



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:46 AM UTC

PDB ID : 2BO7 / pdb_00002bo7
Title : DISSECTION OF MANNOSYLGLYCERATE SYNTHASE: AN ARCHETYPAL MANNOSYLTRANSFERASE
Authors : Flint, J.; Taylor, E.; Yang, M.; Bolam, D.N.; Tailford, L.E.; Martinez-Fleites, C.; Dodson, E.J.; Davis, B.G.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-04-08
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

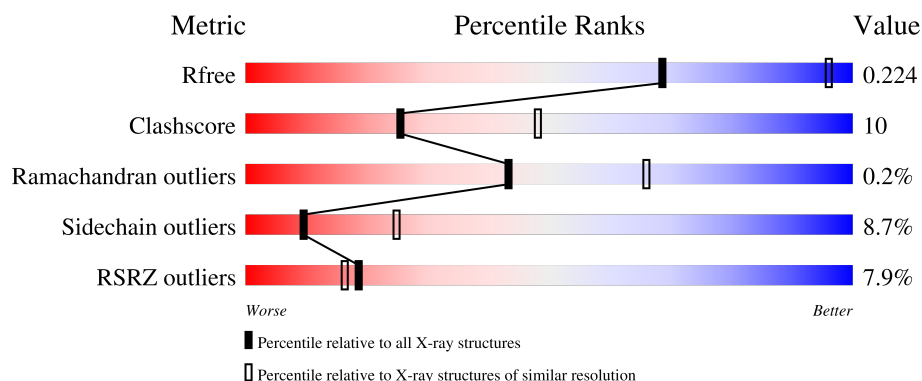
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	397	 4% 75% 15% 5% 5%
1	B	397	 4% 72% 18% 5% 5%
1	C	397	 3% 73% 18% 5% 5%
1	D	397	 9% 75% 15% 5% 5%

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Mol	Chain	Length	Quality of chain
1	E	397	4% 76% 15% • 5%
1	F	397	37% 73% 19% • 5%
1	G	397	6% 75% 15% • 5%
1	H	397	2% 73% 18% • 5%
1	I	397	2% 76% 16% • 5%
1	J	397	4% 73% 18% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31437 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 MANNOSYLGLYCERATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	B	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	C	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	D	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	E	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	F	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	G	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	H	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	I	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			
1	J	376	Total	C	N	O	S	0	0	1
			3102	1983	553	551	15			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	E	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	F	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	G	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	H	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	I	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	J	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Co 1	0	0
3	D	1	Total 1	Co 1	0	0
3	E	1	Total 1	Co 1	0	0
3	F	1	Total 1	Co 1	0	0
3	G	1	Total 1	Co 1	0	0
3	H	1	Total 1	Co 1	0	0
3	I	1	Total 1	Co 1	0	0
3	J	1	Total 1	Co 1	0	0

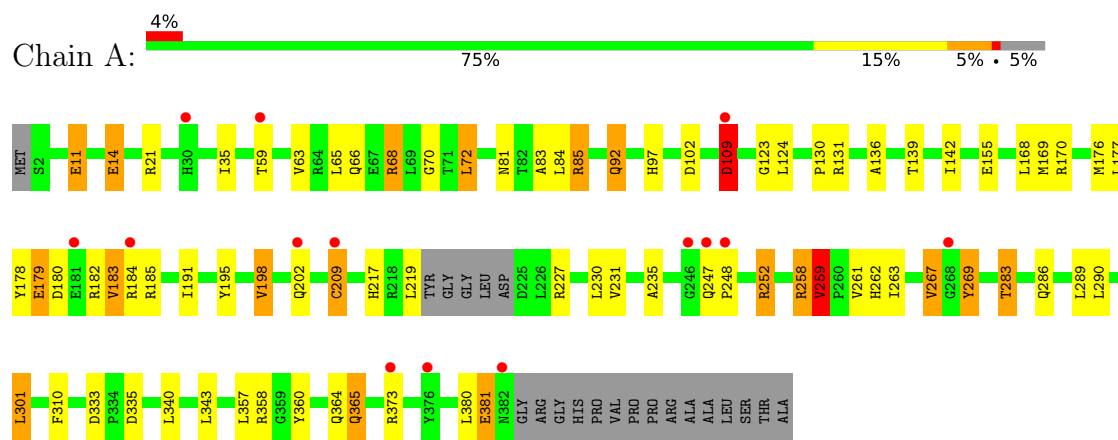
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total 24	O 24	0	0
4	B	27	Total 27	O 27	0	0
4	C	18	Total 18	O 18	0	0
4	D	10	Total 10	O 10	0	0
4	E	10	Total 10	O 10	0	0
4	F	9	Total 9	O 9	0	0
4	G	14	Total 14	O 14	0	0
4	H	2	Total 2	O 2	0	0
4	I	8	Total 8	O 8	0	0
4	J	5	Total 5	O 5	0	0

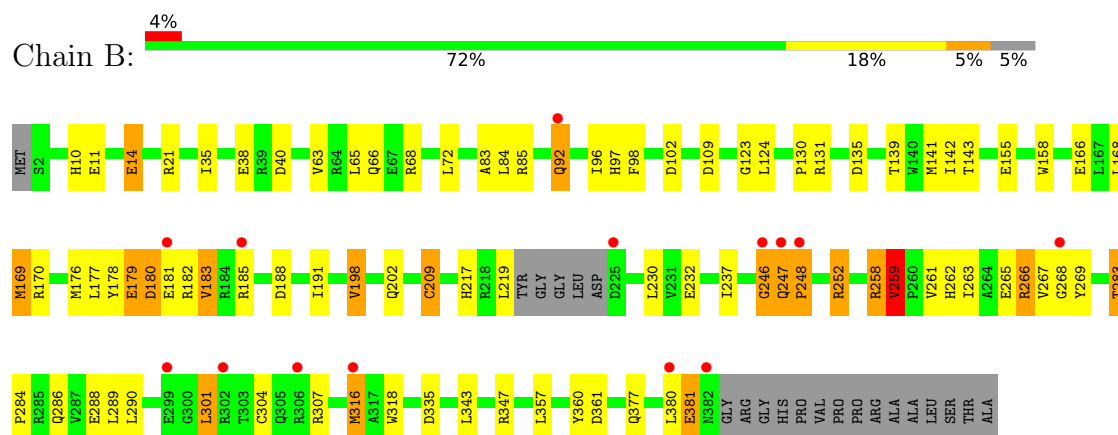
3 Residue-property plots [i](#)

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.

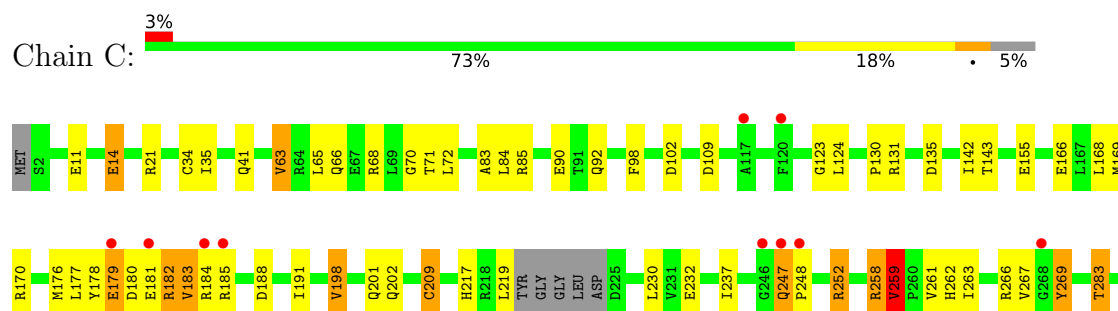
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

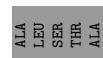
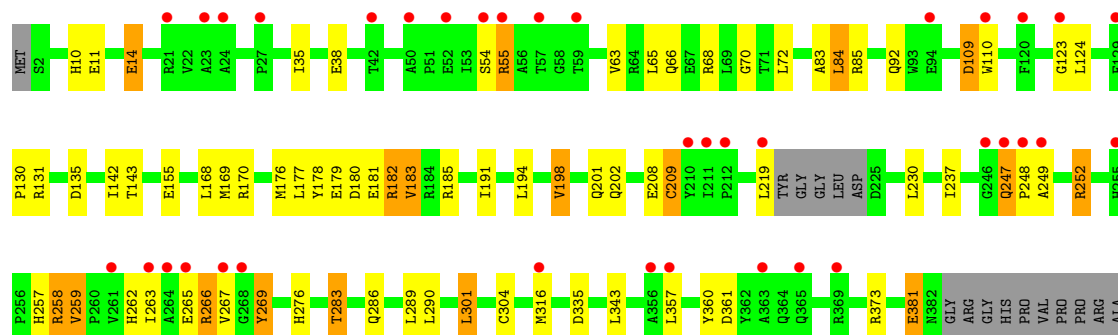
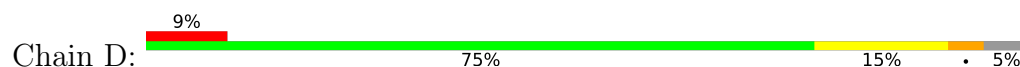


• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

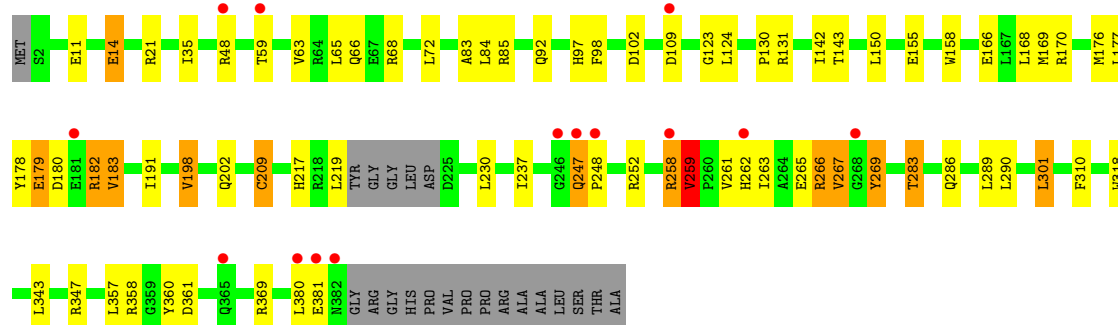
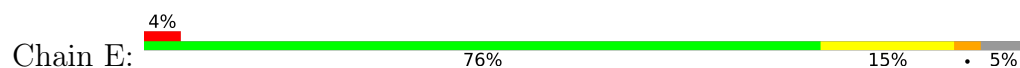




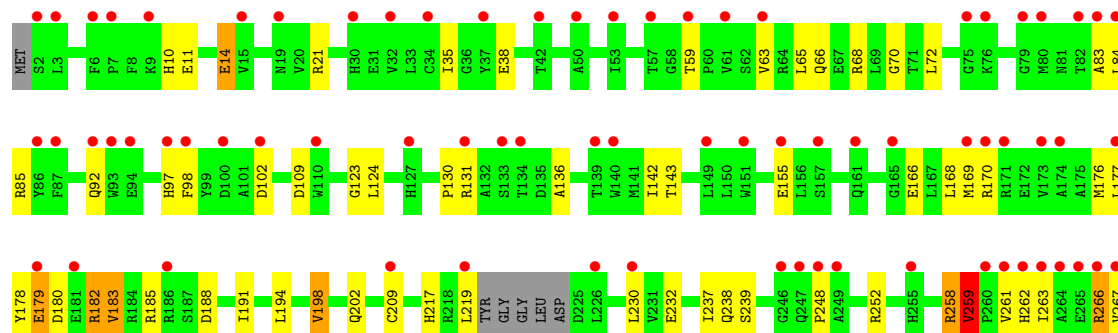
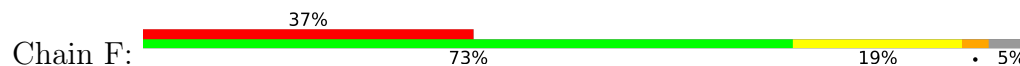
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

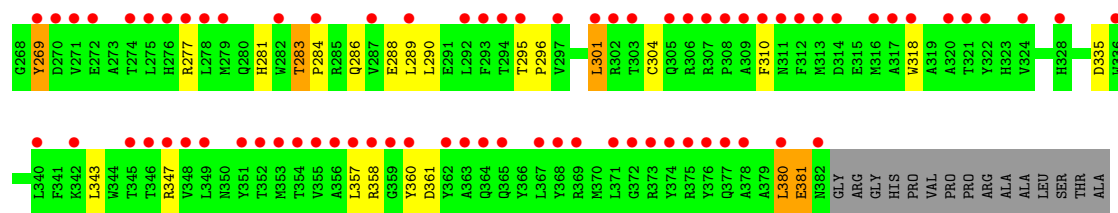


• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

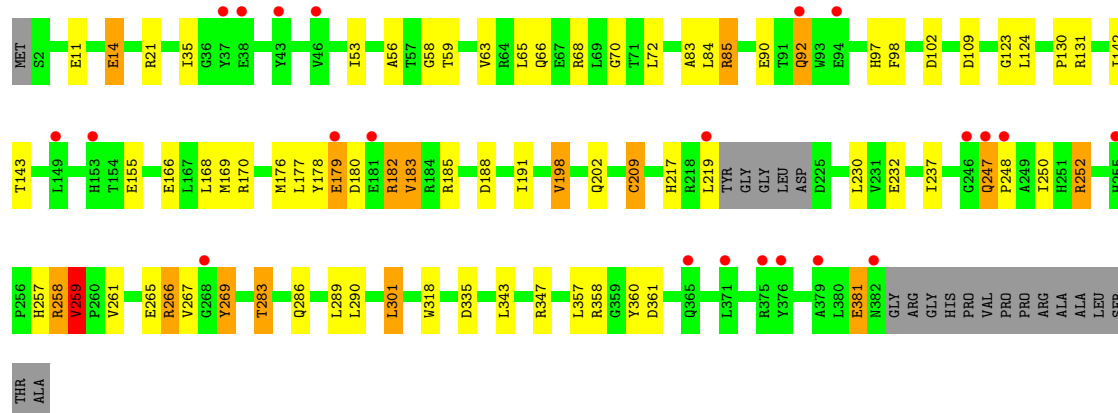
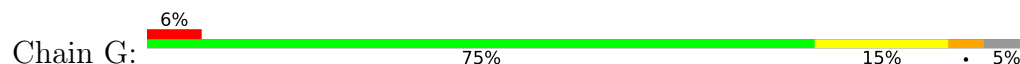


• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

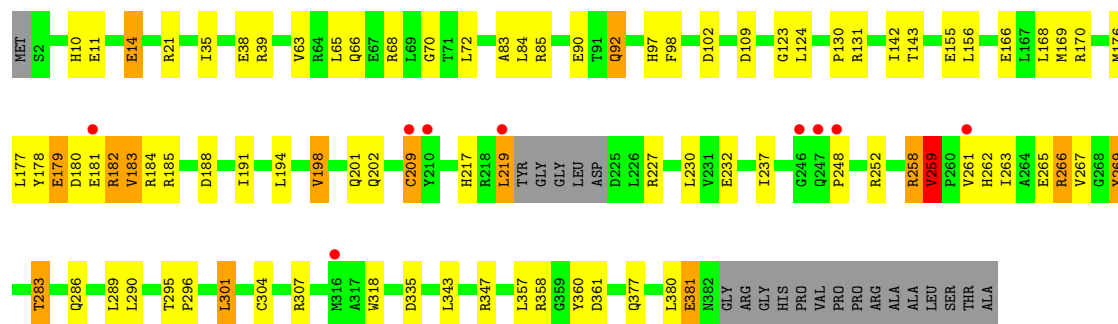




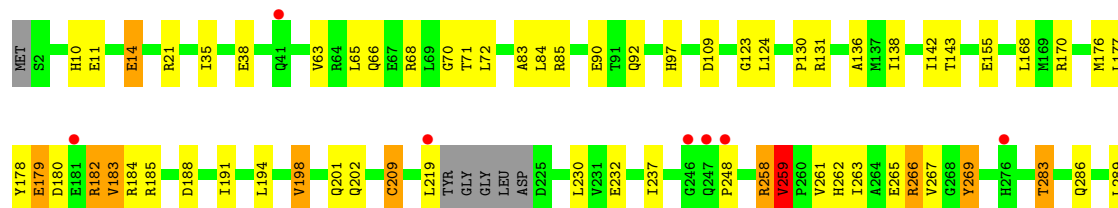
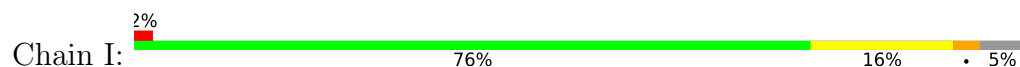
● Molecule 1: MANNOSYLGLYCERATE SYNTHASE

