



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:44 am BST

PDB ID : 5VZ0
Title : Crystal structure of Lactococcus lactis pyruvate carboxylase G746A mutant
in complex with cyclic-di-AMP
Authors : Choi, P.H.; Tong, L.
Deposited on : 2017-05-26
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

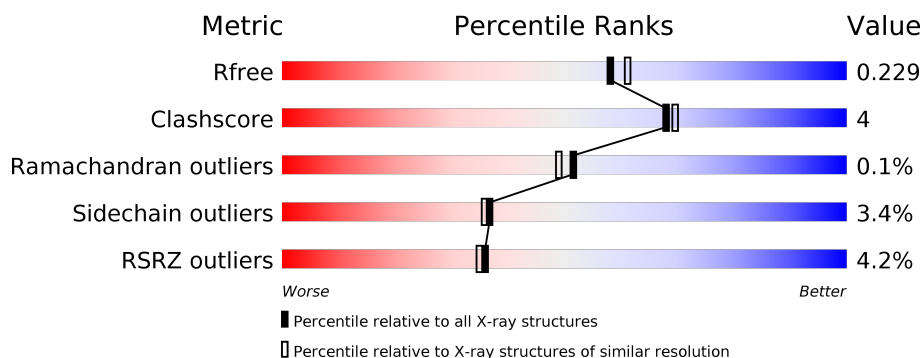
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1144	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
1	B	1144	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>••</div> </div> </div>
1	C	1144	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
1	D	1144	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>••</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36604 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	1139	Total	C	N	O	S	0	0	0
			8918	5654	1537	1692	35			
1	B	1138	Total	C	N	O	S	0	0	0
			8931	5664	1541	1691	35			
1	C	1074	Total	C	N	O	S	0	0	0
			8440	5353	1457	1598	32			
1	D	1137	Total	C	N	O	S	0	1	0
			8922	5659	1537	1690	36			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	746	ALA	GLY	engineered mutation	UNP A0A089XIW4
A	1055	ALA	THR	variant	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	746	ALA	GLY	engineered mutation	UNP A0A089XIW4
B	1055	ALA	THR	variant	UNP A0A089XIW4
C	-6	LEU	-	expression tag	UNP A0A089XIW4
C	-5	VAL	-	expression tag	UNP A0A089XIW4
C	-4	PRO	-	expression tag	UNP A0A089XIW4

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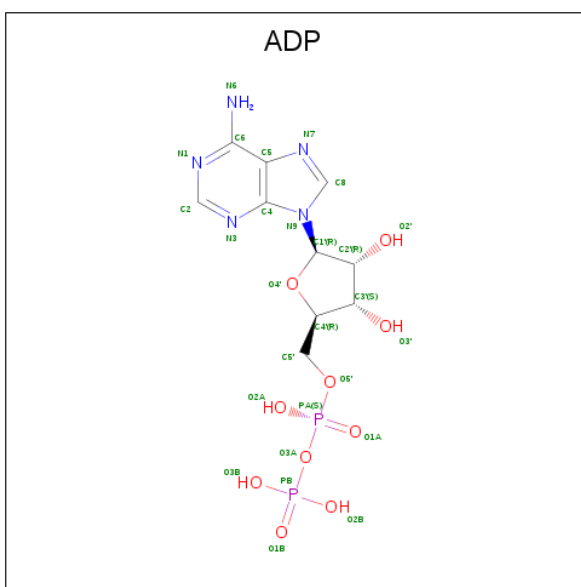
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP A0A089XIW4
C	-2	GLY	-	expression tag	UNP A0A089XIW4
C	-1	SER	-	expression tag	UNP A0A089XIW4
C	0	HIS	-	expression tag	UNP A0A089XIW4
C	746	ALA	GLY	engineered mutation	UNP A0A089XIW4
C	1055	ALA	THR	variant	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	746	ALA	GLY	engineered mutation	UNP A0A089XIW4
D	1055	ALA	THR	variant	UNP A0A089XIW4

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

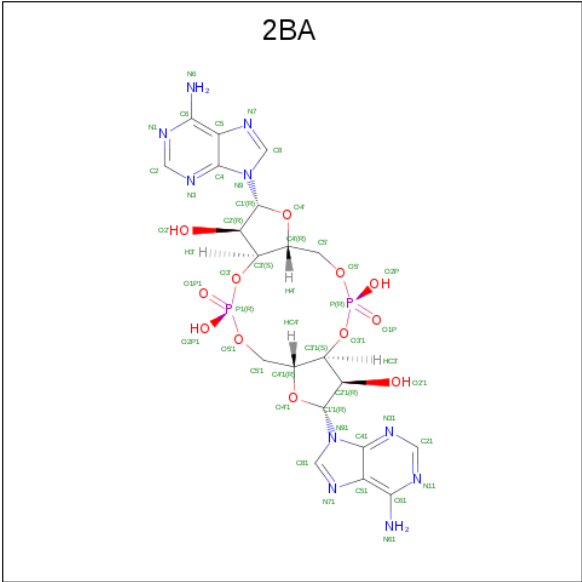


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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-tetraol 5,12-dioxide (three-letter code: 2BA) (formula: C₂₀H₂₄N₁₀O₁₂P₂).



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

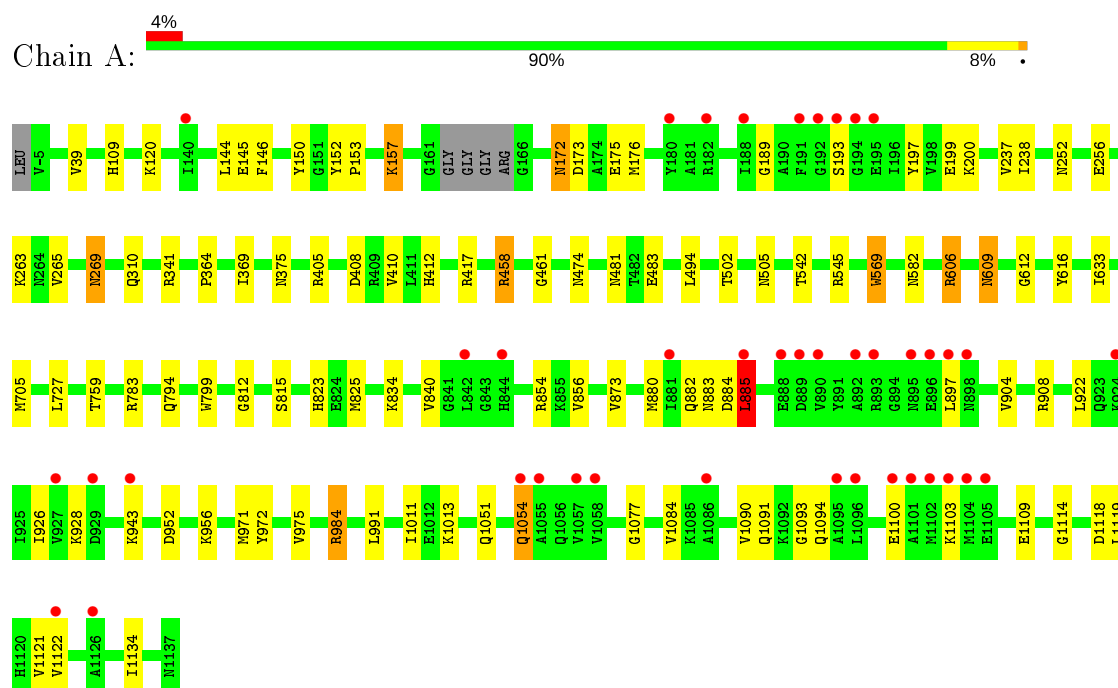
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total	O	0	0
			268	268		
6	B	340	Total	O	0	0
			340	340		
6	C	268	Total	O	0	0
			268	268		
6	D	341	Total	O	0	0
			341	341		

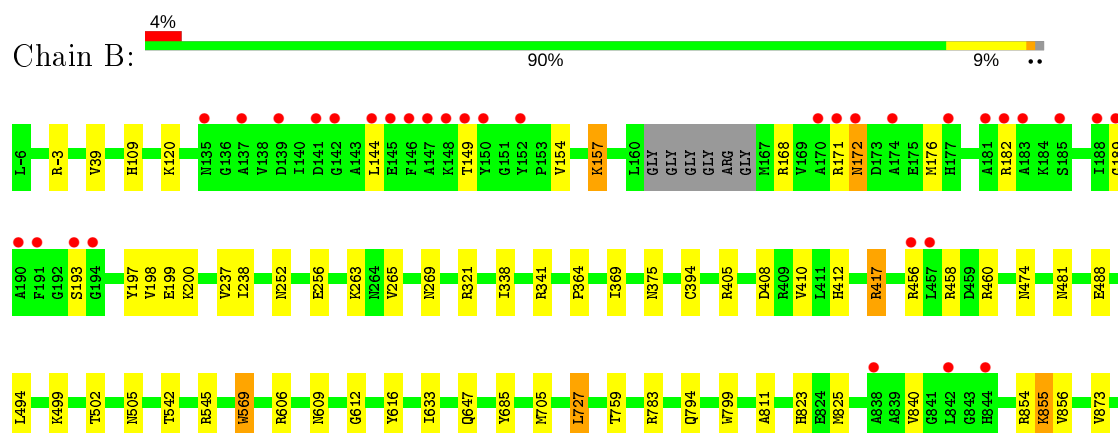
3 Residue-property plots [i](#)

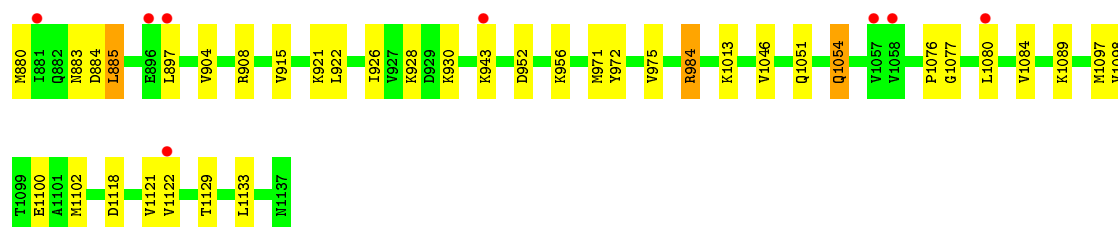
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

