



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 PM UTC

PDB ID : 2BO8 / pdb_00002bo8
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 : 2.80 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:

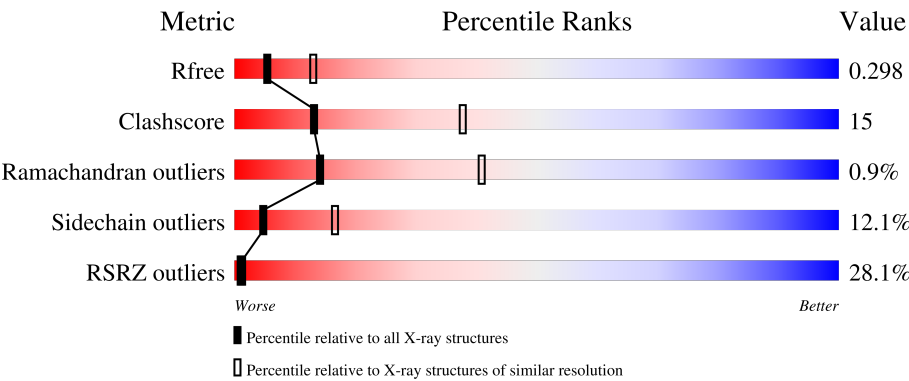
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	59% 59%26%8% . .
1	B	397	59% 62%24%7% . .
1	C	397	12% 70%19%6% . .
1	D	397	16% 70%18%6% . .

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Mol	Chain	Length	Quality of chain
1	E	397	13%69%20%6% . .
1	F	397	32%71%20% . . .
1	G	397	39%63%24%7% . .
1	H	397	12%71%21% . . .
1	I	397	7%70%21% . . .
1	J	397	21%64%23%7% . .



2 Entry composition

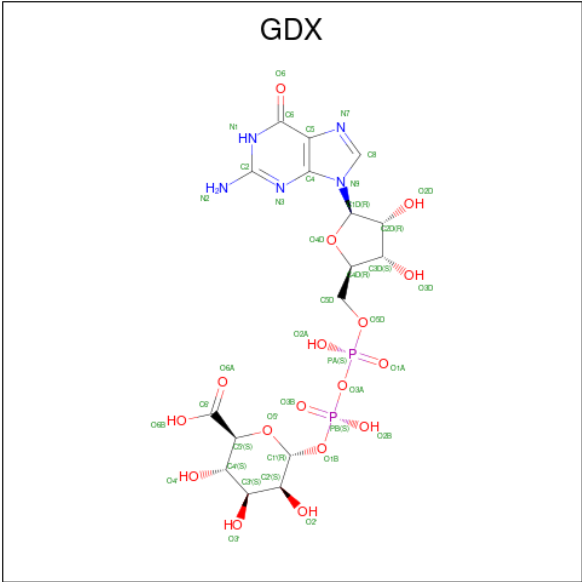
There are 5 unique types of molecules in this entry. The entry contains 32098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	B	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	C	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	D	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	E	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	F	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	G	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	H	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	I	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			
1	J	381	Total	C	N	O	S	0	0	1
			3138	2006	558	559	15			

- Molecule 2 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (CCD ID: GDX) (formula: $C_{16}H_{23}N_5O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	B	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	C	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	D	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	E	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	F	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	G	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	H	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	I	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
2	J	1	Total	C	N	O	P	0	0
			39	16	5	16	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

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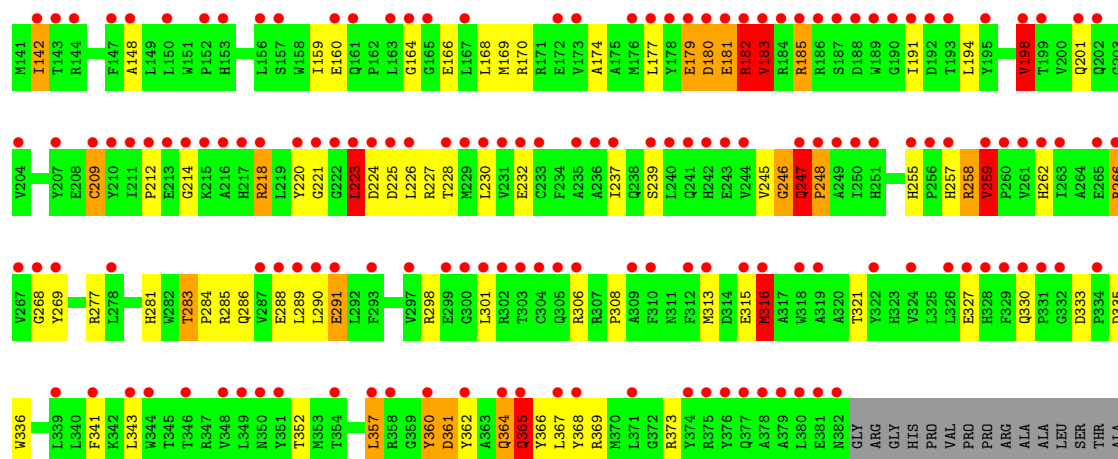
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mn 1	0	0
3	D	1	Total 1	Mn 1	0	0
3	E	1	Total 1	Mn 1	0	0
3	F	1	Total 1	Mn 1	0	0
3	G	1	Total 1	Mn 1	0	0
3	H	1	Total 1	Mn 1	0	0
3	I	1	Total 1	Mn 1	0	0
3	J	1	Total 1	Mn 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

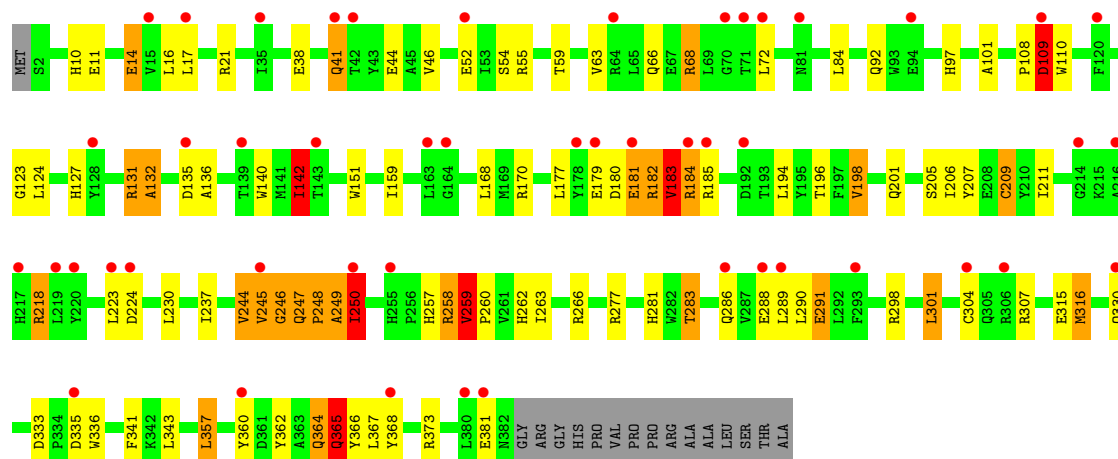
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	G	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	I	1	Total 1	Cl 1	0	0
4	J	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

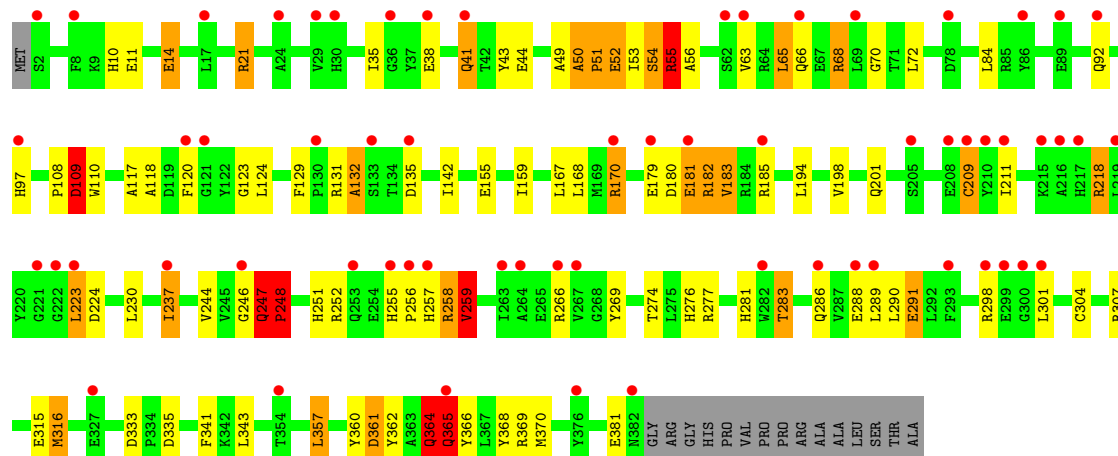
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total 78	O 78	0	0
5	B	80	Total 80	O 80	0	0
5	C	38	Total 38	O 38	0	0
5	D	27	Total 27	O 27	0	0
5	E	34	Total 34	O 34	0	0
5	F	3	Total 3	O 3	0	0
5	G	23	Total 23	O 23	0	0
5	H	6	Total 6	O 6	0	0
5	I	13	Total 13	O 13	0	0
5	J	6	Total 6	O 6	0	0



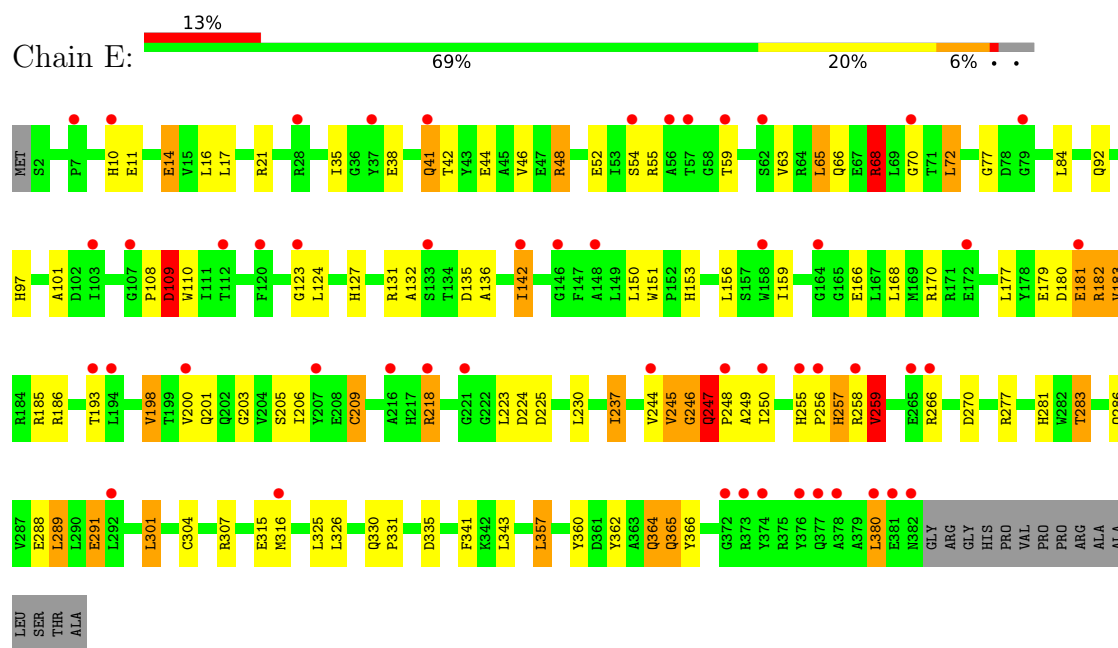
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



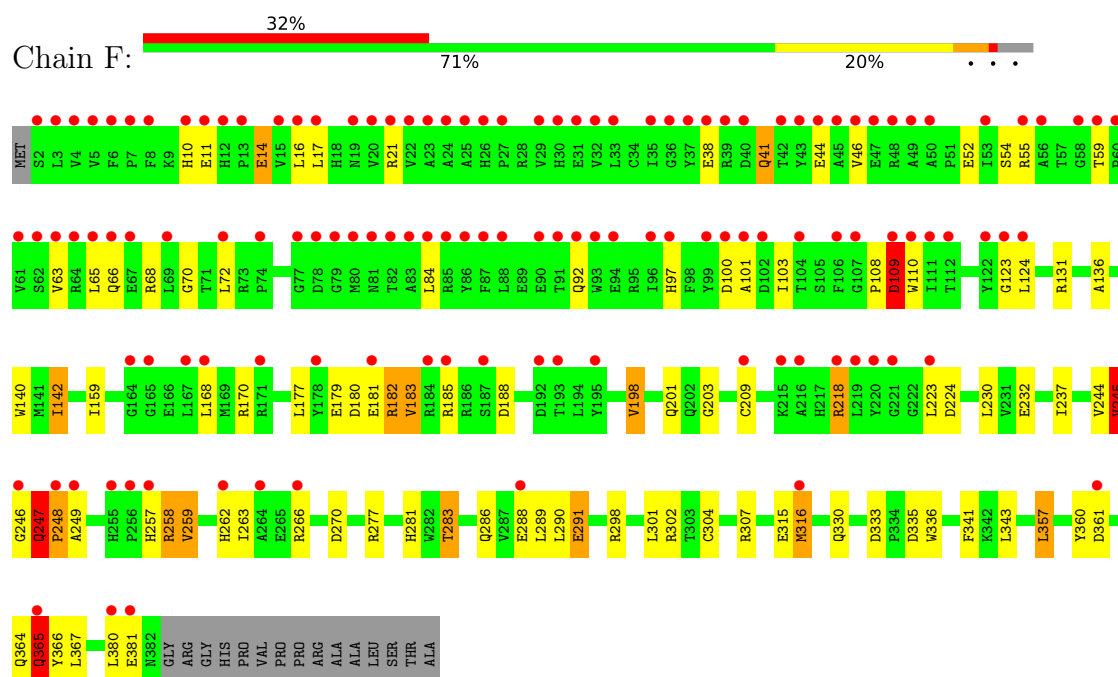
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



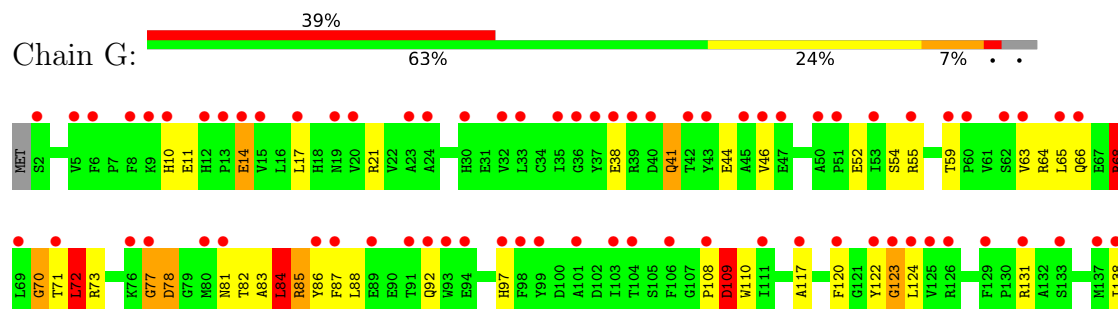
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

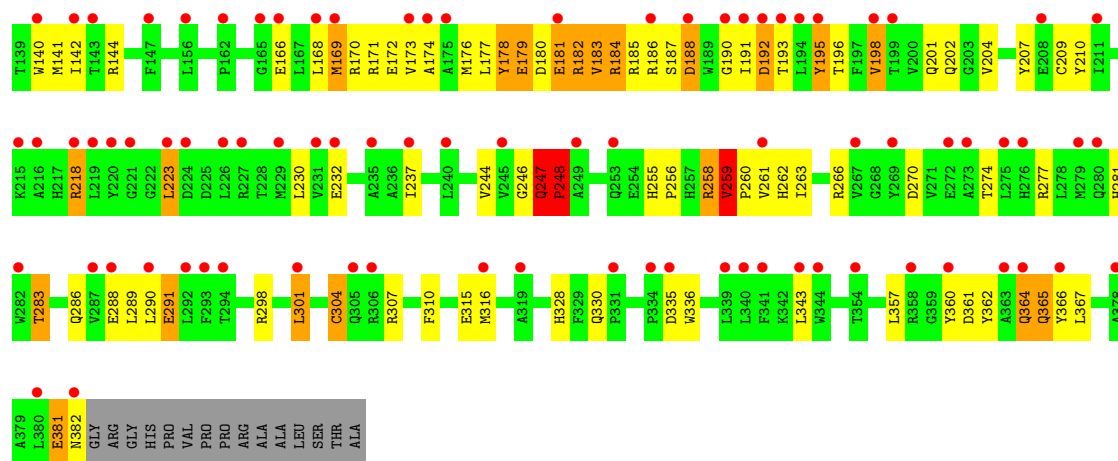


• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

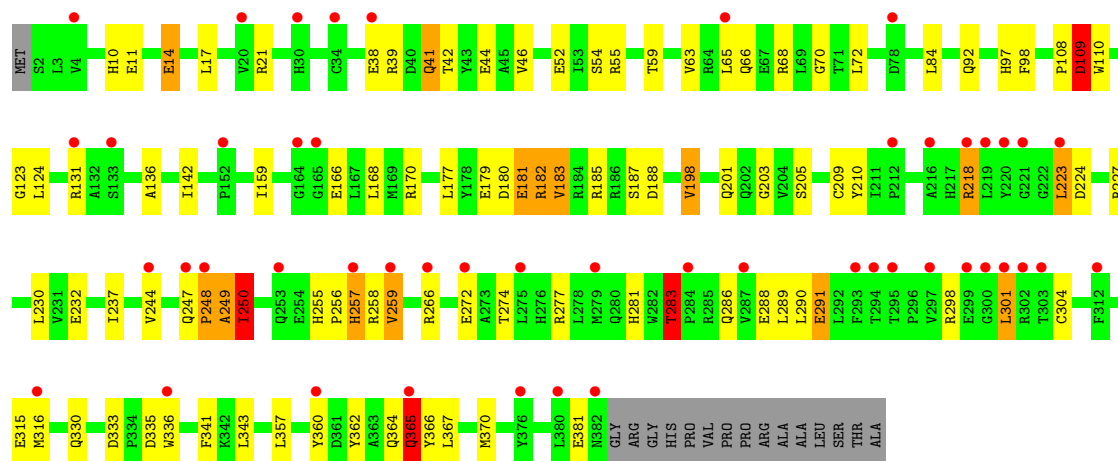


• Molecule 1: MANNOSYLGLYCERATE SYNTHASE

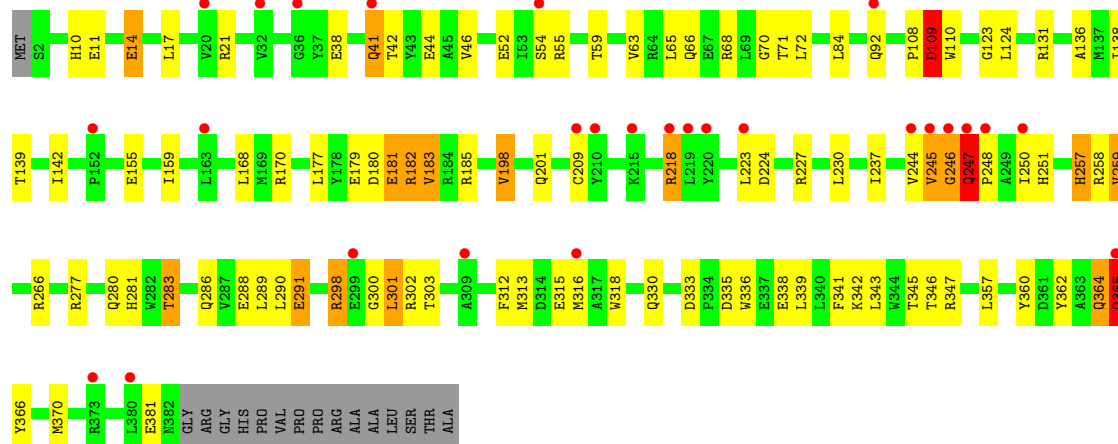




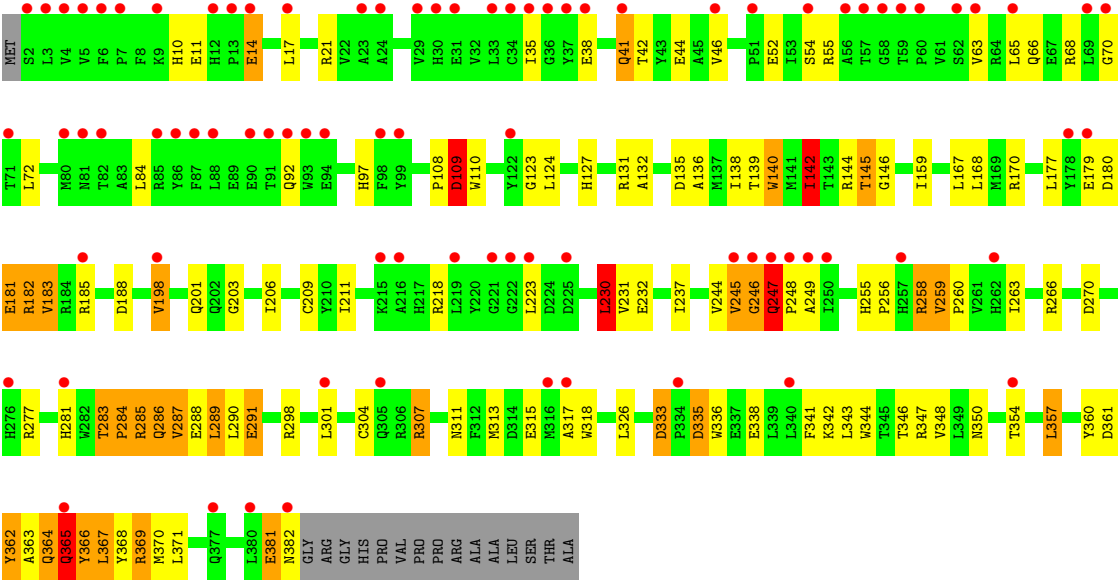
• Molecule 1: MANNOSYLGLYCERATE SYNTHASE



• 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	405.09Å 161.43Å 108.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.12 – 2.80 74.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (74.12-2.80) 97.4 (74.12-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.216 0.287 , 0.298	Depositor DCC
R_{free} test set	8687 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	32098	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: CL, MN, GDX

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	1.77	51/3229 (1.6%)	1.48	37/4394 (0.8%)
1	B	1.78	49/3229 (1.5%)	1.41	16/4394 (0.4%)
1	C	1.23	9/3229 (0.3%)	1.17	9/4394 (0.2%)
1	D	1.29	12/3229 (0.4%)	1.15	9/4394 (0.2%)
1	E	1.16	4/3229 (0.1%)	1.16	9/4394 (0.2%)
1	F	0.86	4/3229 (0.1%)	0.99	4/4394 (0.1%)
1	G	1.41	38/3229 (1.2%)	1.27	23/4394 (0.5%)
1	H	0.91	3/3229 (0.1%)	1.04	6/4394 (0.1%)
1	I	1.04	9/3229 (0.3%)	1.12	5/4394 (0.1%)
1	J	1.41	45/3229 (1.4%)	1.27	30/4394 (0.7%)
All	All	1.32	224/32290 (0.7%)	1.22	148/43940 (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	A	0	2
1	B	0	3
1	C	0	6
1	D	0	3
1	E	0	4
1	F	0	4
1	G	0	4
1	H	0	4
1	I	1	3
1	J	0	3
All	All	1	36

