C81	2.52	108.38	105.74
3	C	1202	ADP	C6-C5-N7	2.48	136.87	132.09
5	A	1204	2BA	C2'1-C1'1-N91	-2.42	107.30	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	ADP	O3'-C3'-C4'	2.40	117.98	111.08
5	A	1204	2BA	C21-N11-C61	2.40	122.67	118.73
5	A	1204	2BA	C51-N71-C81	2.39	107.21	103.45
5	D	1201	2BA	C2'1-C1'1-N91	-2.37	107.43	113.30
3	D	1203	ADP	C2-N3-C4	2.36	117.60	111.83
5	D	1201	2BA	O4'-C1'-N9	2.36	112.62	108.09
3	B	1202	ADP	C2'-C1'-N9	-2.36	107.45	113.30
5	D	1201	2BA	C51-C61-N11	2.35	123.48	117.51
3	B	1202	ADP	C2-N3-C4	2.35	117.56	111.83
5	D	1201	2BA	O3'-P1-O1P1	2.33	117.25	109.81
3	B	1202	ADP	O3B-PB-O2B	2.32	116.50	107.80
3	C	1202	ADP	O2A-PA-O1A	2.30	123.13	112.44
3	B	1202	ADP	N6-C6-N1	2.27	123.43	118.38
5	D	1201	2BA	C51-N71-C81	2.27	107.01	103.45
3	B	1202	ADP	N9-C8-N7	-2.21	110.81	113.94
3	C	1202	ADP	C4-N9-C1'	-2.20	121.49	126.63
3	D	1203	ADP	C2'-C1'-N9	-2.17	107.91	113.30
5	A	1204	2BA	C6-C5-C4	-2.15	114.25	117.18
3	A	1202	ADP	C5-N7-C8	2.14	106.81	103.45
3	A	1202	ADP	N9-C8-N7	-2.12	110.92	113.94
3	A	1202	ADP	O2A-PA-O3A	2.09	112.93	107.27
3	D	1203	ADP	O2A-PA-O1A	2.08	122.14	112.44
5	A	1204	2BA	N9-C8-N7	-2.08	110.98	113.94
3	B	1202	ADP	O2'-C2'-C1'	-2.07	102.97	110.10
3	A	1202	ADP	O3A-PB-O1B	-2.05	100.23	111.04
3	C	1202	ADP	C2'-C1'-N9	-2.05	108.21	113.30
5	D	1201	2BA	O2P1-P1-O5'1	2.04	116.80	107.57
3	A	1202	ADP	C6-C5-C4	-2.02	114.43	117.18
5	D	1201	2BA	C3'1-C2'1-C1'1	2.01	104.31	99.89
5	D	1201	2BA	N61-C61-N11	2.01	122.85	118.38
3	D	1203	ADP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	ADP	PA-O3A-PB-O2B
3	A	1202	ADP	PA-O3A-PB-O3B
3	C	1202	ADP	PA-O3A-PB-O2B
3	D	1203	ADP	C5'-O5'-PA-O1A
3	C	1202	ADP	O4'-C4'-C5'-O5'
3	A	1202	ADP	PB-O3A-PA-O1A