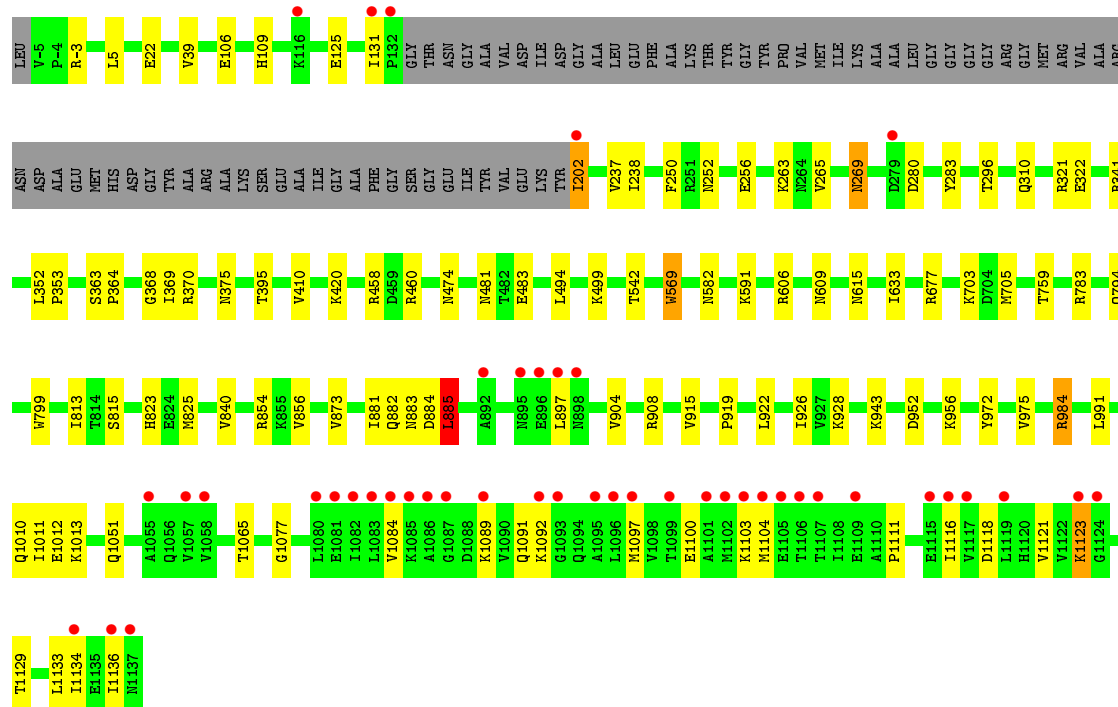
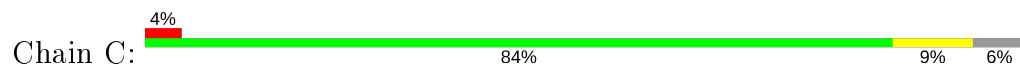


• Molecule 1: Pyruvate carboxylase

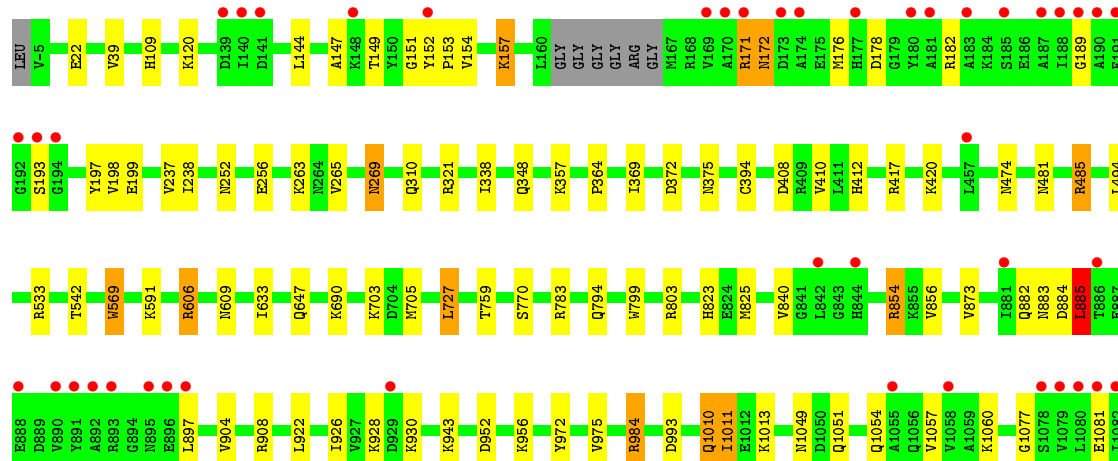
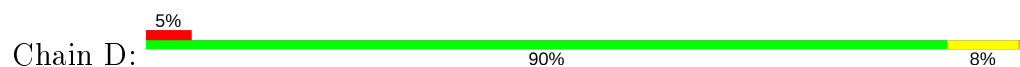


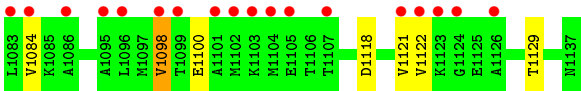


• Molecule 1: Pyruvate carboxylase



• 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	97.16Å 130.39Å 134.27Å 65.99° 88.67° 70.14°	Depositor
Resolution (Å)	48.55 – 2.00 48.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.55-2.00) 92.2 (48.51-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.218 0.202 , 0.229	Depositor DCC
R_{free} test set	17612 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	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	36604	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, 2BA, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/9090	0.80	8/12301 (0.1%)
1	B	0.77	1/9104 (0.0%)	0.83	13/12319 (0.1%)
1	C	0.73	0/8604	0.82	10/11647 (0.1%)
1	D	0.80	1/9098 (0.0%)	0.83	12/12311 (0.1%)
All	All	0.77	2/35896 (0.0%)	0.82	43/48578 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	770	SER	CA-CB	5.81	1.61	1.52
1	B	685	TYR	CE1-CZ	-5.58	1.31	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	984	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	B	341	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	C	-3	ARG	NE-CZ-NH1	-10.49	115.06	120.30
1	A	984	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	C	-3	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	D	984	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	C	984	ARG	NE-CZ-NH1	7.98	124.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	984	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	783	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	783	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	341	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	D	606	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	321	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	783	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	606	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	606	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	606	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	D	1011	ILE	CB-CA-C	-6.82	97.95	111.60
1	C	783	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	545	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	885	LEU	CA-CB-CG	6.24	129.64	115.30
1	A	984	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	D	783	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	D	885	LEU	CA-CB-CG	5.94	128.97	115.30
1	C	885	LEU	CA-CB-CG	5.91	128.90	115.30
1	D	485	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	A	545	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	984	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	984	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	321	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	783	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	-3	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	341	ARG	CG-CD-NE	-5.33	100.60	111.80
1	D	417	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	D	417	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	D	703	LYS	CD-CE-NZ	5.19	123.63	111.70
1	C	341	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	417	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	993	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	-3	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	703	LYS	CD-CE-NZ	5.05	123.31	111.70
1	C	341	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	A	783	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	131	ILE	Peptide

