Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 03:44 pm GMT

PDB ID	:	5CR7
Title	:	Human cytosolic 5'-nucleotidase II in complex with N-(9H-Purin-6-yl)-3-(3-pyrrol-1-ylphenyl)benzamide
Authors	:	Aghajari, N.; Preeti, P.
Deposited on	:	2015-07-22
Resolution	:	2.90 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:

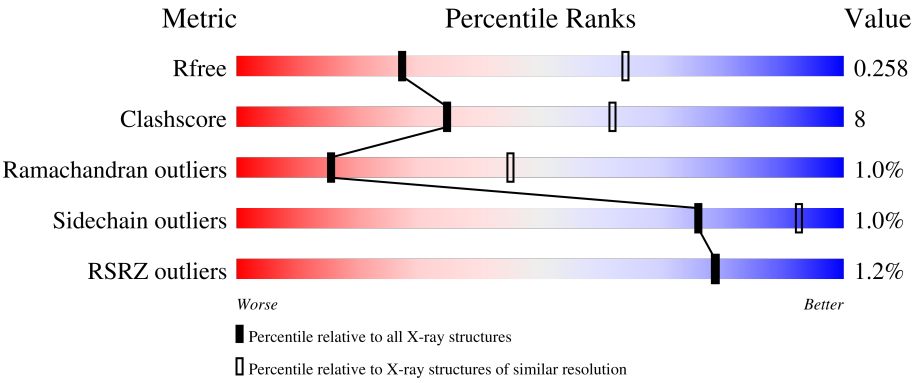
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	554	% 68% 13% •• 17%
1	B	554	% 69% 11% •• 18%

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
3	ACT	A	607	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7854 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 Cytosolic purine 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	4	0
			3757	2428	622	688	19			
1	B	454	Total	C	N	O	S	0	3	0
			3727	2409	617	682	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP P49902
A	-16	SER	-	expression tag	UNP P49902
A	-15	SER	-	expression tag	UNP P49902
A	-14	HIS	-	expression tag	UNP P49902
A	-13	HIS	-	expression tag	UNP P49902
A	-12	HIS	-	expression tag	UNP P49902
A	-11	HIS	-	expression tag	UNP P49902
A	-10	HIS	-	expression tag	UNP P49902
A	-9	HIS	-	expression tag	UNP P49902
A	-8	SER	-	expression tag	UNP P49902
A	-7	SER	-	expression tag	UNP P49902
A	-6	GLY	-	expression tag	UNP P49902
A	-5	LEU	-	expression tag	UNP P49902
A	-4	VAL	-	expression tag	UNP P49902
A	-3	PRO	-	expression tag	UNP P49902
A	-2	ARG	-	expression tag	UNP P49902
A	-1	GLY	-	expression tag	UNP P49902
A	0	SER	-	expression tag	UNP P49902
B	-17	GLY	-	expression tag	UNP P49902
B	-16	SER	-	expression tag	UNP P49902
B	-15	SER	-	expression tag	UNP P49902
B	-14	HIS	-	expression tag	UNP P49902
B	-13	HIS	-	expression tag	UNP P49902
B	-12	HIS	-	expression tag	UNP P49902
B	-11	HIS	-	expression tag	UNP P49902

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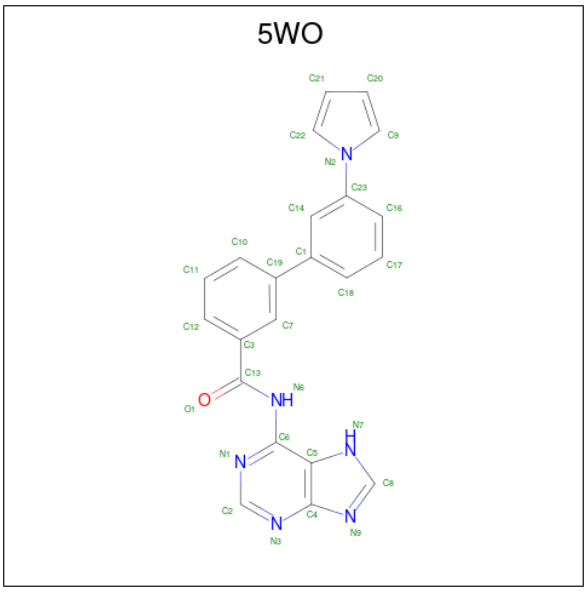
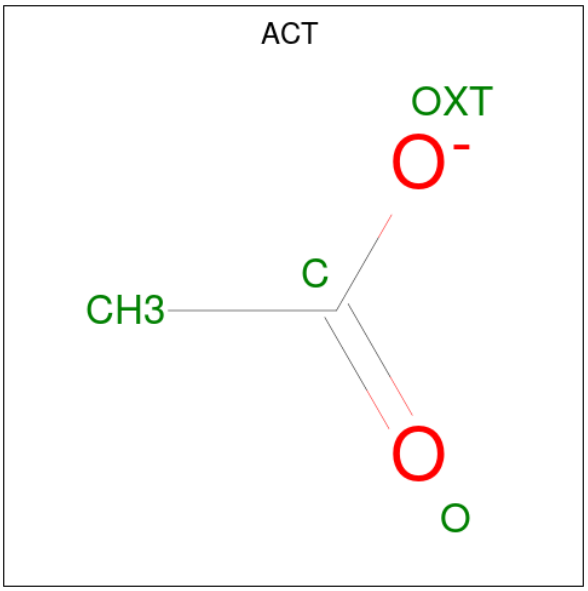
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP P49902
B	-9	HIS	-	expression tag	UNP P49902
B	-8	SER	-	expression tag	UNP P49902
B	-7	SER	-	expression tag	UNP P49902
B	-6	GLY	-	expression tag	UNP P49902
B	-5	LEU	-	expression tag	UNP P49902
B	-4	VAL	-	expression tag	UNP P49902
B	-3	PRO	-	expression tag	UNP P49902
B	-2	ARG	-	expression tag	UNP P49902
B	-1	GLY	-	expression tag	UNP P49902
B	0	SER	-	expression tag	UNP P49902

- Molecule 2 is {N}-(7 {H}-purin-6-yl)-3-(3-pyrrol-1-ylphenyl)benzamide (three-letter code: 5WO) (formula: $C_{22}H_{16}N_6O$).



