Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2022 – 01:12 pm BST

PDB ID	:	7OPA
Title	:	Purine nucleoside phosphorylase(DeoD-type) from H. pylori with 6-benzylthiopurine
Authors	:	Narczyk, M.; Stefanic, Z.
Deposited on	:	2021-05-31
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

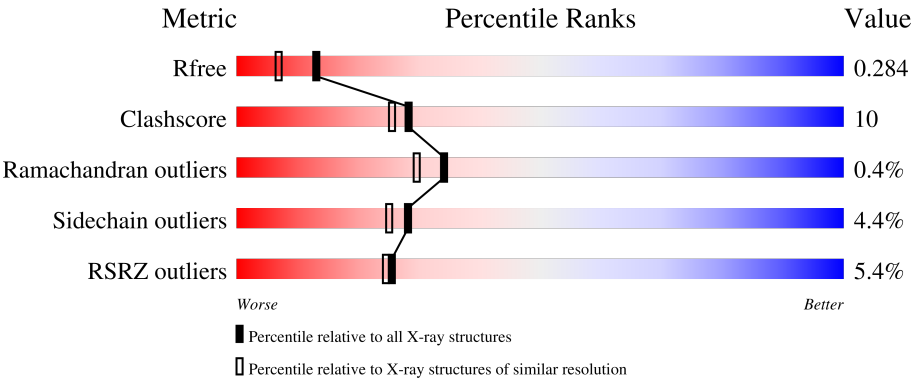
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	233	2% 78% 21%
1	B	233	6% 75% 24%
1	C	233	84% 15%
1	D	233	4% 72% 27%
1	E	233	3% 78% 21%

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Mol	Chain	Length	Quality of chain
1	F	233	77% 21%
1	G	233	12% 70% 27%
1	H	233	80% 18%
1	I	233	11% 73% 25%
1	J	233	3% 78% 21%
1	K	233	8% 77% 22%
1	L	233	15% 70% 28%

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	GOL	B	303	-	-	X	-
2	GOL	F	304	-	-	X	-
2	GOL	H	305	-	-	X	-

2 Entry composition (i)

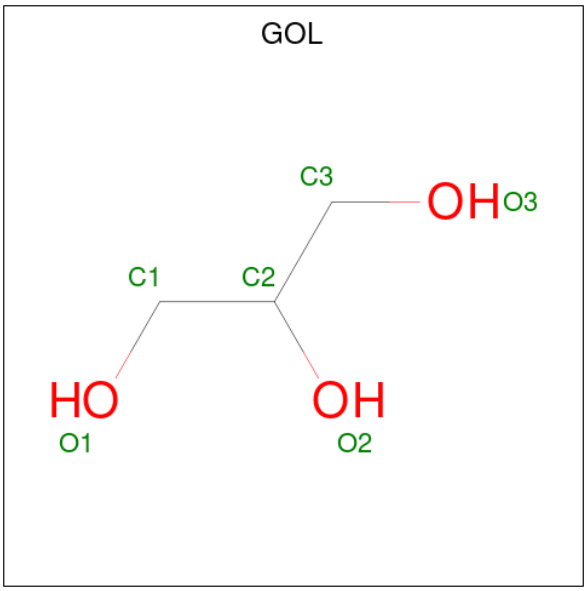
There are 6 unique types of molecules in this entry. The entry contains 22853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine nucleoside phosphorylase DeoD-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	B	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	C	233	Total	C	N	O	S	0	0	0
			1798	1147	302	332	17			
1	D	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	E	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	F	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	G	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	H	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	I	233	Total	C	N	O	S	0	0	0
			1798	1147	302	332	17			
1	J	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	K	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	L	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

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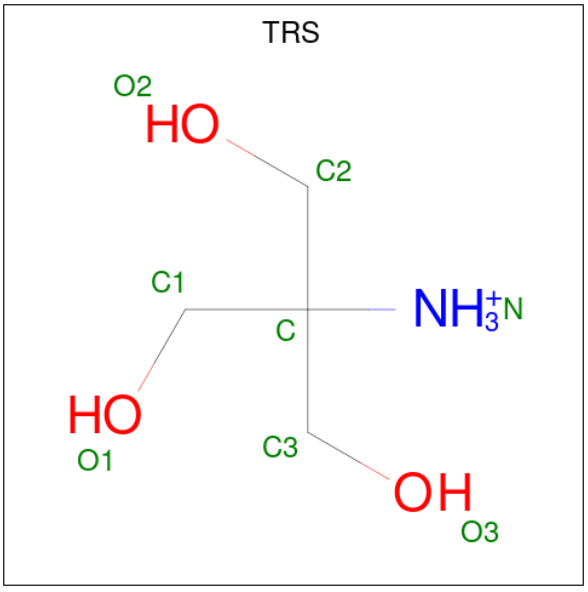
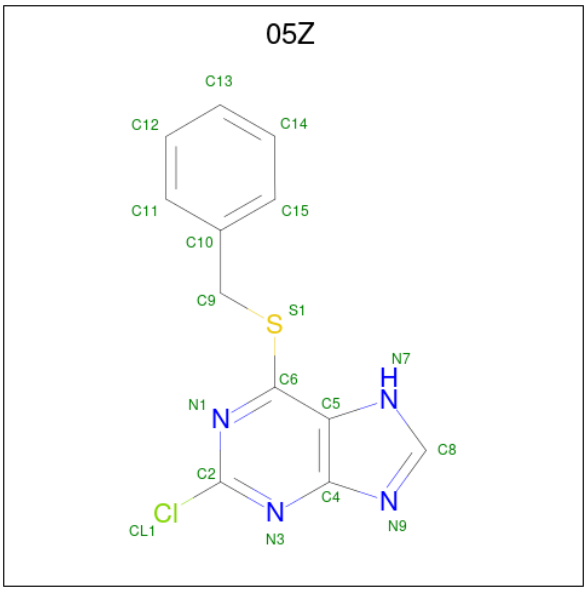
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	K	1	Total C O 6 3 3	0	0
2	K	1	Total C O 6 3 3	0	0
2	K	1	Total C O 6 3 3	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



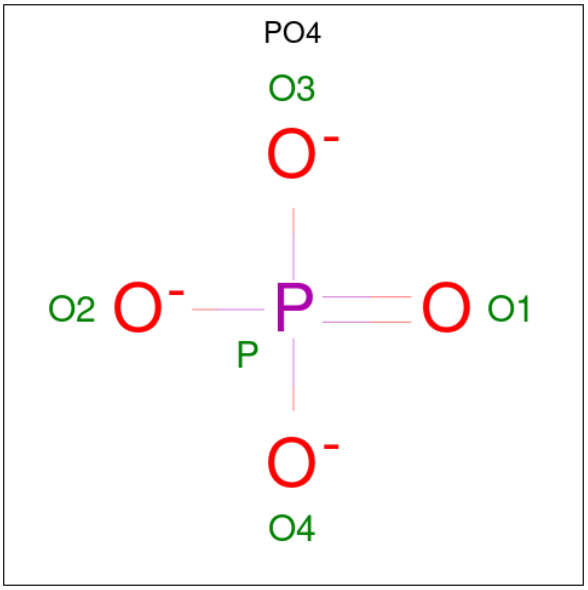
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 8 4 1 3	0	0
3	H	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is 6-benzylthio-2-chloropurine (three-letter code: 05Z) (formula: $C_{12}H_9ClN_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	S	0	0
			17	12	4	1		
4	H	1	Total	C	N	S	0	0
			17	12	4	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	O	P		0	0
			5	4	1			
5	H	1	Total	O	P		0	0
			5	4	1			

- Molecule 6 is water.

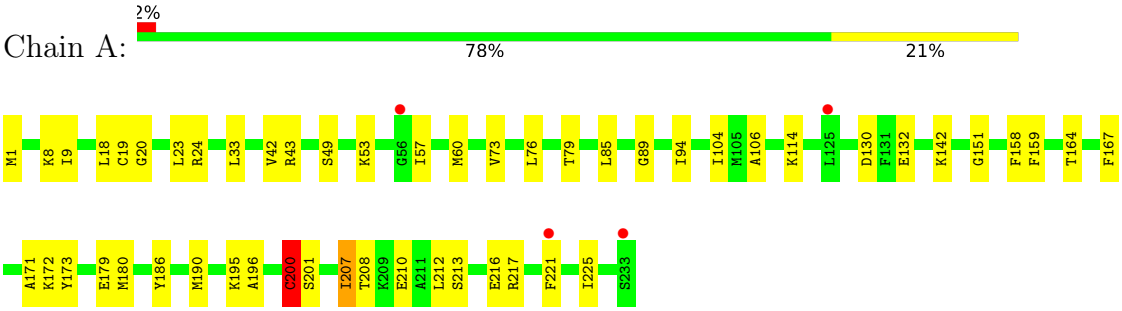
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	106	Total O 106 106	0	0
6	B	70	Total O 70 70	0	0
6	C	115	Total O 115 115	0	0
6	D	81	Total O 81 81	0	0
6	E	73	Total O 73 73	0	0
6	F	153	Total O 153 153	0	0
6	G	52	Total O 52 52	0	0
6	H	130	Total O 130 130	0	0
6	I	59	Total O 59 59	0	0
6	J	96	Total O 96 96	0	0
6	K	78	Total O 78 78	0	0
6	L	44	Total O 44 44	0	0

3 Residue-property plots (i)

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

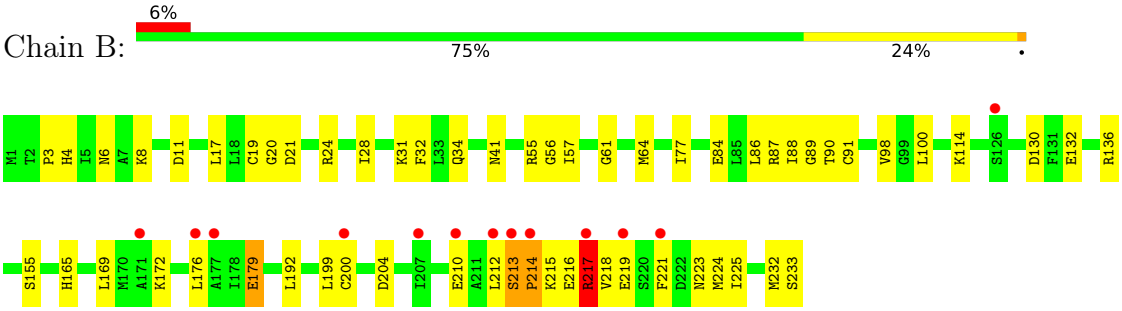
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain A:



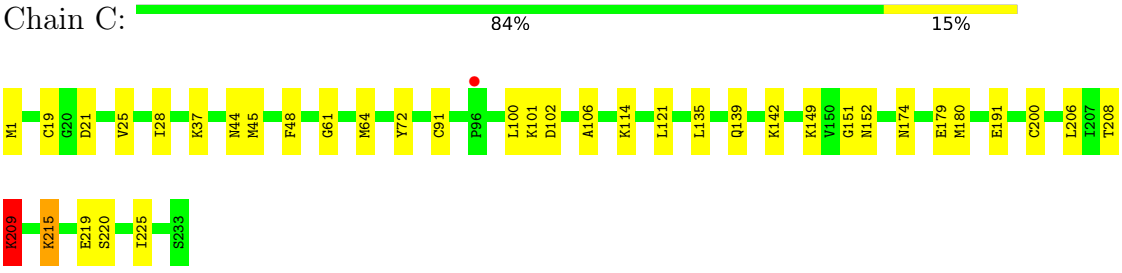
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain B:



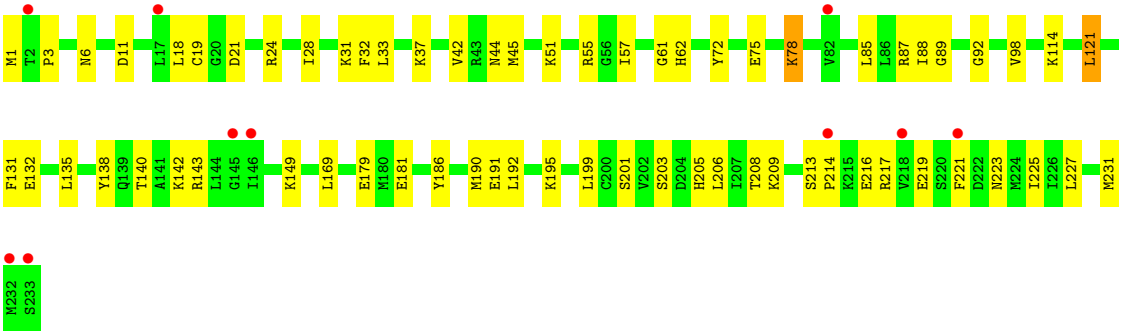
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain C:



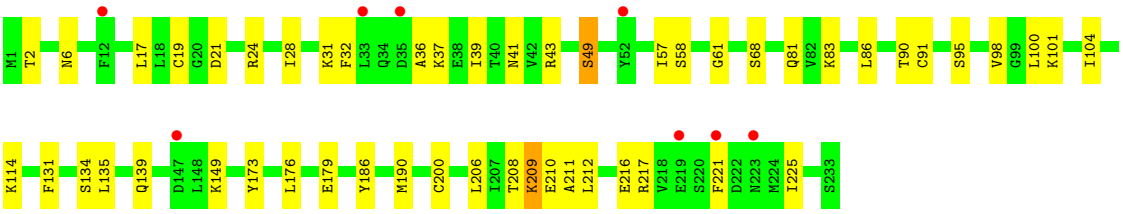
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain D:



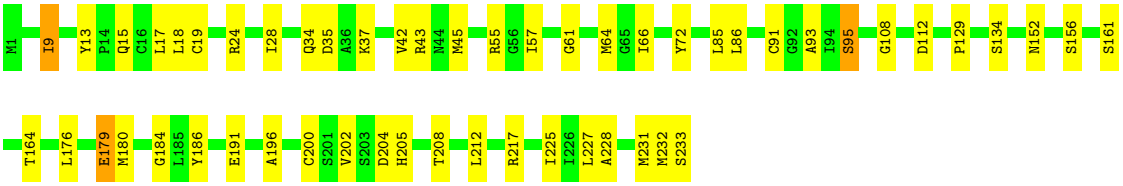
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain E:



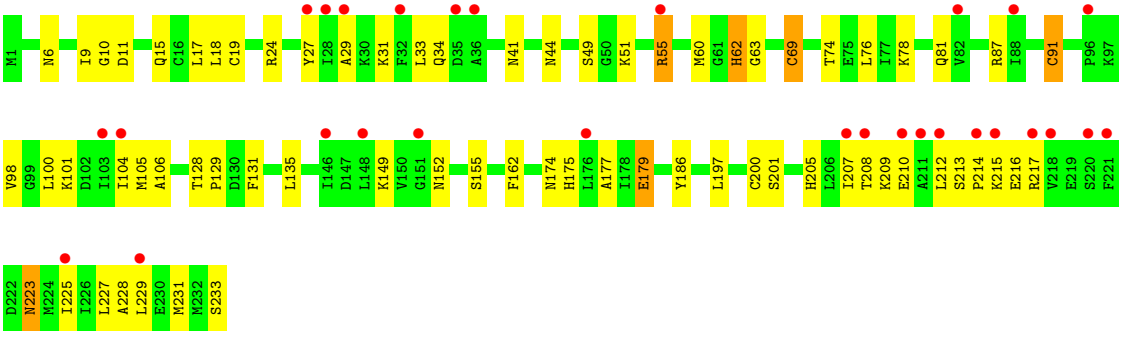
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain F:



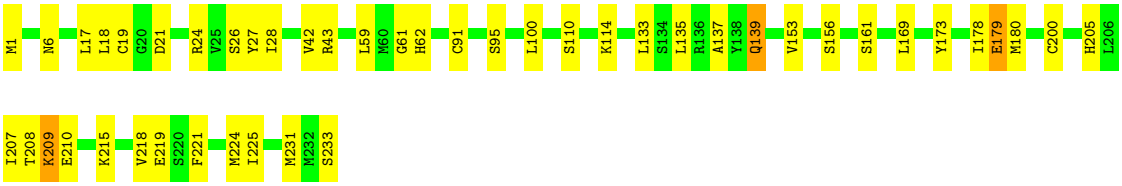
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain G:

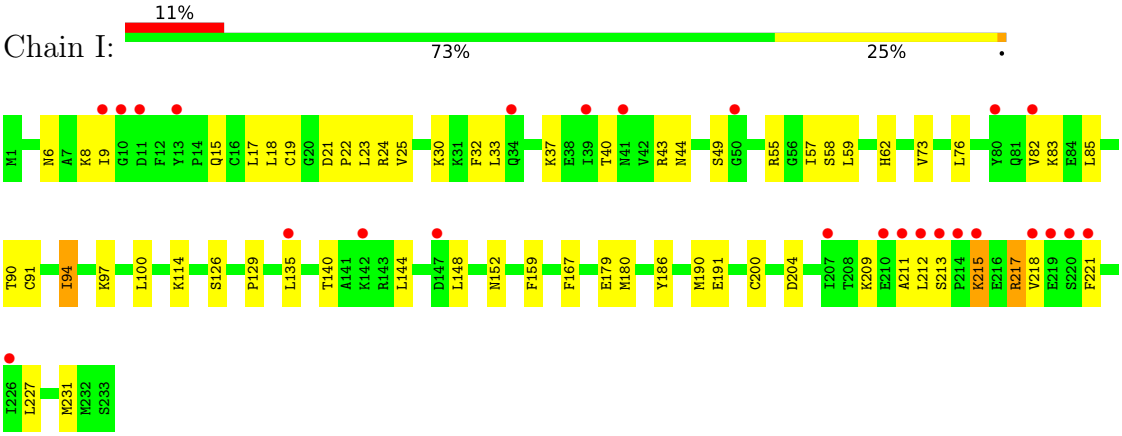


• Molecule 1: Purine nucleoside phosphorylase DeoD-type

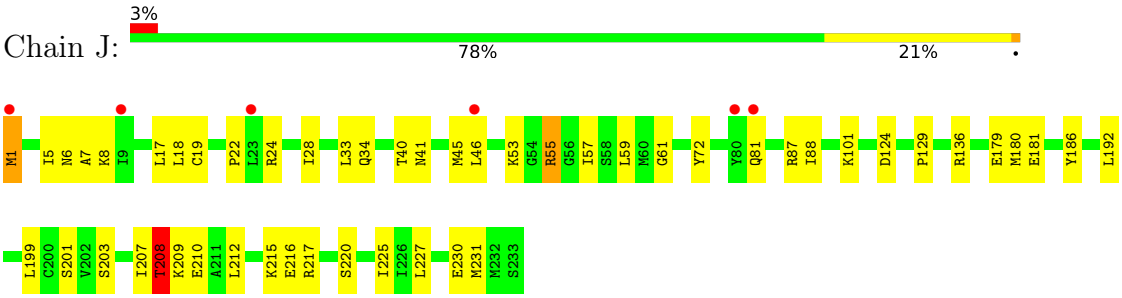
Chain H:



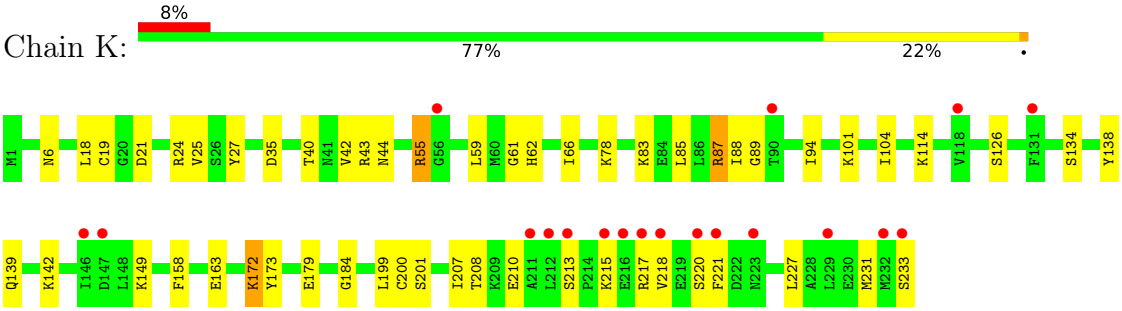
• Molecule 1: Purine nucleoside phosphorylase DeoD-type



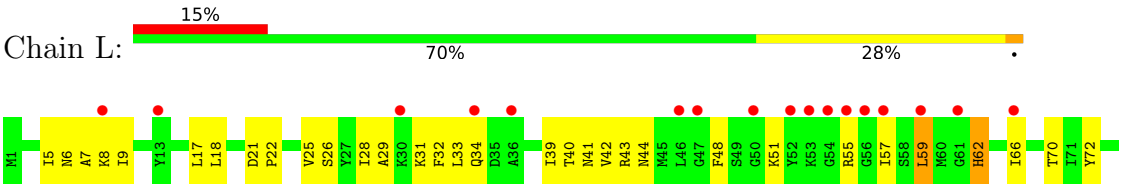
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

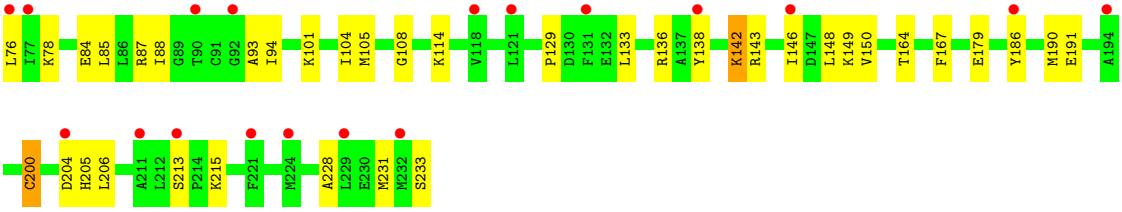


• Molecule 1: Purine nucleoside phosphorylase DeoD-type



• Molecule 1: Purine nucleoside phosphorylase DeoD-type




L76
I77
K78
E84
L85
L86
R87
I88
G89
T90
C91
G92
A93
I94
K101
I104
M105
G108
K114
V118
L121
P129
D130
F131
E132
L133
R136
A137
Y138
K142
R143
I146
D147
L148
K149
V150
T164
F167
E179
Y186
M190
E191
A194
C200
D204
H205
L206
A211
L212
S213
P214
K215
F221
M224
A228
L229
E230
M231
M232
S233

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.56Å 139.00Å 318.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 2.00 49.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.62-2.00) 99.8 (49.62-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.229 , 0.285 0.229 , 0.284	Depositor DCC
R_{free} test set	1999 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22853	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, PO4, 05Z, TRS

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	0.44	1/1833 (0.1%)	0.64	0/2467
1	B	0.40	0/1833	0.62	0/2467
1	C	0.45	0/1829	0.66	0/2462
1	D	0.43	0/1833	0.62	0/2467
1	E	0.38	0/1833	0.62	0/2467
1	F	0.49	0/1833	0.69	0/2467
1	G	0.40	0/1833	0.64	0/2467
1	H	0.49	0/1833	0.73	0/2467
1	I	0.42	0/1829	0.63	0/2462
1	J	0.41	0/1833	0.63	0/2467
1	K	0.41	0/1833	0.63	0/2467
1	L	0.39	0/1833	0.63	0/2467
All	All	0.43	1/21988 (0.0%)	0.65	0/29594

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	CYS	CB-SG	-6.63	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1802	0	1836	34	0
1	B	1802	0	1838	44	0
1	C	1798	0	1834	23	0
1	D	1802	0	1836	44	1
1	E	1802	0	1838	34	0
1	F	1802	0	1838	38	0
1	G	1802	0	1836	53	0
1	H	1802	0	1838	32	1
1	I	1798	0	1834	39	0
1	J	1802	0	1836	29	0
1	K	1802	0	1836	37	0
1	L	1802	0	1836	52	0
2	A	12	0	16	0	0
2	B	18	0	24	5	0
2	C	6	0	8	1	0
2	D	12	0	16	2	0
2	E	6	0	8	0	0
2	F	24	0	31	6	0
2	H	18	0	24	8	0
2	I	6	0	8	0	0
2	K	18	0	23	3	0
3	C	8	0	12	3	0
3	H	8	0	12	1	0
4	C	17	0	0	1	0
4	H	17	0	0	3	0
5	C	5	0	0	0	0
5	H	5	0	0	0	0
6	A	106	0	0	7	0
6	B	70	0	0	3	0
6	C	115	0	0	3	0
6	D	81	0	0	7	0
6	E	73	0	0	1	0
6	F	153	0	0	8	0
6	G	52	0	0	8	0
6	H	130	0	0	2	0
6	I	59	0	0	2	0
6	J	96	0	0	3	0
6	K	78	0	0	3	0
6	L	44	0	0	3	0
All	All	22853	0	22218	431	1

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 10.