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	8918	0	8885	73	0
1	B	8931	0	8911	70	0
1	C	8440	0	8422	66	0
1	D	8922	0	8898	61	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	0	0
3	B	27	0	12	0	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	44	0	22	1	0
5	C	44	0	23	1	0
6	A	268	0	0	8	0
6	B	340	0	0	12	0
6	C	268	0	0	9	0
6	D	341	0	0	10	0
All	All	36604	0	35197	268	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 (268) 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:D:152:TYR:CE2	1:D:172:ASN:HA	1.95	1.00
1:A:612:GLY:HA3	1:A:971:MET:CE	1.96	0.96
1:B:612:GLY:HA3	1:B:971:MET:CE	1.97	0.94
1:A:458:ARG:HG2	1:A:458:ARG:HH11	1.37	0.89
1:A:612:GLY:HA3	1:A:971:MET:HE1	1.59	0.83
1:D:178:ASP:O	1:D:182:ARG:HG3	1.79	0.83
1:B:612:GLY:HA3	1:B:971:MET:HE1	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:LEU:HB2	1:B:1098:VAL:HG13	1.64	0.79
1:B:984:ARG:HD2	6:B:1564:HOH:O	1.84	0.78
1:B:883:ASN:HB2	1:B:885:LEU:HD11	1.65	0.78
1:A:606:ARG:NH1	1:A:609:ASN:HD21	1.84	0.76
1:B:915:VAL:HG23	6:B:1376:HOH:O	1.87	0.74
1:C:1116:ILE:HG21	6:C:1301:HOH:O	1.89	0.73
1:C:677:ARG:HD3	6:C:1337:HOH:O	1.87	0.73
1:D:152:TYR:HB3	1:D:153:PRO:HA	1.70	0.73
1:D:823:HIS:HD2	1:D:825:MET:H	1.37	0.73
1:A:823:HIS:HD2	1:A:825:MET:H	1.37	0.72
1:D:1010:GLN:HG3	6:D:1618:HOH:O	1.87	0.72
1:A:612:GLY:CA	1:A:971:MET:CE	2.69	0.71
1:C:202:ILE:HG22	1:C:202:ILE:O	1.89	0.71
1:C:883:ASN:HB2	1:C:885:LEU:HD21	1.71	0.70
1:B:823:HIS:HD2	1:B:825:MET:H	1.37	0.70
1:C:369:ILE:HD12	1:C:410:VAL:HG21	1.73	0.70
1:A:369:ILE:HD12	1:A:410:VAL:HG21	1.74	0.70
1:B:417:ARG:HD3	6:B:1627:HOH:O	1.92	0.70
6:B:1578:HOH:O	1:C:984:ARG:HD2	1.90	0.69
1:D:369:ILE:HD12	1:D:410:VAL:HG21	1.74	0.69
1:C:582:ASN:HB2	6:C:1459:HOH:O	1.92	0.69
1:B:811:ALA:C	6:B:1332:HOH:O	2.32	0.69
1:C:823:HIS:HD2	1:C:825:MET:H	1.40	0.69
1:D:883:ASN:HB2	1:D:885:LEU:HD21	1.76	0.68
1:B:612:GLY:CA	1:B:971:MET:CE	2.71	0.68
1:B:369:ILE:HD12	1:B:410:VAL:HG21	1.75	0.67
1:B:494:LEU:H	1:B:794:GLN:HE21	1.41	0.67
1:A:461:GLY:HA3	6:A:1313:HOH:O	1.93	0.67
1:C:1123:LYS:H	1:C:1123:LYS:HE3	1.60	0.67
1:C:840:VAL:O	1:C:840:VAL:HG12	1.95	0.67
1:D:984:ARG:HD2	6:D:1497:HOH:O	1.93	0.67
1:A:840:VAL:O	1:A:840:VAL:HG12	1.95	0.66
1:D:840:VAL:HG12	1:D:840:VAL:O	1.95	0.66
1:B:39:VAL:H	1:B:375:ASN:ND2	1.94	0.66
1:B:880:MET:HA	1:B:885:LEU:HD13	1.76	0.65
1:B:840:VAL:HG12	1:B:840:VAL:O	1.95	0.65
1:B:612:GLY:CA	1:B:971:MET:HE1	2.25	0.64
1:A:883:ASN:HB2	1:A:885:LEU:HD21	1.80	0.63
1:B:168:ARG:NH2	1:B:182:ARG:HG3	2.14	0.63
1:D:474:ASN:HD21	1:D:1051:GLN:H	1.47	0.63
1:A:458:ARG:HH11	1:A:458:ARG:CG	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:GLY:CA	1:A:971:MET:HE1	2.29	0.63
1:A:883:ASN:HB2	1:A:885:LEU:CD2	2.30	0.61
1:A:474:ASN:HD21	1:A:1051:GLN:H	1.49	0.61
1:D:39:VAL:H	1:D:375:ASN:ND2	1.98	0.61
1:C:202:ILE:HD11	1:C:283:TYR:CE2	2.36	0.60
1:A:146:PHE:CE1	1:A:150:TYR:CE1	2.90	0.60
1:C:474:ASN:HD21	1:C:1051:GLN:H	1.48	0.60
1:D:1011:ILE:HG22	1:D:1011:ILE:O	2.01	0.60
1:D:647:GLN:NE2	6:D:1302:HOH:O	2.33	0.60
1:A:109:HIS:HE1	1:A:265:VAL:O	1.85	0.60
1:B:474:ASN:HD21	1:B:1051:GLN:H	1.50	0.60
1:B:1054:GLN:HG2	6:B:1417:HOH:O	2.01	0.59
1:C:39:VAL:H	1:C:375:ASN:ND2	2.00	0.58
1:C:1123:LYS:HE3	1:C:1123:LYS:N	2.18	0.58
1:A:364:PRO:HG2	1:A:410:VAL:HG13	1.86	0.58
1:D:364:PRO:HG2	1:D:410:VAL:HG13	1.86	0.57
1:A:494:LEU:H	1:A:794:GLN:HE21	1.51	0.57
1:C:569:TRP:CE3	1:C:633:ILE:HD11	2.39	0.57
1:D:474:ASN:ND2	1:D:1051:GLN:H	2.01	0.57
1:A:582:ASN:CB	6:A:1338:HOH:O	2.52	0.57
1:A:815:SER:HB3	6:B:1387:HOH:O	2.04	0.57
1:D:109:HIS:HE1	1:D:265:VAL:O	1.86	0.57
1:D:494:LEU:H	1:D:794:GLN:HE21	1.52	0.57
1:C:109:HIS:HE1	1:C:265:VAL:O	1.88	0.57
1:B:1097:MET:HE2	1:B:1133:LEU:HD13	1.86	0.57
1:C:202:ILE:O	1:C:202:ILE:CG2	2.53	0.57
1:A:569:TRP:CE3	1:A:633:ILE:HD11	2.40	0.56
1:B:647:GLN:NE2	6:B:1303:HOH:O	2.38	0.56
1:D:152:TYR:CE2	1:D:172:ASN:CA	2.80	0.56
1:A:474:ASN:ND2	1:A:1051:GLN:H	2.04	0.56
1:A:39:VAL:H	1:A:375:ASN:ND2	2.03	0.56
5:B:1201:2BA:HC5A	5:B:1201:2BA:H5'A	1.87	0.56
1:C:321:ARG:HG2	1:C:322:GLU:HG3	1.86	0.56
1:C:569:TRP:CE3	1:C:633:ILE:CD1	2.89	0.56
1:A:582:ASN:HB2	6:A:1338:HOH:O	2.05	0.56
1:C:915:VAL:HG23	6:C:1364:HOH:O	2.06	0.56
1:C:582:ASN:CB	6:C:1459:HOH:O	2.51	0.56
1:C:364:PRO:HG2	1:C:410:VAL:HG13	1.87	0.55
1:C:474:ASN:ND2	1:C:1051:GLN:H	2.04	0.55
1:B:569:TRP:CE3	1:B:633:ILE:HD11	2.41	0.55
1:D:152:TYR:CD2	1:D:172:ASN:HA	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:GLY:O	1:A:1109:GLU:OE1	2.23	0.55
1:B:364:PRO:HG2	1:B:410:VAL:HG13	1.88	0.55
1:A:146:PHE:CE1	1:A:150:TYR:CD1	2.95	0.55
1:B:569:TRP:CE3	1:B:633:ILE:CD1	2.90	0.55
1:A:569:TRP:CE3	1:A:633:ILE:CD1	2.89	0.54
1:B:883:ASN:HB2	1:B:885:LEU:CD1	2.35	0.54
1:D:854:ARG:HG2	6:D:1354:HOH:O	2.06	0.54
1:B:168:ARG:NH2	1:B:182:ARG:CG	2.70	0.54
1:B:811:ALA:CB	6:B:1332:HOH:O	2.54	0.54
1:A:612:GLY:CA	1:A:971:MET:HE2	2.39	0.53
1:B:109:HIS:HE1	1:B:265:VAL:O	1.91	0.53
1:B:922:LEU:HG	1:B:926:ILE:HD12	1.89	0.53
1:C:1092:LYS:HE2	1:C:1111:PRO:O	2.09	0.53
1:D:569:TRP:CE3	1:D:633:ILE:HD11	2.43	0.53
1:D:922:LEU:HG	1:D:926:ILE:HD12	1.91	0.53
1:B:474:ASN:ND2	1:B:1051:GLN:H	2.06	0.53
1:C:883:ASN:HB2	1:C:885:LEU:CD2	2.39	0.53
1:D:481:ASN:HB2	6:D:1626:HOH:O	2.07	0.53
1:A:897:LEU:O	1:A:928:LYS:NZ	2.42	0.53
1:B:885:LEU:H	1:B:885:LEU:HD12	1.75	0.52
1:A:341:ARG:HD3	6:A:1302:HOH:O	2.08	0.52
1:A:952:ASP:OD1	1:A:956:LYS:HE2	2.10	0.52
1:D:883:ASN:HB2	1:D:885:LEU:CD2	2.40	0.52
1:C:883:ASN:CB	1:C:885:LEU:HD21	2.40	0.52
1:D:569:TRP:CE3	1:D:633:ILE:CD1	2.92	0.52
1:B:897:LEU:O	1:B:928:LYS:NZ	2.42	0.51
1:A:458:ARG:NH1	1:A:458:ARG:CG	2.72	0.51
1:D:840:VAL:CG1	1:D:840:VAL:O	2.58	0.51
1:C:840:VAL:O	1:C:840:VAL:CG1	2.58	0.51
1:C:952:ASP:OD1	1:C:956:LYS:HE2	2.11	0.51
1:A:840:VAL:O	1:A:840:VAL:CG1	2.59	0.51
1:B:39:VAL:H	1:B:375:ASN:HD21	1.58	0.51
1:C:897:LEU:O	1:C:928:LYS:NZ	2.42	0.51
1:C:922:LEU:HG	1:C:926:ILE:HD12	1.92	0.51
1:A:922:LEU:HG	1:A:926:ILE:HD12	1.93	0.51
1:D:897:LEU:O	1:D:928:LYS:NZ	2.43	0.51
1:B:840:VAL:CG1	1:B:840:VAL:O	2.58	0.50
1:C:460:ARG:NH1	1:C:1012:GLU:OE1	2.41	0.50
1:C:39:VAL:H	1:C:375:ASN:HD21	1.59	0.50
1:B:885:LEU:N	1:B:885:LEU:HD12	2.27	0.50
1:A:984:ARG:HD2	6:D:1561:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:MET:HE3	1:A:971:MET:HA	1.94	0.49
1:B:971:MET:HA	1:B:971:MET:HE3	1.93	0.49
1:D:147:ALA:O	1:D:151:GLY:HA2	2.12	0.49