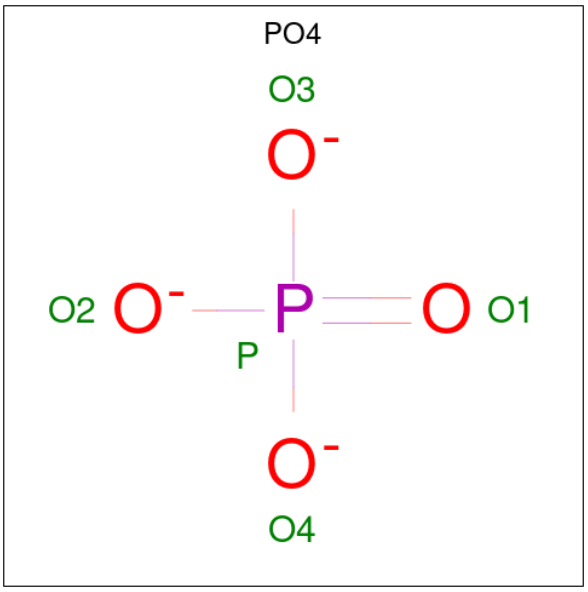
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 29 22 6 1	0	0
2	B	1	Total C N 10 5 5	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

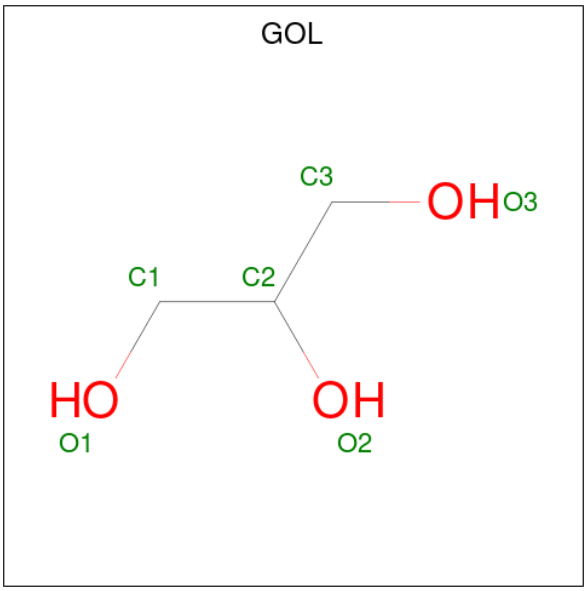


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	127	Total O 127 127	0	0

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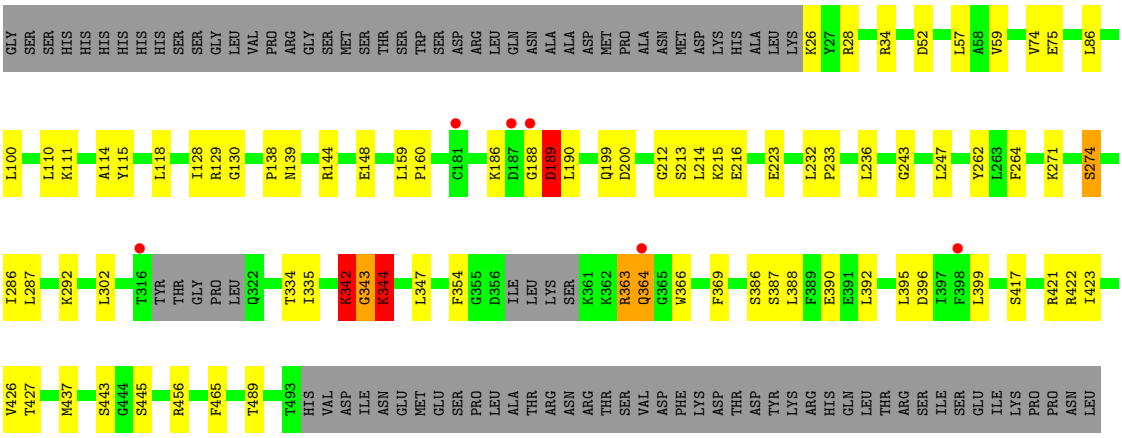
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	71	Total	O	0	0
			71	71		

3 Residue-property plots (i)

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

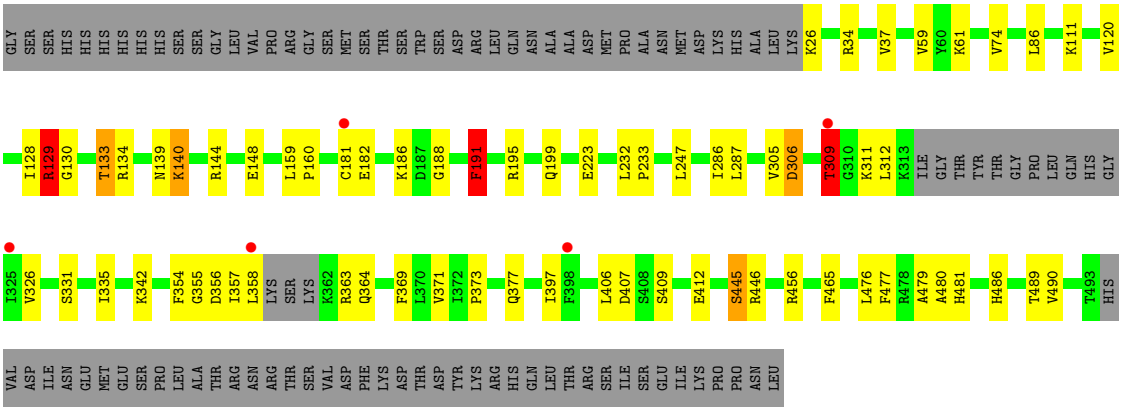
• Molecule 1: Cytosolic purine 5'-nucleotidase

Chain A:



• Molecule 1: Cytosolic purine 5'-nucleotidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.65Å 123.88Å 90.58Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	45.37 – 2.90 45.37 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.37-2.90) 98.3 (45.37-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.265 0.218 , 0.258	Depositor DCC
R_{free} test set	1811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7854	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8443e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACT, MG, PO4, 5WO, GOL