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	72	LEU	C-O	16.80	1.45	1.24
1	J	347	ARG	C-O	15.22	1.42	1.24
1	A	365	GLN	CB-CG	13.14	1.91	1.52
1	J	341	PHE	C-O	12.73	1.40	1.24
1	J	348	VAL	C-O	11.36	1.36	1.24
1	J	368	TYR	N-CA	11.33	1.60	1.46
1	J	231	VAL	CA-CB	11.28	1.68	1.54
1	J	142	ILE	CA-CB	-10.88	1.43	1.55
1	G	188	ASP	CG-OD1	10.87	1.46	1.25
1	G	186	ARG	C-O	10.60	1.36	1.23
1	G	169	MET	CG-SD	10.24	2.06	1.80
1	B	269	TYR	C-O	-10.20	1.11	1.23
1	G	70	GLY	C-O	9.40	1.32	1.24
1	J	347	ARG	N-CA	-9.33	1.35	1.46
1	B	180	ASP	C-O	-9.30	1.12	1.24
1	B	316	MET	CG-SD	9.26	2.03	1.80
1	J	346	THR	CA-C	9.19	1.65	1.52
1	B	352	THR	C-O	-9.08	1.13	1.24
1	G	77	GLY	CA-C	8.97	1.61	1.52
1	A	268	GLY	C-O	8.93	1.33	1.24
1	B	70	GLY	N-CA	8.69	1.51	1.44
1	J	145	THR	C-N	8.55	1.46	1.33
1	B	129	PHE	N-CA	8.54	1.52	1.45
1	G	82	THR	CA-CB	8.51	1.66	1.53
1	D	209	CYS	CB-SG	-8.50	1.53	1.81
1	J	230	LEU	CG-CD1	-8.46	1.24	1.52
1	G	188	ASP	CA-C	8.31	1.64	1.52
1	D	361	ASP	C-O	-8.18	1.14	1.24
1	C	365	GLN	CB-CG	8.12	1.76	1.52
1	G	192	ASP	C-O	8.09	1.34	1.24
1	J	317	ALA	C-O	8.08	1.34	1.24
1	A	313	MET	N-CA	-7.92	1.36	1.46
1	A	346	THR	C-N	7.87	1.43	1.33
1	B	78	ASP	N-CA	-7.72	1.37	1.46
1	J	333	ASP	C-O	-7.71	1.14	1.24
1	B	365	GLN	CB-CG	7.71	1.75	1.52
1	G	184	ARG	C-O	7.66	1.32	1.24
1	A	347	ARG	C-O	7.59	1.32	1.24
1	B	327	GLU	C-O	-7.53	1.14	1.24
1	C	131	ARG	C-O	7.33	1.32	1.23
1	C	183	VAL	CA-CB	7.29	1.64	1.54
1	B	357	LEU	N-CA	-7.26	1.36	1.46
1	A	209	CYS	CB-SG	-7.24	1.57	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	LEU	C-O	-7.23	1.15	1.24
1	A	270	ASP	C-O	7.20	1.32	1.24
1	B	209	CYS	CB-SG	-7.19	1.57	1.81
1	J	366	TYR	CA-C	7.19	1.61	1.52
1	J	369	ARG	C-N	7.19	1.43	1.33
1	G	204	VAL	CA-CB	-7.16	1.45	1.54
1	D	365	GLN	CB-CG	7.14	1.73	1.52
1	A	269	TYR	C-O	-7.11	1.16	1.23
1	A	147	PHE	C-O	-7.08	1.16	1.24
1	J	347	ARG	CZ-NH1	6.95	1.42	1.32
1	B	198	VAL	N-CA	-6.92	1.37	1.46
1	J	370	MET	N-CA	-6.87	1.38	1.46
1	A	373	ARG	CZ-NH1	6.87	1.42	1.32
1	J	369	ARG	C-O	6.87	1.32	1.24
1	J	145	THR	C-O	6.85	1.32	1.24
1	I	209	CYS	CB-SG	-6.84	1.58	1.81
1	J	350	ASN	N-CA	-6.84	1.38	1.46
1	G	71	THR	C-O	6.82	1.32	1.24
1	B	232	GLU	N-CA	-6.82	1.38	1.46
1	J	365	GLN	CB-CG	6.81	1.72	1.52
1	A	306	ARG	CZ-NH1	6.81	1.42	1.32
1	I	381	GLU	C-N	-6.81	1.23	1.33
1	B	223	LEU	CA-C	6.79	1.62	1.52
1	J	354	THR	C-O	6.78	1.32	1.24
1	G	188	ASP	C-O	6.75	1.32	1.24
1	A	269	TYR	N-CA	6.75	1.54	1.46
1	F	365	GLN	CB-CG	6.74	1.72	1.52
1	G	173	VAL	CA-C	6.65	1.61	1.52
1	B	194	LEU	N-CA	-6.65	1.38	1.46
1	D	237	ILE	CA-CB	6.61	1.61	1.54
1	C	209	CYS	CB-SG	-6.60	1.59	1.81
1	H	209	CYS	CB-SG	-6.60	1.59	1.81
1	J	363	ALA	C-O	6.59	1.32	1.24
1	G	172	GLU	C-N	6.57	1.42	1.34
1	C	132	ALA	CA-CB	-6.55	1.43	1.53
1	J	346	THR	C-O	-6.50	1.15	1.24
1	A	222	GLY	CA-C	6.50	1.57	1.52
1	A	346	THR	N-CA	-6.50	1.38	1.46
1	J	346	THR	CB-CG2	-6.47	1.31	1.52
1	A	274	THR	N-CA	-6.45	1.38	1.46
1	B	269	TYR	CA-C	-6.39	1.45	1.52
1	J	336	TRP	C-O	6.38	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	346	THR	CA-C	6.37	1.61	1.52
1	B	148	ALA	CA-CB	-6.37	1.43	1.53
1	B	218	ARG	CA-C	6.37	1.60	1.52
1	J	344	TRP	C-O	-6.35	1.16	1.24
1	G	85	ARG	N-CA	-6.35	1.38	1.46
1	G	193	THR	C-O	6.34	1.31	1.24
1	B	135	ASP	CG-OD2	6.33	1.37	1.25
1	B	268	GLY	C-O	6.30	1.30	1.23
1	D	170	ARG	CZ-NH1	6.30	1.41	1.32
1	A	273	ALA	N-CA	-6.29	1.38	1.46
1	A	268	GLY	C-N	6.29	1.41	1.33
1	J	342	LYS	C-O	-6.25	1.16	1.24
1	J	140	TRP	N-CA	6.23	1.54	1.46
1	J	318	TRP	C-O	6.23	1.31	1.24
1	I	301	LEU	CA-C	6.23	1.61	1.52
1	B	239	SER	C-O	-6.20	1.16	1.24
1	B	333	ASP	CA-C	6.20	1.59	1.52
1	I	300	GLY	N-CA	6.17	1.54	1.45
1	J	347	ARG	C-N	6.14	1.41	1.33
1	D	316	MET	CG-SD	6.13	1.96	1.80
1	G	192	ASP	C-N	6.09	1.42	1.33
1	J	342	LYS	CA-C	6.08	1.61	1.52
1	F	381	GLU	C-N	-6.08	1.24	1.33
1	G	88	LEU	CA-C	6.07	1.60	1.52
1	B	179	GLU	C-O	-6.06	1.16	1.24
1	G	171	ARG	C-N	6.06	1.41	1.33
1	C	207	TYR	N-CA	6.05	1.53	1.46
1	B	367	LEU	CA-C	6.04	1.60	1.52
1	B	97	HIS	N-CA	6.03	1.53	1.46
1	H	381	GLU	C-N	-6.01	1.25	1.33
1	B	70	GLY	C-O	-5.99	1.18	1.23
1	A	135	ASP	CA-C	5.99	1.61	1.53
1	G	172	GLU	C-O	5.98	1.31	1.24
1	G	381	GLU	C-N	-5.97	1.25	1.33
1	J	362	TYR	CA-C	5.96	1.60	1.52
1	J	341	PHE	C-N	5.96	1.41	1.33
1	I	345	THR	C-N	5.94	1.41	1.34
1	A	221	GLY	N-CA	5.93	1.53	1.45
1	A	266	ARG	C-O	5.92	1.31	1.23
1	B	373	ARG	CZ-NH1	5.89	1.41	1.32
1	B	139	THR	C-O	-5.89	1.17	1.24
1	J	338	GLU	CG-CD	5.88	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	SER	N-CA	-5.88	1.38	1.46
1	B	185	ARG	CD-NE	5.87	1.54	1.46
1	A	268	GLY	N-CA	5.86	1.52	1.45
1	B	92	GLN	CA-C	-5.83	1.45	1.52
1	I	346	THR	CA-CB	-5.82	1.43	1.53
1	I	365	GLN	CB-CG	5.82	1.70	1.52
1	G	173	VAL	CA-CB	-5.80	1.47	1.54
1	A	142	ILE	C-O	5.80	1.30	1.23
1	B	132	ALA	CA-CB	-5.79	1.44	1.53
1	J	371	LEU	CB-CG	5.78	1.65	1.53
1	C	381	GLU	C-N	-5.78	1.25	1.33
1	G	172	GLU	N-CA	5.75	1.53	1.46
1	J	146	GLY	N-CA	5.75	1.53	1.45
1	D	120	PHE	CD1-CE1	5.74	1.55	1.38
1	A	222	GLY	N-CA	5.72	1.52	1.45
1	B	368	TYR	N-CA	-5.72	1.39	1.46
1	A	151	TRP	CA-C	-5.70	1.46	1.52
1	A	373	ARG	CZ-NH2	5.68	1.40	1.33
1	B	160	GLU	C-O	-5.67	1.17	1.24
1	A	267	VAL	CA-C	-5.65	1.45	1.52
1	A	295	THR	N-CA	5.65	1.51	1.46
1	G	83	ALA	N-CA	5.64	1.52	1.46
1	B	191	ILE	N-CA	-5.62	1.40	1.46
1	A	274	THR	C-O	-5.62	1.17	1.24
1	G	117	ALA	CA-C	5.62	1.60	1.52
1	G	204	VAL	C-O	5.62	1.30	1.24
1	E	59	THR	CB-CG2	5.60	1.71	1.52
1	B	313	MET	N-CA	-5.59	1.39	1.46
1	G	71	THR	C-N	5.59	1.41	1.33
1	A	355	VAL	C-O	-5.58	1.17	1.24
1	J	381	GLU	C-N	-5.58	1.25	1.33
1	A	263	ILE	CA-CB	5.56	1.62	1.54
1	B	71	THR	CA-CB	5.55	1.62	1.54
1	J	363	ALA	C-N	5.53	1.41	1.33
1	G	172	GLU	CA-C	5.53	1.60	1.52
1	D	120	PHE	CG-CD2	5.52	1.50	1.38
1	A	129	PHE	N-CA	5.51	1.50	1.45
1	H	365	GLN	CB-CG	5.51	1.69	1.52
1	D	381	GLU	C-N	-5.48	1.25	1.33
1	A	253	GLN	N-CA	5.47	1.52	1.46
1	A	11	GLU	CA-C	-5.46	1.45	1.52
1	A	270	ASP	N-CA	5.45	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	VAL	CA-CB	-5.45	1.48	1.54
1	E	237	ILE	C-O	5.44	1.30	1.24
1	J	307	ARG	N-CA	-5.43	1.41	1.46
1	D	129	PHE	C-O	-5.42	1.18	1.24
1	J	362	TYR	N-CA	5.42	1.53	1.46
1	G	82	THR	C-O	5.40	1.30	1.24
1	B	221	GLY	N-CA	5.40	1.53	1.45
1	A	381	GLU	C-N	-5.35	1.25	1.33
1	A	346	THR	C-O	-5.34	1.17	1.24
1	A	131	ARG	CG-CD	5.33	1.68	1.52
1	A	175	ALA	CA-CB	-5.32	1.44	1.53
1	G	123	GLY	C-O	5.31	1.31	1.23
1	A	201	GLN	C-O	-5.29	1.17	1.24
1	G	171	ARG	C-O	5.29	1.30	1.24
1	G	144	ARG	N-CA	-5.26	1.39	1.46
1	B	308	PRO	C-O	-5.25	1.17	1.23
1	A	364	GLN	C-O	-5.25	1.18	1.24
1	A	208	GLU	N-CA	5.24	1.52	1.46
1	E	65	LEU	C-O	-5.24	1.17	1.23
1	J	335	ASP	CG-OD1	5.23	1.35	1.25
1	B	136	ALA	C-O	5.21	1.31	1.23
1	J	335	ASP	CG-OD2	5.21	1.35	1.25
1	I	280	GLN	C-O	5.21	1.30	1.23
1	D	132	ALA	CA-CB	-5.20	1.45	1.53
1	A	358	ARG	CA-C	-5.20	1.45	1.52
1	E	200	VAL	C-O	5.20	1.30	1.24
1	B	228	THR	C-O	-5.18	1.18	1.24
1	A	131	ARG	C-O	5.17	1.30	1.23
1	B	361	ASP	C-O	-5.17	1.18	1.24
1	D	120	PHE	CE1-CZ	5.17	1.54	1.38
1	A	341	PHE	CA-C	5.16	1.59	1.52
1	B	183	VAL	CA-CB	5.16	1.61	1.54
1	A	242	HIS	C-O	-5.15	1.16	1.23
1	A	218	ARG	CA-C	5.15	1.59	1.52
1	G	190	GLY	C-N	5.14	1.40	1.33
1	B	174	ALA	CA-CB	-5.12	1.45	1.53
1	G	316	MET	CG-SD	5.12	1.93	1.80
1	J	139	THR	CA-C	-5.12	1.46	1.52
1	G	84	LEU	CB-CG	5.10	1.63	1.53
1	B	164	GLY	C-O	-5.09	1.18	1.24
1	C	184	ARG	NE-CZ	5.09	1.38	1.33
1	A	239	SER	C-O	5.07	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	209	CYS	CB-SG	-5.07	1.64	1.81
1	B	360	TYR	N-CA	-5.07	1.40	1.46
1	B	316	MET	C-O	-5.06	1.18	1.24
1	F	316	MET	CG-SD	5.06	1.93	1.80
1	A	218	ARG	C-O	5.05	1.30	1.23
1	J	311	ASN	C-O	-5.03	1.17	1.24
1	J	350	ASN	C-O	5.03	1.30	1.24
1	C	316	MET	CG-SD	5.03	1.93	1.80
1	B	212	PRO	C-O	-5.03	1.18	1.24
1	A	221	GLY	C-O	5.02	1.30	1.23
1	G	78	ASP	CA-CB	5.02	1.61	1.53
1	G	196	THR	CA-CB	5.02	1.61	1.53
1	B	220	TYR	N-CA	5.01	1.51	1.45

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	VAL	CB-CA-C	-12.62	98.51	110.88
1	A	346	THR	CA-C-O	-10.75	107.61	119.97
1	A	273	ALA	N-CA-C	-8.89	101.67	111.36
1	B	227	ARG	N-CA-C	8.84	120.53	111.07
1	J	354	THR	CA-C-N	-8.74	114.26	123.08
1	J	354	THR	C-N-CA	-8.74	114.26	123.08
1	B	191	ILE	N-CA-C	8.61	119.40	110.36
1	G	259	VAL	CB-CA-C	-8.35	102.69	110.88
1	G	68	ARG	NE-CZ-NH2	8.13	126.52	119.20
1	J	370	MET	N-CA-C	-7.83	102.82	111.36
1	E	259	VAL	CB-CA-C	-7.75	101.77	110.68
1	A	227	ARG	N-CA-C	7.62	119.37	111.14
1	A	326	LEU	N-CA-C	-7.58	103.02	111.28
1	A	343	LEU	CA-C-O	-7.56	113.07	121.00
1	A	209	CYS	N-CA-CB	-7.51	98.18	110.42
1	G	87	PHE	N-CA-C	7.30	119.87	111.11
1	J	342	LYS	CA-C-O	-7.24	112.81	120.92
1	A	142	ILE	N-CA-C	7.21	118.26	111.48
1	A	259	VAL	CB-CA-C	-7.05	98.52	111.36
1	G	85	ARG	N-CA-C	-6.96	103.62	111.07
1	C	209	CYS	N-CA-CB	-6.95	98.69	110.16
1	A	109	ASP	N-CA-CB	-6.90	98.82	110.49
1	J	365	GLN	N-CA-C	-6.84	102.90	111.11
1	G	81	ASN	CA-C-N	-6.77	111.24	120.44
1	G	81	ASN	C-N-CA	-6.77	111.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	367	LEU	CA-C-N	-6.73	111.27	120.28
1	J	367	LEU	C-N-CA	-6.73	111.27	120.28
1	J	368	TYR	N-CA-C	6.73	118.61	111.28
1	A	364	GLN	CA-C-O	-6.65	113.85	120.70
1	A	241	GLN	N-CA-C	6.63	120.46	112.38
1	I	227	ARG	N-CA-C	6.59	118.13	111.07
1	B	142	ILE	N-CA-C	6.58	117.66	111.48
1	G	210	TYR	CA-C-N	-6.57	118.14	122.60
1	G	210	TYR	C-N-CA	-6.57	118.14	122.60
1	A	347	ARG	NH1-CZ-NH2	6.56	127.82	119.30
1	A	350	ASN	CA-C-O	6.54	127.69	120.82
1	J	366	TYR	N-CA-C	6.54	118.07	111.07
1	G	172	GLU	N-CA-C	6.50	119.20	111.33
1	B	68	ARG	NE-CZ-NH2	6.45	125.01	119.20
1	A	191	ILE	N-CA-C	6.43	117.11	110.36
1	G	82	THR	CA-C-N	-6.40	111.90	120.79
1	G	82	THR	C-N-CA	-6.40	111.90	120.79
1	G	86	TYR	N-CA-C	-6.37	104.26	111.07
1	J	371	LEU	N-CA-C	-6.33	104.46	111.36
1	B	369	ARG	N-CA-C	-6.30	105.08	112.89
1	D	209	CYS	N-CA-CB	-6.19	100.34	110.43
1	E	156	LEU	N-CA-C	6.16	118.50	111.11
1	J	139	THR	N-CA-C	-6.15	104.49	111.07
1	B	285	ARG	N-CA-C	6.08	117.58	111.07
1	A	160	GLU	N-CA-C	6.04	117.53	111.07
1	J	347	ARG	O-C-N	6.04	128.53	122.12
1	G	195	TYR	CA-C-N	-6.02	112.21	120.28
1	G	195	TYR	C-N-CA	-6.02	112.21	120.28
1	E	193	THR	N-CA-C	-6.02	104.63	111.07
1	G	171	ARG	CA-C-N	-5.97	112.20	120.38
1	G	171	ARG	C-N-CA	-5.97	112.20	120.38
1	A	277	ARG	N-CA-C	-5.96	104.90	111.82
1	A	269	TYR	N-CA-C	5.93	117.28	107.73
1	B	118	ALA	N-CA-C	-5.93	104.89	111.36
1	C	365	GLN	N-CA-C	-5.93	103.99	111.11
1	B	259	VAL	CB-CA-C	-5.93	105.07	110.88
1	G	174	ALA	N-CA-C	-5.92	104.96	111.82
1	I	209	CYS	N-CA-CB	-5.88	100.83	110.42
1	B	364	GLN	CA-C-O	-5.88	114.65	120.70
1	J	138	ILE	CB-CG1-CD1	-5.87	101.47	113.80
1	A	198	VAL	N-CA-CB	5.86	119.37	110.58
1	D	68	ARG	NE-CZ-NH2	5.83	124.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	CYS	N-CA-CB	-5.82	100.56	110.16
1	C	206	ILE	N-CA-C	5.82	116.25	108.11
1	A	363	ALA	N-CA-C	-5.81	104.91	112.23
1	J	371	LEU	CA-C-N	5.80	126.53	120.03
1	J	371	LEU	C-N-CA	5.80	126.53	120.03
1	E	68	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	D	259	VAL	CB-CA-C	-5.77	100.87	111.36
1	E	35	ILE	N-CA-C	5.76	116.40	107.99
1	A	182	ARG	N-CA-C	-5.76	105.00	111.28
1	D	55	ARG	N-CA-C	-5.74	108.08	114.62
1	C	196	THR	N-CA-C	-5.73	104.95	111.14
1	C	68	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	A	347	ARG	CA-C-O	5.63	126.73	120.82
1	A	314	ASP	N-CA-C	5.61	117.14	110.19
1	D	109	ASP	N-CA-CB	-5.58	101.05	110.49
1	I	298	ARG	N-CA-C	-5.58	104.84	111.03
1	H	209	CYS	N-CA-CB	-5.57	101.34	110.43
1	A	209	CYS	CB-CA-C	-5.57	101.17	110.19
1	G	209	CYS	N-CA-CB	-5.54	101.87	110.57
1	I	303	THR	CA-C-O	5.51	126.16	119.49
1	G	141	MET	CA-C-N	-5.44	117.39	123.16
1	G	141	MET	C-N-CA	-5.44	117.39	123.16
1	A	343	LEU	O-C-N	5.44	127.69	122.03
1	G	186	ARG	CA-C-N	5.43	128.57	120.31
1	G	186	ARG	C-N-CA	5.43	128.57	120.31
1	H	227	ARG	N-CA-C	5.42	117.00	111.14
1	D	194	LEU	N-CA-C	5.40	116.84	111.07
1	J	347	ARG	CA-C-N	-5.39	113.66	120.56
1	J	347	ARG	C-N-CA	-5.39	113.66	120.56
1	A	347	ARG	N-CA-C	-5.37	105.32	111.07
1	I	138	ILE	N-CA-C	-5.37	105.14	111.00
1	A	211	ILE	N-CA-C	5.37	112.86	107.55
1	D	209	CYS	CB-CA-C	-5.37	100.90	109.75
1	J	346	THR	CA-C-N	5.36	127.46	120.28
1	J	346	THR	C-N-CA	5.36	127.46	120.28
1	J	341	PHE	CA-C-N	-5.34	112.81	120.82
1	J	341	PHE	C-N-CA	-5.34	112.81	120.82
1	J	369	ARG	CA-C-O	-5.34	114.86	120.63
1	A	198	VAL	N-CA-C	5.32	116.09	110.72
1	J	348	VAL	O-C-N	5.31	127.42	121.90
1	C	142	ILE	N-CA-C	5.31	115.81	111.62
1	A	380	LEU	N-CA-CB	5.30	118.50	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	364	GLN	CA-C-O	-5.30	115.25	120.82
1	J	231	VAL	N-CA-CB	5.30	117.75	110.54
1	J	369	ARG	O-C-N	5.29	127.73	122.12
1	J	142	ILE	N-CA-C	5.29	116.11	111.56
1	B	35	ILE	CG1-CB-CG2	-5.27	94.90	110.70
1	J	367	LEU	CA-C-O	5.26	126.85	121.07
1	J	209	CYS	N-CA-CB	-5.24	101.89	110.43
1	E	206	ILE	N-CA-C	5.23	115.43	108.11
1	F	209	CYS	N-CA-CB	-5.21	101.93	110.42
1	F	59	THR	CB-CA-C	5.18	116.41	109.42
1	A	267	VAL	O-C-N	5.18	128.78	123.03
1	A	333	ASP	CA-C-O	5.17	123.15	119.32
1	A	302	ARG	N-CA-C	5.17	116.91	111.28
1	E	209	CYS	N-CA-CB	-5.16	101.49	110.17
1	A	265	GLU	CA-C-N	-5.16	114.49	122.59
1	A	265	GLU	C-N-CA	-5.16	114.49	122.59
1	J	138	ILE	CA-C-O	5.16	126.04	120.47
1	D	269	TYR	N-CA-C	5.15	115.97	108.14
1	B	225	ASP	CB-CA-C	5.15	119.53	110.37
1	B	365	GLN	N-CA-C	-5.14	104.94	111.11
1	C	364	GLN	CA-C-O	-5.13	115.42	120.70
1	C	183	VAL	N-CA-CB	5.13	117.90	110.52
1	G	192	ASP	O-C-N	5.12	128.21	122.22
1	B	182	ARG	CB-CG-CD	-5.09	99.58	111.30
1	H	210	TYR	CA-C-N	-5.09	117.05	122.85
1	H	210	TYR	C-N-CA	-5.09	117.05	122.85
1	J	206	ILE	N-CA-C	5.08	115.22	108.11
1	E	77	GLY	N-CA-C	-5.07	106.62	112.50
1	A	266	ARG	CA-C-N	-5.06	116.56	122.93
1	A	266	ARG	C-N-CA	-5.06	116.56	122.93
1	A	67	GLU	CA-C-N	-5.04	115.72	122.42
1	A	67	GLU	C-N-CA	-5.04	115.72	122.42
1	F	380	LEU	N-CA-C	5.03	117.49	111.71
1	H	283	THR	CA-C-N	-5.03	113.47	119.05
1	H	283	THR	C-N-CA	-5.03	113.47	119.05
1	E	380	LEU	N-CA-C	5.02	116.83	111.36
1	B	321	THR	N-CA-C	-5.01	105.90	111.36
1	B	209	CYS	CB-CA-C	-5.01	101.59	109.80
1	F	142	ILE	N-CA-C	5.00	115.57	111.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	245	VAL	CA

