



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:23 AM UTC

PDB ID : 4QSK / pdb_00004qsk
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 : 2.70 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

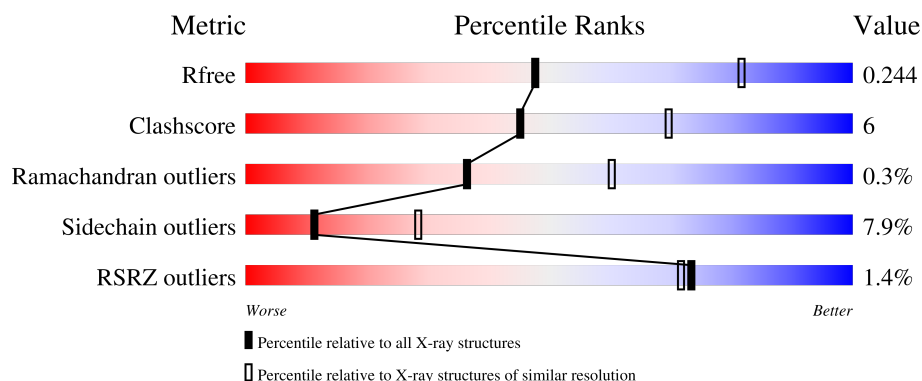
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

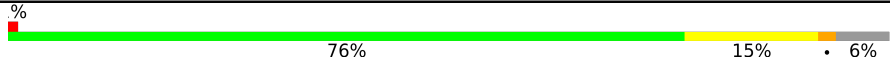
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1147	
1	B	1147	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16959 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.

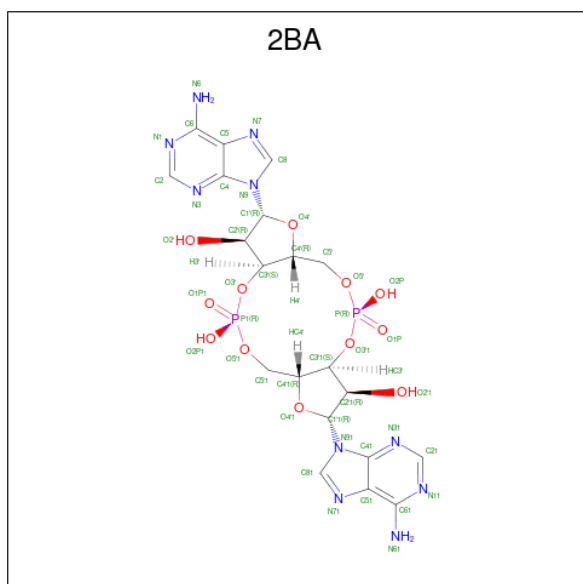
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1073	Total	C	N	O	S	0	0	0
			8438	5355	1433	1609	41			
1	B	1073	Total	C	N	O	S	0	0	0
			8449	5362	1433	1613	41			

There are 2 discrepancies between the modelled and reference sequences:

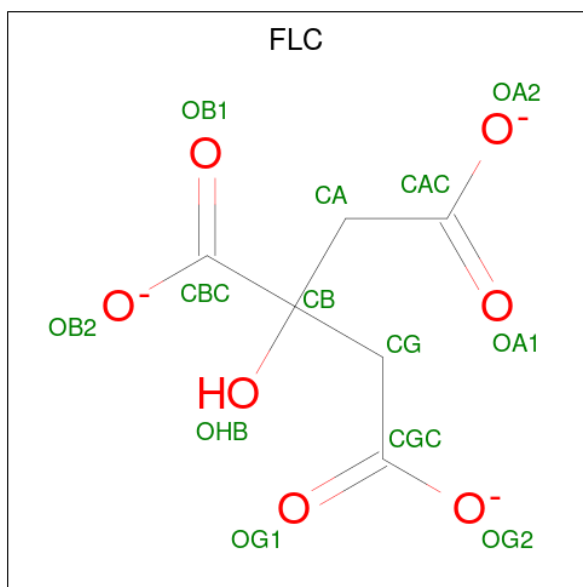
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP W6G6F5
B	0	MET	-	expression tag	UNP W6G6F5

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



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

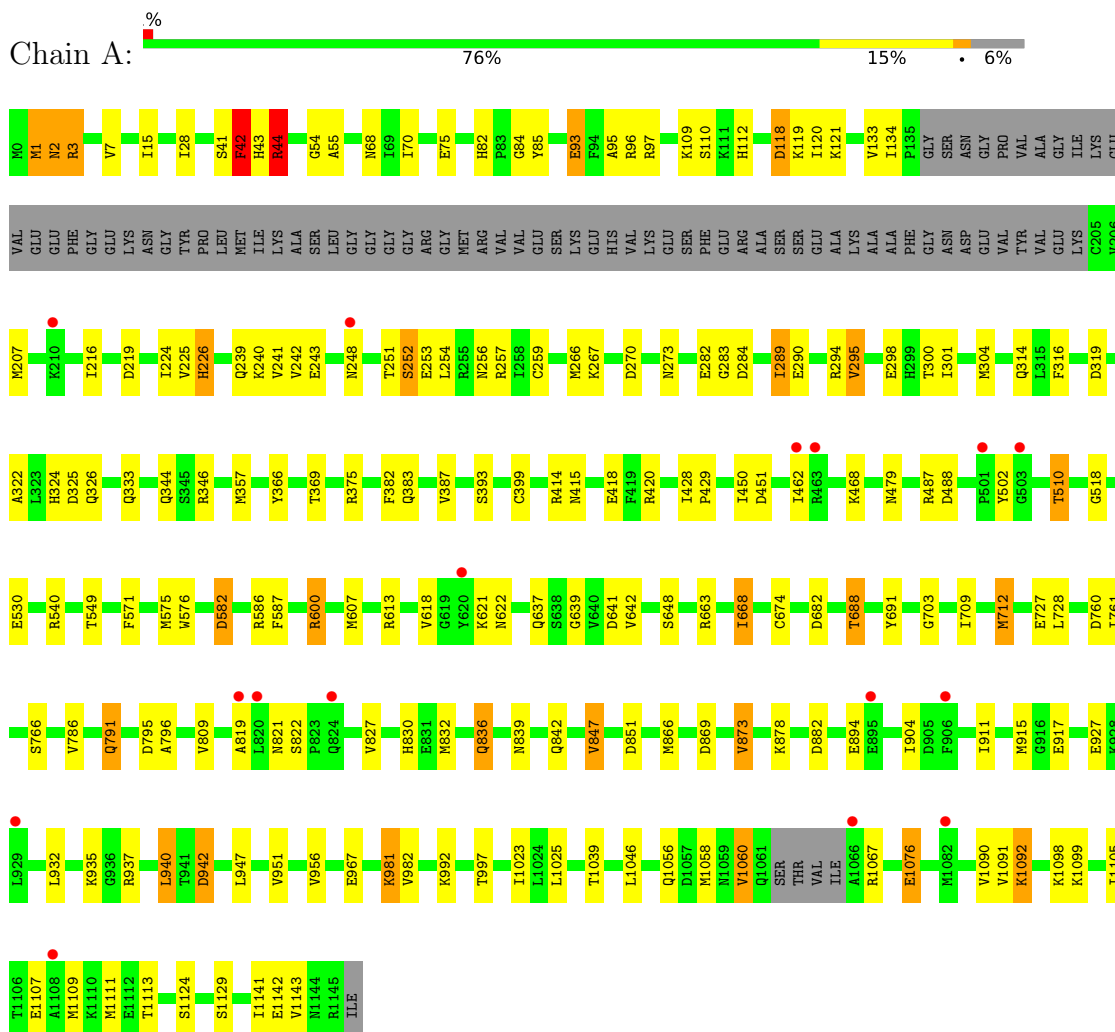
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