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	0.47	6/3854 (0.2%)	0.67	6/5202 (0.1%)
1	B	0.52	6/3822 (0.2%)	0.65	8/5161 (0.2%)
All	All	0.50	12/7676 (0.2%)	0.66	14/10363 (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	2
1	B	0	4
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	THR	CB-CG2	-15.10	1.02	1.52
1	B	191	PHE	CD2-CE2	-11.69	1.15	1.39
1	A	190	LEU	CG-CD2	-9.37	1.17	1.51
1	A	364	GLN	CB-CG	-9.08	1.28	1.52
1	A	364	GLN	CG-CD	-7.84	1.33	1.51
1	A	342	LYS	CD-CE	7.71	1.70	1.51
1	A	387	SER	CB-OG	7.58	1.52	1.42
1	A	344	LYS	CE-NZ	-6.64	1.32	1.49
1	B	129	ARG	CZ-NH2	-6.07	1.25	1.33
1	B	140	LYS	CD-CE	5.64	1.65	1.51
1	B	140	LYS	CE-NZ	5.19	1.62	1.49
1	B	191	PHE	CA-CB	-5.10	1.42	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	LYS	CD-CE-NZ	13.42	142.57	111.70
1	A	190	LEU	CB-CG-CD2	-13.30	88.38	111.00
1	B	129	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	191	PHE	CB-CG-CD2	-8.61	114.77	120.80
1	A	342	LYS	CG-CD-CE	8.11	136.22	111.90
1	B	309	THR	CA-CB-CG2	-7.80	101.48	112.40
1	A	363	ARG	N-CA-C	-7.52	90.70	111.00
1	B	309	THR	OG1-CB-CG2	-6.56	94.92	110.00
1	B	191	PHE	CB-CG-CD1	6.18	125.13	120.80
1	B	129	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	B	130	GLY	N-CA-C	-6.07	97.92	113.10
1	B	133	THR	OG1-CB-CG2	-5.88	96.46	110.00
1	A	190	LEU	CD1-CG-CD2	-5.74	93.29	110.50
1	A	189	ASP	CB-CG-OD2	-5.14	113.67	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	GLU	Peptide
1	A	189	ASP	Peptide
1	B	128	ILE	Peptide
1	B	191	PHE	Sidechain,Mainchain
1	B	480	ALA	Peptide

5.2 Too-close contacts (i)

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	3757	0	3673	69	0
1	B	3727	0	3643	62	0
2	A	29	0	16	5	0
2	B	10	0	3	0	0
3	A	24	0	18	3	0
3	B	16	0	12	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	48	0	64	0	0
6	B	18	0	24	0	0
7	A	127	0	0	2	0
7	B	71	0	0	1	0
All	All	7854	0	7453	126	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 8.