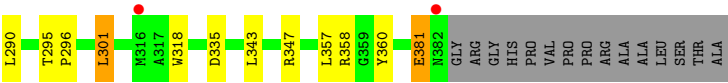


● Molecule 1: MANNOSYLGLYCERATE SYNTHASE

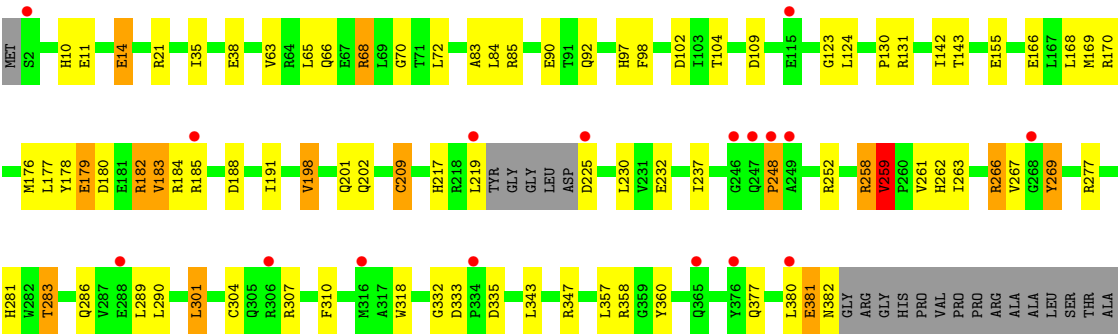


● Molecule 1: MANNOSYLGLYCERATE SYNTHASE





● Molecule 1: MANNOSYLGlycerate SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	406.70Å 162.14Å 108.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	223.61 – 2.95 203.35 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (223.61-2.95) 97.8 (203.35-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.207 , 0.224 0.208 , 0.224	Depositor DCC
R_{free} test set	7443 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31437	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: GDP, CO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.09	4/3191 (0.1%)	1.11	7/4341 (0.2%)
1	B	1.14	6/3191 (0.2%)	1.11	6/4341 (0.1%)
1	C	0.91	2/3191 (0.1%)	1.04	4/4341 (0.1%)
1	D	0.93	3/3191 (0.1%)	1.04	6/4341 (0.1%)
1	E	0.95	1/3191 (0.0%)	1.05	7/4341 (0.2%)
1	F	0.63	1/3191 (0.0%)	0.94	4/4341 (0.1%)
1	G	0.76	2/3191 (0.1%)	0.97	4/4341 (0.1%)
1	H	0.67	1/3191 (0.0%)	0.95	5/4341 (0.1%)
1	I	0.68	1/3191 (0.0%)	0.96	5/4341 (0.1%)
1	J	0.73	1/3191 (0.0%)	0.97	4/4341 (0.1%)
All	All	0.87	22/31910 (0.1%)	1.02	52/43410 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLN	C-O	10.91	1.38	1.23
1	A	373	ARG	NE-CZ	7.94	1.41	1.33
1	B	247	GLN	CA-C	7.43	1.61	1.53
1	B	316	MET	CG-SD	7.15	1.98	1.80
1	I	381	GLU	C-N	-7.03	1.23	1.33
1	D	247	GLN	C-O	6.74	1.32	1.23
1	A	381	GLU	C-N	-6.53	1.24	1.33
1	H	381	GLU	C-N	-6.39	1.24	1.33
1	D	381	GLU	C-N	-6.37	1.24	1.33
1	G	381	GLU	C-N	-6.29	1.24	1.33
1	J	381	GLU	C-N	-6.29	1.24	1.33
1	F	381	GLU	C-N	-6.22	1.24	1.33
1	E	247	GLN	C-O	6.20	1.31	1.23
1	C	381	GLU	C-N	-6.03	1.25	1.33
1	D	373	ARG	NE-CZ	5.90	1.39	1.33
1	C	247	GLN	C-O	5.86	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	GLU	C-N	-5.73	1.25	1.33
1	G	247	GLN	C-O	5.57	1.30	1.23
1	B	248	PRO	N-CA	5.46	1.54	1.47
1	A	365	GLN	CG-CD	5.37	1.65	1.52
1	A	235	ALA	CA-CB	-5.04	1.45	1.53
1	B	246	GLY	CA-C	5.03	1.58	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	VAL	CB-CA-C	-9.68	101.39	110.88
1	D	209	CYS	CB-CA-C	-8.93	95.60	109.89
1	A	259	VAL	CB-CA-C	-8.84	102.22	110.88
1	B	259	VAL	CB-CA-C	-8.23	102.81	110.88
1	A	209	CYS	CB-CA-C	-8.08	96.97	109.89
1	D	191	ILE	N-CA-C	7.62	117.73	110.42
1	B	209	CYS	CB-CA-C	-7.54	97.82	109.89
1	B	191	ILE	N-CA-C	7.49	117.61	110.42
1	J	259	VAL	CB-CA-C	-7.25	103.77	110.88
1	E	191	ILE	N-CA-C	7.21	117.98	110.62
1	E	259	VAL	CB-CA-C	-7.06	103.96	110.88
1	A	191	ILE	N-CA-C	6.98	117.74	110.62
1	C	191	ILE	N-CA-C	6.91	117.67	110.62
1	H	259	VAL	CB-CA-C	-6.79	104.22	110.88
1	I	259	VAL	CB-CA-C	-6.77	104.24	110.88
1	D	269	TYR	N-CA-C	6.66	118.26	108.14
1	F	259	VAL	CB-CA-C	-6.53	104.48	110.88
1	G	259	VAL	CB-CA-C	-6.49	104.52	110.88
1	E	209	CYS	CB-CA-C	-6.39	99.66	109.89
1	C	209	CYS	CB-CA-C	-6.36	98.77	109.65
1	D	109	ASP	N-CA-C	6.35	118.20	111.28
1	J	209	CYS	CB-CA-C	-6.35	99.73	109.89
1	I	269	TYR	N-CA-C	6.22	117.60	108.14
1	E	269	TYR	N-CA-C	6.20	117.57	108.14
1	J	191	ILE	N-CA-C	6.18	116.93	110.62
1	G	191	ILE	N-CA-C	6.16	116.94	110.72
1	F	191	ILE	N-CA-C	6.16	116.90	110.62
1	H	191	ILE	N-CA-C	6.00	116.74	110.62
1	G	209	CYS	CB-CA-C	-5.91	99.55	109.65
1	F	380	LEU	N-CA-C	5.86	117.35	110.97
1	F	269	TYR	N-CA-C	5.79	116.93	108.14
1	C	269	TYR	N-CA-C	5.78	116.92	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	380	LEU	N-CA-C	5.73	118.01	111.02
1	H	209	CYS	CB-CA-C	-5.59	100.94	109.89
1	A	269	TYR	N-CA-C	5.59	116.64	108.14
1	I	191	ILE	N-CA-C	5.54	116.27	110.62
1	E	59	THR	CB-CA-C	5.51	115.97	109.47
1	I	209	CYS	CB-CA-C	-5.47	100.29	109.65
1	G	269	TYR	N-CA-C	5.45	116.42	108.14
1	J	269	TYR	N-CA-C	5.41	116.36	108.14
1	A	109	ASP	N-CA-C	5.29	117.72	111.33
1	A	267	VAL	N-CA-C	5.25	115.41	107.80
1	B	180	ASP	N-CA-C	5.24	116.70	109.15
1	B	141	MET	CA-C-N	-5.22	117.85	122.97
1	B	141	MET	C-N-CA	-5.22	117.85	122.97
1	I	138	ILE	N-CA-C	-5.18	105.49	110.72
1	E	267	VAL	N-CA-C	5.17	115.30	107.80
1	A	59	THR	CB-CA-C	5.15	115.55	109.47
1	H	156	LEU	N-CA-C	5.14	117.29	111.02
1	H	269	TYR	N-CA-C	5.07	115.84	108.14
1	D	208	GLU	CA-C-N	5.05	128.02	120.95
1	D	208	GLU	C-N-CA	5.05	128.02	120.95

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	3102	0	3006	72	1
1	B	3102	0	3006	69	0
1	C	3102	0	3006	72	2
1	D	3102	0	3006	76	2
1	E	3102	0	3006	55	2
1	F	3102	0	3006	69	0
1	G	3102	0	3006	68	1
1	H	3102	0	3006	67	0
1	I	3102	0	3006	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3102	0	3006	60	2
2	A	28	0	12	4	0
2	B	28	0	12	4	0
2	C	28	0	12	4	0
2	D	28	0	12	4	0
2	E	28	0	12	4	0
2	F	28	0	12	4	0
2	G	28	0	12	4	0
2	H	28	0	12	4	0
2	I	28	0	12	5	0
2	J	28	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	24	0	0	5	0
4	B	27	0	0	0	0
4	C	18	0	0	5	0
4	D	10	0	0	5	0
4	E	10	0	0	1	0
4	F	9	0	0	5	0
4	G	14	0	0	9	0
4	H	2	0	0	1	0
4	I	8	0	0	1	0
4	J	5	0	0	3	0
All	All	31437	0	30180	587	5