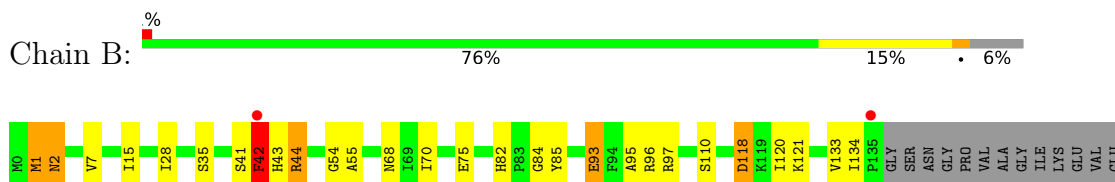
3 Residue-property plots

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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.00Å 146.86Å 96.06Å 90.00° 103.54° 90.00°	Depositor
Resolution (Å)	45.68 – 2.70 45.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.68-2.70) 97.1 (45.68-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.198 , 0.242 0.198 , 0.244	Depositor DCC
R_{free} test set	4086 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16959	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: 2BA, MN, 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	0.85	1/8605 (0.0%)	1.03	12/11659 (0.1%)
1	B	0.93	4/8616 (0.0%)	1.06	22/11673 (0.2%)
All	All	0.89	5/17221 (0.0%)	1.04	34/23332 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	ARG	CA-C	6.37	1.61	1.52
1	B	706	ILE	C-O	-5.37	1.18	1.24
1	A	44	ARG	CA-C	5.33	1.60	1.52
1	B	930	GLN	N-CA	5.25	1.52	1.46
1	B	823	PRO	CA-C	5.04	1.58	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	VAL	N-CA-C	-6.39	106.90	113.10
1	B	802	ILE	N-CA-C	-6.38	104.29	110.42
1	B	42	PHE	CB-CA-C	6.19	122.93	109.99
1	B	1001	THR	CA-C-N	-5.89	112.51	119.05
1	B	1001	THR	C-N-CA	-5.89	112.51	119.05
1	A	518	GLY	CA-C-N	5.88	126.02	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	GLY	C-N-CA	5.88	126.02	119.32
1	B	618	VAL	N-CA-C	-5.85	107.43	113.10
1	B	42	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	911	ILE	N-CA-C	-5.76	104.89	110.42
1	B	809	VAL	N-CA-C	5.64	116.37	110.62
1	A	42	PHE	CB-CA-C	5.61	121.11	109.95
1	A	1023	ILE	N-CA-C	5.58	116.52	108.48
1	B	822	SER	CA-C-N	-5.55	114.23	119.89
1	B	822	SER	C-N-CA	-5.55	114.23	119.89
1	A	822	SER	CA-C-N	-5.53	114.26	119.90
1	A	822	SER	C-N-CA	-5.53	114.26	119.90
1	B	529	GLN	N-CA-C	5.52	117.70	109.59
1	B	911	ILE	N-CA-C	-5.52	105.34	110.53
1	B	688	THR	CB-CA-C	-5.43	101.11	111.48
1	A	42	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	1033	GLU	CA-C-N	-5.33	114.85	120.66
1	B	1033	GLU	C-N-CA	-5.33	114.85	120.66
1	A	1060	VAL	N-CA-C	5.32	116.38	108.23
1	B	585	TYR	N-CA-C	-5.29	104.95	111.40
1	A	809	VAL	N-CA-C	5.25	115.97	110.62
1	B	982	VAL	N-CA-CB	5.16	120.11	110.77
1	B	518	GLY	CA-C-N	5.14	125.18	119.32
1	B	518	GLY	C-N-CA	5.14	125.18	119.32
1	B	507	SER	CA-C-N	-5.11	114.69	119.85
1	B	507	SER	C-N-CA	-5.11	114.69	119.85
1	A	688	THR	CB-CA-C	-5.11	101.72	111.48
1	B	1023	ILE	N-CA-C	5.07	115.78	108.48
1	B	1143	VAL	N-CA-C	5.03	113.62	106.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	621	LYS	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	8438	0	8361	104	0
1	B	8449	0	8378	97	0
2	A	22	0	11	0	1
2	B	22	0	11	0	1
3	A	13	0	5	0	0
3	B	13	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	16959	0	16771	198	2

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 6.