1:B:952:ASP:OD1	1:B:956:LYS:HE2	2.13	0.49
1:D:727:LEU:H	1:D:727:LEU:HD12	1.77	0.49
1:B:1054:GLN:OE1	1:B:1054:GLN:N	2.46	0.49
1:B:811:ALA:HB1	6:B:1332:HOH:O	2.12	0.49
1:C:883:ASN:C	1:C:885:LEU:HD23	2.33	0.49
1:B:168:ARG:HH22	1:B:182:ARG:HG3	1.78	0.48
1:C:494:LEU:H	1:C:794:GLN:HE21	1.62	0.48
1:B:616:TYR:OH	1:B:971:MET:HE3	2.14	0.48
1:D:606:ARG:NH1	1:D:609:ASN:OD1	2.46	0.48
1:D:690:LYS:HE2	6:D:1520:HOH:O	2.12	0.48
1:D:952:ASP:OD1	1:D:956:LYS:HE2	2.13	0.47
1:C:202:ILE:HD11	1:C:283:TYR:CD2	2.49	0.47
1:A:759:THR:HG21	1:A:799:TRP:CD1	2.50	0.47
1:A:172:ASN:HD22	1:A:172:ASN:C	2.18	0.47
1:D:1081:GLU:HB2	1:D:1098:VAL:HG23	1.95	0.47
1:A:1090:VAL:HG22	1:A:1114:GLY:O	2.15	0.47
1:A:812:GLY:HA2	6:A:1557:HOH:O	2.15	0.47
1:B:759:THR:HG21	1:B:799:TRP:CD1	2.50	0.46
1:A:606:ARG:HD3	6:A:1431:HOH:O	2.14	0.46
1:C:1116:ILE:CB	6:C:1301:HOH:O	2.64	0.46
1:A:971:MET:HE3	1:A:971:MET:CA	2.46	0.46
1:A:612:GLY:HA3	1:A:971:MET:HE2	1.91	0.45
1:D:120:LYS:HE2	1:D:199:GLU:OE2	2.16	0.45
1:A:609:ASN:HB2	1:A:616:TYR:CE2	2.52	0.45
1:C:759:THR:HG21	1:C:799:TRP:CD1	2.51	0.45
1:C:904:VAL:O	1:C:908:ARG:HG3	2.16	0.45
1:A:120:LYS:HE2	1:A:199:GLU:OE2	2.16	0.45
1:C:1116:ILE:CG2	6:C:1301:HOH:O	2.57	0.45
1:B:120:LYS:HE2	1:B:199:GLU:OE2	2.17	0.45
1:C:252:ASN:O	1:C:256:GLU:HG2	2.17	0.45
1:D:152:TYR:CD2	1:D:171:ARG:O	2.70	0.45
1:D:1077:GLY:HA3	1:D:1100:GLU:O	2.17	0.45
1:D:147:ALA:O	1:D:151:GLY:N	2.49	0.45
1:C:615:ASN:ND2	6:C:1312:HOH:O	2.49	0.44
1:D:904:VAL:O	1:D:908:ARG:HG3	2.17	0.44
1:A:157:LYS:HE2	1:A:197:TYR:OH	2.18	0.44
1:A:417:ARG:HD3	6:A:1559:HOH:O	2.17	0.44
1:A:1054:GLN:OE1	1:A:1054:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1081:GLU:HB2	1:D:1098:VAL:CG2	2.47	0.44
1:B:612:GLY:CA	1:B:971:MET:HE2	2.47	0.44
1:C:237:VAL:HG12	1:C:238:ILE:HG13	2.00	0.44
1:A:252:ASN:O	1:A:256:GLU:HG2	2.17	0.44
1:B:908:ARG:HD2	1:B:930:LYS:HB2	1.98	0.44
1:C:1097:MET:HE2	1:C:1133:LEU:HD13	2.00	0.44
1:B:856:VAL:HG12	1:B:873:VAL:HG13	2.00	0.44
1:B:904:VAL:O	1:B:908:ARG:HG3	2.17	0.44
1:B:971:MET:HE3	1:B:971:MET:CA	2.48	0.44
1:D:252:ASN:O	1:D:256:GLU:HG2	2.18	0.44
1:B:458:ARG:HE	1:B:458:ARG:HB2	1.25	0.43
1:B:1077:GLY:HA3	1:B:1100:GLU:O	2.18	0.43
1:C:1077:GLY:HA3	1:C:1100:GLU:O	2.17	0.43
1:C:352:LEU:HD12	1:C:353:PRO:HD2	1.99	0.43
1:D:269:ASN:OD1	1:D:310:GLN:HG2	2.19	0.43
1:C:296:THR:HG22	1:C:370:ARG:NH2	2.33	0.43
1:C:883:ASN:O	1:C:885:LEU:HD23	2.19	0.43
1:D:172:ASN:C	1:D:172:ASN:HD22	2.21	0.43
1:A:1091:GLN:H	1:A:1094:GLN:HE21	1.67	0.43
1:A:904:VAL:O	1:A:908:ARG:HG3	2.17	0.43
1:B:460:ARG:HG2	6:B:1604:HOH:O	2.18	0.43
1:D:759:THR:HG21	1:D:799:TRP:CD1	2.52	0.43
1:D:154:VAL:HG13	1:D:198:VAL:HG13	2.00	0.43
1:D:727:LEU:N	1:D:727:LEU:HD12	2.34	0.43
1:A:616:TYR:OH	1:A:971:MET:HE3	2.19	0.43
1:C:813:ILE:HG21	1:D:803:ARG:CZ	2.49	0.43
1:B:157:LYS:HE2	1:B:197:TYR:OH	2.18	0.43
1:B:172:ASN:C	1:B:172:ASN:HD22	2.21	0.43
1:B:609:ASN:HB2	1:B:616:TYR:CE2	2.54	0.43
1:D:533:ARG:HD2	1:D:533:ARG:C	2.39	0.43
1:B:612:GLY:N	1:B:971:MET:HE1	2.33	0.42
1:C:972:TYR:HB3	1:C:975:VAL:HB	2.00	0.42
1:B:237:VAL:HG12	1:B:238:ILE:HG13	2.01	0.42
1:B:338:ILE:O	1:B:394:CYS:HA	2.19	0.42
1:D:338:ILE:O	1:D:394:CYS:HA	2.19	0.42
1:D:39:VAL:H	1:D:375:ASN:HD21	1.63	0.42
1:C:363:SER:HA	1:C:364:PRO:HD3	1.91	0.42
1:D:157:LYS:HE2	1:D:197:TYR:OH	2.19	0.42
5:C:1202:2BA:HC5A	5:C:1202:2BA:H5'A	2.00	0.42
1:A:1119:LEU:HD22	1:A:1134:ILE:HD12	2.02	0.42
1:A:606:ARG:CZ	1:A:609:ASN:HD21	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:HD12	1:B:727:LEU:H	1.84	0.42
1:C:815:SER:HB3	6:D:1336:HOH:O	2.19	0.42
1:A:612:GLY:N	1:A:971:MET:CE	2.82	0.42
1:D:237:VAL:HG12	1:D:238:ILE:HG13	2.01	0.42
1:B:855:LYS:HD2	6:B:1457:HOH:O	2.19	0.42
1:C:883:ASN:CB	1:C:885:LEU:CD2	2.98	0.42
1:A:840:VAL:HG11	1:A:882:GLN:NE2	2.34	0.42
1:C:269:ASN:OD1	1:C:310:GLN:HG2	2.20	0.42
1:B:502:THR:H	1:B:505:ASN:HD22	1.67	0.42
1:B:405:ARG:HD3	1:D:22:GLU:O	2.19	0.42
1:C:840:VAL:HG11	1:C:882:GLN:NE2	2.34	0.42
1:B:408:ASP:O	1:B:412:HIS:HD2	2.03	0.41
1:C:368:GLY:O	1:C:395:THR:HA	2.20	0.41
1:A:856:VAL:HG12	1:A:873:VAL:HG13	2.02	0.41
1:A:972:TYR:HB3	1:A:975:VAL:HB	2.02	0.41
1:B:606:ARG:NH1	1:B:609:ASN:OD1	2.52	0.41
1:B:972:TYR:HB3	1:B:975:VAL:HB	2.02	0.41
1:D:972:TYR:HB3	1:D:975:VAL:HB	2.00	0.41
1:D:408:ASP:O	1:D:412:HIS:HD2	2.03	0.41
1:A:1077:GLY:HA3	1:A:1100:GLU:O	2.20	0.41
1:A:405:ARG:HD3	1:C:22:GLU:O	2.20	0.41
1:A:880:MET:HA	1:A:885:LEU:HD23	2.02	0.41
1:A:883:ASN:C	1:A:885:LEU:HD22	2.41	0.41
1:B:616:TYR:CZ	1:B:971:MET:HE3	2.56	0.41
1:B:502:THR:H	1:B:505:ASN:ND2	2.19	0.41
1:C:991:LEU:HD13	1:C:1011:ILE:HA	2.02	0.41
1:C:677:ARG:CD	6:C:1337:HOH:O	2.59	0.41
1:A:269:ASN:OD1	1:A:310:GLN:HG2	2.21	0.41
1:D:883:ASN:CB	1:D:885:LEU:HD21	2.47	0.41
1:A:502:THR:H	1:A:505:ASN:ND2	2.19	0.41
1:A:582:ASN:CG	6:A:1338:HOH:O	2.60	0.41
1:B:612:GLY:N	1:B:971:MET:CE	2.84	0.41
1:C:106:GLU:H	1:C:109:HIS:HD2	1.69	0.41
1:C:250:PHE:CZ	1:C:280:ASP:HA	2.56	0.41
1:D:591:LYS:HD3	6:D:1373:HOH:O	2.20	0.41
1:D:856:VAL:HG12	1:D:873:VAL:HG13	2.02	0.41
1:D:840:VAL:HG11	1:D:882:GLN:NE2	2.35	0.41
1:A:502:THR:H	1:A:505:ASN:HD22	1.68	0.41
1:A:883:ASN:O	1:A:885:LEU:HD22	2.20	0.41
1:B:154:VAL:HG13	1:B:198:VAL:HG13	2.03	0.41
1:B:252:ASN:O	1:B:256:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG12	1:A:238:ILE:HG13	2.03	0.40
1:A:408:ASP:O	1:A:412:HIS:HD2	2.04	0.40
1:A:152:TYR:HB3	1:A:153:PRO:HA	2.03	0.40
1:C:606:ARG:NH1	1:C:609:ASN:OD1	2.55	0.40
1:D:147:ALA:O	1:D:151:GLY:CA	2.70	0.40
1:D:369:ILE:HD12	1:D:410:VAL:CG2	2.47	0.40
1:A:146:PHE:CZ	1:A:150:TYR:CD1	3.09	0.40
1:A:991:LEU:HD13	1:A:1011:ILE:HA	2.03	0.40
1:C:420:LYS:HD2	1:C:420:LYS:HA	1.92	0.40
1:D:1049:ASN:ND2	6:D:1315:HOH:O	2.47	0.40
1:A:172:ASN:ND2	1:A:175:GLU:H	2.20	0.40
1:B:1046:VAL:HG13	1:C:1065:THR:HB	2.03	0.40
1:C:856:VAL:HG12	1:C:873:VAL:HG13	2.03	0.40
1:C:5:LEU:HD23	1:C:5:LEU:C	2.42	0.40
1:C:881:ILE:HD13	1:C:881:ILE:HA	1.98	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	1135/1144 (99%)	1107 (98%)	27 (2%)	1 (0%)	51	49
1	B	1134/1144 (99%)	1105 (97%)	27 (2%)	2 (0%)	47	44
1	C	1070/1144 (94%)	1043 (98%)	27 (2%)	0	100	100
1	D	1134/1144 (99%)	1104 (97%)	28 (2%)	2 (0%)	47	44
All	All	4473/4576 (98%)	4359 (98%)	109 (2%)	5 (0%)	51	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	ASN
1	D	269	ASN
1	B	189	GLY
1	A	189	GLY
1	D	189	GLY