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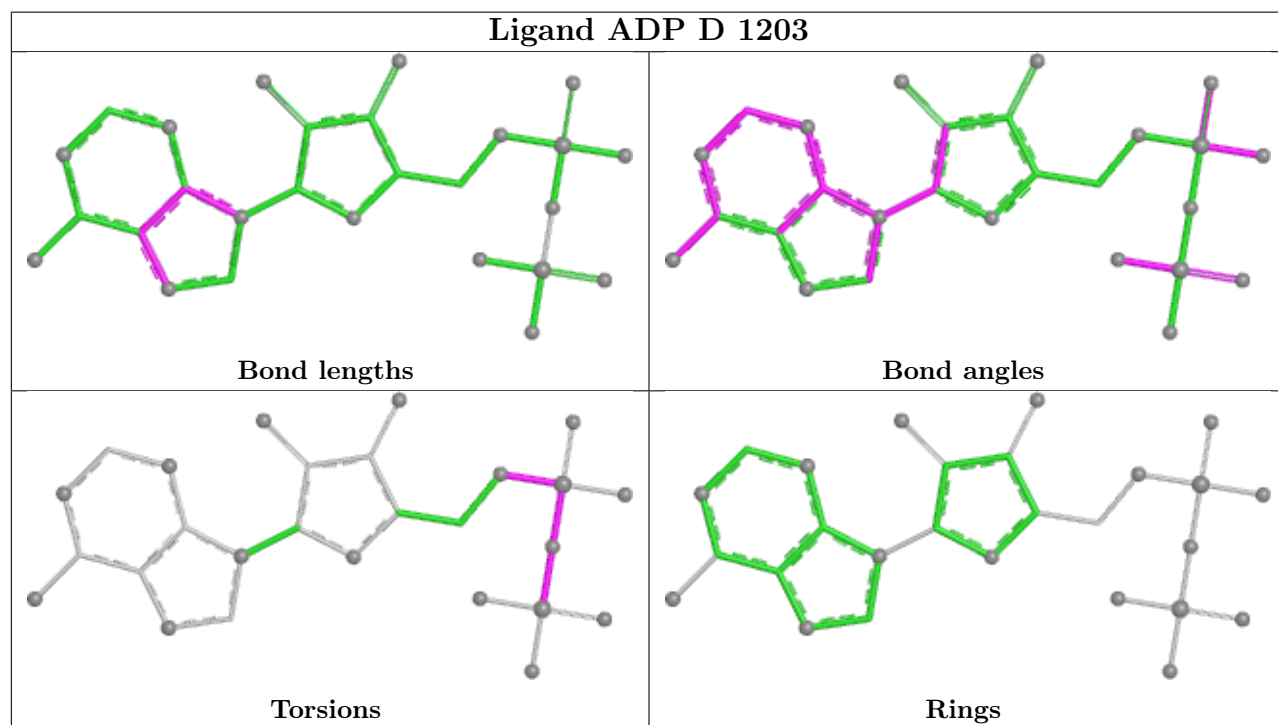
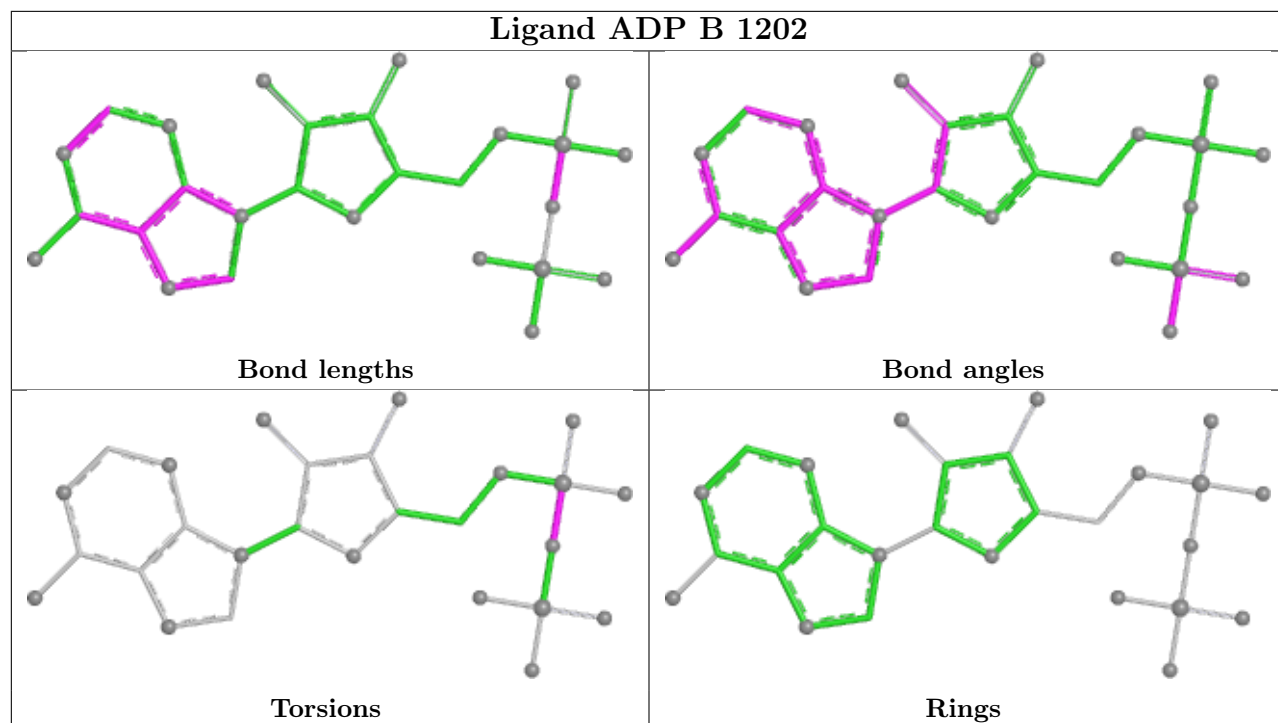
Mol	Chain	Res	Type	Atoms
3	D	1203	ADP	PA-O3A-PB-O1B
3	C	1202	ADP	C3'-C4'-C5'-O5'
3	A	1202	ADP	PB-O3A-PA-O2A
3	B	1202	ADP	PB-O3A-PA-O2A
3	C	1202	ADP	PB-O3A-PA-O1A
3	C	1202	ADP	PA-O3A-PB-O3B
3	D	1203	ADP	PA-O3A-PB-O2B
3	D	1203	ADP	PA-O3A-PB-O3B
3	B	1202	ADP	PB-O3A-PA-O1A
3	C	1202	ADP	PB-O3A-PA-O2A
3	A	1202	ADP	PA-O3A-PB-O1B
3	D	1203	ADP	PB-O3A-PA-O2A