All (198) 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	1.33	1.06
1:B:304:MET:HE1	1:B:399:CYS:HB3	1.35	1.04
1:B:582:ASP:OD2	1:B:586:ARG:NH1	2.01	0.92
1:A:582:ASP:OD2	1:A:586:ARG:NH1	2.03	0.91
1:A:663:ARG:NH1	1:A:703:GLY:O	2.13	0.81
1:B:663:ARG:NH1	1:B:703:GLY:O	2.14	0.80
1:B:510:THR:HG21	1:B:571:PHE:O	1.82	0.80
1:A:904:ILE:O	1:A:935:LYS:NZ	2.14	0.80
1:A:510:THR:HG21	1:A:571:PHE:O	1.86	0.76
1:A:304:MET:HE1	1:A:399:CYS:CB	2.14	0.76
1:B:304:MET:HE1	1:B:399:CYS:CB	2.15	0.73
1:B:644:ARG:NH1	1:B:670:GLU:OE2	2.21	0.72
1:B:42:PHE:HB3	1:B:382:PHE:CE1	2.25	0.72
1:A:226:HIS:CD2	1:A:259:CYS:HB3	2.25	0.72
1:B:226:HIS:CD2	1:B:259:CYS:HB3	2.25	0.71
1:A:295:VAL:HG22	1:A:314:GLN:NE2	2.06	0.70
1:A:366:TYR:H	1:A:383:GLN:HE21	1.40	0.69
1:B:819:ALA:O	1:B:821:ASN:ND2	2.25	0.69
1:B:616:ASN:HB3	1:B:621:LYS:O	1.93	0.69
1:A:42:PHE:HB3	1:A:382:PHE:CE1	2.28	0.68
1:A:819:ALA:O	1:A:821:ASN:ND2	2.26	0.68
1:B:295:VAL:HG22	1:B:314:GLN:NE2	2.08	0.68
1:A:607:MET:HE1	1:A:668:ILE:HD12	1.75	0.68
1:A:674:CYS:HB3	1:A:712:MET:HE1	1.74	0.68
1:A:942:ASP:N	1:A:942:ASP:OD1	2.27	0.68
1:B:366:TYR:H	1:B:383:GLN:HE21	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:LEU:O	1:A:935:LYS:HE3	1.95	0.67
1:B:830:HIS:HD2	1:B:832:MET:H	1.42	0.67
1:A:674:CYS:CB	1:A:712:MET:HE1	2.24	0.67
1:A:830:HIS:HD2	1:A:832:MET:H	1.43	0.67
1:B:607:MET:HE1	1:B:668:ILE:HD12	1.76	0.67
1:A:93:GLU:O	1:A:97:ARG:HB2	1.95	0.66
1:A:54:GLY:H	1:A:68:ASN:HD22	1.43	0.66
1:B:93:GLU:O	1:B:97:ARG:HB2	1.97	0.64
1:B:674:CYS:HB3	1:B:712:MET:HE1	1.77	0.64
1:B:674:CYS:CB	1:B:712:MET:HE1	2.26	0.64
1:A:82:HIS:HD2	1:A:84:GLY:H	1.46	0.64
1:B:942:ASP:N	1:B:942:ASP:OD1	2.31	0.64
1:B:82:HIS:HD2	1:B:84:GLY:H	1.46	0.64
1:A:607:MET:HE1	1:A:668:ILE:CD1	2.28	0.64
1:B:54:GLY:H	1:B:68:ASN:HD22	1.46	0.64
1:B:607:MET:HE1	1:B:668:ILE:CD1	2.28	0.63
1:B:253:GLU:OE2	1:B:257:ARG:HD3	1.97	0.63
1:A:253:GLU:OE2	1:A:257:ARG:HD3	1.98	0.62
1:B:118:ASP:HB3	1:B:121:LYS:HG3	1.82	0.62
1:B:252:SER:O	1:B:256:ASN:ND2	2.31	0.61
1:B:420:ARG:NH1	3:B:1203:FLC:OA1	2.32	0.61
1:A:295:VAL:HG22	1:A:314:GLN:HE22	1.65	0.60
1:A:252:SER:O	1:A:256:ASN:ND2	2.33	0.59
1:B:226:HIS:H	1:B:333:GLN:HE22	1.49	0.59
1:B:54:GLY:O	1:B:55:ALA:C	2.46	0.58
1:B:2:ASN:HB2	1:B:319:ASP:OD2	2.04	0.57
1:B:709:ILE:HD11	1:B:728:LEU:CD1	2.34	0.57
1:A:2:ASN:HB2	1:A:319:ASP:OD2	2.05	0.56
1:A:226:HIS:H	1:A:333:GLN:HE22	1.52	0.56
1:A:369:THR:CG2	1:A:415:ASN:HD22	2.19	0.56
1:A:709:ILE:HD11	1:A:728:LEU:CD1	2.35	0.56
1:B:369:THR:CG2	1:B:415:ASN:HD22	2.18	0.56
1:B:295:VAL:HG22	1:B:314:GLN:HE22	1.69	0.56
1:B:847:VAL:CG1	1:B:847:VAL:O	2.53	0.56
1:A:847:VAL:CG1	1:A:847:VAL:O	2.54	0.56
1:B:878:LYS:NZ	1:B:882:ASP:OD2	2.39	0.55
1:B:243:GLU:OE2	1:B:346:ARG:NH2	2.39	0.55
1:A:369:THR:HG21	1:A:415:ASN:HD22	1.72	0.55
1:B:369:THR:HG21	1:B:415:ASN:HD22	1.72	0.55
1:A:82:HIS:HE1	1:A:314:GLN:OE1	1.89	0.55
1:A:298:GLU:N	1:A:298:GLU:OE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ASN:ND2	1:A:917:GLU:O	2.41	0.53
1:B:607:MET:HE2	1:B:642:VAL:HG23	1.89	0.53
1:A:674:CYS:SG	1:A:712:MET:HE1	2.48	0.53
1:A:878:LYS:NZ	1:A:882:ASP:OD2	2.42	0.53
1:A:243:GLU:OE2	1:A:346:ARG:NH2	2.41	0.53
1:B:118:ASP:CB	1:B:121:LYS:HG3	2.39	0.53
1:A:3:ARG:NH1	1:A:319:ASP:O	2.41	0.52
1:B:298:GLU:O	1:B:301:ILE:HG12	2.09	0.52
1:A:607:MET:HE2	1:A:642:VAL:HG23	1.89	0.52
1:B:82:HIS:HE1	1:B:314:GLN:OE1	1.92	0.52
1:B:298:GLU:N	1:B:298:GLU:OE2	2.42	0.52
1:A:82:HIS:CE1	1:A:314:GLN:OE1	2.63	0.52
1:B:468:LYS:HG2	1:B:992:LYS:O	2.09	0.51
1:A:15:ILE:HB	1:A:85:TYR:CE2	2.45	0.51
1:A:298:GLU:O	1:A:301:ILE:HG12	2.11	0.51
1:B:836:GLN:O	1:B:836:GLN:HG3	2.10	0.50
1:A:468:LYS:HG2	1:A:992:LYS:O	2.10	0.50
1:A:118:ASP:HB3	1:A:121:LYS:HG2	1.92	0.50
1:A:479:ASN:HD21	1:A:1058:MET:H	1.60	0.50
1:B:82:HIS:CE1	1:B:314:GLN:OE1	2.64	0.50
1:B:674:CYS:SG	1:B:712:MET:HE1	2.51	0.50
1:A:836:GLN:O	1:A:836:GLN:HG3	2.11	0.50
1:A:915:MET:O	1:A:940:LEU:HD12	2.12	0.50
1:A:510:THR:HG23	1:A:607:MET:HG3	1.93	0.50
1:A:915:MET:O	1:A:940:LEU:CD1	2.60	0.49
1:B:479:ASN:HD21	1:B:1058:MET:H	1.61	0.49
1:A:600:ARG:NH2	1:A:641:ASP:OD2	2.45	0.49
1:A:54:GLY:O	1:A:55:ALA:C	2.56	0.49
1:B:586:ARG:HD3	1:B:587:PHE:CZ	2.47	0.49
1:B:760:ASP:C	1:B:761:ILE:HG13	2.38	0.49
1:B:600:ARG:NH2	1:B:641:ASP:OD2	2.46	0.48
1:A:95:ALA:O	1:A:96:ARG:C	2.56	0.48
1:B:607:MET:HE2	1:B:642:VAL:CG2	2.43	0.48
1:A:760:ASP:C	1:A:761:ILE:HG13	2.40	0.47
