



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:05 AM UTC

PDB ID : 4QSH / pdb_00004qsh
Title : Crystal Structure of L. monocytogenes Pyruvate Carboxylase in complex with Cyclic-di-AMP
Authors : Choi, P.H.; Tong, L.
Deposited on : 2014-07-04
Resolution : 2.51 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

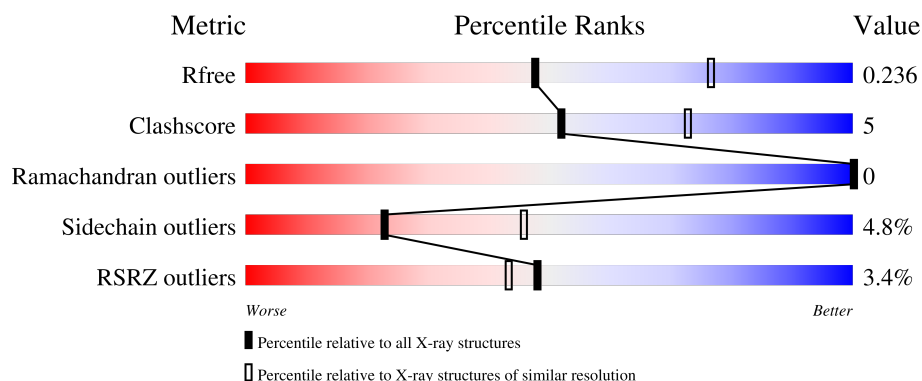
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1148	2% 80% 12% • 7%
1	B	1148	4% 82% 10% • 6%
1	C	1148	5% 81% 12% • 6%
1	D	1148	2% 80% 13% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	2001	-	-	X	-
2	FLC	B	2001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34524 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.

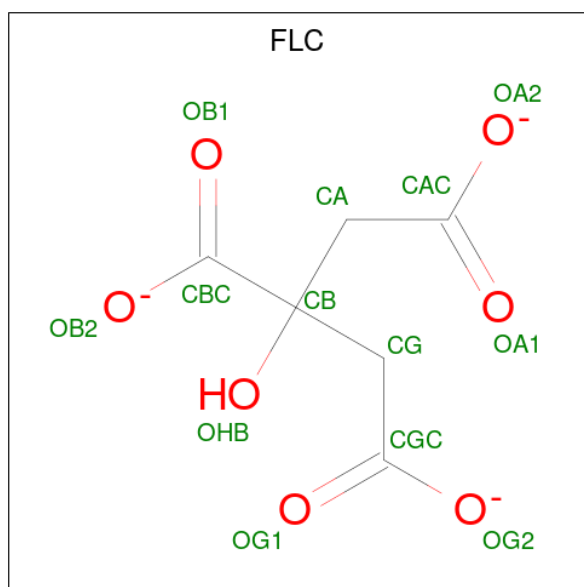
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1072	Total	C	N	O	S	0	0	0
			8447	5361	1435	1612	39			
1	B	1074	Total	C	N	O	S	0	0	0
			8436	5356	1431	1608	41			
1	C	1081	Total	C	N	O	S	0	0	0
			8501	5396	1442	1623	40			
1	D	1072	Total	C	N	O	S	0	0	0
			8446	5363	1431	1611	41			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP W6G6F5
A	0	MET	-	expression tag	UNP W6G6F5
B	-1	HIS	-	expression tag	UNP W6G6F5
B	0	MET	-	expression tag	UNP W6G6F5
C	-1	HIS	-	expression tag	UNP W6G6F5
C	0	MET	-	expression tag	UNP W6G6F5
D	-1	HIS	-	expression tag	UNP W6G6F5
D	0	MET	-	expression tag	UNP W6G6F5

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).

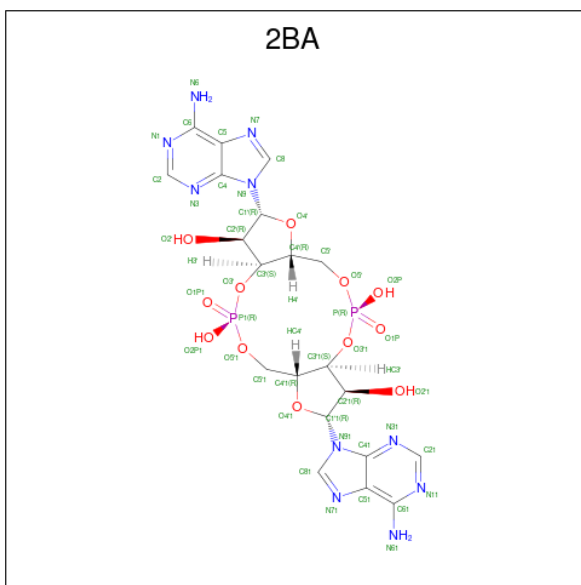


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 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: C₂₀H₂₄N₁₀O₁₂P₂).



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

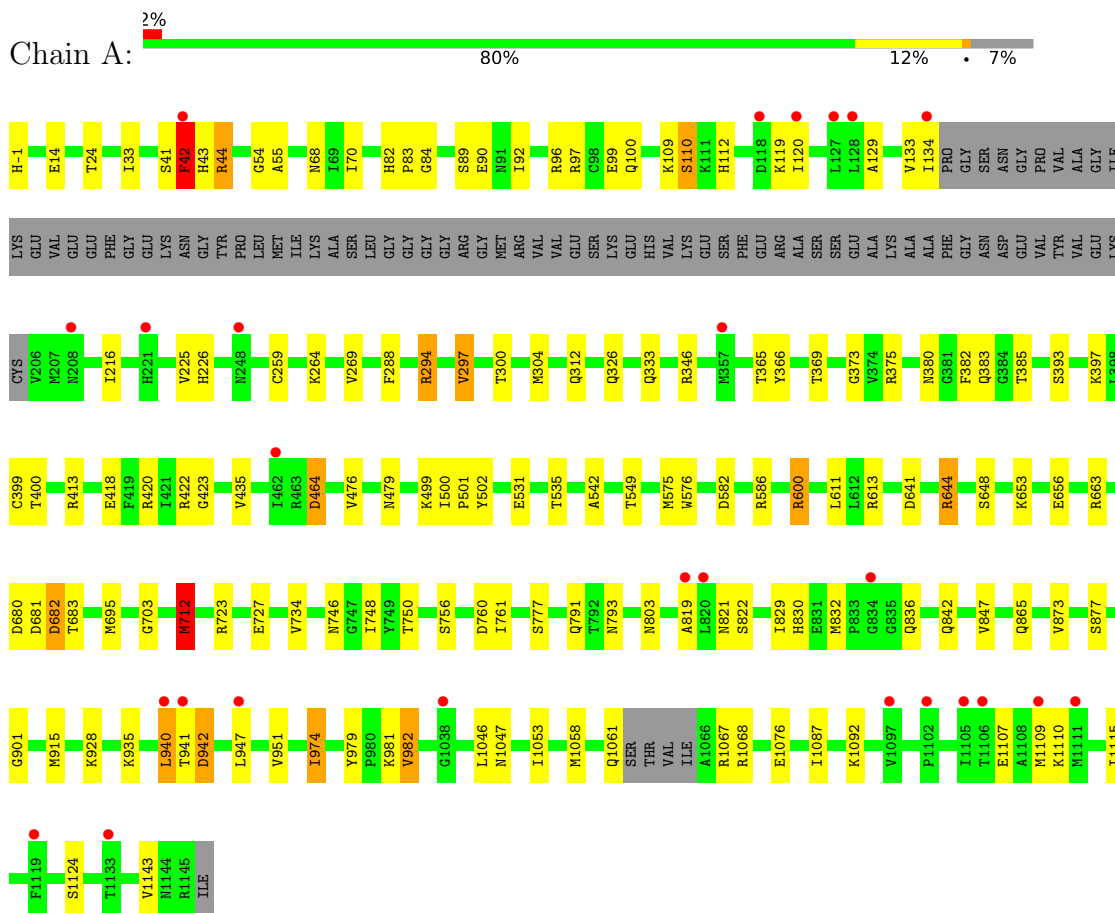
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	163	Total O 163 163	0	0
5	B	79	Total O 79 79	0	0
5	C	82	Total O 82 82	0	0
5	D	182	Total O 182 182	0	0

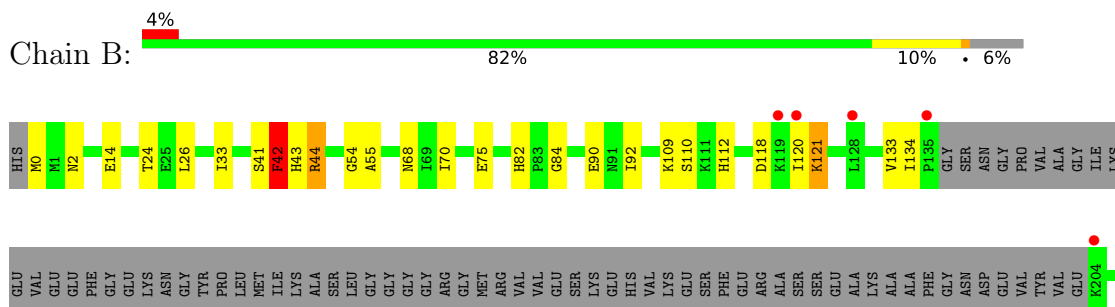
3 Residue-property plots

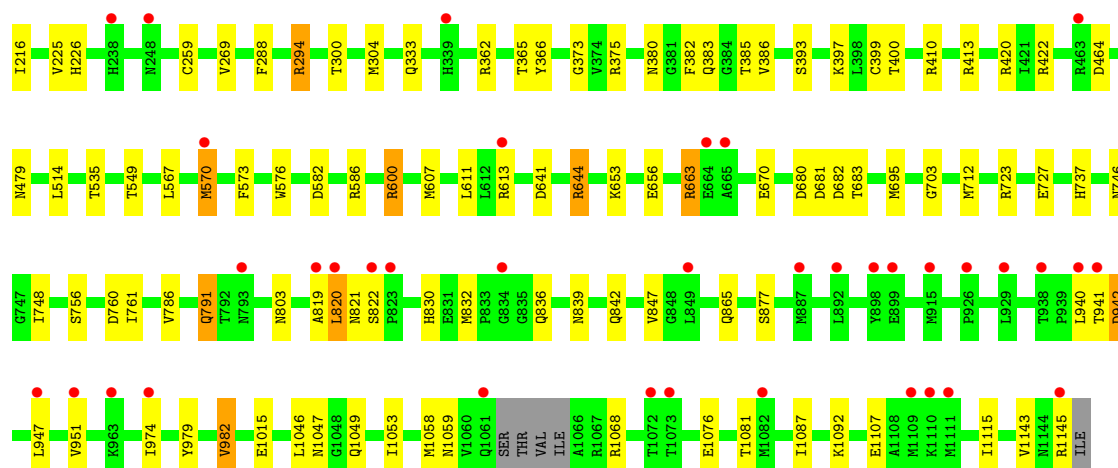
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Pyruvate carboxylase