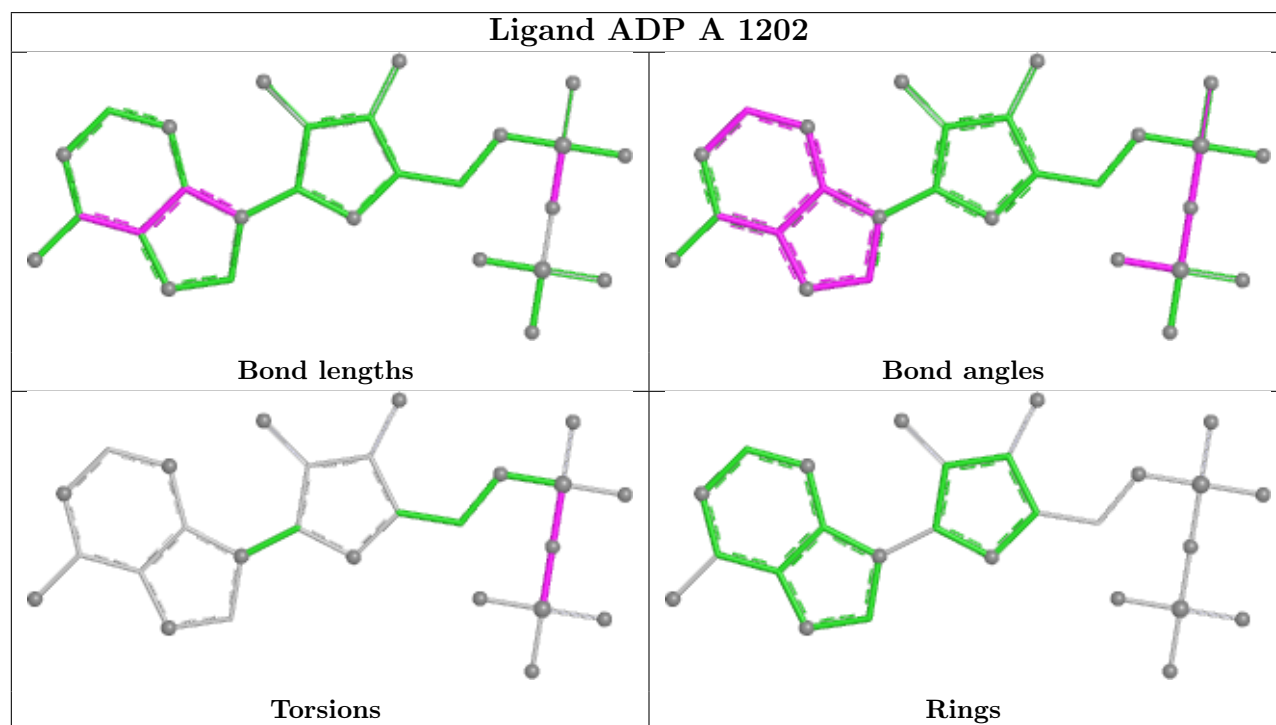
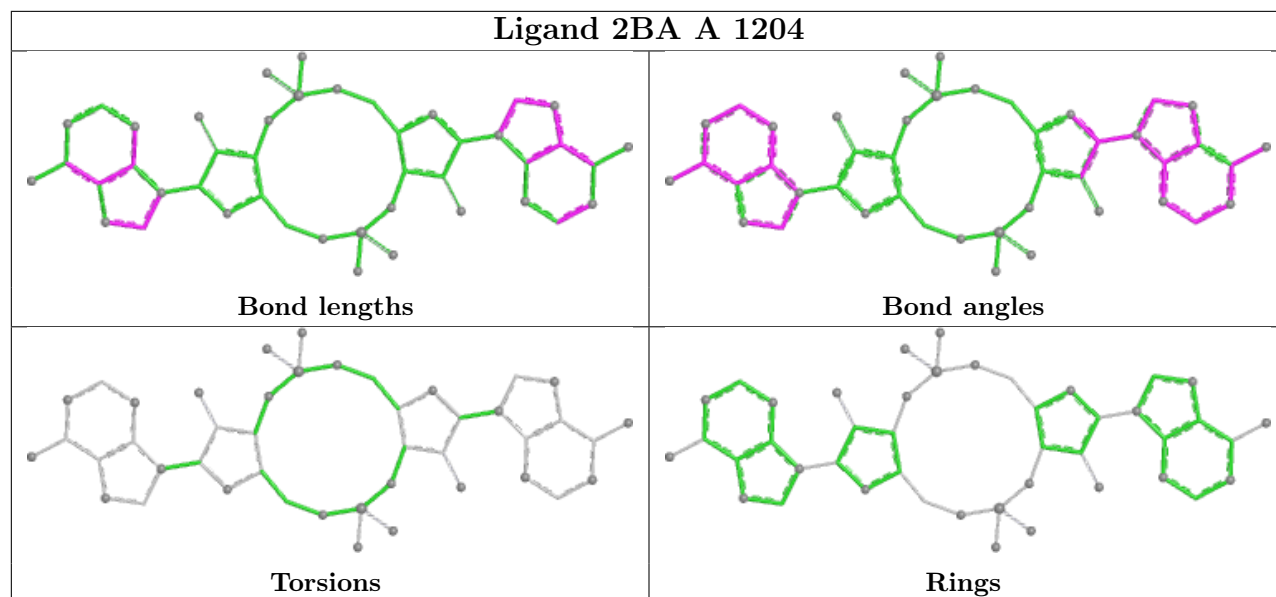
There are no ring outliers.