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 (587) 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:180:ASP:HA	4:F:2006:HOH:O	1.57	1.04
1:A:109:ASP:HB2	4:A:2008:HOH:O	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:HH11	1:B:258:ARG:HG2	1.21	1.02
1:A:176:MET:SD	1:A:202:GLN:HG3	2.00	1.01
1:F:238:GLN:HB3	4:F:2007:HOH:O	1.60	1.01
1:H:258:ARG:HG2	1:H:258:ARG:HH11	1.22	1.01
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.27	0.99
1:J:258:ARG:HG2	1:J:258:ARG:HH11	1.26	0.99
1:E:258:ARG:HG2	1:E:258:ARG:HH11	1.28	0.97
1:D:258:ARG:HH11	1:D:258:ARG:HG2	1.29	0.97
1:G:258:ARG:HG2	1:G:258:ARG:HH11	1.26	0.97
1:I:258:ARG:HH11	1:I:258:ARG:HG2	1.29	0.96
1:G:66:GLN:HE22	2:G:1383:GDP:HN1	1.16	0.94
1:F:66:GLN:HE22	2:F:1383:GDP:HN1	1.14	0.94
1:A:66:GLN:HE22	2:A:1383:GDP:HN1	1.13	0.93
1:F:258:ARG:HG2	1:F:258:ARG:HH11	1.29	0.93
1:E:66:GLN:HE22	2:E:1383:GDP:HN1	1.09	0.92
1:B:85:ARG:HG3	1:B:178:TYR:OH	1.69	0.92
1:H:66:GLN:HE22	2:H:1383:GDP:HN1	1.15	0.91
1:I:66:GLN:HE22	2:I:1383:GDP:HN1	1.10	0.91
1:E:252:ARG:HH12	1:G:248:PRO:HG3	1.34	0.91
1:D:66:GLN:HE22	2:D:1383:GDP:HN1	1.12	0.91
1:B:66:GLN:HE22	2:B:1383:GDP:HN1	1.15	0.90
1:C:258:ARG:HG2	1:C:258:ARG:HH11	1.34	0.90
1:D:249:ALA:HB3	4:D:2004:HOH:O	1.71	0.89
1:B:252:ARG:HH12	1:C:248:PRO:CG	1.86	0.89
1:J:66:GLN:HE22	2:J:1383:GDP:HN1	1.14	0.89
1:C:66:GLN:HE22	2:C:1383:GDP:HN1	1.10	0.88
1:I:85:ARG:HG3	1:I:178:TYR:OH	1.75	0.86
1:H:85:ARG:HG3	1:H:178:TYR:OH	1.77	0.85
1:F:85:ARG:HG3	1:F:178:TYR:OH	1.75	0.84
1:G:85:ARG:HG3	1:G:178:TYR:OH	1.74	0.84
1:D:85:ARG:HG3	1:D:178:TYR:OH	1.79	0.83
1:E:252:ARG:HH12	1:G:248:PRO:CG	1.92	0.82
1:J:85:ARG:HG3	1:J:178:TYR:OH	1.78	0.82
1:A:252:ARG:NH1	1:D:155:GLU:OE1	2.12	0.82
1:C:85:ARG:HG3	1:C:178:TYR:OH	1.79	0.82
1:D:55:ARG:HG2	1:D:55:ARG:HH21	1.44	0.81
1:G:56:ALA:HB3	4:G:2002:HOH:O	1.80	0.80
1:A:85:ARG:HG3	1:A:178:TYR:OH	1.81	0.80
1:B:142:ILE:CD1	1:B:230:LEU:HD11	2.13	0.78
1:H:258:ARG:HG2	1:H:258:ARG:NH1	1.95	0.78
1:J:258:ARG:HG2	1:J:258:ARG:NH1	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:VAL:HG21	1:F:360:TYR:CE1	2.19	0.78
1:C:66:GLN:NE2	2:C:1383:GDP:HN1	1.84	0.76
1:A:248:PRO:CG	1:D:252:ARG:HH12	1.96	0.76
1:I:259:VAL:HG21	1:I:360:TYR:CE1	2.20	0.76
1:B:252:ARG:HH12	1:C:248:PRO:HG3	1.49	0.76
1:G:259:VAL:HG21	1:G:360:TYR:CE1	2.21	0.76
1:E:258:ARG:HG2	1:E:258:ARG:NH1	2.00	0.75
1:F:252:ARG:HH12	1:H:248:PRO:CG	2.01	0.73
1:E:85:ARG:HG3	1:E:178:TYR:OH	1.89	0.73
1:J:259:VAL:HG21	1:J:360:TYR:CE1	2.23	0.73
1:J:283:THR:HG22	1:J:286:GLN:H	1.53	0.72
1:H:259:VAL:HG21	1:H:360:TYR:CE1	2.25	0.72
1:F:258:ARG:HG2	1:F:258:ARG:NH1	2.02	0.71
1:G:56:ALA:CB	4:G:2002:HOH:O	2.35	0.71
1:J:142:ILE:CD1	1:J:230:LEU:HD11	2.21	0.71
1:A:11:GLU:HG3	4:A:2001:HOH:O	1.90	0.71
1:H:176:MET:SD	1:H:202:GLN:HG3	2.31	0.70
1:C:142:ILE:CD1	1:C:230:LEU:HD11	2.21	0.70
1:B:361:ASP:OD1	1:C:258:ARG:HD2	1.90	0.70
1:F:248:PRO:CG	1:H:252:ARG:HH12	2.05	0.70
1:F:252:ARG:HH12	1:H:248:PRO:HG3	1.55	0.70
1:C:176:MET:SD	1:C:202:GLN:HG3	2.32	0.70
1:B:258:ARG:HG2	1:B:258:ARG:NH1	1.94	0.69
1:C:293:PHE:C	4:C:2012:HOH:O	2.35	0.69
1:J:142:ILE:HD12	1:J:230:LEU:CD1	2.23	0.69
1:B:155:GLU:OE1	1:C:252:ARG:NH1	2.25	0.69
1:F:142:ILE:CD1	1:F:230:LEU:HD11	2.23	0.69
1:B:248:PRO:CG	1:C:252:ARG:HH12	2.05	0.69
1:B:283:THR:HG22	1:B:286:GLN:H	1.58	0.69
1:B:248:PRO:HG3	1:C:252:ARG:HH12	1.57	0.69
1:A:259:VAL:HG21	1:A:360:TYR:CE1	2.28	0.68
1:A:123:GLY:HA2	1:A:170:ARG:HD3	1.75	0.68
1:G:358:ARG:HH21	1:H:266:ARG:HA	1.58	0.68
1:I:283:THR:HG22	1:I:286:GLN:H	1.59	0.68
1:F:258:ARG:HD2	1:H:361:ASP:OD1	1.93	0.68
1:F:283:THR:HG22	1:F:286:GLN:H	1.57	0.68
1:E:259:VAL:HG21	1:E:360:TYR:CE1	2.28	0.68
1:A:66:GLN:NE2	2:A:1383:GDP:HN1	1.91	0.68
1:F:176:MET:SD	1:F:202:GLN:HG3	2.34	0.68
1:I:66:GLN:NE2	2:I:1383:GDP:HN1	1.89	0.68
1:I:258:ARG:HG2	1:I:258:ARG:NH1	2.01	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:ASP:HB3	1:H:183:VAL:HG13	1.77	0.67
1:I:176:MET:SD	1:I:202:GLN:HG3	2.34	0.67
1:D:259:VAL:HG21	1:D:360:TYR:CE1	2.29	0.67
1:E:66:GLN:NE2	2:E:1383:GDP:HN1	1.88	0.67
1:F:361:ASP:OD1	1:H:258:ARG:HD2	1.94	0.67
1:F:248:PRO:HG3	1:H:252:ARG:HH12	1.59	0.67
1:H:219:LEU:C	4:H:2002:HOH:O	2.38	0.67
1:I:357:LEU:HD13	1:J:357:LEU:HD13	1.77	0.67
1:B:85:ARG:HG3	1:B:178:TYR:CZ	2.31	0.66
1:G:258:ARG:HG2	1:G:258:ARG:NH1	2.00	0.66
1:J:66:GLN:NE2	2:J:1383:GDP:HN1	1.91	0.66
1:C:184:ARG:NH1	1:C:184:ARG:HG2	2.10	0.66
1:G:142:ILE:CD1	1:G:230:LEU:HD11	2.26	0.66
1:A:248:PRO:HG2	1:D:252:ARG:HH22	1.60	0.66
1:C:259:VAL:HG21	1:C:360:TYR:CE1	2.30	0.66
1:D:176:MET:SD	1:D:202:GLN:HG3	2.36	0.66
1:G:66:GLN:NE2	2:G:1383:GDP:HN1	1.89	0.66
1:A:248:PRO:HG2	1:D:252:ARG:NH2	2.11	0.65
1:B:258:ARG:HH11	1:B:258:ARG:CG	2.02	0.65
1:E:123:GLY:HA2	1:E:170:ARG:HD3	1.78	0.65
1:B:267:VAL:HG12	1:B:269:TYR:H	1.62	0.65
1:F:180:ASP:HB3	1:F:183:VAL:HG13	1.78	0.65
1:D:249:ALA:CA	4:D:2004:HOH:O	2.44	0.65
1:E:248:PRO:HG3	1:G:252:ARG:HH12	1.61	0.65
1:H:142:ILE:CD1	1:H:230:LEU:HD11	2.27	0.64
1:E:361:ASP:OD1	1:G:258:ARG:HD2	1.97	0.64
1:B:180:ASP:HB3	1:B:183:VAL:HG13	1.79	0.64
1:G:85:ARG:HG3	1:G:178:TYR:CZ	2.32	0.64
1:A:358:ARG:HH21	1:B:266:ARG:HA	1.61	0.64
1:D:142:ILE:CD1	1:D:230:LEU:HD11	2.28	0.64
1:E:283:THR:HG22	1:E:286:GLN:H	1.63	0.64
1:B:123:GLY:HA2	1:B:170:ARG:HD3	1.80	0.64
1:I:123:GLY:HA2	1:I:170:ARG:HD3	1.78	0.63
1:A:248:PRO:CG	1:D:252:ARG:HH22	2.10	0.63
1:F:123:GLY:HA2	1:F:170:ARG:HD3	1.80	0.63
1:J:142:ILE:HD12	1:J:230:LEU:HD11	1.79	0.63
1:C:41:GLN:HG3	4:C:2001:HOH:O	1.96	0.63
1:G:123:GLY:HA2	1:G:170:ARG:HD3	1.79	0.63
1:H:123:GLY:HA2	1:H:170:ARG:HD3	1.79	0.63
1:E:266:ARG:HA	1:F:358:ARG:NH2	2.14	0.63
1:A:283:THR:HG22	1:A:286:GLN:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ARG:HG3	1:F:178:TYR:CZ	2.33	0.63
1:C:358:ARG:HH21	1:D:266:ARG:HA	1.63	0.63
1:B:288:GLU:HG3	1:F:284:PRO:HG2	1.81	0.62
1:C:123:GLY:HA2	1:C:170:ARG:HD3	1.81	0.62
1:J:176:MET:SD	1:J:202:GLN:HG3	2.39	0.62
1:H:142:ILE:HD12	1:H:230:LEU:CD1	2.29	0.62
1:G:59:THR:CG2	4:G:2003:HOH:O	2.46	0.62
1:G:176:MET:SD	1:G:202:GLN:HG3	2.39	0.62
1:I:85:ARG:HG3	1:I:178:TYR:CZ	2.33	0.62
1:J:85:ARG:HG3	1:J:178:TYR:CZ	2.34	0.62
1:C:258:ARG:HG2	1:C:258:ARG:NH1	2.04	0.62
1:D:283:THR:HG22	1:D:286:GLN:H	1.63	0.62
1:E:258:ARG:HH11	1:E:258:ARG:CG	2.09	0.62
1:H:258:ARG:HH11	1:H:258:ARG:CG	2.06	0.61
1:H:142:ILE:HD12	1:H:230:LEU:HD11	1.82	0.61
1:A:358:ARG:CD	4:A:2020:HOH:O	2.48	0.61
1:G:283:THR:HG22	1:G:286:GLN:H	1.64	0.61
1:C:358:ARG:CD	4:C:2016:HOH:O	2.48	0.61
1:D:85:ARG:HG3	1:D:178:TYR:CZ	2.35	0.61
1:D:249:ALA:CB	4:D:2004:HOH:O	2.40	0.61
1:H:85:ARG:HG3	1:H:178:TYR:CZ	2.36	0.61
1:B:259:VAL:HG21	1:B:360:TYR:CE1	2.34	0.61
1:C:142:ILE:HD12	1:C:230:LEU:HD11	1.81	0.61
1:A:155:GLU:OE1	1:D:252:ARG:NH1	2.34	0.61
1:B:142:ILE:CD1	1:B:230:LEU:CD1	2.78	0.61
1:C:142:ILE:HD12	1:C:230:LEU:CD1	2.30	0.61
1:B:142:ILE:HD12	1:B:230:LEU:CD1	2.31	0.61
1:H:283:THR:HG22	1:H:286:GLN:H	1.65	0.60
1:J:180:ASP:HB3	1:J:183:VAL:HG13	1.81	0.60
1:B:179:GLU:HA	1:B:179:GLU:OE2	2.00	0.60
1:C:179:GLU:OE2	1:C:179:GLU:HA	2.00	0.60
1:C:180:ASP:HB3	1:C:183:VAL:HG13	1.83	0.60
1:F:66:GLN:NE2	2:F:1383:GDP:HN1	1.94	0.60
1:B:66:GLN:HE21	2:B:1383:GDP:HN21	1.50	0.60
1:A:258:ARG:HH11	1:A:258:ARG:CG	2.09	0.60
1:B:66:GLN:NE2	2:B:1383:GDP:HN1	1.92	0.60
1:A:180:ASP:HB3	1:A:183:VAL:HG13	1.84	0.60
1:C:85:ARG:HG3	1:C:178:TYR:CZ	2.37	0.60
1:D:66:GLN:NE2	2:D:1383:GDP:HN1	1.92	0.60
1:A:176:MET:SD	1:A:202:GLN:CG	2.84	0.59
1:F:142:ILE:HD12	1:F:230:LEU:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ARG:HD3	4:C:2016:HOH:O	2.03	0.59
1:J:123:GLY:HA2	1:J:170:ARG:HD3	1.84	0.59
1:G:58:GLY:C	4:G:2003:HOH:O	2.44	0.59
1:B:142:ILE:HD12	1:B:230:LEU:HD11	1.84	0.59
1:E:142:ILE:HD12	1:E:230:LEU:CD1	2.33	0.59
1:E:248:PRO:CG	1:G:252:ARG:HH12	2.15	0.59
1:J:258:ARG:HH11	1:J:258:ARG:CG	2.08	0.59
1:E:176:MET:SD	1:E:202:GLN:HG3	2.43	0.59
1:H:39:ARG:HB3	1:I:71:THR:HB	1.84	0.59
1:I:180:ASP:HB3	1:I:183:VAL:HG13	1.85	0.59
1:H:66:GLN:NE2	2:H:1383:GDP:HN1	1.93	0.59
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.68	0.59
1:C:283:THR:HG22	1:C:286:GLN:H	1.66	0.59
1:I:142:ILE:CD1	1:I:230:LEU:HD11	2.33	0.58
1:G:142:ILE:HD12	1:G:230:LEU:CD1	2.33	0.58
1:B:181:GLU:OE1	1:B:185:ARG:NH2	2.31	0.58
1:A:248:PRO:HG2	1:D:252:ARG:NH1	2.18	0.58
1:A:258:ARG:HG2	1:A:258:ARG:NH1	2.04	0.58
1:E:155:GLU:OE1	1:E:248:PRO:HB3	2.04	0.58
1:A:14:GLU:CD	1:A:14:GLU:H	2.11	0.58
1:D:180:ASP:HB3	1:D:183:VAL:HG13	1.84	0.58
1:E:142:ILE:CD1	1:E:230:LEU:HD11	2.32	0.58
1:B:252:ARG:HH12	1:C:248:PRO:HG2	1.65	0.58
1:A:168:LEU:HD23	1:A:168:LEU:C	2.29	0.57
1:B:177:LEU:HD23	1:B:198:VAL:HG22	1.86	0.57
1:B:177:LEU:CD2	1:B:198:VAL:HG22	2.35	0.57
1:D:249:ALA:C	4:D:2004:HOH:O	2.47	0.57
1:E:142:ILE:HD12	1:E:230:LEU:HD11	1.86	0.57
1:I:142:ILE:HD12	1:I:230:LEU:CD1	2.34	0.57
1:E:266:ARG:HA	1:F:358:ARG:HH21	1.69	0.57
1:G:180:ASP:HB3	1:G:183:VAL:HG13	1.84	0.57
1:I:142:ILE:HD12	1:I:230:LEU:HD11	1.86	0.57
1:E:85:ARG:HG3	1:E:178:TYR:CZ	2.40	0.57
2:I:1383:GDP:PB	4:I:2008:HOH:O	2.61	0.57
1:J:382:ASN:N	4:J:2005:HOH:O	2.37	0.57
1:D:155:GLU:OE1	1:D:248:PRO:HB3	2.04	0.57
1:G:66:GLN:HE21	2:G:1383:GDP:HN21	1.53	0.57
1:A:248:PRO:HG2	1:D:252:ARG:HH12	1.69	0.57
1:A:258:ARG:HD2	1:D:361:ASP:OD1	2.06	0.56
1:D:123:GLY:HA2	1:D:170:ARG:HD3	1.87	0.56
1:G:290:LEU:HD21	1:G:301:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HD13	1:B:357:LEU:HD13	1.86	0.56
1:D:55:ARG:HG2	1:D:55:ARG:NH2	2.19	0.56
1:F:258:ARG:HH11	1:F:258:ARG:CG	2.13	0.56
1:J:66:GLN:HE21	2:J:1383:GDP:HN21	1.53	0.56
1:C:66:GLN:HE21	2:C:1383:GDP:HN21	1.54	0.56
1:E:358:ARG:HH21	1:F:266:ARG:HA	1.70	0.56
1:F:142:ILE:HD12	1:F:230:LEU:HD11	1.87	0.56
1:A:85:ARG:HG3	1:A:178:TYR:CZ	2.40	0.56
1:A:267:VAL:HG12	1:A:269:TYR:H	1.71	0.55
1:C:358:ARG:NH2	1:D:266:ARG:HA	2.22	0.55
1:G:258:ARG:HH11	1:G:258:ARG:CG	2.10	0.55
1:H:177:LEU:CD2	1:H:198:VAL:HG22	2.37	0.55
1:I:266:ARG:HA	1:J:358:ARG:NH2	2.21	0.55
1:B:284:PRO:HG2	1:F:288:GLU:OE1	2.07	0.55
1:A:227:ARG:NH1	1:A:227:ARG:HG2	2.22	0.54
1:A:290:LEU:HD21	1:A:301:LEU:HD12	1.89	0.54
1:E:267:VAL:HG12	1:E:269:TYR:H	1.73	0.54
1:H:177:LEU:HD23	1:H:198:VAL:HG22	1.88	0.54
1:B:176:MET:SD	1:B:202:GLN:HG3	2.48	0.54
1:B:155:GLU:OE1	1:B:248:PRO:HB3	2.06	0.54
1:C:358:ARG:HD3	1:D:265:GLU:O	2.08	0.54
1:G:358:ARG:HD3	1:H:265:GLU:O	2.06	0.54
1:A:248:PRO:CG	1:D:252:ARG:NH1	2.70	0.54
1:E:290:LEU:HD21	1:E:301:LEU:HD12	1.89	0.54
1:F:142:ILE:CD1	1:F:230:LEU:CD1	2.85	0.54
1:D:142:ILE:HD12	1:D:230:LEU:HD11	1.90	0.54
1:F:290:LEU:HD21	1:F:301:LEU:HD12	1.89	0.54
1:G:142:ILE:HD12	1:G:230:LEU:HD11	1.87	0.54
1:I:177:LEU:CD2	1:I:198:VAL:HG22	2.37	0.54
1:C:290:LEU:HD21	1:C:301:LEU:HD12	1.90	0.54
1:D:258:ARG:HG2	1:D:258:ARG:NH1	2.05	0.54
1:E:180:ASP:HB3	1:E:183:VAL:HG13	1.90	0.54
1:H:290:LEU:HD21	1:H:301:LEU:HD12	1.89	0.54
1:A:142:ILE:CD1	1:A:230:LEU:HD11	2.38	0.54
1:G:35:ILE:HD12	1:G:83:ALA:HB2	1.90	0.54
1:J:182:ARG:NH2	1:J:201:GLN:OE1	2.39	0.53
1:B:66:GLN:NE2	2:B:1383:GDP:HN21	2.05	0.53
1:G:59:THR:HG22	4:G:2003:HOH:O	2.06	0.53
1:A:248:PRO:HG3	1:D:252:ARG:HH12	1.74	0.53
1:A:252:ARG:HH22	1:D:248:PRO:CG	2.22	0.53
1:G:358:ARG:NH2	1:H:266:ARG:HA	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:ASP:HB2	1:H:232:GLU:OE2	2.09	0.53
1:G:59:THR:HG23	4:G:2003:HOH:O	2.08	0.53
1:G:266:ARG:HA	1:H:358:ARG:HH21	1.74	0.53
1:D:290:LEU:HD21	1:D:301:LEU:HD12	1.91	0.53
1:D:55:ARG:HH21	1:D:55:ARG:CG	2.13	0.53
1:J:104:THR:C	4:J:2001:HOH:O	2.51	0.53
1:D:142:ILE:HD12	1:D:230:LEU:CD1	2.39	0.53
1:I:155:GLU:OE1	1:I:248:PRO:HB3	2.09	0.53
1:J:66:GLN:NE2	2:J:1383:GDP:HN21	2.07	0.53
1:E:358:ARG:NH2	1:F:266:ARG:HA	2.24	0.52
1:F:177:LEU:HD23	1:F:198:VAL:HG22	1.91	0.52
1:C:177:LEU:HD23	1:C:198:VAL:HG22	1.90	0.52
1:D:249:ALA:N	4:D:2004:HOH:O	2.42	0.52
1:E:252:ARG:NH1	1:G:248:PRO:CG	2.67	0.52
1:J:177:LEU:CD2	1:J:198:VAL:HG22	2.40	0.52
1:A:179:GLU:OE2	1:A:179:GLU:HA	2.08	0.52
1:A:248:PRO:HG2	1:D:252:ARG:CZ	2.40	0.52
1:D:267:VAL:HG12	1:D:269:TYR:H	1.74	0.52
1:F:155:GLU:OE1	1:F:248:PRO:HB3	2.09	0.52
1:G:267:VAL:HG12	1:G:269:TYR:H	1.75	0.52
1:B:188:ASP:HB2	1:B:232:GLU:OE2	2.10	0.52
1:F:177:LEU:CD2	1:F:198:VAL:HG22	2.39	0.52
1:J:225:ASP:N	4:J:2002:HOH:O	2.43	0.52
1:C:155:GLU:OE1	1:C:248:PRO:HB3	2.08	0.52
1:G:97:HIS:CE1	1:G:168:LEU:HD12	2.45	0.51
1:B:252:ARG:NH1	1:C:248:PRO:HG2	2.24	0.51
1:C:357:LEU:HD13	1:D:357:LEU:HD13	1.91	0.51
1:D:110:TRP:H	1:D:110:TRP:CD1	2.29	0.51
1:H:267:VAL:HG12	1:H:269:TYR:H	1.75	0.51
1:J:290:LEU:HD21	1:J:301:LEU:HD12	1.92	0.51
1:I:266:ARG:HA	1:J:358:ARG:HH21	1.76	0.51
1:I:258:ARG:HH11	1:I:258:ARG:CG	2.13	0.51
1:E:265:GLU:O	1:F:358:ARG:HD3	2.10	0.51
1:F:238:GLN:CB	4:F:2007:HOH:O	2.35	0.51
1:E:357:LEU:HD13	1:F:357:LEU:HD13	1.93	0.51
1:F:180:ASP:OD2	1:F:182:ARG:NH1	2.44	0.51
1:I:290:LEU:HD21	1:I:301:LEU:HD12	1.92	0.51
1:F:283:THR:HG21	1:F:335:ASP:OD2	2.11	0.50
1:G:177:LEU:HD23	1:G:198:VAL:HG22	1.94	0.50
1:I:66:GLN:HE21	2:I:1383:GDP:HN21	1.59	0.50
1:J:35:ILE:HD12	1:J:83:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:THR:HA	1:I:237:ILE:CD1	2.41	0.50
1:A:252:ARG:HH12	1:D:248:PRO:CG	2.24	0.50
1:B:92:GLN:HA	1:B:92:GLN:OE1	2.11	0.50
1:B:130:PRO:C	1:B:131:ARG:HG2	2.36	0.50
1:I:177:LEU:HD23	1:I:198:VAL:HG22	1.93	0.50
1:J:180:ASP:OD2	1:J:182:ARG:NH1	2.44	0.50
1:C:258:ARG:HH11	1:C:258:ARG:CG	2.13	0.50
1:E:66:GLN:HE21	2:E:1383:GDP:HN21	1.58	0.50
1:H:155:GLU:OE1	1:H:248:PRO:HB3	2.12	0.50
1:I:14:GLU:CD	1:I:14:GLU:H	2.19	0.50
1:B:10:HIS:HE1	1:B:38:GLU:OE2	1.94	0.50
1:D:177:LEU:HD23	1:D:198:VAL:HG22	1.93	0.50
1:J:142:ILE:CD1	1:J:230:LEU:CD1	2.84	0.50
1:A:66:GLN:HE21	2:A:1383:GDP:HN21	1.60	0.50
1:I:188:ASP:HB2	1:I:232:GLU:OE2	2.12	0.50
1:J:177:LEU:HD23	1:J:198:VAL:HG22	1.93	0.50
1:A:184:ARG:NH1	1:A:184:ARG:HG2	2.27	0.50
1:B:168:LEU:C	1:B:168:LEU:HD23	2.37	0.50
1:B:290:LEU:HD21	1:B:301:LEU:HD12	1.94	0.50
1:G:142:ILE:CD1	1:G:230:LEU:CD1	2.89	0.50
1:H:35:ILE:HD12	1:H:83:ALA:HB2	1.94	0.50
1:A:262:HIS:CD2	1:A:263:ILE:HG13	2.47	0.49
1:E:258:ARG:HD2	1:G:361:ASP:OD1	2.12	0.49
1:H:142:ILE:CD1	1:H:230:LEU:CD1	2.90	0.49
1:H:143:THR:HA	1:H:237:ILE:CD1	2.40	0.49
1:D:66:GLN:NE2	2:D:1383:GDP:HN21	2.10	0.49
1:I:182:ARG:NH2	1:I:201:GLN:OE1	2.43	0.49
1:J:97:HIS:CE1	1:J:168:LEU:HD12	2.48	0.49
1:B:252:ARG:NH1	1:C:248:PRO:CG	2.66	0.49
1:E:168:LEU:C	1:E:168:LEU:HD23	2.38	0.49
1:C:142:ILE:CD1	1:C:230:LEU:CD1	2.87	0.49
1:E:369:ARG:HH11	1:G:257:HIS:HE1	1.60	0.49
1:A:358:ARG:HD3	1:B:265:GLU:O	2.12	0.49
1:E:158:TRP:CE2	1:G:252:ARG:HD2	2.47	0.49
1:H:180:ASP:OD2	1:H:182:ARG:NH1	2.45	0.49
1:D:130:PRO:C	1:D:131:ARG:HG2	2.38	0.49
1:D:85:ARG:HG3	1:D:178:TYR:HH	1.77	0.49
1:F:59:THR:HG21	4:F:2002:HOH:O	2.11	0.49
1:I:265:GLU:O	1:J:358:ARG:HD3	2.11	0.49
1:B:14:GLU:CD	1:B:14:GLU:H	2.20	0.49
1:B:283:THR:HG21	1:B:335:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:HD3	4:A:2020:HOH:O	2.12	0.49
1:H:97:HIS:CE1	1:H:168:LEU:HD12	2.48	0.49
1:A:142:ILE:HD12	1:A:230:LEU:HD11	1.95	0.48
1:E:177:LEU:HD23	1:E:198:VAL:HG22	1.95	0.48
1:G:177:LEU:CD2	1:G:198:VAL:HG22	2.43	0.48
1:H:143:THR:HA	1:H:237:ILE:HD11	1.95	0.48
1:G:14:GLU:H	1:G:14:GLU:CD	2.20	0.48
1:I:97:HIS:CE1	1:I:168:LEU:HD12	2.48	0.48
1:A:358:ARG:NH2	1:B:266:ARG:HA	2.28	0.48
1:B:143:THR:HA	1:B:237:ILE:CD1	2.43	0.48
1:C:247:GLN:HB2	1:C:248:PRO:HD2	1.95	0.48
1:I:267:VAL:HG12	1:I:269:TYR:H	1.77	0.48
1:J:283:THR:HG21	1:J:335:ASP:OD2	2.13	0.48
1:A:358:ARG:NE	4:A:2020:HOH:O	2.47	0.48
1:D:180:ASP:OD2	1:D:182:ARG:NH1	2.47	0.48
1:D:181:GLU:OE1	1:D:185:ARG:NH2	2.43	0.48
1:E:66:GLN:NE2	2:E:1383:GDP:HN21	2.11	0.48
1:E:179:GLU:OE2	1:E:179:GLU:HA	2.12	0.48
1:E:247:GLN:HB2	1:G:250:ILE:HD11	1.96	0.48
1:D:168:LEU:C	1:D:168:LEU:HD23	2.39	0.48
1:A:142:ILE:HD12	1:A:230:LEU:CD1	2.44	0.48
1:C:177:LEU:CD2	1:C:198:VAL:HG22	2.43	0.48
1:J:267:VAL:HG12	1:J:269:TYR:H	1.77	0.48
1:D:194:LEU:O	1:D:198:VAL:HG13	2.14	0.48
1:F:267:VAL:HG12	1:F:269:TYR:H	1.79	0.47
1:J:85:ARG:HG3	1:J:178:TYR:HH	1.76	0.47
1:C:267:VAL:HG12	1:C:269:TYR:H	1.78	0.47
1:H:66:GLN:NE2	2:H:1383:GDP:HN21	2.13	0.47
1:I:66:GLN:NE2	2:I:1383:GDP:HN21	2.12	0.47
1:C:66:GLN:NE2	2:C:1383:GDP:HN21	2.11	0.47
1:E:14:GLU:H	1:E:14:GLU:CD	2.21	0.47
1:J:143:THR:HA	1:J:237:ILE:CD1	2.43	0.47
1:D:66:GLN:HE21	2:D:1383:GDP:HN21	1.62	0.47
1:F:35:ILE:HD12	1:F:83:ALA:HB2	1.97	0.47
1:I:262:HIS:CD2	1:I:263:ILE:HG13	2.50	0.47
1:A:177:LEU:HD23	1:A:198:VAL:HG22	1.96	0.47
1:C:35:ILE:HD12	1:C:83:ALA:HB2	1.95	0.47
1:C:180:ASP:OD2	1:C:182:ARG:NH1	2.47	0.47
1:D:55:ARG:NH2	1:D:55:ARG:CG	2.70	0.47
1:D:258:ARG:HH11	1:D:258:ARG:CG	2.13	0.47
1:G:66:GLN:NE2	2:G:1383:GDP:HN21	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:ASP:OD2	1:G:182:ARG:NH1	2.47	0.47
1:F:130:PRO:C	1:F:131:ARG:HG2	2.40	0.47
1:G:265:GLU:O	1:H:358:ARG:HD3	2.14	0.47
1:A:81:ASN:ND2	1:A:195:TYR:OH	2.48	0.47
1:D:14:GLU:CD	1:D:14:GLU:H	2.22	0.47
1:H:304:CYS:HA	1:H:307:ARG:O	2.15	0.47
1:I:283:THR:HG21	1:I:335:ASP:OD2	2.14	0.47
1:D:142:ILE:CD1	1:D:230:LEU:CD1	2.93	0.47
1:F:194:LEU:O	1:F:198:VAL:HG13	2.15	0.47
1:F:262:HIS:CD2	1:F:263:ILE:HG13	2.50	0.47
1:H:66:GLN:HE21	2:H:1383:GDP:HN21	1.62	0.47
1:A:155:GLU:OE1	1:A:248:PRO:HB3	2.15	0.46
1:C:181:GLU:OE1	1:C:185:ARG:NH2	2.47	0.46
1:D:130:PRO:O	1:D:131:ARG:HG2	2.15	0.46
1:H:70:GLY:HA2	1:H:185:ARG:HA	1.97	0.46
1:J:168:LEU:C	1:J:168:LEU:HD23	2.40	0.46
1:E:143:THR:HA	1:E:237:ILE:CD1	2.45	0.46
1:F:143:THR:HA	1:F:237:ILE:CD1	2.46	0.46
1:B:40:ASP:OD1	1:B:40:ASP:C	2.59	0.46
1:D:257:HIS:N	1:D:257:HIS:CD2	2.83	0.46
1:D:262:HIS:CD2	1:D:263:ILE:HG13	2.50	0.46
1:E:180:ASP:OD2	1:E:182:ARG:NH1	2.48	0.46
1:G:357:LEU:HD13	1:H:357:LEU:HD13	1.97	0.46
1:J:304:CYS:HA	1:J:307:ARG:O	2.16	0.46
1:E:130:PRO:C	1:E:131:ARG:HG2	2.41	0.46
1:J:130:PRO:C	1:J:131:ARG:HG2	2.41	0.46
1:E:318:TRP:HB2	1:E:347:ARG:HD3	1.97	0.46
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.80	0.46
1:F:66:GLN:HE21	2:F:1383:GDP:HN21	1.63	0.46
1:I:70:GLY:HA2	1:I:185:ARG:HA	1.98	0.46
1:F:66:GLN:NE2	2:F:1383:GDP:HN21	2.15	0.45
1:I:85:ARG:NH2	1:I:90:GLU:OE1	2.50	0.45
1:C:14:GLU:CD	1:C:14:GLU:H	2.23	0.45
1:H:168:LEU:HD23	1:H:168:LEU:C	2.42	0.45
1:J:70:GLY:HA2	1:J:185:ARG:HA	1.98	0.45
1:F:168:LEU:C	1:F:168:LEU:HD23	2.41	0.45
1:J:333:ASP:C	1:J:333:ASP:OD1	2.59	0.45
1:J:377:GLN:O	1:J:380:LEU:HB2	2.17	0.45
1:C:294:THR:N	4:C:2012:HOH:O	2.47	0.45
1:D:247:GLN:HB2	1:D:248:PRO:HD2	1.99	0.45
1:E:102:ASP:CG	1:E:217:HIS:HB2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:PRO:C	1:H:131:ARG:HG2	2.42	0.45
1:I:35:ILE:HD12	1:I:83:ALA:HB2	1.98	0.45
1:B:177:LEU:HD23	1:B:198:VAL:CG2	2.47	0.45
1:G:56:ALA:HB2	4:G:2002:HOH:O	2.12	0.45
1:G:267:VAL:N	4:G:2009:HOH:O	2.35	0.45
1:H:14:GLU:CD	1:H:14:GLU:H	2.24	0.45
1:A:177:LEU:CD2	1:A:198:VAL:HG22	2.46	0.45
1:A:333:ASP:OD1	1:A:333:ASP:C	2.58	0.45
1:B:198:VAL:O	1:B:202:GLN:HG2	2.17	0.45
1:C:307:ARG:HD2	1:D:276:HIS:CD2	2.51	0.45
1:I:179:GLU:OE2	1:I:179:GLU:HA	2.16	0.45
1:I:318:TRP:HB2	1:I:347:ARG:HD3	1.99	0.45
1:J:318:TRP:HB2	1:J:347:ARG:HD3	1.99	0.45
1:A:130:PRO:C	1:A:131:ARG:HG2	2.42	0.45
1:B:97:HIS:CE1	1:B:168:LEU:HD12	2.52	0.45
1:E:97:HIS:CE1	1:E:168:LEU:HD12	2.52	0.45
1:E:177:LEU:CD2	1:E:198:VAL:HG22	2.47	0.45
1:C:130:PRO:C	1:C:131:ARG:HG2	2.42	0.45
1:D:110:TRP:CD1	1:D:110:TRP:N	2.84	0.45
1:H:177:LEU:HD23	1:H:198:VAL:CG2	2.46	0.45
1:C:143:THR:HA	1:C:237:ILE:CD1	2.47	0.44
1:G:130:PRO:C	1:G:131:ARG:HG2	2.42	0.44
1:B:248:PRO:CG	1:C:252:ARG:NH1	2.78	0.44
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.83	0.44
1:B:304:CYS:HA	1:B:307:ARG:O	2.18	0.44
1:C:98:PHE:O	1:C:166:GLU:HA	2.17	0.44
1:G:102:ASP:CG	1:G:217:HIS:HB2	2.42	0.44
1:H:179:GLU:OE2	1:H:179:GLU:HA	2.17	0.44
1:I:177:LEU:HD23	1:I:198:VAL:CG2	2.47	0.44
1:A:198:VAL:O	1:A:202:GLN:HG2	2.17	0.44
1:F:102:ASP:CG	1:F:217:HIS:HB2	2.42	0.44
1:D:177:LEU:CD2	1:D:198:VAL:HG22	2.47	0.44
1:F:239:SER:N	4:F:2007:HOH:O	2.50	0.44
1:B:98:PHE:O	1:B:166:GLU:HA	2.18	0.44
1:C:102:ASP:CG	1:C:217:HIS:HB2	2.43	0.44
1:F:70:GLY:HA2	1:F:185:ARG:HA	2.00	0.44
1:F:301:LEU:HD23	1:F:301:LEU:HA	1.88	0.44
1:I:358:ARG:HH21	1:J:266:ARG:HA	1.83	0.44
1:B:130:PRO:O	1:B:131:ARG:HG2	2.17	0.44
1:C:198:VAL:O	1:C:202:GLN:HG2	2.17	0.44
1:G:155:GLU:OE1	1:G:248:PRO:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:GLU:OE1	1:J:248:PRO:HB3	2.17	0.44
1:A:68:ARG:NH1	1:A:72:LEU:O	2.49	0.44
1:B:262:HIS:CD2	1:B:263:ILE:HG13	2.52	0.43
1:J:102:ASP:CG	1:J:217:HIS:HB2	2.43	0.43
1:F:177:LEU:HD23	1:F:198:VAL:CG2	2.48	0.43
1:G:179:GLU:OE2	1:G:179:GLU:HA	2.18	0.43
1:I:143:THR:HA	1:I:237:ILE:HD11	1.99	0.43
1:J:143:THR:HA	1:J:237:ILE:HD11	2.00	0.43
1:A:35:ILE:HD12	1:A:83:ALA:HB2	2.01	0.43
1:A:66:GLN:NE2	2:A:1383:GDP:HN21	2.15	0.43
1:B:96:ILE:CG2	1:B:169:MET:HG3	2.48	0.43
1:C:377:GLN:O	1:C:380:LEU:HB2	2.18	0.43
1:J:14:GLU:H	1:J:14:GLU:CD	2.27	0.43
1:C:34:CYS:HB2	1:C:63:VAL:HG13	1.99	0.43
1:C:182:ARG:NH2	1:C:201:GLN:OE1	2.46	0.43
1:D:70:GLY:HA2	1:D:185:ARG:HA	2.01	0.43
1:F:179:GLU:OE2	1:F:179:GLU:HA	2.18	0.43
1:G:143:THR:HA	1:G:237:ILE:CD1	2.48	0.43
1:H:194:LEU:O	1:H:198:VAL:HG13	2.18	0.43
1:A:252:ARG:HH12	1:D:248:PRO:HG3	1.83	0.43
1:E:361:ASP:HB2	4:E:2010:HOH:O	2.17	0.43
1:H:318:TRP:HB2	1:H:347:ARG:HD3	1.99	0.43
1:I:130:PRO:C	1:I:131:ARG:HG2	2.44	0.43
1:F:98:PHE:O	1:F:166:GLU:HA	2.19	0.43
1:G:247:GLN:HB2	1:G:248:PRO:HD2	2.01	0.43
1:H:283:THR:HG21	1:H:335:ASP:OD2	2.18	0.43
1:J:179:GLU:OE2	1:J:179:GLU:HA	2.19	0.43
1:A:283:THR:HG21	1:A:335:ASP:OD2	2.18	0.43
1:G:70:GLY:HA2	1:G:185:ARG:HA	2.00	0.43
1:I:142:ILE:CD1	1:I:230:LEU:CD1	2.95	0.43
1:J:277:ARG:CZ	1:J:281:HIS:HD2	2.31	0.43
1:C:85:ARG:NH2	1:C:90:GLU:OE1	2.52	0.43
1:D:135:ASP:CG	1:D:266:ARG:HH11	2.25	0.43
1:C:262:HIS:CD2	1:C:263:ILE:HG13	2.53	0.43
1:F:97:HIS:CE1	1:F:168:LEU:HD12	2.54	0.43
1:G:188:ASP:HB2	1:G:232:GLU:OE2	2.19	0.43
1:J:177:LEU:HD23	1:J:198:VAL:CG2	2.49	0.43
1:B:35:ILE:HD12	1:B:83:ALA:HB2	2.00	0.42
1:B:247:GLN:HB2	1:B:248:PRO:HD2	1.99	0.42
1:C:70:GLY:HA2	1:C:185:ARG:HA	2.01	0.42
1:I:180:ASP:OD2	1:I:182:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASP:CG	1:B:266:ARG:HH11	2.28	0.42
1:C:333:ASP:C	1:C:333:ASP:OD1	2.62	0.42
1:D:143:THR:HA	1:D:237:ILE:CD1	2.48	0.42
1:I:198:VAL:O	1:I:202:GLN:HG2	2.18	0.42
1:D:35:ILE:HD12	1:D:83:ALA:HB2	2.01	0.42
1:F:130:PRO:O	1:F:131:ARG:HG2	2.18	0.42
1:G:318:TRP:HB2	1:G:347:ARG:HD3	2.01	0.42
1:H:98:PHE:O	1:H:166:GLU:HA	2.19	0.42
1:H:262:HIS:CD2	1:H:263:ILE:HG13	2.54	0.42
1:J:85:ARG:NH2	1:J:90:GLU:OE1	2.52	0.42
1:H:182:ARG:NH2	1:H:201:GLN:OE1	2.46	0.42
1:J:262:HIS:CD2	1:J:263:ILE:HG13	2.54	0.42
1:B:143:THR:HA	1:B:237:ILE:HD11	2.00	0.42
1:B:377:GLN:O	1:B:380:LEU:HB2	2.20	0.42
1:G:53:ILE:HA	4:G:2002:HOH:O	2.20	0.42
1:H:227:ARG:NH1	1:H:227:ARG:HG2	2.35	0.42
1:I:168:LEU:C	1:I:168:LEU:HD23	2.44	0.42
1:B:258:ARG:HD2	1:C:361:ASP:OD1	2.19	0.42
1:C:170:ARG:H	1:C:170:ARG:HG2	1.69	0.42
1:C:307:ARG:CD	1:D:276:HIS:CD2	3.03	0.42
1:D:301:LEU:O	1:D:304:CYS:HB2	2.20	0.42
1:E:262:HIS:CD2	1:E:263:ILE:HG13	2.55	0.42
1:F:188:ASP:HB2	1:F:232:GLU:OE2	2.20	0.42
1:C:188:ASP:HB2	1:C:232:GLU:OE2	2.20	0.42
1:J:10:HIS:HE1	1:J:38:GLU:OE2	2.02	0.42
1:B:102:ASP:CG	1:B:217:HIS:HB2	2.45	0.42
1:H:377:GLN:O	1:H:380:LEU:HB2	2.20	0.42
1:A:92:GLN:OE1	1:A:92:GLN:HA	2.20	0.41
1:C:283:THR:HG21	1:C:335:ASP:OD2	2.20	0.41
1:C:318:TRP:HB2	1:C:347:ARG:HD3	2.01	0.41
1:E:35:ILE:HD12	1:E:83:ALA:HB2	2.02	0.41
1:F:14:GLU:CD	1:F:14:GLU:H	2.27	0.41
1:H:39:ARG:CB	1:I:71:THR:HB	2.49	0.41
1:H:102:ASP:CG	1:H:217:HIS:HB2	2.45	0.41
1:B:85:ARG:HE	1:B:85:ARG:HB3	1.67	0.41
1:D:198:VAL:O	1:D:202:GLN:HG2	2.19	0.41
1:H:85:ARG:NH2	1:H:90:GLU:OE1	2.53	0.41
1:A:70:GLY:HA2	1:A:185:ARG:HA	2.03	0.41
1:G:85:ARG:NH2	1:G:90:GLU:OE1	2.53	0.41
1:I:295:THR:HB	1:I:296:PRO:HD3	2.02	0.41
1:F:143:THR:HA	1:F:237:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:HIS:HE1	1:H:38:GLU:OE2	2.03	0.41
1:E:102:ASP:OD2	1:E:217:HIS:HB2	2.21	0.41
1:F:131:ARG:CZ	1:F:136:ALA:HB2	2.50	0.41
1:G:102:ASP:OD2	1:G:217:HIS:HB2	2.21	0.41
1:G:283:THR:HG21	1:G:335:ASP:OD2	2.20	0.41
1:H:184:ARG:NH1	1:H:184:ARG:HG2	2.35	0.41
1:J:184:ARG:NH1	1:J:184:ARG:HG2	2.35	0.41
1:A:170:ARG:H	1:A:170:ARG:HG2	1.74	0.41
1:J:98:PHE:O	1:J:166:GLU:HA	2.20	0.41
1:J:188:ASP:HB2	1:J:232:GLU:OE2	2.21	0.41
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.76	0.41
1:F:301:LEU:O	1:F:304:CYS:HB2	2.21	0.41
1:F:318:TRP:HB2	1:F:347:ARG:HD3	2.03	0.41
1:H:295:THR:HB	1:H:296:PRO:HD3	2.02	0.41
1:A:102:ASP:CG	1:A:217:HIS:HB2	2.46	0.41
1:B:158:TRP:CE2	1:C:252:ARG:HD2	2.56	0.41
1:D:283:THR:HG21	1:D:335:ASP:OD2	2.19	0.41
1:H:181:GLU:OE1	1:H:185:ARG:NH2	2.50	0.41
1:A:130:PRO:O	1:A:131:ARG:HG2	2.21	0.41
1:C:168:LEU:C	1:C:168:LEU:HD23	2.46	0.41
1:E:98:PHE:O	1:E:166:GLU:HA	2.21	0.41
1:E:143:THR:HA	1:E:237:ILE:HD11	2.02	0.41
1:F:10:HIS:HE1	1:F:38:GLU:OE2	2.04	0.41
1:F:380:LEU:HD23	1:F:380:LEU:HA	1.96	0.41
1:I:170:ARG:H	1:I:170:ARG:HG2	1.76	0.41
1:A:131:ARG:CZ	1:A:136:ALA:HB2	2.51	0.41
1:G:98:PHE:O	1:G:166:GLU:HA	2.21	0.41
1:G:168:LEU:C	1:G:168:LEU:HD23	2.45	0.41
1:I:85:ARG:HE	1:I:85:ARG:HB3	1.68	0.41
1:J:142:ILE:HD12	1:J:230:LEU:HD12	1.98	0.41
1:J:142:ILE:HD11	1:J:230:LEU:HD11	2.01	0.41
1:F:252:ARG:HH12	1:H:248:PRO:HG2	1.82	0.40
1:I:131:ARG:CZ	1:I:136:ALA:HB2	2.52	0.40
1:I:194:LEU:O	1:I:198:VAL:HG13	2.21	0.40
1:A:247:GLN:HB2	1:A:248:PRO:HD2	2.03	0.40
1:A:364:GLN:O	1:A:365:GLN:C	2.65	0.40
1:B:318:TRP:HB2	1:B:347:ARG:HD3	2.02	0.40
1:D:10:HIS:HE1	1:D:38:GLU:OE2	2.04	0.40
1:D:84:LEU:HA	1:D:84:LEU:HD12	1.85	0.40
1:F:295:THR:HB	1:F:296:PRO:HD3	2.04	0.40
1:A:97:HIS:CE1	1:A:168:LEU:HD12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ARG:NH1	1:G:248:PRO:HG2	2.35	0.40
1:I:10:HIS:HE1	1:I:38:GLU:OE2	2.04	0.40
1:J:198:VAL:O	1:J:202:GLN:HG2	2.21	0.40
1:C:135:ASP:CG	1:C:266:ARG:HH11	2.30	0.40
1:D:182:ARG:NH2	1:D:201:GLN:OE1	2.46	0.40
1:F:277:ARG:CZ	1:F:281:HIS:HD2	2.35	0.40
1:G:92:GLN:OE1	1:G:92:GLN:HA	2.21	0.40
1:H:92:GLN:OE1	1:H:92:GLN:HA	2.20	0.40
1:A:231:VAL:HG12	1:A:340:LEU:HD23	2.03	0.40
1:E:252:ARG:NH1	1:G:248:PRO:HG3	2.17	0.40
1:I:184:ARG:NH1	1:I:184:ARG:HG2	2.36	0.40