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PRO	Peptide
1	A	247	GLN	Peptide
1	B	108	PRO	Peptide
1	B	246	GLY	Peptide
1	B	247	GLN	Peptide
1	C	108	PRO	Peptide
1	C	244	VAL	Peptide
1	C	246	GLY	Peptide
1	C	247	GLN	Peptide
1	C	248	PRO	Peptide
1	C	249	ALA	Peptide
1	D	108	PRO	Peptide
1	D	247	GLN	Peptide
1	D	248	PRO	Peptide
1	E	108	PRO	Peptide
1	E	245	VAL	Peptide
1	E	246	GLY	Peptide
1	E	247	GLN	Peptide
1	F	108	PRO	Peptide
1	F	245	VAL	Peptide
1	F	247	GLN	Peptide
1	F	248	PRO	Peptide
1	G	108	PRO	Peptide
1	G	246	GLY	Peptide
1	G	247	GLN	Peptide
1	G	248	PRO	Peptide
1	H	108	PRO	Peptide
1	H	248	PRO	Peptide
1	H	249	ALA	Peptide
1	H	250	ILE	Peptide
1	I	108	PRO	Peptide
1	I	246	GLY	Peptide
1	I	247	GLN	Peptide
1	J	108	PRO	Peptide
1	J	246	GLY	Peptide
1	J	247	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3037	109	2
1	B	3138	0	3037	95	1
1	C	3138	0	3037	99	0
1	D	3138	0	3037	106	0
1	E	3138	0	3037	77	0
1	F	3138	0	3037	84	0
1	G	3138	0	3037	111	1
1	H	3138	0	3037	81	0
1	I	3138	0	3037	86	0
1	J	3138	0	3036	104	0
2	A	39	0	20	4	0
2	B	39	0	20	4	0
2	C	39	0	20	3	0
2	D	39	0	20	4	0
2	E	39	0	20	3	0
2	F	39	0	20	3	0
2	G	39	0	20	3	0
2	H	39	0	20	3	0
2	I	39	0	20	3	0
2	J	39	0	20	3	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	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	1	0	0	1	0
4	G	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	1	0
4	I	1	0	0	1	0
4	J	1	0	0	1	0
5	A	78	0	0	17	0
5	B	80	0	0	12	0
5	C	38	0	0	12	0
5	D	27	0	0	3	0
5	E	34	0	0	6	0
5	F	3	0	0	1	0
5	G	23	0	0	9	0
5	H	6	0	0	2	0
5	I	13	0	0	6	0
5	J	6	0	0	0	0
All	All	32098	0	30569	928	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (928) 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:C:365:GLN:CG	1:C:365:GLN:CB	1.76	1.61
1:B:365:GLN:CB	1:B:365:GLN:CG	1.75	1.55
1:B:316:MET:CG	1:B:316:MET:SD	2.03	1.46
1:J:247:GLN:CB	1:J:248:PRO:HD3	1.43	1.44
1:A:365:GLN:CG	1:A:365:GLN:CB	1.91	1.44
1:G:169:MET:CG	1:G:169:MET:SD	2.06	1.42
1:B:247:GLN:HB2	1:B:248:PRO:CD	1.54	1.31
1:F:247:GLN:CG	1:F:248:PRO:HD3	1.62	1.28
1:F:247:GLN:HG2	1:F:248:PRO:CD	1.62	1.27
1:B:247:GLN:HB2	1:B:248:PRO:CG	1.66	1.25
1:J:247:GLN:CG	1:J:248:PRO:HG3	1.68	1.23
1:D:50:ALA:HB3	1:D:51:PRO:CD	1.67	1.22
1:G:178:TYR:CE2	1:G:184:ARG:NH2	2.08	1.21
1:C:365:GLN:HB3	5:C:2032:HOH:O	1.41	1.19
1:E:247:GLN:HB2	1:E:248:PRO:HD2	1.20	1.17
1:J:285:ARG:HG2	1:J:285:ARG:HH11	1.04	1.16
1:I:201:GLN:HE21	1:I:245:VAL:HG11	1.07	1.15
1:I:365:GLN:HB3	5:I:2009:HOH:O	1.46	1.15
1:J:247:GLN:CG	1:J:248:PRO:HD3	1.75	1.14
1:E:247:GLN:HB2	1:E:248:PRO:CD	1.77	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:SER:HA	1:H:250:ILE:CG2	1.80	1.10
1:I:201:GLN:HE21	1:I:245:VAL:CG1	1.63	1.10
1:B:185:ARG:HD3	5:B:2035:HOH:O	1.51	1.10
1:C:244:VAL:HG12	1:C:245:VAL:H	1.11	1.10
1:J:247:GLN:CG	1:J:248:PRO:CD	2.30	1.10
1:J:247:GLN:CB	1:J:248:PRO:CD	2.31	1.09
1:C:109:ASP:HB2	5:C:2008:HOH:O	1.51	1.08
1:J:247:GLN:CG	1:J:248:PRO:CG	2.30	1.08
1:J:247:GLN:HG2	1:J:248:PRO:HG3	1.30	1.08
1:J:247:GLN:HG2	1:J:248:PRO:CG	1.84	1.08
1:D:50:ALA:HB3	1:D:51:PRO:HD3	1.30	1.06
1:I:283:THR:HG22	1:I:286:GLN:H	1.20	1.05
1:J:283:THR:HG21	1:J:335:ASP:OD2	1.55	1.03
1:F:283:THR:HG22	1:F:286:GLN:H	1.23	1.03
1:B:247:GLN:HB2	1:B:248:PRO:HD3	1.31	1.03
1:A:218:ARG:HB3	5:A:2077:HOH:O	1.55	1.02
1:E:283:THR:HG22	1:E:286:GLN:H	1.24	1.02
1:I:201:GLN:NE2	1:I:245:VAL:HG11	1.73	1.02
1:I:246:GLY:C	1:I:247:GLN:HG3	1.86	1.00
1:J:247:GLN:HG3	1:J:248:PRO:HG3	1.41	0.99
1:J:247:GLN:HB3	1:J:248:PRO:HD3	1.01	0.99
1:G:178:TYR:CD2	1:G:184:ARG:NH2	2.29	0.99
1:F:247:GLN:HG2	1:F:248:PRO:HD2	1.43	0.99
1:F:247:GLN:CG	1:F:248:PRO:CD	2.30	0.99
1:G:66:GLN:HE22	2:G:400:GDX:HN1	1.08	0.99
1:A:283:THR:HG22	1:A:286:GLN:H	1.29	0.98
1:H:66:GLN:HE22	2:H:400:GDX:HN1	1.09	0.98
1:G:283:THR:HG22	1:G:286:GLN:H	1.29	0.98
1:C:283:THR:HG22	1:C:286:GLN:H	1.27	0.98
1:D:283:THR:HG22	1:D:286:GLN:H	1.27	0.98
1:J:247:GLN:HB3	1:J:248:PRO:CD	1.93	0.97
1:D:52:GLU:C	1:D:52:GLU:CD	2.33	0.97
1:H:283:THR:HG22	1:H:286:GLN:H	1.28	0.97
1:B:247:GLN:CB	1:B:248:PRO:CD	2.43	0.97
1:I:259:VAL:HG21	1:I:360:TYR:CE1	2.00	0.97
1:D:50:ALA:CB	1:D:51:PRO:CD	2.37	0.96
1:E:109:ASP:HB3	1:E:110:TRP:HD1	1.30	0.96
1:F:66:GLN:HE22	2:F:400:GDX:HN1	1.07	0.96
1:C:250:ILE:HG22	1:C:250:ILE:O	1.63	0.96
1:B:283:THR:HG22	1:B:286:GLN:H	1.32	0.95
1:I:66:GLN:HE22	2:I:400:GDX:HN1	1.08	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:GLN:HG3	1:I:245:VAL:HG11	1.47	0.95
1:C:66:GLN:HE22	2:C:400:GDX:HN1	1.15	0.94
1:E:66:GLN:HE22	2:E:400:GDX:HN1	1.04	0.94
1:J:285:ARG:HG2	1:J:285:ARG:NH1	1.79	0.94
1:I:246:GLY:O	1:I:247:GLN:HG3	1.68	0.93
1:D:66:GLN:HE22	2:D:400:GDX:HN1	1.10	0.93
1:C:247:GLN:HB3	1:C:248:PRO:O	1.68	0.93
1:G:328:HIS:HD2	5:G:2019:HOH:O	1.52	0.93
1:F:247:GLN:CB	1:F:248:PRO:CD	2.46	0.93
1:J:283:THR:HG22	1:J:283:THR:O	1.67	0.92
1:H:205:SER:HA	1:H:250:ILE:HG23	1.52	0.92
1:H:259:VAL:HG21	1:H:360:TYR:CE1	2.05	0.92
1:D:52:GLU:O	1:D:55:ARG:HG2	1.69	0.92
1:D:50:ALA:HB3	1:D:51:PRO:HD2	1.49	0.92
1:J:286:GLN:O	1:J:288:GLU:N	2.01	0.92
1:A:66:GLN:HE22	2:A:400:GDX:HN1	1.18	0.92
1:G:178:TYR:HE2	1:G:184:ARG:NH2	1.66	0.92
1:J:286:GLN:O	1:J:289:LEU:N	2.04	0.90
1:F:245:VAL:O	1:F:245:VAL:HG12	1.69	0.90
1:G:259:VAL:HG21	1:G:360:TYR:CE1	2.07	0.90
1:B:247:GLN:HB3	1:B:248:PRO:HB3	1.51	0.90
1:J:259:VAL:HG21	1:J:360:TYR:CE1	2.06	0.90
1:B:365:GLN:HB3	5:B:2073:HOH:O	1.72	0.89
1:F:247:GLN:CB	1:F:248:PRO:HD3	1.89	0.89
1:B:59:THR:HG21	5:B:2001:HOH:O	1.71	0.89
1:B:247:GLN:CB	1:B:248:PRO:HB3	2.03	0.89
1:J:247:GLN:HG3	1:J:248:PRO:CG	1.99	0.89
1:B:247:GLN:CB	1:B:248:PRO:HD3	2.00	0.89
1:H:205:SER:CA	1:H:250:ILE:CG2	2.50	0.89
1:H:250:ILE:HG23	1:H:250:ILE:O	1.72	0.89
1:B:66:GLN:HE22	2:B:400:GDX:HN1	1.16	0.88
1:J:66:GLN:HE22	2:J:400:GDX:HN1	1.18	0.88
1:F:259:VAL:HG21	1:F:360:TYR:CE1	2.08	0.88
1:D:369:ARG:HD3	5:D:2025:HOH:O	1.73	0.88
1:H:205:SER:CB	1:H:250:ILE:CG2	2.52	0.87
1:C:109:ASP:HB3	1:C:110:TRP:HD1	1.37	0.87
1:G:109:ASP:HB3	1:G:110:TRP:HD1	1.37	0.87
1:I:59:THR:HG21	5:I:2002:HOH:O	1.74	0.87
1:E:247:GLN:CB	1:E:248:PRO:CD	2.45	0.86
1:A:41:GLN:HE21	1:A:41:GLN:HA	1.40	0.86
1:B:247:GLN:HB2	1:B:248:PRO:CB	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ASP:HB3	1:H:110:TRP:HD1	1.40	0.85
1:A:373:ARG:HD2	5:A:2074:HOH:O	1.74	0.85
1:I:109:ASP:HB3	1:I:110:TRP:HD1	1.40	0.85
1:C:244:VAL:CG1	1:C:245:VAL:H	1.90	0.84
1:C:259:VAL:HG21	1:C:360:TYR:CE1	2.11	0.84
1:C:205:SER:HB2	1:C:250:ILE:HG21	1.57	0.84
1:A:369:ARG:HD2	5:A:2072:HOH:O	1.77	0.84
1:J:247:GLN:HG2	1:J:248:PRO:CD	2.06	0.83
1:I:246:GLY:C	1:I:247:GLN:CG	2.44	0.83
1:C:59:THR:HG21	5:C:2004:HOH:O	1.78	0.83
1:G:176:MET:SD	1:G:202:GLN:HG3	2.17	0.83
1:D:369:ARG:CD	5:D:2025:HOH:O	2.24	0.83
1:A:179:GLU:HG3	5:A:2033:HOH:O	1.79	0.83
1:B:247:GLN:CB	1:B:248:PRO:CB	2.56	0.83
1:C:244:VAL:HG12	1:C:245:VAL:N	1.86	0.83
1:J:109:ASP:HB3	1:J:110:TRP:HD1	1.42	0.83
1:F:66:GLN:NE2	2:F:400:GDX:HN1	1.76	0.82
1:B:284:PRO:HB3	1:F:288:GLU:HG3	1.60	0.82
1:F:109:ASP:HB3	1:F:110:TRP:HD1	1.43	0.82
1:B:259:VAL:HG21	1:B:360:TYR:CZ	2.15	0.82
1:C:123:GLY:HA2	1:C:170:ARG:HD3	1.61	0.81
1:C:283:THR:HG21	1:C:335:ASP:OD2	1.81	0.81
1:I:66:GLN:NE2	2:I:400:GDX:HN1	1.77	0.81
1:D:109:ASP:HB3	1:D:110:TRP:HD1	1.45	0.81
1:G:178:TYR:CD2	1:G:178:TYR:O	2.33	0.81
1:C:205:SER:HB2	1:C:250:ILE:CG2	2.11	0.81
1:G:365:GLN:HG3	1:G:366:TYR:N	1.95	0.81
1:H:205:SER:CB	1:H:250:ILE:HG21	2.10	0.81
1:G:178:TYR:HD2	1:G:184:ARG:HH21	1.29	0.81
1:J:259:VAL:HG21	1:J:360:TYR:CZ	2.17	0.80
1:G:59:THR:HG21	5:G:2003:HOH:O	1.78	0.80
1:B:109:ASP:HB3	1:B:110:TRP:HD1	1.44	0.80
1:H:205:SER:HB3	1:H:250:ILE:HG21	1.63	0.80
1:J:283:THR:O	1:J:283:THR:CG2	2.30	0.79
1:A:109:ASP:HB3	1:A:110:TRP:HD1	1.48	0.79
1:B:247:GLN:CB	1:B:248:PRO:CG	2.56	0.79
1:I:246:GLY:O	1:I:247:GLN:CG	2.30	0.79
1:I:259:VAL:HG21	1:I:360:TYR:CZ	2.17	0.79
1:H:283:THR:HG21	1:H:335:ASP:OD2	1.82	0.79
1:D:66:GLN:NE2	2:D:400:GDX:HN1	1.80	0.79
1:F:247:GLN:HG2	1:F:248:PRO:HD3	1.26	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:THR:CG2	5:I:2002:HOH:O	2.29	0.79
1:A:10:HIS:HA	5:A:2002:HOH:O	1.83	0.79
1:B:283:THR:HG21	1:B:335:ASP:OD2	1.83	0.78
1:C:250:ILE:O	1:C:250:ILE:CG2	2.30	0.78
1:I:201:GLN:CG	1:I:245:VAL:HG11	2.14	0.78
1:G:180:ASP:HB3	1:G:183:VAL:HG13	1.65	0.78
1:C:249:ALA:HB1	5:C:2018:HOH:O	1.81	0.78
1:E:66:GLN:NE2	2:E:400:GDX:HN1	1.81	0.78
1:B:142:ILE:CD1	1:B:230:LEU:CD1	2.62	0.78
1:C:41:GLN:HE21	1:C:41:GLN:HA	1.49	0.77
1:D:259:VAL:HG21	1:D:360:TYR:CE1	2.18	0.77
1:H:205:SER:HA	1:H:250:ILE:HG22	1.64	0.77
1:E:123:GLY:HA2	1:E:170:ARG:HD3	1.66	0.77
1:E:259:VAL:HG21	1:E:360:TYR:CE1	2.19	0.77
1:G:66:GLN:NE2	2:G:400:GDX:HN1	1.82	0.77
1:H:66:GLN:NE2	2:H:400:GDX:HN1	1.82	0.77
1:G:178:TYR:CE2	1:G:184:ARG:CZ	2.68	0.76
1:C:66:GLN:NE2	2:C:400:GDX:HN1	1.81	0.76
1:H:205:SER:CA	1:H:250:ILE:HG23	2.15	0.76
1:I:357:LEU:HD13	1:J:357:LEU:HD13	1.68	0.76
1:D:52:GLU:C	1:D:52:GLU:OE2	2.30	0.75
1:J:66:GLN:NE2	2:J:400:GDX:HN1	1.84	0.75
1:B:247:GLN:HB2	1:B:248:PRO:HG3	1.66	0.75
1:B:259:VAL:HG21	1:B:360:TYR:CE1	2.22	0.75
1:A:52:GLU:C	1:A:52:GLU:OE2	2.30	0.74
1:H:205:SER:CB	1:H:250:ILE:HG23	2.17	0.74
1:I:142:ILE:CD1	1:I:230:LEU:HD11	2.16	0.74
1:I:246:GLY:O	1:I:247:GLN:CD	2.30	0.74
1:F:283:THR:HG21	1:F:335:ASP:OD2	1.88	0.74
1:A:66:GLN:NE2	2:A:400:GDX:HN1	1.83	0.74
1:G:41:GLN:HA	1:G:41:GLN:HE21	1.53	0.74
1:G:180:ASP:OD1	1:G:182:ARG:HB2	1.88	0.74
1:H:123:GLY:HA2	1:H:170:ARG:HD3	1.69	0.74
1:A:283:THR:HG21	1:A:335:ASP:OD2	1.88	0.74
1:G:283:THR:HG21	1:G:335:ASP:OD2	1.87	0.74
1:H:259:VAL:HG21	1:H:360:TYR:CZ	2.22	0.74
1:C:205:SER:CB	1:C:250:ILE:HG21	2.19	0.73
1:J:123:GLY:HA2	1:J:170:ARG:HD3	1.70	0.73
1:E:41:GLN:HE21	1:E:41:GLN:HA	1.54	0.73
1:F:180:ASP:HB3	1:F:183:VAL:HG13	1.70	0.73
1:A:267:VAL:HB	5:A:2053:HOH:O	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:LEU:HD13	1:F:357:LEU:HD13	1.70	0.73
1:A:259:VAL:HG21	1:A:360:TYR:CE1	2.23	0.73
1:B:66:GLN:NE2	2:B:400:GDX:HN1	1.86	0.73
1:D:52:GLU:CD	1:D:52:GLU:O	2.31	0.73
1:D:283:THR:HG21	1:D:335:ASP:OD2	1.88	0.73
1:B:123:GLY:HA2	1:B:170:ARG:HD3	1.71	0.72
1:J:286:GLN:O	1:J:287:VAL:C	2.32	0.72
1:E:109:ASP:HB3	1:E:110:TRP:CD1	2.21	0.72
1:F:246:GLY:HA2	1:F:247:GLN:CB	2.20	0.72
1:F:259:VAL:HG21	1:F:360:TYR:CZ	2.24	0.72
1:H:203:GLY:HA2	1:H:249:ALA:HB2	1.71	0.72
1:H:250:ILE:CD1	1:H:250:ILE:C	2.62	0.72
1:I:201:GLN:HG3	1:I:245:VAL:CG1	2.17	0.72
1:F:123:GLY:HA2	1:F:170:ARG:HD3	1.72	0.72
1:A:357:LEU:HD13	1:B:357:LEU:HD13	1.71	0.71
1:J:41:GLN:HE21	1:J:41:GLN:HA	1.55	0.71
1:C:52:GLU:OE1	1:C:55:ARG:NH1	2.23	0.71
1:G:177:LEU:HD23	1:G:198:VAL:HG22	1.71	0.71
1:G:85:ARG:HB2	1:G:178:TYR:HE1	1.56	0.71
1:E:365:GLN:HG3	1:E:366:TYR:N	2.04	0.71
1:B:41:GLN:HE21	1:B:41:GLN:HA	1.55	0.71
1:C:244:VAL:CG1	1:C:245:VAL:N	2.52	0.71
1:F:41:GLN:HE21	1:F:41:GLN:HA	1.55	0.71
1:B:262:HIS:HE1	5:B:2044:HOH:O	1.74	0.70
1:G:178:TYR:O	1:G:178:TYR:HD2	1.72	0.70
1:I:283:THR:HB	1:I:286:GLN:NE2	2.07	0.70
1:C:142:ILE:CD1	1:C:230:LEU:CD1	2.69	0.70
1:G:123:GLY:HA2	1:G:170:ARG:HD3	1.72	0.70
1:G:315:GLU:HB2	5:G:2018:HOH:O	1.90	0.70
1:D:50:ALA:CB	1:D:51:PRO:HD3	2.11	0.70
1:H:250:ILE:C	1:H:250:ILE:HD13	2.15	0.70
1:B:142:ILE:CD1	1:B:230:LEU:HD11	2.22	0.69
1:C:142:ILE:CD1	1:C:230:LEU:HD11	2.22	0.69
1:C:259:VAL:HG21	1:C:360:TYR:CZ	2.27	0.69
1:E:218:ARG:HG2	1:E:218:ARG:HH11	1.57	0.69
1:A:252:ARG:NH1	1:D:155:GLU:OE1	2.26	0.69
1:I:365:GLN:HG3	1:I:366:TYR:N	2.06	0.69
1:I:123:GLY:HA2	1:I:170:ARG:HD3	1.75	0.69
1:A:68:ARG:HD3	5:E:2010:HOH:O	1.93	0.68
1:A:180:ASP:HB3	1:A:183:VAL:HG13	1.76	0.68
1:D:53:ILE:C	1:D:55:ARG:H	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:VAL:HG12	1:E:246:GLY:N	2.09	0.68
1:H:52:GLU:OE1	1:H:55:ARG:NH1	2.27	0.68
1:G:142:ILE:CD1	1:G:230:LEU:HD11	2.24	0.68
1:H:41:GLN:HA	1:H:41:GLN:HE21	1.58	0.68
1:I:41:GLN:HE21	1:I:41:GLN:HA	1.58	0.68
1:I:283:THR:HG21	1:I:335:ASP:OD2	1.94	0.68
1:H:250:ILE:CG2	1:H:250:ILE:O	2.42	0.68
1:D:123:GLY:HA2	1:D:170:ARG:HD3	1.76	0.68
1:D:182:ARG:NH2	1:D:201:GLN:OE1	2.25	0.68
1:J:182:ARG:NH2	1:J:201:GLN:OE1	2.26	0.68
1:A:262:HIS:HE1	5:A:2039:HOH:O	1.77	0.68
1:B:52:GLU:OE1	1:B:55:ARG:NH1	2.27	0.68
1:F:283:THR:HB	1:F:286:GLN:NE2	2.09	0.67
1:E:136:ALA:HA	4:E:1382:CL:CL	2.31	0.67
1:E:283:THR:HG21	1:E:335:ASP:OD2	1.94	0.67
1:I:142:ILE:CD1	1:I:230:LEU:CD1	2.73	0.67
1:J:180:ASP:HB3	1:J:183:VAL:HG13	1.76	0.67
1:D:180:ASP:HB3	1:D:183:VAL:HG13	1.77	0.66
1:F:245:VAL:O	1:F:245:VAL:CG1	2.43	0.66
1:C:109:ASP:CB	5:C:2008:HOH:O	2.24	0.66
1:D:50:ALA:CB	1:D:51:PRO:HD2	2.15	0.66
1:J:246:GLY:H	1:J:247:GLN:HB2	1.60	0.66
1:D:49:ALA:O	1:D:50:ALA:O	2.12	0.66
1:A:142:ILE:CD1	1:A:230:LEU:HD11	2.25	0.66
1:E:182:ARG:NH2	1:E:201:GLN:OE1	2.29	0.66
1:J:285:ARG:NH1	1:J:335:ASP:OD1	2.29	0.66
1:E:218:ARG:HH11	1:E:218:ARG:CG	2.08	0.65
1:B:10:HIS:HE1	1:B:38:GLU:OE2	1.79	0.65
1:A:52:GLU:OE1	1:A:55:ARG:NH1	2.30	0.65
1:C:59:THR:CG2	5:C:2004:HOH:O	2.39	0.65
1:E:180:ASP:HB3	1:E:183:VAL:HG13	1.79	0.65
1:E:259:VAL:HG21	1:E:360:TYR:CZ	2.31	0.65
1:G:52:GLU:OE1	1:G:55:ARG:NH1	2.29	0.65
1:I:52:GLU:OE1	1:I:55:ARG:NH1	2.30	0.65
1:J:283:THR:O	1:J:285:ARG:N	2.30	0.65
1:A:52:GLU:OE2	1:A:53:ILE:N	2.30	0.65
1:D:50:ALA:O	1:D:52:GLU:N	2.30	0.65
1:A:259:VAL:HG21	1:A:360:TYR:CZ	2.32	0.64
1:G:177:LEU:O	1:G:179:GLU:N	2.30	0.64
1:A:142:ILE:CD1	1:A:230:LEU:CD1	2.76	0.64
1:F:244:VAL:HG12	1:F:245:VAL:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:O	1:A:360:TYR:HE2	1.80	0.64
1:C:109:ASP:CG	5:C:2008:HOH:O	2.38	0.64
1:H:205:SER:HB2	1:H:250:ILE:HG23	1.77	0.64
1:F:201:GLN:HG3	1:F:245:VAL:HG22	1.79	0.64
1:G:142:ILE:CD1	1:G:230:LEU:CD1	2.74	0.64
1:J:247:GLN:HG3	1:J:248:PRO:CD	2.24	0.64
1:A:168:LEU:HD23	1:A:168:LEU:C	2.23	0.64
1:G:247:GLN:O	1:G:248:PRO:C	2.41	0.64
1:E:247:GLN:CB	1:E:248:PRO:HD3	2.27	0.64
1:J:52:GLU:OE1	1:J:55:ARG:NH1	2.30	0.64
1:G:109:ASP:HB3	1:G:110:TRP:CD1	2.28	0.64
1:I:364:GLN:HB3	5:I:2010:HOH:O	1.98	0.64
1:C:357:LEU:HD13	1:D:357:LEU:HD13	1.78	0.63
1:G:177:LEU:C	1:G:179:GLU:H	2.06	0.63
1:I:247:GLN:N	1:I:247:GLN:OE1	2.30	0.63
1:B:266:ARG:NH1	5:B:2056:HOH:O	2.32	0.63
1:A:381:GLU:HG2	1:A:382:ASN:N	2.12	0.63
1:J:285:ARG:HH11	1:J:285:ARG:CG	1.92	0.63
1:H:180:ASP:HB3	1:H:183:VAL:HG13	1.78	0.63
1:G:259:VAL:HG21	1:G:360:TYR:CZ	2.32	0.63
1:C:259:VAL:CG2	1:C:360:TYR:CE1	2.81	0.63
1:I:201:GLN:CD	1:I:245:VAL:HG11	2.23	0.63
1:G:180:ASP:CG	1:G:182:ARG:HH11	2.07	0.63
1:G:191:ILE:HG23	1:G:192:ASP:N	2.14	0.63
1:C:109:ASP:HB3	1:C:110:TRP:CD1	2.28	0.63
1:D:41:GLN:HE21	1:D:41:GLN:HA	1.63	0.63
1:E:48:ARG:HD3	5:E:2006:HOH:O	1.98	0.63
1:E:380:LEU:HD23	5:E:2033:HOH:O	1.98	0.63
1:A:123:GLY:HA2	1:A:170:ARG:HD3	1.79	0.62
1:C:249:ALA:HB1	1:C:250:ILE:HB	1.82	0.62
1:H:142:ILE:CD1	1:H:230:LEU:CD1	2.76	0.62
1:F:365:GLN:HG3	1:F:366:TYR:N	2.14	0.62
1:H:142:ILE:CD1	1:H:230:LEU:HD11	2.30	0.62
1:A:142:ILE:HD13	1:A:230:LEU:HD12	1.81	0.62
1:G:169:MET:SD	1:G:169:MET:CB	2.87	0.62
1:E:247:GLN:CB	1:E:248:PRO:HD2	2.11	0.62
1:B:168:LEU:C	1:B:168:LEU:HD23	2.25	0.62
1:B:181:GLU:OE1	1:B:185:ARG:NH2	2.33	0.62
1:F:142:ILE:CD1	1:F:230:LEU:CD1	2.77	0.62
1:H:365:GLN:HG3	1:H:366:TYR:N	2.14	0.62
1:B:365:GLN:NE2	5:B:2075:HOH:O	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:THR:HB	1:C:286:GLN:NE2	2.15	0.61
1:J:285:ARG:NH1	1:J:285:ARG:CG	2.57	0.61
1:D:52:GLU:OE2	1:D:53:ILE:N	2.33	0.61
1:D:50:ALA:O	1:D:51:PRO:C	2.43	0.61
1:D:110:TRP:H	1:D:110:TRP:CD1	2.16	0.61
1:C:180:ASP:HB3	1:C:183:VAL:HG13	1.82	0.61
1:D:369:ARG:HD2	5:D:2025:HOH:O	1.95	0.61
1:I:168:LEU:C	1:I:168:LEU:HD23	2.25	0.61
1:B:283:THR:CG2	1:B:286:GLN:H	2.10	0.61
1:F:52:GLU:OE1	1:F:55:ARG:NH1	2.33	0.61
1:I:259:VAL:CG2	1:I:360:TYR:CE1	2.81	0.61
1:E:52:GLU:OE1	1:E:55:ARG:NH1	2.35	0.60
1:G:304:CYS:HA	1:G:307:ARG:O	2.00	0.60
1:J:247:GLN:HG2	1:J:248:PRO:HD3	1.65	0.60
1:H:168:LEU:HD23	1:H:168:LEU:C	2.27	0.60
1:D:246:GLY:O	1:D:247:GLN:HG2	2.01	0.60
1:A:270:ASP:OD2	1:A:270:ASP:C	2.42	0.60
1:E:277:ARG:CZ	1:E:281:HIS:HD2	2.15	0.60
1:F:142:ILE:CD1	1:F:230:LEU:HD11	2.30	0.60
1:H:136:ALA:HA	4:H:1382:CL:CL	2.38	0.60
1:I:283:THR:HG22	1:I:286:GLN:N	2.05	0.60
1:C:205:SER:HA	1:C:250:ILE:HG22	1.83	0.60
1:D:142:ILE:CD1	1:D:230:LEU:CD1	2.79	0.60
1:D:53:ILE:O	1:D:55:ARG:N	2.32	0.60
1:J:285:ARG:HH12	1:J:335:ASP:HB2	1.66	0.60
1:J:136:ALA:HA	4:J:1382:CL:CL	2.39	0.60
1:J:142:ILE:CD1	1:J:230:LEU:CD1	2.80	0.60
1:D:55:ARG:HG3	1:D:56:ALA:N	2.16	0.59
1:F:283:THR:HG22	1:F:286:GLN:N	2.07	0.59
1:J:283:THR:HG22	1:J:286:GLN:H	1.66	0.59
1:C:365:GLN:HG3	1:C:366:TYR:N	2.17	0.59
1:D:283:THR:HB	1:D:286:GLN:NE2	2.17	0.59
1:B:131:ARG:CB	5:B:2023:HOH:O	2.51	0.59
1:G:283:THR:HB	1:G:286:GLN:NE2	2.18	0.59
1:B:142:ILE:HD11	1:B:230:LEU:HD11	1.85	0.59
1:D:10:HIS:HE1	1:D:38:GLU:OE2	1.86	0.59
1:F:246:GLY:HA2	1:F:247:GLN:CG	2.33	0.59
1:J:10:HIS:HE1	1:J:38:GLU:OE2	1.86	0.59
1:A:142:ILE:HD13	1:A:230:LEU:CD1	2.33	0.58
1:I:365:GLN:NE2	5:I:2011:HOH:O	2.35	0.58
1:H:10:HIS:HE1	1:H:38:GLU:OE2	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:VAL:HG12	1:E:246:GLY:H	1.68	0.58
1:E:180:ASP:OD2	1:E:182:ARG:NH1	2.36	0.58
1:F:109:ASP:HB3	1:F:110:TRP:CD1	2.33	0.58
1:J:201:GLN:HG3	1:J:245:VAL:HG13	1.84	0.58
5:A:2008:HOH:O	1:E:68:ARG:HD3	2.04	0.58
1:F:244:VAL:O	1:F:245:VAL:HG23	2.04	0.58
1:G:177:LEU:CD2	1:G:198:VAL:HG22	2.32	0.58
1:D:142:ILE:CD1	1:D:230:LEU:HD11	2.34	0.58
1:F:246:GLY:HA2	1:F:247:GLN:HG3	1.83	0.58
1:G:177:LEU:C	1:G:179:GLU:N	2.59	0.58
1:G:178:TYR:O	1:G:184:ARG:NH2	2.37	0.58
1:H:182:ARG:NH2	1:H:201:GLN:OE1	2.36	0.58
1:J:315:GLU:HG3	1:J:366:TYR:OH	2.04	0.57
1:D:259:VAL:HG21	1:D:360:TYR:CZ	2.37	0.57
1:D:180:ASP:OD2	1:D:182:ARG:NH1	2.37	0.57
1:H:283:THR:HB	1:H:286:GLN:NE2	2.19	0.57
1:J:365:GLN:HG3	1:J:366:TYR:N	2.19	0.57
1:I:182:ARG:NH2	1:I:201:GLN:OE1	2.34	0.57
1:I:180:ASP:HB3	1:I:183:VAL:HG13	1.85	0.57
1:A:258:ARG:HG3	1:D:361:ASP:OD1	2.05	0.57
1:C:245:VAL:HG13	1:C:245:VAL:O	2.05	0.57
1:F:10:HIS:HE1	1:F:38:GLU:OE2	1.87	0.57
1:D:290:LEU:HB3	1:D:298:ARG:HG3	1.86	0.57
1:G:169:MET:CG	1:G:169:MET:CE	2.83	0.57
1:A:52:GLU:CD	1:A:55:ARG:NH1	2.62	0.57
1:D:49:ALA:O	1:D:50:ALA:C	2.47	0.57
1:G:97:HIS:CE1	1:G:168:LEU:HD12	2.39	0.57
1:G:247:GLN:O	1:G:247:GLN:HG2	2.05	0.57
1:B:131:ARG:HB2	5:B:2023:HOH:O	2.05	0.57
1:A:373:ARG:CD	5:A:2074:HOH:O	2.43	0.56
1:B:288:GLU:O	1:B:291:GLU:HB2	2.05	0.56
1:F:182:ARG:NH2	1:F:201:GLN:OE1	2.38	0.56
1:B:177:LEU:HD23	1:B:198:VAL:HG22	1.86	0.56
1:A:182:ARG:NH2	1:A:201:GLN:OE1	2.36	0.56
1:B:180:ASP:HB3	1:B:183:VAL:HG13	1.87	0.56
1:C:365:GLN:NE2	5:C:2034:HOH:O	2.38	0.56
1:G:365:GLN:HG3	1:G:366:TYR:H	1.69	0.56
1:J:142:ILE:HD13	1:J:230:LEU:HD12	1.88	0.56
1:E:203:GLY:CA	1:E:249:ALA:HB2	2.35	0.56
1:H:109:ASP:HB3	1:H:110:TRP:CD1	2.30	0.56
1:D:257:HIS:N	1:D:257:HIS:CD2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:VAL:CG2	1:G:360:TYR:CE1	2.88	0.56
1:H:59:THR:HG21	5:H:2002:HOH:O	2.05	0.56
1:C:131:ARG:O	1:C:360:TYR:HE2	1.88	0.56
1:G:180:ASP:HB3	1:G:183:VAL:CG1	2.36	0.56
1:I:218:ARG:HG2	1:I:218:ARG:HH11	1.71	0.56
1:B:284:PRO:CB	1:F:288:GLU:HG3	2.32	0.56
1:G:365:GLN:HB3	5:G:2020:HOH:O	2.06	0.56
1:A:66:GLN:HE21	2:A:400:GDX:HN21	1.54	0.55
1:C:205:SER:CB	1:C:250:ILE:CG2	2.80	0.55
1:B:142:ILE:CD1	1:B:230:LEU:HD12	2.35	0.55
1:I:218:ARG:HH11	1:I:218:ARG:CG	2.19	0.55
1:B:66:GLN:HE21	2:B:400:GDX:HN21	1.55	0.55
1:A:224:ASP:HB3	1:A:341:PHE:CZ	2.41	0.55
1:C:315:GLU:HG3	1:C:366:TYR:OH	2.06	0.55
1:J:70:GLY:HA2	1:J:185:ARG:HA	1.89	0.55
1:A:52:GLU:HG2	1:A:55:ARG:HH11	1.70	0.55
1:C:304:CYS:HA	1:C:307:ARG:O	2.07	0.55
1:G:277:ARG:CZ	1:G:281:HIS:HD2	2.20	0.55
1:A:369:ARG:CD	5:A:2072:HOH:O	2.46	0.55
1:D:132:ALA:HB3	1:D:135:ASP:CG	2.32	0.55
1:J:286:GLN:C	1:J:288:GLU:N	2.61	0.55
1:C:142:ILE:HD13	1:C:230:LEU:HD12	1.87	0.55
1:A:179:GLU:CG	5:A:2033:HOH:O	2.48	0.55
1:G:131:ARG:O	1:G:360:TYR:HE2	1.90	0.55
1:B:224:ASP:HB3	1:B:341:PHE:CZ	2.42	0.54
1:D:181:GLU:OE1	1:D:185:ARG:NH2	2.40	0.54
1:D:362:TYR:O	1:D:365:GLN:HG3	2.07	0.54
1:E:288:GLU:O	1:E:291:GLU:HB2	2.07	0.54
1:E:283:THR:HG23	5:E:2029:HOH:O	2.06	0.54
1:J:201:GLN:O	1:J:246:GLY:O	2.24	0.54
1:A:52:GLU:O	1:A:55:ARG:N	2.34	0.54
1:A:223:LEU:O	1:A:226:LEU:HB2	2.07	0.54
1:F:247:GLN:CG	1:F:248:PRO:HD2	2.19	0.54
1:F:97:HIS:CE1	1:F:168:LEU:HD12	2.43	0.54
1:G:138:ILE:HB	4:G:1382:CL:CL	2.44	0.54
1:A:288:GLU:O	1:A:291:GLU:HB2	2.08	0.54
1:J:270:ASP:OD2	1:J:270:ASP:C	2.51	0.54
1:C:182:ARG:NH2	1:C:201:GLN:OE1	2.36	0.54
1:C:290:LEU:HB3	1:C:298:ARG:HG3	1.90	0.54
1:D:110:TRP:HD1	1:D:110:TRP:H	1.53	0.54
1:F:168:LEU:C	1:F:168:LEU:HD23	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ASP:OD2	1:F:182:ARG:NH1	2.41	0.54
1:H:259:VAL:CG2	1:H:360:TYR:CE1	2.86	0.54
1:A:142:ILE:HD11	1:A:230:LEU:HD11	1.91	0.53
1:B:142:ILE:HD13	1:B:230:LEU:HD12	1.89	0.53
1:C:181:GLU:OE1	1:C:185:ARG:NH2	2.40	0.53
1:C:218:ARG:HB3	5:C:2038:HOH:O	2.09	0.53
1:D:50:ALA:O	1:D:53:ILE:N	2.42	0.53
1:D:66:GLN:HE21	2:D:400:GDX:HN21	1.55	0.53
1:E:10:HIS:HE1	1:E:38:GLU:OE2	1.91	0.53
1:E:123:GLY:HA2	1:E:170:ARG:CD	2.38	0.53
1:F:244:VAL:C	1:F:245:VAL:HG23	2.33	0.53
1:G:328:HIS:CD2	5:G:2019:HOH:O	2.40	0.53
1:H:205:SER:HB2	1:H:250:ILE:CG2	2.35	0.53
1:I:180:ASP:OD2	1:I:182:ARG:NH1	2.42	0.53