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	951/956 (100%)	921 (97%)	30 (3%)	39	38
1	B	955/956 (100%)	922 (96%)	33 (4%)	36	35
1	C	908/956 (95%)	878 (97%)	30 (3%)	38	37
1	D	954/956 (100%)	920 (96%)	34 (4%)	35	34
All	All	3768/3824 (98%)	3641 (97%)	127 (3%)	37	36

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	GLU
1	A	157	LYS
1	A	172	ASN
1	A	173	ASP
1	A	176	MET
1	A	193	SER
1	A	200	LYS
1	A	263	LYS
1	A	269	ASN
1	A	458	ARG
1	A	481	ASN
1	A	483	GLU
1	A	542	THR
1	A	569	TRP
1	A	609	ASN
1	A	705	MET

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Mol	Chain	Res	Type
1	A	727	LEU
1	A	834	LYS
1	A	854	ARG
1	A	884	ASP
1	A	885	LEU
1	A	943	LYS
1	A	1013	LYS
1	A	1054	GLN
1	A	1084	VAL
1	A	1103	LYS
1	A	1118	ASP
1	A	1121	VAL
1	A	1122	VAL
1	B	144	LEU
1	B	149	THR
1	B	157	LYS
1	B	171	ARG
1	B	172	ASN
1	B	176	MET
1	B	193	SER
1	B	200	LYS
1	B	263	LYS
1	B	456	ARG
1	B	481	ASN
1	B	488	GLU
1	B	499	LYS
1	B	542	THR
1	B	569	TRP
1	B	705	MET
1	B	727	LEU
1	B	854	ARG
1	B	855	LYS
1	B	884	ASP
1	B	885	LEU
1	B	921	LYS
1	B	943	LYS
1	B	1013	LYS
1	B	1054	GLN
1	B	1076	PRO
1	B	1084	VAL
1	B	1089	LYS
1	B	1102	MET

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Mol	Chain	Res	Type
1	B	1118	ASP
1	B	1121	VAL
1	B	1122	VAL
1	B	1129	THR
1	C	125	GLU
1	C	202	ILE
1	C	263	LYS
1	C	269	ASN
1	C	458	ARG
1	C	481	ASN
1	C	483	GLU
1	C	499	LYS
1	C	542	THR
1	C	569	TRP
1	C	591	LYS
1	C	705	MET
1	C	854	ARG
1	C	884	ASP
1	C	885	LEU
1	C	919	PRO
1	C	943	LYS
1	C	1010	GLN
1	C	1013	LYS
1	C	1084	VAL
1	C	1089	LYS
1	C	1091	GLN
1	C	1103	LYS
1	C	1104	MET
1	C	1118	ASP
1	C	1121	VAL
1	C	1123	LYS
1	C	1129	THR
1	C	1134	ILE
1	C	1136	ILE
1	D	144	LEU
1	D	149	THR
1	D	157	LYS
1	D	171	ARG
1	D	172	ASN
1	D	176	MET
1	D	193	SER
1	D	263	LYS

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Mol	Chain	Res	Type
1	D	321	ARG
1	D	348	GLN
1	D	357	LYS
1	D	372	ASP
1	D	420	LYS
1	D	485	ARG
1	D	542	THR
1	D	569	TRP
1	D	705	MET
1	D	727	LEU
1	D	854	ARG
1	D	884	ASP
1	D	885	LEU
1	D	930	LYS
1	D	943	LYS
1	D	1010	GLN
1	D	1013	LYS
1	D	1054	GLN
1	D	1057	VAL
1	D	1060	LYS
1	D	1084	VAL
1	D	1098	VAL
1	D	1118	ASP
1	D	1121	VAL
1	D	1122	VAL
1	D	1129	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	172	ASN
1	A	219	ASN
1	A	308	GLN
1	A	375	ASN
1	A	412	HIS
1	A	439	GLN
1	A	474	ASN
1	A	481	ASN
1	A	486	HIS
1	A	492	GLN
1	A	505	ASN

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Mol	Chain	Res	Type
1	A	547	GLN
1	A	609	ASN
1	A	615	ASN
1	A	739	ASN
1	A	794	GLN
1	A	817	GLN
1	A	823	HIS
1	A	829	GLN
1	A	913	GLN
1	A	1010	GLN
1	A	1069	ASN
1	A	1094	GLN
1	B	52	GLN
1	B	109	HIS
1	B	172	ASN
1	B	219	ASN
1	B	264	ASN
1	B	308	GLN
1	B	375	ASN
1	B	412	HIS
1	B	439	GLN
1	B	474	ASN
1	B	481	ASN
1	B	492	GLN
1	B	505	ASN
1	B	547	GLN
1	B	615	ASN
1	B	647	GLN
1	B	739	ASN
1	B	794	GLN
1	B	817	GLN
1	B	823	HIS
1	B	829	GLN
1	B	913	GLN
1	B	1010	GLN
1	B	1049	ASN
1	B	1069	ASN
1	B	1094	GLN
1	C	109	HIS
1	C	207	HIS
1	C	219	ASN
1	C	308	GLN

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Mol	Chain	Res	Type
1	C	375	ASN
1	C	412	HIS
1	C	439	GLN
1	C	474	ASN
1	C	481	ASN
1	C	486	HIS
1	C	492	GLN
1	C	505	ASN
1	C	547	GLN
1	C	615	ASN
1	C	647	GLN
1	C	739	ASN
1	C	794	GLN
1	C	817	GLN
1	C	823	HIS
1	C	829	GLN
1	C	940	HIS
1	C	1010	GLN
1	C	1049	ASN
1	C	1094	GLN
1	D	109	HIS
1	D	172	ASN
1	D	219	ASN
1	D	308	GLN
1	D	375	ASN
1	D	412	HIS
1	D	439	GLN
1	D	474	ASN
1	D	486	HIS
1	D	492	GLN
1	D	505	ASN
1	D	547	GLN
1	D	615	ASN
1	D	739	ASN
1	D	794	GLN
1	D	817	GLN
1	D	823	HIS
1	D	829	GLN
1	D	980	GLN
1	D	1069	ASN
1	D	1094	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	2BA	C	1202	-	44,50,50	1.60	6 (13%)	50,78,78	1.71	8 (16%)
3	ADP	B	1203	4	24,29,29	1.39	4 (16%)	29,45,45	1.40	4 (13%)
3	ADP	A	1202	4	24,29,29	1.19	3 (12%)	29,45,45	1.32	4 (13%)
5	2BA	B	1201	-	44,50,50	1.42	7 (15%)	50,78,78	1.41	9 (18%)
3	ADP	D	1202	4	24,29,29	1.08	2 (8%)	29,45,45	1.64	5 (17%)

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	2BA	C	1202	-	-	1/22/62/62	0/6/7/7
3	ADP	B	1203	4	-	1/12/32/32	0/3/3/3
3	ADP	A	1202	4	-	2/12/32/32	0/3/3/3
5	2BA	B	1201	-	-	0/22/62/62	0/6/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	1202	4	-	4/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1202	2BA	C2'-C1'1	-5.85	1.44	1.53
5	B	1201	2BA	C2'-C1'	-3.66	1.48	1.53
5	C	1202	2BA	C2'-C1'	-3.45	1.48	1.53
3	B	1203	ADP	C2'-C1'	-3.38	1.48	1.53
3	A	1202	ADP	O4'-C1'	2.87	1.45	1.41
3	B	1203	ADP	C2-N3	2.84	1.36	1.32
5	B	1201	2BA	P1-O3'	2.80	1.67	1.60
5	B	1201	2BA	C5-N7	-2.74	1.29	1.39
5	C	1202	2BA	O3'1-C3'1	-2.66	1.34	1.44
3	A	1202	ADP	C5-C4	2.65	1.47	1.40
5	C	1202	2BA	C2'-C3'	2.62	1.58	1.52
5	B	1201	2BA	C4-N3	2.60	1.39	1.35
3	B	1203	ADP	C5-C4	2.59	1.47	1.40
5	C	1202	2BA	P-O3'1	2.55	1.67	1.60
3	D	1202	ADP	C5-C4	2.49	1.47	1.40
5	B	1201	2BA	C5-C4	2.44	1.47	1.40
3	A	1202	ADP	C2-N3	2.41	1.36	1.32
5	B	1201	2BA	O3'-C3'	-2.24	1.35	1.44
3	D	1202	ADP	O4'-C1'	2.17	1.44	1.41
5	C	1202	2BA	C51-C41	2.14	1.46	1.40
3	B	1203	ADP	C2-N1	2.13	1.37	1.33
5	B	1201	2BA	C51-C41	2.02	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1202	2BA	N31-C21-N11	-4.63	121.44	128.68
5	C	1202	2BA	N3-C2-N1	-4.53	121.59	128.68
3	A	1202	ADP	PA-O3A-PB	-3.98	119.18	132.83
3	D	1202	ADP	PA-O3A-PB	-3.91	119.41	132.83
5	C	1202	2BA	C21-N11-C61	3.91	125.44	118.75
5	B	1201	2BA	N3-C2-N1	-3.77	122.78	128.68
3	D	1202	ADP	N3-C2-N1	-3.55	123.14	128.68
5	C	1202	2BA	O2P1-P1-O5'1	3.23	122.77	107.75
5	B	1201	2BA	N31-C21-N11	-3.12	123.80	128.68
5	B	1201	2BA	N6-C6-N1	2.92	124.63	118.57
3	B	1203	ADP	N6-C6-N1	2.87	124.53	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1201	2BA	O5'-P-O1P	-2.86	97.90	109.07
5	C	1202	2BA	C2-N1-C6	2.81	123.57	118.75
5	B	1201	2BA	C2'1-C3'1-C4'1	-2.80	98.25	103.22
3	A	1202	ADP	C4-C5-N7	-2.68	106.60	109.40
3	B	1203	ADP	N3-C2-N1	-2.67	124.50	128.68
5	B	1201	2BA	C2-N1-C6	2.66	123.30	118.75
3	A	1202	ADP	N3-C2-N1	-2.63	124.56	128.68
5	C	1202	2BA	C2'-C3'-C4'	-2.57	98.67	103.22
3	D	1202	ADP	C2-N1-C6	2.54	123.10	118.75
5	B	1201	2BA	C5-C6-N6	-2.51	116.53	120.35
5	C	1202	2BA	N6-C6-N1	2.50	123.76	118.57
3	B	1203	ADP	PA-O3A-PB	-2.48	124.31	132.83
3	D	1202	ADP	O3B-PB-O1B	2.39	120.05	110.68
3	D	1202	ADP	O3B-PB-O3A	-2.18	97.32	104.64
3	A	1202	ADP	O3B-PB-O2B	2.14	115.82	107.64
5	C	1202	2BA	O4'1-C4'1-C3'1	-2.13	100.31	104.87
5	B	1201	2BA	O2'-C2'-C3'	-2.11	105.17	111.17
5	B	1201	2BA	C1'1-N91-C41	-2.04	123.05	126.64
3	B	1203	ADP	O3B-PB-O2B	2.03	115.40	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1202	ADP	C5'-O5'-PA-O1A
3	D	1202	ADP	C5'-O5'-PA-O3A
3	A	1202	ADP	PB-O3A-PA-O2A
3	D	1202	ADP	PB-O3A-PA-O1A
3	B	1203	ADP	PB-O3A-PA-O2A
3	A	1202	ADP	PB-O3A-PA-O1A
3	D	1202	ADP	C5'-O5'-PA-O2A
5	C	1202	2BA	C3'1-C4'1-C5'1-O5'1