1:A:241:VAL:HG12	1:A:242:VAL:HG23	1.94	0.47
1:A:607:MET:HE2	1:A:642:VAL:CG2	2.44	0.47
1:B:95:ALA:O	1:B:96:ARG:C	2.56	0.47
1:A:289:ILE:HG13	1:A:290:GLU:HB2	1.95	0.47
1:B:15:ILE:HB	1:B:85:TYR:CE2	2.49	0.47
1:B:133:VAL:HG12	1:B:134:ILE:N	2.30	0.47
1:A:133:VAL:HG12	1:A:134:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:ASN:ND2	1:B:917:GLU:O	2.43	0.47
1:B:241:VAL:HG12	1:B:242:VAL:HG23	1.95	0.46
1:A:1090:VAL:HG12	1:A:1090:VAL:O	2.16	0.46
1:B:324:HIS:O	1:B:325:ASP:C	2.59	0.46
1:B:289:ILE:HG13	1:B:290:GLU:HB2	1.97	0.46
1:B:1090:VAL:HG12	1:B:1090:VAL:O	2.16	0.46
1:B:510:THR:HG23	1:B:607:MET:HG3	1.98	0.45
1:B:847:VAL:O	1:B:847:VAL:HG12	2.15	0.45
1:A:225:VAL:CG1	1:A:226:HIS:N	2.80	0.45
1:A:942:ASP:OD2	1:A:947:LEU:HD21	2.17	0.45
1:B:1124:SER:HB3	1:B:1142:GLU:HB3	1.99	0.45
1:A:600:ARG:HG2	1:A:639:GLY:HA3	1.99	0.45
1:B:96:ARG:HH11	1:B:96:ARG:HG2	1.82	0.45
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.82	0.45
1:A:786:VAL:O	1:A:791:GLN:NE2	2.48	0.45
1:A:847:VAL:O	1:A:847:VAL:HG12	2.16	0.45
1:B:225:VAL:CG1	1:B:226:HIS:N	2.81	0.44
1:B:369:THR:OG1	1:B:415:ASN:ND2	2.50	0.44
1:A:324:HIS:O	1:A:325:ASP:C	2.61	0.44
1:A:1:MET:HE3	1:A:319:ASP:HB2	2.00	0.44
1:A:1098:LYS:O	1:A:1099:LYS:C	2.60	0.44
1:A:1124:SER:HB3	1:A:1142:GLU:HB3	2.00	0.44
1:A:41:SER:OG	1:A:43:HIS:HD2	2.00	0.44
1:A:1046:LEU:C	1:A:1046:LEU:HD23	2.43	0.44
1:B:300:THR:HG22	1:B:375:ARG:CZ	2.47	0.44
1:B:786:VAL:O	1:B:791:GLN:NE2	2.50	0.43
1:B:620:TYR:CZ	1:B:621:LYS:HD3	2.53	0.43
1:A:502:TYR:CE1	1:B:75:GLU:HG2	2.53	0.43
1:B:219:ASP:OD2	1:B:322:ALA:HA	2.18	0.43
1:A:575:MET:C	1:A:575:MET:SD	3.02	0.43
1:B:224:ILE:HD12	1:B:267:LYS:HA	2.00	0.43
1:B:1076:GLU:HG3	1:B:1143:VAL:O	2.19	0.43
1:A:44:ARG:NH2	1:B:1015:GLU:OE2	2.51	0.43
1:A:3:ARG:NH1	1:A:3:ARG:HB2	2.34	0.43
1:B:41:SER:OG	1:B:43:HIS:HD2	2.01	0.43
1:B:544:GLN:HG3	1:B:549:THR:OG1	2.19	0.43
1:B:1039:THR:HA	1:B:1056:GLN:HA	2.00	0.43
1:B:1:MET:HE3	1:B:319:ASP:HB2	2.01	0.43
1:A:240:LYS:HB2	1:A:346:ARG:HH22	1.84	0.43
1:A:301:ILE:HA	1:A:304:MET:HE3	2.00	0.43
1:B:295:VAL:CG2	1:B:314:GLN:HE22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:THR:HG22	1:A:375:ARG:CZ	2.49	0.42
1:A:344:GLN:HG3	1:A:399:CYS:SG	2.59	0.42
1:A:75:GLU:HG2	1:B:502:TYR:CE1	2.54	0.42
1:A:414:ARG:NH1	1:A:418:GLU:OE1	2.50	0.42
1:B:1:MET:HE1	1:B:316:PHE:CD1	2.54	0.42
1:B:240:LYS:HB2	1:B:346:ARG:HH22	1.85	0.42
1:B:729:LYS:HD3	1:B:736:ILE:HD12	2.02	0.42
1:A:7:VAL:HG23	1:A:28:ILE:HG21	2.00	0.42
1:B:600:ARG:HG2	1:B:639:GLY:HA3	2.01	0.42
1:A:207:MET:HB2	1:A:282:GLU:OE2	2.20	0.42
1:A:795:ASP:O	1:A:796:ALA:C	2.63	0.42
1:B:7:VAL:HG23	1:B:28:ILE:HG21	2.00	0.42
1:A:981:LYS:HB2	1:A:981:LYS:HE3	1.88	0.42
1:A:1076:GLU:HG3	1:A:1143:VAL:O	2.20	0.42
1:B:1098:LYS:O	1:B:1099:LYS:C	2.62	0.42
1:A:224:ILE:HD12	1:A:267:LYS:HA	2.01	0.41
1:A:830:HIS:CD2	1:A:832:MET:HG3	2.55	0.41
1:A:866:MET:SD	1:A:894:GLU:HG3	2.60	0.41
1:B:616:ASN:CB	1:B:621:LYS:O	2.63	0.41
1:A:219:ASP:OD2	1:A:322:ALA:HA	2.19	0.41
1:A:369:THR:OG1	1:A:415:ASN:ND2	2.53	0.41
1:A:586:ARG:HD3	1:A:587:PHE:CZ	2.54	0.41
1:B:344:GLN:HG3	1:B:399:CYS:SG	2.61	0.41
1:B:414:ARG:NH1	1:B:418:GLU:OE1	2.52	0.41
1:B:830:HIS:CD2	1:B:832:MET:HG3	2.55	0.41
1:A:1039:THR:HA	1:A:1056:GLN:HA	2.02	0.41
1:B:575:MET:C	1:B:575:MET:SD	3.04	0.41
1:B:591:ASP:HA	1:B:592:PRO:HD2	1.92	0.41
1:A:226:HIS:NE2	1:A:259:CYS:HB3	2.35	0.41
1:A:295:VAL:CG2	1:A:314:GLN:HE22	2.29	0.41
1:B:226:HIS:NE2	1:B:259:CYS:HB3	2.35	0.41
1:A:109:LYS:H	1:A:112:HIS:HD2	1.69	0.41
1:B:688:THR:O	1:B:691:TYR:HB3	2.20	0.41
1:B:740:THR:HG22	1:B:751:TYR:CE1	2.55	0.41
1:B:874:THR:HA	1:B:875:PRO:HA	1.91	0.41
1:A:1:MET:HE1	1:A:316:PHE:CD1	2.56	0.41
1:B:207:MET:HB2	1:B:282:GLU:OE2	2.21	0.41
1:B:288:PHE:CD1	1:B:288:PHE:C	2.98	0.41
1:B:866:MET:SD	1:B:894:GLU:HG3	2.61	0.41
1:A:1091:VAL:C	1:A:1092:LYS:HD2	2.46	0.41
1:A:118:ASP:CB	1:A:121:LYS:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HG13	1:A:266:MET:HG3	2.04	0.40
1:A:282:GLU:O	1:A:284:ASP:N	2.54	0.40
1:A:428:ILE:O	1:A:429:PRO:C	2.64	0.40
1:A:688:THR:O	1:A:691:TYR:HB3	2.21	0.40
1:A:648:SER:HA	1:A:873:VAL:HG13	2.03	0.40
1:A:540:ARG:HD2	1:A:540:ARG:C	2.47	0.40
1:A:487:ARG:O	1:A:488:ASP:C	2.65	0.40
1:B:35:SER:OG	1:B:391:TYR:OH	2.38	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2000:2BA:P	2:A:2000:2BA:O3'[2_757]	1.79	0.41
2:B:1202:2BA:P	2:B:1202:2BA:O3'[2_757]	1.82	0.38