All (126) 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:342:LYS:HG2	1:A:364:GLN:NE2	1.65	1.12
1:A:342:LYS:HG2	1:A:364:GLN:HE22	1.01	1.09
1:A:342:LYS:CG	1:A:364:GLN:HE22	1.73	1.02
1:A:344:LYS:HD2	1:A:344:LYS:H	1.29	0.97
1:B:186:LYS:HD2	1:B:191:PHE:HA	1.46	0.97
1:B:129:ARG:HB3	1:B:133:THR:OG1	1.69	0.92
1:B:186:LYS:NZ	1:B:191:PHE:HB2	1.83	0.92
1:A:186:LYS:NZ	1:A:189:ASP:OD2	2.03	0.91
1:B:354:PHE:O	1:B:456:ARG:NH2	2.03	0.91
1:B:129:ARG:HH21	1:B:140:LYS:CD	1.85	0.89
1:A:216:GLU:N	1:A:216:GLU:OE1	2.08	0.86
1:A:216:GLU:H	1:A:216:GLU:CD	1.78	0.84
1:B:134:ARG:HD2	1:B:140:LYS:HE3	1.61	0.83
1:A:344:LYS:HZ2	1:A:364:GLN:HE21	1.26	0.83
1:A:344:LYS:NZ	1:A:364:GLN:NE2	2.28	0.81
1:A:344:LYS:NZ	1:A:364:GLN:HE21	1.80	0.79
1:B:342:LYS:NZ	1:B:364:GLN:O	2.16	0.78
1:A:344:LYS:HD2	1:A:344:LYS:N	2.02	0.74
1:A:344:LYS:HZ2	1:A:364:GLN:NE2	1.85	0.73
1:A:363:ARG:C	1:A:364:GLN:HA	2.09	0.73
1:B:407:ASP:OD1	1:B:409:SER:OG	2.07	0.72
1:A:364:GLN:O	1:B:139:ASN:ND2	2.24	0.71
1:B:186:LYS:HZ2	1:B:191:PHE:HB2	1.55	0.71
1:A:342:LYS:HG2	1:A:364:GLN:CD	2.09	0.71
1:A:28:ARG:HH21	3:A:607:ACT:H1	1.59	0.68
2:A:601:5WO:C7	2:A:601:5WO:N1	2.56	0.68
1:A:396:ASP:OD2	1:B:26:LYS:NZ	2.26	0.67
1:B:181:CYS:SG	1:B:182:GLU:N	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HH21	1:B:140:LYS:HD3	1.57	0.66
1:A:445:SER:HA	1:B:481:HIS:CE1	2.30	0.66
1:A:302:LEU:HD22	1:A:334:THR:HG21	1.79	0.65
1:B:129:ARG:NH2	1:B:140:LYS:HD3	2.12	0.64
1:A:114:ALA:O	1:A:144:ARG:NH1	2.30	0.64
1:B:129:ARG:NH2	1:B:140:LYS:CD	2.60	0.63
1:B:134:ARG:NH1	1:B:140:LYS:HD2	2.14	0.63
1:A:186:LYS:HZ1	1:A:189:ASP:CG	1.99	0.61
1:B:129:ARG:HH21	1:B:140:LYS:CE	2.13	0.61
1:A:354:PHE:O	1:A:456:ARG:NH2	2.34	0.61
1:A:215:LYS:N	1:A:216:GLU:OE1	2.34	0.60
2:A:601:5WO:N1	2:A:601:5WO:H7	2.17	0.59
1:A:344:LYS:HZ3	1:A:364:GLN:NE2	1.98	0.59
1:B:129:ARG:NH2	1:B:140:LYS:CE	2.66	0.58
1:B:134:ARG:CZ	1:B:140:LYS:HD2	2.32	0.58
1:A:52:ASP:OD1	1:A:292:LYS:NZ	2.36	0.58
1:A:364:GLN:C	1:B:139:ASN:HD21	2.08	0.58
1:B:186:LYS:HZ1	1:B:191:PHE:HB2	1.64	0.57
1:B:309:THR:HG21	1:B:311:LYS:HB2	1.87	0.57
1:B:129:ARG:CB	1:B:133:THR:OG1	2.48	0.56
1:A:422:ARG:O	1:A:426:VAL:HG23	2.07	0.55
1:B:61:LYS:NZ	1:B:223:GLU:O	2.34	0.55
1:A:399:LEU:HD21	1:B:476:LEU:HD23	1.88	0.55
1:B:186:LYS:HD2	1:B:191:PHE:CA	2.29	0.55
1:B:309:THR:HG21	1:B:311:LYS:HD2	1.87	0.55
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.90	0.54
1:B:306:ASP:OD2	1:B:309:THR:HB	2.07	0.54
1:B:134:ARG:CD	1:B:140:LYS:HE3	2.34	0.54
1:A:34:ARG:NH1	1:B:489:THR:O	2.41	0.53
1:A:213:SER:C	1:A:216:GLU:OE1	2.47	0.53
1:A:363:ARG:C	1:A:364:GLN:CA	2.76	0.53
1:A:188:GLY:O	1:A:189:ASP:HB2	2.09	0.52
1:A:363:ARG:O	1:A:364:GLN:HA	2.08	0.52
1:A:342:LYS:HG2	1:A:364:GLN:OE1	2.10	0.52
1:A:247:LEU:HD23	1:A:286:ILE:HG23	1.91	0.51
1:A:213:SER:HA	1:A:216:GLU:CD	2.31	0.51
1:A:26:LYS:HB2	1:B:397:ILE:HD13	1.92	0.50
1:B:232:LEU:HB3	1:B:233:PRO:HD3	1.93	0.50
1:B:287:LEU:HD13	1:B:335:ILE:HD11	1.92	0.50
1:A:271:LYS:O	1:A:274:SER:HB3	2.12	0.50
1:B:445:SER:HB2	1:B:446:ARG:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ASP:OD2	1:B:309:THR:CB	2.60	0.49
2:A:601:5WO:H1	7:A:702:HOH:O	2.12	0.49
1:B:309:THR:CG2	1:B:311:LYS:HD2	2.42	0.49
1:B:186:LYS:CE	1:B:191:PHE:HB2	2.43	0.48
1:B:37:VAL:HG12	1:B:479:ALA:HA	1.95	0.48
1:A:236:LEU:HD12	1:A:264:PHE:HZ	1.79	0.48
1:B:195:ARG:HH12	1:B:199:GLN:HG2	1.79	0.47
1:A:159:LEU:HB2	1:A:160:PRO:HD3	1.97	0.47
1:A:110:LEU:HD13	1:A:118:LEU:HD11	1.96	0.47
1:A:388:LEU:O	1:A:392:LEU:HD13	2.15	0.47
2:A:601:5WO:H7	2:A:601:5WO:C6	2.44	0.47
1:B:129:ARG:HB3	1:B:133:THR:HG1	1.77	0.46
1:B:129:ARG:HH21	1:B:140:LYS:CG	2.27	0.46
1:B:309:THR:CG2	1:B:311:LYS:HB2	2.46	0.46
1:B:306:ASP:HB3	1:B:309:THR:HB	1.97	0.46
1:A:344:LYS:HZ2	1:A:364:GLN:CG	2.29	0.45
1:B:247:LEU:HD23	1:B:286:ILE:HG23	1.97	0.45
1:B:406:LEU:HD11	1:B:412:GLU:OE1	2.16	0.45
1:A:243:GLY:HA2	3:A:602:ACT:H1	1.96	0.45
1:B:305:VAL:HG22	1:B:312:LEU:HD23	1.99	0.45
1:A:364:GLN:O	1:A:364:GLN:HG2	2.16	0.45
1:A:395:LEU:HD23	1:A:423:ILE:HG13	1.99	0.45
1:B:74:VAL:HG13	1:B:86:LEU:HB3	1.98	0.45
1:A:427:THR:HG23	7:A:704:HOH:O	2.17	0.45
1:B:37:VAL:HG21	1:B:477:PHE:HB3	1.99	0.45
1:B:355:GLY:HA2	1:B:456:ARG:NH2	2.31	0.44
1:A:347:LEU:HD11	1:A:369:PHE:HB2	1.97	0.44
1:A:128:ILE:HG22	1:A:129:ARG:N	2.33	0.44
1:B:129:ARG:NH2	1:B:140:LYS:NZ	2.65	0.44
1:A:343:GLY:HA2	1:A:366:TRP:HD1	1.82	0.44
1:B:159:LEU:HB2	1:B:160:PRO:HD3	2.00	0.43
1:B:356:ASP:HB3	1:B:357:ILE:H	1.41	0.43
1:A:57:LEU:HD23	1:A:465:PHE:CZ	2.53	0.43
1:A:212:GLY:O	1:A:216:GLU:OE2	2.35	0.43
1:B:134:ARG:HH11	1:B:140:LYS:HE3	1.84	0.43
1:A:417:SER:O	1:A:421:ARG:HG3	2.18	0.43
1:A:115:TYR:CD1	1:B:456:ARG:HG3	2.54	0.43
1:A:223:GLU:HG2	1:A:262:TYR:HE1	1.83	0.43
1:B:111:LYS:HB3	1:B:120:VAL:HB	2.00	0.42
1:A:100:LEU:HD21	1:A:437:MET:HE2	2.01	0.42
1:A:129:ARG:HG3	1:A:130:GLY:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:NZ	1:A:189:ASP:CG	2.65	0.42
1:B:486:HIS:O	1:B:490:VAL:HG13	2.19	0.42
1:B:371:VAL:HG12	1:B:373:PRO:HD3	2.00	0.41
1:A:74:VAL:HG13	1:A:86:LEU:HB3	2.02	0.41
1:B:357:ILE:HG22	1:B:358:LEU:N	2.35	0.41
1:A:59:VAL:HB	2:A:601:5WO:H5	1.85	0.41
1:B:59:VAL:N	7:B:702:HOH:O	2.39	0.41
1:B:369:PHE:CE1	1:B:465:PHE:HA	2.56	0.41
1:A:28:ARG:NH2	3:A:607:ACT:H1	2.30	0.41
1:A:138:PRO:O	1:A:139:ASN:HB2	2.21	0.41
1:A:386:SER:O	1:A:390:GLU:HG3	2.21	0.41
1:A:199[B]:GLN:HG3	1:A:200:ASP:N	2.36	0.41
1:A:489:THR:O	1:B:34:ARG:NH1	2.53	0.41
1:A:111:LYS:HE2	1:A:443:SER:HB2	2.03	0.40
1:A:287:LEU:HD13	1:A:335:ILE:HD11	2.02	0.40
1:A:214:LEU:N	1:A:216:GLU:OE1	2.54	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	455/554 (82%)	424 (93%)	28 (6%)	3 (1%)	22	54
1	B	451/554 (81%)	421 (93%)	24 (5%)	6 (1%)	12	37
All	All	906/1108 (82%)	845 (93%)	52 (6%)	9 (1%)	15	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ARG
1	A	189	ASP