All (431) 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:F:15:GLN:O	6:F:401:HOH:O	1.91	0.89
1:B:89:GLY:HA3	2:B:303:GOL:H31	1.58	0.85
1:I:213:SER:HB3	1:I:217:ARG:HB2	1.59	0.84
1:C:200:CYS:SG	6:C:431:HOH:O	2.41	0.78
1:H:6:ASN:HB2	1:H:42:VAL:HG23	1.64	0.78
1:L:29:ALA:HA	1:L:33:LEU:HD23	1.65	0.78
1:B:87:ARG:NH1	2:B:303:GOL:O3	2.18	0.77
1:K:55:ARG:HD3	1:K:233:SER:HA	1.66	0.77
1:I:19:CYS:SG	1:I:24:ARG:NE	2.57	0.77
1:A:212:LEU:O	1:A:217:ARG:NH1	2.18	0.77
1:B:20:GLY:H	2:B:303:GOL:H32	1.51	0.75
1:J:33:LEU:HD11	1:J:59:LEU:HD11	1.67	0.75
1:I:114:LYS:HB2	1:L:114:LYS:HB2	1.69	0.74
1:G:213:SER:N	1:G:216:GLU:OE1	2.17	0.74
1:E:206:LEU:O	1:E:209:LYS:NZ	2.21	0.73
1:L:186:TYR:O	1:L:190:MET:HG3	1.88	0.73
1:E:91:CYS:SG	1:E:200:CYS:HB3	2.29	0.72
1:I:18:LEU:HD11	1:I:85:LEU:HB3	1.71	0.72
1:J:34:GLN:NE2	6:J:301:HOH:O	2.22	0.72
1:I:186:TYR:O	1:I:190:MET:HG3	1.92	0.70
1:H:1:MET:N	6:H:403:HOH:O	2.21	0.69
1:J:208:THR:O	1:J:210:GLU:N	2.24	0.69
1:I:19:CYS:SG	1:I:24:ARG:NH2	2.65	0.69
1:L:78:LYS:N	6:L:302:HOH:O	2.24	0.69
1:K:172:LYS:NZ	6:K:403:HOH:O	2.25	0.69
1:G:19:CYS:SG	6:G:336:HOH:O	2.51	0.68
1:I:212:LEU:HD13	1:I:217:ARG:HG2	1.76	0.68
1:F:24:ARG:NH1	6:F:402:HOH:O	2.28	0.67
1:L:129:PRO:HG3	1:L:186:TYR:CZ	2.30	0.67
1:G:205:HIS:HB3	1:G:210:GLU:OE1	1.95	0.67
1:F:57:ILE:HA	6:F:401:HOH:O	1.94	0.66
1:I:76:LEU:HD22	1:I:82:VAL:HG21	1.76	0.66
1:D:1:MET:N	6:D:405:HOH:O	2.29	0.66
1:B:221:PHE:O	1:B:225:ILE:HG12	1.94	0.66
1:B:165:HIS:O	6:B:401:HOH:O	2.13	0.65
1:I:91:CYS:SG	1:I:200:CYS:HB3	2.35	0.65
1:G:162:PHE:CD1	2:H:305:GOL:H2	2.31	0.65
1:B:84:GLU:OE2	6:B:402:HOH:O	2.14	0.65
1:D:208:THR:OG1	6:D:401:HOH:O	2.15	0.65
1:A:171:ALA:O	6:A:401:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:N	6:C:403:HOH:O	2.29	0.64
1:H:114:LYS:HB2	1:K:114:LYS:HB2	1.80	0.64
1:F:179:GLU:HA	2:F:301:GOL:H32	1.80	0.63
1:J:1:MET:SD	1:J:1:MET:N	2.69	0.63
1:D:223:ASN:ND2	6:D:406:HOH:O	2.32	0.63
1:G:155:SER:HA	1:G:179:GLU:O	1.99	0.63
1:L:7:ALA:HB2	1:L:40:THR:HG22	1.81	0.62
1:A:42:VAL:HG12	1:A:43:ARG:HG3	1.80	0.62
1:J:6:ASN:ND2	1:J:41:ASN:OD1	2.32	0.62
1:H:19:CYS:HB3	1:H:24:ARG:NH1	2.15	0.62
1:G:207:ILE:HG13	1:G:208:THR:HG23	1.82	0.61
1:D:31:LYS:HD3	1:D:32:PHE:CE2	2.36	0.61
1:E:100:LEU:HD11	1:E:210:GLU:HB3	1.83	0.60
1:H:169:LEU:HD11	2:H:305:GOL:H31	1.84	0.60
1:C:1:MET:N	6:C:405:HOH:O	2.34	0.60
1:L:6:ASN:ND2	1:L:41:ASN:OD1	2.35	0.60
1:J:212:LEU:HD22	1:J:216:GLU:HB3	1.83	0.60
1:B:218:VAL:HA	1:B:221:PHE:HB2	1.83	0.60
1:D:98:VAL:HG12	1:D:149:LYS:HG3	1.84	0.59
1:A:186:TYR:O	1:A:190:MET:HG3	2.02	0.58
1:F:42:VAL:HG12	1:F:43:ARG:HG3	1.85	0.58
1:G:9:ILE:HD12	1:G:10:GLY:H	1.67	0.58
1:G:6:ASN:ND2	1:G:41:ASN:OD1	2.35	0.58
2:H:304:GOL:H11	1:K:78:LYS:NZ	2.17	0.58
1:F:161:SER:N	2:F:304:GOL:H11	2.18	0.58
1:I:32:PHE:N	6:I:401:HOH:O	2.22	0.58
1:D:205:HIS:HB3	6:D:401:HOH:O	2.03	0.57
1:G:128:THR:O	6:G:302:HOH:O	2.17	0.57
1:I:15:GLN:HE22	1:I:55:ARG:HH21	1.50	0.57
1:L:33:LEU:HD11	1:L:57:ILE:HD11	1.87	0.57
1:G:91:CYS:HB2	1:G:177:ALA:HB1	1.86	0.57
1:L:5:ILE:HG22	1:L:7:ALA:H	1.69	0.57
1:G:15:GLN:NE2	6:G:307:HOH:O	2.36	0.57
1:K:138:TYR:OH	1:K:142:LYS:HE2	2.05	0.57
1:L:39:ILE:HG13	1:L:40:THR:HG23	1.86	0.57
1:B:24:ARG:HH12	2:B:303:GOL:H2	1.69	0.56
1:C:21:ASP:OD1	1:F:43:ARG:HA	2.05	0.56
1:B:55:ARG:HD2	1:B:233:SER:HA	1.87	0.56
1:G:205:HIS:HE1	1:G:207:ILE:HG12	1.70	0.56
1:I:22:PRO:HG2	1:L:44:ASN:HB2	1.87	0.56
1:J:101:LYS:HG3	1:J:212:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ASN:N	1:G:223:ASN:OD1	2.36	0.56
1:E:6:ASN:ND2	1:E:41:ASN:OD1	2.39	0.56
2:F:303:GOL:HO1	2:F:304:GOL:HO2	1.53	0.56
1:G:212:LEU:HB3	1:G:216:GLU:HB2	1.87	0.56
1:C:102:ASP:OD1	1:C:149:LYS:NZ	2.39	0.56
1:D:213:SER:O	1:D:217:ARG:N	2.35	0.56
1:G:11:ASP:OD2	6:G:303:HOH:O	2.18	0.56
1:L:136:ARG:HD3	1:L:231:MET:O	2.06	0.56
1:A:20:GLY:O	6:A:402:HOH:O	2.18	0.56
1:A:94:ILE:O	1:A:207:ILE:HD11	2.06	0.55
1:D:24:ARG:HH22	1:D:89:GLY:HA2	1.72	0.55
1:D:221:PHE:O	1:D:225:ILE:HG12	2.06	0.55
1:H:91:CYS:SG	1:H:200:CYS:HB3	2.46	0.55
1:L:18:LEU:HD11	1:L:85:LEU:HB3	1.88	0.55
1:A:104:ILE:HB	1:A:200:CYS:HB3	1.89	0.55
1:H:135:LEU:O	1:H:139:GLN:HG2	2.07	0.55
1:J:129:PRO:HB3	1:J:186:TYR:CZ	2.42	0.55
1:D:186:TYR:O	1:D:190:MET:HG3	2.06	0.55
1:K:42:VAL:HG12	1:K:43:ARG:HG3	1.87	0.55
1:I:73:VAL:HG13	1:I:85:LEU:HD22	1.88	0.55
1:B:100:LEU:HD11	1:B:210:GLU:HB3	1.88	0.54
1:H:137:ALA:HB2	1:H:231:MET:HE1	1.88	0.54
1:K:208:THR:OG1	1:K:210:GLU:OE1	2.26	0.54
1:L:42:VAL:HG12	1:L:43:ARG:HG3	1.88	0.54
1:G:74:THR:O	1:G:78:LYS:HG2	2.07	0.54
1:L:17:LEU:HB2	1:L:59:LEU:HD12	1.88	0.54
1:L:17:LEU:HD12	1:L:88:ILE:HD13	1.90	0.54
1:L:191:GLU:OE2	6:L:301:HOH:O	2.18	0.54
1:I:227:LEU:O	1:I:231:MET:HG2	2.08	0.54
1:H:218:VAL:HG23	1:H:219:GLU:HG3	1.89	0.54
2:C:303:GOL:H11	1:F:64:MET:SD	2.47	0.54
1:E:100:LEU:HD13	1:E:212:LEU:HD23	1.89	0.54
1:G:62:HIS:HE1	1:G:87:ARG:HD2	1.72	0.54
1:K:101:LYS:HG2	1:K:220:SER:HB2	1.90	0.54
1:J:55:ARG:NH2	6:J:309:HOH:O	2.32	0.53
1:K:227:LEU:O	1:K:231:MET:HG2	2.08	0.53
1:F:19:CYS:O	1:F:61:GLY:HA2	2.08	0.53
1:D:6:ASN:HB2	1:D:42:VAL:HG23	1.90	0.53
1:F:66:ILE:HG23	1:F:184:GLY:HA3	1.89	0.53
1:J:5:ILE:HG22	1:J:7:ALA:H	1.73	0.53
1:C:91:CYS:SG	1:C:200:CYS:HB3	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:CYS:O	1:K:61:GLY:HA2	2.09	0.53
1:J:45:MET:HG2	1:J:72:TYR:CZ	2.44	0.53
1:G:104:ILE:HA	1:G:149:LYS:O	2.09	0.53
1:E:19:CYS:O	1:E:61:GLY:HA2	2.09	0.53
1:G:60:MET:HG2	1:G:76:LEU:HD11	1.89	0.53
1:A:79:THR:OG1	6:A:404:HOH:O	2.19	0.52
1:B:91:CYS:SG	1:B:200:CYS:HB3	2.49	0.52
1:D:214:PRO:HA	1:D:217:ARG:HB2	1.91	0.52
1:F:164:THR:CG2	2:F:304:GOL:H12	2.39	0.52
1:D:88:ILE:HA	1:D:199:LEU:O	2.09	0.52
1:G:17:LEU:HD11	1:G:228:ALA:HB1	1.91	0.52
1:L:6:ASN:HB2	1:L:40:THR:HA	1.92	0.52
1:H:178:ILE:HG22	4:H:302:05Z:C8	2.40	0.52
1:A:19:CYS:SG	1:A:24:ARG:NH1	2.83	0.52
1:F:55:ARG:NH2	6:F:411:HOH:O	2.42	0.52
1:H:156:SER:OG	2:H:303:GOL:H32	2.11	0.51
1:A:24:ARG:HH12	1:A:89:GLY:HA2	1.74	0.51
1:C:206:LEU:HD21	4:C:302:05Z:S1	2.50	0.51
1:E:186:TYR:O	1:E:190:MET:HG3	2.09	0.51
1:L:26:SER:HA	1:L:48:PHE:CE2	2.45	0.51
1:F:227:LEU:O	1:F:231:MET:HG3	2.11	0.51
1:L:22:PRO:HA	1:L:25:VAL:HG23	1.92	0.51
1:I:33:LEU:N	6:I:401:HOH:O	2.15	0.51
1:J:208:THR:O	1:J:208:THR:OG1	2.18	0.51
1:J:53:LYS:NZ	1:J:230:GLU:OE1	2.37	0.51
1:L:51:LYS:HA	1:L:55:ARG:O	2.10	0.51
1:L:143:ARG:HG2	1:L:143:ARG:HH11	1.76	0.51
1:L:72:TYR:O	1:L:76:LEU:HG	2.11	0.51
1:B:87:ARG:NH2	1:B:179:GLU:OE1	2.43	0.51
1:B:136:ARG:NH2	6:B:402:HOH:O	2.41	0.51
1:L:17:LEU:HD11	1:L:228:ALA:HB1	1.92	0.51
1:F:28:ILE:HG12	1:F:225:ILE:HD13	1.93	0.51
1:G:51:LYS:HA	1:G:55:ARG:O	2.11	0.51
1:K:94:ILE:HA	1:K:207:ILE:HG12	1.94	0.51
1:G:174:ASN:ND2	6:G:311:HOH:O	2.45	0.50
1:L:104:ILE:HA	1:L:149:LYS:O	2.11	0.50
1:E:221:PHE:O	1:E:225:ILE:HG12	2.10	0.50
1:A:9:ILE:O	6:A:403:HOH:O	2.19	0.50
1:F:95:SER:HB3	1:F:176:LEU:HA	1.93	0.50
1:K:163:GLU:HB2	2:K:303:GOL:H2	1.92	0.50
1:D:28:ILE:HD11	1:D:225:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:GLU:HA	4:H:302:05Z:N9	2.25	0.50
1:J:19:CYS:O	1:J:61:GLY:HA2	2.11	0.50
1:K:35:ASP:OD1	6:K:401:HOH:O	2.19	0.50
1:A:210:GLU:HA	6:A:417:HOH:O	2.11	0.50
1:I:44:ASN:HB2	1:L:22:PRO:HG2	1.94	0.50
1:B:77:ILE:HG21	1:B:192:LEU:HB3	1.94	0.50
1:I:58:SER:O	1:I:59:LEU:HD23	2.11	0.50
1:K:139:GLN:NE2	6:K:410:HOH:O	2.44	0.50
1:D:19:CYS:O	1:D:61:GLY:HA2	2.12	0.50
1:E:211:ALA:HB1	1:E:217:ARG:NH2	2.27	0.50
1:G:34:GLN:NE2	6:G:306:HOH:O	2.33	0.50
1:K:18:LEU:HD11	1:K:85:LEU:HB3	1.94	0.50
1:L:104:ILE:HB	1:L:200:CYS:HB3	1.94	0.49
1:D:33:LEU:HD11	1:D:57:ILE:HD11	1.95	0.49
1:H:221:PHE:HB3	1:H:224:MET:HE2	1.94	0.49
1:A:60:MET:HG2	1:A:76:LEU:HD11	1.93	0.49
1:C:19:CYS:O	1:C:61:GLY:HA2	2.13	0.49
1:G:131:PHE:CE2	1:L:105:MET:HE1	2.47	0.49
1:H:19:CYS:O	1:H:61:GLY:HA2	2.12	0.49
1:J:6:ASN:OD1	1:J:40:THR:HA	2.12	0.49
1:L:164:THR:HA	1:L:167:PHE:CE1	2.48	0.49
1:B:19:CYS:O	1:B:61:GLY:HA2	2.12	0.49
1:I:19:CYS:SG	1:I:24:ARG:CZ	3.00	0.49
1:L:94:ILE:HG23	1:L:206:LEU:HD12	1.95	0.49
1:B:100:LEU:HD22	1:B:212:LEU:HG	1.94	0.48
1:B:213:SER:N	1:B:214:PRO:HD3	2.28	0.48
1:E:95:SER:HB2	1:E:176:LEU:HA	1.95	0.48
1:D:45:MET:HG2	1:D:72:TYR:CZ	2.48	0.48
1:G:98:VAL:HG12	1:G:149:LYS:HG3	1.95	0.48
1:K:163:GLU:OE1	2:K:303:GOL:O2	2.31	0.48
1:F:15:GLN:HG3	1:F:232:MET:CE	2.43	0.48
1:L:26:SER:O	1:L:29:ALA:N	2.46	0.48
1:D:221:PHE:CZ	1:D:225:ILE:HD11	2.49	0.48
1:G:149:LYS:NZ	6:G:312:HOH:O	2.46	0.48
1:B:130:ASP:OD2	1:B:132:GLU:HB2	2.13	0.48
1:D:78:LYS:HD3	2:D:302:GOL:O3	2.13	0.48
1:F:180:MET:HG3	2:F:301:GOL:H12	1.95	0.48
1:B:114:LYS:HB2	1:E:114:LYS:HB2	1.95	0.48
1:D:21:ASP:OD2	6:D:402:HOH:O	2.20	0.48
1:E:49:SER:HA	1:E:58:SER:HA	1.95	0.48
1:E:221:PHE:CE2	1:E:225:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:203:SER:HA	1:J:212:LEU:HD12	1.95	0.48
1:B:21:ASP:OD1	1:E:43:ARG:HA	2.14	0.48
1:I:129:PRO:HB3	1:I:186:TYR:CZ	2.48	0.48
1:J:136:ARG:NH2	6:J:316:HOH:O	2.46	0.48
1:D:3:PRO:HD2	1:D:75:GLU:OE2	2.13	0.48
1:I:15:GLN:NE2	1:I:55:ARG:HH21	2.11	0.48
1:F:91:CYS:SG	1:F:200:CYS:HB2	2.54	0.47
1:H:43:ARG:HA	1:K:21:ASP:OD1	2.14	0.47
1:E:31:LYS:HB3	1:E:32:PHE:CD2	2.50	0.47
1:B:6:ASN:ND2	1:B:41:ASN:OD1	2.47	0.47
1:G:29:ALA:HA	1:G:33:LEU:HD12	1.95	0.47
1:G:55:ARG:HE	1:G:233:SER:HA	1.79	0.47
