



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 01:42 AM EDT

PDB ID : 4OHF / pdb_00004ohf
Title : Crystal structure of cytosolic nucleotidase II (LPG0095) in complex with GMP from *Legionella pneumophila*, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET LGR1
Authors : Srinivisan, B.; Forouhar, F.; Shukla, A.; Sampangi, C.; Kulkarni, S.; Abashidze, M.; Seetharaman, J.; Lew, S.; Mao, L.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.M.; Tong, L.; Balaram, H.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2014-01-17
Resolution : 2.53 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

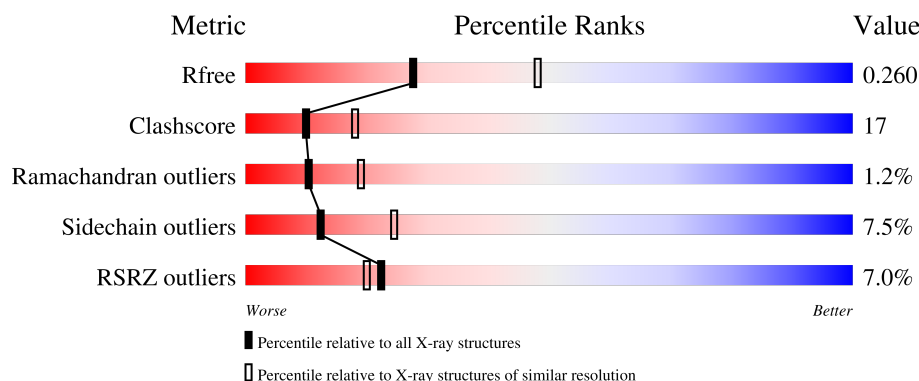
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

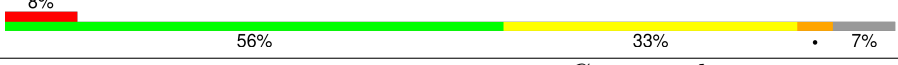
The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	470	
1	B	470	
1	C	470	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	470	5% 63% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15143 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 IMP-GMP specific 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3736	2405	628	690	13			
1	B	458	Total	C	N	O	S	0	0	0
			3752	2412	630	697	13			
1	C	438	Total	C	N	O	S	0	0	0
			3594	2319	605	658	12			
1	D	456	Total	C	N	O	S	0	0	0
			3742	2405	631	693	13			

There are 44 discrepancies between the modelled and reference sequences:

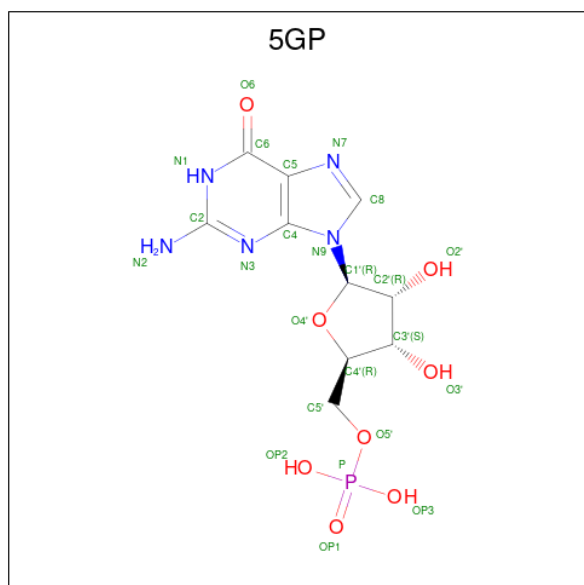
Chain	Residue	Modelled	Actual	Comment	Reference
A	459A	ALA	-	expression tag	UNP Q5ZZB6
A	459B	ALA	-	expression tag	UNP Q5ZZB6
A	459C	ALA	-	expression tag	UNP Q5ZZB6
A	460	LEU	-	expression tag	UNP Q5ZZB6
A	461	GLU	-	expression tag	UNP Q5ZZB6
A	462	HIS	-	expression tag	UNP Q5ZZB6
A	463	HIS	-	expression tag	UNP Q5ZZB6
A	464	HIS	-	expression tag	UNP Q5ZZB6
A	465	HIS	-	expression tag	UNP Q5ZZB6
A	466	HIS	-	expression tag	UNP Q5ZZB6
A	467	HIS	-	expression tag	UNP Q5ZZB6
B	460	ALA	-	expression tag	UNP Q5ZZB6
B	461	ALA	-	expression tag	UNP Q5ZZB6
B	462	ALA	-	expression tag	UNP Q5ZZB6
B	463	LEU	-	expression tag	UNP Q5ZZB6
B	464	GLU	-	expression tag	UNP Q5ZZB6
B	465	HIS	-	expression tag	UNP Q5ZZB6
B	466	HIS	-	expression tag	UNP Q5ZZB6
B	467	HIS	-	expression tag	UNP Q5ZZB6
B	468	HIS	-	expression tag	UNP Q5ZZB6
B	469	HIS	-	expression tag	UNP Q5ZZB6

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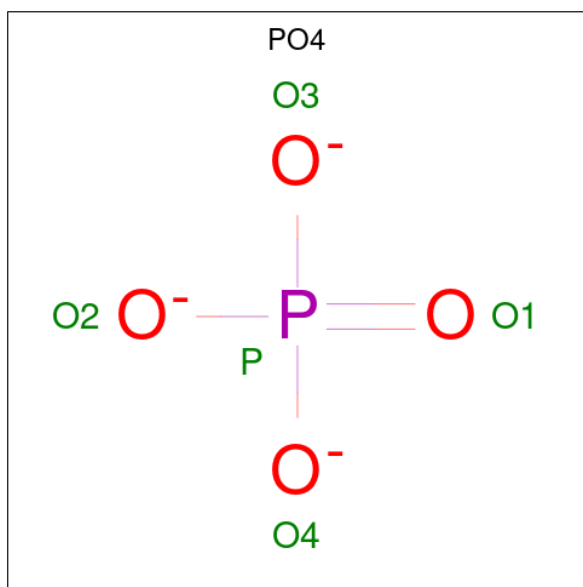
Chain	Residue	Modelled	Actual	Comment	Reference
B	470	HIS	-	expression tag	UNP Q5ZZB6
C	460	ALA	-	expression tag	UNP Q5ZZB6
C	461	ALA	-	expression tag	UNP Q5ZZB6
C	462	ALA	-	expression tag	UNP Q5ZZB6
C	463	LEU	-	expression tag	UNP Q5ZZB6
C	464	GLU	-	expression tag	UNP Q5ZZB6
C	465	HIS	-	expression tag	UNP Q5ZZB6
C	466	HIS	-	expression tag	UNP Q5ZZB6
C	467	HIS	-	expression tag	UNP Q5ZZB6
C	468	HIS	-	expression tag	UNP Q5ZZB6
C	469	HIS	-	expression tag	UNP Q5ZZB6
C	470	HIS	-	expression tag	UNP Q5ZZB6
D	460	ALA	-	expression tag	UNP Q5ZZB6
D	461	ALA	-	expression tag	UNP Q5ZZB6
D	462	ALA	-	expression tag	UNP Q5ZZB6
D	463	LEU	-	expression tag	UNP Q5ZZB6
D	464	GLU	-	expression tag	UNP Q5ZZB6
D	465	HIS	-	expression tag	UNP Q5ZZB6
D	466	HIS	-	expression tag	UNP Q5ZZB6
D	467	HIS	-	expression tag	UNP Q5ZZB6
D	468	HIS	-	expression tag	UNP Q5ZZB6
D	469	HIS	-	expression tag	UNP Q5ZZB6
D	470	HIS	-	expression tag	UNP Q5ZZB6

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	67	Total O 67 67	0	0
5	C	48	Total O 48 48	0	0
5	D	58	Total O 58 58	0	0

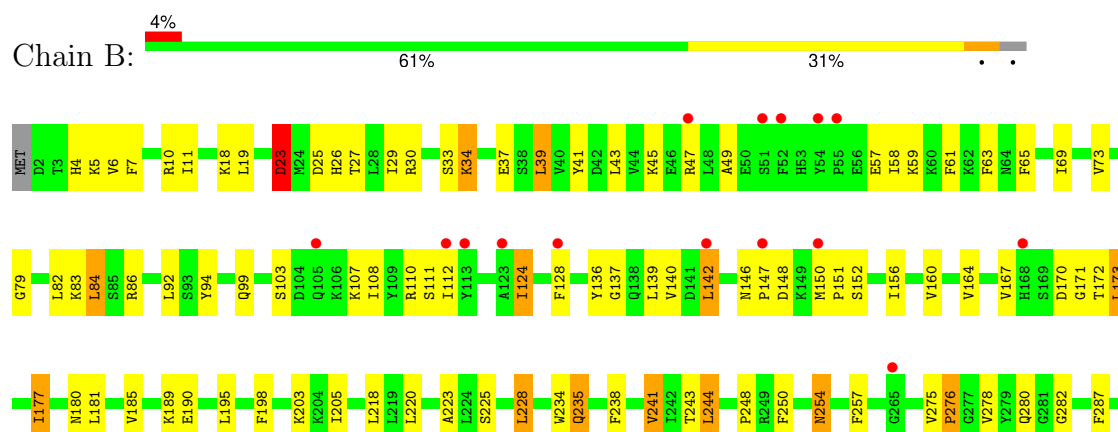
3 Residue-property plots [i](#)

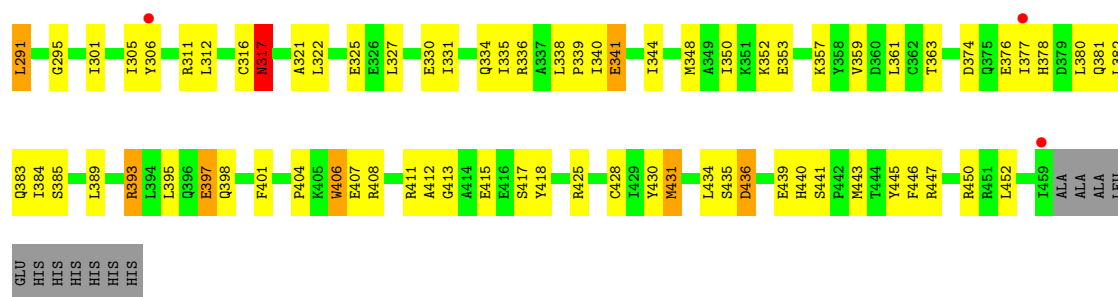
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytosolic IMP-GMP specific 5'-nucleotidase