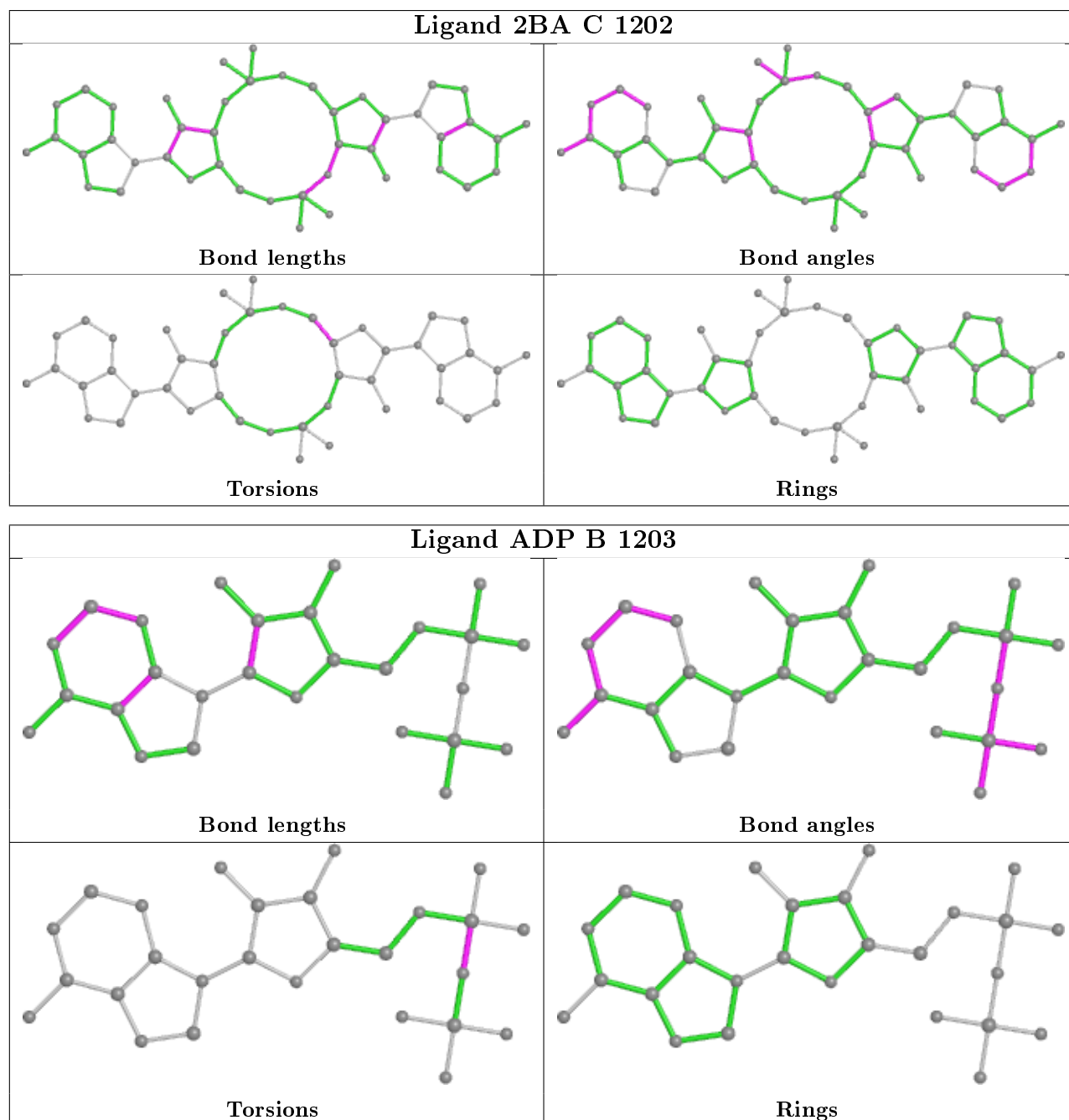
There are no ring outliers.

2 monomers are involved in 2 short contacts:

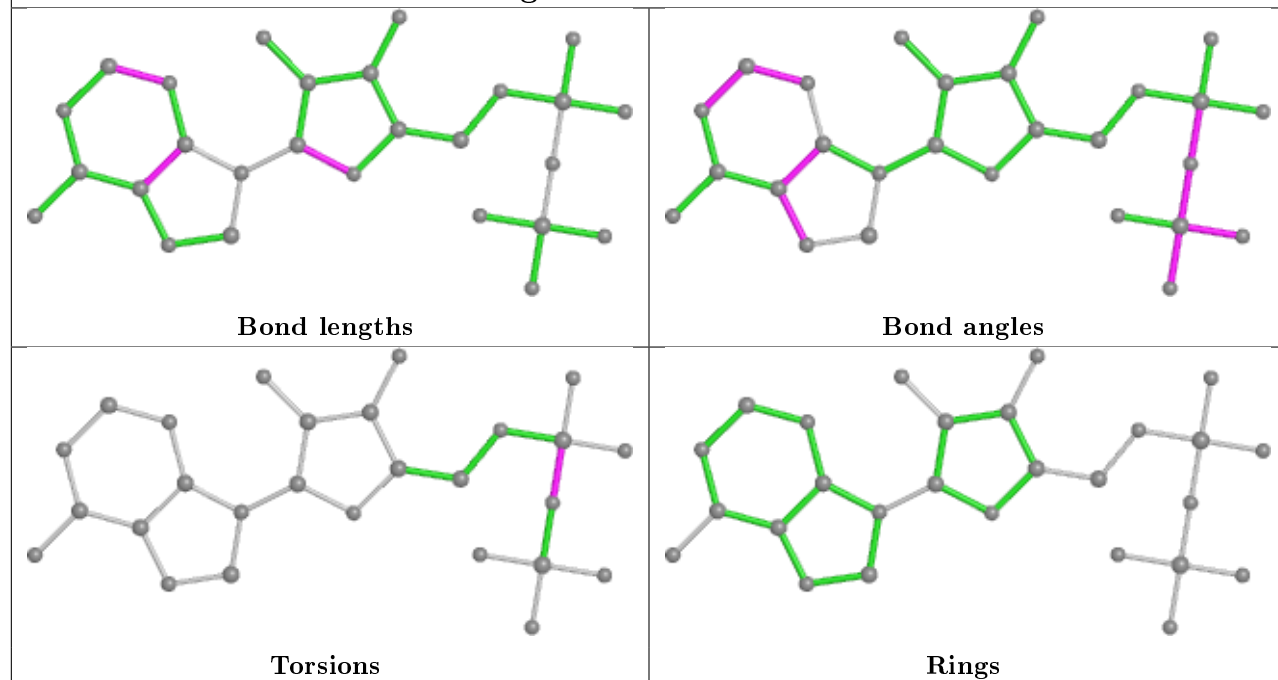
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1202	2BA	1	0
5	B	1201	2BA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

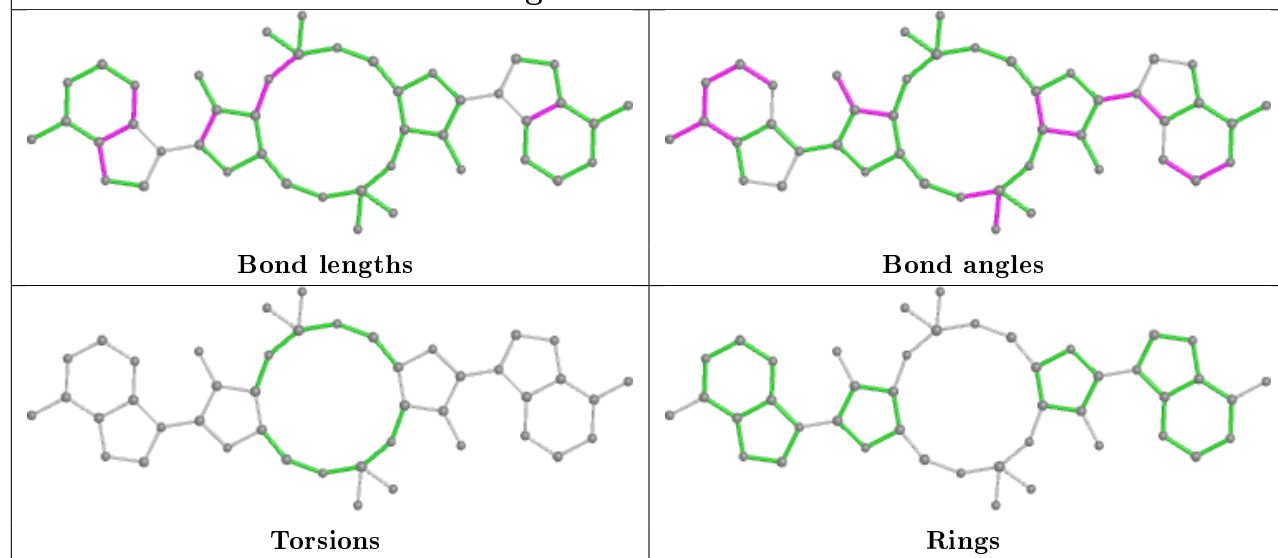
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