1:C:177:LEU:HD23	1:C:198:VAL:HG22	1.90	0.53
1:F:70:GLY:HA2	1:F:185:ARG:HA	1.91	0.53
1:G:290:LEU:HB3	1:G:298:ARG:HG3	1.90	0.53
1:D:131:ARG:O	1:D:360:TYR:HE2	1.91	0.53
1:D:132:ALA:HB3	1:D:135:ASP:OD2	2.09	0.53
1:H:59:THR:CG2	5:H:2002:HOH:O	2.56	0.53
1:I:277:ARG:CZ	1:I:281:HIS:HD2	2.22	0.53
1:J:259:VAL:CG2	1:J:360:TYR:CE1	2.87	0.53
1:C:184:ARG:NH1	1:C:184:ARG:HG2	2.23	0.53
1:D:142:ILE:HD13	1:D:230:LEU:HD12	1.90	0.53
1:F:244:VAL:CG1	1:F:245:VAL:N	2.71	0.53
1:H:257:HIS:N	1:H:257:HIS:CD2	2.76	0.53
1:I:131:ARG:O	1:I:360:TYR:HE2	1.91	0.53
1:D:53:ILE:C	1:D:55:ARG:N	2.64	0.53
1:C:180:ASP:OD2	1:C:182:ARG:NH1	2.42	0.52
1:E:151:TRP:CD1	1:E:245:VAL:HG23	2.44	0.52
1:E:304:CYS:HA	1:E:307:ARG:O	2.09	0.52
1:A:180:ASP:OD1	1:A:182:ARG:HB2	2.07	0.52
1:B:258:ARG:HH21	1:C:258:ARG:HE	1.56	0.52
1:C:142:ILE:HD13	1:C:230:LEU:CD1	2.38	0.52
1:G:142:ILE:HD11	1:G:230:LEU:HD11	1.90	0.52
1:G:182:ARG:NH2	1:G:201:GLN:OE1	2.40	0.52
1:C:123:GLY:HA2	1:C:170:ARG:CD	2.35	0.52
1:C:10:HIS:HE1	1:C:38:GLU:OE2	1.92	0.52
1:G:85:ARG:HB2	1:G:178:TYR:CE1	2.42	0.52
1:F:136:ALA:HA	4:F:1382:CL:CL	2.46	0.52
1:I:109:ASP:HB3	1:I:110:TRP:CD1	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:177:LEU:HB3	1:G:183:VAL:HG21	1.92	0.52
1:I:142:ILE:HD11	1:I:230:LEU:HD11	1.92	0.52
1:I:155:GLU:HG3	1:I:251:HIS:ND1	2.24	0.52
1:A:14:GLU:CD	1:A:14:GLU:H	2.17	0.52
1:D:52:GLU:O	1:D:55:ARG:CG	2.51	0.52
1:E:283:THR:HB	1:E:286:GLN:NE2	2.25	0.52
1:J:246:GLY:N	1:J:247:GLN:HB2	2.25	0.52
1:A:91:THR:HG1	1:A:93:TRP:CD1	2.28	0.51
1:B:262:HIS:CE1	5:B:2044:HOH:O	2.55	0.51
1:A:49:ALA:O	1:A:53:ILE:HG13	2.11	0.51
1:H:14:GLU:CD	1:H:14:GLU:H	2.19	0.51
1:I:181:GLU:OE1	1:I:185:ARG:NH2	2.44	0.51
1:A:10:HIS:HE1	1:A:38:GLU:OE2	1.93	0.51
1:J:283:THR:CG2	1:J:335:ASP:OD2	2.45	0.51
1:J:304:CYS:HA	1:J:307:ARG:O	2.10	0.51
1:A:215:LYS:HE2	5:A:2078:HOH:O	2.11	0.51
1:E:131:ARG:O	1:E:360:TYR:HE2	1.94	0.51
1:H:301:LEU:O	1:H:304:CYS:HB2	2.10	0.51
1:A:362:TYR:O	1:A:365:GLN:HG3	2.10	0.51
1:C:136:ALA:HA	4:C:1382:CL:CL	2.48	0.51
1:C:168:LEU:HD23	1:C:168:LEU:C	2.36	0.51
1:D:168:LEU:C	1:D:168:LEU:HD23	2.36	0.51
1:F:315:GLU:HG3	1:F:366:TYR:OH	2.11	0.51
1:H:70:GLY:HA2	1:H:185:ARG:HA	1.92	0.51
1:H:180:ASP:OD2	1:H:182:ARG:NH1	2.44	0.51
1:G:70:GLY:HA2	1:G:185:ARG:HA	1.92	0.51
1:A:70:GLY:HA2	1:A:185:ARG:HA	1.93	0.50
1:C:262:HIS:HE1	5:C:2020:HOH:O	1.93	0.50
1:F:330:GLN:HB2	1:F:336:TRP:CD1	2.46	0.50
1:G:177:LEU:HD23	1:G:198:VAL:CG2	2.38	0.50
1:G:178:TYR:CD2	1:G:178:TYR:C	2.88	0.50
1:B:109:ASP:HB3	1:B:110:TRP:CD1	2.35	0.50
1:B:142:ILE:HD13	1:B:230:LEU:CD1	2.41	0.50
1:H:110:TRP:CD1	1:H:110:TRP:H	2.29	0.50
1:B:283:THR:HB	1:B:286:GLN:NE2	2.26	0.50
1:D:97:HIS:CE1	1:D:168:LEU:HD12	2.47	0.50
1:D:109:ASP:HB3	1:D:110:TRP:CD1	2.37	0.50
1:H:288:GLU:O	1:H:291:GLU:HB2	2.11	0.50
1:H:290:LEU:HB3	1:H:298:ARG:HG3	1.93	0.50
1:I:257:HIS:N	1:I:257:HIS:CD2	2.79	0.50
1:A:245:VAL:O	1:A:246:GLY:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:HIS:N	1:E:257:HIS:CD2	2.79	0.50
1:F:110:TRP:CD1	1:F:110:TRP:H	2.29	0.50
1:H:123:GLY:HA2	1:H:170:ARG:CD	2.41	0.50
1:C:97:HIS:CE1	1:C:168:LEU:HD12	2.45	0.50
1:E:246:GLY:O	1:E:247:GLN:O	2.30	0.50
1:A:68:ARG:HD2	5:A:2009:HOH:O	2.11	0.50
1:G:247:GLN:O	1:G:247:GLN:CG	2.60	0.50
1:A:365:GLN:HG3	1:A:366:TYR:N	2.27	0.50
1:B:246:GLY:O	1:B:247:GLN:O	2.30	0.50
1:D:50:ALA:N	1:D:51:PRO:HD2	2.23	0.50
1:F:142:ILE:HD13	1:F:230:LEU:HD12	1.94	0.50
1:I:10:HIS:HE1	1:I:38:GLU:OE2	1.95	0.50
1:I:247:GLN:O	1:I:248:PRO:O	2.30	0.50
1:J:381:GLU:HG2	1:J:382:ASN:N	2.26	0.50
1:B:70:GLY:HA2	1:B:185:ARG:HA	1.93	0.50
1:D:51:PRO:O	1:D:55:ARG:HB3	2.12	0.50
1:G:247:GLN:O	1:G:248:PRO:O	2.30	0.50
1:G:288:GLU:O	1:G:291:GLU:HB2	2.12	0.50
1:J:283:THR:O	1:J:284:PRO:C	2.54	0.50
1:D:142:ILE:HD13	1:D:230:LEU:CD1	2.42	0.49
1:G:123:GLY:HA2	1:G:170:ARG:CD	2.38	0.49
1:I:110:TRP:CD1	1:I:110:TRP:H	2.29	0.49
1:H:142:ILE:HD13	1:H:230:LEU:HD12	1.94	0.49
1:H:142:ILE:HD13	1:H:230:LEU:CD1	2.42	0.49
1:H:181:GLU:OE1	1:H:185:ARG:NH2	2.45	0.49
1:J:66:GLN:HE21	2:J:400:GDX:HN21	1.59	0.49
1:J:123:GLY:HA2	1:J:170:ARG:CD	2.41	0.49
1:A:318:TRP:HB2	1:A:347:ARG:HD3	1.92	0.49
1:D:304:CYS:HA	1:D:307:ARG:O	2.12	0.49
1:F:244:VAL:O	1:F:245:VAL:CG2	2.59	0.49
1:G:14:GLU:H	1:G:14:GLU:CD	2.20	0.49
1:B:245:VAL:HG12	1:B:245:VAL:O	2.12	0.49
1:D:315:GLU:HG3	1:D:366:TYR:OH	2.12	0.49
1:I:247:GLN:OE1	1:I:247:GLN:O	2.30	0.49
1:J:168:LEU:C	1:J:168:LEU:HD23	2.37	0.49
1:A:260:PRO:HG2	1:A:263:ILE:HD12	1.93	0.49
1:D:52:GLU:O	1:D:52:GLU:OE1	2.30	0.49
1:D:365:GLN:HG3	1:D:366:TYR:N	2.26	0.49
1:G:77:GLY:O	1:G:78:ASP:C	2.55	0.49
1:G:168:LEU:C	1:G:168:LEU:HD23	2.38	0.49
1:J:142:ILE:CD1	1:J:230:LEU:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:TYR:O	1:A:365:GLN:CG	2.61	0.49
1:B:131:ARG:CZ	5:B:2018:HOH:O	2.59	0.49
1:D:70:GLY:HA2	1:D:185:ARG:HA	1.95	0.49
1:F:66:GLN:HE21	2:F:400:GDX:HN21	1.61	0.49
1:I:246:GLY:O	1:I:247:GLN:OE1	2.30	0.49
1:A:277:ARG:CZ	1:A:281:HIS:HD2	2.25	0.49
1:D:246:GLY:C	1:D:247:GLN:CG	2.85	0.49
1:I:290:LEU:HB3	1:I:298:ARG:HG3	1.93	0.49
1:A:267:VAL:C	5:A:2053:HOH:O	2.56	0.49
1:B:177:LEU:CD2	1:B:198:VAL:HG22	2.43	0.49
1:A:41:GLN:HE21	1:A:41:GLN:CA	2.10	0.48
1:E:16:LEU:HD13	1:E:101:ALA:HB1	1.95	0.48
1:I:14:GLU:CD	1:I:14:GLU:H	2.21	0.48
1:B:315:GLU:HG3	1:B:366:TYR:OH	2.14	0.48
1:D:288:GLU:O	1:D:291:GLU:HB2	2.12	0.48
1:I:312:PHE:CE2	1:I:313:MET:HB2	2.48	0.48
1:H:218:ARG:HH11	1:H:218:ARG:CG	2.26	0.48
1:C:247:GLN:HA	1:C:248:PRO:HD2	1.43	0.48
1:C:362:TYR:O	1:C:365:GLN:HG3	2.12	0.48
1:D:315:GLU:HG2	1:D:370:MET:HG3	1.94	0.48
1:C:184:ARG:HA	1:C:184:ARG:HD3	1.70	0.48
1:D:110:TRP:CD1	1:D:110:TRP:N	2.80	0.48
1:G:255:HIS:CD2	1:G:256:PRO:HD2	2.48	0.48
1:J:109:ASP:HB3	1:J:110:TRP:CD1	2.32	0.48
1:J:142:ILE:CD1	1:J:230:LEU:HD12	2.43	0.48
1:A:50:ALA:O	1:A:54:SER:OG	2.32	0.48
1:B:362:TYR:O	1:B:365:GLN:HG3	2.14	0.48
1:A:315:GLU:HG3	1:A:366:TYR:OH	2.14	0.48
1:D:255:HIS:CD2	1:D:256:PRO:HD2	2.49	0.48
1:F:247:GLN:HB3	1:F:248:PRO:CD	2.41	0.48
1:B:17:LEU:HD21	1:B:46:VAL:HA	1.96	0.48
1:C:132:ALA:HB3	1:C:135:ASP:OD2	2.13	0.48
1:E:218:ARG:CG	1:E:218:ARG:NH1	2.71	0.48
1:G:10:HIS:HE1	1:G:38:GLU:OE2	1.96	0.48
1:I:70:GLY:HA2	1:I:185:ARG:HA	1.96	0.48
1:J:17:LEU:HD21	1:J:46:VAL:HA	1.96	0.48
1:D:333:ASP:OD1	1:D:333:ASP:C	2.55	0.48
1:E:17:LEU:HD21	1:E:46:VAL:HA	1.96	0.48
1:F:14:GLU:CD	1:F:14:GLU:H	2.21	0.48
1:C:262:HIS:CD2	1:C:263:ILE:HG13	2.48	0.47
1:E:205:SER:HB2	1:E:250:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LEU:HD21	1:F:46:VAL:HA	1.96	0.47
1:F:257:HIS:N	1:F:257:HIS:CD2	2.82	0.47
1:G:270:ASP:C	1:G:270:ASP:OD2	2.57	0.47
1:H:39:ARG:HB2	1:I:71:THR:HB	1.95	0.47
1:H:255:HIS:CD2	1:H:256:PRO:HD2	2.49	0.47
1:J:110:TRP:CD1	1:J:110:TRP:H	2.32	0.47
1:A:110:TRP:CD1	1:A:110:TRP:H	2.30	0.47
1:C:257:HIS:N	1:C:257:HIS:CD2	2.82	0.47
1:G:362:TYR:O	1:G:365:GLN:HG3	2.14	0.47
1:J:333:ASP:C	1:J:333:ASP:OD1	2.56	0.47
1:A:258:ARG:HH21	1:D:258:ARG:HE	1.63	0.47
1:A:262:HIS:CE1	5:A:2039:HOH:O	2.59	0.47
1:C:177:LEU:CD2	1:C:198:VAL:HG22	2.44	0.47
1:C:244:VAL:C	1:C:245:VAL:HG12	2.39	0.47
1:E:142:ILE:CD1	1:E:230:LEU:HD11	2.44	0.47
1:E:315:GLU:HG3	1:E:366:TYR:OH	2.14	0.47
1:G:188:ASP:HB2	1:G:232:GLU:OE2	2.15	0.47
1:G:357:LEU:HD13	1:H:357:LEU:HD13	1.96	0.47
1:I:142:ILE:HD13	1:I:230:LEU:CD1	2.44	0.47
1:A:315:GLU:HG2	1:A:370:MET:HG3	1.96	0.47
1:B:142:ILE:HD12	1:B:230:LEU:CD1	2.44	0.47
1:C:218:ARG:HH11	1:C:218:ARG:CG	2.28	0.47
1:F:270:ASP:OD2	1:F:270:ASP:C	2.57	0.47
1:F:288:GLU:O	1:F:291:GLU:HB2	2.14	0.47
1:A:258:ARG:HE	1:D:258:ARG:HH21	1.63	0.47
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.80	0.47
1:A:258:ARG:HH22	1:A:361:ASP:CG	2.22	0.47
1:D:132:ALA:N	1:D:135:ASP:OD2	2.40	0.47
1:G:181:GLU:OE1	1:G:185:ARG:NH2	2.48	0.47
1:A:247:GLN:HA	1:A:248:PRO:HD3	1.39	0.47
1:A:368:TYR:CD2	1:D:255:HIS:CE1	3.03	0.47
1:C:17:LEU:HD21	1:C:46:VAL:HA	1.97	0.47
1:C:247:GLN:CB	1:C:248:PRO:O	2.52	0.47
1:C:277:ARG:CZ	1:C:281:HIS:HD2	2.28	0.47
1:D:277:ARG:CZ	1:D:281:HIS:HD2	2.28	0.47
1:E:177:LEU:CD2	1:E:198:VAL:HG22	2.45	0.47
1:J:258:ARG:HH22	1:J:361:ASP:CG	2.23	0.47
1:B:132:ALA:HB3	1:B:135:ASP:OD2	2.15	0.47
1:E:14:GLU:H	1:E:14:GLU:CD	2.23	0.47
1:H:142:ILE:HD11	1:H:230:LEU:HD11	1.97	0.47
1:G:191:ILE:CG2	1:G:192:ASP:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:TYR:HA	5:G:2012:HOH:O	2.14	0.47
1:H:97:HIS:CE1	1:H:168:LEU:HD12	2.50	0.47
1:J:283:THR:O	1:J:286:GLN:N	2.48	0.47
1:J:285:ARG:NH1	1:J:335:ASP:HB2	2.29	0.47
1:B:66:GLN:NE2	2:B:400:GDX:HN21	2.12	0.46
1:C:151:TRP:CD1	1:C:245:VAL:HG11	2.49	0.46
1:C:288:GLU:O	1:C:291:GLU:HB2	2.15	0.46
1:D:14:GLU:CD	1:D:14:GLU:H	2.23	0.46
1:H:223:LEU:HD22	1:H:274:THR:HG21	1.96	0.46
1:I:288:GLU:O	1:I:291:GLU:HB2	2.15	0.46
1:G:330:GLN:HB2	1:G:336:TRP:CD1	2.50	0.46
1:G:17:LEU:HD21	1:G:46:VAL:HA	1.96	0.46
1:G:84:LEU:HB3	1:G:178:TYR:HD1	1.81	0.46
1:I:136:ALA:HA	4:I:1382:CL:CL	2.53	0.46
1:J:188:ASP:HB2	1:J:232:GLU:OE2	2.15	0.46
1:A:155:GLU:OE1	1:D:252:ARG:NH1	2.47	0.46
1:C:110:TRP:O	1:C:127:HIS:HE1	1.99	0.46
1:J:97:HIS:CE1	1:J:168:LEU:HD12	2.51	0.46
1:C:66:GLN:HE21	2:C:400:GDX:HN21	1.64	0.46
1:D:21:ARG:HD3	1:D:53:ILE:HG12	1.97	0.46
1:G:310:PHE:CZ	1:H:272:GLU:HB2	2.51	0.46
1:G:362:TYR:O	1:G:365:GLN:CG	2.64	0.46
1:I:246:GLY:C	1:I:247:GLN:CD	2.81	0.46
1:J:180:ASP:OD2	1:J:182:ARG:NH1	2.48	0.46
1:J:366:TYR:CD1	1:J:366:TYR:C	2.93	0.46
1:A:364:GLN:O	1:A:365:GLN:C	2.59	0.46
1:B:16:LEU:HD13	1:B:101:ALA:HB1	1.96	0.46
1:D:218:ARG:HH11	1:D:218:ARG:CG	2.29	0.46
1:A:97:HIS:CE1	1:A:168:LEU:HD12	2.51	0.46
1:A:110:TRP:O	1:A:127:HIS:HE1	1.98	0.46
1:B:39:ARG:NE	5:B:2004:HOH:O	2.48	0.46
1:C:14:GLU:CD	1:C:14:GLU:H	2.24	0.46
1:F:142:ILE:HD11	1:F:230:LEU:HD11	1.97	0.46
1:F:203:GLY:HA2	1:F:249:ALA:HB2	1.98	0.46
1:I:318:TRP:HB2	1:I:347:ARG:HD3	1.97	0.46
1:J:14:GLU:H	1:J:14:GLU:CD	2.23	0.46
1:A:52:GLU:O	1:A:53:ILE:C	2.59	0.46
1:A:181:GLU:HG3	1:A:182:ARG:N	2.26	0.46
1:A:277:ARG:HA	1:A:280:GLN:OE1	2.16	0.46
1:E:177:LEU:HD23	1:E:198:VAL:HG22	1.97	0.46
1:F:131:ARG:O	1:F:360:TYR:HE2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LEU:HB2	1:E:151:TRP:CE3	2.51	0.46
1:H:188:ASP:HB2	1:H:232:GLU:OE2	2.16	0.46
1:A:180:ASP:OD2	1:A:182:ARG:NH1	2.49	0.45
1:B:259:VAL:CG2	1:B:360:TYR:CE1	2.97	0.45
1:C:373:ARG:NH1	5:C:2037:HOH:O	2.39	0.45
1:G:85:ARG:CB	1:G:178:TYR:HE1	2.25	0.45
1:I:180:ASP:OD1	1:I:182:ARG:HB2	2.16	0.45
1:A:135:ASP:O	1:A:136:ALA:HB3	2.15	0.45
1:B:224:ASP:HB3	1:B:341:PHE:HZ	1.80	0.45
1:F:304:CYS:HA	1:F:307:ARG:O	2.17	0.45
1:G:110:TRP:CD1	1:G:110:TRP:H	2.34	0.45
1:H:66:GLN:HE21	2:H:400:GDX:HN21	1.64	0.45
1:I:333:ASP:OD1	1:I:333:ASP:C	2.59	0.45
1:J:285:ARG:HG2	1:J:335:ASP:OD1	2.16	0.45
1:A:127:HIS:HA	1:A:209:CYS:HB3	1.98	0.45
1:B:306:ARG:HG2	5:F:2001:HOH:O	2.15	0.45
1:F:142:ILE:CD1	1:F:230:LEU:HD12	2.47	0.45
1:F:291:GLU:OE1	1:F:302:ARG:NH2	2.48	0.45
1:G:110:TRP:CD1	1:G:110:TRP:N	2.85	0.45
1:I:338:GLU:HG3	1:I:342:LYS:NZ	2.32	0.45
1:A:140:TRP:CD2	1:A:367:LEU:HD13	2.51	0.45
1:C:201:GLN:NE2	1:C:244:VAL:O	2.41	0.45
1:G:177:LEU:O	1:G:178:TYR:C	2.60	0.45
1:H:110:TRP:CD1	1:H:110:TRP:N	2.84	0.45
1:J:290:LEU:HB3	1:J:298:ARG:HG3	1.97	0.45
1:G:362:TYR:CD2	1:G:362:TYR:C	2.95	0.45
1:I:17:LEU:HD21	1:I:46:VAL:HA	1.98	0.45
1:I:110:TRP:CD1	1:I:110:TRP:N	2.84	0.45
1:H:333:ASP:C	1:H:333:ASP:OD1	2.59	0.45
1:I:66:GLN:NE2	2:I:400:GDX:N1	2.57	0.45
1:A:29:VAL:O	1:A:59:THR:HG21	2.17	0.45
1:A:66:GLN:NE2	2:A:400:GDX:HN21	2.13	0.45
1:D:259:VAL:CG2	1:D:360:TYR:CE1	2.95	0.45
1:F:259:VAL:CG2	1:F:360:TYR:CE1	2.91	0.45
1:G:68:ARG:NH1	1:G:187:SER:OG	2.50	0.45
1:B:258:ARG:HH22	1:B:361:ASP:CG	2.25	0.45
1:B:258:ARG:HE	1:C:258:ARG:HH21	1.63	0.45
1:G:260:PRO:HA	5:G:2016:HOH:O	2.17	0.45
1:J:177:LEU:HD23	1:J:198:VAL:HG22	1.99	0.45
1:A:109:ASP:HB3	1:A:110:TRP:CD1	2.38	0.44
1:E:245:VAL:CG1	1:E:246:GLY:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:ASP:OD1	1:F:333:ASP:C	2.60	0.44
1:H:17:LEU:HD21	1:H:46:VAL:HA	1.99	0.44
1:A:215:LYS:CE	5:A:2078:HOH:O	2.65	0.44
1:B:255:HIS:CE1	1:C:368:TYR:CD2	3.06	0.44
1:C:110:TRP:CD1	1:C:110:TRP:H	2.35	0.44
1:C:142:ILE:HD11	1:C:230:LEU:HD11	1.96	0.44
1:F:123:GLY:HA2	1:F:170:ARG:CD	2.43	0.44
1:I:315:GLU:HG2	1:I:370:MET:HG3	1.98	0.44
1:B:257:HIS:N	1:B:257:HIS:CD2	2.84	0.44
1:F:262:HIS:CD2	1:F:263:ILE:HG13	2.53	0.44
1:H:70:GLY:HA3	1:H:187:SER:HB3	2.00	0.44
1:H:218:ARG:HH11	1:H:218:ARG:HG2	1.82	0.44
1:I:247:GLN:O	1:I:248:PRO:C	2.60	0.44
1:E:132:ALA:HB3	1:E:135:ASP:OD2	2.17	0.44
1:G:301:LEU:HD23	1:G:301:LEU:HA	1.84	0.44
1:J:177:LEU:CD2	1:J:198:VAL:HG22	2.47	0.44
1:H:131:ARG:HA	1:H:131:ARG:HD2	1.87	0.44
1:J:131:ARG:O	1:J:360:TYR:HE2	2.01	0.44
1:J:203:GLY:HA2	1:J:249:ALA:HB2	1.99	0.44
1:B:365:GLN:HG3	1:B:366:TYR:N	2.33	0.44
1:C:218:ARG:HH11	1:C:218:ARG:HG2	1.83	0.44
1:E:142:ILE:CD1	1:E:230:LEU:CD1	2.95	0.44
1:B:136:ALA:HA	4:B:1382:CL:CL	2.54	0.44
1:E:110:TRP:O	1:E:127:HIS:HE1	2.01	0.44
1:J:365:GLN:HG3	1:J:366:TYR:H	1.82	0.44
1:C:307:ARG:HD2	1:D:276:HIS:CD2	2.53	0.44
1:D:123:GLY:HA2	1:D:170:ARG:CD	2.45	0.44
1:J:142:ILE:HD11	1:J:230:LEU:HD11	2.00	0.44
1:A:283:THR:HB	1:A:286:GLN:NE2	2.33	0.44
1:E:225:ASP:HB3	5:E:2024:HOH:O	2.18	0.44
1:J:144:ARG:O	1:J:145:THR:C	2.61	0.44
1:A:110:TRP:CD1	1:A:110:TRP:N	2.87	0.43
1:A:365:GLN:HB3	5:A:2066:HOH:O	2.18	0.43
1:C:245:VAL:HA	1:C:246:GLY:HA3	1.89	0.43
1:E:255:HIS:CD2	1:E:256:PRO:HD2	2.53	0.43
1:G:66:GLN:HE21	2:G:400:GDX:HN21	1.66	0.43
1:G:166:GLU:N	1:G:166:GLU:CD	2.77	0.43
1:G:218:ARG:CG	1:G:218:ARG:HH11	2.31	0.43
1:G:223:LEU:HD22	1:G:274:THR:HG21	1.99	0.43
1:G:364:GLN:O	1:G:365:GLN:C	2.61	0.43
1:J:277:ARG:CZ	1:J:281:HIS:HD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD21	1:A:46:VAL:HA	2.00	0.43
1:A:257:HIS:N	1:A:257:HIS:CD2	2.84	0.43
1:F:177:LEU:CD2	1:F:198:VAL:HG22	2.48	0.43
1:G:122:TYR:CG	1:G:207:TYR:HB2	2.53	0.43
1:B:35:ILE:HG23	1:B:35:ILE:HD12	1.32	0.43
1:B:290:LEU:HB3	1:B:298:ARG:HG3	2.00	0.43
1:I:338:GLU:HG3	1:I:342:LYS:HZ2	1.84	0.43
1:B:362:TYR:C	1:B:362:TYR:CD2	2.96	0.43
1:B:365:GLN:CG	1:B:365:GLN:CA	2.84	0.43
1:E:97:HIS:CE1	1:E:168:LEU:HD12	2.53	0.43
1:E:365:GLN:HG3	1:E:366:TYR:H	1.82	0.43
1:H:98:PHE:O	1:H:166:GLU:HA	2.18	0.43
1:A:123:GLY:HA2	1:A:170:ARG:CD	2.47	0.43
1:D:52:GLU:OE2	1:D:53:ILE:HA	2.18	0.43
1:E:301:LEU:HD23	1:E:301:LEU:HA	1.82	0.43
1:H:315:GLU:HG3	1:H:366:TYR:OH	2.19	0.43
1:I:364:GLN:O	1:I:365:GLN:C	2.61	0.43
1:B:180:ASP:OD1	1:B:182:ARG:HD3	2.18	0.43
1:C:110:TRP:CD1	1:C:110:TRP:N	2.87	0.43
1:C:260:PRO:HG2	1:C:263:ILE:HD12	2.00	0.43
1:F:258:ARG:HH22	1:F:361:ASP:CG	2.27	0.43
1:G:41:GLN:HE21	1:G:41:GLN:CA	2.23	0.43
1:J:245:VAL:HA	1:J:246:GLY:HA3	1.53	0.43
1:A:52:GLU:HG2	1:A:55:ARG:NH1	2.32	0.43
1:F:142:ILE:HD13	1:F:230:LEU:CD1	2.47	0.43
1:J:142:ILE:HD13	1:J:230:LEU:CD1	2.48	0.43
1:J:255:HIS:CD2	1:J:256:PRO:HD2	2.54	0.43
1:J:288:GLU:O	1:J:291:GLU:HB2	2.19	0.43
1:J:289:LEU:HD12	1:J:289:LEU:HA	1.91	0.43
1:J:362:TYR:O	1:J:365:GLN:HG3	2.19	0.43
1:E:259:VAL:CG2	1:E:360:TYR:CE1	2.97	0.43
1:I:142:ILE:HD13	1:I:230:LEU:HD12	2.01	0.43
1:J:131:ARG:HA	1:J:131:ARG:HD2	1.84	0.43
1:C:140:TRP:CZ3	1:C:367:LEU:HB3	2.54	0.43
1:E:330:GLN:O	1:E:331:PRO:C	2.59	0.43
1:H:177:LEU:HD23	1:H:198:VAL:HG22	2.00	0.43
1:H:180:ASP:OD1	1:H:182:ARG:HB2	2.19	0.43
1:J:313:MET:O	1:J:313:MET:HG3	2.18	0.43
1:F:246:GLY:CA	1:F:247:GLN:CB	2.96	0.42
1:F:277:ARG:CZ	1:F:281:HIS:HD2	2.32	0.42
1:A:368:TYR:CD2	1:D:255:HIS:ND1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:GLU:N	1:E:166:GLU:CD	2.77	0.42
1:F:100:ASP:O	1:F:103:ILE:HD12	2.19	0.42
1:G:258:ARG:HH22	1:G:361:ASP:CG	2.26	0.42
1:I:364:GLN:CB	5:I:2010:HOH:O	2.61	0.42
1:A:248:PRO:CG	1:D:252:ARG:HH12	2.32	0.42
1:C:262:HIS:CE1	5:C:2020:HOH:O	2.69	0.42
1:E:224:ASP:HB3	1:E:341:PHE:CZ	2.55	0.42
1:H:177:LEU:CD2	1:H:198:VAL:HG22	2.48	0.42
1:I:366:TYR:CD1	1:I:366:TYR:C	2.96	0.42
1:D:218:ARG:HH11	1:D:218:ARG:HG2	1.83	0.42
1:F:109:ASP:HB3	1:F:110:TRP:H	1.60	0.42
1:F:177:LEU:HD23	1:F:198:VAL:HG22	2.01	0.42
1:G:381:GLU:HG2	1:G:382:ASN:N	2.34	0.42
1:I:362:TYR:O	1:I:365:GLN:HG3	2.19	0.42
1:J:140:TRP:CD2	1:J:367:LEU:HD13	2.54	0.42
1:A:255:HIS:ND1	1:D:368:TYR:CD2	2.88	0.42
1:B:110:TRP:O	1:B:127:HIS:HE1	2.02	0.42
1:C:330:GLN:HB2	1:C:336:TRP:CD1	2.54	0.42
1:D:117:ALA:O	1:D:118:ALA:C	2.61	0.42
1:F:110:TRP:CD1	1:F:110:TRP:N	2.87	0.42
1:G:64:ARG:HG2	5:G:2004:HOH:O	2.18	0.42
1:G:72:LEU:HB3	1:G:73:ARG:H	1.62	0.42
1:I:312:PHE:HE2	1:I:313:MET:HE2	1.84	0.42
1:A:176:MET:SD	1:A:176:MET:C	3.02	0.42
1:D:52:GLU:OE2	1:D:53:ILE:CA	2.68	0.42
1:D:66:GLN:NE2	2:D:400:GDX:HN21	2.16	0.42
1:F:16:LEU:HD13	1:F:101:ALA:HB1	2.01	0.42
1:G:140:TRP:CD2	1:G:367:LEU:HD13	2.54	0.42
1:I:246:GLY:C	1:I:247:GLN:OE1	2.61	0.42
1:A:248:PRO:CB	1:D:252:ARG:HH12	2.32	0.42
1:B:131:ARG:O	1:B:360:TYR:HE2	2.03	0.42
1:C:301:LEU:HD23	1:C:301:LEU:HA	1.84	0.42
1:E:153:HIS:HE1	1:G:120:PHE:O	2.02	0.42
1:E:181:GLU:OE1	1:E:185:ARG:NH2	2.53	0.42
1:E:246:GLY:C	1:E:247:GLN:O	2.63	0.42
1:H:218:ARG:NH1	1:H:218:ARG:HB3	2.34	0.42
1:H:367:LEU:O	1:H:370:MET:HB3	2.20	0.42
1:J:110:TRP:O	1:J:127:HIS:HE1	2.03	0.42
1:J:364:GLN:O	1:J:365:GLN:C	2.60	0.42
1:E:203:GLY:HA2	1:E:249:ALA:HB2	2.00	0.42
1:A:131:ARG:HA	1:A:131:ARG:HD2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:HD12	1:D:35:ILE:HG23	1.66	0.42
1:H:362:TYR:CD2	1:H:362:TYR:C	2.98	0.42
1:J:201:GLN:HA	1:J:245:VAL:CG1	2.50	0.42
1:A:218:ARG:HG2	1:A:218:ARG:HH11	1.84	0.41
1:D:246:GLY:O	1:D:247:GLN:CG	2.66	0.41
1:E:270:ASP:OD2	1:E:270:ASP:C	2.62	0.41
1:F:218:ARG:HH11	1:F:218:ARG:CG	2.33	0.41
1:A:333:ASP:OD1	1:A:333:ASP:C	2.63	0.41
1:D:132:ALA:CB	1:D:135:ASP:OD2	2.68	0.41
1:D:224:ASP:HB3	1:D:341:PHE:CZ	2.55	0.41
1:D:362:TYR:CD2	1:D:362:TYR:C	2.98	0.41
1:G:176:MET:HE3	1:G:176:MET:HB3	1.76	0.41
1:J:10:HIS:CE1	1:J:38:GLU:OE2	2.71	0.41
1:J:181:GLU:OE1	1:J:185:ARG:NH2	2.53	0.41
1:B:98:PHE:O	1:B:166:GLU:HA	2.21	0.41
1:C:224:ASP:HB3	1:C:341:PHE:CZ	2.55	0.41
1:D:142:ILE:HD11	1:D:230:LEU:HD11	2.02	0.41
1:E:362:TYR:O	1:E:365:GLN:HG3	2.20	0.41
1:I:224:ASP:HB3	1:I:341:PHE:CZ	2.55	0.41
1:J:326:LEU:HD23	1:J:326:LEU:HA	1.91	0.41
1:B:123:GLY:HA2	1:B:170:ARG:CD	2.46	0.41
1:B:330:GLN:HB2	1:B:336:TRP:CD1	2.54	0.41
1:G:176:MET:CE	1:G:202:GLN:HG3	2.50	0.41
1:G:191:ILE:HD11	1:G:195:TYR:CE1	2.56	0.41
1:G:315:GLU:HG3	1:G:366:TYR:OH	2.19	0.41
1:H:362:TYR:O	1:H:365:GLN:HG3	2.19	0.41
1:A:218:ARG:HH11	1:A:218:ARG:CG	2.33	0.41
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.93	0.41
1:B:50:ALA:O	1:B:51:PRO:C	2.63	0.41
1:D:251:HIS:C	1:D:252:ARG:HG2	2.45	0.41
1:F:188:ASP:HB2	1:F:232:GLU:OE2	2.21	0.41
1:H:224:ASP:HB3	1:H:341:PHE:CZ	2.56	0.41
1:H:277:ARG:CZ	1:H:281:HIS:HD2	2.33	0.41
1:A:35:ILE:HD12	1:A:35:ILE:HG23	1.65	0.41
1:E:325:LEU:O	1:E:326:LEU:C	2.64	0.41
1:G:247:GLN:O	1:G:247:GLN:OE1	2.38	0.41
1:H:330:GLN:HB2	1:H:336:TRP:CD1	2.56	0.41
1:I:259:VAL:H	1:I:259:VAL:HG23	1.56	0.41
1:B:258:ARG:NH2	1:B:361:ASP:OD1	2.54	0.41
1:E:72:LEU:HB3	5:E:2021:HOH:O	2.21	0.41
1:B:14:GLU:CD	1:B:14:GLU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ILE:CD1	1:G:230:LEU:HD12	2.50	0.41
1:I:136:ALA:HB1	1:I:139:THR:HB	2.02	0.41
1:B:168:LEU:HD23	1:B:169:MET:N	2.35	0.41
1:B:223:LEU:O	1:B:226:LEU:HB2	2.21	0.41
1:B:277:ARG:CZ	1:B:281:HIS:HD2	2.33	0.41
1:C:131:ARG:HA	1:C:131:ARG:HD2	1.82	0.41
1:D:223:LEU:HD22	1:D:274:THR:HG21	2.03	0.41
1:D:362:TYR:O	1:D:365:GLN:CG	2.69	0.41
1:G:261:VAL:N	5:G:2016:HOH:O	2.29	0.41
1:B:283:THR:HG22	1:B:286:GLN:N	2.16	0.41
1:F:244:VAL:CG1	1:F:245:VAL:H	2.33	0.41
1:G:177:LEU:O	1:G:180:ASP:N	2.54	0.41
1:A:283:THR:CG2	1:A:286:GLN:H	2.16	0.40
1:C:16:LEU:HD13	1:C:101:ALA:HB1	2.04	0.40
1:D:43:TYR:CE2	1:D:65:LEU:HD13	2.56	0.40
1:D:364:GLN:O	1:D:365:GLN:C	2.63	0.40
1:E:289:LEU:HD12	1:E:289:LEU:HA	1.97	0.40
1:F:140:TRP:CD2	1:F:367:LEU:HD13	2.56	0.40
1:H:247:GLN:HA	1:H:248:PRO:HD2	1.63	0.40
1:I:291:GLU:OE1	1:I:302:ARG:NH2	2.54	0.40
1:J:35:ILE:HD12	1:J:35:ILE:HG23	1.79	0.40
1:B:182:ARG:NH2	1:B:201:GLN:OE1	2.43	0.40
1:C:333:ASP:OD1	1:C:333:ASP:C	2.65	0.40
1:D:131:ARG:HA	1:D:131:ARG:HD2	1.82	0.40
1:D:247:GLN:HA	1:D:248:PRO:HD2	1.32	0.40
1:F:290:LEU:HB3	1:F:298:ARG:HG3	2.01	0.40
1:C:194:LEU:O	1:C:198:VAL:HG13	2.22	0.40
1:C:362:TYR:CD2	1:C:362:TYR:C	2.99	0.40
1:E:70:GLY:HA2	1:E:185:ARG:HA	2.02	0.40
1:E:168:LEU:C	1:E:168:LEU:HD23	2.46	0.40
1:I:177:LEU:CD2	1:I:198:VAL:HG22	2.52	0.40
1:A:168:LEU:C	1:A:168:LEU:CD2	2.93	0.40
1:B:97:HIS:CE1	1:B:168:LEU:HD12	2.57	0.40
1:F:110:TRP:HD1	1:F:110:TRP:H	1.68	0.40
1:H:315:GLU:HG2	1:H:370:MET:HG3	2.02	0.40
1:J:110:TRP:CD1	1:J:110:TRP:N	2.88	0.40
1:J:132:ALA:HB3	1:J:135:ASP:CG	2.46	0.40
1:J:260:PRO:HG2	1:J:263:ILE:HD12	2.03	0.40
1:A:50:ALA:O	1:A:51:PRO:C	2.63	0.40
1:A:251:HIS:C	1:A:252:ARG:HG2	2.47	0.40
1:B:214:GLY:CA	5:B:2016:HOH:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:GLN:HE21	2:E:400:GDX:HN21	1.69	0.40
1:E:364:GLN:O	1:E:365:GLN:C	2.65	0.40
1:F:224:ASP:HB3	1:F:341:PHE:CZ	2.57	0.40
1:G:262:HIS:CD2	1:G:263:ILE:HG13	2.56	0.40
1:I:330:GLN:HB2	1:I:336:TRP:CD1	2.57	0.40
1:I:339:LEU:HA	1:I:339:LEU:HD12	1.89	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:O	1:G:179:GLU:OE2[1_554]	1.86	0.34
1:A:181:GLU:OE2	1:B:64:ARG:NH2[3_545]	2.17	0.03