All (5) 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:CD	1:E:150:LEU:O[1_554]	1.25	0.95
1:A:380:LEU:O	1:G:179:GLU:OE2[1_554]	2.09	0.11
1:C:71:THR:OG1	1:J:332:GLY:O[3_556]	2.09	0.11
1:D:55:ARG:CD	1:E:150:LEU:C[1_554]	2.15	0.05
1:C:332:GLY:O	1:J:68:ARG:NH2[3_556]	2.19	0.01

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	372/397 (94%)	362 (97%)	9 (2%)	1 (0%)	36	59
1	B	372/397 (94%)	361 (97%)	9 (2%)	2 (0%)	24	49
1	C	372/397 (94%)	362 (97%)	10 (3%)	0	100	100
1	D	372/397 (94%)	361 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	372/397 (94%)	361 (97%)	10 (3%)	1 (0%)	36	59
1	F	372/397 (94%)	362 (97%)	9 (2%)	1 (0%)	36	59
1	G	372/397 (94%)	359 (96%)	13 (4%)	0	100	100
1	H	372/397 (94%)	361 (97%)	11 (3%)	0	100	100
1	I	372/397 (94%)	361 (97%)	11 (3%)	0	100	100
1	J	372/397 (94%)	363 (98%)	7 (2%)	2 (0%)	24	49
All	All	3720/3970 (94%)	3613 (97%)	100 (3%)	7 (0%)	43	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	A	310	PHE
1	B	246	GLY
1	E	310	PHE
1	F	310	PHE
1	J	310	PHE
1	J	248	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	323/338 (96%)	294 (91%)	29 (9%)	9	24
1	B	323/338 (96%)	293 (91%)	30 (9%)	8	23
1	C	323/338 (96%)	295 (91%)	28 (9%)	9	25
1	D	323/338 (96%)	294 (91%)	29 (9%)	9	24
1	E	323/338 (96%)	295 (91%)	28 (9%)	9	25
1	F	323/338 (96%)	296 (92%)	27 (8%)	10	26
1	G	323/338 (96%)	294 (91%)	29 (9%)	9	24
1	H	323/338 (96%)	296 (92%)	27 (8%)	10	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	323/338 (96%)	297 (92%)	26 (8%)	11	28
1	J	323/338 (96%)	295 (91%)	28 (9%)	9	25
All	All	3230/3380 (96%)	2949 (91%)	281 (9%)	9	25

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	GLU
1	A	21	ARG
1	A	63	VAL
1	A	65	LEU
1	A	68	ARG
1	A	72	LEU
1	A	84	LEU
1	A	85	ARG
1	A	92	GLN
1	A	109	ASP
1	A	124	LEU
1	A	139	THR
1	A	169	MET
1	A	179	GLU
1	A	182	ARG
1	A	183	VAL
1	A	198	VAL
1	A	209	CYS
1	A	219	LEU
1	A	252	ARG
1	A	258	ARG
1	A	259	VAL
1	A	261	VAL
1	A	283	THR
1	A	289	LEU
1	A	301	LEU
1	A	343	LEU
1	A	381	GLU
1	B	11	GLU
1	B	14	GLU
1	B	21	ARG
1	B	63	VAL
1	B	65	LEU

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Mol	Chain	Res	Type
1	B	68	ARG
1	B	72	LEU
1	B	84	LEU
1	B	92	GLN
1	B	109	ASP
1	B	124	LEU
1	B	139	THR
1	B	169	MET
1	B	179	GLU
1	B	182	ARG
1	B	183	VAL
1	B	198	VAL
1	B	209	CYS
1	B	219	LEU
1	B	252	ARG
1	B	258	ARG
1	B	259	VAL
1	B	261	VAL
1	B	266	ARG
1	B	283	THR
1	B	289	LEU
1	B	301	LEU
1	B	316	MET
1	B	343	LEU
1	B	381	GLU
1	C	11	GLU
1	C	14	GLU
1	C	21	ARG
1	C	63	VAL
1	C	65	LEU
1	C	68	ARG
1	C	72	LEU
1	C	84	LEU
1	C	92	GLN
1	C	109	ASP
1	C	124	LEU
1	C	169	MET
1	C	179	GLU
1	C	182	ARG
1	C	183	VAL
1	C	198	VAL
1	C	209	CYS