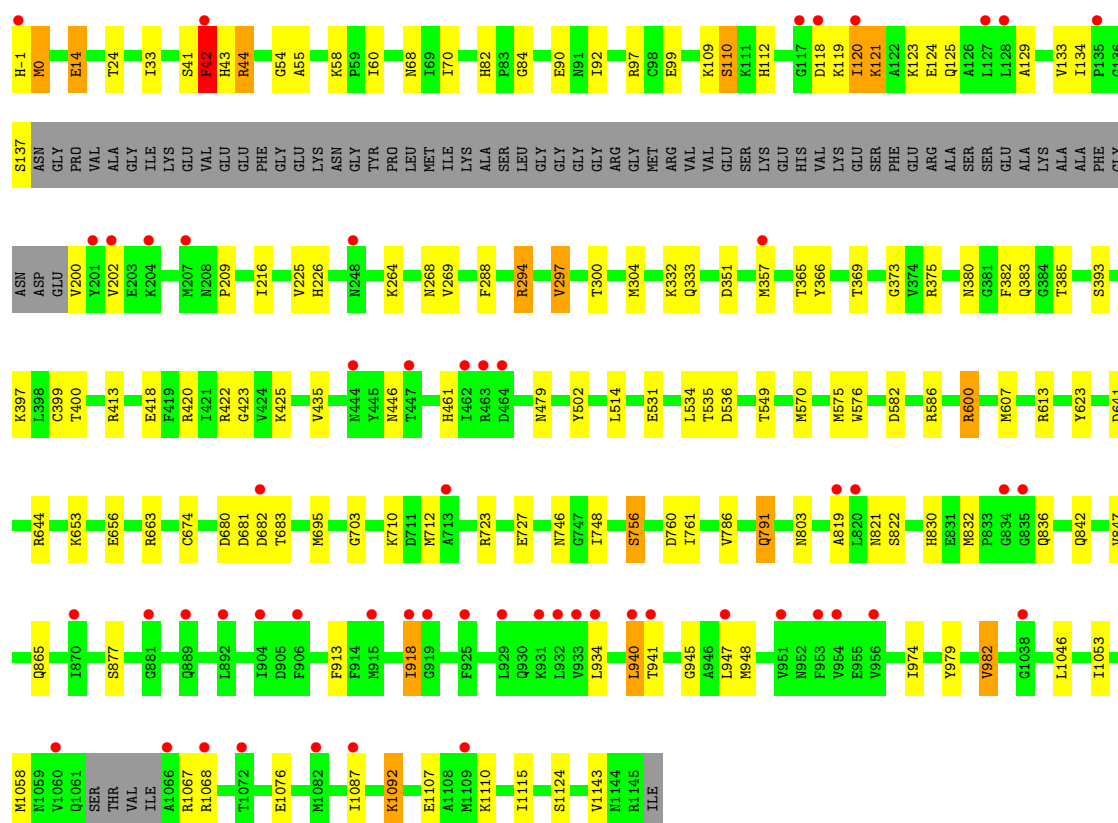
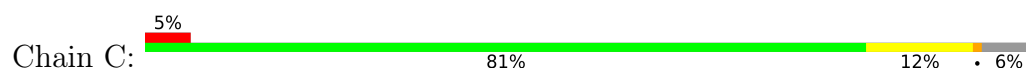


• Molecule 1: Pyruvate carboxylase

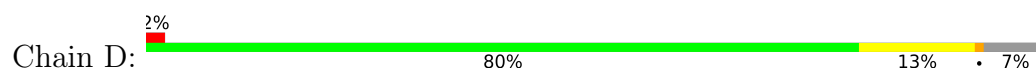




• Molecule 1: Pyruvate carboxylase



• Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.78Å 153.30Å 221.24Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	49.80 – 2.51 49.80 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.80-2.51) 96.9 (49.80-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.233 0.200 , 0.236	Depositor DCC
R_{free} test set	10520 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34524	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% 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: MN, 2BA, FLC

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	1.06	3/8614 (0.0%)	1.05	15/11669 (0.1%)
1	B	0.93	1/8603 (0.0%)	1.02	9/11658 (0.1%)
1	C	0.93	0/8670	1.01	12/11747 (0.1%)
1	D	1.08	6/8613 (0.1%)	1.05	13/11666 (0.1%)
All	All	1.00	10/34500 (0.0%)	1.03	49/46740 (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	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	718	PRO	CA-CB	6.54	1.63	1.53
1	D	995	ASP	CA-C	6.08	1.60	1.53
1	D	558	GLN	C-O	-5.77	1.16	1.24
1	A	829	ILE	C-O	-5.69	1.17	1.23
1	B	1015	GLU	C-O	-5.42	1.17	1.24
1	A	793	ASN	N-CA	5.29	1.51	1.46
1	D	1015	GLU	C-O	-5.16	1.18	1.24
1	A	542	ALA	N-CA	5.12	1.52	1.46
1	D	31	VAL	N-CA	-5.10	1.39	1.46
1	D	976	TYR	N-CA	5.04	1.52	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	MET	CA-CB-CG	-8.82	96.46	114.10
1	C	822	SER	CA-C-N	-7.81	111.56	119.92
1	C	822	SER	C-N-CA	-7.81	111.56	119.92
1	A	822	SER	CA-C-N	-7.44	111.96	119.92
1	A	822	SER	C-N-CA	-7.44	111.96	119.92
1	A	476	VAL	CB-CA-C	-7.31	102.27	112.14
1	A	793	ASN	N-CA-C	7.15	120.65	112.57
1	B	822	SER	CA-C-N	-7.03	112.39	119.92
1	B	822	SER	C-N-CA	-7.03	112.39	119.92
1	D	822	SER	CA-C-N	-6.78	112.66	119.92
1	D	822	SER	C-N-CA	-6.78	112.66	119.92
1	A	940	LEU	N-CA-C	-6.49	100.09	110.14
1	A	100	GLN	CB-CA-C	-6.45	99.72	110.68
1	C	803	ASN	N-CA-C	6.27	118.12	111.28
1	A	803	ASN	N-CA-C	6.14	118.77	111.71
1	B	803	ASN	N-CA-C	6.09	118.71	111.71
1	D	803	ASN	N-CA-C	5.98	118.59	111.71
1	C	461	HIS	N-CA-C	-5.98	100.75	110.20
1	C	42	PHE	CB-CA-C	5.81	121.51	109.95
1	C	0	MET	N-CA-CB	-5.79	101.65	110.33
1	B	570	MET	CG-SD-CE	-5.77	88.21	100.90
1	C	423	GLY	N-CA-C	-5.76	107.63	114.48
1	A	712	MET	CG-SD-CE	5.75	113.56	100.90
1	A	648	SER	N-CA-C	5.74	119.80	112.34
1	C	42	PHE	CA-CB-CG	5.71	119.50	113.80
1	C	297	VAL	CB-CA-C	-5.70	104.59	111.88
1	C	940	LEU	N-CA-C	-5.70	101.31	110.14
1	D	989	MET	CG-SD-CE	-5.67	88.43	100.90
1	A	42	PHE	CA-CB-CG	5.64	119.44	113.80
1	D	42	PHE	CB-CA-C	5.62	121.14	109.95
1	D	648	SER	N-CA-C	5.55	119.56	112.34
1	A	1124	SER	CA-C-O	5.55	121.16	117.94
1	C	1124	SER	CA-C-O	5.52	121.14	117.94
1	D	940	LEU	N-CA-C	-5.51	101.61	110.14
1	D	802	ILE	N-CA-C	-5.45	105.06	110.62
1	B	42	PHE	CB-CA-C	5.42	120.74	109.95
1	D	1081	THR	N-CA-C	-5.41	105.82	112.90
1	B	1081	THR	N-CA-C	-5.35	105.89	112.90
1	A	42	PHE	CB-CA-C	5.32	120.53	109.95
1	A	423	GLY	N-CA-C	-5.29	107.92	113.58
1	B	386	VAL	CB-CA-C	-5.28	104.93	111.32
1	A	297	VAL	CB-CA-C	-5.25	105.16	111.88
1	A	712	MET	CB-CG-SD	5.19	128.28	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	PHE	CA-CB-CG	5.18	118.98	113.80
1	D	500	ILE	CA-C-N	-5.16	114.45	119.76
1	D	500	ILE	C-N-CA	-5.16	114.45	119.76
1	D	42	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	14	GLU	N-CA-CB	-5.07	102.38	109.94
1	D	571	PHE	N-CA-C	-5.06	105.66	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	682	ASP	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	8447	0	8377	83	0
1	B	8436	0	8357	82	0
1	C	8501	0	8419	99	0
1	D	8446	0	8392	88	0
2	A	13	0	5	4	0
2	B	13	0	5	5	0
2	C	13	0	5	1	0
2	D	13	0	5	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	46	0	0
4	C	44	0	23	0	0
5	A	163	0	0	14	0
5	B	79	0	0	5	0
5	C	82	0	0	7	0
5	D	182	0	0	12	0
All	All	34524	0	33634	343	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 5.