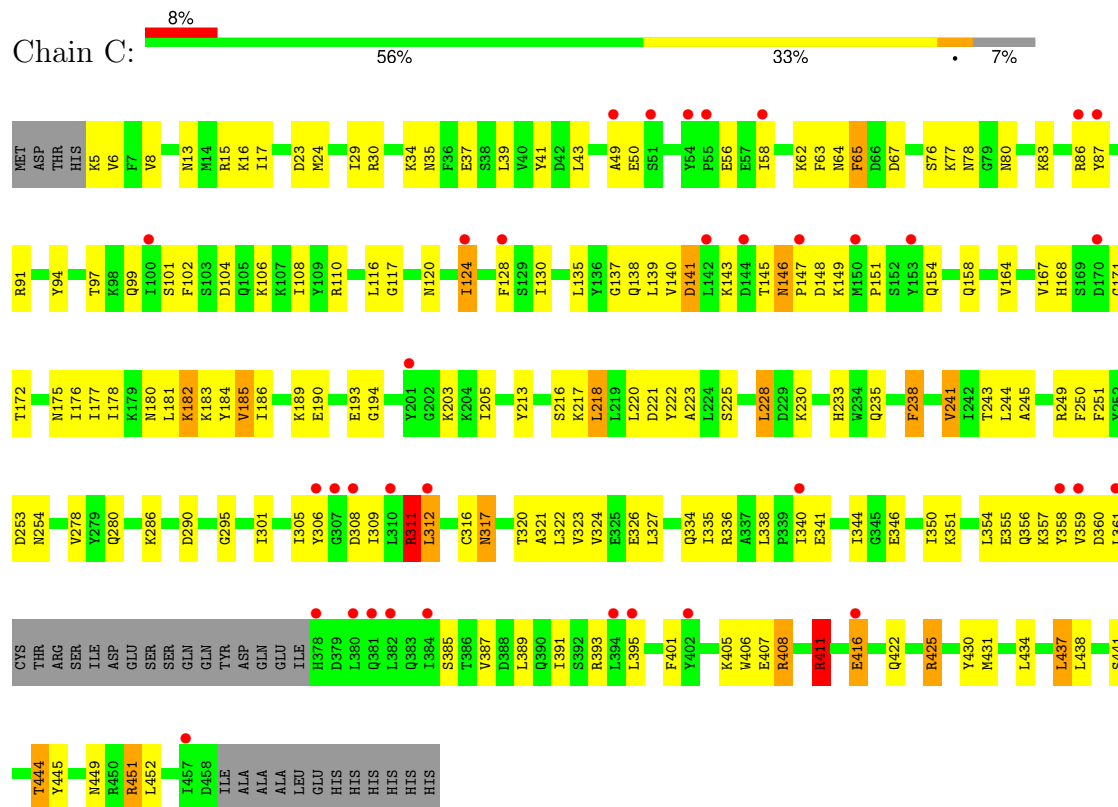


- Molecule 1: Cytosolic IMP-GMP specific 5'-nucleotidase

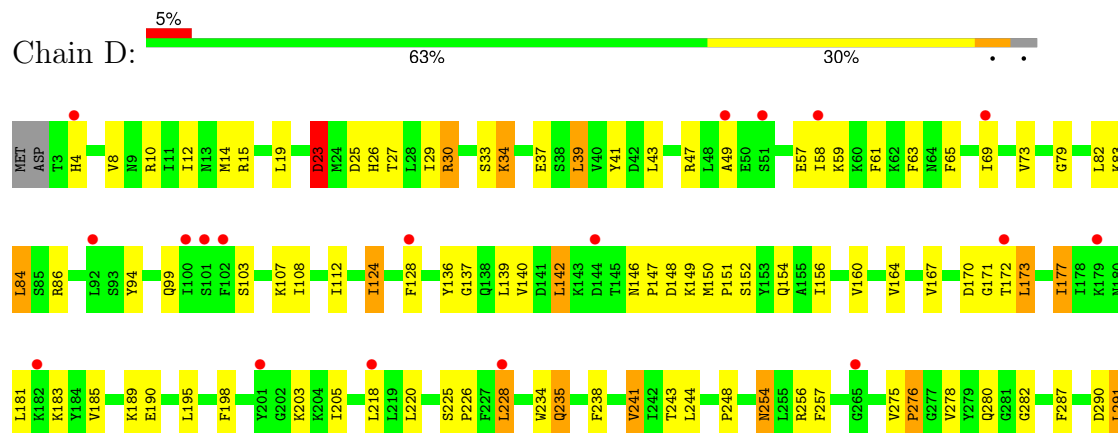


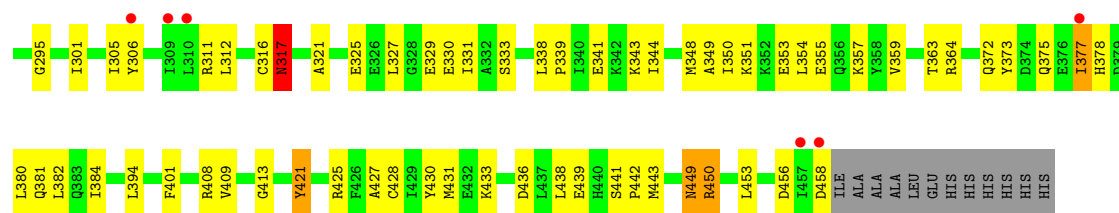


- Molecule 1: Cytosolic IMP-GMP specific 5'-nucleotidase



- Molecule 1: Cytosolic IMP-GMP specific 5'-nucleotidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.33Å 92.72Å 161.89Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	44.70 – 2.53 44.70 – 2.53	Depositor EDS
% Data completeness (in resolution range)	92.8 (44.70-2.53) 92.9 (44.70-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.54Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.231 , 0.272 0.220 , 0.260	Depositor DCC
R_{free} test set	7158 reflections (9.40%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15143	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, 5GP

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	0.46	0/3814	0.97	22/5139 (0.4%)
1	B	0.47	0/3831	0.92	15/5165 (0.3%)
1	C	0.44	0/3670	0.97	19/4944 (0.4%)
1	D	0.45	0/3821	0.93	14/5150 (0.3%)
All	All	0.46	0/15136	0.95	70/20398 (0.3%)

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	D	0	1

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	ARG	NE-CZ-NH2	8.37	126.74	119.20
1	A	411	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	A	411	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	C	311	ARG	NE-CZ-NH1	-7.94	113.56	121.50
1	C	91	ARG	NE-CZ-NH2	7.87	126.28	119.20
1	A	457	ILE	N-CA-C	-7.77	103.66	113.22
1	C	91	ARG	NE-CZ-NH1	-7.65	113.85	121.50
1	D	171	GLY	N-CA-C	-7.38	104.86	115.27
1	D	428	CYS	N-CA-C	-7.24	103.42	111.82
1	B	171	GLY	N-CA-C	-7.14	105.47	115.32
1	D	108	ILE	N-CA-C	7.06	117.17	110.53
1	A	249	ARG	NE-CZ-NH2	6.93	125.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	ARG	NE-CZ-NH2	-6.85	113.04	119.20
1	B	108	ILE	N-CA-C	6.80	116.92	110.53
1	A	249	ARG	NE-CZ-NH1	-6.75	114.75	121.50
1	A	91	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	C	411	ARG	CD-NE-CZ	6.55	133.57	124.40
1	C	23	ASP	N-CA-C	-6.45	100.73	110.28
1	C	171	GLY	N-CA-C	-6.34	106.57	115.32
1	D	23	ASP	N-CA-C	-6.34	100.89	110.28
1	A	23	ASP	N-CA-C	-6.30	100.24	110.20
1	A	251	PHE	N-CA-C	6.24	118.16	111.36
1	A	171	GLY	N-CA-C	-6.21	106.75	115.32
1	D	408	ARG	N-CA-C	6.16	119.16	110.23
1	B	23	ASP	N-CA-C	-6.13	101.20	110.28
1	C	251	PHE	N-CA-C	6.10	118.01	111.36
1	A	91	ARG	CD-NE-CZ	6.01	132.82	124.40
1	A	311	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	C	408	ARG	N-CA-C	5.90	118.83	110.50
1	C	311	ARG	CD-NE-CZ	5.89	132.64	124.40
1	B	82	LEU	N-CA-C	5.87	119.11	109.72
1	A	311	ARG	CD-NE-CZ	5.87	132.61	124.40
1	D	238	PHE	N-CA-C	5.82	118.38	108.90
1	C	117	GLY	N-CA-C	-5.70	107.59	114.66
1	A	403	ASN	CA-C-N	5.65	125.49	119.28
1	A	403	ASN	C-N-CA	5.65	125.49	119.28
1	C	91	ARG	CD-NE-CZ	5.64	132.30	124.40
1	B	428	CYS	N-CA-C	-5.63	105.13	112.23
1	C	411	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	D	427	ALA	N-CA-C	5.61	117.66	108.52
1	B	436	ASP	N-CA-C	-5.57	105.11	111.07
1	B	238	PHE	N-CA-C	5.57	117.97	108.90
1	D	413	GLY	N-CA-C	-5.56	101.91	111.47
1	B	413	GLY	N-CA-C	-5.52	104.66	111.45
1	A	411	ARG	CD-NE-CZ	5.49	132.09	124.40
1	B	33	SER	N-CA-C	5.49	117.70	111.11
1	A	117	GLY	N-CA-C	-5.46	107.89	114.66
1	D	82	LEU	N-CA-C	5.42	118.40	109.72
1	A	8	VAL	N-CA-C	5.40	116.09	108.36
1	A	91	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	238	PHE	N-CA-C	5.34	117.60	108.90
1	D	33	SER	N-CA-C	5.34	117.51	111.11
1	C	8	VAL	N-CA-C	5.30	115.93	108.36
1	B	112	ILE	N-CA-C	-5.28	107.25	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	ARG	N-CA-C	5.24	117.89	110.50
1	D	8	VAL	N-CA-C	5.24	115.40	107.80
1	A	427	ALA	N-CA-C	5.21	117.74	109.24
1	B	406	TRP	N-CA-C	5.20	121.34	114.12
1	C	238	PHE	N-CA-C	5.16	117.32	108.90
1	A	311	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	D	112	ILE	N-CA-C	-5.11	107.44	113.42
1	C	434	LEU	N-CA-C	5.10	116.84	111.28
1	D	425	ARG	N-CA-C	5.08	116.90	111.36
1	B	244	LEU	N-CA-C	-5.08	104.39	111.30
1	C	249	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	D	256	ARG	N-CA-C	5.03	117.35	110.55
1	B	223	ALA	N-CA-C	5.03	119.42	113.28
1	A	434	LEU	N-CA-C	5.02	117.41	111.33
1	C	223	ALA	N-CA-C	5.02	119.46	113.23
1	B	434	LEU	N-CA-C	5.00	117.39	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	421	TYR	Sidechain

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	3736	0	3739	142	0
1	B	3752	0	3744	125	0
1	C	3594	0	3610	141	0
1	D	3742	0	3740	122	0
2	A	24	0	12	0	0
2	C	24	0	12	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	55	0	0	2	0
5	B	67	0	0	4	0
5	C	48	0	0	2	0
5	D	58	0	0	3	0
All	All	15143	0	14857	517	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 17.