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Mol	Chain	Res	Type
1	C	219	LEU
1	C	252	ARG
1	C	258	ARG
1	C	259	VAL
1	C	261	VAL
1	C	283	THR
1	C	289	LEU
1	C	301	LEU
1	C	316	MET
1	C	343	LEU
1	C	381	GLU
1	D	11	GLU
1	D	14	GLU
1	D	54	SER
1	D	55	ARG
1	D	63	VAL
1	D	65	LEU
1	D	68	ARG
1	D	72	LEU
1	D	84	LEU
1	D	92	GLN
1	D	109	ASP
1	D	124	LEU
1	D	169	MET
1	D	179	GLU
1	D	182	ARG
1	D	183	VAL
1	D	198	VAL
1	D	209	CYS
1	D	219	LEU
1	D	252	ARG
1	D	258	ARG
1	D	259	VAL
1	D	266	ARG
1	D	283	THR
1	D	289	LEU
1	D	301	LEU
1	D	316	MET
1	D	343	LEU
1	D	381	GLU
1	E	11	GLU
1	E	14	GLU

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Mol	Chain	Res	Type
1	E	21	ARG
1	E	48	ARG
1	E	63	VAL
1	E	65	LEU
1	E	68	ARG
1	E	72	LEU
1	E	84	LEU
1	E	92	GLN
1	E	109	ASP
1	E	124	LEU
1	E	169	MET
1	E	179	GLU
1	E	182	ARG
1	E	183	VAL
1	E	198	VAL
1	E	209	CYS
1	E	219	LEU
1	E	258	ARG
1	E	259	VAL
1	E	261	VAL
1	E	266	ARG
1	E	283	THR
1	E	289	LEU
1	E	301	LEU
1	E	343	LEU
1	E	381	GLU
1	F	11	GLU
1	F	14	GLU
1	F	21	ARG
1	F	63	VAL
1	F	65	LEU
1	F	68	ARG
1	F	72	LEU
1	F	84	LEU
1	F	92	GLN
1	F	109	ASP
1	F	124	LEU
1	F	169	MET
1	F	179	GLU
1	F	182	ARG
1	F	183	VAL
1	F	198	VAL

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Mol	Chain	Res	Type
1	F	209	CYS
1	F	219	LEU
1	F	258	ARG
1	F	259	VAL
1	F	261	VAL
1	F	266	ARG
1	F	283	THR
1	F	289	LEU
1	F	301	LEU
1	F	343	LEU
1	F	381	GLU
1	G	11	GLU
1	G	14	GLU
1	G	21	ARG
1	G	63	VAL
1	G	65	LEU
1	G	68	ARG
1	G	72	LEU
1	G	84	LEU
1	G	85	ARG
1	G	92	GLN
1	G	109	ASP
1	G	124	LEU
1	G	169	MET
1	G	179	GLU
1	G	182	ARG
1	G	183	VAL
1	G	198	VAL
1	G	209	CYS
1	G	219	LEU
1	G	252	ARG
1	G	258	ARG
1	G	259	VAL
1	G	261	VAL
1	G	266	ARG
1	G	283	THR
1	G	289	LEU
1	G	301	LEU
1	G	343	LEU
1	G	381	GLU
1	H	11	GLU
1	H	14	GLU

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Mol	Chain	Res	Type
1	H	21	ARG
1	H	63	VAL
1	H	65	LEU
1	H	68	ARG
1	H	72	LEU
1	H	84	LEU
1	H	92	GLN
1	H	109	ASP
1	H	124	LEU
1	H	169	MET
1	H	179	GLU
1	H	182	ARG
1	H	183	VAL
1	H	198	VAL
1	H	209	CYS
1	H	219	LEU
1	H	258	ARG
1	H	259	VAL
1	H	261	VAL
1	H	266	ARG
1	H	283	THR
1	H	289	LEU
1	H	301	LEU
1	H	343	LEU
1	H	381	GLU
1	I	11	GLU
1	I	14	GLU
1	I	21	ARG
1	I	63	VAL
1	I	65	LEU
1	I	68	ARG
1	I	72	LEU
1	I	84	LEU
1	I	92	GLN
1	I	109	ASP
1	I	124	LEU
1	I	179	GLU
1	I	182	ARG
1	I	183	VAL
1	I	198	VAL
1	I	209	CYS
1	I	219	LEU

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Mol	Chain	Res	Type
1	I	258	ARG
1	I	259	VAL
1	I	261	VAL
1	I	266	ARG
1	I	283	THR
1	I	289	LEU
1	I	301	LEU
1	I	343	LEU
1	I	381	GLU
1	J	11	GLU
1	J	14	GLU
1	J	21	ARG
1	J	63	VAL
1	J	65	LEU
1	J	68	ARG
1	J	72	LEU
1	J	84	LEU
1	J	92	GLN
1	J	109	ASP
1	J	124	LEU
1	J	169	MET
1	J	179	GLU
1	J	182	ARG
1	J	183	VAL
1	J	198	VAL
1	J	209	CYS
1	J	219	LEU
1	J	252	ARG
1	J	258	ARG
1	J	259	VAL
1	J	261	VAL
1	J	266	ARG
1	J	283	THR
1	J	289	LEU
1	J	301	LEU
1	J	343	LEU
1	J	381	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS

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Mol	Chain	Res	Type
1	A	30	HIS
1	A	66	GLN
1	A	81	ASN
1	A	253	GLN
1	A	257	HIS
1	A	281	HIS
1	A	328	HIS
1	B	10	HIS
1	B	30	HIS
1	B	66	GLN
1	B	81	ASN
1	B	153	HIS
1	B	276	HIS
1	B	281	HIS
1	B	328	HIS
1	C	10	HIS
1	C	66	GLN
1	C	81	ASN
1	C	257	HIS
1	C	276	HIS
1	C	281	HIS
1	D	10	HIS
1	D	30	HIS
1	D	66	GLN
1	D	81	ASN
1	D	257	HIS
1	D	276	HIS
1	D	281	HIS
1	D	365	GLN
1	E	10	HIS
1	E	30	HIS
1	E	66	GLN
1	E	81	ASN
1	E	153	HIS
1	E	257	HIS
1	E	281	HIS
1	E	328	HIS
1	E	330	GLN
1	F	10	HIS
1	F	30	HIS
1	F	66	GLN
1	F	81	ASN

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Mol	Chain	Res	Type
1	F	257	HIS
1	F	276	HIS
1	F	281	HIS
1	F	365	GLN
1	G	10	HIS
1	G	30	HIS
1	G	66	GLN
1	G	81	ASN
1	G	257	HIS
1	G	281	HIS
1	H	10	HIS
1	H	30	HIS
1	H	66	GLN
1	H	81	ASN
1	H	253	GLN
1	H	257	HIS
1	H	281	HIS
1	H	365	GLN
1	I	10	HIS
1	I	30	HIS
1	I	66	GLN
1	I	81	ASN
1	I	257	HIS
1	I	281	HIS
1	I	365	GLN
1	J	10	HIS
1	J	30	HIS
1	J	66	GLN
1	J	81	ASN
1	J	255	HIS
1	J	281	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 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	GDP	D	1383	3	29,30,30	1.17	3 (10%)	45,47,47	1.71	7 (15%)
2	GDP	H	1383	3	29,30,30	1.17	3 (10%)	45,47,47	1.71	8 (17%)
2	GDP	A	1383	3	29,30,30	1.33	4 (13%)	45,47,47	1.79	8 (17%)
2	GDP	J	1383	3	29,30,30	1.14	4 (13%)	45,47,47	1.64	7 (15%)
2	GDP	I	1383	3	29,30,30	1.11	3 (10%)	45,47,47	1.75	8 (17%)
2	GDP	E	1383	3	29,30,30	1.30	3 (10%)	45,47,47	1.71	8 (17%)
2	GDP	C	1383	3	29,30,30	1.22	4 (13%)	45,47,47	1.68	6 (13%)
2	GDP	F	1383	3	29,30,30	1.11	3 (10%)	45,47,47	1.74	7 (15%)
2	GDP	G	1383	3	29,30,30	1.16	3 (10%)	45,47,47	1.83	8 (17%)
2	GDP	B	1383	3	29,30,30	1.24	4 (13%)	45,47,47	1.68	8 (17%)

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	GDP	D	1383	3	-	3/16/32/32	0/3/3/3
2	GDP	H	1383	3	-	5/16/32/32	0/3/3/3
2	GDP	A	1383	3	-	3/16/32/32	0/3/3/3
2	GDP	J	1383	3	-	3/16/32/32	0/3/3/3
2	GDP	I	1383	3	-	3/16/32/32	0/3/3/3
2	GDP	E	1383	3	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	C	1383	3	-	3/16/32/32	0/3/3/3
2	GDP	F	1383	3	-	5/16/32/32	0/3/3/3
2	GDP	G	1383	3	-	4/16/32/32	0/3/3/3
2	GDP	B	1383	3	-	4/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1383	GDP	PA-O3A	-3.92	1.55	1.59
2	E	1383	GDP	C6-N1	-3.43	1.32	1.38
2	E	1383	GDP	C5-C4	3.28	1.47	1.38
2	C	1383	GDP	C5-C4	3.20	1.47	1.38
2	H	1383	GDP	C5-C4	3.10	1.47	1.38
2	D	1383	GDP	C5-C4	3.06	1.47	1.38
2	J	1383	GDP	C5-C4	3.03	1.47	1.38
2	F	1383	GDP	C5-C4	3.01	1.47	1.38
2	A	1383	GDP	C5-C4	3.01	1.47	1.38
2	B	1383	GDP	C5-C4	2.99	1.46	1.38
2	I	1383	GDP	C5-C4	2.92	1.46	1.38
2	G	1383	GDP	C5-C4	2.90	1.46	1.38
2	D	1383	GDP	C6-N1	-2.80	1.33	1.38
2	B	1383	GDP	C5-N7	-2.72	1.33	1.39
2	C	1383	GDP	C5-N7	-2.62	1.33	1.39
2	G	1383	GDP	C6-N1	-2.53	1.34	1.38
2	H	1383	GDP	C6-N1	-2.52	1.34	1.38
2	B	1383	GDP	C6-N1	-2.51	1.34	1.38
2	C	1383	GDP	C4-N9	-2.35	1.32	1.38
2	H	1383	GDP	C4-N9	-2.29	1.32	1.38
2	I	1383	GDP	C6-N1	-2.25	1.34	1.38
2	A	1383	GDP	C5-N7	-2.23	1.34	1.39
2	B	1383	GDP	C4-N9	-2.23	1.32	1.38
2	E	1383	GDP	C5-N7	-2.23	1.34	1.39
2	F	1383	GDP	C5-N7	-2.22	1.34	1.39
2	A	1383	GDP	C6-N1	-2.21	1.34	1.38
2	F	1383	GDP	C6-N1	-2.21	1.34	1.38
2	J	1383	GDP	C6-N1	-2.20	1.34	1.38
2	J	1383	GDP	C5-N7	-2.17	1.34	1.39
2	D	1383	GDP	C5-N7	-2.15	1.34	1.39
2	J	1383	GDP	C4-N9	-2.15	1.32	1.38
2	C	1383	GDP	C6-N1	-2.14	1.34	1.38
2	I	1383	GDP	C5-N7	-2.14	1.34	1.39
2	G	1383	GDP	C5-N7	-2.09	1.34	1.39

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1383	GDP	C5-C4-N3	-6.00	118.84	128.39
2	E	1383	GDP	C5-C4-N3	-5.67	119.36	128.39
2	I	1383	GDP	C5-C4-N3	-5.62	119.44	128.39
2	H	1383	GDP	C5-C4-N3	-5.60	119.48	128.39
2	A	1383	GDP	C5-C4-N3	-5.48	119.67	128.39
2	D	1383	GDP	C5-C4-N3	-5.47	119.68	128.39
2	F	1383	GDP	C5-C4-N3	-5.35	119.87	128.39
2	G	1383	GDP	C2-N3-C4	5.27	121.37	112.30
2	J	1383	GDP	C5-C4-N3	-5.07	120.31	128.39
2	B	1383	GDP	C5-C4-N3	-5.02	120.41	128.39
2	C	1383	GDP	C5-C4-N3	-4.97	120.49	128.39
2	I	1383	GDP	C2-N3-C4	4.95	120.83	112.30
2	A	1383	GDP	C2-N3-C4	4.69	120.37	112.30
2	F	1383	GDP	C2-N3-C4	4.69	120.37	112.30
2	H	1383	GDP	C2-N3-C4	4.55	120.14	112.30
2	D	1383	GDP	C2-N3-C4	4.55	120.14	112.30
2	J	1383	GDP	C2-N3-C4	4.53	120.10	112.30
2	I	1383	GDP	N9-C4-N3	4.35	134.64	125.95
2	H	1383	GDP	N9-C4-N3	4.32	134.58	125.95
2	G	1383	GDP	N9-C4-N3	4.27	134.50	125.95
2	F	1383	GDP	N9-C4-N3	4.18	134.32	125.95
2	E	1383	GDP	C2-N3-C4	4.12	119.39	112.30
2	E	1383	GDP	N9-C4-N3	4.04	134.03	125.95
2	J	1383	GDP	N9-C4-N3	4.04	134.02	125.95
2	B	1383	GDP	O3B-PB-O3A	4.01	118.08	104.64
2	A	1383	GDP	N9-C4-N3	4.00	133.95	125.95
2	B	1383	GDP	N9-C4-N3	3.91	133.78	125.95
2	B	1383	GDP	C2-N3-C4	3.89	119.00	112.30
2	D	1383	GDP	N9-C4-N3	3.87	133.69	125.95
2	C	1383	GDP	N9-C4-N3	3.86	133.66	125.95
2	C	1383	GDP	C2-N3-C4	3.79	118.82	112.30
2	G	1383	GDP	C6-C5-N7	3.77	137.16	130.29
2	A	1383	GDP	O3B-PB-O3A	3.54	116.52	104.64
2	C	1383	GDP	C6-C5-N7	3.53	136.72	130.29
2	E	1383	GDP	C6-C5-N7	3.51	136.67	130.29
2	C	1383	GDP	O3B-PB-O3A	3.51	116.39	104.64
2	I	1383	GDP	C6-C5-N7	3.48	136.62	130.29
2	F	1383	GDP	C6-C5-N7	3.43	136.53	130.29
2	H	1383	GDP	C6-C5-N7	3.40	136.48	130.29
2	D	1383	GDP	C6-C5-N7	3.26	136.23	130.29
2	J	1383	GDP	O3B-PB-O3A	3.17	115.25	104.64
2	J	1383	GDP	C6-C5-N7	3.16	136.03	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1383	GDP	C4-C5-N7	-3.02	105.88	110.67
2	A	1383	GDP	C6-C5-N7	3.02	135.78	130.29
2	F	1383	GDP	O3B-PB-O3A	2.96	114.55	104.64
2	D	1383	GDP	O3B-PB-O3A	2.95	114.54	104.64
2	H	1383	GDP	C4-C5-N7	-2.82	106.21	110.67
2	G	1383	GDP	C4-C5-N7	-2.81	106.22	110.67
2	B	1383	GDP	C6-C5-N7	2.79	135.38	130.29
2	I	1383	GDP	O3B-PB-O3A	2.77	113.92	104.64
2	G	1383	GDP	O3B-PB-O3A	2.68	113.61	104.64
2	I	1383	GDP	C4-C5-N7	-2.66	106.45	110.67
2	A	1383	GDP	O6-C6-C5	-2.65	119.53	126.53
2	A	1383	GDP	C4-C5-N7	-2.64	106.48	110.67
2	F	1383	GDP	O6-C6-C5	-2.62	119.63	126.53
2	D	1383	GDP	C4-C5-N7	-2.52	106.67	110.67
2	C	1383	GDP	C4-C5-N7	-2.52	106.68	110.67
2	E	1383	GDP	O3B-PB-O3A	2.47	112.92	104.64
2	F	1383	GDP	C4-C5-N7	-2.31	107.01	110.67
2	B	1383	GDP	O6-C6-C5	-2.31	120.43	126.53
2	B	1383	GDP	C4-C5-N7	-2.30	107.03	110.67
2	E	1383	GDP	C8-N7-C5	2.28	108.33	104.26
2	A	1383	GDP	C8-N7-C5	2.15	108.09	104.26
2	I	1383	GDP	O6-C6-C5	-2.15	120.86	126.53
2	J	1383	GDP	O6-C6-C5	-2.13	120.90	126.53
2	H	1383	GDP	C8-N9-C4	2.13	110.02	106.03
2	H	1383	GDP	O3B-PB-O3A	2.10	111.69	104.64
2	H	1383	GDP	O6-C6-C5	-2.10	120.99	126.53
2	B	1383	GDP	O3'-C3'-C4'	-2.10	105.06	111.08
2	I	1383	GDP	C8-N7-C5	2.09	107.98	104.26
2	J	1383	GDP	O3A-PA-O1A	2.07	116.92	110.70
2	E	1383	GDP	O3'-C3'-C4'	-2.07	105.15	111.08
2	G	1383	GDP	C5-C6-N1	2.06	118.50	113.25
2	D	1383	GDP	O6-C6-C5	-2.05	121.13	126.53
2	G	1383	GDP	C8-N7-C5	2.03	107.88	104.26

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1383	GDP	PA-O3A-PB-O3B
2	B	1383	GDP	PA-O3A-PB-O3B
2	C	1383	GDP	PA-O3A-PB-O3B
2	D	1383	GDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
2	E	1383	GDP	PA-O3A-PB-O3B
2	F	1383	GDP	PA-O3A-PB-O3B
2	G	1383	GDP	PA-O3A-PB-O3B
2	H	1383	GDP	PA-O3A-PB-O3B
2	I	1383	GDP	PA-O3A-PB-O3B
2	J	1383	GDP	PA-O3A-PB-O3B
2	F	1383	GDP	PB-O3A-PA-O1A
2	F	1383	GDP	PA-O3A-PB-O1B
2	H	1383	GDP	PA-O3A-PB-O1B
2	A	1383	GDP	PA-O3A-PB-O2B
2	B	1383	GDP	PA-O3A-PB-O2B
2	C	1383	GDP	PA-O3A-PB-O2B
2	D	1383	GDP	PA-O3A-PB-O2B
2	E	1383	GDP	PA-O3A-PB-O2B
2	F	1383	GDP	PA-O3A-PB-O2B
2	G	1383	GDP	PA-O3A-PB-O2B
2	H	1383	GDP	PA-O3A-PB-O2B
2	I	1383	GDP	PA-O3A-PB-O2B
2	J	1383	GDP	PA-O3A-PB-O2B
2	A	1383	GDP	PB-O3A-PA-O2A
2	C	1383	GDP	PB-O3A-PA-O2A
2	D	1383	GDP	PB-O3A-PA-O2A
2	E	1383	GDP	PB-O3A-PA-O2A
2	G	1383	GDP	PB-O3A-PA-O1A
2	G	1383	GDP	PB-O3A-PA-O2A
2	H	1383	GDP	PB-O3A-PA-O1A
2	H	1383	GDP	PB-O3A-PA-O2A
2	I	1383	GDP	PB-O3A-PA-O2A
2	J	1383	GDP	PB-O3A-PA-O2A
2	B	1383	GDP	PA-O3A-PB-O1B
2	B	1383	GDP	PB-O3A-PA-O2A
2	F	1383	GDP	PB-O3A-PA-O2A

There are no ring outliers.