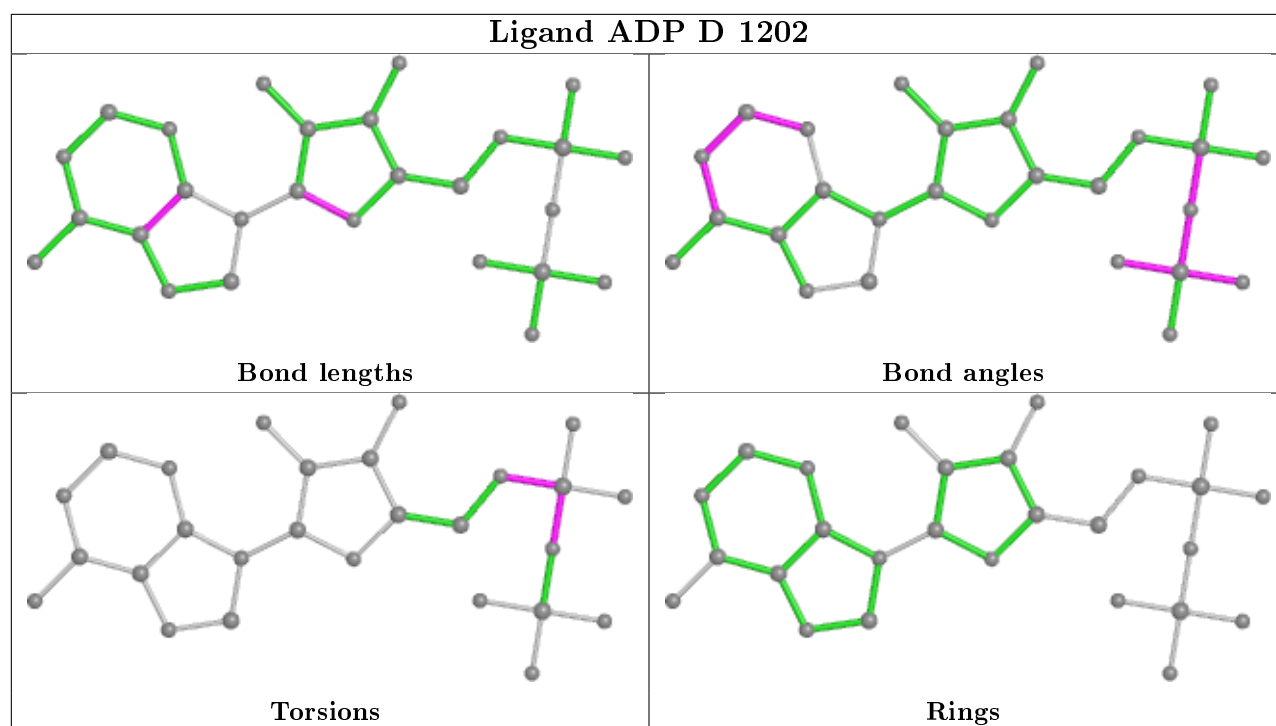


Ligand ADP A 1202



Ligand 2BA B 1201





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	1139/1144 (99%)	-0.09	41 (3%)	42	42	13, 37, 79, 124	0
1	B	1138/1144 (99%)	-0.21	41 (3%)	42	42	13, 35, 77, 109	0
1	C	1074/1144 (93%)	-0.15	45 (4%)	36	35	16, 38, 78, 124	0
1	D	1137/1144 (99%)	-0.11	62 (5%)	25	24	14, 34, 83, 128	0
All	All	4488/4576 (98%)	-0.14	189 (4%)	36	35	13, 36, 80, 128	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	ILE	7.0
1	B	135	ASN	6.0
1	B	191	PHE	5.8
1	D	187	ALA	5.6
1	A	1102	MET	5.5
1	C	1086	ALA	5.5
1	A	194	GLY	5.3
1	C	1084	VAL	5.3
1	D	189	GLY	5.2
1	C	1089	LYS	5.1
1	C	1057	VAL	5.0
1	D	1102	MET	4.8
1	D	1083	LEU	4.7
1	C	1087	GLY	4.7
1	B	150	TYR	4.7
1	B	194	GLY	4.6
1	B	148	LYS	4.5
1	B	190	ALA	4.5
1	B	149	THR	4.4
1	C	1080	LEU	4.4
1	A	191	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	457	LEU	4.4
1	C	1083	LEU	4.3
1	C	1103	LYS	4.3
1	C	1104	MET	4.3
1	A	1058	VAL	4.1
1	D	1081	GLU	4.1
1	C	1093	GLY	3.9
1	A	1055	ALA	3.9
1	D	1080	LEU	3.9
1	D	1101	ALA	3.9
1	A	1057	VAL	3.9
1	A	1103	LYS	3.9
1	B	177	HIS	3.9
1	B	174	ALA	3.8
1	B	152	TYR	3.7
1	A	182	ARG	3.7
1	B	141	ASP	3.7
1	A	881	ILE	3.7
1	A	897	LEU	3.7
1	D	929	ASP	3.6
1	D	892	ALA	3.6
1	C	202	ILE	3.6
1	B	146	PHE	3.6
1	A	1095	ALA	3.6
1	B	171	ARG	3.6
1	D	1103	LYS	3.6
1	A	193	SER	3.5
1	B	137	ALA	3.5
1	D	1122	VAL	3.5
1	B	144	LEU	3.5
1	C	1095	ALA	3.5
1	C	1085	LYS	3.4
1	A	1122	VAL	3.4
1	C	1058	VAL	3.4
1	A	1086	ALA	3.3
1	B	147	ALA	3.3
1	A	929	ASP	3.3
1	D	192	GLY	3.3
1	D	181	ALA	3.3
1	D	190	ALA	3.3
1	C	1124	GLY	3.3
1	C	1082	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	1106	THR	3.2
1	B	189	GLY	3.2
1	A	898	ASN	3.2
1	D	191	PHE	3.2
1	D	171	ARG	3.2
1	C	1136	ILE	3.2
1	C	1102	MET	3.1
1	D	194	GLY	3.1
1	D	1058	VAL	3.1
1	B	881	ILE	3.1
1	A	1104	MET	3.1
1	D	1123	LYS	3.1
1	C	896	GLU	3.1
1	D	1082	ILE	3.1
1	D	1055	ALA	3.1
1	C	1105	GLU	3.1
1	C	1101	ALA	3.0
1	D	139	ASP	3.0
1	A	842	LEU	3.0
1	B	897	LEU	3.0
1	A	844	HIS	3.0
1	D	896	GLU	3.0
1	C	895	ASN	3.0
1	C	1107	THR	2.9
1	D	1124	GLY	2.9
1	C	892	ALA	2.9
1	D	141	ASP	2.9
1	D	891	TYR	2.9
1	D	1104	MET	2.9
1	C	1096	LEU	2.9
1	D	1107	THR	2.9
1	D	1079	VAL	2.9
1	B	142	GLY	2.9
1	D	1126	ALA	2.9
1	A	885	LEU	2.9
1	A	895	ASN	2.9
1	B	1122	VAL	2.9
1	C	132	PRO	2.9
1	A	1105	GLU	2.9
1	C	1116	ILE	2.8
1	A	192	GLY	2.8
1	B	139	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1100	GLU	2.8
1	C	116	LYS	2.8
1	A	892	ALA	2.8
1	D	148	LYS	2.7
1	D	177	HIS	2.7
1	A	1126	ALA	2.7
1	D	174	ALA	2.7
1	D	1098	VAL	2.7
1	D	844	HIS	2.6
1	A	927	VAL	2.6
1	A	893	ARG	2.6
1	C	1055	ALA	2.6
1	B	182	ARG	2.6
1	A	1101	ALA	2.6
1	A	195	GLU	2.6
1	B	456	ARG	2.6
1	D	1105	GLU	2.6
1	B	457	LEU	2.6
1	A	943	LYS	2.6
1	A	188	ILE	2.6
1	D	140	ILE	2.6
1	C	898	ASN	2.6
1	D	897	LEU	2.6
1	D	1084	VAL	2.5
1	D	185	SER	2.5
1	C	1134	ILE	2.5
1	D	888	GLU	2.5
1	A	180	TYR	2.5
1	D	173	ASP	2.5
1	B	1080	LEU	2.5
1	D	1095	ALA	2.5
1	B	185	SER	2.5
1	D	1096	LEU	2.5
1	B	170	ALA	2.5
1	B	1057	VAL	2.5
1	D	152	TYR	2.5
1	C	1081	GLU	2.5
1	C	1097	MET	2.4
1	A	890	VAL	2.4
1	B	1058	VAL	2.4
1	A	140	ILE	2.4
1	C	1099	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	279	ASP	2.4
1	D	1121	VAL	2.4
1	C	897	LEU	2.3
1	C	1115	GLU	2.3
1	C	1119	LEU	2.3
1	B	896	GLU	2.3
1	C	1109	GLU	2.3
1	C	1137	ASN	2.3
1	D	169	VAL	2.3
1	D	183	ALA	2.3
1	C	131	ILE	2.3
1	B	842	LEU	2.2
1	C	1123	LYS	2.2
1	B	181	ALA	2.2
1	A	896	GLU	2.2
1	B	172	ASN	2.2
1	B	943	LYS	2.2
1	D	886	THR	2.2
1	D	895	ASN	2.2
1	D	1086	ALA	2.2
1	D	1078	SER	2.2
1	B	145	GLU	2.2
1	B	838	ALA	2.2
1	D	881	ILE	2.1
1	D	842	LEU	2.1
1	A	889	ASP	2.1
1	C	1092	LYS	2.1
1	B	193	SER	2.1
1	D	893	ARG	2.1
1	D	890	VAL	2.1
1	A	1096	LEU	2.1
1	D	180	TYR	2.1
1	B	188	ILE	2.1
1	A	1054	GLN	2.1
1	D	193	SER	2.0
1	B	183	ALA	2.0
1	C	1117	VAL	2.0
1	A	888	GLU	2.0
1	A	924	LYS	2.0
1	D	170	ALA	2.0
1	D	1099	THR	2.0
1	B	844	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