1:G:81:GLN:HA	6:G:314:HOH:O	2.14	0.47
1:I:135:LEU:HD21	1:K:138:TYR:CE2	2.50	0.47
1:A:85:LEU:O	1:A:196:ALA:HA	2.15	0.47
1:A:173:TYR:CE2	1:F:191:GLU:HB2	2.50	0.47
1:I:94:ILE:HD11	1:I:167:PHE:CD2	2.50	0.47
1:L:84:GLU:HG2	1:L:133:LEU:HD11	1.96	0.47
1:D:92:GLY:HA3	1:D:206:LEU:HD21	1.96	0.47
1:E:131:PHE:O	1:E:134:SER:OG	2.23	0.47
1:I:152:ASN:HD21	1:K:126:SER:HB3	1.79	0.47
1:B:88:ILE:HG22	1:B:199:LEU:HB2	1.96	0.47
1:C:106:ALA:HA	1:C:151:GLY:O	2.15	0.47
1:D:209:LYS:N	6:D:401:HOH:O	2.47	0.47
1:E:17:LEU:HD13	1:E:57:ILE:HD11	1.97	0.47
1:E:100:LEU:HB3	1:E:212:LEU:HD21	1.97	0.47
1:F:164:THR:HG21	2:F:304:GOL:H12	1.97	0.47
1:G:62:HIS:CD2	1:G:69:CYS:HB2	2.49	0.47
1:H:180:MET:HB2	3:H:301:TRS:H31	1.97	0.47
1:I:191:GLU:HB2	1:K:173:TYR:CE2	2.50	0.47
1:K:158:PHE:CD2	2:K:303:GOL:H12	2.50	0.47
1:J:227:LEU:O	1:J:231:MET:HG2	2.14	0.47
1:E:31:LYS:HB3	1:E:32:PHE:CE2	2.50	0.47
1:J:17:LEU:HD23	1:J:18:LEU:H	1.80	0.47
1:E:208:THR:O	1:E:210:GLU:N	2.48	0.46
1:G:214:PRO:HA	1:G:217:ARG:HD2	1.97	0.46
1:L:8:LYS:HD2	1:L:9:ILE:H	1.79	0.46
1:A:114:LYS:HB2	1:D:114:LYS:HB2	1.96	0.46
1:H:21:ASP:OD1	1:K:43:ARG:HA	2.15	0.46
1:D:131:PHE:CE2	1:D:135:LEU:HD11	2.50	0.46
1:J:59:LEU:HD12	1:J:59:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:HD23	1:D:121:LEU:HD11	1.98	0.46
1:I:25:VAL:HG13	1:I:59:LEU:HB3	1.97	0.46
1:F:37:LYS:NZ	6:F:409:HOH:O	2.39	0.46
1:I:100:LEU:HD13	1:I:212:LEU:HG	1.97	0.46
1:I:23:LEU:HD21	1:L:44:ASN:OD1	2.15	0.46
1:K:66:ILE:HG23	1:K:184:GLY:HA3	1.97	0.46
1:L:164:THR:HG22	1:L:167:PHE:CZ	2.51	0.46
1:E:37:LYS:O	1:E:39:ILE:HG23	2.16	0.46
1:H:18:LEU:HB3	1:H:62:HIS:HD2	1.81	0.46
1:I:17:LEU:HB2	1:I:59:LEU:HD22	1.98	0.46
1:I:140:THR:HG22	1:I:227:LEU:HD12	1.98	0.46
1:G:60:MET:HE3	1:G:60:MET:HA	1.98	0.46
1:A:172:LYS:NZ	6:A:416:HOH:O	2.50	0.45
1:B:8:LYS:O	1:B:11:ASP:HB2	2.15	0.45
1:B:20:GLY:HA3	2:B:303:GOL:H11	1.98	0.45
1:B:89:GLY:H	1:B:224:MET:HE3	1.80	0.45
1:G:128:THR:HG21	1:L:108:GLY:HA3	1.99	0.45
1:H:233:SER:O	6:H:402:HOH:O	2.20	0.45
1:J:8:LYS:HB2	1:J:8:LYS:HE2	1.68	0.45
1:K:19:CYS:SG	1:K:24:ARG:NH2	2.88	0.45
1:K:24:ARG:HD2	1:K:221:PHE:CZ	2.51	0.45
1:L:31:LYS:HB3	1:L:32:PHE:CD1	2.52	0.45
1:F:17:LEU:HD12	1:F:86:LEU:O	2.17	0.45
1:C:135:LEU:O	1:C:139:GLN:HG3	2.16	0.45
1:C:191:GLU:HB2	1:E:173:TYR:CE1	2.51	0.45
1:E:135:LEU:O	1:E:139:GLN:HG3	2.16	0.45
1:F:15:GLN:HG2	6:F:401:HOH:O	2.17	0.45
1:A:221:PHE:HD2	1:A:225:ILE:HD11	1.80	0.45
1:B:3:PRO:HB2	1:B:4:HIS:CE1	2.51	0.45
1:D:51:LYS:HA	1:D:55:ARG:O	2.17	0.45
1:G:129:PRO:HB3	1:G:186:TYR:CE1	2.52	0.45
1:B:216:GLU:HA	1:B:219:GLU:HG2	1.98	0.45
1:B:17:LEU:HD23	1:B:86:LEU:O	2.17	0.45
1:B:28:ILE:HD11	1:B:225:ILE:HD12	1.98	0.45
1:G:131:PHE:CD2	1:L:150:VAL:HG11	2.52	0.45
1:H:205:HIS:CD2	1:H:207:ILE:HG13	2.52	0.45
1:F:85:LEU:O	1:F:196:ALA:HA	2.17	0.45
1:H:208:THR:O	1:H:209:LYS:HG3	2.16	0.45
1:L:34:GLN:O	1:L:51:LYS:N	2.48	0.45
1:B:55:ARG:HG2	1:B:56:GLY:H	1.82	0.45
1:B:57:ILE:HD12	1:B:232:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:MET:HG2	3:C:301:TRS:C3	2.46	0.45
1:C:64:MET:HG2	3:C:301:TRS:H32	1.98	0.45
1:B:34:GLN:HA	1:B:34:GLN:NE2	2.32	0.45
1:K:88:ILE:HA	1:K:199:LEU:O	2.16	0.45
1:F:228:ALA:O	1:F:231:MET:HB2	2.17	0.44
1:J:28:ILE:HG12	1:J:225:ILE:HD13	2.00	0.44
1:A:23:LEU:HD21	1:D:44:ASN:N	2.31	0.44
1:D:31:LYS:HD3	1:D:32:PHE:CZ	2.51	0.44
1:D:138:TYR:CE1	1:D:142:LYS:HE3	2.52	0.44
1:H:180:MET:HG3	4:H:302:05Z:N9	2.32	0.44
1:H:215:LYS:HE3	1:H:219:GLU:OE1	2.17	0.44
1:I:140:THR:O	1:I:144:LEU:HG	2.17	0.44
1:C:180:MET:HB2	3:C:301:TRS:H21	2.00	0.44
1:D:140:THR:HG23	1:D:143:ARG:NH2	2.32	0.44
1:D:213:SER:OG	1:D:216:GLU:HB2	2.18	0.44
1:E:81:GLN:O	1:E:83:LYS:HE2	2.16	0.44
1:E:104:ILE:HA	1:E:149:LYS:O	2.18	0.44
1:D:18:LEU:HD11	1:D:85:LEU:HB3	2.00	0.44
1:B:31:LYS:HG2	1:B:32:PHE:CE1	2.53	0.44
1:F:18:LEU:HD11	1:F:85:LEU:HD23	2.00	0.44
1:E:100:LEU:O	1:E:101:LYS:HB2	2.18	0.44
1:G:106:ALA:O	1:G:129:PRO:HG3	2.18	0.44
1:G:135:LEU:HD21	1:L:138:TYR:CD2	2.53	0.44
1:H:110:SER:HB3	1:J:124:ASP:O	2.17	0.44
1:D:192:LEU:HD21	2:D:302:GOL:O3	2.18	0.44
1:A:24:ARG:HD2	1:A:221:PHE:CZ	2.52	0.44
1:A:164:THR:HA	1:A:167:PHE:CE1	2.53	0.44
1:D:227:LEU:O	1:D:231:MET:HG2	2.17	0.43
1:F:15:GLN:HG3	1:F:232:MET:HE3	1.99	0.43
1:J:33:LEU:HD11	1:J:59:LEU:CD1	2.41	0.43
1:D:11:ASP:OD1	6:D:403:HOH:O	2.20	0.43
1:D:142:LYS:HA	1:D:142:LYS:HD3	1.79	0.43
1:B:89:GLY:N	1:B:224:MET:HE3	2.32	0.43
1:F:34:GLN:NE2	6:F:420:HOH:O	2.51	0.43
1:G:215:LYS:H	1:G:215:LYS:HG3	1.40	0.43
1:A:130:ASP:CG	1:A:195:LYS:HG2	2.39	0.43
1:G:162:PHE:HD1	2:H:305:GOL:H2	1.82	0.43
1:I:83:LYS:HD2	1:I:83:LYS:HA	1.57	0.43
1:B:217:ARG:HG3	1:B:218:VAL:H	1.84	0.43
1:E:98:VAL:HG21	1:E:104:ILE:HD11	2.00	0.43
2:H:304:GOL:H11	1:K:78:LYS:HZ2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:TYR:CZ	1:G:31:LYS:HD2	2.53	0.43
1:H:28:ILE:HG12	1:H:225:ILE:HD13	2.01	0.43
1:I:43:ARG:HA	1:L:21:ASP:OD1	2.18	0.43
1:A:43:ARG:HA	1:D:21:ASP:OD1	2.18	0.43
1:I:159:PHE:HD1	1:I:180:MET:HE3	1.83	0.43
1:B:90:THR:H	1:B:90:THR:HG1	1.59	0.43
1:C:152:ASN:HB2	1:C:174:ASN:O	2.19	0.43
1:C:209:LYS:HB2	1:C:209:LYS:HE2	1.53	0.43
1:E:86:LEU:HD12	1:E:86:LEU:HA	1.83	0.43
1:K:83:LYS:HD2	1:K:83:LYS:HA	1.61	0.43
1:G:17:LEU:HD12	1:G:17:LEU:HA	1.90	0.43
1:F:45:MET:HG2	1:F:72:TYR:CZ	2.54	0.42
1:G:152:ASN:HB3	1:G:175:HIS:CD2	2.54	0.42
1:H:100:LEU:HD13	1:H:210:GLU:HB3	2.01	0.42
1:H:173:TYR:HE1	2:H:305:GOL:HO3	1.67	0.42
1:I:100:LEU:CD1	1:I:212:LEU:HG	2.49	0.42
1:K:104:ILE:HA	1:K:149:LYS:O	2.18	0.42
1:B:3:PRO:HB2	1:B:4:HIS:ND1	2.34	0.42
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.84	0.42
1:I:204:ASP:OD1	1:I:211:ALA:HA	2.19	0.42
1:L:55:ARG:HA	1:L:55:ARG:HD2	1.79	0.42
1:D:216:GLU:HA	1:D:219:GLU:HG2	2.02	0.42
1:I:148:LEU:HD23	1:I:148:LEU:HA	1.85	0.42
1:K:18:LEU:HB3	1:K:62:HIS:HD2	1.84	0.42
1:C:101:LYS:HE2	1:C:220:SER:HB3	2.01	0.42
1:C:215:LYS:O	1:C:219:GLU:HG3	2.19	0.42
1:E:95:SER:OG	6:E:401:HOH:O	2.21	0.42
1:E:212:LEU:HD13	1:E:216:GLU:HB3	2.01	0.42
1:F:129:PRO:HB3	1:F:186:TYR:CZ	2.54	0.42
1:G:129:PRO:HB3	1:G:186:TYR:CZ	2.53	0.42
1:H:133:LEU:HD23	1:H:133:LEU:HA	1.80	0.42
1:J:24:ARG:O	1:J:28:ILE:HG13	2.19	0.42
1:C:45:MET:HG2	1:C:72:TYR:CZ	2.54	0.42
1:E:24:ARG:HD2	1:E:221:PHE:CE2	2.55	0.42
1:F:108:GLY:HA3	1:F:152:ASN:OD1	2.20	0.42
1:G:100:LEU:HB3	1:G:212:LEU:HD21	2.01	0.42
1:K:24:ARG:O	1:K:27:TYR:HB3	2.19	0.42
1:L:136:ARG:NH2	6:L:318:HOH:O	2.51	0.42
1:A:53:LYS:N	6:A:408:HOH:O	2.38	0.42
1:C:28:ILE:HG12	1:C:225:ILE:HD13	2.01	0.42
1:L:142:LYS:HB3	1:L:142:LYS:HE2	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:LEU:O	1:G:231:MET:HG2	2.20	0.42
1:A:73:VAL:HG13	1:A:85:LEU:HD22	2.01	0.42
1:F:93:ALA:HB2	1:F:202:VAL:CG1	2.50	0.42
1:F:112:ASP:OD1	1:F:156:SER:HA	2.20	0.42
1:J:19:CYS:HG	1:J:24:ARG:HH21	1.66	0.42
1:J:88:ILE:HA	1:J:199:LEU:O	2.20	0.42
1:L:17:LEU:HD13	1:L:17:LEU:HA	1.94	0.42
1:A:132:GLU:H	1:A:132:GLU:CD	2.16	0.42
1:G:24:ARG:O	1:G:27:TYR:HB3	2.20	0.42
1:G:100:LEU:HD11	1:G:210:GLU:HB2	2.02	0.41
1:G:217:ARG:H	1:G:217:ARG:HG3	1.65	0.41
1:J:180:MET:HB2	1:J:181:GLU:OE2	2.20	0.41
1:G:62:HIS:CE1	1:G:87:ARG:HD2	2.53	0.41
1:K:215:LYS:O	1:K:218:VAL:HG12	2.20	0.41
1:A:158:PHE:C	1:A:180:MET:HE3	2.40	0.41
1:G:225:ILE:HG22	1:G:229:LEU:HD12	2.03	0.41
1:I:6:ASN:OD1	1:I:40:THR:HA	2.20	0.41
1:K:89:GLY:O	1:K:200:CYS:HA	2.20	0.41
1:L:148:LEU:HD12	1:L:148:LEU:HA	1.81	0.41
1:B:98:VAL:HG13	1:B:176:LEU:HD22	2.03	0.41
1:D:203:SER:HB2	1:D:217:ARG:NH1	2.36	0.41
1:F:205:HIS:ND1	1:F:208:THR:HG23	2.36	0.41
1:H:17:LEU:HB2	1:H:59:LEU:HD23	2.01	0.41
1:B:57:ILE:HD11	1:B:232:MET:HB3	2.03	0.41
1:A:106:ALA:HA	1:A:151:GLY:O	2.21	0.41
1:C:114:LYS:HE2	1:F:112:ASP:O	2.20	0.41
1:F:212:LEU:HD23	1:F:212:LEU:HA	1.85	0.41
1:I:21:ASP:OD1	1:L:43:ARG:HA	2.20	0.41
1:J:22:PRO:HB3	1:J:46:LEU:H	1.85	0.41
1:L:28:ILE:HG22	1:L:59:LEU:HD21	2.02	0.41
1:K:6:ASN:OD1	1:K:40:THR:HA	2.21	0.41
1:G:18:LEU:HD23	1:G:60:MET:HB3	2.02	0.41
1:G:62:HIS:HD2	1:G:63:GLY:O	2.02	0.41
1:H:207:ILE:HG13	1:H:208:THR:H	1.85	0.41
1:L:66:ILE:O	1:L:70:THR:OG1	2.27	0.41
1:A:33:LEU:CD2	1:A:57:ILE:HD11	2.50	0.41
1:A:208:THR:HG22	1:A:210:GLU:HG2	2.02	0.41
1:B:64:MET:O	1:E:68:SER:HB2	2.21	0.41
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.90	0.41
1:D:225:ILE:HG12	1:D:225:ILE:H	1.63	0.41
1:G:105:MET:HG3	1:G:197:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:VAL:HG13	1:K:59:LEU:HB3	2.01	0.41
1:K:62:HIS:NE2	1:K:87:ARG:HD2	2.36	0.41
1:A:159:PHE:N	1:A:180:MET:HE3	2.35	0.41
1:C:25:VAL:HG12	1:C:48:PHE:CD2	2.56	0.41
1:A:19:CYS:SG	1:A:24:ARG:CZ	3.09	0.40
1:B:172:LYS:HE2	1:D:191:GLU:HG2	2.03	0.40
1:A:213:SER:O	1:A:216:GLU:N	2.54	0.40
1:D:132:GLU:OE2	1:D:195:LYS:NZ	2.54	0.40
1:E:24:ARG:O	1:E:28:ILE:HG13	2.21	0.40
1:L:62:HIS:NE2	1:L:87:ARG:HD2	2.36	0.40
1:B:155:SER:HA	1:B:179:GLU:O	2.21	0.40
1:F:13:TYR:HB2	6:F:401:HOH:O	2.20	0.40
1:H:161:SER:OG	2:H:303:GOL:H2	2.21	0.40
1:H:218:VAL:CG2	1:H:219:GLU:HG3	2.52	0.40
1:L:93:ALA:HB3	1:L:205:HIS:CD2	2.57	0.40
1:A:221:PHE:CD2	1:A:225:ILE:HD11	2.55	0.40
1:E:21:ASP:O	1:E:24:ARG:HB3	2.21	0.40
1:F:9:ILE:H	1:F:9:ILE:HG12	1.72	0.40
1:I:212:LEU:HD22	1:I:217:ARG:CZ	2.51	0.40
1:K:213:SER:O	1:K:217:ARG:N	2.49	0.40
1:D:87:ARG:NH2	1:D:181:GLU:OE1	2.54	0.40
1:L:5:ILE:HG23	1:L:40:THR:HG21	2.03	0.40