10 monomers are involved in 41 short contacts:

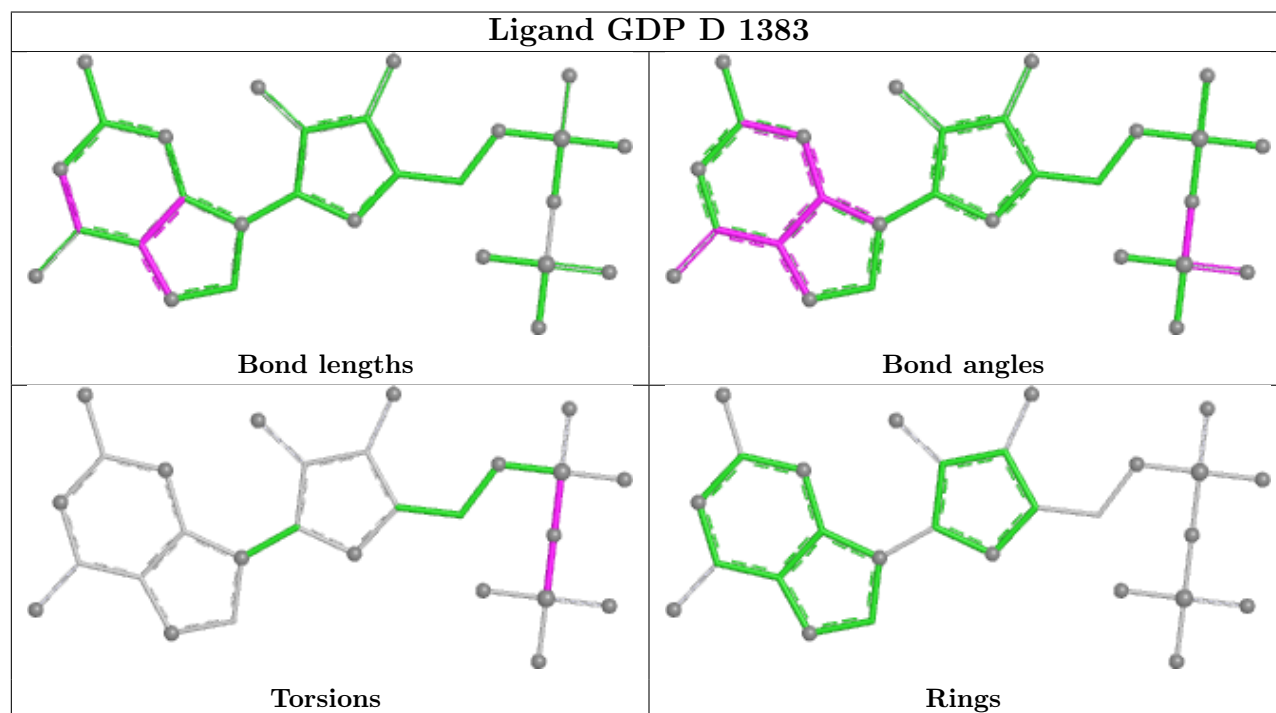
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1383	GDP	4	0
2	H	1383	GDP	4	0
2	A	1383	GDP	4	0
2	J	1383	GDP	4	0
2	I	1383	GDP	5	0

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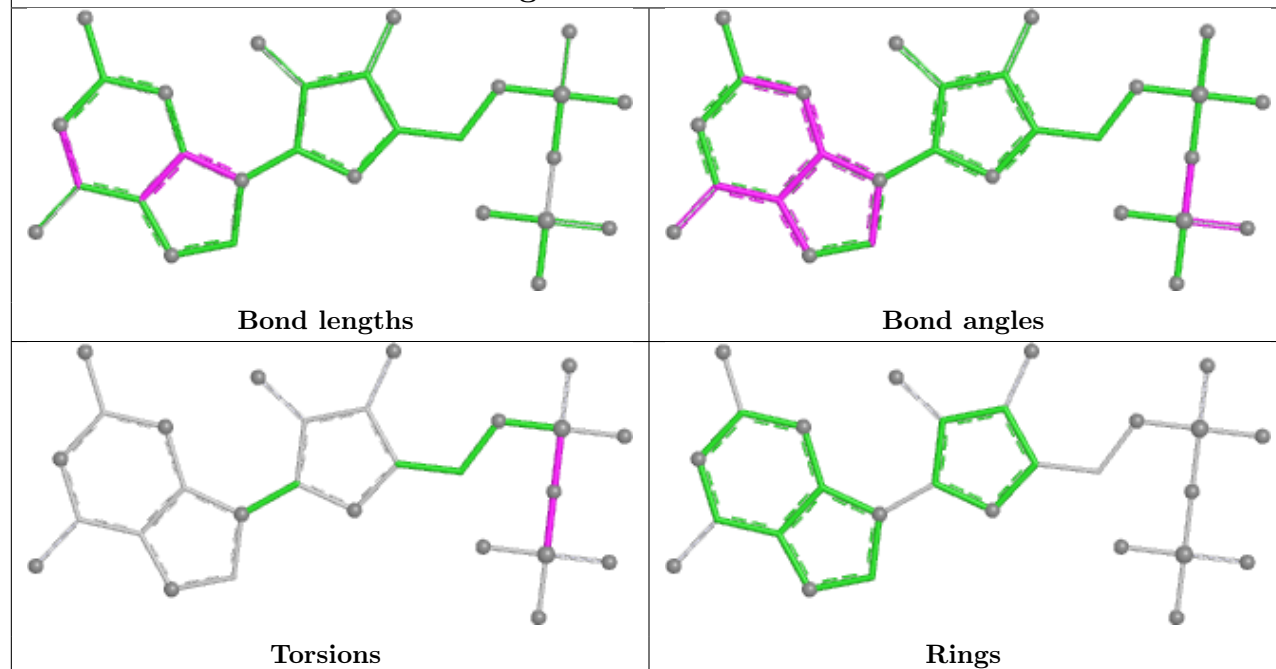
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1383	GDP	4	0
2	C	1383	GDP	4	0
2	F	1383	GDP	4	0
2	G	1383	GDP	4	0
2	B	1383	GDP	4	0

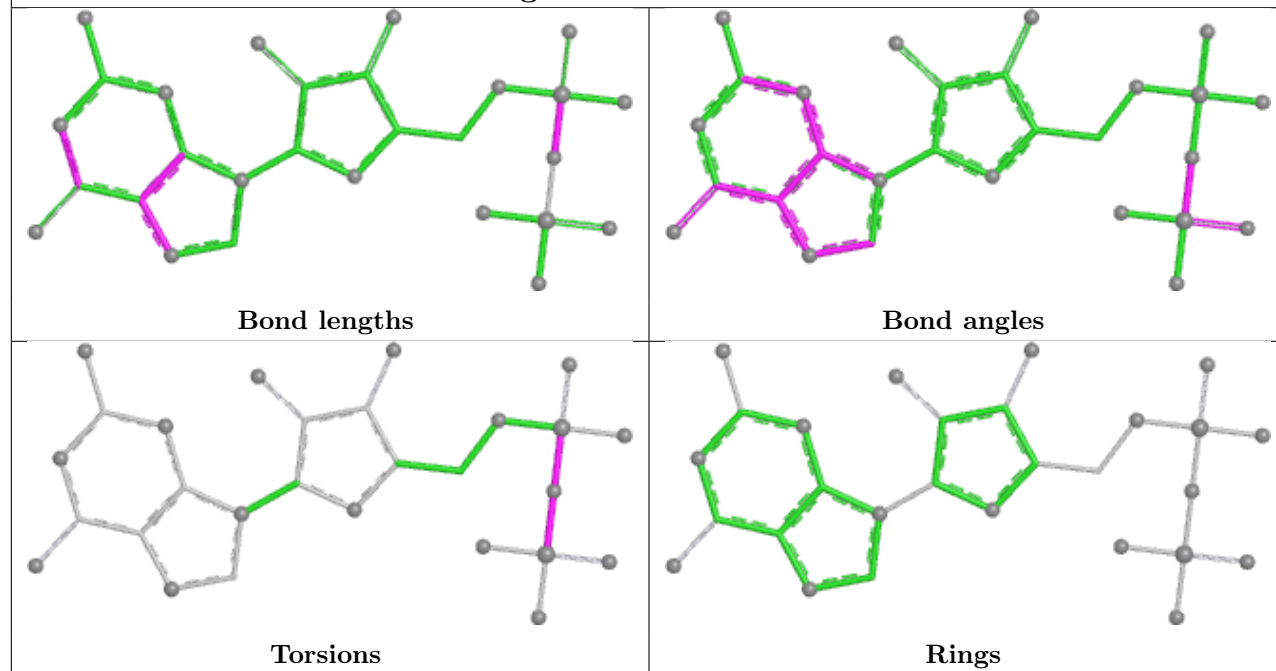
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

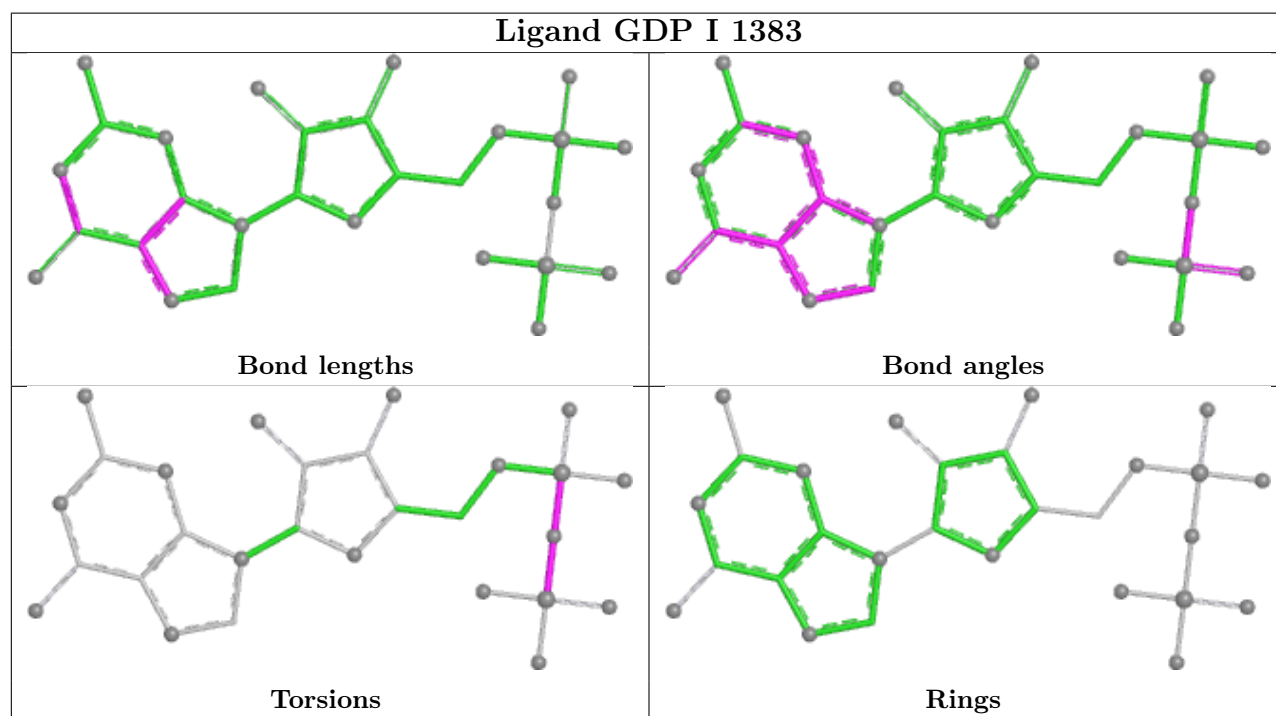
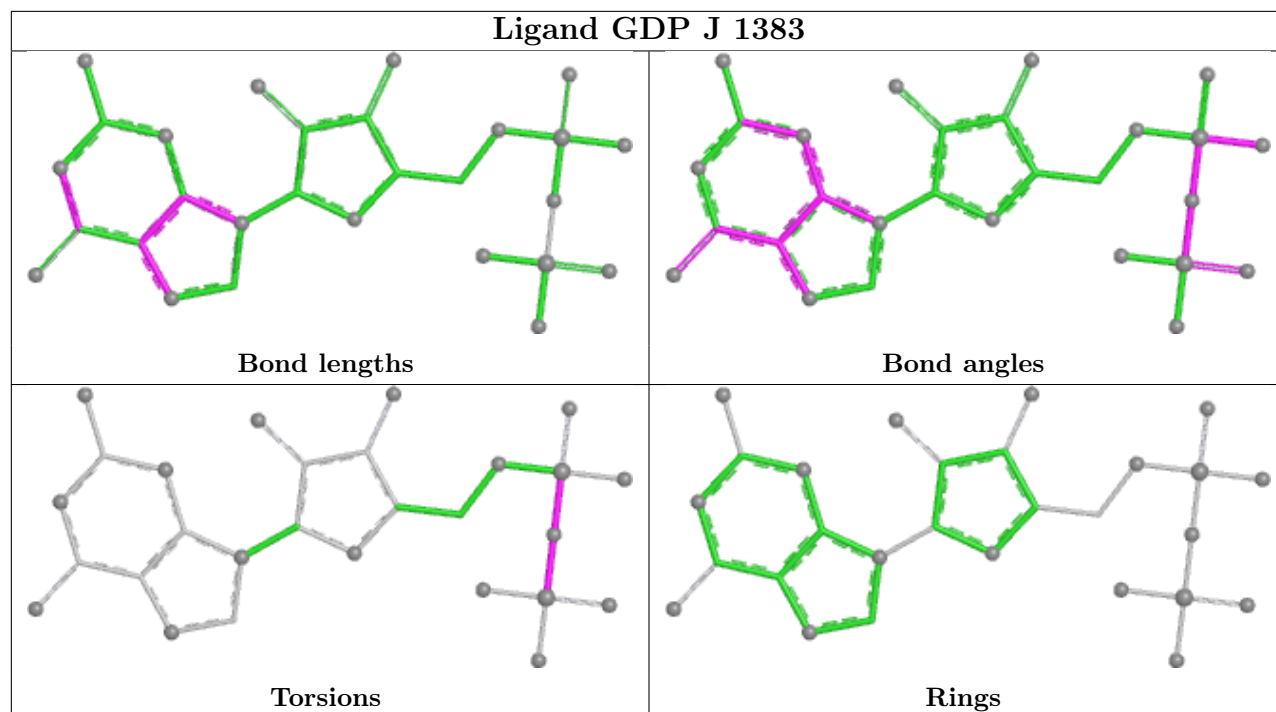


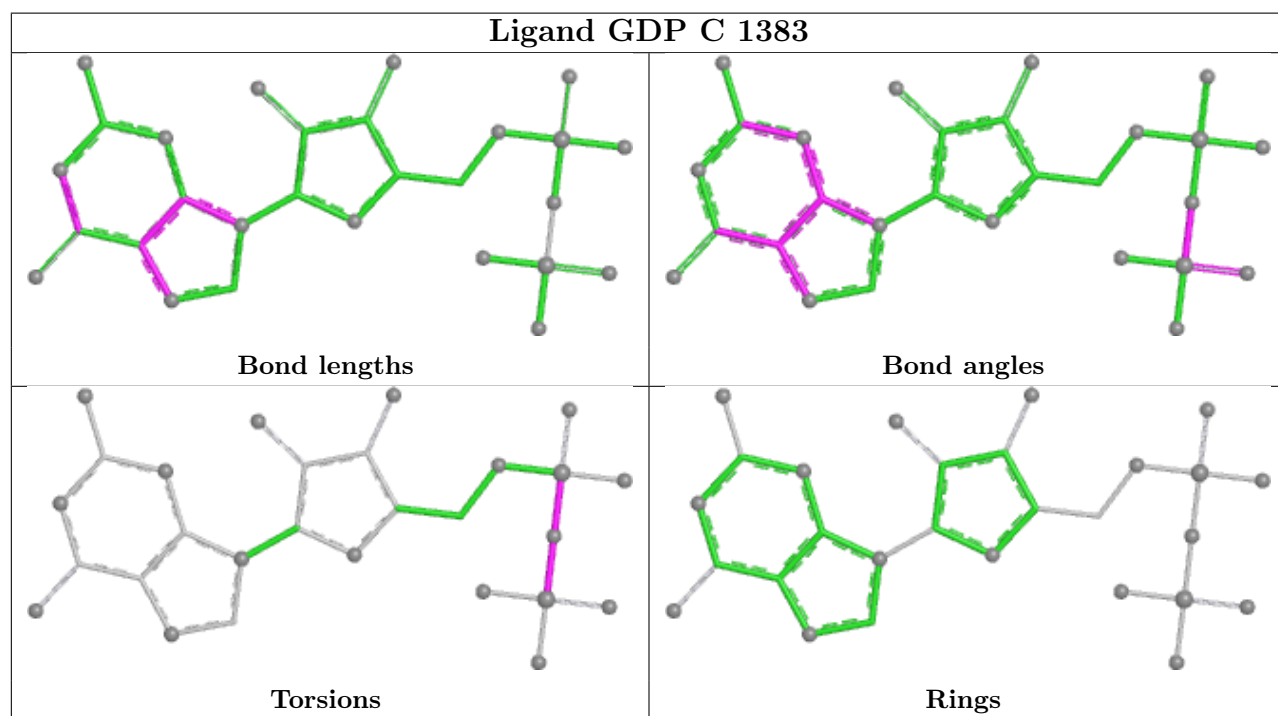
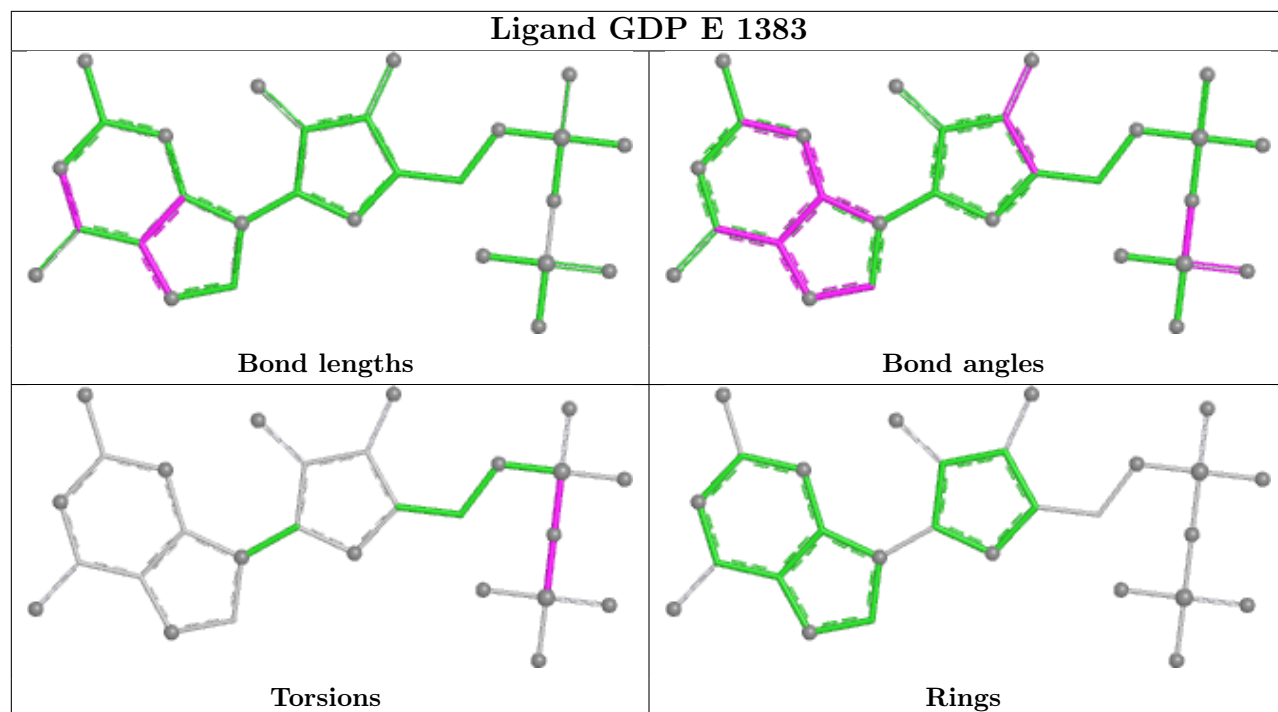
Ligand GDP H 1383