All (343) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:MET:HE1	1:A:399:CYS:HB3	1.32	1.12
1:C:304:MET:HE1	1:C:399:CYS:HB3	1.32	1.10
1:A:97:ARG:HD3	5:A:2174:HOH:O	1.53	1.08
1:B:304:MET:HE1	1:B:399:CYS:HB3	1.33	1.07
1:D:304:MET:HE1	1:D:399:CYS:HB3	1.34	1.04
1:C:125:GLN:OE1	5:C:1359:HOH:O	1.83	0.95
1:A:723:ARG:HD3	5:A:2115:HOH:O	1.71	0.90
1:C:945:GLY:HA2	1:C:948:MET:HE2	1.53	0.90
1:B:582:ASP:OD2	1:B:586:ARG:NH1	2.08	0.87
1:A:582:ASP:OD2	1:A:586:ARG:NH1	2.08	0.86
1:D:582:ASP:OD2	1:D:586:ARG:NH1	2.07	0.86
1:C:582:ASP:OD2	1:C:586:ARG:NH1	2.08	0.85
1:A:499:LYS:HA	5:A:2163:HOH:O	1.76	0.85
1:C:420:ARG:NH1	2:C:1202:FLC:OA1	2.12	0.82
1:C:82:HIS:HD2	1:C:84:GLY:H	1.28	0.81
1:D:82:HIS:HD2	1:D:84:GLY:H	1.29	0.80
1:C:710:LYS:HG2	1:C:712:MET:HE3	1.61	0.80
1:D:0:MET:HE1	1:D:26:LEU:HD22	1.64	0.80
1:B:663:ARG:NH1	1:B:703:GLY:O	2.13	0.79
1:B:82:HIS:HD2	1:B:84:GLY:H	1.29	0.79
1:B:567:LEU:HB3	1:B:570:MET:HE2	1.66	0.78
1:C:663:ARG:NH1	1:C:703:GLY:O	2.17	0.78
1:A:82:HIS:HD2	1:A:84:GLY:H	1.30	0.78
1:A:663:ARG:NH1	1:A:703:GLY:O	2.17	0.77
1:D:663:ARG:NH1	1:D:703:GLY:O	2.17	0.77
1:B:1145:ARG:O	5:B:2162:HOH:O	2.02	0.77
1:C:120:ILE:HD12	1:C:124:GLU:OE2	1.85	0.76
1:A:1047:ASN:HD22	2:A:2001:FLC:HG1	1.49	0.76
1:C:756:SER:OG	5:C:1323:HOH:O	2.05	0.73
1:D:830:HIS:HD2	1:D:832:MET:H	1.38	0.71
1:C:304:MET:HE1	1:C:399:CYS:CB	2.17	0.70
1:C:351:ASP:OD2	1:C:425:LYS:HD2	1.92	0.70
1:C:674:CYS:SG	1:C:712:MET:HE1	2.31	0.70
1:D:723:ARG:HD3	5:D:2214:HOH:O	1.90	0.70
1:D:304:MET:HE1	1:D:399:CYS:CB	2.19	0.69
1:C:54:GLY:H	1:C:68:ASN:HD22	1.41	0.69
1:A:502:TYR:OH	1:B:75:GLU:OE1	2.04	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:MET:HE1	1:B:399:CYS:CB	2.19	0.68
1:D:42:PHE:HB3	1:D:382:PHE:CE1	2.27	0.68
1:C:42:PHE:HB3	1:C:382:PHE:CE1	2.28	0.68
1:A:304:MET:HE1	1:A:399:CYS:CB	2.17	0.68
1:A:226:HIS:H	1:A:333:GLN:HE22	1.41	0.68
1:C:226:HIS:H	1:C:333:GLN:HE22	1.40	0.68
1:C:297:VAL:HG23	5:C:1303:HOH:O	1.94	0.68
1:A:42:PHE:HB3	1:A:382:PHE:CE1	2.29	0.67
1:A:830:HIS:HD2	1:A:832:MET:H	1.43	0.67
1:C:945:GLY:HA2	1:C:948:MET:CE	2.25	0.67
1:B:14:GLU:CD	1:B:397:LYS:HE3	2.19	0.67
1:C:14:GLU:CD	1:C:397:LYS:HE3	2.20	0.67
1:C:120:ILE:CD1	1:C:124:GLU:OE2	2.44	0.66
1:B:42:PHE:HB3	1:B:382:PHE:CE1	2.30	0.66
1:C:268:ASN:ND2	5:C:1359:HOH:O	2.28	0.66
1:B:479:ASN:HD21	1:B:1058:MET:H	1.43	0.66
1:B:54:GLY:H	1:B:68:ASN:HD22	1.42	0.65
1:C:120:ILE:O	1:C:124:GLU:HG3	1.96	0.65
1:B:226:HIS:H	1:B:333:GLN:HE22	1.44	0.65
1:B:1049:GLN:HE22	2:B:2001:FLC:HG2	1.61	0.65
1:C:830:HIS:HD2	1:C:832:MET:H	1.45	0.64
1:C:118:ASP:HB2	1:C:121:LYS:HD3	1.77	0.64
1:A:90:GLU:OE2	1:A:294:ARG:HD3	1.98	0.64
1:C:918:ILE:HD13	1:C:918:ILE:C	2.23	0.64
1:D:54:GLY:H	1:D:68:ASN:HD22	1.44	0.64
1:B:830:HIS:HD2	1:B:832:MET:H	1.42	0.64
1:B:0:MET:CE	1:B:26:LEU:HD22	2.28	0.64
1:B:1049:GLN:NE2	2:B:2001:FLC:HG2	2.12	0.64
1:A:54:GLY:H	1:A:68:ASN:HD22	1.43	0.64
1:D:226:HIS:H	1:D:333:GLN:HE22	1.43	0.63
1:D:14:GLU:CD	1:D:397:LYS:HE3	2.23	0.63
1:B:362:ARG:NH1	5:B:2163:HOH:O	2.32	0.63
1:D:479:ASN:HD21	1:D:1058:MET:H	1.45	0.63
1:B:90:GLU:OE2	1:B:294:ARG:HD3	1.99	0.63
1:B:366:TYR:H	1:B:383:GLN:HE21	1.47	0.63
1:A:14:GLU:CD	1:A:397:LYS:HE3	2.24	0.62
1:C:90:GLU:OE2	1:C:294:ARG:HD3	1.98	0.62
1:D:514:LEU:HD22	1:D:607:MET:CE	2.29	0.62
1:D:366:TYR:H	1:D:383:GLN:HE21	1.48	0.62
1:B:570:MET:CE	1:B:573:PHE:CE1	2.83	0.62
1:B:54:GLY:H	1:B:68:ASN:ND2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:MET:HE2	1:B:641:ASP:HB3	1.82	0.61
1:C:514:LEU:HD22	1:C:607:MET:CE	2.30	0.61
1:A:479:ASN:HD21	1:A:1058:MET:H	1.49	0.61
1:C:674:CYS:CB	1:C:712:MET:HE1	2.30	0.61
1:B:514:LEU:HD22	1:B:607:MET:CE	2.31	0.61
1:B:746:ASN:HD22	1:C:748:ILE:HG21	1.66	0.60
1:A:24:THR:O	1:B:413:ARG:NH2	2.35	0.60
1:C:24:THR:O	1:D:413:ARG:NH2	2.35	0.60
1:C:54:GLY:H	1:C:68:ASN:ND2	1.98	0.60
1:D:499:LYS:HB3	5:D:2166:HOH:O	2.02	0.60
1:D:90:GLU:OE2	1:D:294:ARG:HD3	2.01	0.60
1:D:464:ASP:OD1	1:D:464:ASP:N	2.34	0.60
1:C:366:TYR:H	1:C:383:GLN:HE21	1.50	0.59
1:D:1087:ILE:HD11	1:D:1107:GLU:HB2	1.84	0.59
1:A:41:SER:OG	1:A:43:HIS:HD2	1.86	0.59
1:C:607:MET:HE2	1:C:641:ASP:HB3	1.85	0.59
1:C:1087:ILE:HD11	1:C:1107:GLU:HB2	1.84	0.59
1:A:54:GLY:H	1:A:68:ASN:ND2	2.00	0.59
1:B:570:MET:HE1	1:B:573:PHE:HE1	1.68	0.59
1:D:54:GLY:H	1:D:68:ASN:ND2	2.00	0.59
1:C:118:ASP:HB2	1:C:121:LYS:CD	2.34	0.58
1:A:297:VAL:HG23	5:A:2155:HOH:O	2.04	0.58
1:C:413:ARG:NH2	1:D:24:THR:O	2.36	0.58
1:B:420:ARG:NH1	2:B:2001:FLC:OG2	2.36	0.57
1:A:366:TYR:H	1:A:383:GLN:HE21	1.52	0.57
1:A:413:ARG:NH2	1:B:24:THR:O	2.37	0.57
1:B:1087:ILE:HD11	1:B:1107:GLU:HB2	1.85	0.57
1:C:786:VAL:O	1:C:791:GLN:NE2	2.38	0.57
1:D:294:ARG:NH2	5:D:2157:HOH:O	2.36	0.57
1:A:1087:ILE:HD11	1:A:1107:GLU:HB2	1.85	0.57
1:D:607:MET:HE2	1:D:641:ASP:HB3	1.84	0.57
1:C:479:ASN:HD21	1:C:1058:MET:H	1.52	0.57
1:C:41:SER:OG	1:C:43:HIS:HD2	1.88	0.56
1:A:1046:LEU:HD23	1:A:1046:LEU:C	2.30	0.56
1:B:570:MET:HE3	1:B:573:PHE:CE1	2.40	0.56
1:C:1067:ARG:HG2	5:C:1319:HOH:O	2.04	0.56
1:C:1076:GLU:HG2	1:C:1143:VAL:O	2.06	0.56
1:C:1046:LEU:HD23	1:C:1046:LEU:C	2.30	0.56
1:B:14:GLU:CD	1:B:397:LYS:CE	2.79	0.56
1:B:1076:GLU:HG2	1:B:1143:VAL:O	2.06	0.56
1:C:109:LYS:H	1:C:112:HIS:HD2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ASP:OD1	1:B:464:ASP:N	2.37	0.56
1:C:536:ASP:HB2	1:C:570:MET:HE2	1.87	0.56
1:B:786:VAL:O	1:B:791:GLN:NE2	2.40	0.55
1:C:99:GLU:OE1	1:C:110:SER:OG	2.24	0.55
1:C:14:GLU:CD	1:C:397:LYS:CE	2.80	0.55
1:A:1076:GLU:HG2	1:A:1143:VAL:O	2.06	0.55
1:D:1076:GLU:HG2	1:D:1143:VAL:O	2.06	0.55
1:B:109:LYS:H	1:B:112:HIS:HD2	1.55	0.54
1:C:502:TYR:OH	1:D:75:GLU:OE1	2.17	0.54
1:D:14:GLU:CD	1:D:397:LYS:CE	2.81	0.54
1:A:748:ILE:HG21	1:D:746:ASN:HD22	1.72	0.54
1:C:674:CYS:SG	1:C:712:MET:CE	2.96	0.54
1:B:570:MET:HE1	1:B:573:PHE:CE1	2.42	0.54
1:B:748:ILE:HG21	1:C:746:ASN:HD22	1.72	0.54
1:C:536:ASP:CB	1:C:570:MET:HE2	2.38	0.54
1:D:0:MET:HE1	1:D:26:LEU:CD2	2.37	0.54
1:C:913:PHE:HD1	1:C:918:ILE:HD11	1.71	0.54
1:D:41:SER:OG	1:D:43:HIS:HD2	1.91	0.54
1:A:1067:ARG:HG2	5:A:2135:HOH:O	2.07	0.54
1:B:942:ASP:OD1	1:B:942:ASP:N	2.41	0.53
1:A:99:GLU:OE1	1:A:110:SER:OG	2.25	0.53
1:D:514:LEU:HB2	1:D:607:MET:HE3	1.91	0.53
1:B:41:SER:OG	1:B:43:HIS:HD2	1.92	0.53
1:B:663:ARG:HA	5:B:2137:HOH:O	2.07	0.53
1:B:820:LEU:N	1:B:820:LEU:HD23	2.23	0.53
1:C:534:LEU:O	1:C:570:MET:HE3	2.08	0.53
1:A:746:ASN:HD22	1:D:748:ILE:HG21	1.74	0.53
1:C:847:VAL:HG12	1:C:847:VAL:O	2.08	0.53
1:A:681:ASP:OD1	1:A:683:THR:HB	2.08	0.53
1:D:300:THR:HG22	1:D:375:ARG:NH2	2.24	0.53
1:A:847:VAL:O	1:A:847:VAL:CG1	2.57	0.53
1:A:847:VAL:O	1:A:847:VAL:HG12	2.08	0.53
1:B:681:ASP:OD1	1:B:683:THR:HB	2.08	0.52
1:C:847:VAL:O	1:C:847:VAL:CG1	2.57	0.52
1:C:623:TYR:N	1:C:948:MET:HE1	2.25	0.52
1:D:681:ASP:OD1	1:D:683:THR:HB	2.08	0.52
1:D:847:VAL:O	1:D:847:VAL:CG1	2.57	0.52
1:D:847:VAL:O	1:D:847:VAL:HG12	2.08	0.52
1:D:109:LYS:H	1:D:112:HIS:HD2	1.56	0.52
1:B:1046:LEU:C	1:B:1046:LEU:HD23	2.34	0.51
1:A:14:GLU:CD	1:A:397:LYS:CE	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:VAL:HG12	1:B:847:VAL:O	2.09	0.51
1:C:121:LYS:HA	1:C:124:GLU:CD	2.36	0.51
1:C:681:ASP:OD1	1:C:683:THR:HB	2.10	0.51
1:B:300:THR:HG22	1:B:375:ARG:NH2	2.26	0.51
1:B:514:LEU:HB2	1:B:607:MET:HE3	1.93	0.51
1:B:847:VAL:O	1:B:847:VAL:CG1	2.58	0.51
1:D:1046:LEU:C	1:D:1046:LEU:HD23	2.36	0.51
1:A:109:LYS:H	1:A:112:HIS:HD2	1.59	0.50
1:A:133:VAL:HG12	1:A:134:ILE:N	2.27	0.50
1:A:380:ASN:O	1:A:385:THR:HG21	2.12	0.50
1:C:380:ASN:O	1:C:385:THR:HG21	2.11	0.50
1:A:935:LYS:HE2	5:A:2209:HOH:O	2.12	0.50
1:D:133:VAL:HG12	1:D:134:ILE:N	2.27	0.50
1:D:836:GLN:OE1	1:D:877:SER:HB2	2.12	0.50
1:A:836:GLN:OE1	1:A:877:SER:HB2	2.12	0.50
1:C:514:LEU:HD22	1:C:607:MET:HE3	1.94	0.50
1:D:410:ARG:NH2	5:D:2101:HOH:O	2.36	0.50