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Mol	Chain	Res	Type
1	A	343	GLY
1	A	344	LYS
1	B	188	GLY
1	B	363	ARG
1	B	129	ARG
1	B	326	VAL
1	B	306	ASP

5.3.2 Protein sidechains (i)

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	407/496 (82%)	403 (99%)	4 (1%)	76 92
1	B	405/496 (82%)	399 (98%)	6 (2%)	65 87
All	All	812/992 (82%)	802 (99%)	10 (1%)	76 91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75[A]	GLU
1	A	75[B]	GLU
1	A	274	SER
1	A	342	LYS
1	B	148	GLU
1	B	309	THR
1	B	331	SER
1	B	377[A]	GLN
1	B	377[B]	GLN
1	B	445	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN

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Mol	Chain	Res	Type
1	B	139	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
6	GOL	A	616	-	5,5,5	0.37	0	5,5,5	0.37	0
6	GOL	A	615	-	5,5,5	0.37	0	5,5,5	0.15	0
2	5WO	A	601	-	30,33,33	2.32	11 (36%)	34,46,46	3.31	15 (44%)
6	GOL	A	611	-	5,5,5	0.35	0	5,5,5	0.23	0
6	GOL	A	612	-	5,5,5	0.35	0	5,5,5	0.40	0
3	ACT	A	604	-	3,3,3	0.74	0	3,3,3	1.35	0
3	ACT	A	603	-	3,3,3	0.77	0	3,3,3	1.46	0
6	GOL	A	617	-	5,5,5	0.37	0	5,5,5	0.30	0
4	PO4	A	608	5	4,4,4	0.93	0	6,6,6	0.46	0
6	GOL	B	612	-	5,5,5	0.40	0	5,5,5	0.24	0
6	GOL	B	610	-	5,5,5	0.34	0	5,5,5	0.26	0
2	5WO	B	601	-	9,11,33	2.49	4 (44%)	7,15,46	3.06	4 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACT	B	604	-	3,3,3	0.75	0	3,3,3	1.31	0
6	GOL	B	611	-	5,5,5	0.37	0	5,5,5	0.25	0
6	GOL	A	618	-	5,5,5	0.35	0	5,5,5	0.49	0
4	PO4	A	609	-	4,4,4	0.88	0	6,6,6	0.43	0
3	ACT	B	602	-	3,3,3	0.78	0	3,3,3	1.29	0
4	PO4	B	606	5	4,4,4	0.96	0	6,6,6	0.36	0
6	GOL	A	614	-	5,5,5	0.37	0	5,5,5	0.44	0
3	ACT	A	606	-	3,3,3	0.76	0	3,3,3	1.36	0
3	ACT	B	605	-	3,3,3	0.74	0	3,3,3	1.40	0
6	GOL	A	613	-	5,5,5	0.36	0	5,5,5	0.21	0
3	ACT	A	607	-	3,3,3	0.76	0	3,3,3	1.43	0
3	ACT	A	602	-	3,3,3	0.75	0	3,3,3	1.45	0
3	ACT	B	603	-	3,3,3	0.76	0	3,3,3	1.41	0
3	ACT	A	605	-	3,3,3	0.76	0	3,3,3	1.39	0
4	PO4	B	608	-	4,4,4	0.90	0	6,6,6	0.41	0
4	PO4	B	607	-	4,4,4	0.96	0	6,6,6	0.50	0

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
6	GOL	B	611	-	-	0/4/4/4	-
6	GOL	A	613	-	-	2/4/4/4	-
6	GOL	A	618	-	-	2/4/4/4	-
6	GOL	A	616	-	-	4/4/4/4	-
6	GOL	A	615	-	-	2/4/4/4	-
2	5WO	A	601	-	-	5/16/22/22	0/5/5/5
6	GOL	A	611	-	-	0/4/4/4	-
6	GOL	A	612	-	-	0/4/4/4	-
6	GOL	B	612	-	-	2/4/4/4	-
6	GOL	B	610	-	-	0/4/4/4	-
2	5WO	B	601	-	-	-	0/2/2/5
6	GOL	A	614	-	-	2/4/4/4	-
6	GOL	A	617	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	5WO	C23-N2	-7.17	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	5WO	C2-N3	5.10	1.40	1.32
2	A	601	5WO	C9-N2	-3.91	1.33	1.39
2	A	601	5WO	C3-C13	-3.88	1.42	1.50
2	A	601	5WO	C22-N2	-3.81	1.33	1.39
2	A	601	5WO	C19-C1	-3.79	1.39	1.49
2	A	601	5WO	C2-N3	3.37	1.37	1.32
2	B	601	5WO	C2-N1	3.33	1.40	1.33
2	B	601	5WO	C5-C4	-2.63	1.34	1.40
2	B	601	5WO	C6-C5	-2.42	1.34	1.43
2	A	601	5WO	C9-C20	-2.26	1.33	1.38
2	A	601	5WO	C2-N1	2.24	1.38	1.33
2	A	601	5WO	C5-C4	-2.18	1.35	1.40
2	A	601	5WO	C21-C20	-2.12	1.33	1.40
2	A	601	5WO	C4-N3	-2.10	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	5WO	C2-N1-C6	11.50	126.45	116.59
2	A	601	5WO	N3-C2-N1	-8.84	114.86	128.68
2	B	601	5WO	N3-C2-N1	-6.86	117.96	128.68
2	A	601	5WO	C19-C7-C3	5.63	127.19	121.09
2	A	601	5WO	C12-C3-C7	-4.36	114.08	119.24
2	A	601	5WO	C18-C1-C19	-3.97	114.48	121.36
2	A	601	5WO	C3-C13-N6	3.45	123.51	115.92
2	A	601	5WO	C4-C5-N7	-3.21	106.05	109.40
2	A	601	5WO	C9-N2-C23	-3.17	121.18	126.33
2	A	601	5WO	C14-C1-C19	3.11	126.00	120.86
2	B	601	5WO	C2-N3-C4	2.84	120.11	113.45
2	A	601	5WO	C10-C19-C1	2.74	126.10	121.36
2	A	601	5WO	C7-C19-C1	-2.62	116.53	120.86
2	A	601	5WO	O1-C13-C3	-2.51	116.45	120.94
2	A	601	5WO	C22-N2-C23	2.26	130.00	126.33
2	A	601	5WO	C10-C19-C7	-2.17	115.10	118.16
2	A	601	5WO	C2-N3-C4	2.16	118.52	113.45
2	B	601	5WO	C5-C6-N6	-2.12	117.13	120.35
2	B	601	5WO	C4-C5-N7	-2.07	107.24	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	5WO	C3-C13-N6-C6
2	A	601	5WO	O1-C13-N6-C6
6	A	614	GOL	C1-C2-C3-O3
6	A	615	GOL	O1-C1-C2-C3
6	A	616	GOL	O1-C1-C2-C3
6	A	616	GOL	C1-C2-C3-O3
6	A	617	GOL	C1-C2-C3-O3
6	A	616	GOL	O2-C2-C3-O3
6	A	613	GOL	O1-C1-C2-C3
6	A	618	GOL	O1-C1-C2-C3
6	B	612	GOL	C1-C2-C3-O3
6	A	615	GOL	O1-C1-C2-O2
6	A	617	GOL	O2-C2-C3-O3
6	A	614	GOL	O2-C2-C3-O3
6	A	618	GOL	O1-C1-C2-O2
6	B	612	GOL	O2-C2-C3-O3
6	A	616	GOL	O1-C1-C2-O2
2	A	601	5WO	C18-C1-C19-C7
2	A	601	5WO	O1-C13-C3-C12
2	A	601	5WO	N6-C13-C3-C12
6	A	613	GOL	O1-C1-C2-O2