All (517) 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:441:SER:O	1:A:444:THR:HG22	1.58	1.02
1:C:441:SER:O	1:C:444:THR:HG22	1.59	1.01
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.29	0.96
1:B:311:ARG:HH11	1:B:311:ARG:HG3	1.29	0.95
1:B:235:GLN:H	1:B:235:GLN:HE21	0.98	0.94
1:D:235:GLN:HE21	1:D:235:GLN:H	1.00	0.93
1:D:235:GLN:H	1:D:235:GLN:NE2	1.69	0.89
1:B:235:GLN:H	1:B:235:GLN:NE2	1.70	0.89
1:C:334:GLN:HE22	1:D:456:ASP:HA	1.39	0.87
1:C:305:ILE:HD13	1:C:422:GLN:HB3	1.56	0.85
1:A:13:ASN:HD22	1:A:16:LYS:HD3	1.44	0.83
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.44	0.81
1:C:13:ASN:HD22	1:C:16:LYS:HD3	1.44	0.80
1:A:189:LYS:HE2	1:A:193:GLU:OE1	1.82	0.79
1:C:189:LYS:HE2	1:C:193:GLU:OE1	1.81	0.79
1:A:230:LYS:H	1:A:230:LYS:HD2	1.48	0.78
1:B:344:ILE:HG22	1:B:348:MET:HE2	1.66	0.78
1:C:83:LYS:NZ	1:C:407:GLU:HG3	1.98	0.77
1:D:235:GLN:HE21	1:D:235:GLN:N	1.81	0.76
1:B:235:GLN:HE21	1:B:235:GLN:N	1.80	0.76
1:C:24:MET:HE1	1:C:216:SER:CB	2.16	0.76
1:C:83:LYS:HZ2	1:C:407:GLU:HG3	1.51	0.75
1:A:24:MET:HE1	1:A:216:SER:HB3	1.67	0.75
1:A:241:VAL:CG1	1:A:278:VAL:HG22	2.17	0.74
1:B:49:ALA:HB2	1:B:58:ILE:HD11	1.70	0.74
1:C:24:MET:HE1	1:C:216:SER:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:MET:HE1	1:A:216:SER:CB	2.17	0.74
1:C:241:VAL:CG1	1:C:278:VAL:HG22	2.18	0.73
1:B:359:VAL:O	1:B:363:THR:HG23	1.89	0.73
1:C:64:ASN:HB3	1:C:67:ASP:OD2	1.89	0.73
1:C:387:VAL:O	1:C:391:ILE:HG12	1.88	0.73
1:A:357:LYS:O	1:A:361:LEU:HD13	1.90	0.72
1:A:230:LYS:HD2	1:A:230:LYS:N	2.05	0.72
1:C:360:ASP:O	1:C:361:LEU:HD23	1.88	0.71
1:D:49:ALA:HB2	1:D:58:ILE:HD11	1.71	0.71
1:A:64:ASN:HB3	1:A:67:ASP:OD2	1.90	0.70
1:A:441:SER:OG	1:B:363:THR:HG21	1.90	0.70
1:A:29:ILE:HD11	1:A:220:LEU:HD23	1.74	0.70
1:C:29:ILE:HD11	1:C:220:LEU:HD23	1.72	0.70
1:A:327:LEU:O	1:A:331:ILE:HG12	1.92	0.70
1:A:305:ILE:HD13	1:A:422:GLN:HB3	1.73	0.69
1:A:334:GLN:HG2	1:A:402:TYR:OH	1.91	0.69
1:C:451:ARG:NE	1:C:451:ARG:H	1.89	0.69
1:D:449:ASN:N	1:D:449:ASN:HD22	1.90	0.69
1:B:124:ILE:HD12	1:B:124:ILE:H	1.58	0.68
1:D:248:PRO:HB3	1:D:306:TYR:HB3	1.75	0.68
1:A:124:ILE:HD12	1:A:124:ILE:H	1.59	0.68
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.58	0.68
1:C:124:ILE:HD12	1:C:124:ILE:H	1.58	0.68
1:D:311:ARG:HG3	1:D:311:ARG:NH1	2.05	0.67
1:D:449:ASN:ND2	1:D:449:ASN:H	1.93	0.67
1:A:30:ARG:CZ	1:A:186:ILE:HD11	2.25	0.67
1:B:248:PRO:HB3	1:B:306:TYR:HB3	1.76	0.67
1:A:360:ASP:O	1:A:363:THR:HG22	1.94	0.67
1:D:124:ILE:HD12	1:D:124:ILE:H	1.59	0.66
1:A:13:ASN:ND2	1:A:16:LYS:HD3	2.10	0.66
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.60	0.66
1:C:13:ASN:ND2	1:C:16:LYS:HD3	2.11	0.66
1:D:442:PRO:O	1:D:443:MET:HE2	1.96	0.66
1:A:49:ALA:HB2	1:A:58:ILE:HD11	1.78	0.65
1:D:241:VAL:CG1	1:D:278:VAL:HG22	2.26	0.65
1:A:431:MET:HE2	1:A:437:LEU:HB2	1.79	0.65
1:C:86:ARG:HD2	1:C:87:TYR:CZ	2.31	0.65
1:C:451:ARG:HD2	1:C:451:ARG:O	1.96	0.65
1:C:30:ARG:CZ	1:C:186:ILE:HD11	2.27	0.65
1:C:449:ASN:O	1:C:451:ARG:NH1	2.30	0.65
1:C:336:ARG:HB3	1:C:401:PHE:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:HB2	1:C:58:ILE:HD11	1.77	0.65
1:D:128:PHE:CD1	1:D:164:VAL:HG11	2.32	0.65
1:C:295:GLY:HA3	1:C:317:ASN:HD21	1.62	0.64
1:D:339:PRO:O	1:D:343:LYS:HG2	1.97	0.64
1:A:330:GLU:O	1:A:334:GLN:HG3	1.96	0.64
1:D:61:PHE:HE1	1:D:139:LEU:HD23	1.63	0.64
1:A:228:LEU:HD21	1:A:234:TRP:HA	1.80	0.64
1:B:317:ASN:C	1:B:317:ASN:HD22	2.05	0.64
1:C:182:LYS:NZ	1:C:182:LYS:HB3	2.12	0.64
1:B:311:ARG:HG3	1:B:311:ARG:NH1	2.06	0.64
1:B:61:PHE:HE1	1:B:139:LEU:HD23	1.62	0.64
1:D:330:GLU:HG2	5:D:627:HOH:O	1.97	0.64
1:A:77:LYS:HB2	1:A:120:ASN:OD1	1.98	0.64
1:A:30:ARG:NH2	1:A:186:ILE:HD11	2.13	0.63
1:A:295:GLY:HA3	1:A:317:ASN:HD21	1.63	0.63
1:A:86:ARG:HD2	1:A:87:TYR:CZ	2.33	0.63
1:B:241:VAL:CG1	1:B:278:VAL:HG22	2.29	0.63
1:B:128:PHE:CD1	1:B:164:VAL:HG11	2.34	0.63
1:D:142:LEU:HD12	1:D:150:MET:SD	2.39	0.63
1:D:350:ILE:O	1:D:354:LEU:HD23	1.98	0.63
1:D:449:ASN:HD22	1:D:449:ASN:H	1.44	0.62
1:A:17:ILE:O	1:A:203:LYS:HE3	1.99	0.62
1:A:182:LYS:NZ	1:A:182:LYS:HB3	2.14	0.62
1:B:377:ILE:HD12	1:B:378:HIS:N	2.14	0.62
1:D:225:SER:HA	1:D:228:LEU:HD22	1.82	0.62
1:D:344:ILE:O	1:D:348:MET:HG3	1.99	0.62
1:A:178:ILE:HD11	1:A:218:LEU:HB3	1.82	0.62
1:B:142:LEU:HD12	1:B:150:MET:SD	2.41	0.61
1:B:225:SER:HA	1:B:228:LEU:HD22	1.81	0.61
1:D:244:LEU:HB2	1:D:280:GLN:HG3	1.82	0.61
1:D:317:ASN:C	1:D:317:ASN:HD22	2.08	0.61
1:B:311:ARG:HH11	1:B:311:ARG:CG	2.09	0.61
1:C:77:LYS:HB2	1:C:120:ASN:OD1	1.99	0.61
1:A:380:LEU:O	1:A:384:ILE:HG12	2.00	0.61
1:C:41:TYR:CE1	1:C:63:PHE:HB2	2.36	0.60
1:A:295:GLY:HA3	1:A:317:ASN:ND2	2.17	0.60
1:B:327:LEU:O	1:B:331:ILE:HG12	2.01	0.60
1:C:17:ILE:O	1:C:203:LYS:HE3	2.00	0.60
1:C:178:ILE:HD11	1:C:218:LEU:HB3	1.83	0.60
1:C:431:MET:HE2	1:C:437:LEU:HB2	1.82	0.60
1:C:30:ARG:NH2	1:C:186:ILE:HD11	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:C	1:B:317:ASN:ND2	2.58	0.60
1:A:41:TYR:CE1	1:A:63:PHE:HB2	2.37	0.59
1:C:225:SER:HA	1:C:228:LEU:HD22	1.83	0.59
1:B:295:GLY:HA3	1:B:317:ASN:HD21	1.67	0.59
1:D:195:LEU:HD22	1:D:205:ILE:HD13	1.84	0.59
1:A:286:LYS:NZ	1:A:290:ASP:OD2	2.36	0.59
1:C:305:ILE:HD13	1:C:422:GLN:CB	2.31	0.59
1:C:140:VAL:HA	1:C:143:LYS:HB3	1.85	0.59
1:C:295:GLY:HA3	1:C:317:ASN:ND2	2.17	0.59
1:C:301:ILE:HG12	1:C:321:ALA:HB3	1.85	0.59
1:C:336:ARG:HB3	1:C:401:PHE:CD2	2.38	0.59
1:C:451:ARG:C	1:C:452:LEU:HD12	2.27	0.59
1:D:441:SER:C	1:D:443:MET:H	2.09	0.58
1:D:295:GLY:HA3	1:D:317:ASN:HD21	1.68	0.58
1:D:359:VAL:O	1:D:363:THR:HG23	2.02	0.58
1:D:327:LEU:O	1:D:331:ILE:HG12	2.02	0.58
1:C:451:ARG:H	1:C:451:ARG:CZ	2.16	0.58
1:A:241:VAL:HG13	1:A:278:VAL:HG22	1.85	0.58
1:A:454:ALA:O	1:A:457:ILE:HG23	2.03	0.58
1:C:241:VAL:HG13	1:C:278:VAL:HG22	1.86	0.58
1:D:317:ASN:C	1:D:317:ASN:ND2	2.60	0.57
1:A:205:ILE:HG22	1:A:238:PHE:HD1	1.68	0.57
1:A:175:ASN:O	1:A:178:ILE:HG22	2.05	0.57
1:B:336:ARG:O	1:B:401:PHE:CE2	2.57	0.57
1:B:374:ASP:O	1:B:377:ILE:HG13	2.04	0.57
1:B:195:LEU:HD22	1:B:205:ILE:HD13	1.86	0.57
1:A:451:ARG:HH11	1:A:451:ARG:CG	2.17	0.57
1:B:244:LEU:HB2	1:B:280:GLN:HG3	1.87	0.57
1:C:309:ILE:HG21	1:C:425:ARG:CG	2.34	0.57
1:A:143:LYS:HD2	1:A:143:LYS:O	2.04	0.56
1:C:221:ASP:O	1:C:225:SER:HB2	2.05	0.56
1:D:29:ILE:HD11	1:D:220:LEU:HD23	1.87	0.56
1:A:35:ASN:HD22	1:A:183:LYS:HG2	1.70	0.56
1:C:35:ASN:HD22	1:C:183:LYS:HG2	1.70	0.56
1:A:140:VAL:HA	1:A:143:LYS:HB3	1.87	0.56
1:A:451:ARG:HG3	1:A:451:ARG:NH1	2.18	0.56
1:B:146:ASN:HD22	1:B:146:ASN:C	2.13	0.56
1:B:254:ASN:H	1:B:254:ASN:HD22	1.53	0.56
1:C:175:ASN:O	1:C:178:ILE:HG22	2.06	0.56
1:D:4:HIS:HB3	1:D:436:ASP:HA	1.88	0.56
1:D:39:LEU:HD22	1:D:43:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ILE:HD13	1:B:395:LEU:HD23	1.87	0.55
1:B:406:TRP:O	1:B:407:GLU:HB2	2.05	0.55
1:C:177:ILE:HG22	1:C:184:TYR:CD2	2.42	0.55
1:D:311:ARG:HH11	1:D:311:ARG:CG	2.08	0.55
1:D:354:LEU:HB3	1:D:384:ILE:CG1	2.37	0.55
1:D:73:VAL:HG21	1:D:84:LEU:HD22	1.88	0.55
1:D:235:GLN:NE2	1:D:235:GLN:N	2.49	0.55
1:C:94:TYR:CE2	1:C:405:LYS:HE3	2.41	0.55
1:D:275:VAL:O	1:D:276:PRO:C	2.50	0.55
1:C:143:LYS:HD2	1:C:143:LYS:O	2.07	0.55
1:B:73:VAL:HG21	1:B:84:LEU:HD22	1.89	0.54
1:C:180:ASN:HB2	5:C:621:HOH:O	2.05	0.54
1:B:441:SER:C	1:B:443:MET:H	2.16	0.54
1:D:373:TYR:O	1:D:377:ILE:HG23	2.08	0.54
1:C:244:LEU:HD12	1:C:280:GLN:CD	2.33	0.54
1:D:37:GLU:HG3	1:D:65:PHE:HE2	1.72	0.54
1:B:34:LYS:NZ	1:B:34:LYS:HB3	2.22	0.54
1:B:39:LEU:HD22	1:B:43:LEU:HG	1.89	0.54
1:A:408:ARG:HG2	1:A:408:ARG:HH21	1.73	0.54
1:D:146:ASN:C	1:D:146:ASN:HD22	2.16	0.54
1:D:128:PHE:CE1	1:D:164:VAL:HG11	2.42	0.54
1:A:441:SER:CB	1:B:363:THR:HG21	2.38	0.54
1:B:37:GLU:HG3	1:B:65:PHE:HE2	1.71	0.54