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	379/397 (96%)	357 (94%)	16 (4%)	6 (2%)	7	27
1	B	379/397 (96%)	363 (96%)	13 (3%)	3 (1%)	16	44
1	C	379/397 (96%)	363 (96%)	13 (3%)	3 (1%)	16	44
1	D	379/397 (96%)	360 (95%)	14 (4%)	5 (1%)	9	31
1	E	379/397 (96%)	363 (96%)	14 (4%)	2 (0%)	24	55
1	F	379/397 (96%)	364 (96%)	13 (3%)	2 (0%)	24	55
1	G	379/397 (96%)	359 (95%)	15 (4%)	5 (1%)	9	31
1	H	379/397 (96%)	365 (96%)	12 (3%)	2 (0%)	24	55
1	I	379/397 (96%)	366 (97%)	11 (3%)	2 (0%)	24	55
1	J	379/397 (96%)	353 (93%)	22 (6%)	4 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3790/3970 (96%)	3613 (95%)	143 (4%)	34 (1%)	14	41

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ASP
1	B	109	ASP
1	B	247	GLN
1	B	248	PRO
1	C	109	ASP
1	C	245	VAL
1	D	50	ALA
1	D	51	PRO
1	D	109	ASP
1	E	109	ASP
1	E	247	GLN
1	F	109	ASP
1	G	109	ASP
1	G	248	PRO
1	H	109	ASP
1	H	250	ILE
1	I	109	ASP
1	I	247	GLN
1	J	109	ASP
1	J	284	PRO
1	J	286	GLN
1	J	287	VAL
1	A	52	GLU
1	A	53	ILE
1	A	223	LEU
1	D	54	SER
1	D	248	PRO
1	F	245	VAL
1	G	178	TYR
1	A	246	GLY
1	G	72	LEU
1	G	304	CYS
1	C	250	ILE
1	A	186	ARG