1:B:836:GLN:OE1	1:B:877:SER:HB2	2.12	0.50
1:A:1047:ASN:ND2	2:A:2001:FLC:HG1	2.24	0.49
1:A:653:LYS:O	1:A:656:GLU:HG2	2.13	0.49
1:B:133:VAL:HG12	1:B:134:ILE:N	2.27	0.49
1:D:297:VAL:HG23	5:D:2157:HOH:O	2.13	0.49
1:D:380:ASN:O	1:D:385:THR:HG21	2.12	0.49
1:D:479:ASN:ND2	1:D:1058:MET:H	2.11	0.49
1:C:710:LYS:HG2	1:C:712:MET:CE	2.38	0.49
1:B:373:GLY:O	1:B:400:THR:HA	2.13	0.49
1:B:653:LYS:O	1:B:656:GLU:HG2	2.13	0.48
1:A:819:ALA:HB3	5:A:2202:HOH:O	2.13	0.48
1:B:0:MET:HE1	1:B:26:LEU:HD22	1.94	0.48
1:D:499:LYS:HG3	5:D:2167:HOH:O	2.13	0.48
1:A:464:ASP:OD2	1:A:464:ASP:N	2.38	0.48
1:D:216:ILE:HG13	1:D:266:MET:HG3	1.95	0.48
1:D:514:LEU:HD22	1:D:607:MET:HE3	1.95	0.48
1:B:0:MET:HE2	1:B:26:LEU:HD22	1.95	0.48
1:C:653:LYS:O	1:C:656:GLU:HG2	2.13	0.48
1:C:836:GLN:OE1	1:C:877:SER:HB2	2.13	0.48
1:B:380:ASN:O	1:B:385:THR:HG21	2.13	0.48
1:C:514:LEU:HB2	1:C:607:MET:HE3	1.94	0.48
1:B:14:GLU:CG	1:B:397:LYS:HE3	2.44	0.48
1:D:300:THR:HG22	1:D:375:ARG:CZ	2.44	0.48
1:B:479:ASN:ND2	1:B:1058:MET:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:THR:HB	1:C:422:ARG:HB2	1.96	0.47
1:B:82:HIS:CD2	1:B:84:GLY:H	2.20	0.47
1:B:33:ILE:O	1:B:43:HIS:HE1	1.96	0.47
1:C:373:GLY:O	1:C:400:THR:HA	2.14	0.47
1:D:0:MET:CE	1:D:26:LEU:HD22	2.40	0.47
1:D:653:LYS:O	1:D:656:GLU:HG2	2.14	0.47
1:A:979:TYR:HB3	1:A:982:VAL:HG22	1.97	0.47
1:B:514:LEU:HD22	1:B:607:MET:HE3	1.95	0.47
1:B:567:LEU:HB3	1:B:570:MET:CE	2.41	0.47
1:C:600:ARG:HA	1:C:600:ARG:HD3	1.63	0.47
1:D:14:GLU:CG	1:D:397:LYS:HE3	2.45	0.47
1:D:942:ASP:OD1	1:D:942:ASP:N	2.47	0.47
2:A:2001:FLC:CBC	2:A:2001:FLC:OG2	2.59	0.47
1:C:14:GLU:CG	1:C:397:LYS:HE3	2.45	0.47
1:D:128:LEU:HD12	1:D:128:LEU:O	2.15	0.47
1:A:294:ARG:NH2	5:A:2155:HOH:O	2.48	0.47
1:B:1047:ASN:HD22	2:B:2001:FLC:HG1	1.80	0.47
1:C:133:VAL:HG12	1:C:134:ILE:N	2.29	0.47
1:D:365:THR:HB	1:D:422:ARG:HB2	1.97	0.47
1:D:760:ASP:C	1:D:761:ILE:HG13	2.40	0.47
1:C:300:THR:HG22	1:C:375:ARG:CZ	2.45	0.46
1:D:819:ALA:N	5:D:2216:HOH:O	2.46	0.46
1:D:979:TYR:HB3	1:D:982:VAL:HG22	1.97	0.46
1:A:373:GLY:O	1:A:400:THR:HA	2.15	0.46
1:A:600:ARG:NH2	1:A:641:ASP:OD2	2.48	0.46
2:D:2001:FLC:CBC	2:D:2001:FLC:OA1	2.61	0.46
1:C:674:CYS:HB3	1:C:712:MET:HE1	1.96	0.46
1:A:300:THR:HG22	1:A:375:ARG:NH2	2.30	0.46
1:D:971:LYS:HA	1:D:974:ILE:HG22	1.97	0.46
1:B:979:TYR:HB3	1:B:982:VAL:HG22	1.97	0.46
1:D:33:ILE:O	1:D:43:HIS:HE1	1.98	0.46
1:B:819:ALA:N	5:B:2147:HOH:O	2.49	0.46
1:D:82:HIS:CD2	1:D:84:GLY:H	2.20	0.46
1:B:300:THR:HG22	1:B:375:ARG:CZ	2.46	0.46
1:C:979:TYR:HB3	1:C:982:VAL:HG22	1.98	0.45
1:B:365:THR:HB	1:B:422:ARG:HB2	1.97	0.45
1:A:712:MET:HG2	1:A:873:VAL:HB	1.99	0.45
1:B:611:LEU:HD12	1:B:644:ARG:HG2	1.99	0.45
1:C:33:ILE:O	1:C:43:HIS:HE1	1.99	0.45
1:D:226:HIS:CD2	1:D:259:CYS:HB3	2.52	0.45
1:D:373:GLY:O	1:D:400:THR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:THR:HG22	1:C:375:ARG:NH2	2.32	0.45
1:D:600:ARG:HA	1:D:600:ARG:HD3	1.64	0.45
1:A:112:HIS:HE1	1:A:269:VAL:O	2.00	0.44
1:A:346:ARG:HB2	5:A:2236:HOH:O	2.17	0.44
1:A:365:THR:HB	1:A:422:ARG:HB2	1.99	0.44
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.82	0.44
1:C:288:PHE:CD1	1:C:288:PHE:C	2.95	0.44
1:D:819:ALA:O	1:D:821:ASN:ND2	2.51	0.44
1:D:819:ALA:HB3	5:D:2216:HOH:O	2.18	0.44
1:A:288:PHE:CD1	1:A:288:PHE:C	2.95	0.44
1:A:575:MET:SD	1:A:575:MET:C	3.00	0.44
1:B:746:ASN:ND2	1:C:748:ILE:HG21	2.32	0.44
1:D:613:ARG:NH2	5:D:2251:HOH:O	2.50	0.44
1:B:600:ARG:HA	1:B:600:ARG:HD3	1.65	0.44
1:C:760:ASP:C	1:C:761:ILE:HG13	2.43	0.44
1:A:500:ILE:N	5:A:2163:HOH:O	2.38	0.44
1:B:680:ASP:OD1	1:B:723:ARG:NH1	2.51	0.44
1:D:601:LYS:HE3	5:D:2140:HOH:O	2.17	0.44
1:A:33:ILE:O	1:A:43:HIS:HE1	2.00	0.44
1:B:600:ARG:NH2	1:B:641:ASP:OD2	2.51	0.44
1:C:112:HIS:HE1	1:C:269:VAL:O	2.00	0.44
1:A:14:GLU:CG	1:A:397:LYS:HE3	2.48	0.44
1:B:112:HIS:HE1	1:B:269:VAL:O	2.01	0.44
1:C:97:ARG:HH11	1:C:97:ARG:HG3	1.83	0.44
1:C:1092:LYS:HB2	1:C:1092:LYS:HE2	1.73	0.44
1:A:300:THR:HG22	1:A:375:ARG:CZ	2.47	0.43
1:A:600:ARG:HD3	1:A:600:ARG:HA	1.64	0.43
1:D:420:ARG:NH1	2:D:2001:FLC:OA1	2.47	0.43
1:D:499:LYS:CG	5:D:2167:HOH:O	2.66	0.43
1:D:611:LEU:HD12	1:D:644:ARG:HG2	2.00	0.43
1:A:734:VAL:HG12	5:A:2146:HOH:O	2.19	0.43
1:B:118:ASP:HB3	1:B:121:LYS:CD	2.47	0.43
1:D:97:ARG:HG3	1:D:97:ARG:HH11	1.83	0.43
1:A:1067:ARG:CD	5:A:2135:HOH:O	2.66	0.43
1:C:600:ARG:NH2	1:C:641:ASP:OD2	2.51	0.43
1:D:670:GLU:OE1	1:D:737:HIS:ND1	2.51	0.43
1:A:819:ALA:O	1:A:821:ASN:ND2	2.51	0.43
1:B:819:ALA:HB3	5:B:2147:HOH:O	2.18	0.43
1:B:288:PHE:CD1	1:B:288:PHE:C	2.96	0.43
1:B:819:ALA:O	1:B:821:ASN:ND2	2.52	0.43
1:C:54:GLY:O	1:C:55:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:ASP:OD1	1:C:723:ARG:NH1	2.51	0.43
1:D:536:ASP:HA	1:D:764:VAL:O	2.19	0.43
1:B:44:ARG:O	1:B:44:ARG:HG2	2.17	0.43
1:A:44:ARG:O	1:A:44:ARG:HG2	2.19	0.42
1:D:112:HIS:HE1	1:D:269:VAL:O	2.01	0.42
1:A:369:THR:HG22	1:A:418:GLU:HG2	2.02	0.42
1:C:123:LYS:HD2	1:C:133:VAL:CG1	2.49	0.42
1:D:680:ASP:OD1	1:D:723:ARG:NH1	2.53	0.42
1:A:54:GLY:O	1:A:55:ALA:C	2.61	0.42
1:A:680:ASP:OD1	1:A:723:ARG:NH1	2.53	0.42
1:A:942:ASP:OD1	1:A:942:ASP:N	2.52	0.42
1:A:83:PRO:HB2	1:A:89:SER:HA	2.02	0.42
1:C:369:THR:HG22	1:C:418:GLU:HG2	2.02	0.42
1:D:393:SER:O	1:D:394:LEU:C	2.63	0.42
1:D:1013:THR:HG22	5:D:2274:HOH:O	2.19	0.42
1:C:60:ILE:HB	5:C:1305:HOH:O	2.19	0.42
1:B:54:GLY:O	1:B:55:ALA:C	2.63	0.42
1:D:1037:ASP:OD1	1:D:1037:ASP:C	2.63	0.42
1:D:54:GLY:O	1:D:55:ALA:C	2.63	0.41
1:D:600:ARG:NH2	1:D:641:ASP:OD2	2.52	0.41
1:A:420:ARG:NH1	2:A:2001:FLC:OG2	2.52	0.41
1:C:819:ALA:O	1:C:821:ASN:ND2	2.53	0.41
1:D:575:MET:SD	1:D:575:MET:C	3.03	0.41
1:B:760:ASP:C	1:B:761:ILE:HG13	2.44	0.41
1:C:623:TYR:C	1:C:948:MET:CE	2.94	0.41
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.33	0.41
1:C:575:MET:SD	1:C:575:MET:C	3.04	0.41
2:B:2001:FLC:OG2	2:B:2001:FLC:CBC	2.68	0.41
1:D:97:ARG:HG3	1:D:97:ARG:NH1	2.36	0.41
1:D:805:TYR:CZ	1:D:809:VAL:HG21	2.56	0.41
1:C:0:MET:HE3	1:C:0:MET:HB2	1.91	0.41
1:C:479:ASN:ND2	1:C:1058:MET:H	2.16	0.41
1:C:1067:ARG:CD	5:C:1319:HOH:O	2.68	0.41
1:A:760:ASP:C	1:A:761:ILE:HG13	2.45	0.41
1:C:129:ALA:O	1:C:264:LYS:HD3	2.21	0.41
1:D:44:ARG:HH11	1:D:44:ARG:CG	2.34	0.41
1:D:129:ALA:O	1:D:264:LYS:HD3	2.21	0.41
1:A:312:GLN:HE22	1:B:410:ARG:HH21	1.69	0.41
1:A:830:HIS:CD2	1:A:832:MET:HG3	2.56	0.41
1:A:915:MET:HE2	5:A:2210:HOH:O	2.20	0.41
1:C:44:ARG:O	1:C:44:ARG:HG2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:PRO:O	1:C:446:ASN:HB2	2.21	0.41
1:C:623:TYR:C	1:C:948:MET:HE1	2.45	0.41
1:A:777:SER:HB3	5:A:2111:HOH:O	2.21	0.41
1:B:670:GLU:OE1	1:B:737:HIS:ND1	2.50	0.41
1:C:332:LYS:O	1:C:333:GLN:C	2.64	0.41
1:A:226:HIS:CD2	1:A:259:CYS:HB3	2.55	0.40
1:A:974:ILE:HD13	1:A:974:ILE:N	2.36	0.40
1:D:209:PRO:O	1:D:446:ASN:HB2	2.21	0.40
1:A:479:ASN:ND2	1:A:1058:MET:H	2.17	0.40
1:A:901:GLY:O	1:A:935:LYS:NZ	2.54	0.40
1:A:500:ILE:O	1:A:501:PRO:C	2.62	0.40
1:C:58:LYS:H	1:C:58:LYS:HG3	1.67	0.40
1:C:682:ASP:OD1	1:C:682:ASP:N	2.54	0.40
1:A:611:LEU:HD12	1:A:644:ARG:HG2	2.03	0.40
1:B:226:HIS:CD2	1:B:259:CYS:HB3	2.57	0.40
1:C:934:LEU:HD23	1:C:934:LEU:HA	1.84	0.40
1:D:44:ARG:O	1:D:44:ARG:HG2	2.19	0.40
1:D:682:ASP:OD1	1:D:682:ASP:N	2.53	0.40
1:A:129:ALA:O	1:A:264:LYS:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1066/1148 (93%)	1026 (96%)	40 (4%)	0	100	100
1	B	1068/1148 (93%)	1027 (96%)	41 (4%)	0	100	100
1	C	1075/1148 (94%)	1034 (96%)	41 (4%)	0	100	100
1	D	1066/1148 (93%)	1021 (96%)	45 (4%)	0	100	100
All	All	4275/4592 (93%)	4108 (96%)	167 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	919/983 (94%)	871 (95%)	48 (5%)	21	42
1	B	916/983 (93%)	875 (96%)	41 (4%)	24	49
1	C	924/983 (94%)	882 (96%)	42 (4%)	24	49
1	D	921/983 (94%)	875 (95%)	46 (5%)	22	44
All	All	3680/3932 (94%)	3503 (95%)	177 (5%)	23	46