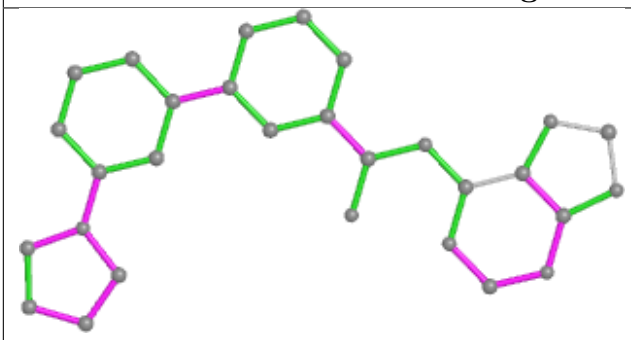
There are no ring outliers.

3 monomers are involved in 8 short contacts:

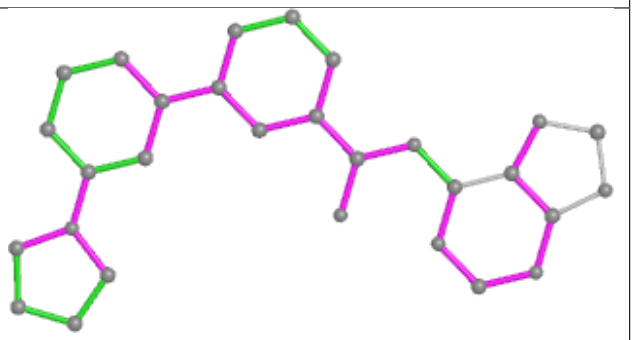
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	5WO	5	0
3	A	607	ACT	2	0
3	A	602	ACT	1	0

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 then 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.