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	1067/1147 (93%)	1004 (94%)	60 (6%)	3 (0%)	36	60
1	B	1067/1147 (93%)	1007 (94%)	57 (5%)	3 (0%)	36	60
All	All	2134/2294 (93%)	2011 (94%)	117 (6%)	6 (0%)	36	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	GLY
1	B	283	GLY
1	A	273	ASN
1	B	273	ASN

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Mol	Chain	Res	Type
1	A	869	ASP
1	B	869	ASP

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	917/982 (93%)	845 (92%)	72 (8%)	11	28
1	B	920/982 (94%)	846 (92%)	74 (8%)	11	28
All	All	1837/1964 (94%)	1691 (92%)	146 (8%)	11	28

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASN
1	A	3	ARG
1	A	42	PHE
1	A	44	ARG
1	A	70	ILE
1	A	93	GLU
1	A	110	SER
1	A	118	ASP
1	A	119	LYS
1	A	120	ILE
1	A	226	HIS
1	A	239	GLN
1	A	248	ASN
1	A	251	THR
1	A	252	SER
1	A	254	LEU
1	A	270	ASP
1	A	289	ILE
1	A	294	ARG
1	A	295	VAL

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	357	MET
1	A	387	VAL
1	A	393	SER
1	A	420	ARG
1	A	450	ILE
1	A	451	ASP
1	A	462	ILE
1	A	510	THR
1	A	530	GLU
1	A	549	THR
1	A	576	TRP
1	A	582	ASP
1	A	600	ARG
1	A	613	ARG
1	A	637	GLN
1	A	668	ILE
1	A	682	ASP
1	A	712	MET
1	A	727	GLU
1	A	766	SER
1	A	791	GLN
1	A	827	VAL
1	A	836	GLN
1	A	839	ASN
1	A	842	GLN
1	A	847	VAL
1	A	851	ASP
1	A	873	VAL
1	A	927	GLU
1	A	937	ARG
1	A	940	LEU
1	A	942	ASP
1	A	951	VAL
1	A	956	VAL
1	A	967	GLU
1	A	981	LYS
1	A	982	VAL
1	A	997	THR
1	A	1025	LEU
1	A	1060	VAL
1	A	1067	ARG

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Mol	Chain	Res	Type
1	A	1076	GLU
1	A	1092	LYS
1	A	1105	ILE
1	A	1107	GLU
1	A	1109	MET
1	A	1111	MET
1	A	1113	THR
1	A	1129	SER
1	A	1141	ILE
1	B	1	MET
1	B	2	ASN
1	B	42	PHE
1	B	44	ARG
1	B	70	ILE
1	B	93	GLU
1	B	110	SER
1	B	118	ASP
1	B	120	ILE
1	B	213	GLU
1	B	226	HIS
1	B	239	GLN
1	B	248	ASN
1	B	251	THR
1	B	252	SER
1	B	254	LEU
1	B	270	ASP
1	B	289	ILE
1	B	294	ARG
1	B	295	VAL
1	B	326	GLN
1	B	357	MET
1	B	387	VAL
1	B	393	SER
1	B	420	ARG
1	B	450	ILE
1	B	451	ASP
1	B	462	ILE
1	B	507	SER
1	B	510	THR
1	B	530	GLU
1	B	549	THR
1	B	576	TRP