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	42	PHE
1	A	44	ARG
1	A	70	ILE
1	A	92	ILE
1	A	96	ARG
1	A	110	SER
1	A	119	LYS
1	A	120	ILE
1	A	216	ILE
1	A	225	VAL
1	A	294	ARG
1	A	326	GLN
1	A	393	SER
1	A	435	VAL
1	A	464	ASP
1	A	531	GLU
1	A	535	THR
1	A	549	THR
1	A	576	TRP
1	A	600	ARG
1	A	613	ARG

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Mol	Chain	Res	Type
1	A	644	ARG
1	A	682	ASP
1	A	695	MET
1	A	712	MET
1	A	727	GLU
1	A	750	THR
1	A	756	SER
1	A	791	GLN
1	A	842	GLN
1	A	865	GLN
1	A	928	LYS
1	A	940	LEU
1	A	941	THR
1	A	942	ASP
1	A	947	LEU
1	A	951	VAL
1	A	974	ILE
1	A	981	LYS
1	A	982	VAL
1	A	1053	ILE
1	A	1061	GLN
1	A	1068	ARG
1	A	1092	LYS
1	A	1109	MET
1	A	1110	LYS
1	A	1115	ILE
1	B	2	ASN
1	B	42	PHE
1	B	44	ARG
1	B	70	ILE
1	B	92	ILE
1	B	110	SER
1	B	120	ILE
1	B	121	LYS
1	B	216	ILE
1	B	225	VAL
1	B	294	ARG
1	B	393	SER
1	B	535	THR
1	B	549	THR
1	B	576	TRP
1	B	600	ARG

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Mol	Chain	Res	Type
1	B	613	ARG
1	B	644	ARG
1	B	663	ARG
1	B	682	ASP
1	B	695	MET
1	B	712	MET
1	B	727	GLU
1	B	756	SER
1	B	791	GLN
1	B	820	LEU
1	B	839	ASN
1	B	842	GLN
1	B	865	GLN
1	B	940	LEU
1	B	941	THR
1	B	942	ASP
1	B	947	LEU
1	B	951	VAL
1	B	974	ILE
1	B	982	VAL
1	B	1053	ILE
1	B	1059	ASN
1	B	1068	ARG
1	B	1092	LYS
1	B	1115	ILE
1	C	-1	HIS
1	C	42	PHE
1	C	44	ARG
1	C	70	ILE
1	C	92	ILE
1	C	110	SER
1	C	119	LYS
1	C	120	ILE
1	C	121	LYS
1	C	137	SER
1	C	200	VAL
1	C	202	VAL
1	C	216	ILE
1	C	225	VAL
1	C	294	ARG
1	C	357	MET
1	C	393	SER

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Mol	Chain	Res	Type
1	C	435	VAL
1	C	531	GLU
1	C	535	THR
1	C	549	THR
1	C	576	TRP
1	C	600	ARG
1	C	613	ARG
1	C	644	ARG
1	C	695	MET
1	C	727	GLU
1	C	756	SER
1	C	791	GLN
1	C	842	GLN
1	C	865	GLN
1	C	918	ILE
1	C	940	LEU
1	C	941	THR
1	C	947	LEU
1	C	974	ILE
1	C	982	VAL
1	C	1053	ILE
1	C	1068	ARG
1	C	1092	LYS
1	C	1110	LYS
1	C	1115	ILE
1	D	42	PHE
1	D	44	ARG
1	D	60	ILE
1	D	70	ILE
1	D	92	ILE
1	D	110	SER
1	D	120	ILE
1	D	128	LEU
1	D	225	VAL
1	D	294	ARG
1	D	357	MET
1	D	393	SER
1	D	425	LYS
1	D	435	VAL
1	D	531	GLU
1	D	535	THR
1	D	549	THR

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Mol	Chain	Res	Type
1	D	576	TRP
1	D	600	ARG
1	D	613	ARG
1	D	644	ARG
1	D	695	MET
1	D	712	MET
1	D	727	GLU
1	D	756	SER
1	D	791	GLN
1	D	824	GLN
1	D	839	ASN
1	D	842	GLN
1	D	865	GLN
1	D	874	THR
1	D	927	GLU
1	D	928	LYS
1	D	940	LEU
1	D	941	THR
1	D	942	ASP
1	D	947	LEU
1	D	951	VAL
1	D	981	LYS
1	D	982	VAL
1	D	1053	ILE
1	D	1059	ASN
1	D	1068	ARG
1	D	1092	LYS
1	D	1110	LYS
1	D	1115	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	68	ASN
1	A	82	HIS
1	A	112	HIS
1	A	239	GLN
1	A	248	ASN
1	A	292	ASN
1	A	312	GLN
1	A	333	GLN

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Mol	Chain	Res	Type
1	A	355	ASN
1	A	383	GLN
1	A	415	ASN
1	A	479	ASN
1	A	589	ASN
1	A	602	GLN
1	A	746	ASN
1	A	821	ASN
1	A	830	HIS
1	A	839	ASN
1	A	843	GLN
1	A	1047	ASN
1	A	1061	GLN
1	B	43	HIS
1	B	68	ASN
1	B	82	HIS
1	B	112	HIS
1	B	292	ASN
1	B	312	GLN
1	B	333	GLN
1	B	355	ASN
1	B	383	GLN
1	B	415	ASN
1	B	479	ASN
1	B	529	GLN
1	B	589	ASN
1	B	602	GLN
1	B	746	ASN
1	B	821	ASN
1	B	824	GLN
1	B	830	HIS
1	B	841	GLN
1	B	843	GLN
1	B	1049	GLN
1	C	43	HIS
1	C	68	ASN
1	C	82	HIS
1	C	112	HIS
1	C	292	ASN
1	C	312	GLN
1	C	333	GLN
1	C	354	ASN