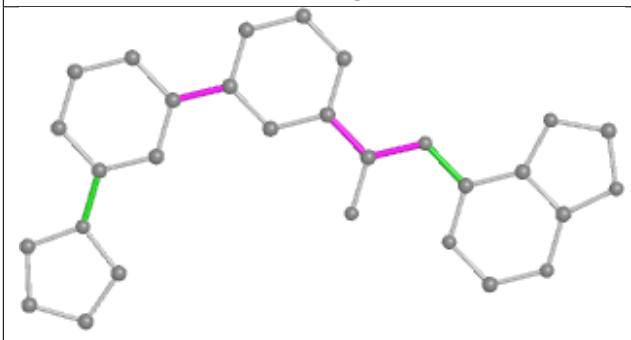
Ligand 5WO A 601



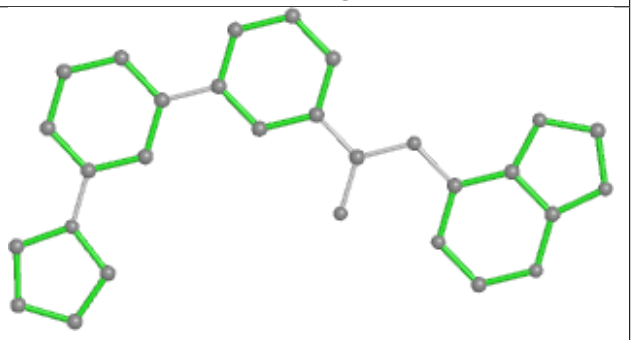
Bond lengths



Bond angles

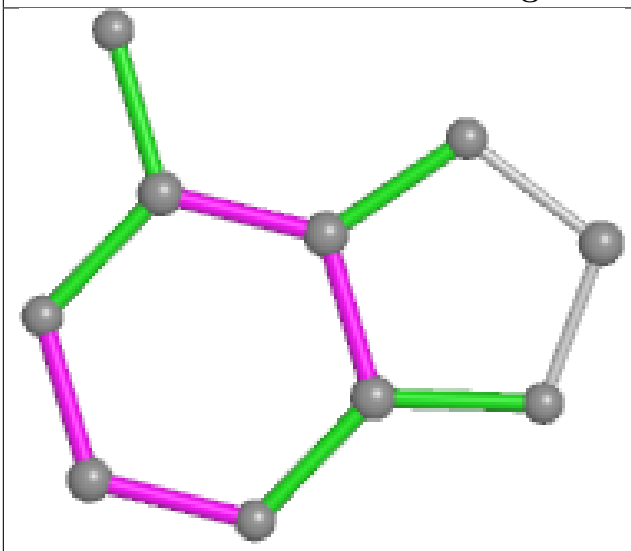


Torsions

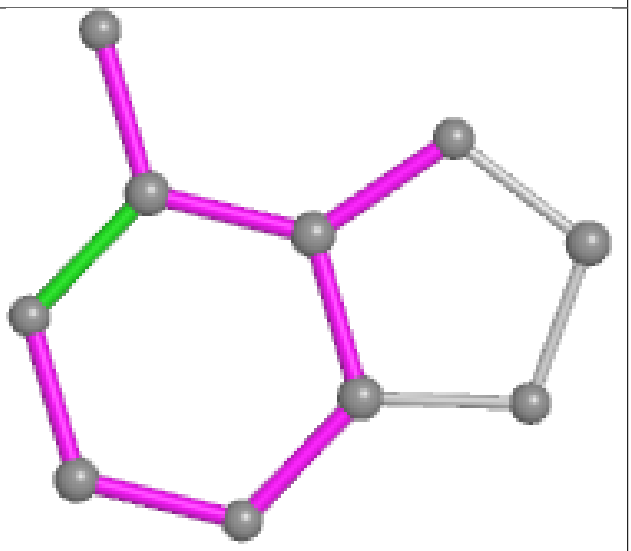


Rings

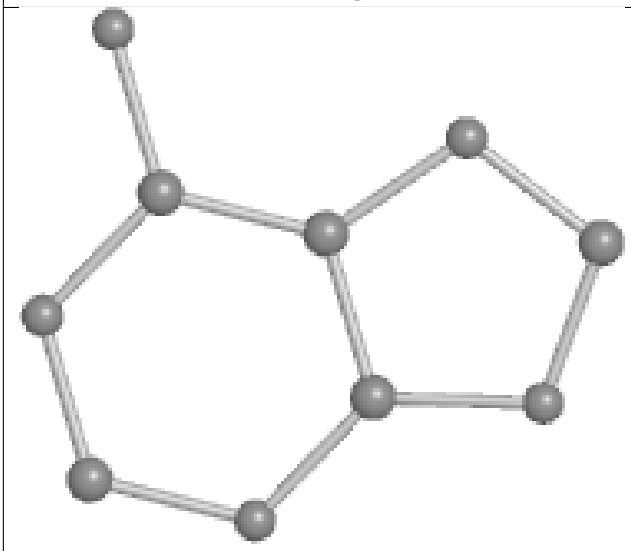
Ligand 5WO B 601



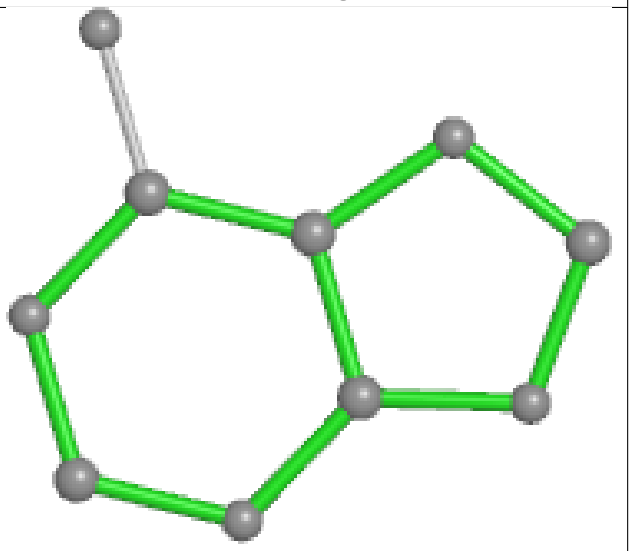
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	363:ARG	C	364:GLN	N	2.89

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, 95^{th} 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	459/554 (82%)	-0.26	6 (1%)	77	77	10, 26, 57, 82	0
1	B	454/554 (81%)	-0.26	5 (1%)	80	80	9, 28, 58, 73	0
All	All	913/1108 (82%)	-0.26	11 (1%)	79	79	9, 27, 58, 82	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	4.9
1	B	358	LEU	3.2
1	A	188	GLY	3.0
1	B	181	CYS	3.0
1	A	181	CYS	2.9
1	A	398	PHE	2.7
1	A	316	THR	2.6
1	A	364	GLN	2.6
1	B	309	THR	2.4
1	B	398	PHE	2.3
1	B	325	ILE	2.3

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 monosaccharides in this entry.

6.4 Ligands (i)

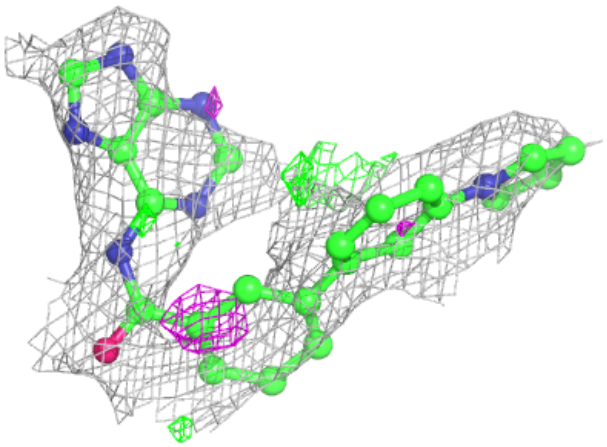
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