1:C:335:ILE:O	1:C:338:LEU:HB2	2.07	0.54
1:A:102:PHE:HB3	5:A:641:HOH:O	2.07	0.54
1:C:286:LYS:NZ	1:C:290:ASP:OD2	2.40	0.54
1:D:301:ILE:HG12	1:D:321:ALA:HB3	1.89	0.53
1:A:221:ASP:O	1:A:225:SER:HB2	2.08	0.53
1:C:351:LYS:O	1:C:355:GLU:HB2	2.08	0.53
1:D:341:GLU:O	1:D:344:ILE:HG13	2.09	0.53
1:A:177:ILE:HG22	1:A:184:TYR:CD2	2.44	0.53
1:A:244:LEU:HD12	1:A:280:GLN:CD	2.33	0.53
1:B:275:VAL:O	1:B:276:PRO:C	2.52	0.53
1:D:137:GLY:O	1:D:140:VAL:HG22	2.09	0.53
1:B:146:ASN:O	1:B:148:ASP:N	2.38	0.53
1:C:205:ILE:HD12	1:C:205:ILE:N	2.23	0.53
1:A:402:TYR:O	1:A:403:ASN:C	2.52	0.53
1:D:254:ASN:HD22	1:D:254:ASN:H	1.55	0.53
1:A:138:GLN:HA	1:A:141:ASP:HB2	1.92	0.52
1:A:301:ILE:HG12	1:A:321:ALA:HB3	1.90	0.52
1:A:354:LEU:HB3	1:A:384:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:CE2	1:B:99:GLN:HB2	2.44	0.52
1:C:146:ASN:C	1:C:146:ASN:HD22	2.17	0.52
1:B:4:HIS:HD1	1:B:436:ASP:HA	1.75	0.52
1:B:128:PHE:CE1	1:B:164:VAL:HG11	2.43	0.52
1:D:344:ILE:HG22	1:D:394:LEU:HB3	1.90	0.52
1:C:205:ILE:HG22	1:C:238:PHE:HD1	1.75	0.52
1:A:452:LEU:HA	1:A:455:HIS:HB3	1.92	0.52
1:C:244:LEU:HB2	1:C:280:GLN:HG3	1.91	0.52
1:C:316:CYS:O	1:C:317:ASN:HB3	2.08	0.52
1:D:34:LYS:NZ	1:D:34:LYS:HB3	2.25	0.52
1:D:86:ARG:HB2	1:D:421:TYR:HB2	1.92	0.51
1:B:124:ILE:HD12	1:B:124:ILE:N	2.24	0.51
1:B:322:LEU:O	1:B:430:TYR:HA	2.11	0.51
1:A:146:ASN:C	1:A:146:ASN:HD22	2.18	0.51
1:C:182:LYS:HB3	1:C:182:LYS:HZ2	1.76	0.51
1:C:309:ILE:HG21	1:C:425:ARG:HG2	1.93	0.51
1:A:94:TYR:CE2	1:A:405:LYS:HE3	2.46	0.51
1:D:164:VAL:O	1:D:167:VAL:HG12	2.11	0.51
1:B:235:GLN:NE2	1:B:235:GLN:N	2.50	0.51
1:D:124:ILE:HD12	1:D:124:ILE:N	2.25	0.51
1:B:331:ILE:O	1:B:335:ILE:HG13	2.10	0.50
1:C:146:ASN:HD21	1:C:148:ASP:HB2	1.76	0.50
1:A:354:LEU:HB3	1:A:384:ILE:CD1	2.41	0.50
1:C:138:GLN:HA	1:C:141:ASP:HB2	1.93	0.50
1:D:295:GLY:HA3	1:D:317:ASN:ND2	2.26	0.50
1:A:146:ASN:HD21	1:A:148:ASP:HB2	1.77	0.50
1:B:137:GLY:O	1:B:140:VAL:HG22	2.11	0.50
1:A:172:THR:O	1:A:176:ILE:HG12	2.11	0.50
1:C:172:THR:O	1:C:176:ILE:HG12	2.11	0.50
1:A:408:ARG:HG2	1:A:408:ARG:NH2	2.26	0.50
1:A:178:ILE:HG12	1:A:218:LEU:HD23	1.93	0.50
1:A:365:SER:O	1:A:369:SER:HA	2.12	0.50
1:B:295:GLY:HA3	1:B:317:ASN:ND2	2.25	0.50
1:C:177:ILE:O	1:C:181:LEU:HD23	2.12	0.50
1:B:301:ILE:HG12	1:B:321:ALA:HB3	1.93	0.50
1:C:359:VAL:C	1:C:361:LEU:H	2.20	0.50
1:A:86:ARG:HA	1:A:418:TYR:HA	1.94	0.49
1:A:244:LEU:HB2	1:A:280:GLN:HG3	1.93	0.49
1:B:29:ILE:HD11	1:B:220:LEU:HD23	1.93	0.49
1:B:198:PHE:O	1:B:203:LYS:HB2	2.12	0.49
1:B:311:ARG:NH1	1:B:311:ARG:CG	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG11	1:D:278:VAL:HG22	1.93	0.49
1:A:177:ILE:O	1:A:181:LEU:HD23	2.12	0.49
1:A:450:ARG:O	1:A:453:LEU:HB3	2.12	0.49
1:B:6:VAL:HG22	1:B:431:MET:HE2	1.94	0.49
1:C:309:ILE:HG21	1:C:425:ARG:HG3	1.94	0.49
1:A:37:GLU:OE1	1:A:130:ILE:HB	2.12	0.49
1:A:331:ILE:HG22	1:A:335:ILE:HD13	1.93	0.49
1:B:164:VAL:O	1:B:167:VAL:HG12	2.12	0.49
1:D:4:HIS:CD2	1:D:439:GLU:HG3	2.48	0.49
1:B:344:ILE:CG2	1:B:348:MET:HE2	2.40	0.49
1:C:37:GLU:OE1	1:C:130:ILE:HB	2.12	0.49
1:B:23:ASP:O	1:B:27:THR:HB	2.13	0.49
1:B:92:LEU:HD11	1:B:406:TRP:CE3	2.47	0.49
1:C:178:ILE:HG12	1:C:218:LEU:HD23	1.95	0.49
1:B:412:ALA:HB2	1:B:417:SER:HA	1.94	0.49
1:D:203:LYS:HZ3	1:D:443:MET:HE2	1.77	0.49
1:B:160:VAL:O	1:B:164:VAL:HG23	2.13	0.49
1:B:389:LEU:O	1:B:393:ARG:HG3	2.11	0.49
1:D:94:TYR:CE2	1:D:99:GLN:HB2	2.47	0.49
1:D:344:ILE:HD12	1:D:344:ILE:C	2.36	0.49
1:A:146:ASN:CG	1:A:149:LYS:HG2	2.38	0.48
1:C:94:TYR:OH	1:C:405:LYS:HG3	2.13	0.48
1:D:312:LEU:C	1:D:312:LEU:HD23	2.38	0.48
1:A:316:CYS:O	1:A:317:ASN:HB3	2.13	0.48
1:A:41:TYR:CD1	1:A:63:PHE:HB2	2.49	0.48
1:B:11:ILE:HA	1:B:446:PHE:O	2.12	0.48
1:A:137:GLY:O	1:A:140:VAL:HG22	2.14	0.48
1:D:160:VAL:O	1:D:164:VAL:HG23	2.13	0.48
1:C:146:ASN:CG	1:C:149:LYS:HG2	2.39	0.48
1:D:195:LEU:CD2	1:D:205:ILE:HD13	2.43	0.48
1:B:407:GLU:HB3	5:B:652:HOH:O	2.14	0.48
1:C:177:ILE:HG22	1:C:184:TYR:CG	2.48	0.48
1:C:441:SER:OG	1:D:363:THR:HG21	2.14	0.48
1:A:449:ASN:C	1:A:451:ARG:H	2.21	0.48
1:C:441:SER:O	1:C:444:THR:CG2	2.47	0.48
1:A:24:MET:HE2	1:A:220:LEU:CG	2.44	0.48
1:B:330:GLU:HG2	5:B:603:HOH:O	2.13	0.48
1:B:350:ILE:O	1:B:353:GLU:HB2	2.13	0.48
1:C:101:SER:HB3	1:C:104:ASP:OD1	2.14	0.48
1:A:452:LEU:HD11	1:B:411:ARG:CZ	2.44	0.47
1:A:224:LEU:O	1:A:228:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:MET:HE2	1:C:220:LEU:CG	2.44	0.47
1:B:7:PHE:HE2	1:B:327:LEU:HD13	1.79	0.47
1:B:19:LEU:HD11	1:B:291:LEU:HD22	1.97	0.47
1:B:124:ILE:H	1:B:124:ILE:CD1	2.19	0.47
1:C:41:TYR:CD1	1:C:63:PHE:HB2	2.49	0.47
1:C:316:CYS:O	1:C:317:ASN:CB	2.61	0.47
1:D:25:ASP:O	1:D:26:HIS:HB2	2.14	0.47
1:A:205:ILE:HD12	1:A:205:ILE:N	2.30	0.47
1:B:4:HIS:O	1:B:440:HIS:HE1	1.97	0.47
1:B:287:PHE:CE1	1:B:291:LEU:HD13	2.50	0.47
1:C:338:LEU:O	1:C:341:GLU:HB3	2.14	0.47
1:C:324:VAL:O	1:C:327:LEU:HB2	2.15	0.47
1:A:24:MET:HE2	1:A:220:LEU:HG	1.96	0.47
1:A:177:ILE:HG22	1:A:184:TYR:CG	2.50	0.47
1:B:79:GLY:HA2	1:B:136:TYR:OH	2.15	0.47
1:D:79:GLY:HA2	1:D:136:TYR:OH	2.15	0.47
1:D:173:LEU:O	1:D:177:ILE:HG23	2.14	0.47
1:C:233:HIS:HA	5:C:623:HOH:O	2.15	0.47
1:C:146:ASN:C	1:C:148:ASP:H	2.23	0.47
1:D:316:CYS:O	1:D:317:ASN:ND2	2.47	0.47
1:A:368:GLU:O	1:A:369:SER:C	2.57	0.47
1:A:459:ILE:HG22	1:B:335:ILE:HG12	1.95	0.47
1:C:385:SER:O	1:C:389:LEU:HD13	2.16	0.46
1:B:341:GLU:OE2	1:B:398:GLN:NE2	2.48	0.46
1:D:23:ASP:O	1:D:27:THR:HB	2.14	0.46
1:A:146:ASN:C	1:A:148:ASP:H	2.23	0.46
1:A:225:SER:HA	1:A:228:LEU:HD22	1.98	0.46
1:B:312:LEU:C	1:B:312:LEU:HD23	2.40	0.46
1:A:101:SER:HB3	1:A:104:ASP:OD1	2.15	0.46
1:A:344:ILE:HD13	1:A:395:LEU:HD23	1.97	0.46
1:A:86:ARG:HB2	1:A:421:TYR:HB2	1.97	0.46
1:A:384:ILE:O	1:A:387:VAL:HG12	2.16	0.46
1:B:381:GLN:NE2	1:B:382:LEU:HD12	2.31	0.46
1:D:198:PHE:CE2	1:D:438:LEU:HA	2.50	0.46
1:B:195:LEU:CD2	1:B:205:ILE:HD13	2.45	0.46
1:C:124:ILE:HD12	1:C:124:ILE:N	2.30	0.46
1:C:320:THR:N	3:C:503:PO4:O2	2.45	0.46
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.29	0.46
1:D:146:ASN:O	1:D:148:ASP:N	2.39	0.46
1:D:433:LYS:HA	5:D:612:HOH:O	2.16	0.46
1:A:13:ASN:HD21	1:A:15:ARG:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ARG:NH2	1:D:373:TYR:OH	2.49	0.46
1:A:182:LYS:HB3	1:A:182:LYS:HZ3	1.81	0.46
1:A:190:GLU:CD	1:A:190:GLU:H	2.24	0.46
1:A:441:SER:O	1:A:444:THR:CG2	2.48	0.46
1:B:316:CYS:O	1:B:317:ASN:ND2	2.49	0.46
1:C:24:MET:HE2	1:C:220:LEU:HG	1.97	0.46
1:A:356:GLN:OE1	1:B:5:LYS:NZ	2.49	0.45
1:A:185:VAL:HG22	1:A:222:TYR:HE2	1.81	0.45
1:B:430:TYR:C	1:B:431:MET:HE3	2.42	0.45
1:C:406:TRP:O	1:C:407:GLU:CG	2.63	0.45
1:A:229:ASP:HA	1:C:230:LYS:HG3	1.97	0.45
1:A:286:LYS:HD2	5:A:633:HOH:O	2.17	0.45
1:C:137:GLY:O	1:C:140:VAL:HG22	2.16	0.45
1:D:311:ARG:NH1	1:D:311:ARG:CG	2.70	0.45
1:A:102:PHE:CE2	1:A:106:LYS:HE3	2.52	0.45
1:B:146:ASN:C	1:B:148:ASP:H	2.24	0.45
1:B:173:LEU:O	1:B:177:ILE:HG23	2.16	0.45
1:C:102:PHE:CE2	1:C:106:LYS:HE3	2.51	0.45
1:D:19:LEU:HD11	1:D:291:LEU:HD22	1.98	0.45
1:A:97:THR:HG22	1:A:97:THR:O	2.17	0.45
1:A:376:GLU:OE2	1:A:376:GLU:HA	2.15	0.45
1:B:241:VAL:HG11	1:B:278:VAL:HG22	1.98	0.45
1:B:257:PHE:CE1	1:B:282:GLY:HA3	2.52	0.45
1:C:102:PHE:O	1:C:106:LYS:HG2	2.17	0.45
1:A:316:CYS:O	1:A:317:ASN:CB	2.65	0.45
1:C:393:ARG:CB	1:C:393:ARG:NH2	2.80	0.45
1:A:43:LEU:HB3	1:A:167:VAL:HG21	1.99	0.45
1:A:185:VAL:HG22	1:A:222:TYR:CE2	2.52	0.45
1:B:435:SER:O	1:B:439:GLU:HB2	2.17	0.45
1:C:43:LEU:HB3	1:C:167:VAL:HG21	1.99	0.45
1:C:340:ILE:O	1:C:344:ILE:HG13	2.16	0.45
1:C:357:LYS:O	1:C:360:ASP:HB2	2.17	0.45
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.76	0.45
1:B:86:ARG:HA	1:B:418:TYR:HA	1.99	0.45
1:D:198:PHE:O	1:D:203:LYS:HB2	2.17	0.45