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Mol	Chain	Res	Type
1	C	383	GLN
1	C	415	ASN
1	C	479	ASN
1	C	505	GLN
1	C	529	GLN
1	C	589	ASN
1	C	602	GLN
1	C	746	ASN
1	C	821	ASN
1	C	830	HIS
1	C	839	ASN
1	C	843	GLN
1	C	1049	GLN
1	D	43	HIS
1	D	68	ASN
1	D	82	HIS
1	D	112	HIS
1	D	292	ASN
1	D	312	GLN
1	D	333	GLN
1	D	355	ASN
1	D	383	GLN
1	D	415	ASN
1	D	479	ASN
1	D	505	GLN
1	D	529	GLN
1	D	589	ASN
1	D	602	GLN
1	D	746	ASN
1	D	821	ASN
1	D	830	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	2BA	A	2004	-	50,50,50	1.55	12 (24%)	74,78,78	2.63	30 (40%)
2	FLC	B	2001	-	12,12,12	1.27	1 (8%)	17,17,17	1.81	5 (29%)
4	2BA	A	2003	-	50,50,50	1.61	9 (18%)	74,78,78	2.21	25 (33%)
2	FLC	A	2001	-	12,12,12	1.46	2 (16%)	17,17,17	1.74	4 (23%)
4	2BA	C	1201	-	50,50,50	1.48	6 (12%)	74,78,78	2.10	26 (35%)
2	FLC	D	2001	-	12,12,12	1.13	1 (8%)	17,17,17	1.95	7 (41%)
2	FLC	C	1202	-	12,12,12	1.23	2 (16%)	17,17,17	2.40	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2BA	A	2004	-	-	4/30/62/62	0/6/7/7
2	FLC	B	2001	-	-	1/16/16/16	-
4	2BA	A	2003	-	-	7/30/62/62	0/6/7/7
2	FLC	A	2001	-	-	7/16/16/16	-
4	2BA	C	1201	-	-	2/30/62/62	0/6/7/7
2	FLC	D	2001	-	-	2/16/16/16	-
2	FLC	C	1202	-	-	4/16/16/16	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1201	2BA	C5-C4	4.60	1.47	1.39
4	C	1201	2BA	C51-C41	4.46	1.47	1.39
4	A	2003	2BA	C5-C4	4.12	1.46	1.39
4	A	2004	2BA	C5-C4	4.09	1.46	1.39
4	A	2004	2BA	C51-C41	3.81	1.45	1.39
4	C	1201	2BA	C5-N7	-3.77	1.32	1.39
4	A	2003	2BA	C5-N7	-3.39	1.32	1.39
4	A	2003	2BA	C8-N7	3.35	1.38	1.31
4	A	2004	2BA	O2'-C2'	3.20	1.50	1.43
4	A	2003	2BA	C51-N71	-3.18	1.33	1.39
4	A	2003	2BA	C51-C41	2.98	1.44	1.39
4	C	1201	2BA	C4-N9	-2.97	1.31	1.37
4	A	2004	2BA	C5-C6	2.66	1.48	1.41
4	A	2003	2BA	C41-N91	-2.54	1.32	1.37
2	C	1202	FLC	OB1-CBC	2.48	1.29	1.22
2	C	1202	FLC	CA-CB	2.46	1.57	1.54
4	A	2003	2BA	C5-C6	2.44	1.47	1.41
4	C	1201	2BA	C51-N71	-2.41	1.34	1.39
4	A	2003	2BA	C81-N71	2.37	1.36	1.31
4	A	2004	2BA	O4'-C1'	2.33	1.47	1.42
4	A	2003	2BA	C4-N9	-2.32	1.32	1.37
4	A	2004	2BA	C1'1-N91	2.31	1.52	1.46
4	C	1201	2BA	C51-C61	2.29	1.47	1.41
2	A	2001	FLC	OB1-CBC	2.27	1.29	1.22
2	D	2001	FLC	OG1-CGC	2.24	1.29	1.22
2	B	2001	FLC	OA1-CAC	2.23	1.29	1.22
4	A	2004	2BA	O4'1-C1'1	2.21	1.47	1.42
4	A	2004	2BA	C8-N7	2.21	1.35	1.31
4	A	2004	2BA	C51-N71	-2.09	1.35	1.39
4	A	2004	2BA	C41-N91	-2.05	1.33	1.37
4	A	2004	2BA	C81-N71	2.05	1.35	1.31
4	A	2004	2BA	C1'-N9	2.04	1.52	1.46
2	A	2001	FLC	OHB-CB	2.02	1.47	1.43

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	2BA	C5-C4-N3	-6.37	117.95	126.72
4	A	2004	2BA	N3-C4-N9	5.80	137.04	127.17
4	A	2003	2BA	N31-C21-N11	-5.80	119.80	128.58
4	A	2004	2BA	N31-C21-N11	-5.71	119.93	128.58
4	A	2004	2BA	C2'-C3'-C4'	5.55	112.96	103.24
4	A	2003	2BA	C5-C4-N3	-5.41	119.27	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1201	2BA	C51-C41-N31	-5.20	119.56	126.72
4	A	2003	2BA	N3-C2-N1	-5.18	120.74	128.58
4	C	1201	2BA	N31-C21-N11	-5.12	120.83	128.58
4	A	2004	2BA	C2-N3-C4	4.97	123.97	111.83
4	A	2004	2BA	C51-C41-N31	-4.94	119.92	126.72
4	C	1201	2BA	N31-C41-N91	4.82	135.36	127.17
4	A	2004	2BA	N3-C2-N1	-4.76	121.38	128.58
2	C	1202	FLC	OA1-CAC-CA	-4.76	109.48	122.95
4	A	2004	2BA	O4'-C1'-N9	-4.62	99.21	108.09
4	A	2003	2BA	C2-N3-C4	4.56	122.98	111.83
4	C	1201	2BA	C5-C4-N3	-4.54	120.47	126.72
4	A	2004	2BA	C21-N31-C41	4.52	122.86	111.83
4	A	2004	2BA	O2'-C2'-C1'	4.48	125.54	110.10
2	C	1202	FLC	OA2-CAC-CA	4.46	128.47	114.35
4	C	1201	2BA	N3-C4-N9	4.35	134.56	127.17
4	C	1201	2BA	N3-C2-N1	-4.25	122.15	128.58
4	C	1201	2BA	C21-N31-C41	4.20	122.08	111.83
4	A	2003	2BA	O3'1-P-O1P	4.15	123.08	109.81
4	A	2004	2BA	O4'1-C1'1-N91	4.11	115.98	108.09
2	B	2001	FLC	OB2-CBC-CB	4.08	120.96	113.14
2	A	2001	FLC	CA-CB-CBC	4.04	118.98	110.03
2	C	1202	FLC	OG1-CGC-CG	-4.02	111.56	122.95
4	A	2003	2BA	N3-C4-N9	3.96	133.91	127.17
4	A	2004	2BA	C4-N9-C8	3.96	109.89	105.74
4	A	2004	2BA	N31-C41-N91	3.88	133.76	127.17
4	A	2003	2BA	N31-C41-N91	3.85	133.72	127.17
4	A	2003	2BA	C51-C61-N61	-3.84	113.77	123.29
4	A	2003	2BA	C21-N31-C41	3.78	121.07	111.83
2	D	2001	FLC	OB2-CBC-CB	3.75	120.34	113.14
4	A	2004	2BA	N9-C8-N7	-3.64	108.77	113.94
2	C	1202	FLC	CB-CA-CAC	-3.64	103.96	113.92
2	D	2001	FLC	OG1-CGC-CG	-3.53	112.97	122.95
4	A	2004	2BA	C5-N7-C8	3.39	108.77	103.45
4	A	2004	2BA	C2'-C1'-N9	3.35	121.63	113.30
4	C	1201	2BA	C2-N3-C4	3.33	119.96	111.83
4	A	2003	2BA	O4'-C1'-N9	-3.30	101.76	108.09
4	A	2003	2BA	C51-C41-N31	-3.29	122.18	126.72
4	A	2003	2BA	O2'1-C2'1-C3'1	-3.25	102.10	111.19
4	C	1201	2BA	C3'-C2'-C1'	3.20	106.92	99.89
2	B	2001	FLC	OB1-CBC-CB	-3.08	116.14	122.09
4	A	2004	2BA	C6-C5-N7	3.07	138.01	132.09
4	C	1201	2BA	O4'-C1'-N9	3.04	113.92	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	2BA	C5-C6-N6	-3.03	115.78	123.29
4	A	2003	2BA	N61-C61-N11	3.02	125.09	118.38
4	A	2004	2BA	C61-C51-C41	-3.00	113.08	117.18
4	A	2003	2BA	C2'-C3'-C4'	-3.00	97.99	103.24
4	A	2003	2BA	C6-C5-N7	2.99	137.85	132.09
4	A	2003	2BA	C41-N91-C81	2.96	108.84	105.74
4	C	1201	2BA	C21-N11-C61	2.88	123.45	118.73
4	A	2004	2BA	C61-C51-N71	2.87	137.62	132.09
2	C	1202	FLC	CG-CB-CBC	2.85	116.34	110.03
4	C	1201	2BA	N6-C6-N1	2.83	124.69	118.38
4	A	2004	2BA	O2P1-P1-O1P1	2.74	125.18	112.44
4	A	2003	2BA	C61-C51-C41	-2.71	113.48	117.18
4	C	1201	2BA	C41-N91-C81	2.70	108.58	105.74
4	A	2004	2BA	O3'1-C3'1-C4'1	2.70	119.54	110.03
4	A	2004	2BA	C4-C5-N7	-2.65	107.55	110.58
4	A	2004	2BA	C4-N9-C1'	-2.63	120.48	126.63
4	A	2004	2BA	O3'1-P-O1P	-2.58	101.57	109.81
2	C	1202	FLC	OG2-CGC-CG	2.57	122.49	114.35
4	A	2004	2BA	O2P1-P1-O3'	-2.55	96.30	106.70
2	B	2001	FLC	OHB-CB-CG	-2.55	103.57	109.38
4	C	1201	2BA	C2'-C3'-C4'	-2.49	98.87	103.24
2	B	2001	FLC	CA-CB-CBC	2.49	115.55	110.03
4	C	1201	2BA	C2-N1-C6	2.49	122.82	118.73
2	D	2001	FLC	OA1-CAC-CA	-2.44	116.04	122.95
2	D	2001	FLC	OB1-CBC-CB	-2.44	117.37	122.09
2	D	2001	FLC	CB-CA-CAC	-2.38	107.42	113.92
4	A	2003	2BA	C4-C5-N7	-2.36	107.88	110.58
2	A	2001	FLC	OB1-CBC-CB	-2.35	117.54	122.09
4	A	2003	2BA	N9-C8-N7	-2.34	110.61	113.94
4	C	1201	2BA	O3'-P1-O1P1	-2.33	102.35	109.81
4	C	1201	2BA	C5-C6-N6	-2.31	117.57	123.29
4	C	1201	2BA	C61-C51-N71	2.28	136.50	132.09
4	A	2004	2BA	O5'-P-O1P	2.27	117.94	108.94
4	C	1201	2BA	O2P-P-O1P	2.26	122.98	112.44
2	A	2001	FLC	CG-CB-CBC	-2.25	105.05	110.03
2	A	2001	FLC	CB-CG-CGC	-2.24	107.80	113.92
4	C	1201	2BA	C2'1-C3'1-C4'1	-2.23	99.33	103.24
4	A	2003	2BA	O2P1-P1-O1P1	2.21	122.74	112.44
4	C	1201	2BA	C51-N71-C81	2.20	106.91	103.45
4	A	2003	2BA	C21-N11-C61	2.18	122.31	118.73
4	C	1201	2BA	P1-O5'1-C5'1	-2.16	108.95	121.35
4	A	2003	2BA	C41-N91-C1'1	-2.16	121.58	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	2BA	C6-C5-C4	-2.15	114.25	117.18
4	C	1201	2BA	O2P1-P1-O1P1	2.14	122.40	112.44
4	A	2003	2BA	C4-N9-C8	2.10	107.94	105.74
4	A	2003	2BA	C5-N7-C8	2.10	106.75	103.45
4	C	1201	2BA	C2'-C1'-N9	-2.09	108.12	113.30
2	D	2001	FLC	OA2-CAC-CA	2.08	120.94	114.35
4	C	1201	2BA	O2P1-P1-O5'1	-2.08	98.16	107.57
4	C	1201	2BA	C41-C51-N71	-2.06	108.23	110.58
4	A	2004	2BA	P1-O5'1-C5'1	2.04	133.06	121.35
2	B	2001	FLC	CB-CG-CGC	-2.04	108.36	113.92
2	D	2001	FLC	OG2-CGC-CG	2.04	120.80	114.35
4	A	2004	2BA	C2'1-C3'1-C4'1	2.03	106.79	103.24
4	A	2004	2BA	C6-C5-C4	-2.00	114.44	117.18