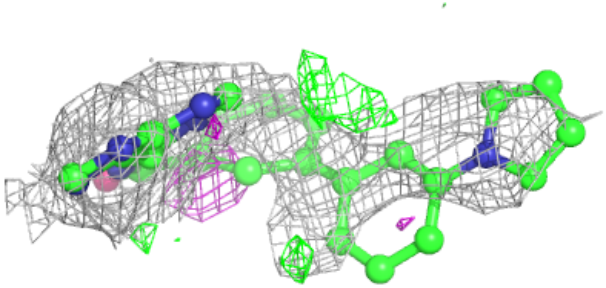
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	615	6/6	0.68	0.21	41,58,65,70	0
6	GOL	A	618	6/6	0.70	0.31	42,45,52,58	0
3	ACT	A	603	4/4	0.77	0.24	54,58,61,79	0
2	5WO	A	601	29/29	0.79	0.33	38,66,95,96	0
4	PO4	B	608	5/5	0.81	0.21	41,49,59,79	0
3	ACT	A	605	4/4	0.83	0.23	29,55,55,57	0
6	GOL	A	616	6/6	0.84	0.20	50,52,57,58	0
3	ACT	A	606	4/4	0.84	0.25	23,44,46,48	0
3	ACT	B	603	4/4	0.85	0.20	42,43,60,63	0
6	GOL	A	617	6/6	0.86	0.26	48,54,63,65	0
3	ACT	A	607	4/4	0.88	0.33	34,38,40,52	0
6	GOL	A	614	6/6	0.88	0.25	27,35,48,52	0
6	GOL	A	612	6/6	0.90	0.18	16,30,41,45	0
3	ACT	A	604	4/4	0.90	0.22	24,31,47,55	0
3	ACT	B	602	4/4	0.91	0.21	32,38,41,50	0
6	GOL	B	610	6/6	0.91	0.17	40,45,49,51	0
2	5WO	B	601	10/29	0.92	0.20	23,26,32,32	0
6	GOL	B	611	6/6	0.92	0.16	36,46,50,50	0
6	GOL	B	612	6/6	0.92	0.25	29,39,50,63	0
3	ACT	A	602	4/4	0.93	0.14	13,36,45,49	0
3	ACT	B	605	4/4	0.93	0.17	36,39,45,49	0
6	GOL	A	611	6/6	0.94	0.14	24,39,44,46	0
3	ACT	B	604	4/4	0.95	0.12	30,31,37,44	0
6	GOL	A	613	6/6	0.95	0.14	31,36,38,38	0
5	MG	B	609	1/1	0.97	0.27	6,6,6,6	0
4	PO4	B	606	5/5	0.97	0.14	9,11,19,21	0
4	PO4	A	608	5/5	0.97	0.14	12,13,17,24	0
5	MG	A	610	1/1	0.97	0.25	3,3,3,3	0
4	PO4	B	607	5/5	0.98	0.13	15,18,20,21	0
4	PO4	A	609	5/5	0.99	0.09	11,15,21,31	0

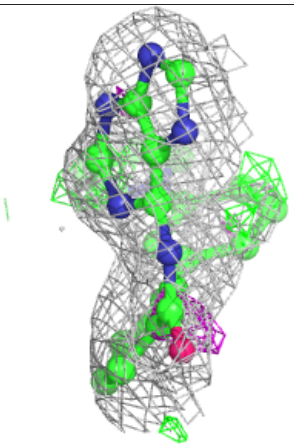
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5WO A 601:

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

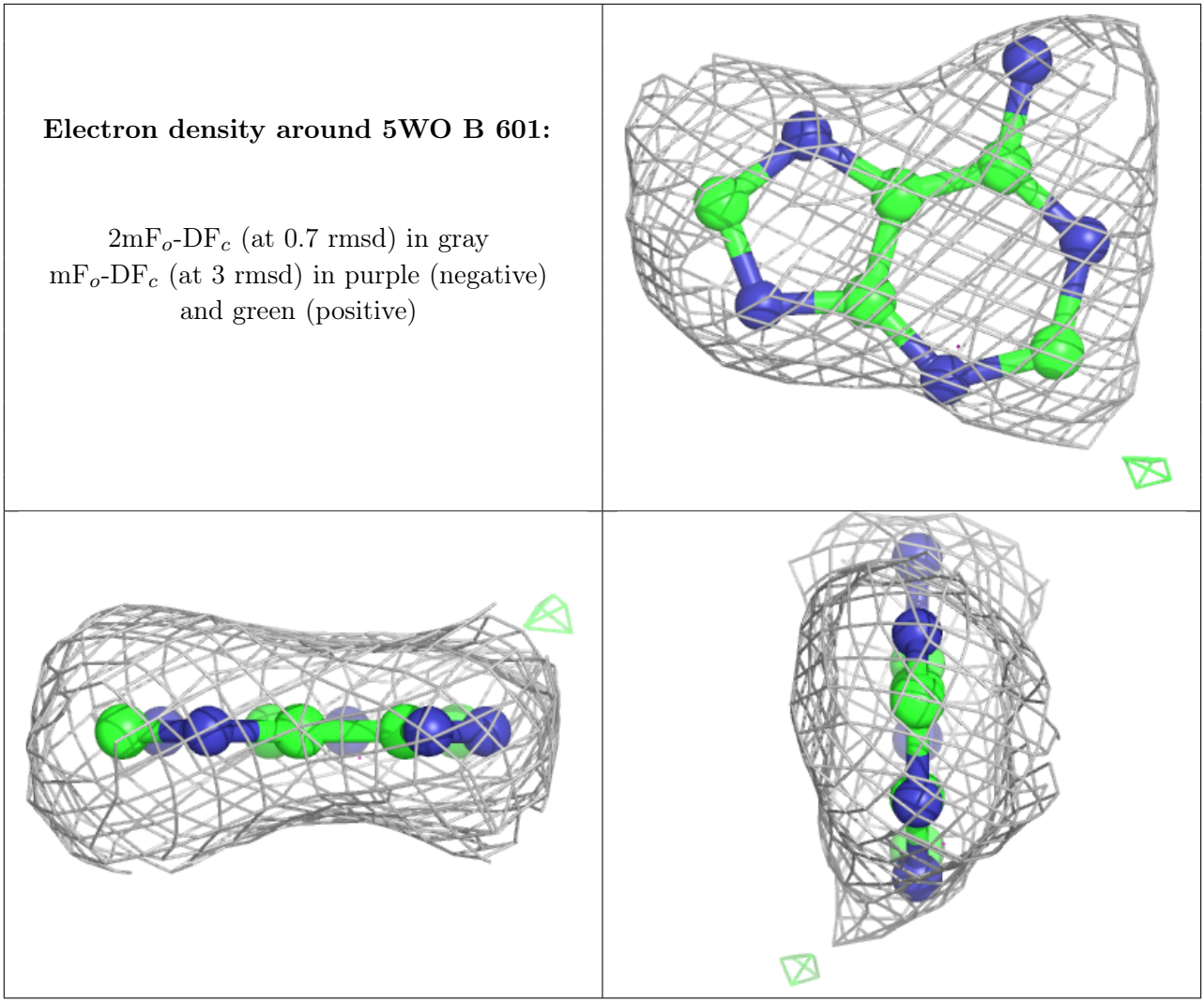






Electron density around 5WO B 601:

$2mF_o$-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.