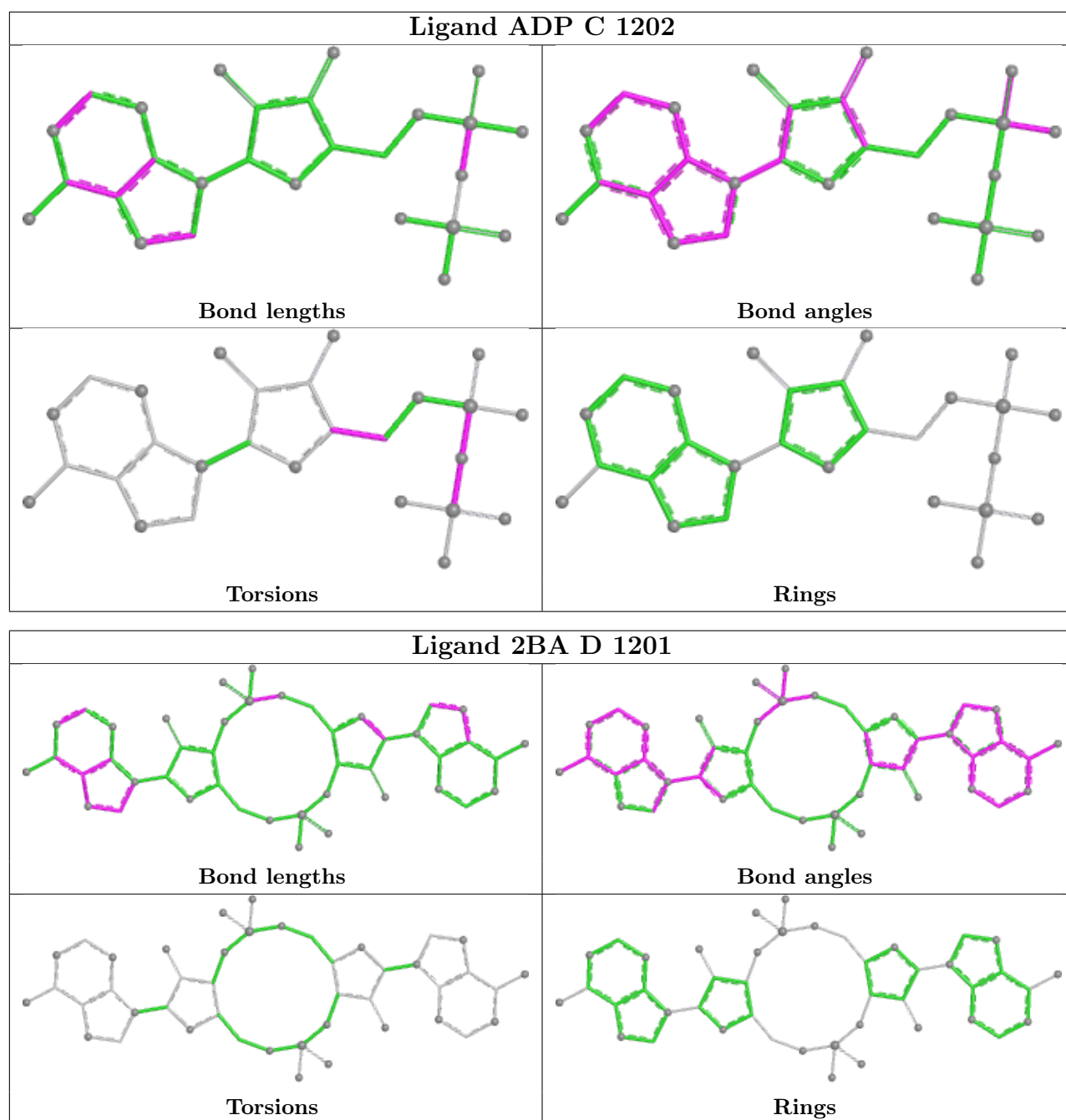
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	ADP	1	0
3	C	1202	ADP	3	0
5	D	1201	2BA	1	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	1144/1145 (99%)	0.05	35 (3%)	51	53	12, 35, 79, 126	0
1	B	1142/1145 (99%)	-0.03	38 (3%)	49	51	12, 33, 78, 108	0
1	C	1083/1145 (94%)	0.06	43 (3%)	42	44	14, 35, 77, 113	0
1	D	1144/1145 (99%)	-0.02	33 (2%)	53	56	15, 34, 82, 111	0
All	All	4513/4580 (98%)	0.01	149 (3%)	49	51	12, 34, 80, 126	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	LEU	5.1
1	A	163	GLY	5.0
1	D	164	GLY	4.1
1	A	194	GLY	4.0
1	C	201	TYR	4.0
1	C	202	ILE	3.9
1	D	165	ARG	3.9
1	C	840	VAL	3.8
1	B	839	ALA	3.8
1	B	147	ALA	3.7
1	A	811	ALA	3.6
1	C	134	THR	3.6
1	A	191	PHE	3.5
1	C	457	LEU	3.3
1	D	811	ALA	3.3
1	A	844	HIS	3.3
1	C	839	ALA	3.2
1	A	1059	ALA	3.2
1	A	162	GLY	3.2
1	B	191	PHE	3.2
1	D	1102	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	613	TYR	3.1
1	A	839	ALA	3.0
1	B	838	ALA	3.0
1	B	827	GLY	3.0
1	B	-6	LEU	2.9
1	C	1084	VAL	2.9
1	D	896	GLU	2.9
1	D	615	ASN	2.9
1	B	144	LEU	2.9
1	A	164	GLY	2.8
1	A	1057	VAL	2.8
1	C	-6	LEU	2.8
1	C	197	TYR	2.8
1	B	615	ASN	2.7
1	A	1086	ALA	2.7
1	A	1058	VAL	2.7
1	A	1102	MET	2.7
1	A	457	LEU	2.7
1	C	1086	ALA	2.7
1	B	881	ILE	2.7
1	C	1093	GLY	2.7
1	C	456	ARG	2.7
1	B	150	TYR	2.7
1	B	840	VAL	2.7
1	C	1090	VAL	2.7
1	B	135	ASN	2.6
1	A	814	THR	2.6
1	B	842	LEU	2.6
1	B	166	GLY	2.6
1	B	146	PHE	2.6
1	C	1112	PHE	2.6
1	A	1122	VAL	2.6
1	D	840	VAL	2.6
1	C	828	GLY	2.5
1	A	187	ALA	2.5
1	B	811	ALA	2.5
1	C	1068	PRO	2.5
1	C	811	ALA	2.5
1	B	143	ALA	2.5
1	D	812	GLY	2.5
1	D	894	GLY	2.5
1	B	846	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	188	ILE	2.4
1	C	198	VAL	2.4
1	D	457	LEU	2.4
1	C	1111	PRO	2.4
1	D	892	ALA	2.4
1	C	132	PRO	2.4
1	C	131	ILE	2.4
1	D	897	LEU	2.4
1	B	613	TYR	2.4
1	C	1076	PRO	2.4
1	D	190	ALA	2.4
1	A	1080	LEU	2.4
1	A	1096	LEU	2.4
1	D	456	ARG	2.4
1	C	1101	ALA	2.3
1	C	890	VAL	2.3
1	C	1098	VAL	2.3
1	D	191	PHE	2.3
1	C	896	GLU	2.3
1	D	433	GLU	2.3
1	C	613	TYR	2.3
1	A	1101	ALA	2.3
1	C	892	ALA	2.3
1	D	833	LEU	2.3
1	C	1088	ASP	2.3
1	B	841	GLY	2.3
1	A	190	ALA	2.3
1	A	838	ALA	2.3
1	C	1058	VAL	2.3
1	D	162	GLY	2.2
1	C	1082	ILE	2.2
1	C	1116	ILE	2.2
1	D	846	PHE	2.2
1	D	1104	MET	2.2
1	A	813	ILE	2.2
1	A	1082	ILE	2.2
1	B	1057	VAL	2.2
1	B	879	PHE	2.2
1	B	-7	GLY	2.2
1	A	186	GLU	2.2
1	B	140	ILE	2.2
1	C	1083	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1057	VAL	2.2
1	D	822	MET	2.2
1	C	129	PRO	2.2
1	A	1103	LYS	2.2
1	B	183	ALA	2.2
1	D	193	SER	2.2
1	C	459	ASP	2.1
1	D	844	HIS	2.1
1	A	843	GLY	2.1
1	D	166	GLY	2.1
1	C	1136	ILE	2.1
1	D	842	LEU	2.1
1	A	817	GLN	2.1
1	B	844	HIS	2.1
1	B	137	ALA	2.1
1	D	839	ALA	2.1
1	D	1101	ALA	2.1
1	A	1075	MET	2.1
1	B	822	MET	2.1
1	B	160	LEU	2.1
1	B	896	GLU	2.1
1	C	1080	LEU	2.1
1	B	138	VAL	2.1
1	C	114	GLY	2.1
1	D	194	GLY	2.1
1	A	815	SER	2.1
1	B	149	THR	2.1
1	B	482	THR	2.1
1	D	174	ALA	2.1
1	D	1126	ALA	2.1
1	A	140	ILE	2.1
1	B	898	ASN	2.1
1	C	844	HIS	2.1
1	C	932	VAL	2.1
1	B	162	GLY	2.1
1	B	877	ALA	2.0
1	A	897	LEU	2.0
1	B	1080	LEU	2.0
1	A	456	ARG	2.0
1	A	837	ALA	2.0
1	D	183	ALA	2.0
1	C	884	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	459	ASP	2.0
1	C	117	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](#)