1:A:34:LYS:HE3	1:A:65:PHE:HB2	1.98	0.44
1:C:124:ILE:H	1:C:124:ILE:CD1	2.24	0.44
1:D:183:LYS:O	1:D:183:LYS:HG2	2.17	0.44
1:D:305:ILE:HD12	1:D:305:ILE:N	2.33	0.44
1:D:441:SER:C	1:D:443:MET:N	2.74	0.44
1:C:146:ASN:OD1	1:C:149:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ASN:N	1:D:449:ASN:ND2	2.52	0.44
1:A:375:GLN:O	1:A:378:HIS:HB3	2.17	0.44
1:B:374:ASP:HA	1:B:377:ILE:HG12	1.99	0.44
1:D:257:PHE:CE1	1:D:282:GLY:HA3	2.52	0.44
1:C:13:ASN:HD21	1:C:15:ARG:HB2	1.82	0.44
1:C:245:ALA:O	1:C:250:PHE:HB2	2.17	0.44
1:C:344:ILE:HD13	1:C:395:LEU:HD23	2.00	0.44
1:A:62:LYS:HG2	1:A:63:PHE:N	2.32	0.44
1:B:243:THR:O	1:B:244:LEU:C	2.61	0.44
1:C:94:TYR:CZ	1:C:405:LYS:HG3	2.52	0.44
1:C:128:PHE:CE1	1:C:164:VAL:HG11	2.53	0.44
1:A:205:ILE:HG22	1:A:238:PHE:CD1	2.50	0.44
1:B:177:ILE:HD12	1:B:181:LEU:HD23	1.99	0.44
1:B:344:ILE:O	1:B:348:MET:HG3	2.17	0.44
1:C:6:VAL:HG22	1:C:431:MET:CE	2.48	0.44
1:C:78:ASN:HB2	1:C:80:ASN:ND2	2.32	0.44
1:C:154:GLN:O	1:C:158:GLN:HG3	2.18	0.44
1:D:287:PHE:CE1	1:D:291:LEU:HD13	2.53	0.44
1:A:102:PHE:O	1:A:106:LYS:HG2	2.18	0.44
1:A:128:PHE:CE1	1:A:164:VAL:HG11	2.53	0.44
1:A:213:TYR:CE2	1:A:217:LYS:HD2	2.53	0.44
1:D:312:LEU:HD23	1:D:312:LEU:O	2.17	0.44
1:A:392:SER:HB3	1:B:447:ARG:NH2	2.33	0.44
1:D:244:LEU:HD12	1:D:280:GLN:CD	2.42	0.44
1:A:104:ASP:O	1:A:108:ILE:HG13	2.18	0.44
1:C:145:THR:O	1:C:146:ASN:HB2	2.18	0.44
1:C:253:ASP:OD2	1:C:254:ASN:N	2.47	0.44
1:D:152:SER:O	1:D:156:ILE:HG13	2.18	0.44
1:A:87:TYR:CD2	1:B:425:ARG:HG3	2.52	0.43
1:A:408:ARG:HH21	1:A:408:ARG:CG	2.31	0.43
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.80	0.43
1:C:34:LYS:HE3	1:C:65:PHE:HB2	2.00	0.43
1:C:312:LEU:HD23	1:C:312:LEU:O	2.18	0.43
1:D:377:ILE:HG13	1:D:378:HIS:N	2.33	0.43
1:A:145:THR:O	1:A:146:ASN:HB2	2.18	0.43
1:A:452:LEU:HD13	1:A:452:LEU:O	2.17	0.43
1:B:152:SER:O	1:B:156:ILE:HG13	2.18	0.43
1:B:305:ILE:N	1:B:305:ILE:HD12	2.32	0.43
1:D:14:MET:O	1:D:203:LYS:NZ	2.46	0.43
1:A:154:GLN:O	1:A:158:GLN:HG3	2.18	0.43
1:D:15:ARG:HD3	1:D:443:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASN:HD22	1:D:254:ASN:N	2.12	0.43
1:A:78:ASN:HB2	1:A:80:ASN:ND2	2.33	0.43
1:B:39:LEU:HD13	1:B:173:LEU:HD23	2.00	0.43
1:D:354:LEU:HB3	1:D:384:ILE:HG13	2.01	0.43
1:B:18:LYS:NZ	5:B:662:HOH:O	2.51	0.43
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.19	0.43
1:C:135:LEU:O	1:C:139:LEU:HD13	2.18	0.43
1:D:43:LEU:HB3	1:D:167:VAL:HG21	1.99	0.43
1:A:6:VAL:HG13	1:A:431:MET:HE3	2.01	0.43
1:C:62:LYS:HG2	1:C:63:PHE:N	2.34	0.43
1:C:97:THR:O	1:C:97:THR:HG22	2.19	0.43
1:C:358:TYR:CE2	1:D:441:SER:HA	2.54	0.43
1:C:393:ARG:HB3	1:C:393:ARG:HH21	1.83	0.43
1:C:178:ILE:HD12	1:C:181:LEU:HD21	2.01	0.43
1:C:354:LEU:HD23	1:C:357:LYS:HD2	2.00	0.43
1:D:146:ASN:C	1:D:148:ASP:H	2.24	0.43
1:A:30:ARG:HG2	1:A:30:ARG:NH1	2.31	0.43
1:A:253:ASP:OD2	1:A:254:ASN:N	2.47	0.43
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.84	0.43
1:A:146:ASN:OD1	1:A:149:LYS:HG2	2.18	0.43
1:B:103:SER:O	1:B:107:LYS:HG2	2.19	0.43
1:B:330:GLU:O	1:B:334:GLN:HG3	2.19	0.43
1:C:451:ARG:HD2	1:C:451:ARG:C	2.43	0.43
1:B:25:ASP:O	1:B:26:HIS:HB2	2.18	0.43
1:B:190:GLU:H	1:B:190:GLU:CD	2.27	0.43
1:B:254:ASN:HD22	1:B:254:ASN:N	2.10	0.43
1:C:213:TYR:CE2	1:C:217:LYS:HD2	2.54	0.43
1:C:356:GLN:NE2	1:C:359:VAL:HG21	2.34	0.43
1:D:39:LEU:HD13	1:D:173:LEU:HD23	2.01	0.43
1:B:45:LYS:HD2	1:B:61:PHE:HB2	2.01	0.42
1:C:64:ASN:HD22	1:C:67:ASP:CG	2.27	0.42
1:D:47:ARG:NH2	1:D:170:ASP:OD2	2.48	0.42
1:A:178:ILE:HD12	1:A:178:ILE:HA	1.93	0.42
1:A:178:ILE:HD12	1:A:181:LEU:HD21	2.00	0.42
1:B:340:ILE:O	1:B:344:ILE:HG13	2.20	0.42
1:A:94:TYR:CZ	1:A:99:GLN:HB2	2.54	0.42
1:A:241:VAL:HG11	1:A:278:VAL:HG22	2.00	0.42
1:B:10:ARG:HG3	1:B:10:ARG:HH11	1.84	0.42
1:B:340:ILE:HD12	1:B:397:GLU:HG2	2.00	0.42
1:C:308:ASP:OD2	1:C:311:ARG:HB2	2.19	0.42
1:C:401:PHE:CD1	1:C:401:PHE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ILE:HD12	1:D:181:LEU:HD23	2.01	0.42
1:D:243:THR:O	1:D:280:GLN:HA	2.20	0.42
1:D:349:ALA:O	1:D:353:GLU:HG3	2.19	0.42
1:A:19:LEU:CD2	1:A:291:LEU:HD13	2.49	0.42
1:C:190:GLU:CD	1:C:190:GLU:H	2.28	0.42
1:D:333:SER:HB3	1:D:401:PHE:O	2.19	0.42
1:C:146:ASN:C	1:C:146:ASN:ND2	2.78	0.42
1:C:185:VAL:HG22	1:C:222:TYR:HE2	1.84	0.42
1:D:450:ARG:O	1:D:450:ARG:HG3	2.19	0.42
1:B:41:TYR:CE1	1:B:63:PHE:HB2	2.54	0.42
1:B:340:ILE:CD1	1:B:397:GLU:HG2	2.50	0.42
1:D:338:LEU:N	1:D:339:PRO:HD2	2.35	0.42
1:A:351:LYS:NZ	1:B:445:TYR:O	2.51	0.42
1:B:357:LYS:HD2	1:B:380:LEU:HD11	2.01	0.42
1:C:243:THR:O	1:C:280:GLN:HA	2.20	0.42
1:D:241:VAL:HG13	1:D:278:VAL:HG22	1.99	0.42
1:D:329:GLU:O	1:D:330:GLU:C	2.62	0.42
1:B:47:ARG:NH2	1:B:170:ASP:OD2	2.50	0.42
1:B:441:SER:C	1:B:443:MET:N	2.78	0.42
1:D:225:SER:HB2	1:D:226:PRO:HD3	2.02	0.42
1:B:380:LEU:O	1:B:384:ILE:HG13	2.20	0.42
1:D:58:ILE:HG13	1:D:59:LYS:N	2.35	0.42
1:D:377:ILE:C	1:D:377:ILE:HD12	2.45	0.42
1:D:380:LEU:O	1:D:381:GLN:C	2.63	0.42
1:B:110:ARG:O	1:B:111:SER:HB2	2.20	0.41
1:B:338:LEU:O	1:B:339:PRO:C	2.61	0.41
1:C:185:VAL:HG22	1:C:222:TYR:CE2	2.55	0.41
1:C:346:GLU:O	1:C:350:ILE:HG12	2.20	0.41
1:D:316:CYS:O	1:D:317:ASN:CG	2.62	0.41
1:B:177:ILE:HD12	1:B:177:ILE:C	2.45	0.41
1:D:57:GLU:OE1	1:D:57:GLU:HA	2.20	0.41
1:D:103:SER:O	1:D:107:LYS:HG2	2.19	0.41
1:D:154:GLN:HE21	1:D:154:GLN:HB2	1.65	0.41
1:D:290:ASP:HA	5:D:652:HOH:O	2.20	0.41
1:A:124:ILE:H	1:A:124:ILE:CD1	2.24	0.41
1:A:245:ALA:O	1:A:250:PHE:HB2	2.19	0.41
1:B:228:LEU:HD21	1:B:234:TRP:HA	2.03	0.41
1:B:243:THR:O	1:B:280:GLN:HA	2.20	0.41
1:C:37:GLU:OE2	1:C:128:PHE:HA	2.20	0.41
1:D:12:ILE:HG23	1:D:12:ILE:O	2.20	0.41
1:D:41:TYR:CE1	1:D:63:PHE:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:THR:O	1:D:244:LEU:C	2.64	0.41
1:A:76:SER:HB2	1:A:154:GLN:HA	2.02	0.41
1:B:58:ILE:HG13	1:B:59:LYS:N	2.36	0.41
1:C:104:ASP:O	1:C:108:ILE:HG13	2.20	0.41
1:C:322:LEU:O	1:C:430:TYR:HA	2.20	0.41
1:D:316:CYS:O	1:D:317:ASN:CB	2.68	0.41
1:B:254:ASN:HD22	1:B:254:ASN:C	2.29	0.41
1:C:13:ASN:HB2	1:C:445:TYR:CE2	2.55	0.41
1:D:190:GLU:H	1:D:190:GLU:CD	2.28	0.41
1:D:228:LEU:HD21	1:D:234:TRP:HA	2.03	0.41
1:D:327:LEU:HD11	1:D:430:TYR:CE2	2.55	0.41
1:A:312:LEU:HD23	1:A:312:LEU:O	2.20	0.41
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.89	0.41
1:A:135:LEU:O	1:A:139:LEU:HD13	2.19	0.41
1:A:225:SER:C	1:A:227:PHE:H	2.28	0.41
1:A:182:LYS:HB3	1:A:182:LYS:HZ2	1.85	0.41
1:B:10:ARG:HG3	1:B:10:ARG:NH1	2.36	0.41
1:B:254:ASN:N	1:B:254:ASN:ND2	2.69	0.41
1:B:376:GLU:O	1:B:380:LEU:HD23	2.21	0.41
1:C:76:SER:HB2	1:C:154:GLN:HA	2.03	0.41
1:C:94:TYR:CZ	1:C:99:GLN:HB2	2.55	0.41
1:C:416:GLU:CD	1:C:416:GLU:H	2.28	0.41
1:D:351:LYS:NZ	1:D:355:GLU:OE2	2.54	0.41
1:A:228:LEU:HD21	1:A:234:TRP:CA	2.49	0.41
1:A:452:LEU:HA	1:A:452:LEU:HD22	1.75	0.41
1:B:250:PHE:CD2	1:B:250:PHE:C	2.98	0.41
1:B:404:PRO:HG2	5:B:625:HOH:O	2.21	0.41
1:C:83:LYS:NZ	1:C:411:ARG:O	2.54	0.41
1:C:194:GLY:HA3	1:C:438:LEU:HB3	2.02	0.41
1:C:326:GLU:OE1	1:C:326:GLU:N	2.45	0.40
1:B:6:VAL:HG13	1:B:431:MET:CE	2.51	0.40
1:D:146:ASN:OD1	1:D:149:LYS:HG2	2.21	0.40
1:D:330:GLU:OE2	1:D:409:VAL:N	2.51	0.40
1:A:373:TYR:CZ	1:A:376:GLU:HG2	2.56	0.40
1:D:30:ARG:HH11	1:D:30:ARG:HG2	1.86	0.40
1:A:229:ASP:OD1	1:C:230:LYS:HE3	2.22	0.40
1:A:460:LEU:C	1:A:462:HIS:N	2.76	0.40
1:C:24:MET:HE2	1:C:220:LEU:HD11	2.03	0.40
1:C:393:ARG:NH2	1:C:393:ARG:HB2	2.36	0.40
1:A:452:LEU:O	1:A:455:HIS:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	451/470 (96%)	419 (93%)	25 (6%)	7 (2%)	7	13
1	B	456/470 (97%)	429 (94%)	22 (5%)	5 (1%)	11	21
1	C	434/470 (92%)	401 (92%)	28 (6%)	5 (1%)	10	19
1	D	454/470 (97%)	426 (94%)	23 (5%)	5 (1%)	11	21
All	All	1795/1880 (96%)	1675 (93%)	98 (6%)	22 (1%)	10	19