All (1) 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)
1:D:55:ARG:NH2	1:H:27:TYR:OH[3_645]	2.00	0.20

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	231/233 (99%)	221 (96%)	10 (4%)	0	100 100
1	B	231/233 (99%)	213 (92%)	15 (6%)	3 (1%)	12 6
1	C	231/233 (99%)	218 (94%)	12 (5%)	1 (0%)	34 30
1	D	231/233 (99%)	221 (96%)	10 (4%)	0	100 100
1	E	231/233 (99%)	215 (93%)	13 (6%)	3 (1%)	12 6
1	F	231/233 (99%)	221 (96%)	10 (4%)	0	100 100
1	G	231/233 (99%)	218 (94%)	12 (5%)	1 (0%)	34 30
1	H	231/233 (99%)	222 (96%)	9 (4%)	0	100 100
1	I	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	34 30
1	J	231/233 (99%)	217 (94%)	11 (5%)	3 (1%)	12 6
1	K	231/233 (99%)	224 (97%)	7 (3%)	0	100 100
1	L	231/233 (99%)	215 (93%)	16 (7%)	0	100 100
All	All	2772/2796 (99%)	2620 (94%)	140 (5%)	12 (0%)	34 30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	209	LYS
1	B	214	PRO
1	E	209	LYS
1	G	101	LYS
1	E	36	ALA
1	E	49	SER
1	I	215	LYS
1	J	208	THR
1	B	217	ARG
1	C	209	LYS
1	J	207	ILE
1	B	213	SER