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	326/338 (96%)	287 (88%)	39 (12%)	5	17
1	B	326/338 (96%)	287 (88%)	39 (12%)	5	17
1	C	326/338 (96%)	288 (88%)	38 (12%)	5	18
1	D	326/338 (96%)	284 (87%)	42 (13%)	4	14
1	E	326/338 (96%)	283 (87%)	43 (13%)	4	14
1	F	326/338 (96%)	290 (89%)	36 (11%)	6	20
1	G	326/338 (96%)	292 (90%)	34 (10%)	7	22
1	H	326/338 (96%)	288 (88%)	38 (12%)	5	18
1	I	326/338 (96%)	286 (88%)	40 (12%)	4	16
1	J	326/338 (96%)	282 (86%)	44 (14%)	4	13
All	All	3260/3380 (96%)	2867 (88%)	393 (12%)	5	16

All (393) 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	41	GLN
1	A	44	GLU
1	A	53	ILE
1	A	54	SER
1	A	55	ARG
1	A	63	VAL
1	A	65	LEU
1	A	68	ARG
1	A	72	LEU
1	A	84	LEU
1	A	91	THR
1	A	92	GLN
1	A	109	ASP

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	131	ARG
1	A	159	ILE
1	A	181	GLU
1	A	182	ARG
1	A	183	VAL
1	A	198	VAL
1	A	218	ARG
1	A	223	LEU
1	A	237	ILE
1	A	244	VAL
1	A	247	GLN
1	A	258	ARG
1	A	259	VAL
1	A	266	ARG
1	A	270	ASP
1	A	283	THR
1	A	289	LEU
1	A	301	LEU
1	A	343	LEU
1	A	357	LEU
1	A	364	GLN
1	A	365	GLN
1	B	11	GLU
1	B	14	GLU
1	B	21	ARG
1	B	41	GLN
1	B	42	THR
1	B	44	GLU
1	B	48	ARG
1	B	54	SER
1	B	63	VAL
1	B	65	LEU
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	131	ARG
1	B	159	ILE
1	B	179	GLU

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Mol	Chain	Res	Type
1	B	181	GLU
1	B	182	ARG
1	B	183	VAL
1	B	198	VAL
1	B	209	CYS
1	B	218	ARG
1	B	223	LEU
1	B	237	ILE
1	B	247	GLN
1	B	258	ARG
1	B	259	VAL
1	B	266	ARG
1	B	283	THR
1	B	289	LEU
1	B	291	GLU
1	B	301	LEU
1	B	316	MET
1	B	343	LEU
1	B	364	GLN
1	B	365	GLN
1	C	11	GLU
1	C	14	GLU
1	C	21	ARG
1	C	41	GLN
1	C	44	GLU
1	C	54	SER
1	C	63	VAL
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	142	ILE
1	C	159	ILE
1	C	179	GLU
1	C	181	GLU
1	C	182	ARG
1	C	183	VAL
1	C	198	VAL
1	C	209	CYS
1	C	211	ILE

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Mol	Chain	Res	Type
1	C	218	ARG
1	C	223	LEU
1	C	237	ILE
1	C	250	ILE
1	C	258	ARG
1	C	259	VAL
1	C	266	ARG
1	C	283	THR
1	C	289	LEU
1	C	291	GLU
1	C	301	LEU
1	C	316	MET
1	C	343	LEU
1	C	357	LEU
1	C	364	GLN
1	C	365	GLN
1	D	11	GLU
1	D	14	GLU
1	D	21	ARG
1	D	41	GLN
1	D	44	GLU
1	D	52	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	159	ILE
1	D	167	LEU
1	D	179	GLU
1	D	181	GLU
1	D	182	ARG
1	D	183	VAL
1	D	198	VAL
1	D	209	CYS
1	D	211	ILE
1	D	218	ARG

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Mol	Chain	Res	Type
1	D	223	LEU
1	D	237	ILE
1	D	244	VAL
1	D	247	GLN
1	D	258	ARG
1	D	259	VAL
1	D	266	ARG
1	D	283	THR
1	D	289	LEU
1	D	291	GLU
1	D	301	LEU
1	D	316	MET
1	D	343	LEU
1	D	357	LEU
1	D	364	GLN
1	D	365	GLN
1	E	11	GLU
1	E	14	GLU
1	E	21	ARG
1	E	41	GLN
1	E	42	THR
1	E	44	GLU
1	E	48	ARG
1	E	54	SER
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	142	ILE
1	E	159	ILE
1	E	179	GLU
1	E	181	GLU
1	E	182	ARG
1	E	183	VAL
1	E	186	ARG
1	E	198	VAL
1	E	209	CYS
1	E	218	ARG

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Mol	Chain	Res	Type
1	E	223	LEU
1	E	237	ILE
1	E	244	VAL
1	E	247	GLN
1	E	257	HIS
1	E	258	ARG
1	E	259	VAL
1	E	266	ARG
1	E	283	THR
1	E	289	LEU
1	E	291	GLU
1	E	301	LEU
1	E	316	MET
1	E	343	LEU
1	E	357	LEU
1	E	364	GLN
1	E	365	GLN
1	F	11	GLU
1	F	14	GLU
1	F	21	ARG
1	F	41	GLN
1	F	44	GLU
1	F	54	SER
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	159	ILE
1	F	179	GLU
1	F	181	GLU
1	F	182	ARG
1	F	183	VAL
1	F	198	VAL
1	F	218	ARG
1	F	223	LEU
1	F	237	ILE
1	F	247	GLN
1	F	258	ARG

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Mol	Chain	Res	Type
1	F	259	VAL
1	F	266	ARG
1	F	283	THR
1	F	289	LEU
1	F	291	GLU
1	F	301	LEU
1	F	316	MET
1	F	343	LEU
1	F	357	LEU
1	F	364	GLN
1	F	365	GLN
1	G	11	GLU
1	G	14	GLU
1	G	21	ARG
1	G	41	GLN
1	G	44	GLU
1	G	54	SER
1	G	63	VAL
1	G	65	LEU
1	G	68	ARG
1	G	72	LEU
1	G	84	LEU
1	G	92	GLN
1	G	109	ASP
1	G	124	LEU
1	G	179	GLU
1	G	181	GLU
1	G	182	ARG
1	G	183	VAL
1	G	198	VAL
1	G	218	ARG
1	G	223	LEU
1	G	237	ILE
1	G	244	VAL
1	G	247	GLN
1	G	258	ARG
1	G	259	VAL
1	G	266	ARG
1	G	283	THR
1	G	289	LEU
1	G	291	GLU
1	G	301	LEU

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Mol	Chain	Res	Type
1	G	343	LEU
1	G	364	GLN
1	G	365	GLN
1	H	11	GLU
1	H	14	GLU
1	H	21	ARG
1	H	41	GLN
1	H	42	THR
1	H	44	GLU
1	H	54	SER
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	159	ILE
1	H	179	GLU
1	H	181	GLU
1	H	182	ARG
1	H	183	VAL
1	H	198	VAL
1	H	218	ARG
1	H	223	LEU
1	H	237	ILE
1	H	244	VAL
1	H	250	ILE
1	H	257	HIS
1	H	258	ARG
1	H	259	VAL
1	H	266	ARG
1	H	283	THR
1	H	289	LEU
1	H	291	GLU
1	H	301	LEU
1	H	316	MET
1	H	343	LEU
1	H	364	GLN
1	H	365	GLN
1	I	11	GLU

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Mol	Chain	Res	Type
1	I	14	GLU
1	I	21	ARG
1	I	41	GLN
1	I	42	THR
1	I	44	GLU
1	I	54	SER
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	159	ILE
1	I	179	GLU
1	I	181	GLU
1	I	182	ARG
1	I	183	VAL
1	I	198	VAL
1	I	218	ARG
1	I	223	LEU
1	I	237	ILE
1	I	244	VAL
1	I	245	VAL
1	I	247	GLN
1	I	250	ILE
1	I	257	HIS
1	I	258	ARG
1	I	259	VAL
1	I	266	ARG
1	I	283	THR
1	I	289	LEU
1	I	291	GLU
1	I	301	LEU
1	I	316	MET
1	I	343	LEU
1	I	364	GLN
1	I	365	GLN
1	J	11	GLU
1	J	14	GLU
1	J	21	ARG

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Mol	Chain	Res	Type
1	J	41	GLN
1	J	42	THR
1	J	44	GLU
1	J	54	SER
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	142	ILE
1	J	159	ILE
1	J	167	LEU
1	J	179	GLU
1	J	181	GLU
1	J	182	ARG
1	J	183	VAL
1	J	198	VAL
1	J	211	ILE
1	J	218	ARG
1	J	223	LEU
1	J	230	LEU
1	J	237	ILE
1	J	244	VAL
1	J	245	VAL
1	J	247	GLN
1	J	258	ARG
1	J	259	VAL
1	J	266	ARG
1	J	283	THR
1	J	285	ARG
1	J	289	LEU
1	J	291	GLU
1	J	301	LEU
1	J	343	LEU
1	J	357	LEU
1	J	364	GLN
1	J	365	GLN
1	J	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	41	GLN
1	A	66	GLN
1	A	81	ASN
1	A	127	HIS
1	A	153	HIS
1	A	202	GLN
1	A	242	HIS
1	A	262	HIS
1	A	281	HIS
1	B	10	HIS
1	B	30	HIS
1	B	41	GLN
1	B	66	GLN
1	B	81	ASN
1	B	161	GLN
1	B	255	HIS
1	B	281	HIS
1	C	10	HIS
1	C	41	GLN
1	C	66	GLN
1	C	81	ASN
1	C	127	HIS
1	C	161	GLN
1	C	202	GLN
1	C	255	HIS
1	C	257	HIS
1	C	276	HIS
1	C	281	HIS
1	D	10	HIS
1	D	30	HIS
1	D	41	GLN
1	D	66	GLN
1	D	81	ASN
1	D	161	GLN
1	D	202	GLN
1	D	217	HIS
1	D	255	HIS
1	D	262	HIS
1	D	276	HIS
1	D	281	HIS
1	E	10	HIS

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Mol	Chain	Res	Type
1	E	30	HIS
1	E	41	GLN
1	E	66	GLN
1	E	81	ASN
1	E	153	HIS
1	E	161	GLN
1	E	238	GLN
1	E	255	HIS
1	E	262	HIS
1	E	276	HIS
1	E	281	HIS
1	F	10	HIS
1	F	41	GLN
1	F	66	GLN
1	F	81	ASN
1	F	161	GLN
1	F	255	HIS
1	F	262	HIS
1	F	276	HIS
1	F	281	HIS
1	G	10	HIS
1	G	41	GLN
1	G	66	GLN
1	G	81	ASN
1	G	161	GLN
1	G	238	GLN
1	G	257	HIS
1	G	262	HIS
1	G	281	HIS
1	H	10	HIS
1	H	30	HIS
1	H	41	GLN
1	H	66	GLN
1	H	81	ASN
1	H	127	HIS
1	H	161	GLN
1	H	202	GLN
1	H	255	HIS
1	H	257	HIS
1	H	262	HIS
1	H	276	HIS
1	H	281	HIS

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Mol	Chain	Res	Type
1	I	10	HIS
1	I	30	HIS
1	I	41	GLN
1	I	66	GLN
1	I	81	ASN
1	I	161	GLN
1	I	202	GLN
1	I	255	HIS
1	I	257	HIS
1	I	262	HIS
1	I	276	HIS
1	I	281	HIS
1	I	286	GLN
1	J	10	HIS
1	J	30	HIS
1	J	41	GLN
1	J	66	GLN
1	J	81	ASN
1	J	127	HIS
1	J	161	GLN
1	J	202	GLN
1	J	255	HIS
1	J	257	HIS
1	J	262	HIS
1	J	276	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 20 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	GDX	J	400	3	40,42,43	1.27	4 (10%)	59,65,67	1.54	8 (13%)
2	GDX	I	400	3	40,42,43	1.33	5 (12%)	59,65,67	1.63	12 (20%)
2	GDX	C	400	3	40,42,43	1.16	4 (10%)	59,65,67	1.72	13 (22%)
2	GDX	A	400	3	40,42,43	1.72	7 (17%)	59,65,67	1.87	14 (23%)
2	GDX	D	400	3	40,42,43	1.51	6 (15%)	59,65,67	1.69	12 (20%)
2	GDX	B	400	3	40,42,43	2.30	10 (25%)	59,65,67	1.78	13 (22%)
2	GDX	E	400	3	40,42,43	1.61	6 (15%)	59,65,67	1.74	12 (20%)
2	GDX	G	400	3	40,42,43	1.84	10 (25%)	59,65,67	1.51	9 (15%)
2	GDX	F	400	3	40,42,43	1.70	5 (12%)	59,65,67	1.69	8 (13%)
2	GDX	H	400	3	40,42,43	1.08	2 (5%)	59,65,67	1.73	10 (16%)

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	GDX	J	400	3	-	2/22/59/61	0/4/4/4
2	GDX	I	400	3	-	2/22/59/61	0/4/4/4
2	GDX	C	400	3	-	2/22/59/61	0/4/4/4
2	GDX	A	400	3	-	2/22/59/61	0/4/4/4
2	GDX	D	400	3	-	2/22/59/61	0/4/4/4
2	GDX	B	400	3	-	2/22/59/61	0/4/4/4
2	GDX	E	400	3	-	3/22/59/61	0/4/4/4
2	GDX	G	400	3	-	3/22/59/61	0/4/4/4
2	GDX	F	400	3	-	2/22/59/61	0/4/4/4
2	GDX	H	400	3	-	2/22/59/61	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	GDX	PA-O3A	-8.75	1.50	1.59
2	B	400	GDX	PB-O3A	-7.31	1.51	1.59
2	F	400	GDX	PB-O3A	6.76	1.66	1.59
2	A	400	GDX	O5'-C5'	6.24	1.53	1.43
2	G	400	GDX	O5'-C5'	6.04	1.53	1.43
2	E	400	GDX	O5'-C5'	5.34	1.52	1.43
2	G	400	GDX	PA-O3A	5.08	1.65	1.59
2	A	400	GDX	PB-O3A	-4.91	1.54	1.59
2	F	400	GDX	O5'-C5'	4.58	1.51	1.43
2	D	400	GDX	O5'-C5'	4.38	1.50	1.43
2	D	400	GDX	C5-N7	-4.10	1.30	1.39
2	I	400	GDX	PB-O3A	4.09	1.63	1.59
2	J	400	GDX	PA-O3A	3.82	1.63	1.59
2	B	400	GDX	PA-O5D	3.64	1.73	1.59
2	E	400	GDX	C5-N7	-3.55	1.31	1.39
2	B	400	GDX	O5'-C5'	3.47	1.49	1.43
2	G	400	GDX	C5-N7	-3.39	1.32	1.39
2	H	400	GDX	C5-N7	-3.33	1.32	1.39
2	E	400	GDX	O5'-C1'	3.30	1.50	1.41
2	D	400	GDX	PB-O3A	3.22	1.63	1.59
2	I	400	GDX	C5-N7	-3.19	1.32	1.39
2	F	400	GDX	PA-O3A	3.09	1.62	1.59
2	E	400	GDX	PB-O2B	-3.08	1.41	1.55
2	J	400	GDX	C5-N7	-3.05	1.33	1.39
2	F	400	GDX	C5-N7	-2.89	1.33	1.39
2	B	400	GDX	PB-O1B	2.85	1.67	1.59
2	C	400	GDX	O5'-C5'	2.78	1.48	1.43
2	C	400	GDX	C5-N7	-2.78	1.33	1.39
2	D	400	GDX	PA-O3A	2.75	1.62	1.59
2	I	400	GDX	PA-O3A	2.67	1.62	1.59
2	A	400	GDX	PB-O1B	2.64	1.67	1.59
2	G	400	GDX	PB-O1B	2.62	1.67	1.59
2	E	400	GDX	O2'-C2'	2.60	1.49	1.43
2	I	400	GDX	O5'-C5'	2.59	1.47	1.43
2	B	400	GDX	C5-N7	-2.59	1.33	1.39
2	D	400	GDX	O2'-C2'	2.56	1.49	1.43
2	A	400	GDX	C4-N9	-2.52	1.31	1.38
2	A	400	GDX	C5-N7	-2.51	1.34	1.39
2	D	400	GDX	C5-C6	-2.47	1.35	1.44
2	G	400	GDX	C4'-C5'	2.45	1.56	1.52
2	B	400	GDX	C5-C6	-2.37	1.35	1.44
2	G	400	GDX	O5'-C1'	2.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	GDX	PA-O2A	-2.27	1.44	1.55
2	E	400	GDX	C4-N9	-2.24	1.32	1.38
2	J	400	GDX	O5'-C5'	2.22	1.47	1.43
2	A	400	GDX	O5'-C1'	2.20	1.47	1.41
2	G	400	GDX	O6A-C6'	2.19	1.28	1.20
2	G	400	GDX	O2'-C2'	2.17	1.48	1.43
2	G	400	GDX	C4-N9	-2.17	1.32	1.38
2	C	400	GDX	PA-O2A	-2.16	1.45	1.55
2	C	400	GDX	PB-O3A	2.14	1.61	1.59
2	B	400	GDX	C8-N9	-2.11	1.32	1.37
2	I	400	GDX	C4-N9	-2.10	1.32	1.38
2	H	400	GDX	PB-O1B	2.08	1.65	1.59
2	J	400	GDX	PB-O3A	2.08	1.61	1.59
2	B	400	GDX	O2'-C2'	2.04	1.48	1.43
2	G	400	GDX	PA-O5D	2.04	1.67	1.59
2	A	400	GDX	C4'-C5'	2.03	1.56	1.52
2	F	400	GDX	C4-N9	-2.02	1.32	1.38