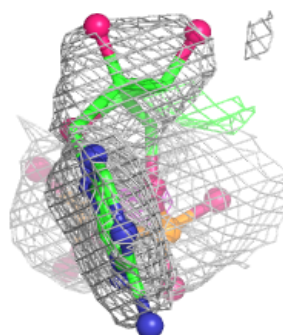
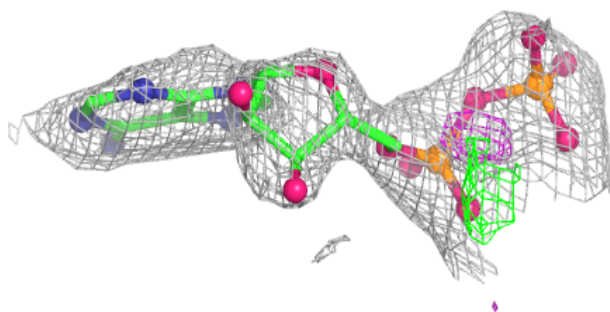
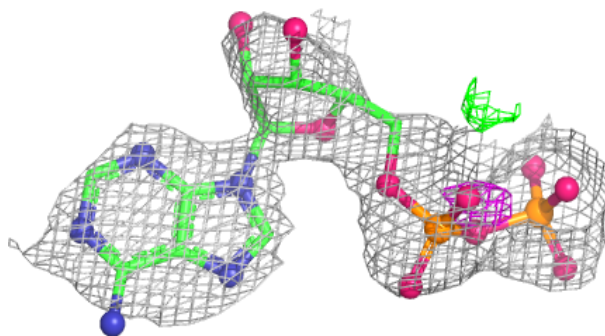
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	C	1202	27/27	0.87	0.10	59,67,73,77	0
3	ADP	D	1203	27/27	0.93	0.08	34,46,56,57	0
4	MG	C	1203	1/1	0.93	0.09	47,47,47,47	0
4	MG	D	1204	1/1	0.95	0.11	31,31,31,31	0
3	ADP	A	1202	27/27	0.96	0.06	35,41,59,66	0
3	ADP	B	1202	27/27	0.96	0.06	35,39,61,65	0
2	MN	B	1201	1/1	0.96	0.05	50,50,50,50	0
4	MG	A	1203	1/1	0.97	0.04	35,35,35,35	0
2	MN	C	1201	1/1	0.98	0.04	45,45,45,45	0
4	MG	B	1203	1/1	0.98	0.03	31,31,31,31	0
2	MN	D	1202	1/1	0.98	0.03	45,45,45,45	0
2	MN	A	1201	1/1	0.98	0.03	50,50,50,50	0
5	2BA	A	1204	44/44	0.98	0.05	14,19,20,22	0
5	2BA	D	1201	44/44	0.99	0.04	14,18,22,25	0