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	PRO
1	A	368	GLU
1	C	151	PRO
1	A	50	GLU
1	A	229	ASP
1	D	450	ARG
1	B	147	PRO
1	B	317	ASN
1	C	50	GLU
1	C	65	PHE
1	D	147	PRO
1	D	317	ASN
1	A	65	PHE
1	B	151	PRO
1	B	452	LEU
1	D	151	PRO
1	A	146	ASN
1	C	146	ASN
1	C	147	PRO
1	A	147	PRO
1	B	276	PRO
1	D	276	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/421 (97%)	377 (92%)	32 (8%)	11	23
1	B	411/421 (98%)	379 (92%)	32 (8%)	11	23
1	C	392/421 (93%)	366 (93%)	26 (7%)	15	30
1	D	410/421 (97%)	379 (92%)	31 (8%)	12	24
All	All	1622/1684 (96%)	1501 (92%)	121 (8%)	12	24

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	39	LEU
1	A	56	GLU
1	A	91	ARG
1	A	110	ARG
1	A	116	LEU
1	A	124	ILE
1	A	141	ASP
1	A	168	HIS
1	A	182	LYS
1	A	185	VAL
1	A	218	LEU
1	A	235	GLN
1	A	306	TYR
1	A	311	ARG
1	A	312	LEU
1	A	317	ASN
1	A	323	VAL
1	A	338	LEU
1	A	352	LYS
1	A	363	THR
1	A	373	TYR
1	A	382	LEU
1	A	388	ASP