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GDX	C1'-O5'-C5'	-6.63	105.48	113.08
2	F	400	GDX	O5'-C1'-O1B	-5.94	103.61	111.36
2	H	400	GDX	C2-N3-C4	5.63	122.00	112.30
2	E	400	GDX	O1B-C1'-C2'	5.63	118.69	108.38
2	B	400	GDX	O1B-C1'-C2'	5.55	118.55	108.38
2	A	400	GDX	C2-N3-C4	5.21	121.27	112.30
2	D	400	GDX	O1B-C1'-C2'	5.20	117.91	108.38
2	J	400	GDX	C2-N3-C4	4.88	120.70	112.30
2	C	400	GDX	O1B-C1'-C2'	4.83	117.23	108.38
2	H	400	GDX	C5-C4-N3	-4.81	120.73	128.39
2	C	400	GDX	C2-N3-C4	4.76	120.50	112.30
2	I	400	GDX	C2-N3-C4	4.67	120.34	112.30
2	C	400	GDX	C5-C4-N3	-4.61	121.05	128.39
2	I	400	GDX	C5-C4-N3	-4.57	121.12	128.39
2	J	400	GDX	C5-C4-N3	-4.56	121.13	128.39
2	E	400	GDX	C2-N3-C4	4.54	120.11	112.30
2	F	400	GDX	C2-N3-C4	4.52	120.09	112.30
2	F	400	GDX	O1B-C1'-C2'	4.52	116.66	108.38
2	D	400	GDX	C2-N3-C4	4.51	120.08	112.30
2	A	400	GDX	C5-C4-N3	-4.49	121.24	128.39
2	E	400	GDX	O5'-C1'-C2'	-4.47	101.19	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	GDX	C5-C4-N3	-4.40	121.39	128.39
2	E	400	GDX	C5-C4-N3	-4.39	121.40	128.39
2	G	400	GDX	C2-N3-C4	4.38	119.84	112.30
2	D	400	GDX	C5-C4-N3	-4.28	121.57	128.39
2	I	400	GDX	O5'-C1'-C2'	-4.25	101.64	110.37
2	H	400	GDX	O1B-C1'-C2'	4.11	115.91	108.38
2	G	400	GDX	O5'-C1'-O1B	-4.10	106.00	111.36
2	B	400	GDX	O1B-PB-O3B	-4.01	96.99	109.81
2	G	400	GDX	C5-C4-N3	-3.89	122.20	128.39
2	D	400	GDX	O5'-C1'-C2'	-3.77	102.62	110.37
2	J	400	GDX	O1B-C1'-C2'	3.62	115.01	108.38
2	I	400	GDX	O1B-C1'-C2'	3.44	114.67	108.38
2	B	400	GDX	C2-N3-C4	3.42	118.19	112.30
2	H	400	GDX	O5'-C1'-C2'	-3.41	103.36	110.37
2	J	400	GDX	O5'-C1'-C2'	-3.35	103.48	110.37
2	H	400	GDX	C2-N1-C6	-3.28	119.17	125.11
2	I	400	GDX	C2-N1-C6	-3.25	119.22	125.11
2	B	400	GDX	C1'-O5'-C5'	-3.23	109.38	113.08
2	B	400	GDX	O2B-PB-O3B	3.21	127.39	112.44
2	C	400	GDX	O5'-C1'-C2'	-3.20	103.79	110.37
2	H	400	GDX	N9-C4-N3	3.14	132.23	125.95
2	A	400	GDX	O1B-PB-O3B	-3.09	99.94	109.81
2	G	400	GDX	C1'-O5'-C5'	-3.07	109.56	113.08
2	F	400	GDX	C2-N1-C6	-3.06	119.55	125.11
2	B	400	GDX	O2A-PA-O3A	3.01	115.40	107.27
2	F	400	GDX	N9-C4-N3	2.99	131.94	125.95
2	B	400	GDX	C5-C4-N3	-2.98	123.64	128.39
2	A	400	GDX	O4'-C4'-C3'	-2.98	103.36	110.38
2	G	400	GDX	O5'-C1'-C2'	-2.96	104.29	110.37
2	I	400	GDX	C1'-O5'-C5'	-2.95	109.70	113.08
2	D	400	GDX	O5'-C1'-O1B	-2.94	107.52	111.36
2	E	400	GDX	N9-C4-N3	2.94	131.83	125.95
2	C	400	GDX	N9-C4-N3	2.84	131.64	125.95
2	E	400	GDX	C3'-C4'-C5'	-2.80	106.94	110.26
2	A	400	GDX	O3A-PA-O1A	2.79	119.11	110.70
2	A	400	GDX	N9-C4-N3	2.78	131.51	125.95
2	C	400	GDX	O4D-C1D-C2D	-2.69	100.86	106.62
2	D	400	GDX	O2B-PB-O3A	2.64	114.42	107.27
2	B	400	GDX	O2A-PA-O5D	-2.64	95.62	107.57
2	I	400	GDX	N9-C4-N3	2.63	131.20	125.95
2	D	400	GDX	N9-C4-N3	2.60	131.16	125.95
2	A	400	GDX	O5'-C1'-C2'	-2.60	105.04	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	400	GDX	C2-N1-C6	-2.58	120.43	125.11
2	B	400	GDX	C4'-C3'-C2'	-2.57	106.32	110.83
2	J	400	GDX	N9-C4-N3	2.54	131.04	125.95
2	F	400	GDX	O6-C6-C5	-2.54	119.82	126.53
2	A	400	GDX	N1-C2-N3	-2.53	118.69	123.32
2	B	400	GDX	O5'-C1'-O1B	-2.50	108.09	111.36
2	B	400	GDX	N9-C4-N3	2.48	130.92	125.95
2	C	400	GDX	C1'-O5'-C5'	-2.47	110.25	113.08
2	H	400	GDX	C5-C6-N1	2.45	119.48	113.25
2	A	400	GDX	C6-C5-N7	2.44	134.73	130.29
2	H	400	GDX	O5'-C1'-O1B	-2.43	108.19	111.36
2	E	400	GDX	C1'-O5'-C5'	-2.37	110.36	113.08
2	G	400	GDX	N9-C4-N3	2.37	130.69	125.95
2	H	400	GDX	O6-C6-C5	-2.33	120.39	126.53
2	C	400	GDX	C4'-C5'-C6'	-2.32	108.70	112.56
2	C	400	GDX	O5'-C1'-O1B	-2.27	108.40	111.36
2	A	400	GDX	O4D-C1D-C2D	-2.25	101.79	106.62
2	E	400	GDX	C4'-C5'-C6'	-2.25	108.82	112.56
2	J	400	GDX	O5'-C1'-O1B	-2.24	108.43	111.36
2	B	400	GDX	N9-C8-N7	-2.22	109.29	113.40
2	C	400	GDX	O4D-C4D-C5D	-2.21	102.26	109.33
2	E	400	GDX	O4D-C1D-C2D	-2.20	101.90	106.62
2	A	400	GDX	O1B-C1'-C2'	2.20	112.41	108.38
2	A	400	GDX	C4-C5-N7	-2.19	107.20	110.67
2	I	400	GDX	C4-C5-N7	-2.19	107.20	110.67
2	C	400	GDX	C2-N1-C6	-2.17	121.17	125.11
2	D	400	GDX	C2-N1-C6	-2.16	121.19	125.11
2	D	400	GDX	O6-C6-C5	-2.15	120.85	126.53
2	E	400	GDX	PB-O1B-C1'	2.15	129.97	121.21
2	J	400	GDX	O4D-C1D-N9	-2.15	103.49	108.36
2	D	400	GDX	N9-C8-N7	-2.14	109.43	113.40
2	H	400	GDX	O4D-C1D-C2D	-2.14	102.03	106.62
2	E	400	GDX	C5-C6-N1	2.14	118.70	113.25
2	E	400	GDX	O4D-C4D-C5D	-2.14	102.48	109.33
2	C	400	GDX	N2-C2-N1	2.13	121.26	116.76
2	F	400	GDX	C1'-O5'-C5'	-2.11	110.66	113.08
2	A	400	GDX	C5-C6-N1	2.11	118.62	113.25
2	I	400	GDX	O4D-C1D-N9	-2.11	103.58	108.36
2	G	400	GDX	O2B-PB-O3A	2.10	112.96	107.27
2	G	400	GDX	O4'-C4'-C5'	2.09	114.94	110.36
2	I	400	GDX	O4D-C1D-C2D	-2.08	102.17	106.62
2	B	400	GDX	O5'-C1'-C2'	-2.05	106.16	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	400	GDX	O2B-PB-O3B	2.05	121.97	112.44
2	D	400	GDX	C8-N7-C5	2.04	107.90	104.26
2	D	400	GDX	N1-C2-N3	-2.02	119.62	123.32
2	I	400	GDX	C5-C6-N1	2.01	118.36	113.25
2	C	400	GDX	C4-C5-N7	-2.01	107.49	110.67
2	I	400	GDX	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	GDX	O5'-C1'-O1B-PB
2	A	400	GDX	C2'-C1'-O1B-PB
2	B	400	GDX	O5'-C1'-O1B-PB
2	B	400	GDX	C2'-C1'-O1B-PB
2	C	400	GDX	O5'-C1'-O1B-PB
2	C	400	GDX	C2'-C1'-O1B-PB
2	D	400	GDX	O5'-C1'-O1B-PB
2	D	400	GDX	C2'-C1'-O1B-PB
2	E	400	GDX	O5'-C1'-O1B-PB
2	E	400	GDX	C2'-C1'-O1B-PB
2	E	400	GDX	C4'-C5'-C6'-O6A
2	F	400	GDX	O5'-C1'-O1B-PB
2	F	400	GDX	C2'-C1'-O1B-PB
2	G	400	GDX	C1'-O1B-PB-O3B
2	G	400	GDX	O5'-C1'-O1B-PB
2	G	400	GDX	C2'-C1'-O1B-PB
2	H	400	GDX	O5'-C1'-O1B-PB
2	H	400	GDX	C2'-C1'-O1B-PB
2	I	400	GDX	O5'-C1'-O1B-PB
2	I	400	GDX	C2'-C1'-O1B-PB
2	J	400	GDX	O5'-C1'-O1B-PB
2	J	400	GDX	C2'-C1'-O1B-PB

There are no ring outliers.

10 monomers are involved in 33 short contacts:

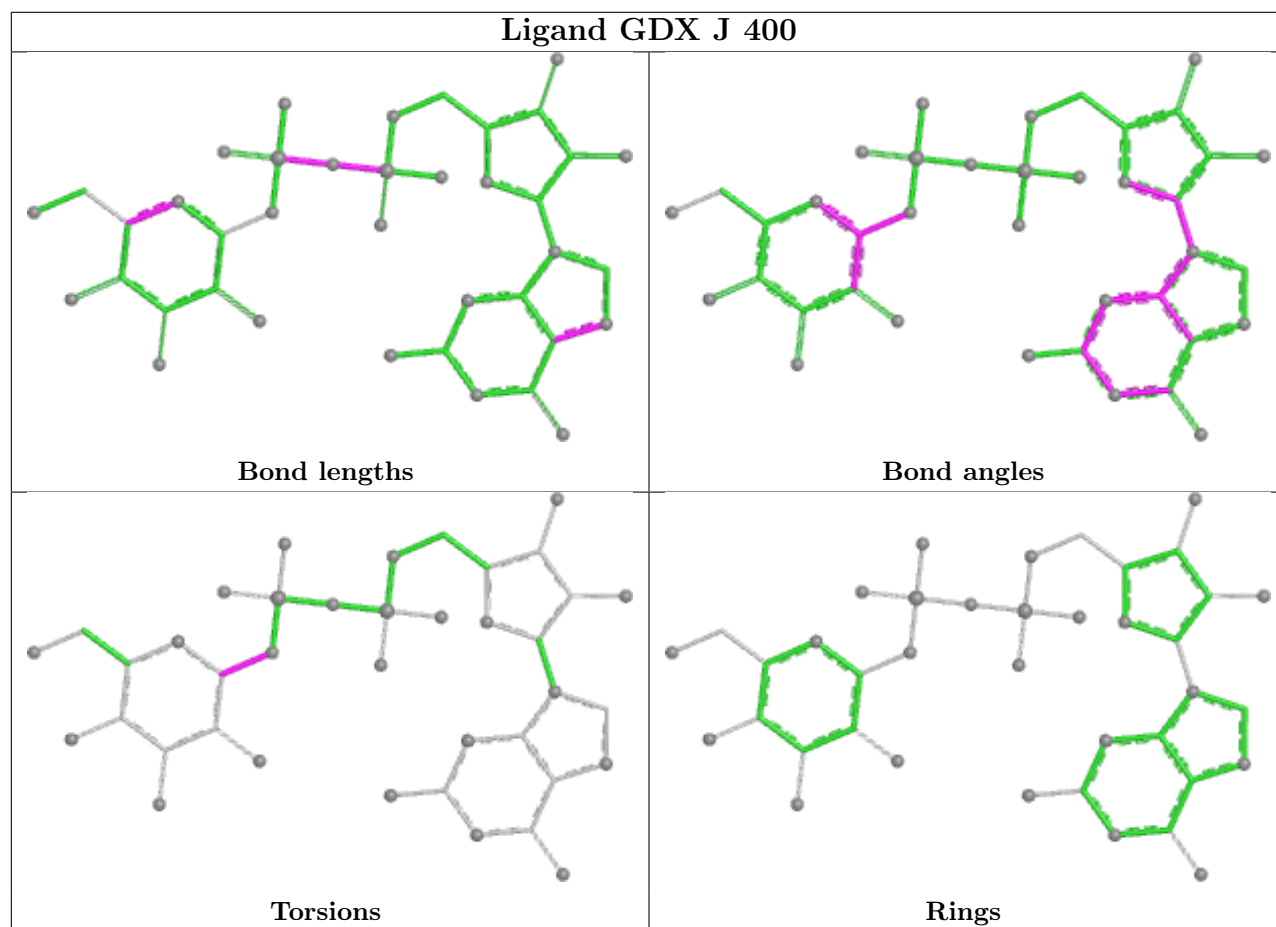
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	400	GDX	3	0
2	I	400	GDX	3	0
2	C	400	GDX	3	0

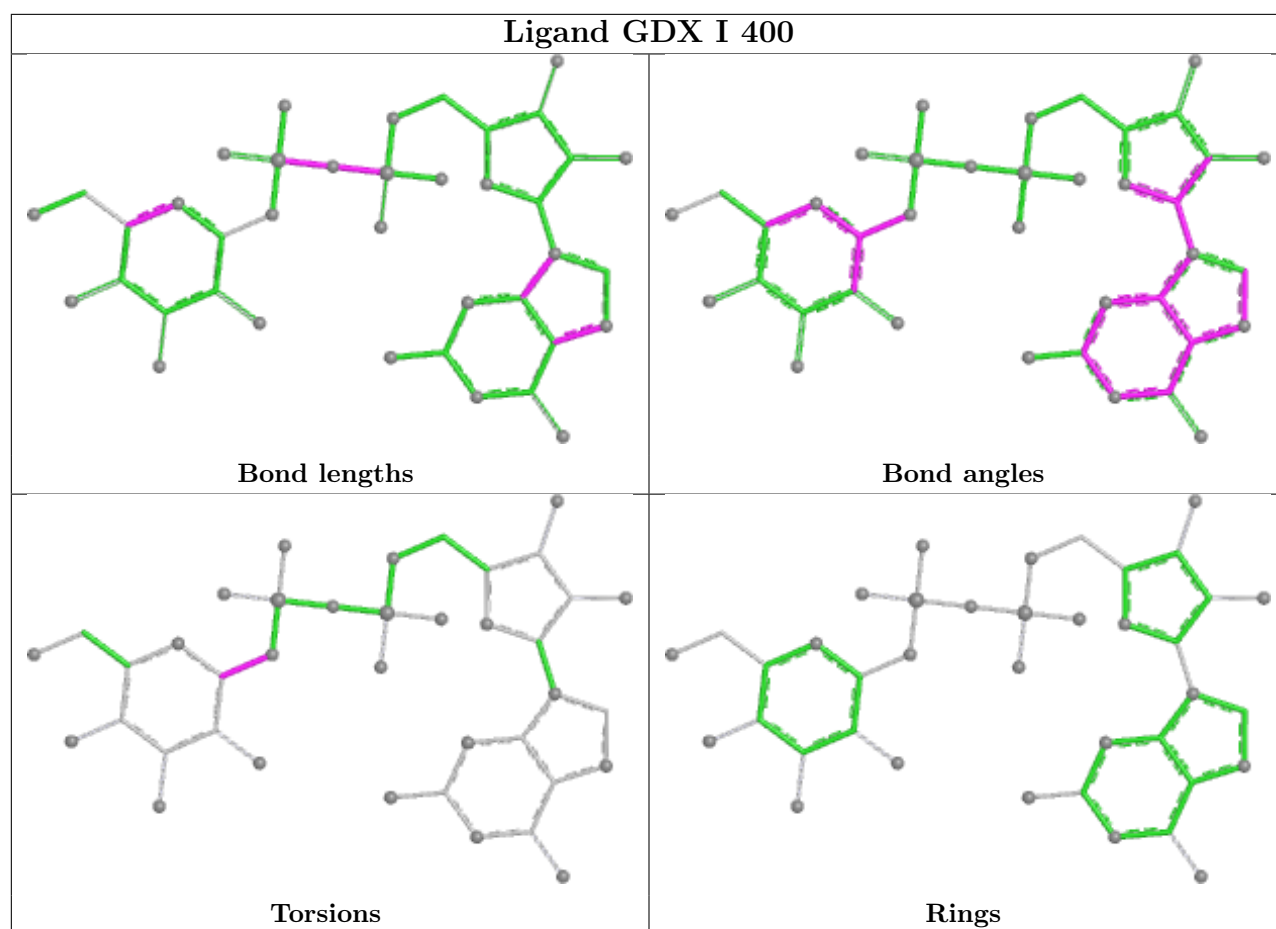
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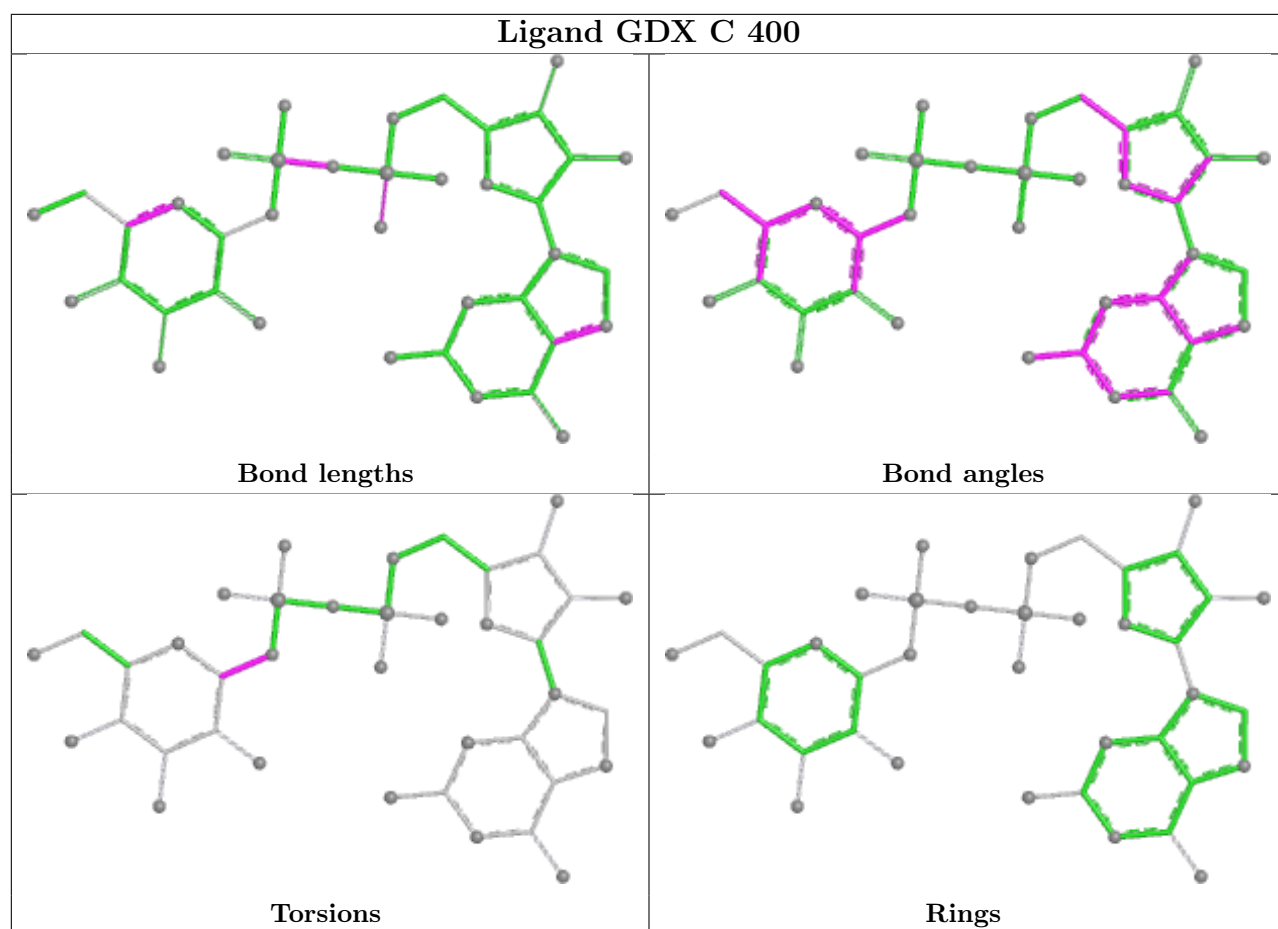
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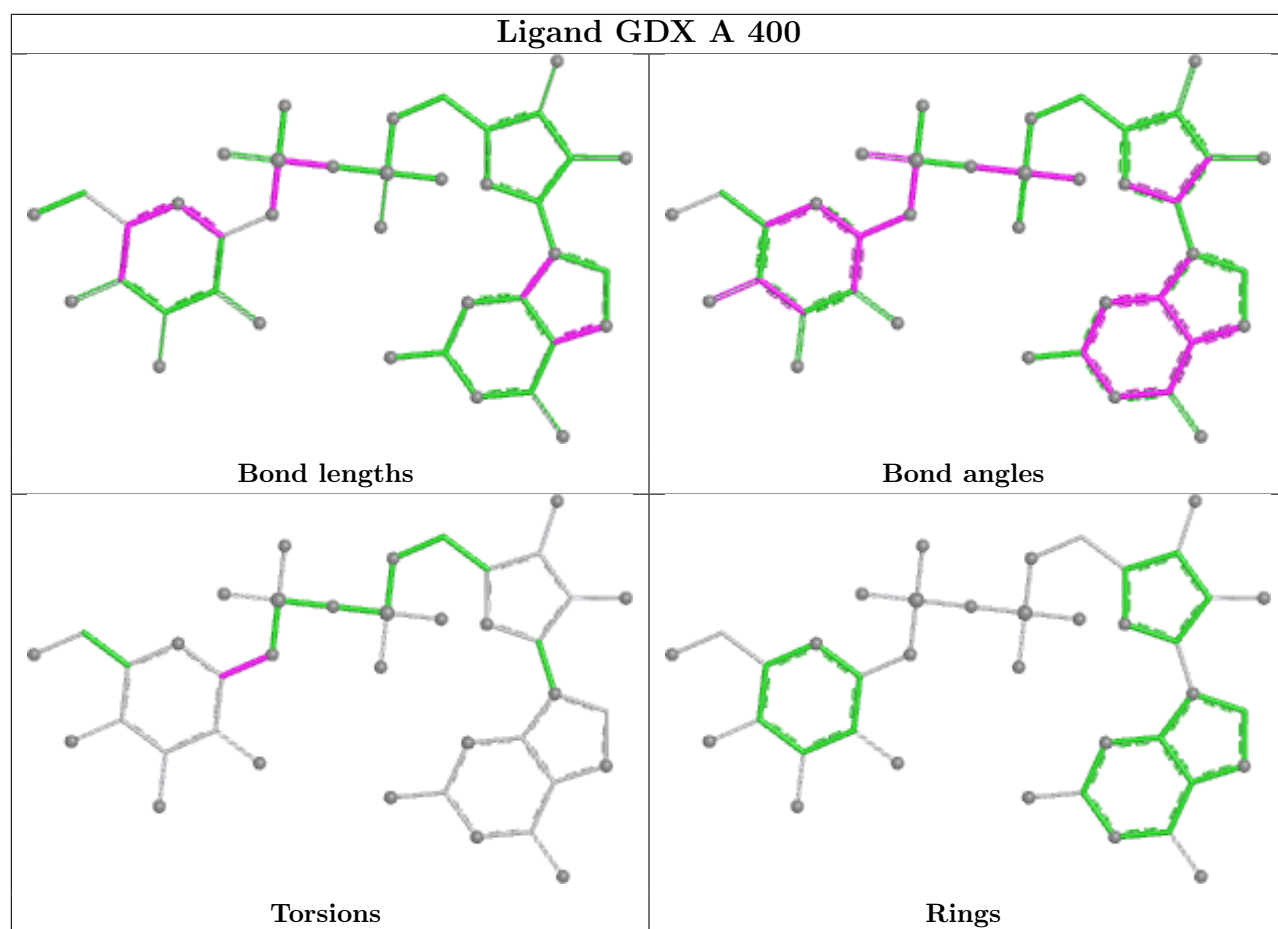
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	GDX	4	0
2	D	400	GDX	4	0
2	B	400	GDX	4	0
2	E	400	GDX	3	0
2	G	400	GDX	3	0
2	F	400	GDX	3	0
2	H	400	GDX	3	0