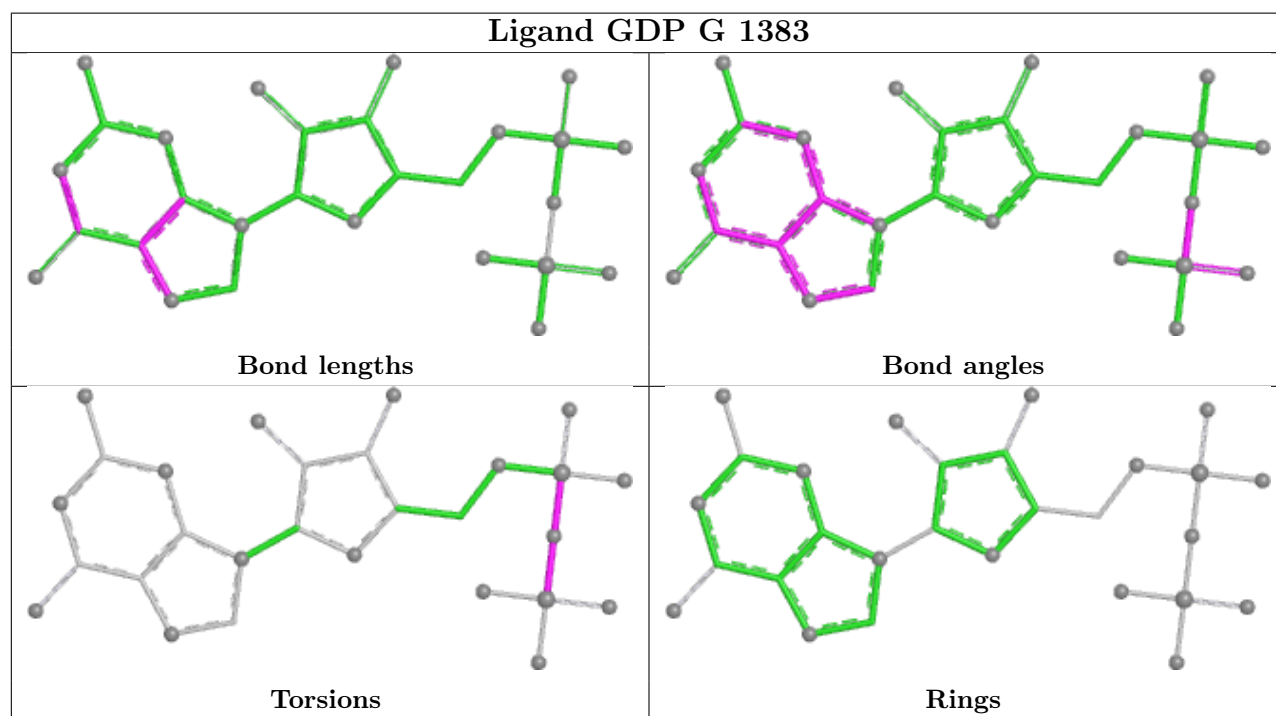
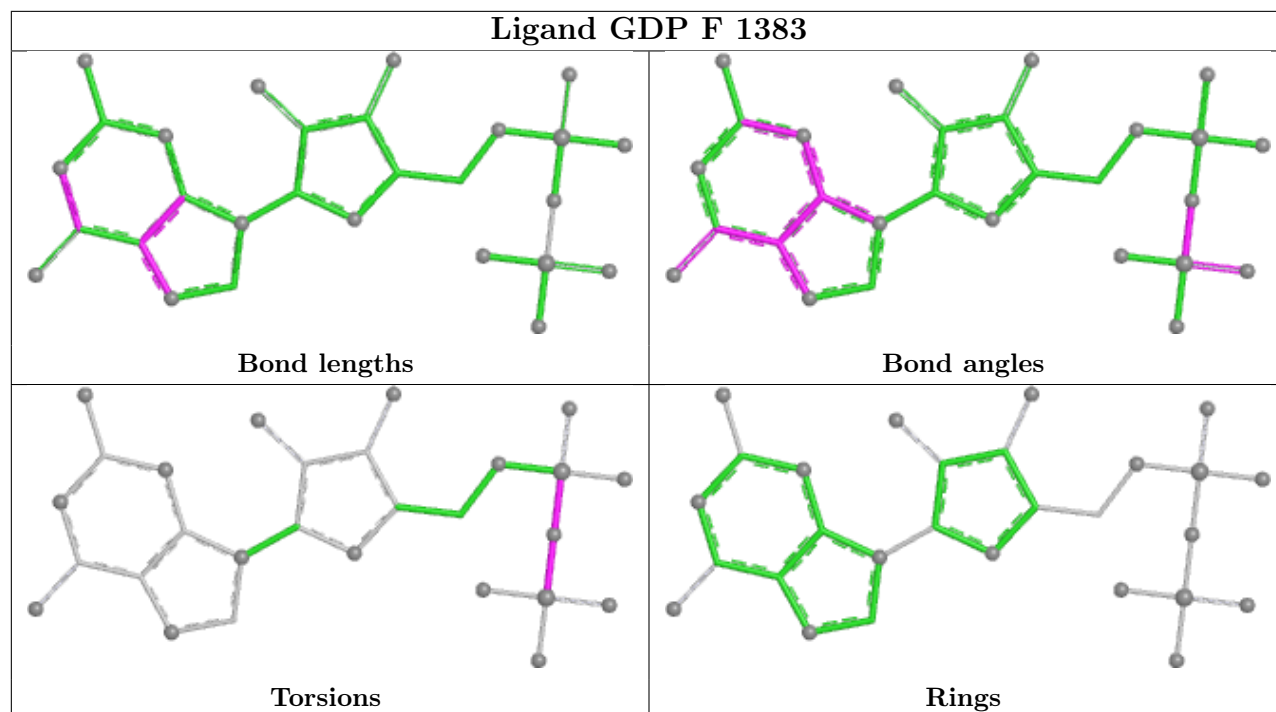


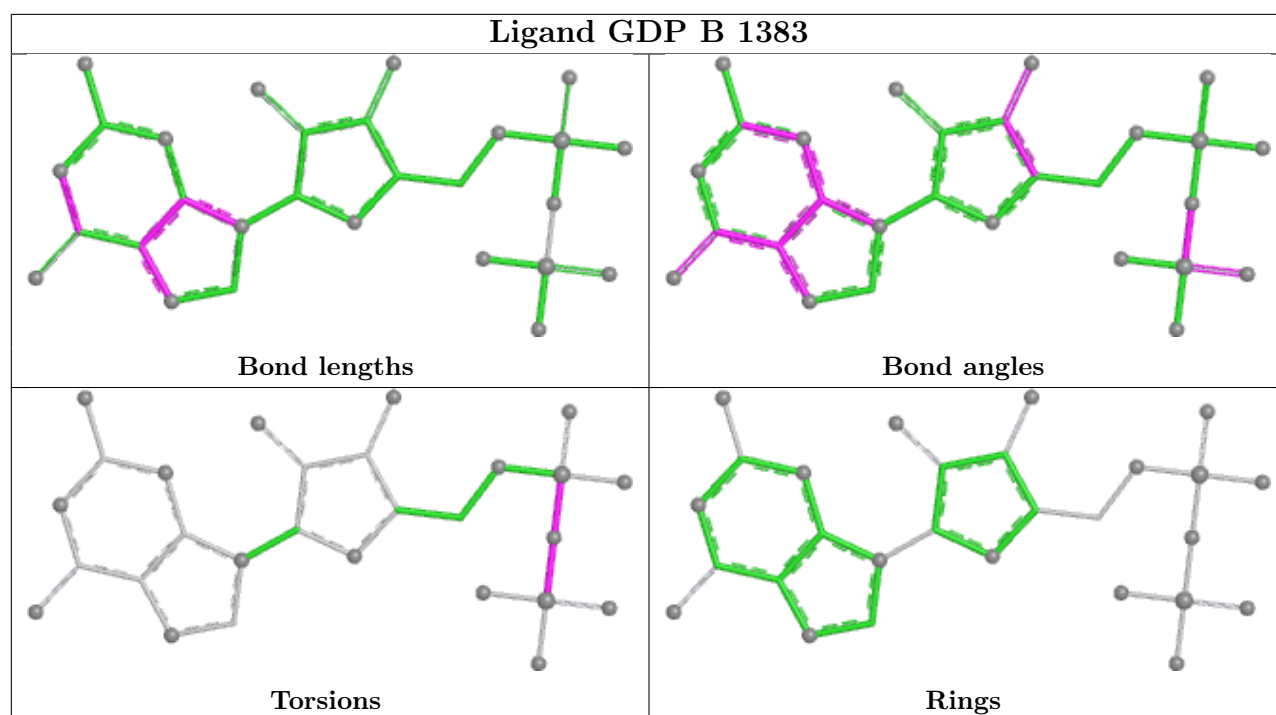
Ligand GDP A 1383











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	376/397 (94%)	0.24	14 (3%)	45	37	62, 63, 65, 67	0
1	B	376/397 (94%)	0.25	14 (3%)	45	37	62, 63, 65, 67	0
1	C	376/397 (94%)	0.57	13 (3%)	47	40	62, 63, 65, 67	0
1	D	376/397 (94%)	0.88	37 (9%)	13	12	62, 63, 65, 67	0
1	E	376/397 (94%)	0.41	14 (3%)	45	37	62, 63, 65, 67	0
1	F	376/397 (94%)	1.87	148 (39%)	1	0	62, 63, 65, 67	0
1	G	376/397 (94%)	0.85	22 (5%)	28	23	62, 63, 65, 67	0
1	H	376/397 (94%)	0.45	9 (2%)	59	51	62, 63, 65, 67	0
1	I	376/397 (94%)	0.42	9 (2%)	59	51	62, 63, 65, 67	0
1	J	376/397 (94%)	0.40	17 (4%)	38	31	62, 63, 65, 67	0
All	All	3760/3970 (94%)	0.63	297 (7%)	18	16	62, 63, 65, 67	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	382	ASN	10.2
1	B	247	GLN	8.0
1	B	248	PRO	7.6
1	D	248	PRO	7.1
1	E	247	GLN	7.0
1	G	246	GLY	6.4
1	C	181	GLU	6.2
1	F	248	PRO	6.2
1	E	248	PRO	5.9
1	I	248	PRO	5.9
1	J	248	PRO	5.8
1	E	246	GLY	5.8
1	D	247	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	247	GLN	5.8
1	F	219	LEU	5.6
1	G	248	PRO	5.5
1	F	76	LYS	5.3
1	I	246	GLY	5.3
1	F	311	ASN	5.3
1	D	268	GLY	5.2
1	F	92	GLN	5.2
1	C	382	ASN	5.2
1	F	309	ALA	5.1
1	F	356	ALA	5.1
1	F	312	PHE	5.0
1	D	120	PHE	4.9
1	A	247	GLN	4.7
1	F	261	VAL	4.7
1	F	357	LEU	4.7
1	F	353	MET	4.6
1	F	382	ASN	4.6
1	F	307	ARG	4.6
1	B	382	ASN	4.5
1	H	246	GLY	4.4
1	B	181	GLU	4.4
1	B	246	GLY	4.3
1	C	184	ARG	4.3
1	F	359	GLY	4.3
1	F	275	LEU	4.2
1	I	247	GLN	4.2
1	F	376	TYR	4.2
1	F	308	PRO	4.1
1	B	225	ASP	4.1
1	F	324	VAL	4.0
1	G	92	GLN	4.0
1	C	247	GLN	4.0
1	F	278	LEU	3.9
1	C	248	PRO	3.9
1	F	6	PHE	3.9
1	G	382	ASN	3.9
1	C	365	GLN	3.9
1	C	246	GLY	3.9
1	F	310	PHE	3.8
1	F	306	ARG	3.8
1	J	225	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	255	HIS	3.8
1	H	247	GLN	3.7
1	F	297	VAL	3.7
1	H	248	PRO	3.7
1	F	97	HIS	3.7
1	F	264	ALA	3.7
1	I	382	ASN	3.7
1	F	305	GLN	3.7
1	F	94	GLU	3.7
1	F	293	PHE	3.6
1	F	265	GLU	3.6
1	F	53	ILE	3.6
1	F	352	THR	3.6
1	F	110	TRP	3.6
1	F	345	THR	3.6
1	F	349	LEU	3.6
1	F	42	THR	3.6
1	D	52	GLU	3.5
1	G	94	GLU	3.5
1	G	247	GLN	3.5
1	F	269	TYR	3.5
1	F	272	GLU	3.5
1	J	247	GLN	3.4
1	D	261	VAL	3.4
1	J	365	GLN	3.4
1	F	348	VAL	3.4
1	F	34	CYS	3.4
1	C	185	ARG	3.4
1	F	354	THR	3.4
1	F	9	LYS	3.4
1	F	351	TYR	3.4
1	F	374	TYR	3.4
1	F	301	LEU	3.4
1	J	334	PRO	3.4
1	G	365	GLN	3.4
1	F	371	LEU	3.3
1	E	181	GLU	3.3
1	F	294	THR	3.3
1	G	179	GLU	3.3
1	F	133	SER	3.3
1	F	316	MET	3.3
1	J	316	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	262	HIS	3.3
1	F	367	LEU	3.2
1	C	179	GLU	3.2
1	A	109	ASP	3.2
1	F	271	VAL	3.2
1	F	377	GLN	3.2
1	D	110	TRP	3.2
1	F	360	TYR	3.2
1	A	268	GLY	3.1
1	F	134	THR	3.1
1	F	380	LEU	3.1
1	F	362	TYR	3.1
1	F	279	MET	3.1
1	A	202	GLN	3.1
1	F	365	GLN	3.1
1	G	376	TYR	3.1
1	J	246	GLY	3.1
1	F	358	ARG	3.1
1	B	380	LEU	3.1
1	D	249	ALA	3.0
1	F	83	ALA	3.0
1	F	2	SER	3.0
1	D	246	GLY	3.0
1	F	37	TYR	3.0
1	F	19	ASN	3.0
1	F	340	LEU	3.0
1	G	153	HIS	3.0
1	F	266	ARG	2.9
1	E	365	GLN	2.9
1	F	246	GLY	2.9
1	F	355	VAL	2.9
1	F	263	ILE	2.9
1	B	268	GLY	2.9
1	G	43	TYR	2.9
1	G	268	GLY	2.9
1	F	303	THR	2.9
1	F	369	ARG	2.9
1	F	177	LEU	2.9
1	D	365	GLN	2.9
1	A	376	TYR	2.9
1	G	37	TYR	2.9
1	F	179	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	15	VAL	2.8
1	J	2	SER	2.8
1	F	93	TRP	2.8
1	F	318	TRP	2.8
1	F	170	ARG	2.8
1	F	87	PHE	2.8
1	G	181	GLU	2.8
1	A	382	ASN	2.8
1	F	100	ASP	2.8
1	C	268	GLY	2.8
1	J	268	GLY	2.8
1	D	59	THR	2.8
1	F	364	GLN	2.7
1	G	219	LEU	2.7
1	F	321	THR	2.7
1	F	372	GLY	2.7
1	D	21	ARG	2.7
1	F	292	LEU	2.7
1	I	219	LEU	2.7
1	F	127	HIS	2.7
1	F	328	HIS	2.7
1	E	59	THR	2.7
1	F	79	GLY	2.7
1	D	265	GLU	2.7
1	F	61	VAL	2.7
1	H	261	VAL	2.7
1	D	129	PHE	2.6
1	F	30	HIS	2.6
1	A	59	THR	2.6
1	F	378	ALA	2.6
1	F	287	VAL	2.6
1	F	320	ALA	2.6
1	F	131	ARG	2.6
1	F	284	PRO	2.6
1	D	219	LEU	2.6
1	F	346	THR	2.6
1	E	381	GLU	2.6
1	D	356	ALA	2.6
1	F	157	SER	2.5
1	F	84	LEU	2.5
1	F	80	MET	2.5
1	C	377	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	23	ALA	2.5
1	E	48	ARG	2.5
1	D	255	HIS	2.5
1	F	102	ASP	2.5
1	F	277	ARG	2.5
1	F	276	HIS	2.5
1	D	357	LEU	2.5
1	F	75	GLY	2.5
1	F	165	GLY	2.5
1	F	282	TRP	2.5
1	H	219	LEU	2.5
1	J	380	LEU	2.5
1	F	173	VAL	2.5
1	C	120	PHE	2.5
1	A	373	ARG	2.5
1	F	373	ARG	2.5
1	F	302	ARG	2.5
1	F	169	MET	2.5
1	D	54	SER	2.5
1	J	288	GLU	2.5
1	F	226	LEU	2.4
1	F	289	LEU	2.4
1	F	336	TRP	2.4
1	F	313	MET	2.4
1	F	3	LEU	2.4
1	H	316	MET	2.4
1	F	7	PRO	2.4
1	E	268	GLY	2.4
1	G	46	VAL	2.4
1	F	368	TYR	2.4
1	D	316	MET	2.3
1	F	255	HIS	2.3
1	F	295	THR	2.3
1	F	270	ASP	2.3
1	D	264	ALA	2.3
1	J	115	GLU	2.3
1	I	41	GLN	2.3
1	F	230	LEU	2.3
1	D	57	THR	2.3
1	D	211	ILE	2.3
1	F	139	THR	2.3
1	J	306	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	63	VAL	2.3
1	F	98	PHE	2.3
1	F	50	ALA	2.3
1	F	363	ALA	2.3
1	G	38	GLU	2.3
1	F	209	CYS	2.3
1	D	263	ILE	2.3
1	F	262	HIS	2.3
1	F	57	THR	2.3
1	B	302	ARG	2.3
1	D	210	TYR	2.3
1	D	369	ARG	2.3
1	E	258	ARG	2.3
1	A	248	PRO	2.3
1	F	260	PRO	2.3
1	D	363	ALA	2.3
1	B	92	GLN	2.3
1	B	185	ARG	2.3
1	F	375	ARG	2.3
1	H	210	TYR	2.3
1	D	267	VAL	2.3
1	F	267	VAL	2.3
1	F	317	ALA	2.2
1	J	249	ALA	2.2
1	B	306	ARG	2.2
1	G	375	ARG	2.2
1	H	209	CYS	2.2
1	D	123	GLY	2.2
1	A	181	GLU	2.2
1	F	342	LYS	2.2
1	A	30	HIS	2.2
1	D	55	ARG	2.2
1	F	314	ASP	2.2
1	J	219	LEU	2.2
1	E	109	ASP	2.2
1	F	82	THR	2.2
1	F	140	TRP	2.2
1	A	246	GLY	2.2
1	F	322	TYR	2.2
1	D	42	THR	2.2
1	F	59	THR	2.2
1	H	181	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	185	ARG	2.1
1	D	212	PRO	2.1
1	B	316	MET	2.1
1	D	50	ALA	2.1
1	F	249	ALA	2.1
1	F	347	ARG	2.1
1	F	161	GLN	2.1
1	F	274	THR	2.1
1	E	380	LEU	2.1
1	F	171	ARG	2.1
1	G	379	ALA	2.1
1	J	376	TYR	2.1
1	A	209	CYS	2.1
1	F	181	GLU	2.1
1	F	32	VAL	2.1
1	F	149	LEU	2.1
1	G	371	LEU	2.1
1	A	184	ARG	2.1
1	C	117	ALA	2.1
1	D	24	ALA	2.1
1	F	155	GLU	2.1
1	I	276	HIS	2.0
1	F	174	ALA	2.0
1	B	299	GLU	2.0
1	I	181	GLU	2.0
1	D	27	PRO	2.0
1	G	149	LEU	2.0
1	F	186	ARG	2.0
1	D	94	GLU	2.0
1	F	151	TRP	2.0
1	I	316	MET	2.0
1	F	86	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