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Mol	Chain	Res	Type
1	A	408	ARG
1	A	416	GLU
1	A	425	ARG
1	A	437	LEU
1	A	444	THR
1	A	449	ASN
1	A	451	ARG
1	A	452	LEU
1	B	23	ASP
1	B	30	ARG
1	B	34	LYS
1	B	39	LEU
1	B	69	ILE
1	B	83	LYS
1	B	84	LEU
1	B	124	ILE
1	B	142	LEU
1	B	172	THR
1	B	173	LEU
1	B	177	ILE
1	B	180	ASN
1	B	185	VAL
1	B	189	LYS
1	B	218	LEU
1	B	228	LEU
1	B	235	GLN
1	B	241	VAL
1	B	254	ASN
1	B	291	LEU
1	B	317	ASN
1	B	325	GLU
1	B	341	GLU
1	B	352	LYS
1	B	383	GLN
1	B	385	SER
1	B	393	ARG
1	B	397	GLU
1	B	415	GLU
1	B	431	MET
1	B	450	ARG
1	C	5	LYS
1	C	39	LEU

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Mol	Chain	Res	Type
1	C	56	GLU
1	C	110	ARG
1	C	116	LEU
1	C	124	ILE
1	C	141	ASP
1	C	168	HIS
1	C	182	LYS
1	C	185	VAL
1	C	218	LEU
1	C	228	LEU
1	C	235	GLN
1	C	241	VAL
1	C	306	TYR
1	C	311	ARG
1	C	312	LEU
1	C	317	ASN
1	C	323	VAL
1	C	408	ARG
1	C	411	ARG
1	C	416	GLU
1	C	425	ARG
1	C	437	LEU
1	C	444	THR
1	C	451	ARG
1	D	23	ASP
1	D	30	ARG
1	D	34	LYS
1	D	39	LEU
1	D	69	ILE
1	D	83	LYS
1	D	84	LEU
1	D	124	ILE
1	D	142	LEU
1	D	172	THR
1	D	173	LEU
1	D	177	ILE
1	D	185	VAL
1	D	189	LYS
1	D	218	LEU
1	D	228	LEU
1	D	235	GLN
1	D	241	VAL

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Mol	Chain	Res	Type
1	D	254	ASN
1	D	291	LEU
1	D	317	ASN
1	D	325	GLU
1	D	357	LYS
1	D	372	GLN
1	D	375	GLN
1	D	377	ILE
1	D	382	LEU
1	D	431	MET
1	D	449	ASN
1	D	453	LEU
1	D	458	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	ASN
1	A	64	ASN
1	A	78	ASN
1	A	138	GLN
1	A	154	GLN
1	A	180	ASN
1	A	246	ASN
1	A	383	GLN
1	A	455	HIS
1	B	138	GLN
1	B	154	GLN
1	B	235	GLN
1	B	246	ASN
1	B	254	ASN
1	B	271	HIS
1	B	317	ASN
1	B	381	GLN
1	B	399	ASN
1	C	13	ASN
1	C	35	ASN
1	C	64	ASN
1	C	78	ASN
1	C	138	GLN
1	C	154	GLN

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Mol	Chain	Res	Type
1	C	180	ASN
1	C	246	ASN
1	C	334	GLN
1	C	356	GLN
1	C	383	GLN
1	C	390	GLN
1	C	399	ASN
1	D	138	GLN
1	D	154	GLN
1	D	180	ASN
1	D	235	GLN
1	D	246	ASN
1	D	254	ASN
1	D	271	HIS
1	D	317	ASN
1	D	372	GLN
1	D	375	GLN
1	D	381	GLN
1	D	390	GLN
1	D	449	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5GP	A	501	-	26,26,26	1.24	4 (15%)	39,40,40	1.67	8 (20%)
2	5GP	C	501	-	26,26,26	1.26	3 (11%)	39,40,40	1.74	8 (20%)
3	PO4	A	503	-	4,4,4	1.68	0	6,6,6	0.45	0
3	PO4	B	501	4	4,4,4	1.77	1 (25%)	6,6,6	0.45	0
3	PO4	B	502	-	4,4,4	1.80	2 (50%)	6,6,6	0.43	0
3	PO4	C	503	-	4,4,4	1.82	2 (50%)	6,6,6	0.46	0
3	PO4	D	502	-	4,4,4	1.56	0	6,6,6	0.46	0
3	PO4	A	502	-	4,4,4	1.86	2 (50%)	6,6,6	0.46	0
3	PO4	C	502	4	4,4,4	1.89	3 (75%)	6,6,6	0.46	0
3	PO4	D	501	4	4,4,4	1.71	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
2	5GP	A	501	-	-	2/10/26/26	0/3/3/3
2	5GP	C	501	-	-	3/10/26/26	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	5GP	C2-N3	2.69	1.39	1.33
2	C	501	5GP	C1'-N9	2.59	1.54	1.47
2	A	501	5GP	C2-N3	2.53	1.39	1.33
3	C	502	PO4	P-O4	-2.31	1.47	1.54
2	A	501	5GP	O4'-C1'	2.30	1.47	1.42
3	A	502	PO4	P-O3	-2.27	1.48	1.54
3	B	501	PO4	P-O2	-2.21	1.48	1.54
3	C	503	PO4	P-O2	-2.18	1.48	1.54
3	A	502	PO4	P-O4	-2.14	1.48	1.54
3	C	503	PO4	P-O3	-2.09	1.48	1.54
2	A	501	5GP	C1'-N9	2.07	1.53	1.47
2	A	501	5GP	O2'-C2'	2.06	1.48	1.43
3	B	502	PO4	P-O4	-2.05	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	PO4	P-O3	-2.04	1.48	1.54
3	C	502	PO4	P-O2	-2.03	1.48	1.54
3	B	502	PO4	P-O3	-2.02	1.48	1.54
2	C	501	5GP	O2'-C2'	2.01	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	5GP	C5-C4-N3	-4.74	120.84	128.39
2	A	501	5GP	C5-C4-N3	-4.56	121.14	128.39
2	A	501	5GP	C2-N3-C4	4.43	119.93	112.30
2	C	501	5GP	C2-N3-C4	4.34	119.78	112.30
2	C	501	5GP	C4'-O4'-C1'	-3.50	101.73	109.47
2	C	501	5GP	O6-C6-C5	-2.69	119.44	126.53
2	C	501	5GP	N9-C4-N3	2.65	131.24	125.95
2	A	501	5GP	O6-C6-C5	-2.61	119.64	126.53
2	A	501	5GP	C6-C5-N7	2.54	134.92	130.29
2	A	501	5GP	C4'-O4'-C1'	-2.49	103.96	109.47
2	A	501	5GP	N9-C4-N3	2.48	130.91	125.95
2	C	501	5GP	C5-C6-N1	2.47	119.55	113.25
2	A	501	5GP	C5-C6-N1	2.46	119.50	113.25
2	A	501	5GP	O4'-C4'-C5'	2.43	117.12	109.33
2	C	501	5GP	C6-C5-N7	2.40	134.66	130.29
2	C	501	5GP	O4'-C4'-C5'	2.27	116.59	109.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

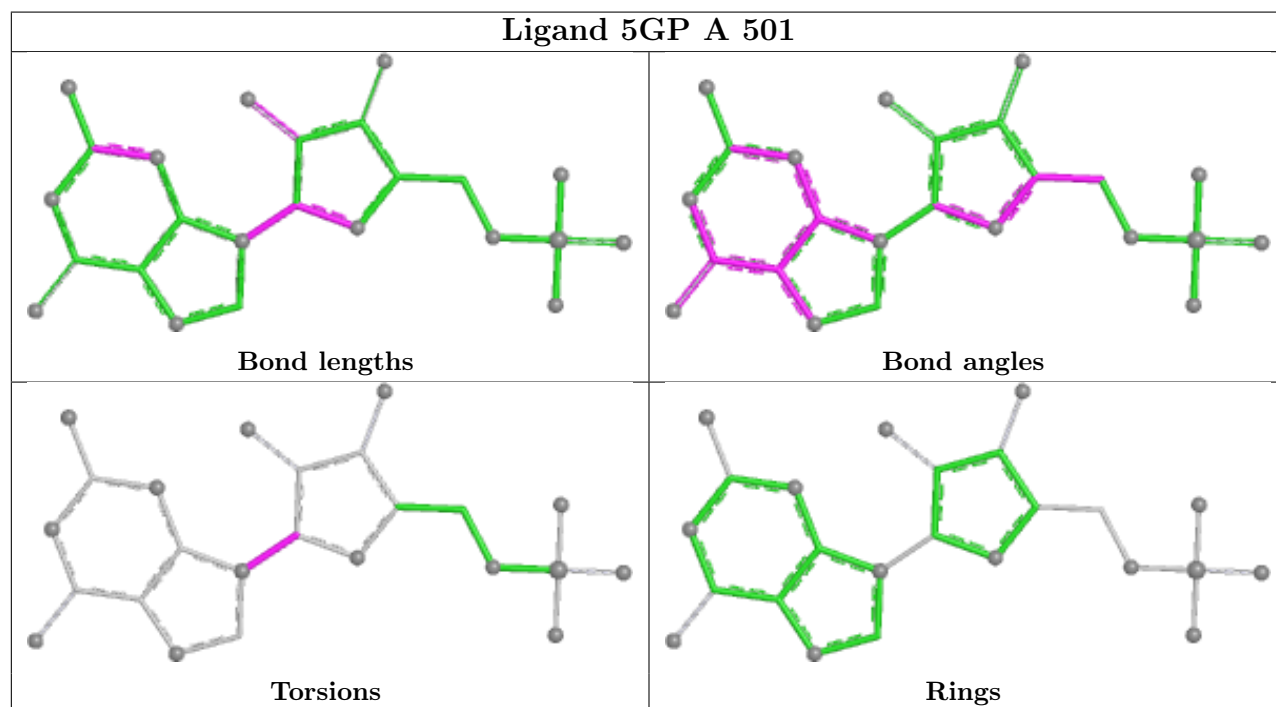
Mol	Chain	Res	Type	Atoms
2	C	501	5GP	O4'-C1'-N9-C8
2	C	501	5GP	O4'-C1'-N9-C4
2	A	501	5GP	O4'-C1'-N9-C4
2	A	501	5GP	O4'-C1'-N9-C8
2	C	501	5GP	C4'-C5'-O5'-P