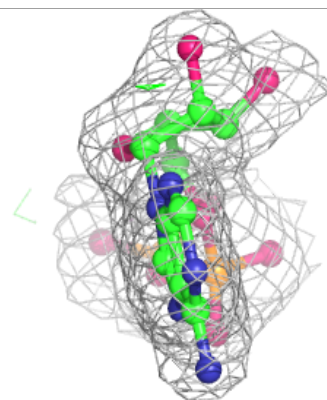
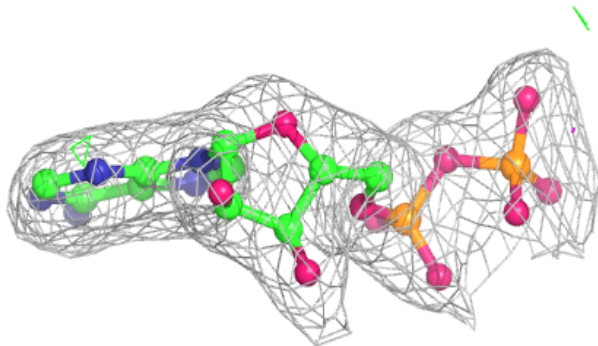
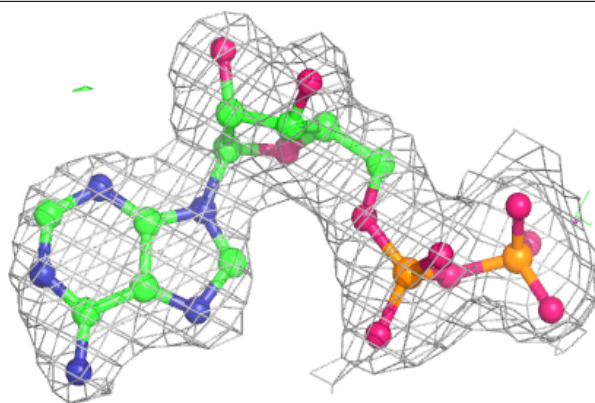
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	1203	1/1	0.94	0.10	48,48,48,48	0
4	MG	D	1203	1/1	0.95	0.11	36,36,36,36	0
3	ADP	D	1202	27/27	0.95	0.08	38,47,59,63	0
3	ADP	A	1202	27/27	0.95	0.08	35,47,66,81	0
3	ADP	B	1203	27/27	0.96	0.08	35,43,60,65	0
4	MG	B	1204	1/1	0.97	0.07	34,34,34,34	0
5	2BA	C	1202	44/44	0.98	0.11	15,21,27,29	0
2	MN	C	1201	1/1	0.99	0.10	32,32,32,32	0
5	2BA	B	1201	44/44	0.99	0.11	16,20,27,30	0
2	MN	B	1202	1/1	0.99	0.08	33,33,33,33	0
2	MN	D	1201	1/1	1.00	0.07	33,33,33,33	0
2	MN	A	1201	1/1	1.00	0.10	35,35,35,35	0

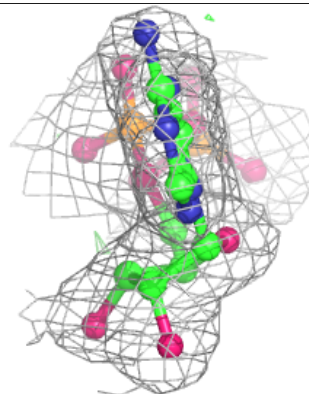
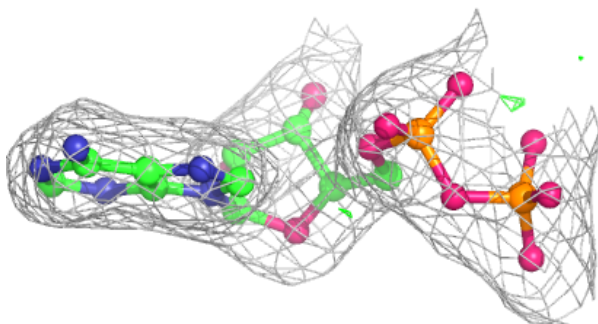
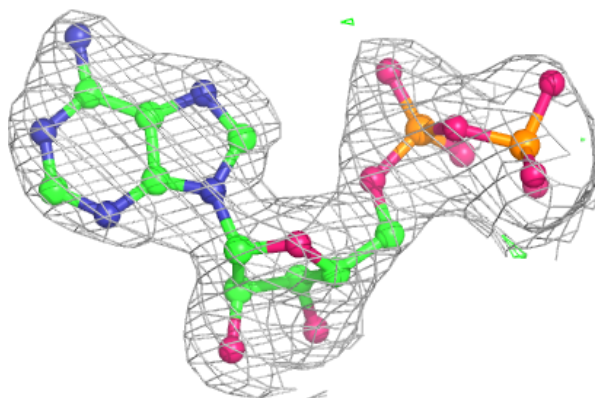
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 1202:

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

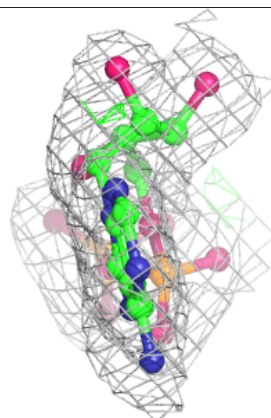
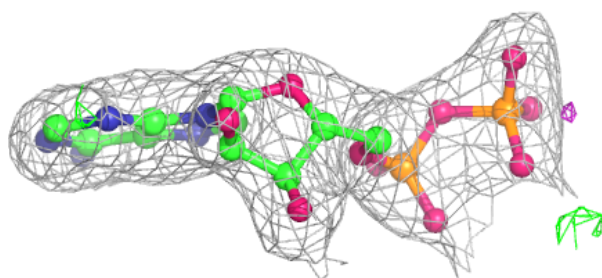
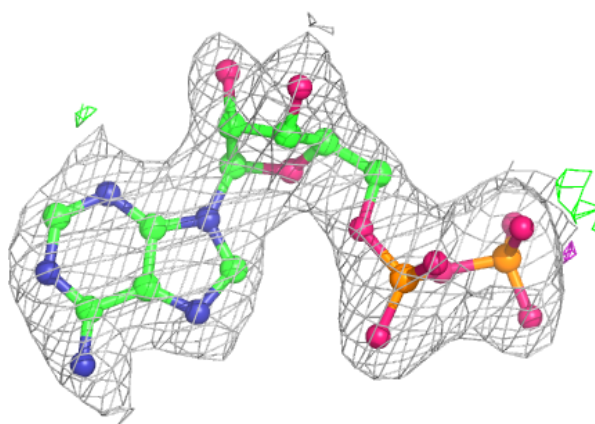
**Electron density around ADP A 1202:**

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

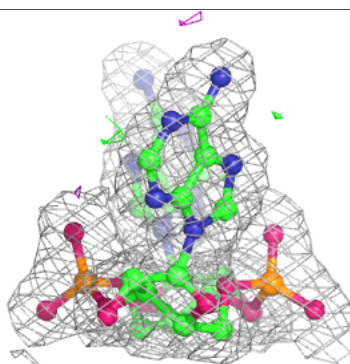
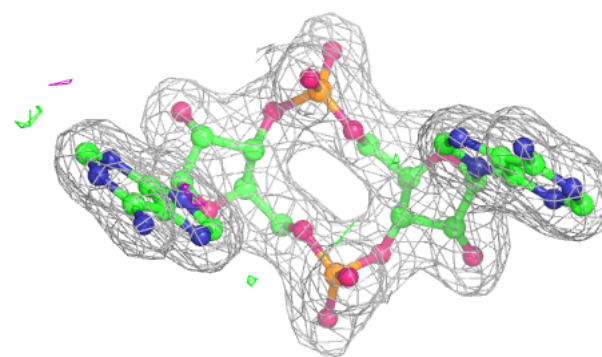
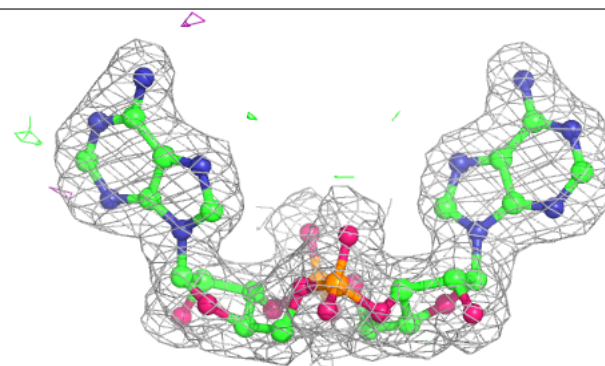


Electron density around ADP B 1203:

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

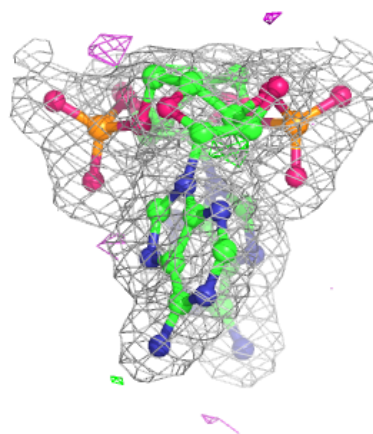
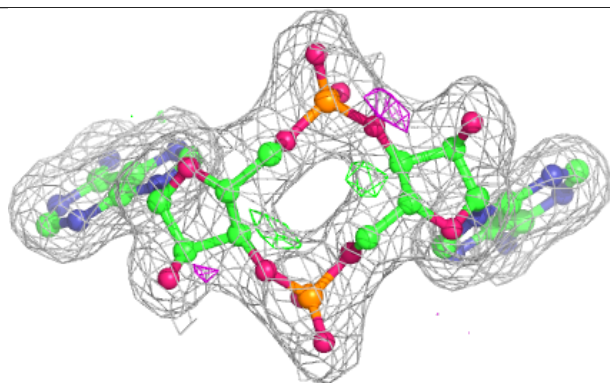
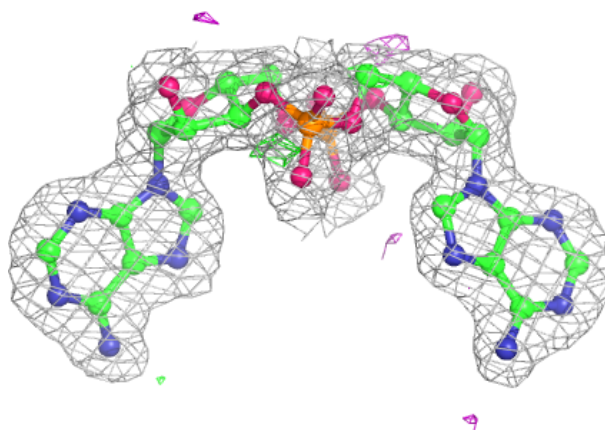
**Electron density around 2BA C 1202:**

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



Electron density around 2BA B 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.