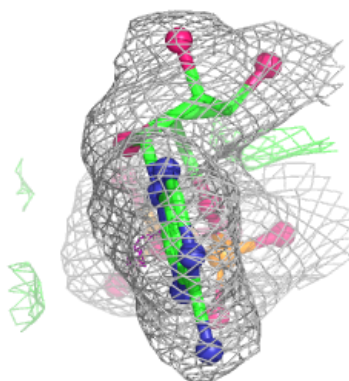
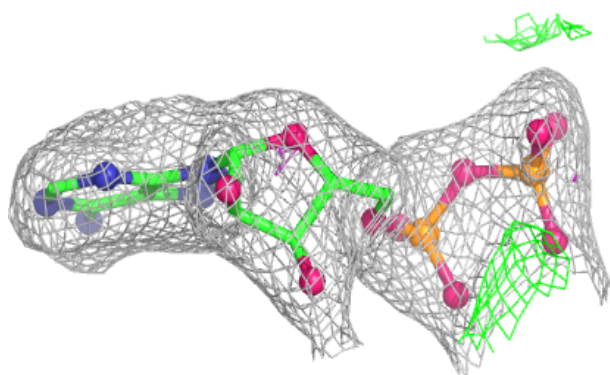
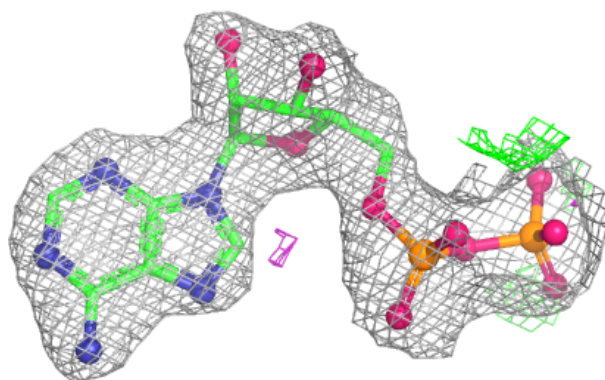
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 1202:

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

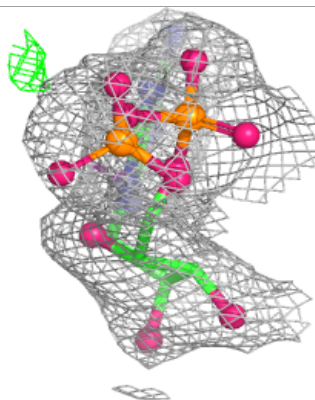
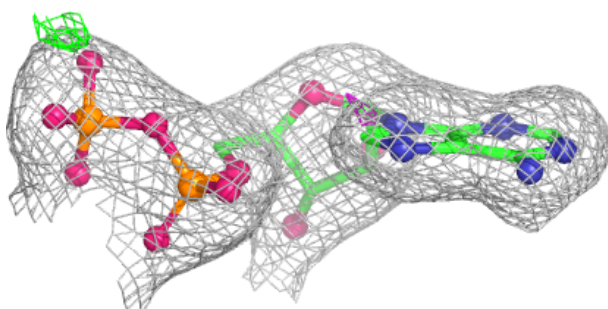
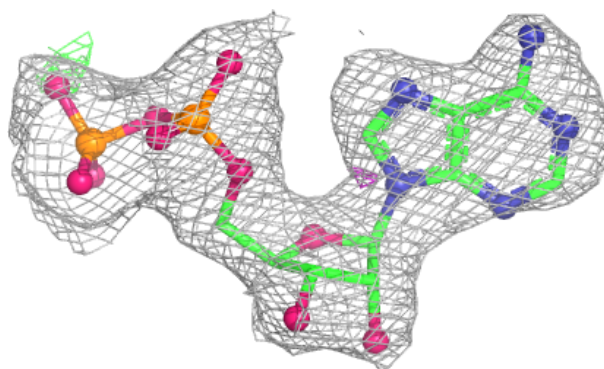
**Electron density around ADP D 1203:**

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

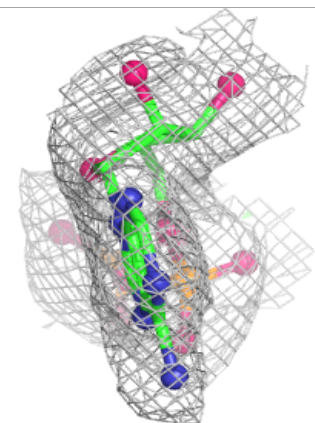
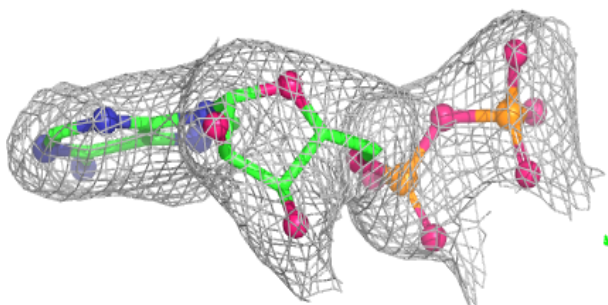
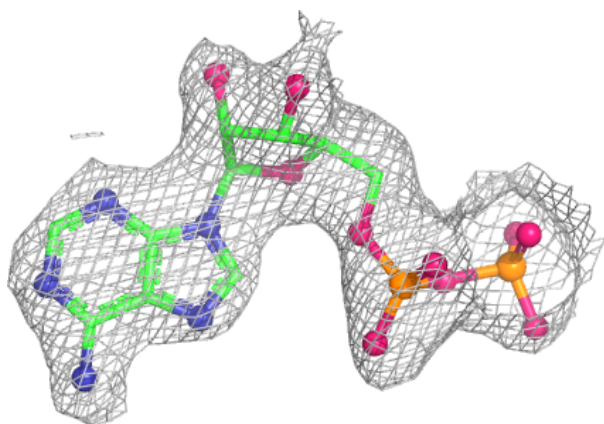