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	FLC	CAC-CA-CB-OHB
4	A	2004	2BA	C2'-C1'-N9-C8
4	A	2003	2BA	C2'1-C3'1-O3'1-P
2	A	2001	FLC	CAC-CA-CB-CBC
2	A	2001	FLC	CAC-CA-CB-CG
4	A	2004	2BA	C2'-C1'-N9-C4
4	A	2003	2BA	C4'-C3'-O3'-P1
4	A	2003	2BA	C4'1-C3'1-O3'1-P
4	C	1201	2BA	O4'1-C4'1-C5'1-O5'1
4	A	2004	2BA	C5'-O5'-P-O1P
4	C	1201	2BA	C3'1-C4'1-C5'1-O5'1
2	A	2001	FLC	CA-CB-CBC-OB2
2	C	1202	FLC	CBC-CB-CG-CGC
2	C	1202	FLC	OHB-CB-CG-CGC
4	A	2003	2BA	C2'-C3'-O3'-P1
2	A	2001	FLC	CB-CG-CGC-OG2
2	A	2001	FLC	CB-CG-CGC-OG1
4	A	2004	2BA	O4'-C4'-C5'-O5'
4	A	2003	2BA	C3'1-O3'1-P-O1P
4	A	2003	2BA	C3'1-O3'1-P-O2P
4	A	2003	2BA	C3'-O3'-P1-O2P1
2	A	2001	FLC	OHB-CB-CBC-OB2
2	D	2001	FLC	CB-CG-CGC-OG1
2	D	2001	FLC	CB-CG-CGC-OG2

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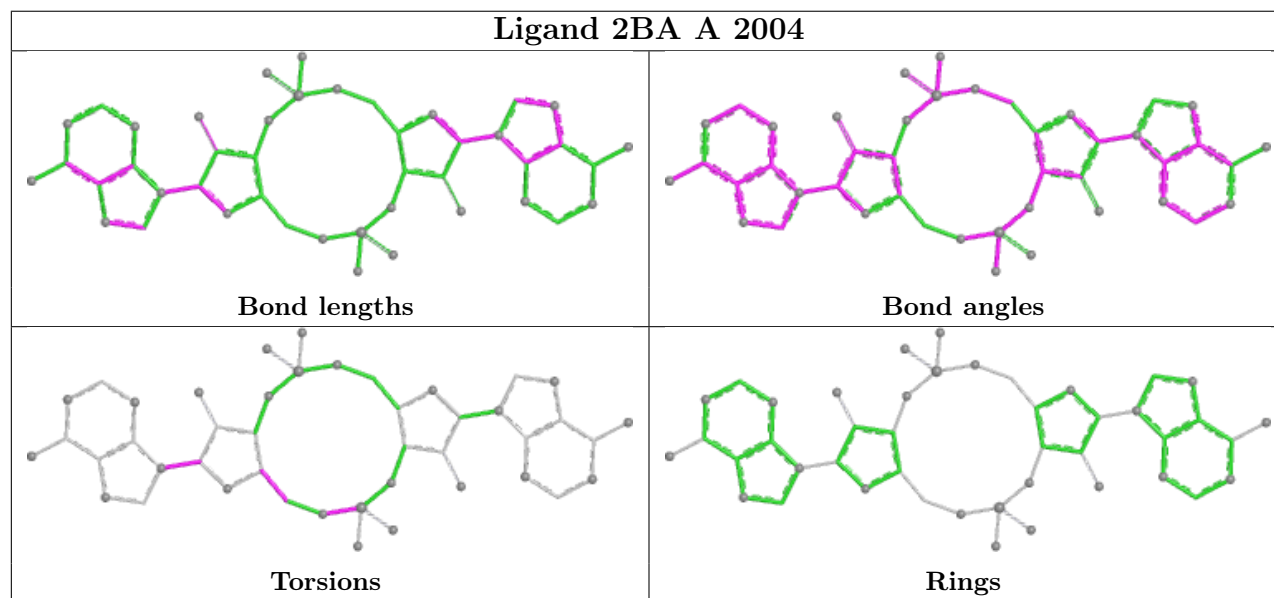
Mol	Chain	Res	Type	Atoms
2	C	1202	FLC	CB-CG-CGC-OG1
2	B	2001	FLC	CB-CG-CGC-OG1
2	C	1202	FLC	CB-CG-CGC-OG2

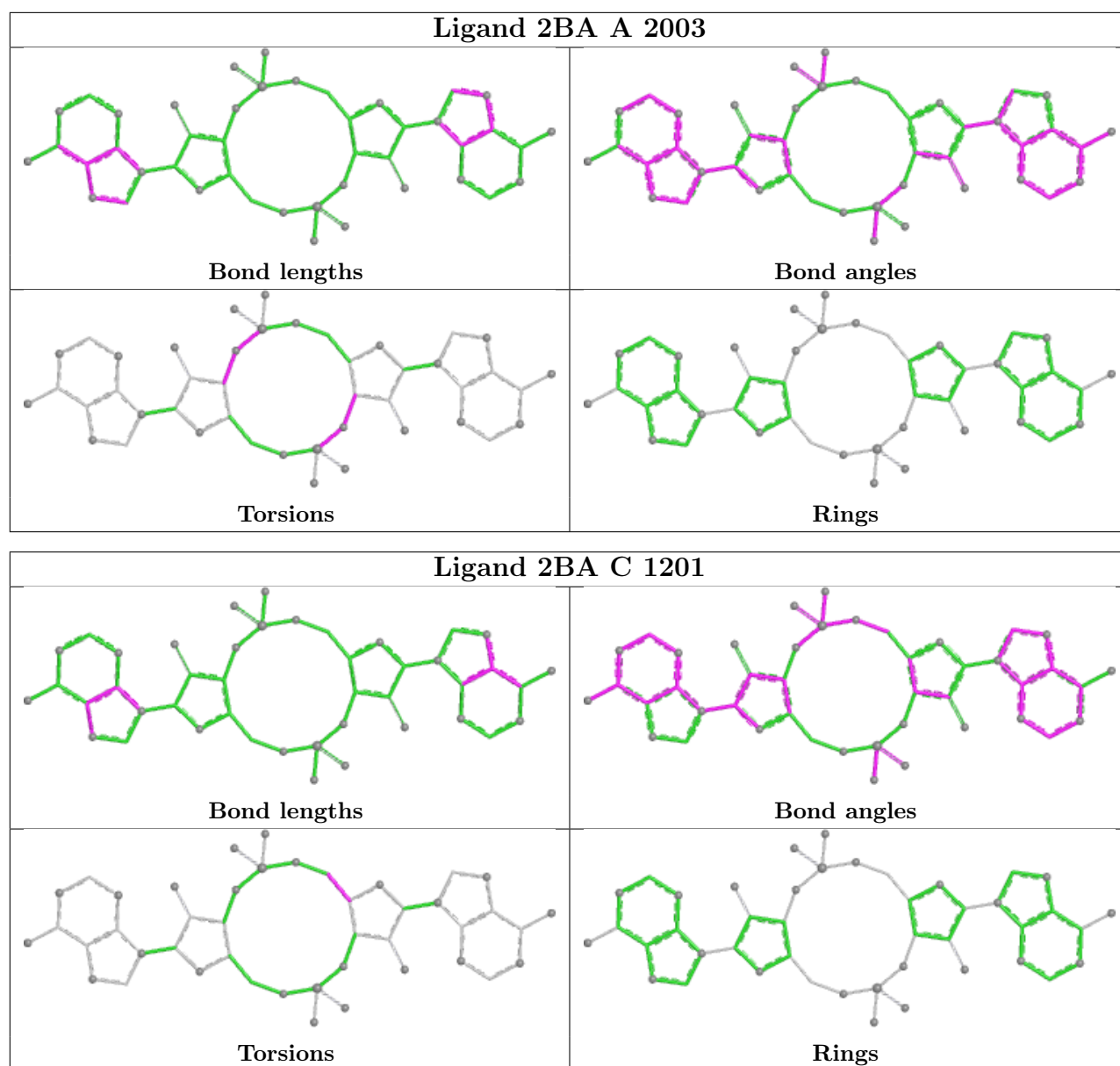
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	FLC	5	0
2	A	2001	FLC	4	0
2	D	2001	FLC	2	0
2	C	1202	FLC	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	1072/1148 (93%)	0.10	26 (2%) 59 55	17, 47, 86, 120	0
1	B	1074/1148 (93%)	0.31	42 (3%) 43 38	34, 56, 100, 128	0
1	C	1081/1148 (94%)	0.34	55 (5%) 33 29	30, 57, 98, 130	0
1	D	1072/1148 (93%)	0.00	25 (2%) 61 57	20, 45, 84, 123	0
All	All	4299/4592 (93%)	0.19	148 (3%) 48 43	17, 51, 94, 130	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	820	LEU	5.7
1	C	933	VAL	4.6
1	C	820	LEU	4.5
1	A	118	ASP	4.4
1	D	820	LEU	4.1
1	A	947	LEU	3.9
1	B	822	SER	3.9
1	A	120	ILE	3.7
1	B	947	LEU	3.7
1	A	820	LEU	3.6
1	C	929	LEU	3.5
1	C	932	LEU	3.5
1	C	940	LEU	3.4
1	C	462	ILE	3.4
1	B	793	ASN	3.4
1	D	1066	ALA	3.4
1	A	940	LEU	3.3
1	C	918	ILE	3.3
1	C	954	VAL	3.3
1	C	135	PRO	3.2
1	C	202	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	941	THR	3.2
1	C	904	ILE	3.2
1	D	463	ARG	3.1
1	B	248	ASN	3.1
1	C	834	GLY	3.1
1	D	1072	THR	3.0
1	D	1109	MET	3.0
1	C	1109	MET	3.0
1	D	1082	MET	3.0
1	D	205	CYS	3.0
1	B	613	ARG	3.0
1	A	128	LEU	3.0
1	C	819	ALA	3.0
1	A	134	ILE	2.9
1	B	951	VAL	2.9
1	C	951	VAL	2.9
1	C	463	ARG	2.8
1	C	947	LEU	2.8
1	A	462	ILE	2.8
1	D	462	ILE	2.8
1	B	570	MET	2.8
1	C	357	MET	2.8
1	C	713	ALA	2.8
1	C	906	PHE	2.7
1	A	1105	ILE	2.7
1	D	135	PRO	2.7
1	C	1038	GLY	2.7
1	C	204	LYS	2.7
1	B	128	LEU	2.7
1	D	1145	ARG	2.7
1	A	941	THR	2.7
1	A	1102	PRO	2.6
1	C	953	PHE	2.6
1	D	120	ILE	2.6
1	C	881	GLY	2.6
1	D	206	VAL	2.6
1	B	940	LEU	2.6
1	D	793	ASN	2.6
1	D	822	SER	2.6
1	C	118	ASP	2.5
1	D	1111	MET	2.5
1	A	42	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	934	LEU	2.5
1	C	1087	ILE	2.5
1	B	892	LEU	2.5
1	B	119	LYS	2.5
1	B	1111	MET	2.5
1	A	834	GLY	2.5
1	B	834	GLY	2.5
1	A	248	ASN	2.4
1	A	1111	MET	2.4
1	B	849	LEU	2.4
1	C	1082	MET	2.4
1	D	210	LYS	2.4
1	C	117	GLY	2.4
1	D	947	LEU	2.4
1	A	357	MET	2.4
1	A	1109	MET	2.4
1	B	887	MET	2.4
1	B	204	LYS	2.4
1	D	1108	ALA	2.4
1	C	835	GLY	2.3
1	B	974	ILE	2.3
1	D	940	LEU	2.3
1	C	207	MET	2.3
1	C	447	THR	2.3
1	C	919	GLY	2.3
1	C	1068	ARG	2.3
1	D	207	MET	2.3
1	A	127	LEU	2.3
1	B	135	PRO	2.3
1	B	463	ARG	2.3
1	B	938	THR	2.3
1	B	120	ILE	2.3
1	C	892	LEU	2.3
1	D	1105	ILE	2.3
1	C	915	MET	2.3
1	B	963	LYS	2.3
1	C	42	PHE	2.3
1	B	929	LEU	2.2
1	A	1119	PHE	2.2
1	C	925	PHE	2.2
1	A	208	ASN	2.2
1	B	898	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	127	LEU	2.2
1	D	819	ALA	2.2
1	B	1109	MET	2.2
1	B	823	PRO	2.2
1	A	221	HIS	2.2
1	D	0	MET	2.2
1	C	870	ILE	2.2
1	C	682	ASP	2.2
1	C	956	VAL	2.1
1	B	238	HIS	2.1
1	B	339	HIS	2.1
1	B	665	ALA	2.1
1	A	1133	THR	2.1
1	C	201	TYR	2.1
1	B	1110	LYS	2.1
1	B	915	MET	2.1
1	A	1038	GLY	2.1
1	C	931	LYS	2.1
1	D	1075	PRO	2.1
1	C	889	GLN	2.1
1	A	819	ALA	2.1
1	B	941	THR	2.1
1	B	664	GLU	2.1
1	B	926	PRO	2.1
1	C	1060	VAL	2.1
1	C	1066	ALA	2.1
1	C	444	ASN	2.1
1	B	1073	THR	2.1
1	D	248	ASN	2.0
1	C	120	ILE	2.0
1	C	464	ASP	2.0
1	B	1061	GLN	2.0
1	A	1097	VAL	2.0
1	B	1145	ARG	2.0
1	B	819	ALA	2.0
1	B	899	GLU	2.0
1	C	128	LEU	2.0
1	C	248	ASN	2.0
1	A	1106	THR	2.0
1	B	1072	THR	2.0
1	C	1072	THR	2.0
1	B	1082	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	-1	HIS	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](#)