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	196/196 (100%)	187 (95%)	9 (5%)	27 23
1	B	196/196 (100%)	191 (97%)	5 (3%)	46 48
1	C	195/196 (100%)	187 (96%)	8 (4%)	30 28
1	D	196/196 (100%)	189 (96%)	7 (4%)	35 34
1	E	196/196 (100%)	193 (98%)	3 (2%)	65 69
1	F	196/196 (100%)	188 (96%)	8 (4%)	30 28
1	G	196/196 (100%)	185 (94%)	11 (6%)	21 17
1	H	196/196 (100%)	190 (97%)	6 (3%)	40 40
1	I	195/196 (100%)	178 (91%)	17 (9%)	10 6
1	J	196/196 (100%)	184 (94%)	12 (6%)	18 14
1	K	196/196 (100%)	189 (96%)	7 (4%)	35 34
1	L	196/196 (100%)	185 (94%)	11 (6%)	21 17
All	All	2350/2352 (100%)	2246 (96%)	104 (4%)	28 25

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	18	LEU
1	A	49	SER
1	A	142	LYS
1	A	179	GLU
1	A	200	CYS
1	A	201	SER
1	A	207	ILE
1	B	179	GLU
1	B	204	ASP
1	B	215	LYS
1	B	217	ARG
1	B	223	ASN
1	C	37	LYS
1	C	44	ASN
1	C	121	LEU
1	C	142	LYS
1	C	179	GLU
1	C	208	THR
1	C	209	LYS
1	C	215	LYS

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Mol	Chain	Res	Type
1	D	37	LYS
1	D	62	HIS
1	D	78	LYS
1	D	121	LEU
1	D	169	LEU
1	D	179	GLU
1	D	201	SER
1	E	2	THR
1	E	90	THR
1	E	179	GLU
1	F	9	ILE
1	F	35	ASP
1	F	95	SER
1	F	134	SER
1	F	179	GLU
1	F	204	ASP
1	F	217	ARG
1	F	233	SER
1	G	44	ASN
1	G	49	SER
1	G	55	ARG
1	G	62	HIS
1	G	69	CYS
1	G	91	CYS
1	G	179	GLU
1	G	200	CYS
1	G	201	SER
1	G	209	LYS
1	G	223	ASN
1	H	26	SER
1	H	95	SER
1	H	139	GLN
1	H	153	VAL
1	H	179	GLU
1	H	209	LYS
1	I	8	LYS
1	I	9	ILE
1	I	30	LYS
1	I	37	LYS
1	I	49	SER
1	I	57	ILE
1	I	62	HIS

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Mol	Chain	Res	Type
1	I	90	THR
1	I	94	ILE
1	I	97	LYS
1	I	126	SER
1	I	179	GLU
1	I	209	LYS
1	I	215	LYS
1	I	217	ARG
1	I	218	VAL
1	I	221	PHE
1	J	1	MET
1	J	55	ARG
1	J	57	ILE
1	J	81	GLN
1	J	87	ARG
1	J	179	GLU
1	J	192	LEU
1	J	201	SER
1	J	208	THR
1	J	215	LYS
1	J	217	ARG
1	J	220	SER
1	K	44	ASN
1	K	55	ARG
1	K	87	ARG
1	K	134	SER
1	K	172	LYS
1	K	179	GLU
1	K	201	SER
1	L	59	LEU
1	L	62	HIS
1	L	101	LYS
1	L	142	LYS
1	L	146	ILE
1	L	179	GLU
1	L	200	CYS
1	L	204	ASP
1	L	213	SER
1	L	215	LYS
1	L	233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	139	GLN
1	D	223	ASN
1	E	122	ASN
1	E	223	ASN
1	G	62	HIS
1	G	205	HIS
1	H	205	HIS
1	I	15	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	H	306	-	4,4,4	0.73	0	6,6,6	0.88	0
3	TRS	C	301	-	7,7,7	0.29	0	9,9,9	0.60	0
2	GOL	K	301	-	5,5,5	1.16	0	5,5,5	0.97	0
2	GOL	H	303	-	5,5,5	1.21	1 (20%)	5,5,5	0.68	0
2	GOL	B	303	-	5,5,5	0.87	0	5,5,5	1.19	0
2	GOL	F	304	-	5,5,5	1.35	0	5,5,5	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	F	301	-	5,5,5	1.15	1 (20%)	5,5,5	0.97	0
2	GOL	B	301	-	5,5,5	0.98	0	5,5,5	0.84	0
2	GOL	D	301	-	5,5,5	0.86	0	5,5,5	1.04	0
2	GOL	D	302	-	5,5,5	1.12	0	5,5,5	1.04	0
2	GOL	K	302	-	5,5,5	0.98	0	5,5,5	1.04	0
2	GOL	I	301	-	5,5,5	0.86	0	5,5,5	0.99	0
2	GOL	A	302	-	5,5,5	0.87	0	5,5,5	1.00	0
3	TRS	H	301	-	7,7,7	0.30	0	9,9,9	1.02	1 (11%)
2	GOL	H	305	-	5,5,5	1.25	1 (20%)	5,5,5	1.05	0
2	GOL	C	303	-	5,5,5	1.46	1 (20%)	5,5,5	0.70	0
2	GOL	A	301	-	5,5,5	0.96	0	5,5,5	1.05	0
4	05Z	H	302	-	17,19,20	1.62	1 (5%)	17,25,27	2.63	6 (35%)
2	GOL	E	301	-	5,5,5	0.93	0	5,5,5	0.86	0
2	GOL	K	303	-	5,5,5	1.44	1 (20%)	5,5,5	0.73	0
2	GOL	B	302	-	5,5,5	1.19	0	5,5,5	0.85	0
5	PO4	C	304	-	4,4,4	0.57	0	6,6,6	0.72	0
2	GOL	F	303	-	5,5,5	0.98	0	5,5,5	0.95	0
2	GOL	F	302	-	5,5,5	1.31	1 (20%)	5,5,5	0.93	0
4	05Z	C	302	-	17,19,20	1.81	2 (11%)	17,25,27	2.68	6 (35%)
2	GOL	H	304	-	5,5,5	1.34	0	5,5,5	0.77	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
3	TRS	C	301	-	-	5/9/9/9	-
2	GOL	K	301	-	-	1/4/4/4	-
2	GOL	H	303	-	-	2/4/4/4	-
2	GOL	B	303	-	-	0/4/4/4	-
2	GOL	F	304	-	-	0/4/4/4	-
2	GOL	F	301	-	-	2/4/4/4	-
2	GOL	B	301	-	-	1/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	D	302	-	-	4/4/4/4	-
2	GOL	K	302	-	-	0/4/4/4	-
2	GOL	I	301	-	-	2/4/4/4	-
2	GOL	A	302	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	H	301	-	-	6/9/9/9	-
2	GOL	H	305	-	-	3/4/4/4	-
2	GOL	C	303	-	-	4/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
4	05Z	H	302	-	-	1/4/5/5	0/3/3/3
2	GOL	E	301	-	-	1/4/4/4	-
2	GOL	K	303	-	-	2/4/4/4	-
2	GOL	B	302	-	-	2/4/4/4	-
2	GOL	F	303	-	-	4/4/4/4	-
2	GOL	F	302	-	-	2/4/4/4	-
4	05Z	C	302	-	-	3/4/5/5	0/3/3/3
2	GOL	H	304	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	302	05Z	C6-S1	6.30	1.84	1.76
4	H	302	05Z	C6-S1	5.41	1.82	1.76
2	C	303	GOL	C3-C2	2.53	1.62	1.51
2	F	302	GOL	O2-C2	-2.51	1.35	1.43
2	K	303	GOL	O2-C2	-2.33	1.36	1.43
4	C	302	05Z	C6-N1	2.26	1.36	1.33
2	F	301	GOL	C3-C2	2.16	1.60	1.51
2	H	303	GOL	O2-C2	-2.11	1.37	1.43
2	H	305	GOL	C1-C2	2.05	1.60	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	302	05Z	N3-C2-N1	-6.75	118.13	128.68
4	C	302	05Z	C9-S1-C6	6.30	110.09	101.52
4	C	302	05Z	N3-C2-N1	-6.28	118.87	128.68
4	H	302	05Z	C9-S1-C6	5.31	108.74	101.52
4	H	302	05Z	C2-N3-C4	3.81	122.38	113.45
4	C	302	05Z	C2-N3-C4	3.68	122.07	113.45
4	C	302	05Z	S1-C6-N1	3.17	125.00	117.85
4	H	302	05Z	C2-N1-C6	3.11	123.24	116.36
4	C	302	05Z	C2-N1-C6	2.77	122.49	116.36
4	H	302	05Z	S1-C6-N1	2.77	124.08	117.85
4	C	302	05Z	C5-C6-S1	-2.18	115.69	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	302	05Z	C10-C9-S1	2.14	119.01	110.62
3	H	301	TRS	C3-C-C2	-2.05	104.45	110.81