Electron density around ADP A 1202:

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

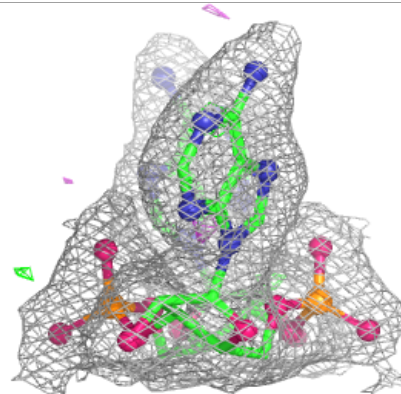
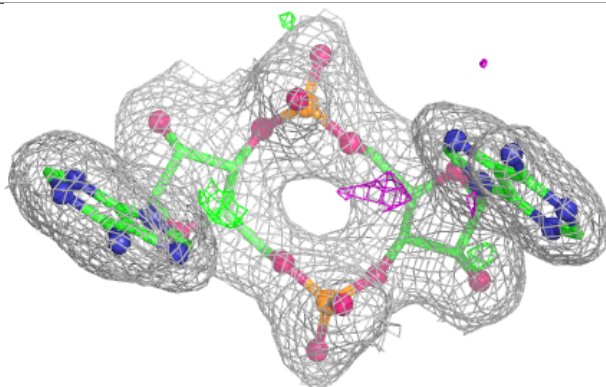
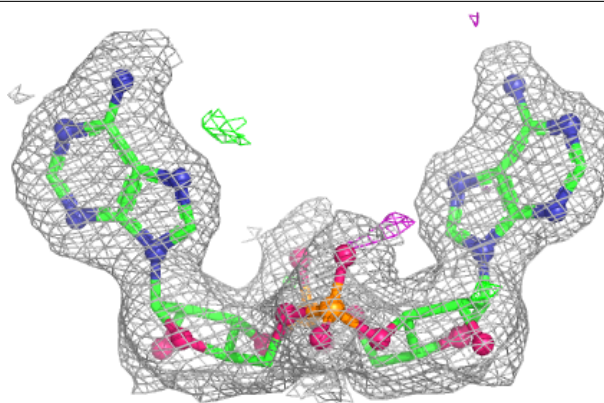
**Electron density around ADP B 1202:**

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

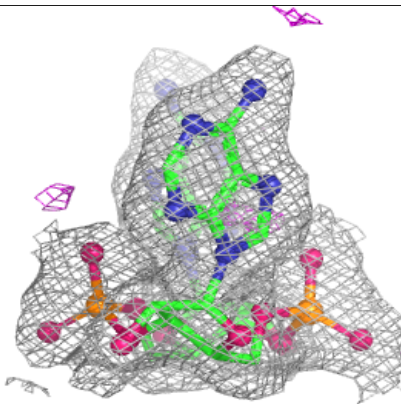
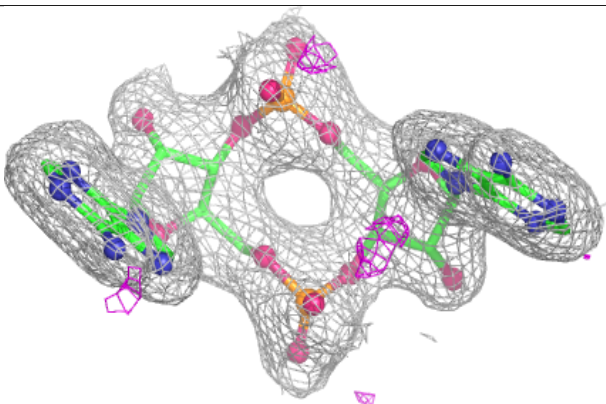
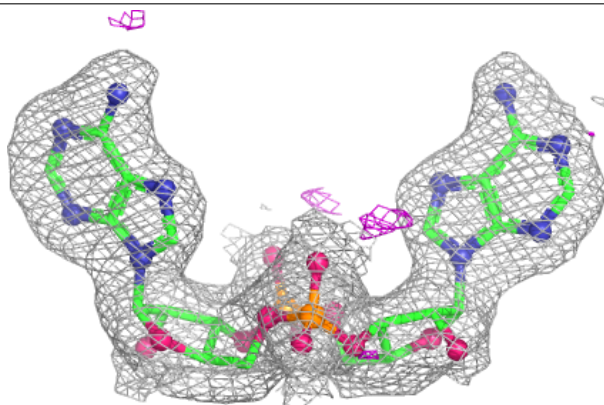


Electron density around 2BA A 1204:

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

**Electron density around 2BA D 1201:**

$2mF_o-DF_c$ (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.