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Mol	Chain	Res	Type
1	B	582	ASP
1	B	600	ARG
1	B	613	ARG
1	B	616	ASN
1	B	621	LYS
1	B	637	GLN
1	B	668	ILE
1	B	682	ASP
1	B	712	MET
1	B	727	GLU
1	B	766	SER
1	B	791	GLN
1	B	827	VAL
1	B	836	GLN
1	B	839	ASN
1	B	842	GLN
1	B	847	VAL
1	B	851	ASP
1	B	873	VAL
1	B	899	GLU
1	B	927	GLU
1	B	937	ARG
1	B	940	LEU
1	B	942	ASP
1	B	951	VAL
1	B	956	VAL
1	B	967	GLU
1	B	981	LYS
1	B	982	VAL
1	B	997	THR
1	B	1025	LEU
1	B	1060	VAL
1	B	1067	ARG
1	B	1076	GLU
1	B	1105	ILE
1	B	1107	GLU
1	B	1109	MET
1	B	1111	MET
1	B	1113	THR
1	B	1129	SER
1	B	1141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

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	223	ASN
1	A	292	ASN
1	A	312	GLN
1	A	326	GLN
1	A	333	GLN
1	A	383	GLN
1	A	415	ASN
1	A	479	ASN
1	A	602	GLN
1	A	746	ASN
1	A	797	GLN
1	A	804	HIS
1	A	821	ASN
1	A	830	HIS
1	A	890	ASN
1	B	36	GLN
1	B	43	HIS
1	B	68	ASN
1	B	82	HIS
1	B	112	HIS
1	B	223	ASN
1	B	292	ASN
1	B	312	GLN
1	B	326	GLN
1	B	333	GLN
1	B	383	GLN
1	B	415	ASN
1	B	479	ASN
1	B	602	GLN
1	B	746	ASN
1	B	797	GLN
1	B	821	ASN
1	B	830	HIS
1	B	890	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	2BA	B	1202	-	21,24,50	1.59	4 (19%)	30,35,78	1.82	8 (26%)
3	FLC	A	2001	-	12,12,12	1.50	1 (8%)	17,17,17	2.10	7 (41%)
3	FLC	B	1203	-	12,12,12	1.22	0	17,17,17	2.03	4 (23%)
2	2BA	A	2000	-	21,24,50	1.64	5 (23%)	30,35,78	1.94	9 (30%)

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
2	2BA	B	1202	-	-	0/7/25/62	0/3/3/7
3	FLC	A	2001	-	-	2/16/16/16	-
3	FLC	B	1203	-	-	0/16/16/16	-
2	2BA	A	2000	-	-	0/7/25/62	0/3/3/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	2BA	C5-C4	4.28	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1202	2BA	C5-C4	4.11	1.46	1.39
3	A	2001	FLC	CG-CB	3.45	1.58	1.54
2	A	2000	2BA	C5-N7	-3.05	1.33	1.39
2	B	1202	2BA	C8-N7	2.96	1.37	1.31
2	A	2000	2BA	C5-C6	2.62	1.48	1.41
2	B	1202	2BA	C5-N7	-2.58	1.34	1.39
2	B	1202	2BA	C4-N9	-2.45	1.32	1.37
2	A	2000	2BA	C4-N9	-2.26	1.33	1.37
2	A	2000	2BA	C8-N7	2.00	1.35	1.31

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	2BA	C5-C4-N3	-5.51	119.13	126.72
3	B	1203	FLC	OB2-CBC-CB	5.46	123.61	113.14
3	A	2001	FLC	OHB-CB-CA	-4.25	99.67	109.38
2	A	2000	2BA	N3-C4-N9	4.11	134.16	127.17
2	B	1202	2BA	C4-N9-C8	3.99	109.93	105.74
2	A	2000	2BA	C2-N3-C4	3.59	120.59	111.83
2	B	1202	2BA	N3-C4-N9	3.57	133.23	127.17
2	B	1202	2BA	N3-C2-N1	-3.54	123.23	128.58
2	A	2000	2BA	C4-C5-N7	-3.29	106.82	110.58
2	B	1202	2BA	C5-C4-N3	-3.27	122.22	126.72
2	A	2000	2BA	N3-C2-N1	-3.26	123.65	128.58
3	A	2001	FLC	CG-CB-CA	3.25	117.66	109.31
3	B	1203	FLC	OG1-CGC-CG	-3.21	113.86	122.95
3	A	2001	FLC	OB2-CBC-CB	3.13	119.14	113.14
2	B	1202	2BA	C4-N9-C1'	-2.82	120.05	126.63
3	B	1203	FLC	OG2-CGC-CG	2.80	123.23	114.35
2	A	2000	2BA	C5-N7-C8	2.69	107.67	103.45
3	A	2001	FLC	OG2-CGC-CG	2.66	122.77	114.35
3	B	1203	FLC	OB1-CBC-CB	-2.62	117.01	122.09
3	A	2001	FLC	OA2-CAC-CA	2.52	122.34	114.35
2	B	1202	2BA	N9-C8-N7	-2.43	110.49	113.94
2	B	1202	2BA	C2-N3-C4	2.41	117.71	111.83
2	B	1202	2BA	C5-C6-N6	-2.32	117.55	123.29
3	A	2001	FLC	OA2-CAC-OA1	-2.30	117.42	123.33
2	A	2000	2BA	C6-C5-N7	2.18	136.29	132.09
2	A	2000	2BA	N9-C8-N7	-2.14	110.90	113.94
2	A	2000	2BA	C4-N9-C8	2.06	107.90	105.74
3	A	2001	FLC	OG2-CGC-OG1	-2.02	118.13	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