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	A	302	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-C3
2	B	302	GOL	O1-C1-C2-O2
2	B	302	GOL	O1-C1-C2-C3
2	C	303	GOL	O1-C1-C2-C3
2	D	301	GOL	C1-C2-C3-O3
2	D	302	GOL	O1-C1-C2-C3
2	D	302	GOL	C1-C2-C3-O3
2	F	303	GOL	C1-C2-C3-O3
2	H	303	GOL	C1-C2-C3-O3
2	H	305	GOL	O1-C1-C2-C3
3	C	301	TRS	N-C-C3-O3
3	H	301	TRS	N-C-C1-O1
3	H	301	TRS	C2-C-C3-O3
3	H	301	TRS	N-C-C3-O3
2	H	303	GOL	O2-C2-C3-O3
2	B	301	GOL	C1-C2-C3-O3
2	C	303	GOL	C1-C2-C3-O3
2	F	302	GOL	O1-C1-C2-C3
2	H	305	GOL	C1-C2-C3-O3
2	I	301	GOL	O1-C1-C2-C3
2	K	303	GOL	C1-C2-C3-O3
2	C	303	GOL	O2-C2-C3-O3
2	D	301	GOL	O2-C2-C3-O3
2	H	305	GOL	O1-C1-C2-O2
3	C	301	TRS	C3-C-C2-O2
3	H	301	TRS	C2-C-C1-O1
4	C	302	05Z	N1-C6-S1-C9
2	C	303	GOL	O1-C1-C2-O2
2	D	302	GOL	O2-C2-C3-O3
2	F	303	GOL	O2-C2-C3-O3
4	C	302	05Z	C15-C10-C9-S1
2	K	303	GOL	O2-C2-C3-O3
4	C	302	05Z	C11-C10-C9-S1

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Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O2-C2-C3-O3
2	F	303	GOL	O1-C1-C2-O2
3	C	301	TRS	C1-C-C2-O2
3	C	301	TRS	C2-C-C3-O3
3	H	301	TRS	C3-C-C1-O1
3	H	301	TRS	C1-C-C3-O3
4	H	302	05Z	N1-C6-S1-C9
2	D	302	GOL	O1-C1-C2-O2
2	F	302	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-O2
2	I	301	GOL	O1-C1-C2-O2
2	F	303	GOL	O1-C1-C2-C3
3	C	301	TRS	N-C-C2-O2
2	A	302	GOL	C1-C2-C3-O3
2	F	301	GOL	C1-C2-C3-O3
2	K	301	GOL	O1-C1-C2-C3
2	E	301	GOL	O2-C2-C3-O3
2	F	301	GOL	O1-C1-C2-O2

There are no ring outliers.

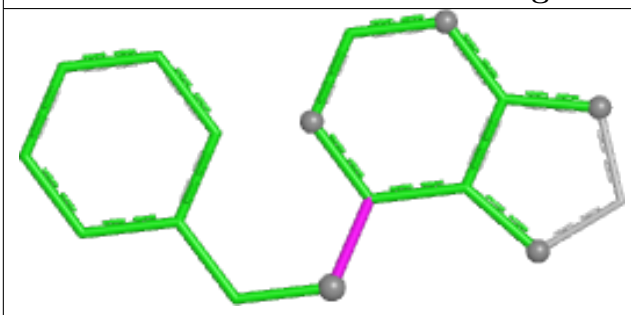
14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	TRS	3	0
2	H	303	GOL	2	0
2	B	303	GOL	5	0
2	F	304	GOL	4	0
2	F	301	GOL	2	0
2	D	302	GOL	2	0
3	H	301	TRS	1	0
2	H	305	GOL	4	0
2	C	303	GOL	1	0
4	H	302	05Z	3	0
2	K	303	GOL	3	0
2	F	303	GOL	1	0
4	C	302	05Z	1	0
2	H	304	GOL	2	0

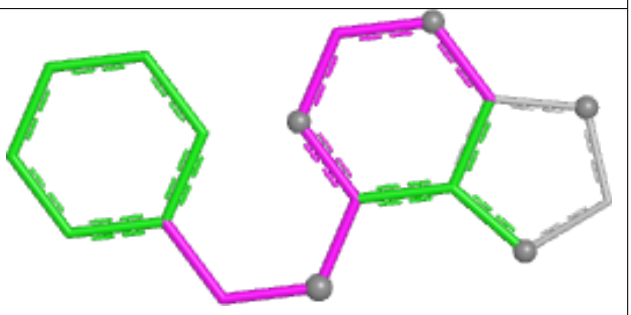
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