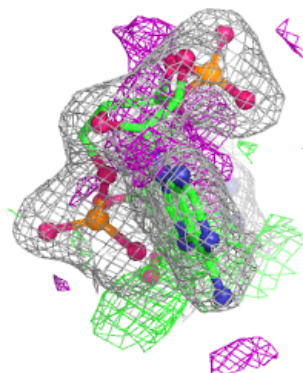
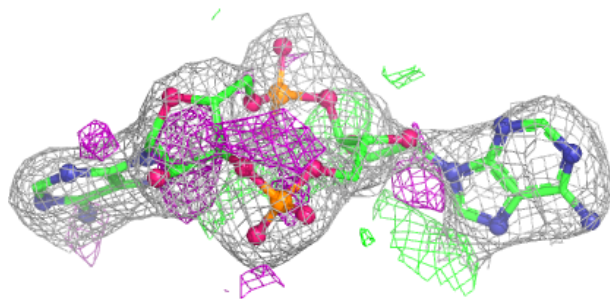
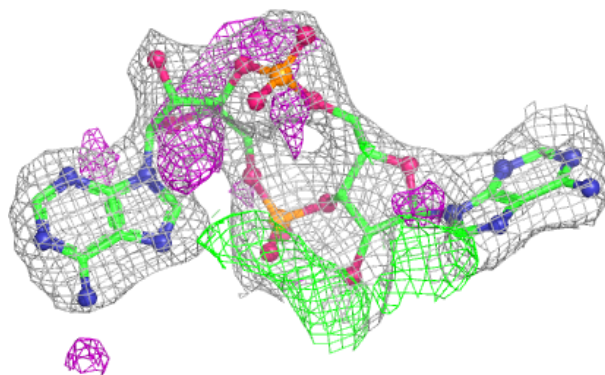
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	2BA	A	2004	44/44	0.83	0.13	35,71,86,94	0
2	FLC	B	2001	13/13	0.86	0.11	46,53,59,69	0
2	FLC	C	1202	13/13	0.88	0.10	47,54,59,62	0
2	FLC	A	2001	13/13	0.90	0.10	43,55,59,62	0
2	FLC	D	2001	13/13	0.92	0.08	41,46,56,59	0
3	MN	B	2002	1/1	0.93	0.08	94,94,94,94	0
3	MN	A	2002	1/1	0.93	0.07	72,72,72,72	0
3	MN	D	2002	1/1	0.95	0.07	75,75,75,75	0
3	MN	C	1203	1/1	0.97	0.05	85,85,85,85	0
4	2BA	C	1201	44/44	0.97	0.07	33,49,59,65	0
4	2BA	A	2003	44/44	0.98	0.05	21,32,38,44	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.

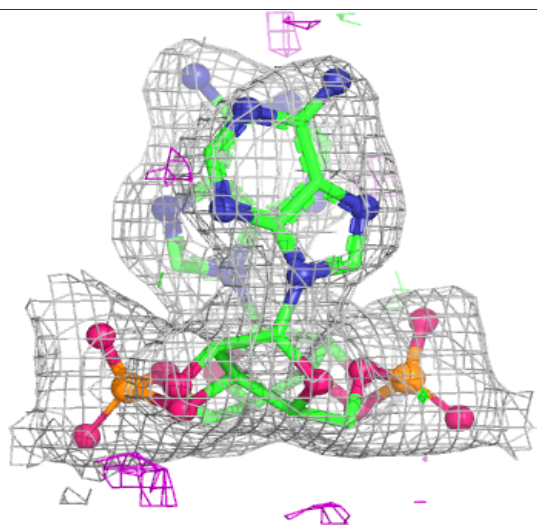
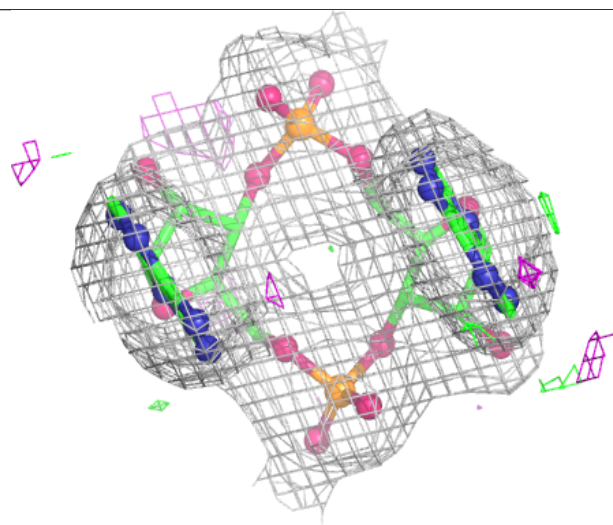
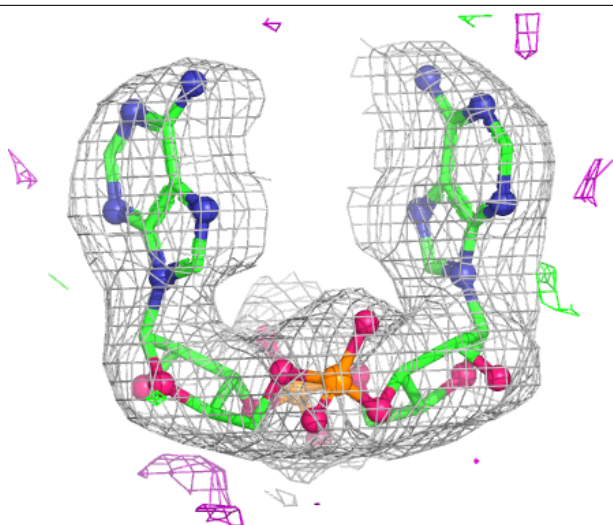
Electron density around 2BA A 2004:

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



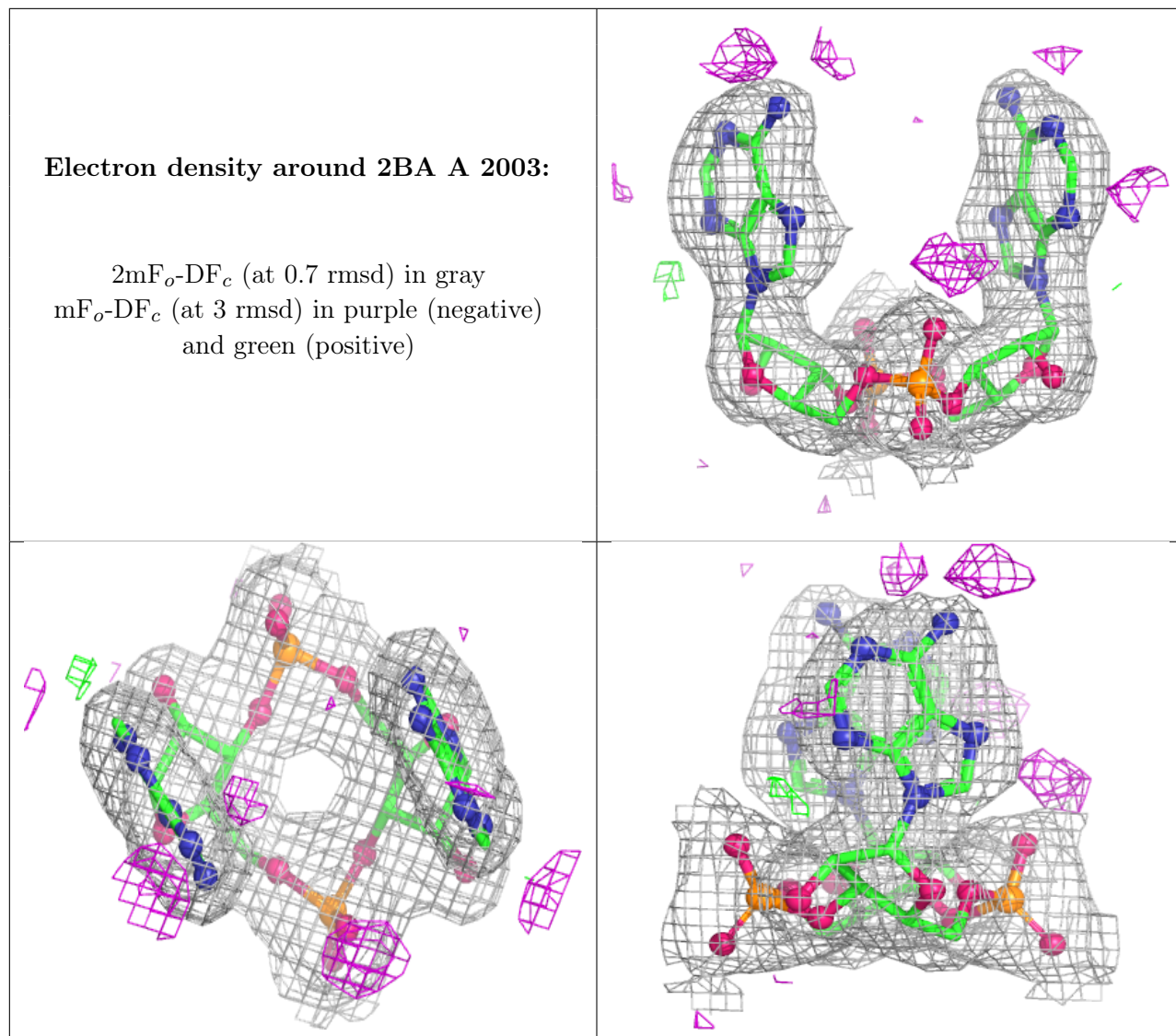
Electron density around 2BA C 1201:

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



Electron density around 2BA A 2003:

$2mF_o-DF_c$ (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.