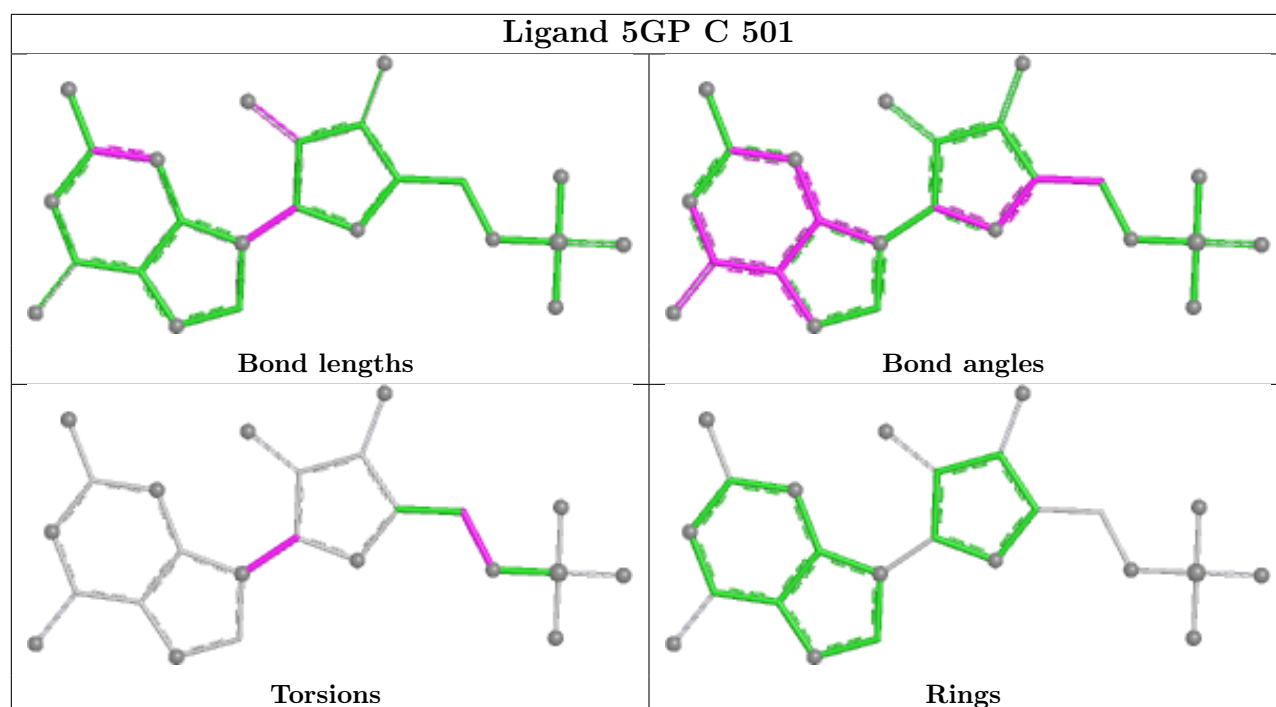
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/470 (96%)	0.62	48 (10%) 11 10	37, 57, 100, 109	0
1	B	458/470 (97%)	0.46	18 (3%) 43 39	32, 53, 81, 92	0
1	C	438/470 (93%)	0.63	36 (8%) 17 15	36, 62, 98, 119	0
1	D	456/470 (97%)	0.51	24 (5%) 32 29	35, 56, 83, 97	0
All	All	1807/1880 (96%)	0.55	126 (6%) 22 20	32, 56, 93, 119	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	TYR	5.0
1	A	459	ILE	4.8
1	A	306	TYR	4.3
1	A	157	ALA	4.2
1	A	363	THR	4.0
1	A	457	ILE	3.9
1	A	460	LEU	3.8
1	A	373	TYR	3.8
1	C	306	TYR	3.7
1	B	306	TYR	3.7
1	A	54	TYR	3.7
1	D	218	LEU	3.6
1	B	128	PHE	3.5
1	D	100	ILE	3.5
1	B	150	MET	3.4
1	A	366	ILE	3.4
1	B	377	ILE	3.4
1	C	384	ILE	3.4
1	B	459	ILE	3.3
1	C	310	LEU	3.3
1	A	128	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	3.2
1	C	100	ILE	3.1
1	C	457	ILE	3.1
1	A	231	GLY	3.1
1	C	395	LEU	3.1
1	A	177	ILE	3.0
1	B	147	PRO	3.0
1	A	362	CYS	3.0
1	C	380	LEU	2.9
1	C	307	GLY	2.9
1	A	150	MET	2.9
1	B	51	SER	2.9
1	C	402	TYR	2.9
1	B	52	PHE	2.8
1	A	453	LEU	2.8
1	D	4	HIS	2.8
1	A	310	LEU	2.8
1	C	55	PRO	2.7
1	C	359	VAL	2.7
1	A	52	PHE	2.7
1	D	228	LEU	2.7
1	A	145	THR	2.7
1	A	100	ILE	2.7
1	D	310	LEU	2.7
1	A	154	GLN	2.7
1	A	456	ASP	2.6
1	D	128	PHE	2.6
1	D	377	ILE	2.6
1	A	462	HIS	2.6
1	A	58	ILE	2.6
1	A	142	LEU	2.6
1	D	457	ILE	2.5
1	A	102	PHE	2.5
1	C	382	LEU	2.5
1	B	47	ARG	2.5
1	A	309	ILE	2.5
1	D	179	LYS	2.5
1	A	55	PRO	2.5
1	C	124	ILE	2.5
1	A	173	LEU	2.5
1	A	230	LYS	2.5
1	A	155	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	172	THR	2.5
1	C	147	PRO	2.4
1	C	416	GLU	2.4
1	D	58	ILE	2.4
1	B	142	LEU	2.4
1	C	49	ALA	2.4
1	A	452	LEU	2.4
1	A	455	HIS	2.4
1	C	358	TYR	2.4
1	D	201	TYR	2.4
1	C	150	MET	2.4
1	A	454	ALA	2.4
1	D	101	SER	2.4
1	C	340	ILE	2.4
1	D	92	LEU	2.4
1	A	312	LEU	2.3
1	A	147	PRO	2.3
1	A	51	SER	2.3
1	D	51	SER	2.3
1	D	265	GLY	2.3
1	C	312	LEU	2.3
1	D	182	LYS	2.3
1	B	112	ILE	2.3
1	D	102	PHE	2.3
1	B	168	HIS	2.2
1	C	378	HIS	2.2
1	A	62	LYS	2.2
1	C	170	ASP	2.2
1	A	53	HIS	2.2
1	B	54	TYR	2.2
1	C	87	TYR	2.2
1	B	265	GLY	2.2
1	C	144	ASP	2.2
1	D	458	ASP	2.2
1	A	316	CYS	2.2
1	C	128	PHE	2.2
1	B	123	ALA	2.1
1	C	142	LEU	2.1
1	C	54	TYR	2.1
1	C	86	ARG	2.1
1	A	229	ASP	2.1
1	A	48	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	309	ILE	2.1
1	C	58	ILE	2.1
1	A	222	TYR	2.1
1	C	51	SER	2.1
1	B	55	PRO	2.1
1	A	61	PHE	2.1
1	D	49	ALA	2.1
1	C	361	LEU	2.1
1	A	97	THR	2.1
1	A	367	ASP	2.1
1	C	201	TYR	2.1
1	C	308	ASP	2.1
1	B	105	GLN	2.0
1	C	381	GLN	2.0
1	A	140	VAL	2.0
1	B	113	TYR	2.0
1	C	153	TYR	2.0
1	D	144	ASP	2.0
1	C	394	LEU	2.0
1	A	314	LYS	2.0
1	D	69	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5GP	C	501	24/24	0.78	0.14	78,91,106,106	0
2	5GP	A	501	24/24	0.80	0.15	78,90,104,104	0

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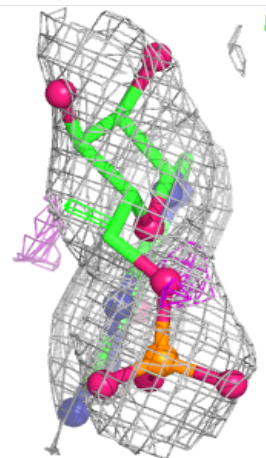
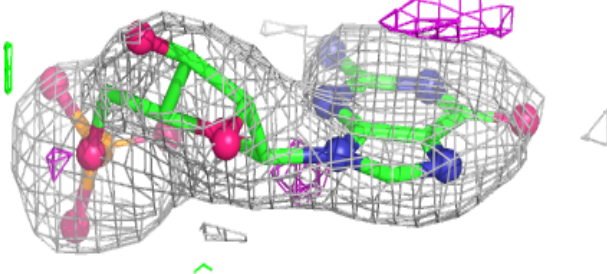
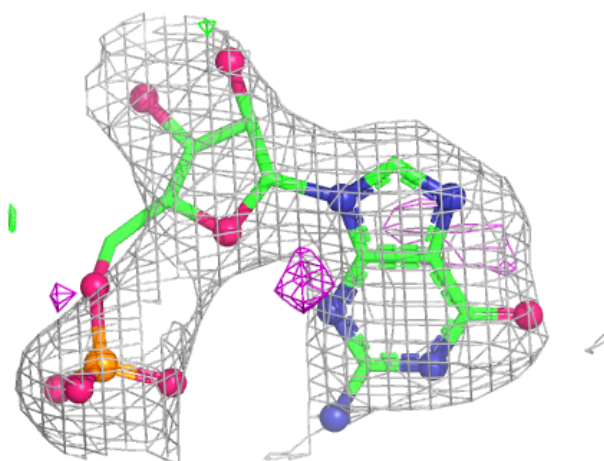
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	503	1/1	0.91	0.09	44,44,44,44	0
3	PO4	D	502	5/5	0.93	0.11	69,69,71,72	0
3	PO4	A	503	5/5	0.93	0.13	83,84,85,85	0
3	PO4	C	503	5/5	0.94	0.13	75,76,78,78	0
3	PO4	B	502	5/5	0.95	0.11	66,68,70,71	0
4	MG	D	503	1/1	0.95	0.09	62,62,62,62	0
4	MG	C	504	1/1	0.97	0.04	69,69,69,69	0
3	PO4	A	502	5/5	0.98	0.05	49,49,52,53	0
3	PO4	D	501	5/5	0.98	0.07	52,54,56,56	0
3	PO4	B	501	5/5	0.99	0.06	38,41,42,45	0
3	PO4	C	502	5/5	0.99	0.05	46,48,50,50	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.

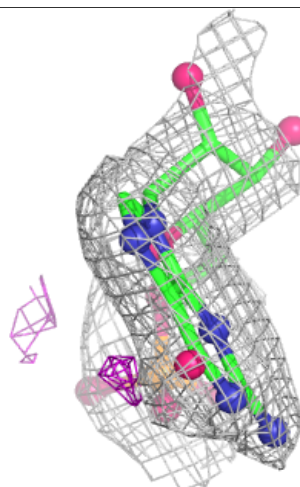
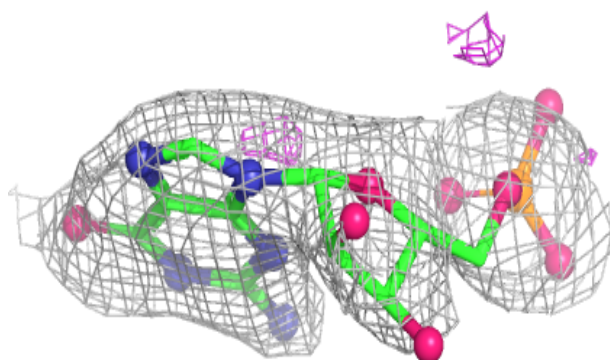
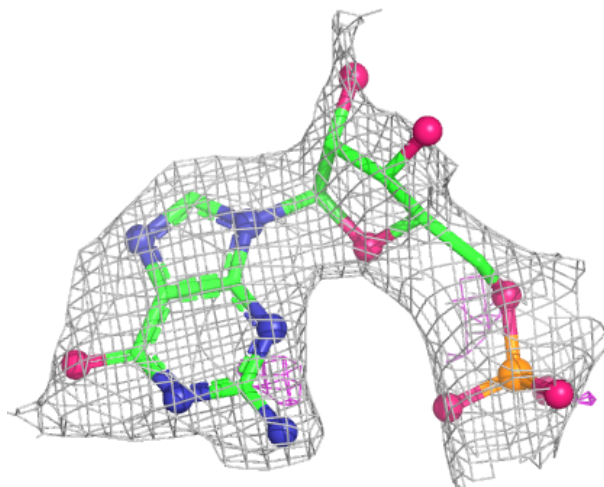
Electron density around 5GP C 501:

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 5GP A 501:

$2mF_o-DF_c$ (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.