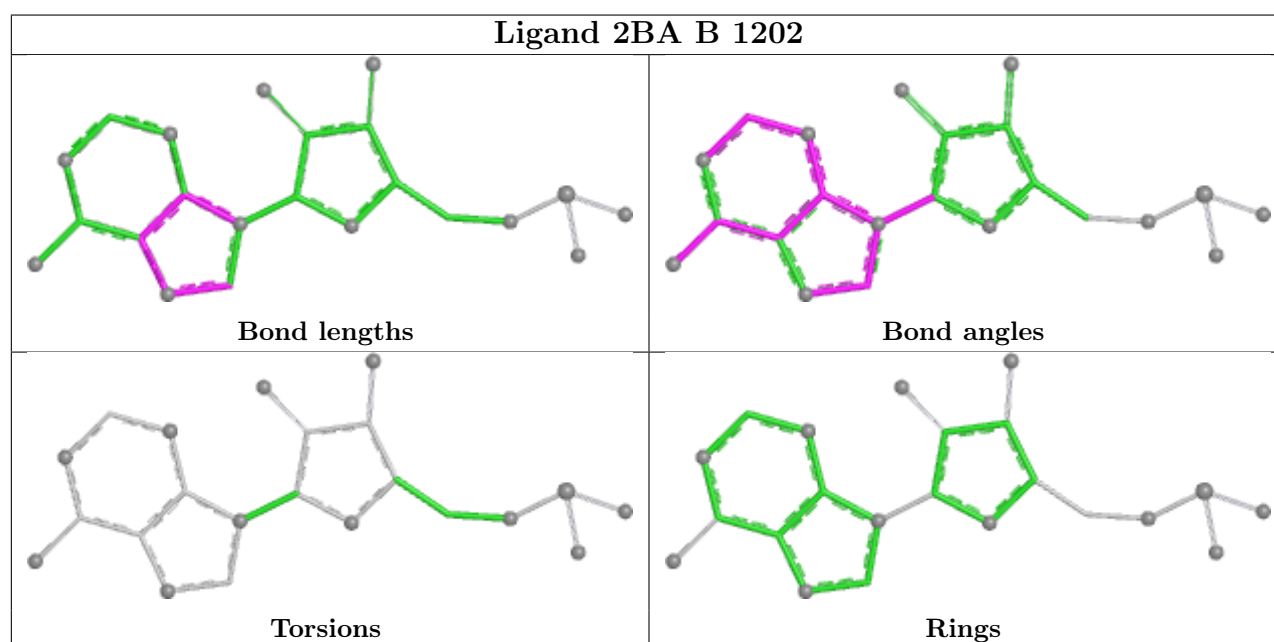
Mol	Chain	Res	Type	Atoms
3	A	2001	FLC	CB-CG-CGC-OG2
3	A	2001	FLC	CB-CG-CGC-OG1

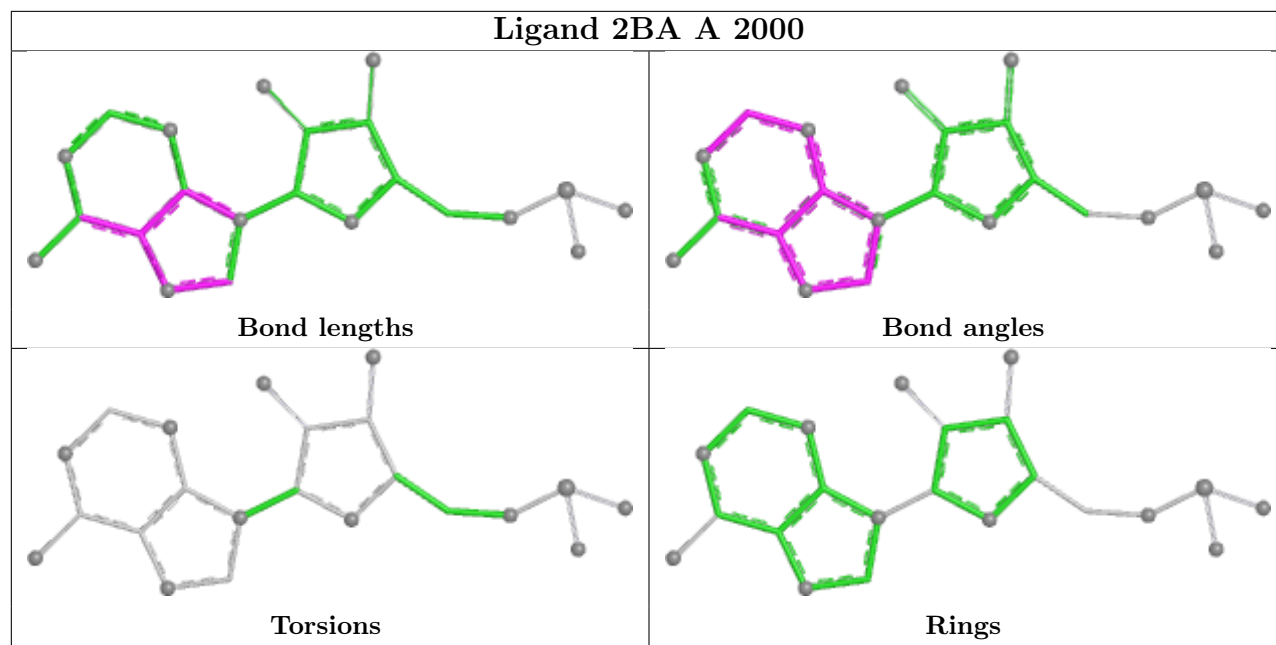
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1202	2BA	0	1
3	B	1203	FLC	1	0
2	A	2000	2BA	0	1

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	1073/1147 (93%)	0.01	16 (1%) 72 70	47, 73, 115, 152	0
1	B	1073/1147 (93%)	-0.18	14 (1%) 75 73	34, 64, 104, 140	0
All	All	2146/2294 (93%)	-0.08	30 (1%) 73 72	34, 68, 109, 152	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	LEU	4.7
1	B	820	LEU	4.0
1	A	462	ILE	3.5
1	B	1108	ALA	3.5
1	A	1108	ALA	3.4
1	A	929	LEU	3.3
1	A	620	TYR	3.2
1	B	501	PRO	3.1
1	A	248	ASN	2.9
1	B	42	PHE	2.9
1	A	501	PRO	2.8
1	B	1066	ALA	2.8
1	A	1066	ALA	2.6
1	B	822	SER	2.4
1	A	824	GLN	2.4
1	B	463	ARG	2.4
1	A	210	LYS	2.4
1	B	1111	MET	2.2
1	A	503	GLY	2.2
1	B	1109	MET	2.2
1	B	135	PRO	2.2
1	B	620	TYR	2.2
1	A	819	ALA	2.1
1	B	248	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	906	PHE	2.1
1	A	463	ARG	2.1
1	A	1082	MET	2.1
1	A	895	GLU	2.0
1	B	824	GLN	2.0
1	B	1145	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