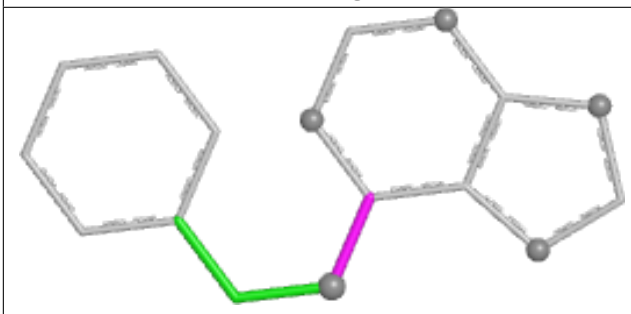
Ligand 05Z H 302



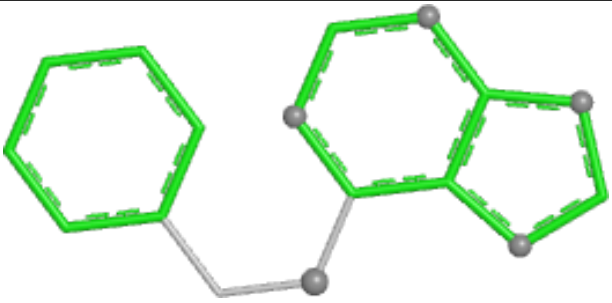
Bond lengths



Bond angles

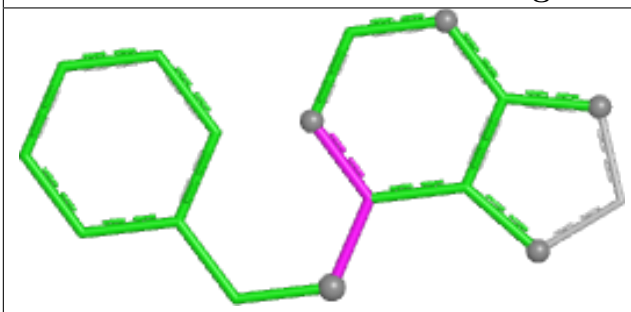


Torsions

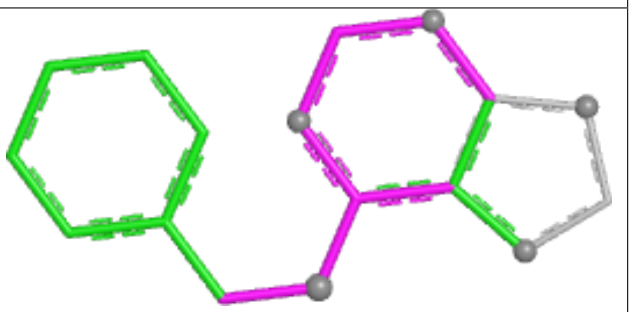


Rings

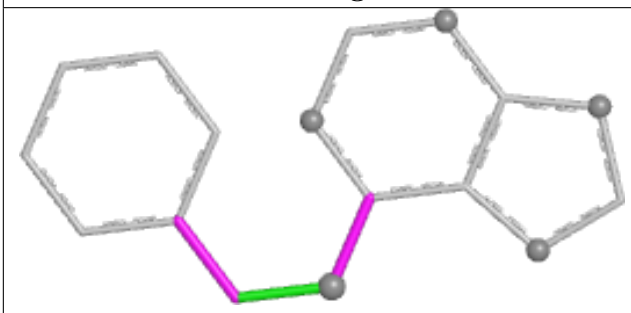
Ligand 05Z C 302



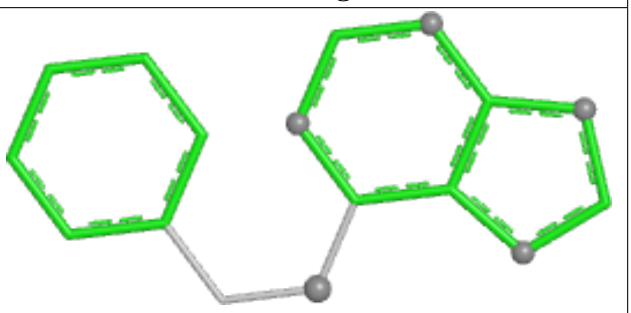
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	233/233 (100%)	0.18	4 (1%) 70 68	24, 39, 58, 67	0
1	B	233/233 (100%)	0.71	13 (5%) 24 23	29, 47, 75, 108	0
1	C	233/233 (100%)	0.15	1 (0%) 92 92	24, 35, 55, 66	0
1	D	233/233 (100%)	0.52	10 (4%) 35 34	24, 44, 60, 72	0
1	E	233/233 (100%)	0.55	8 (3%) 45 44	27, 45, 66, 80	0
1	F	233/233 (100%)	0.26	0 100 100	21, 31, 46, 57	0
1	G	233/233 (100%)	0.93	29 (12%) 4 3	34, 54, 76, 87	0
1	H	233/233 (100%)	0.22	0 100 100	20, 32, 49, 65	0
1	I	233/233 (100%)	0.99	25 (10%) 6 5	32, 53, 82, 113	0
1	J	233/233 (100%)	0.36	6 (2%) 56 54	27, 40, 60, 71	0
1	K	233/233 (100%)	0.52	19 (8%) 11 11	26, 40, 68, 88	0
1	L	233/233 (100%)	1.19	35 (15%) 2 2	36, 59, 74, 79	0
All	All	2796/2796 (100%)	0.55	150 (5%) 25 24	20, 43, 67, 113	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	57	ILE	8.1
1	B	212	LEU	6.9
1	B	213	SER	6.8
1	I	214	PRO	6.8
1	I	215	LYS	6.7
1	I	221	PHE	6.3
1	I	211	ALA	6.1
1	I	210	GLU	5.8
1	G	207	ILE	5.6
1	I	212	LEU	5.4
1	L	56	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	L	221	PHE	4.8
1	I	218	VAL	4.6
1	I	10	GLY	4.5
1	I	219	GLU	4.3
1	G	217	ARG	4.1
1	D	232	MET	4.1
1	L	211	ALA	3.9
1	K	221	PHE	3.8
1	G	214	PRO	3.8
1	G	221	PHE	3.8
1	G	211	ALA	3.8
1	E	33	LEU	3.7
1	G	212	LEU	3.7
1	J	1	MET	3.7
1	E	221	PHE	3.5
1	K	212	LEU	3.4
1	D	82	VAL	3.4
1	D	214	PRO	3.2
1	J	81	GLN	3.2
1	L	54	GLY	3.2
1	E	219	GLU	3.2
1	K	213	SER	3.1
1	L	59	LEU	3.1
1	I	207	ILE	3.1
1	G	88	ILE	3.0
1	K	217	ARG	3.0
1	L	52	TYR	3.0
1	K	215	LYS	3.0
1	I	220	SER	3.0
1	B	221	PHE	3.0
1	L	138	TYR	2.9
1	I	213	SER	2.9
1	L	232	MET	2.9
1	L	92	GLY	2.8
1	K	211	ALA	2.8
1	E	35	ASP	2.8
1	I	135	LEU	2.8
1	G	229	LEU	2.8
1	G	96	PRO	2.7
1	L	224	MET	2.7
1	G	35	ASP	2.7
1	K	223	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	176	LEU	2.7
1	I	147	ASP	2.7
1	L	146	ILE	2.7
1	L	194	ALA	2.7
1	G	55	ARG	2.7
1	G	218	VAL	2.7
1	C	96	PRO	2.7
1	B	210	GLU	2.6
1	B	177	ALA	2.6
1	L	131	PHE	2.6
1	L	61	GLY	2.6
1	D	146	ILE	2.6
1	G	29	ALA	2.6
1	K	232	MET	2.6
1	B	176	LEU	2.6
1	L	36	ALA	2.6
1	E	223	ASN	2.6
1	I	82	VAL	2.6
1	G	36	ALA	2.6
1	K	220	SER	2.6
1	K	218	VAL	2.5
1	G	208	THR	2.5
1	G	148	LEU	2.5
1	G	28	ILE	2.5
1	I	9	ILE	2.5
1	G	151	GLY	2.5
1	E	147	ASP	2.5
1	L	204	ASP	2.5
1	D	221	PHE	2.5
1	L	8	LYS	2.5
1	B	214	PRO	2.4
1	G	210	GLU	2.4
1	B	217	ARG	2.4
1	B	219	GLU	2.4
1	A	221	PHE	2.4
1	K	233	SER	2.4
1	I	11	ASP	2.4
1	L	121	LEU	2.4
1	G	146	ILE	2.4
1	E	12	PHE	2.3
1	G	32	PHE	2.3
1	L	76	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	30	LYS	2.3
1	G	225	ILE	2.3
1	G	27	TYR	2.3
1	K	216	GLU	2.3
1	L	34	GLN	2.3
1	K	146	ILE	2.3
1	L	55	ARG	2.3
1	B	200	CYS	2.3
1	B	207	ILE	2.3
1	I	226	ILE	2.3
1	I	41	ASN	2.3
1	K	131	PHE	2.3
1	D	233	SER	2.3
1	G	104	ILE	2.2
1	L	77	ILE	2.2
1	I	50	GLY	2.2
1	K	56	GLY	2.2
1	L	47	GLY	2.2
1	I	13	TYR	2.2
1	K	147	ASP	2.2
1	E	52	TYR	2.2
1	G	82	VAL	2.2
1	D	2	THR	2.2
1	L	213	SER	2.2
1	I	39	ILE	2.1
1	L	66	ILE	2.1
1	J	80	TYR	2.1
1	G	215	LYS	2.1
1	I	142	LYS	2.1
1	L	50	GLY	2.1
1	L	186	TYR	2.1
1	B	126	SER	2.1
1	G	103	ILE	2.1
1	A	125	LEU	2.1
1	J	46	LEU	2.1
1	L	229	LEU	2.1
1	D	218	VAL	2.1
1	K	118	VAL	2.1
1	L	53	LYS	2.1
1	A	56	GLY	2.1
1	B	171	ALA	2.1
1	A	233	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	17	LEU	2.1
1	G	220	SER	2.1
1	J	23	LEU	2.1
1	I	80	TYR	2.1
1	L	13	TYR	2.1
1	J	9	ILE	2.0
1	L	46	LEU	2.0
1	L	118	VAL	2.0
1	I	34	GLN	2.0
1	K	229	LEU	2.0
1	K	90	THR	2.0
1	L	90	THR	2.0
1	D	145	GLY	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 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
2	GOL	H	304	6/6	0.70	0.30	40,45,48,55	0
2	GOL	C	303	6/6	0.73	0.24	40,49,52,54	0
2	GOL	D	302	6/6	0.75	0.27	43,51,56,56	0
2	GOL	H	305	6/6	0.76	0.24	43,45,51,57	0
2	GOL	B	301	6/6	0.78	0.15	54,55,57,58	0
2	GOL	B	302	6/6	0.78	0.22	54,57,61,61	0
2	GOL	F	303	6/6	0.80	0.18	47,49,50,52	0
2	GOL	K	302	6/6	0.81	0.19	44,47,53,53	0
4	05Z	H	302	17/18	0.81	0.20	27,41,57,58	0
4	05Z	C	302	17/18	0.82	0.26	34,43,61,61	0

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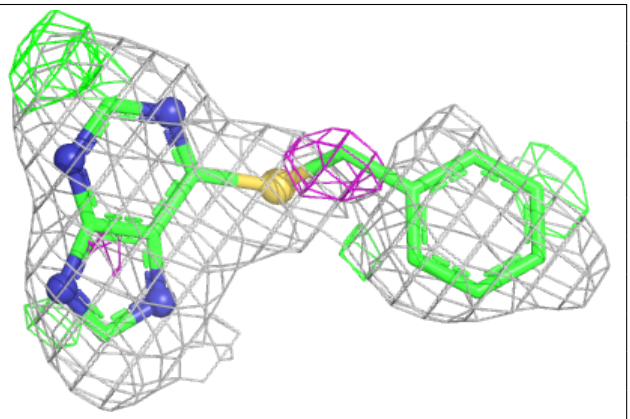
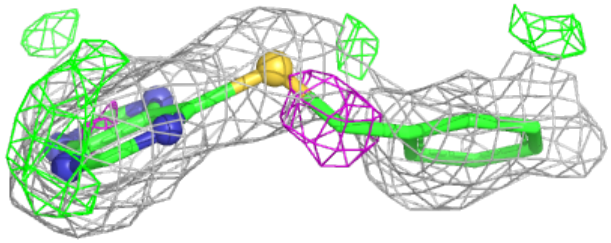
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	303	6/6	0.83	0.16	53,56,58,60	0
2	GOL	I	301	6/6	0.84	0.16	50,56,61,63	0
3	TRS	H	301	8/8	0.84	0.17	27,33,34,39	0
2	GOL	A	302	6/6	0.85	0.21	44,46,52,53	0
2	GOL	E	301	6/6	0.85	0.17	48,52,53,57	0
2	GOL	F	302	6/6	0.87	0.22	42,44,51,52	0
2	GOL	K	301	6/6	0.87	0.10	40,44,47,48	0
2	GOL	K	303	6/6	0.88	0.31	33,36,41,43	0
2	GOL	H	303	6/6	0.89	0.24	33,37,41,44	0
2	GOL	D	301	6/6	0.89	0.27	46,49,55,58	0
2	GOL	F	304	6/6	0.91	0.26	41,44,45,52	0
2	GOL	A	301	6/6	0.92	0.15	41,43,47,47	0
2	GOL	F	301	6/6	0.92	0.20	36,40,48,48	0
3	TRS	C	301	8/8	0.92	0.12	33,35,36,36	0
5	PO4	C	304	5/5	0.97	0.08	34,35,41,42	0
5	PO4	H	306	5/5	0.97	0.11	31,32,34,35	0

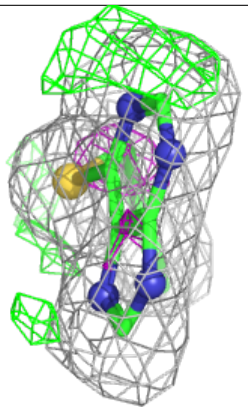
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 05Z H 302:

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

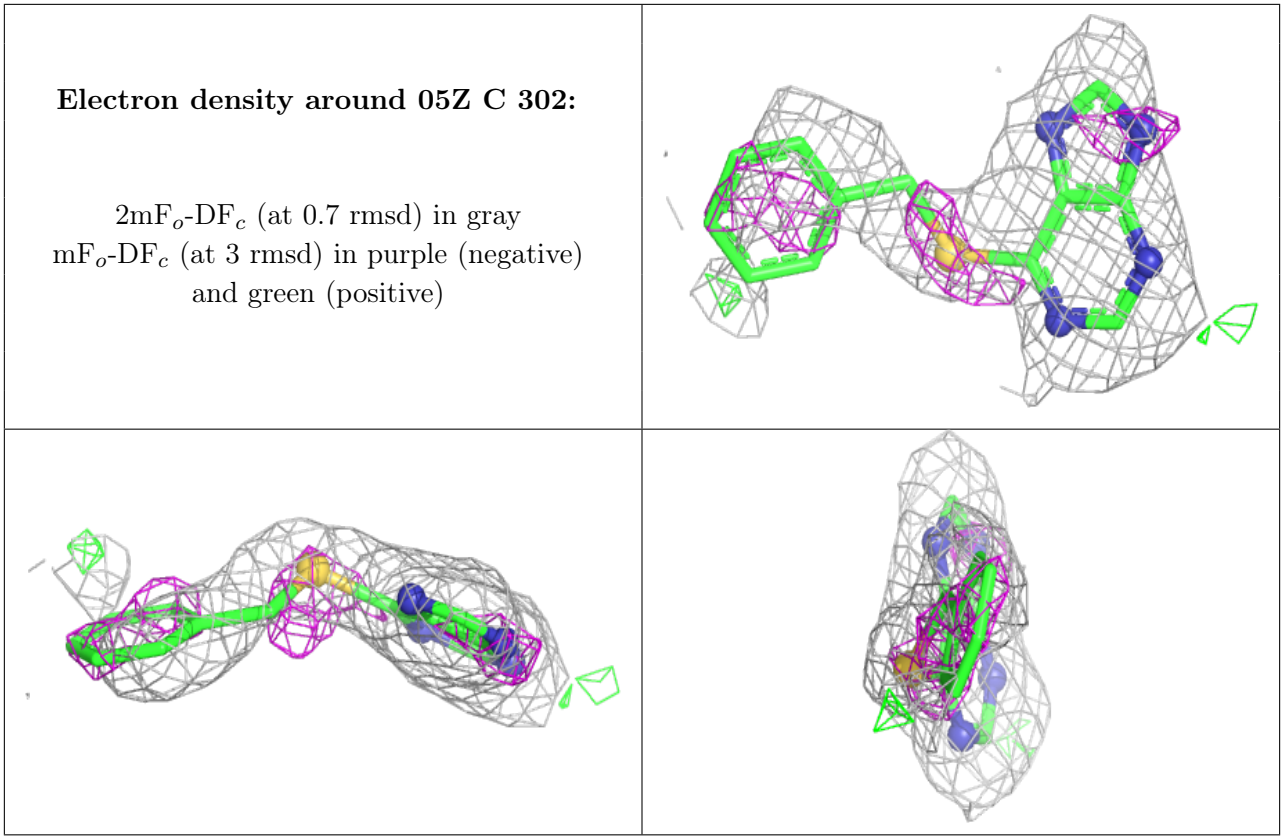






Electron density around 05Z C 302:

$2mF_o$-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.