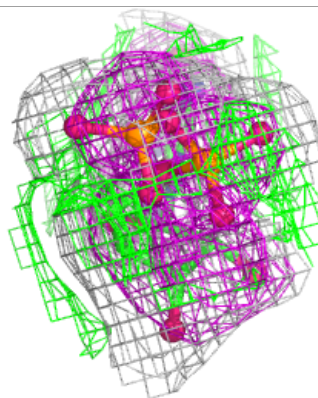
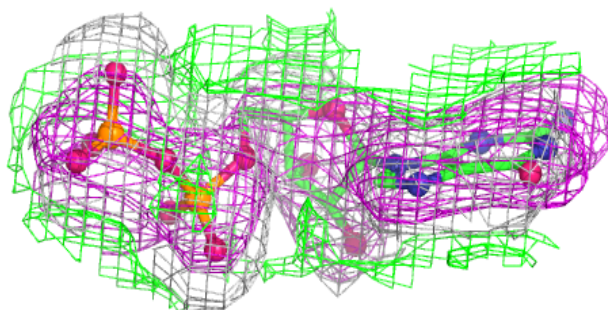
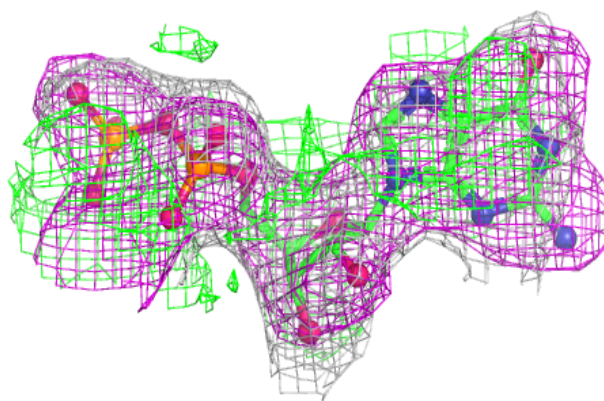
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	GDP	F	1383	28/28	0.55	0.22	63,63,64,65	0
2	GDP	J	1383	28/28	0.81	0.17	62,63,64,66	0
2	GDP	H	1383	28/28	0.82	0.16	63,63,64,65	0
2	GDP	I	1383	28/28	0.83	0.16	63,63,64,66	0
2	GDP	G	1383	28/28	0.86	0.16	63,63,64,65	0
2	GDP	D	1383	28/28	0.93	0.12	62,63,64,66	0
3	CO	F	1384	1/1	0.93	0.19	66,66,66,66	0
2	GDP	C	1383	28/28	0.94	0.10	62,63,64,66	0
3	CO	A	1384	1/1	0.95	0.06	67,67,67,67	0
3	CO	D	1384	1/1	0.95	0.09	68,68,68,68	0
3	CO	E	1384	1/1	0.95	0.07	67,67,67,67	0
2	GDP	E	1383	28/28	0.95	0.09	62,63,64,66	0
2	GDP	A	1383	28/28	0.96	0.08	62,63,64,66	0
3	CO	B	1384	1/1	0.96	0.06	67,67,67,67	0
3	CO	C	1384	1/1	0.96	0.07	67,67,67,67	0
3	CO	G	1384	1/1	0.96	0.10	66,66,66,66	0
2	GDP	B	1383	28/28	0.97	0.08	62,63,64,66	0
3	CO	H	1384	1/1	0.98	0.10	67,67,67,67	0
3	CO	I	1384	1/1	0.98	0.10	67,67,67,67	0
3	CO	J	1384	1/1	0.98	0.10	67,67,67,67	0

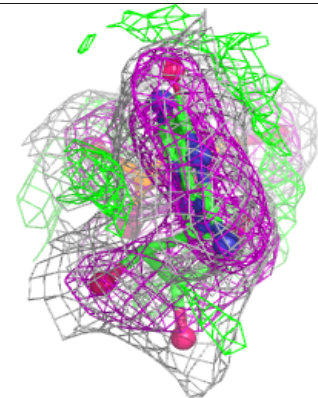
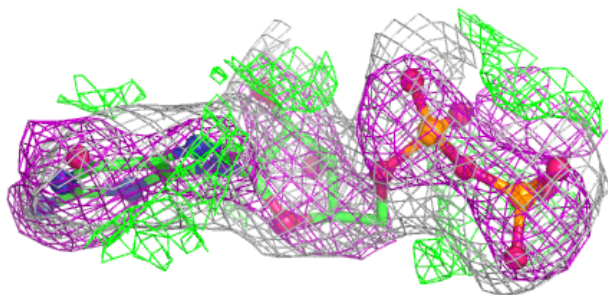
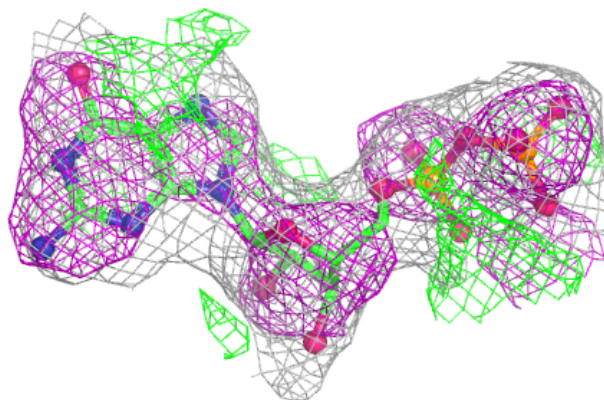
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP F 1383:

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

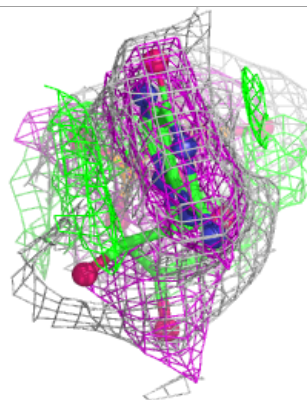
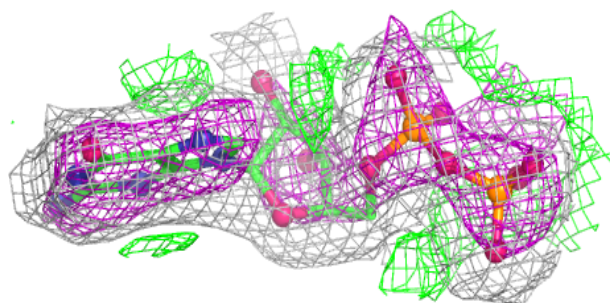
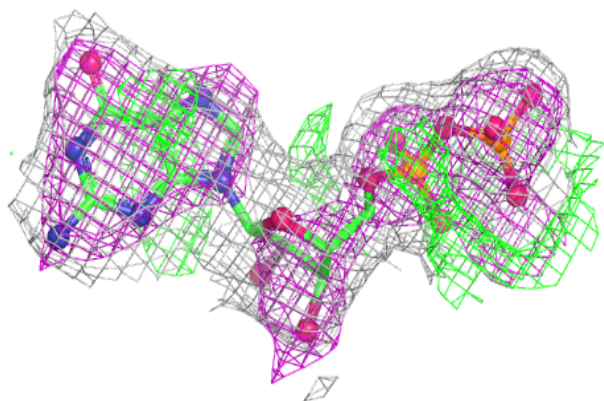
**Electron density around GDP J 1383:**

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

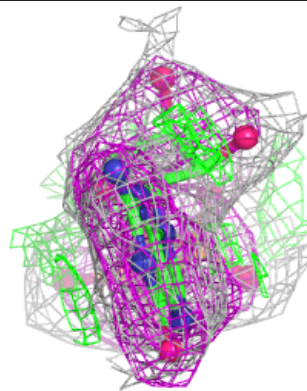
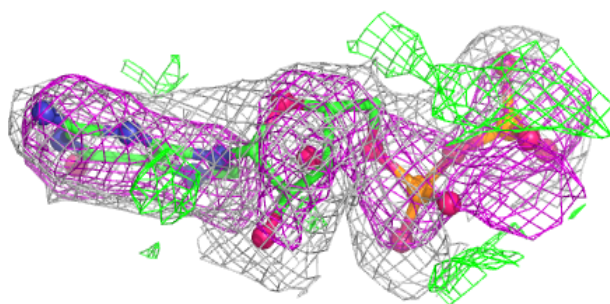
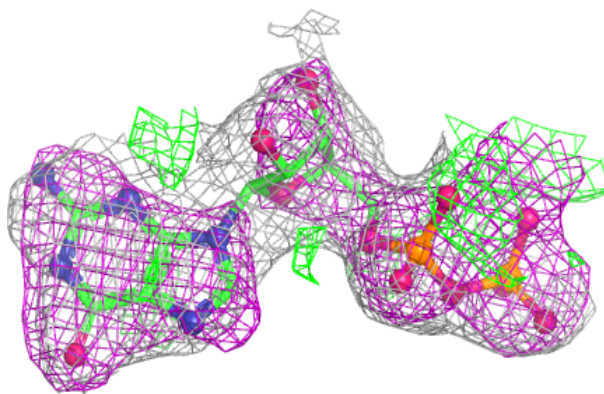


Electron density around GDP H 1383:

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

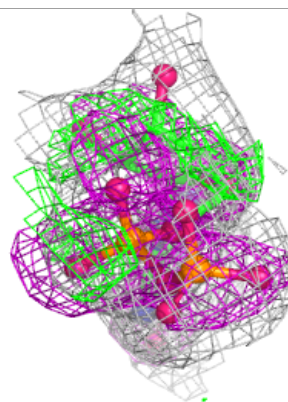
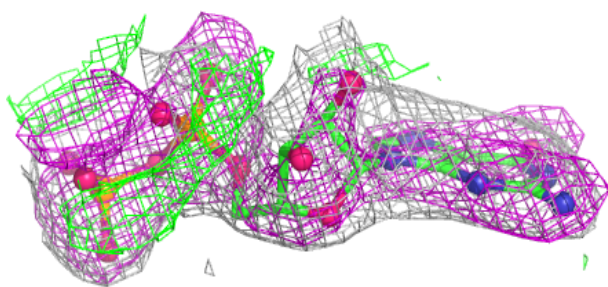
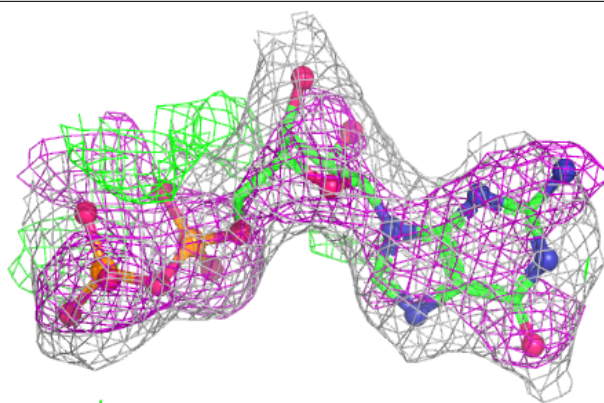
**Electron density around GDP I 1383:**

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

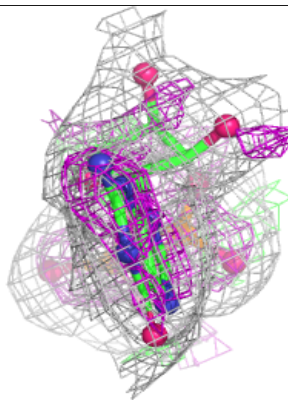
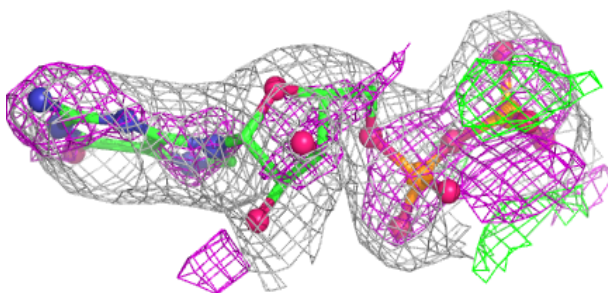
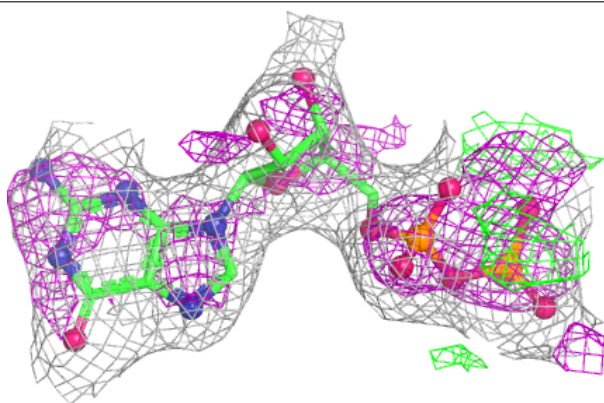


Electron density around GDP G 1383:

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

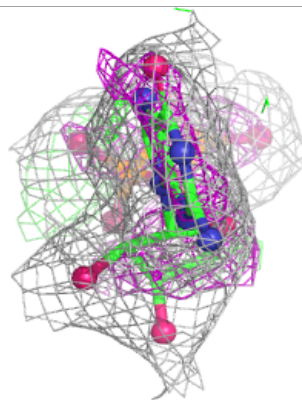
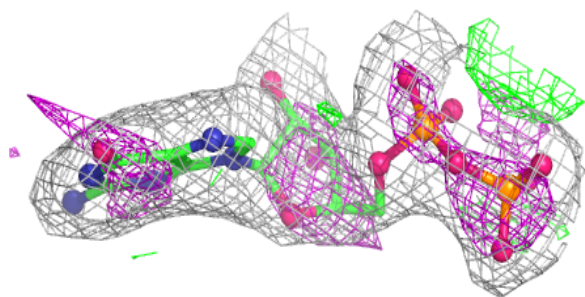
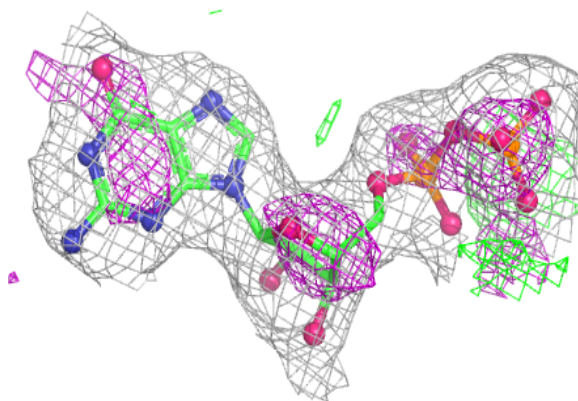
**Electron density around GDP D 1383:**

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

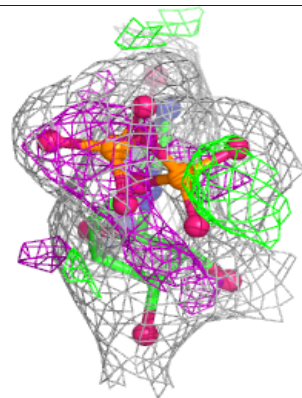
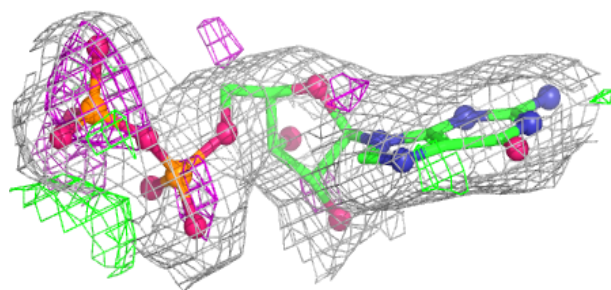
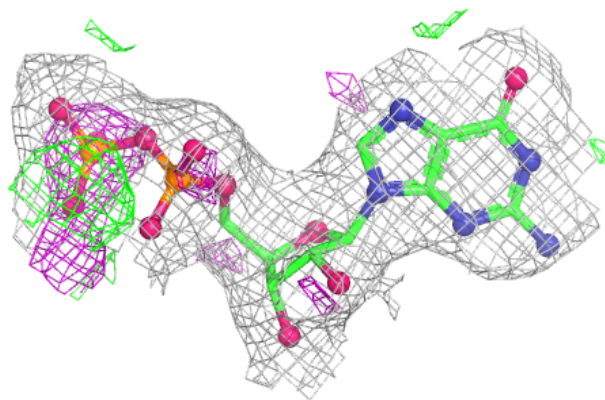


Electron density around GDP C 1383:

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

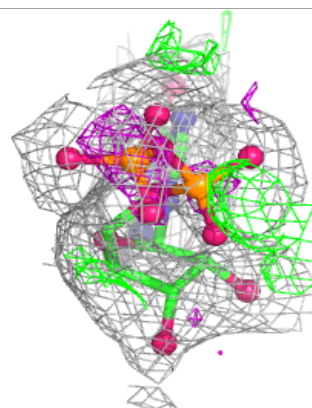
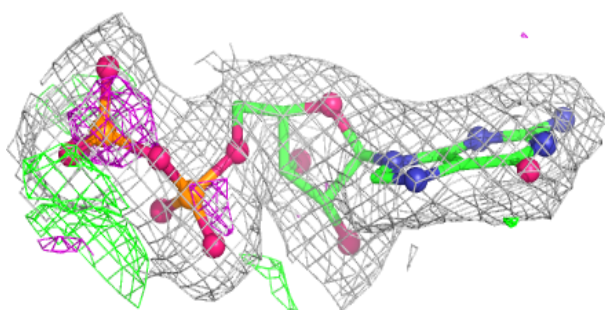
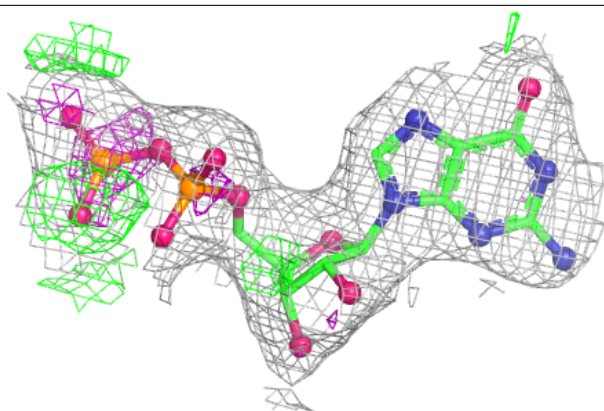
**Electron density around GDP E 1383:**

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

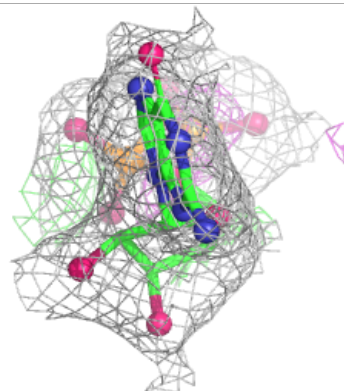
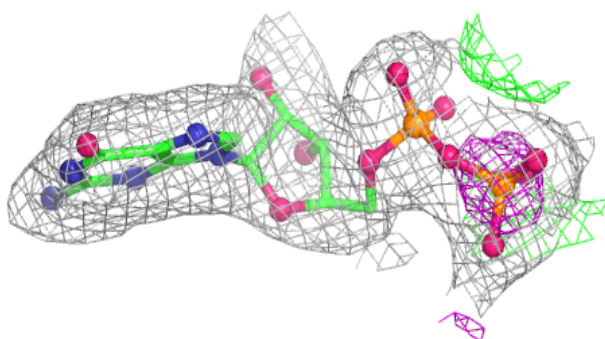
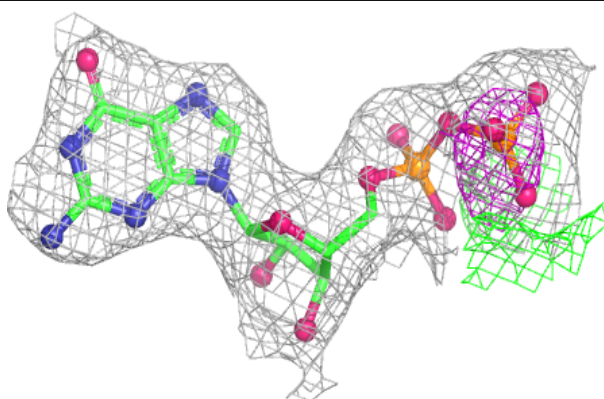


Electron density around GDP A 1383:

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

**Electron density around GDP B 1383:**

$2mF_o-DF_c$ (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.