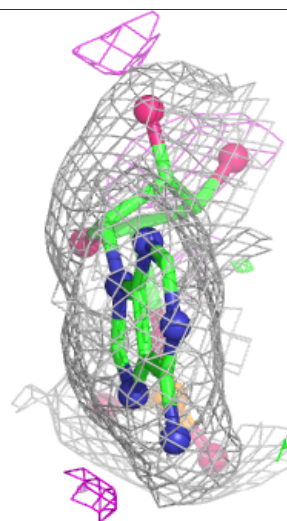
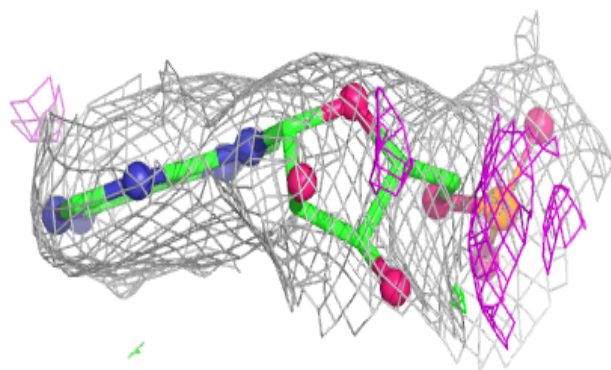
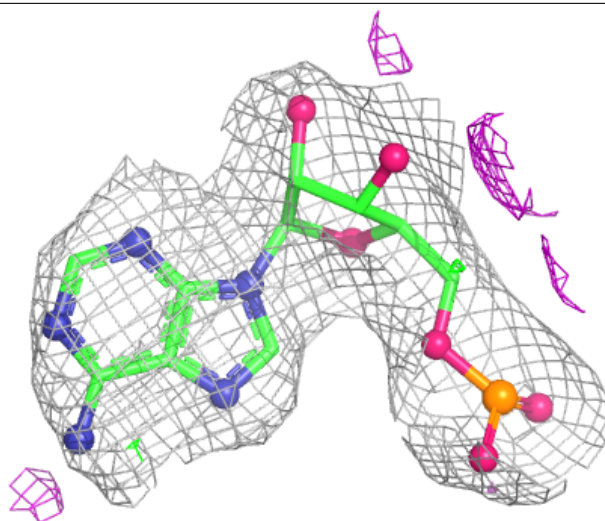
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

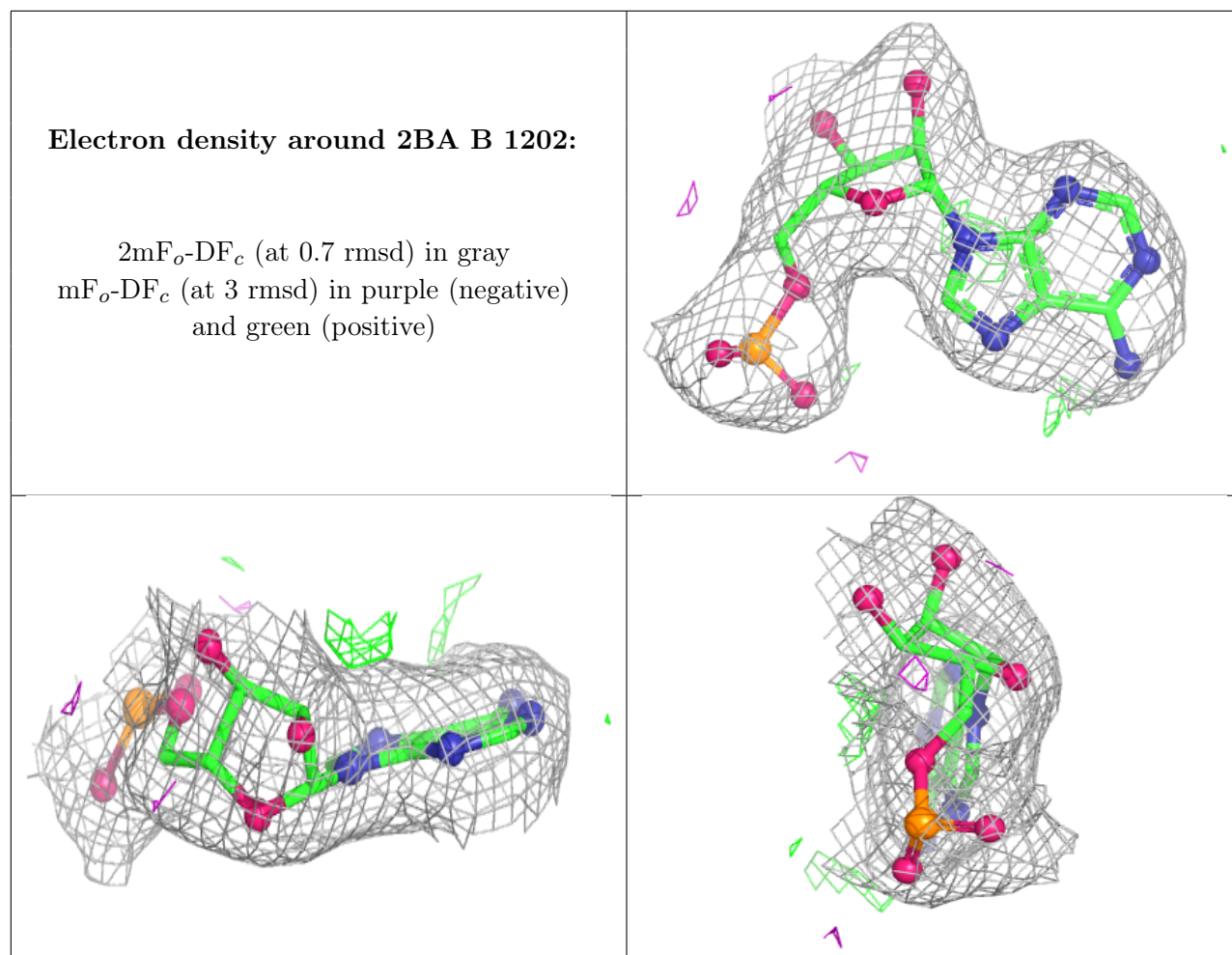
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FLC	A	2001	13/13	0.85	0.10	73,82,88,91	0
3	FLC	B	1203	13/13	0.90	0.10	64,78,86,87	0
2	2BA	A	2000	22/44	0.97	0.07	52,62,76,79	0
2	2BA	B	1202	22/44	0.98	0.06	41,49,53,54	0
4	MN	A	2002	1/1	0.98	0.05	91,91,91,91	0
4	MN	B	1201	1/1	0.99	0.05	65,65,65,65	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 2000:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.