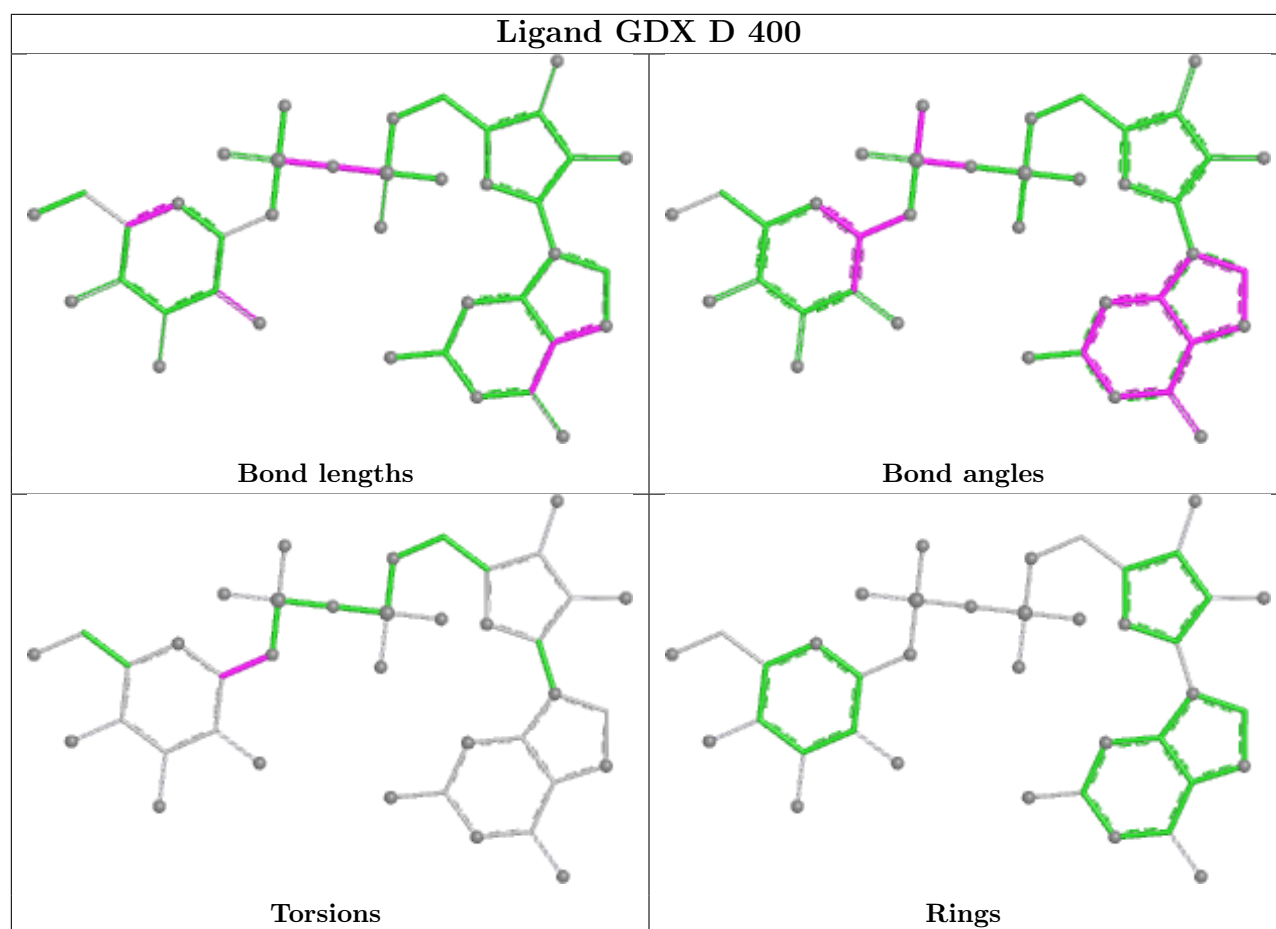
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

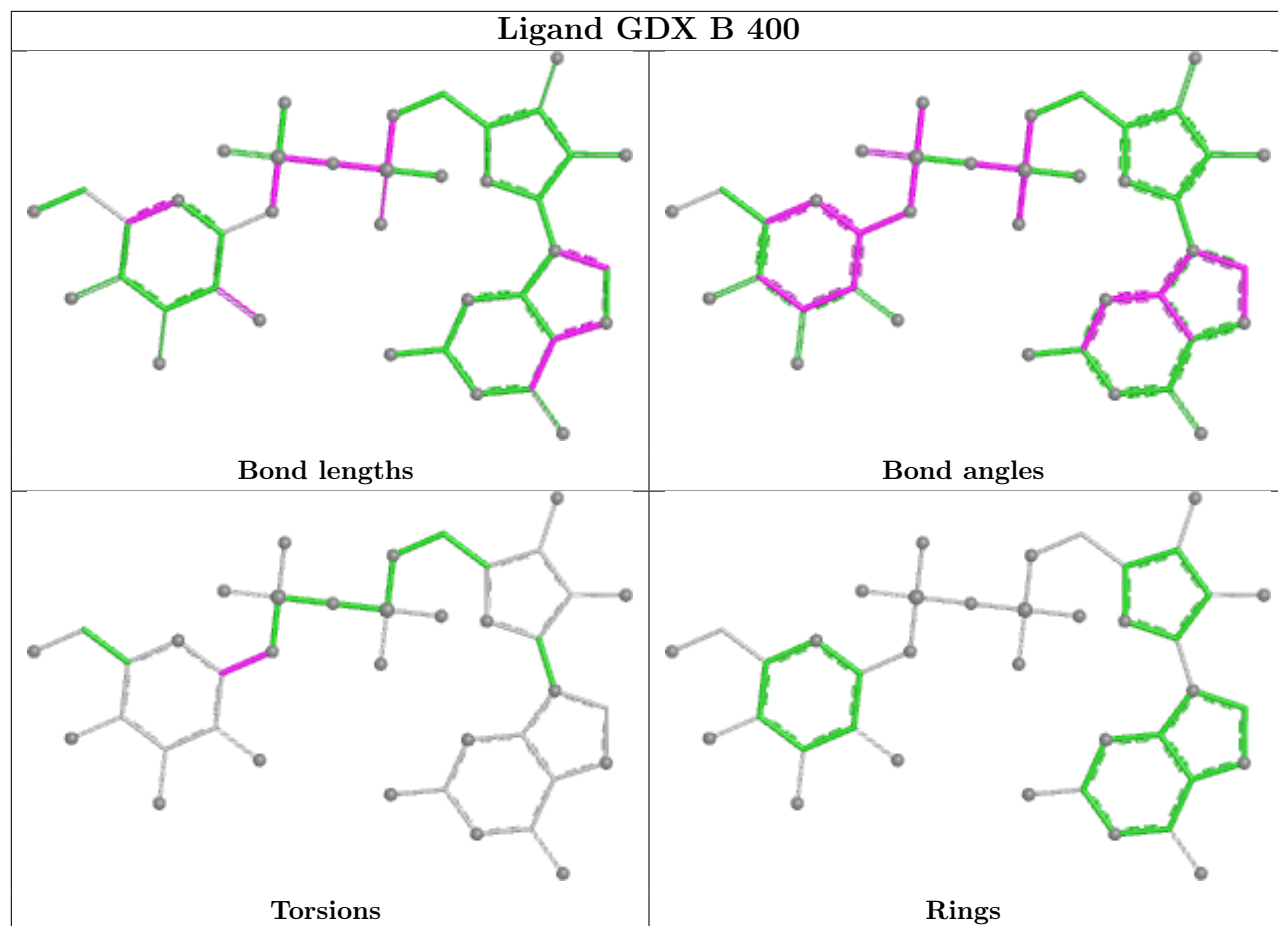


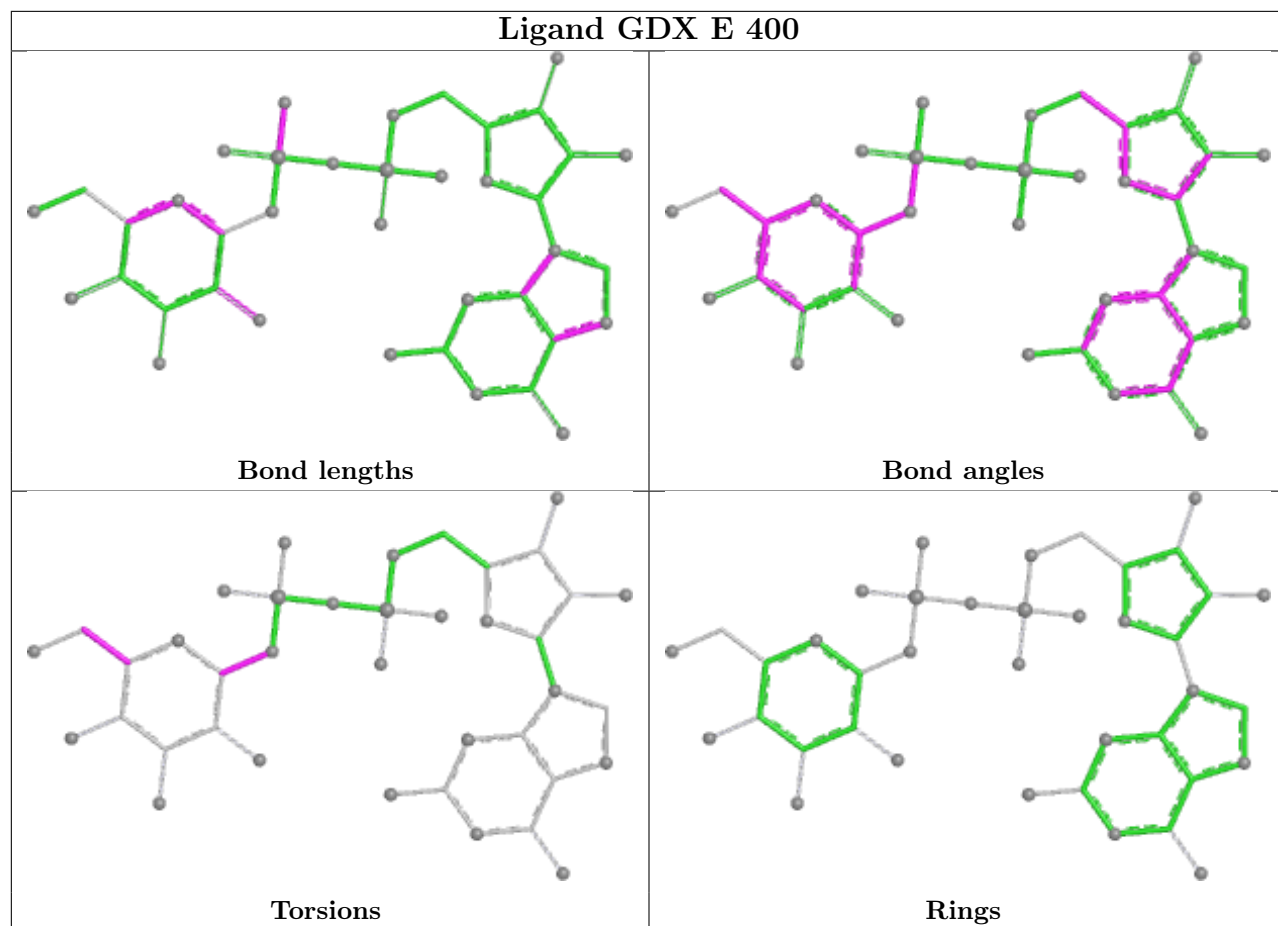


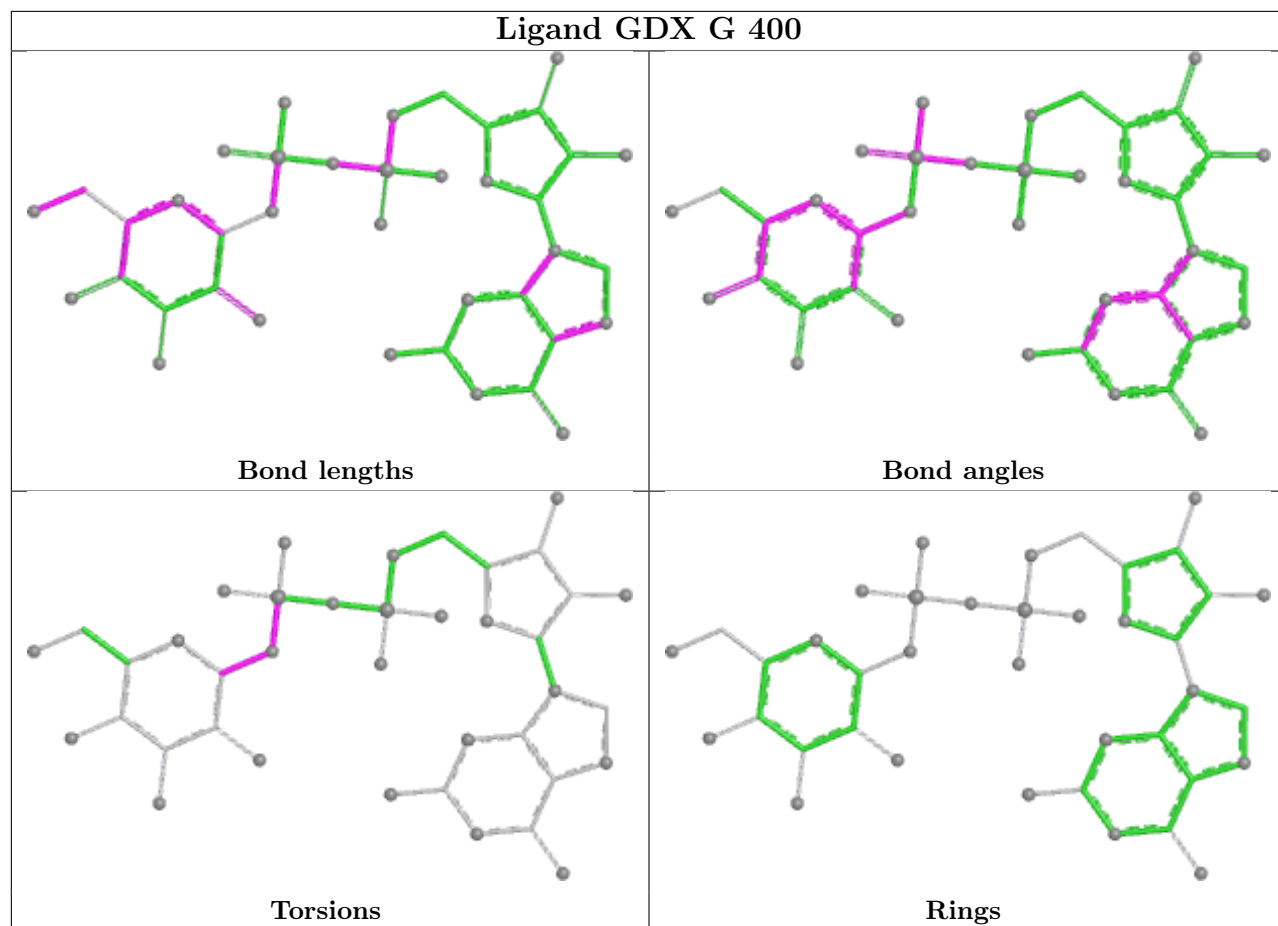


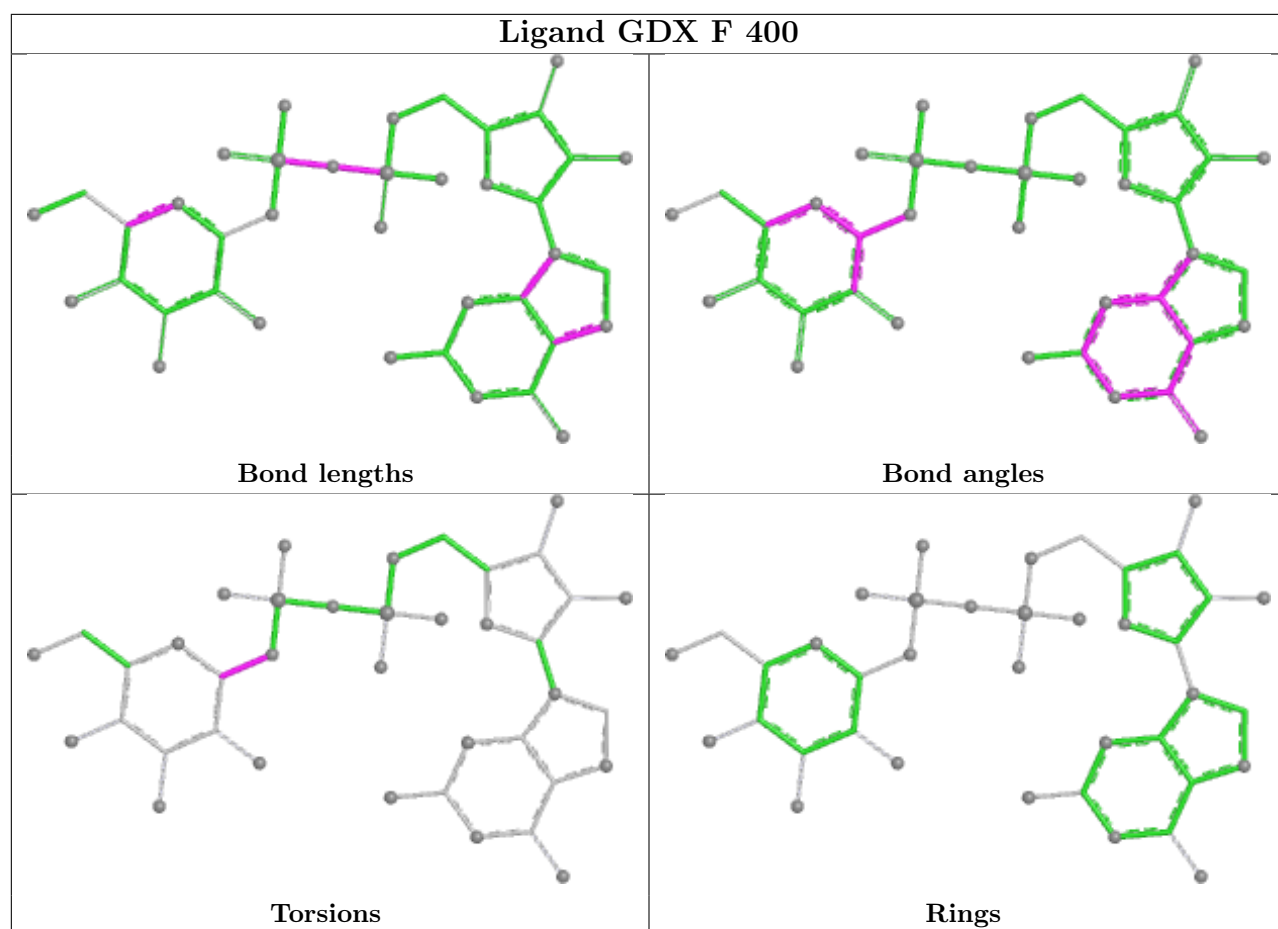


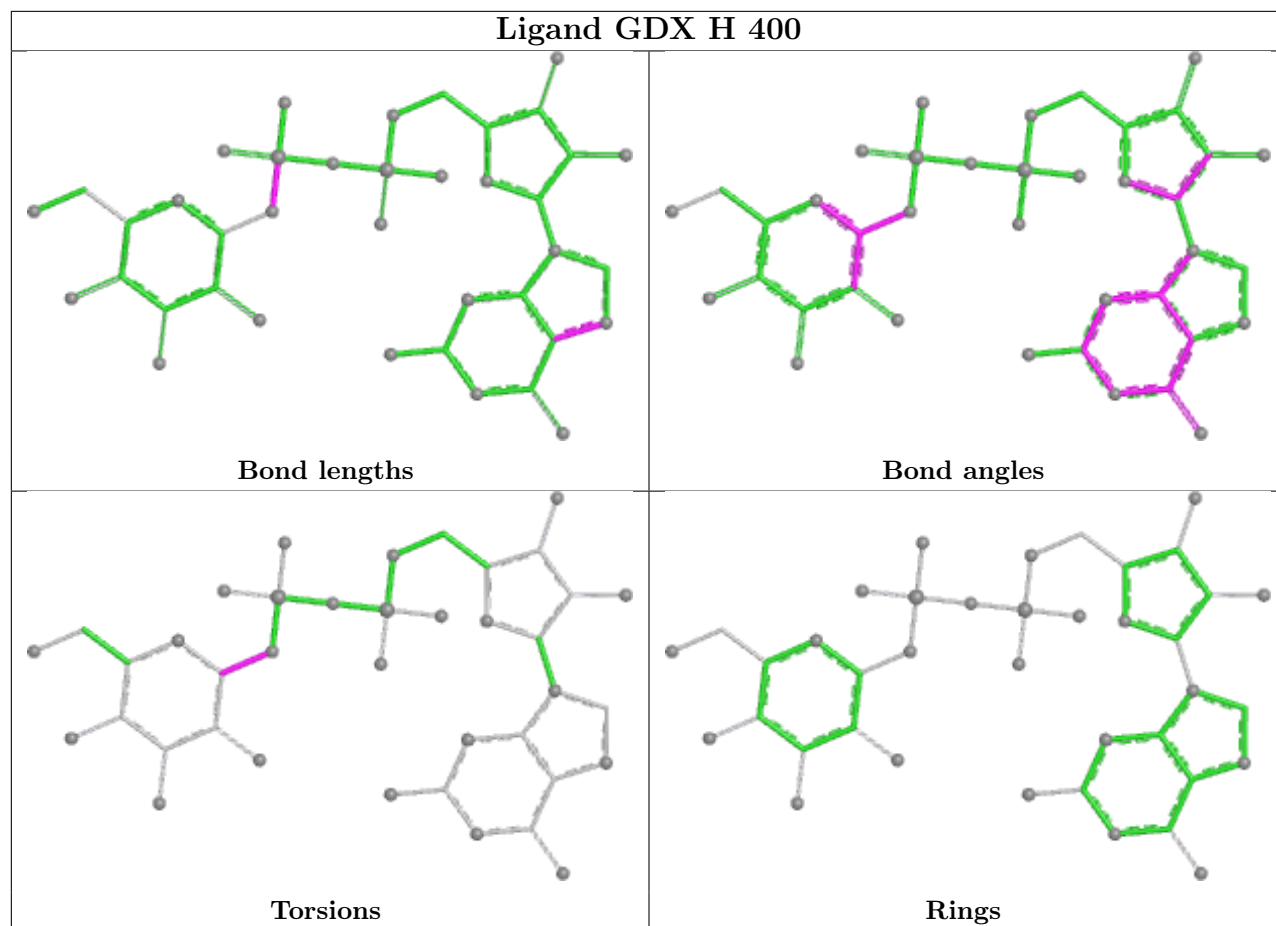












5.7 Other polymers [i](#)

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	381/397 (95%)	2.34	234 (61%) 0 0	50, 57, 67, 83	0
1	B	381/397 (95%)	2.27	233 (61%) 0 0	49, 57, 67, 83	0
1	C	381/397 (95%)	1.15	48 (12%) 8 6	50, 57, 67, 83	0
1	D	381/397 (95%)	1.25	63 (16%) 4 3	50, 57, 67, 83	0
1	E	381/397 (95%)	1.24	51 (13%) 7 5	50, 57, 67, 83	0
1	F	381/397 (95%)	1.70	128 (33%) 1 1	50, 57, 67, 83	0
1	G	381/397 (95%)	1.87	156 (40%) 0 0	50, 57, 67, 83	0
1	H	381/397 (95%)	1.18	48 (12%) 8 6	50, 57, 67, 83	0
1	I	381/397 (95%)	1.01	27 (7%) 22 16	50, 57, 67, 83	0
1	J	381/397 (95%)	1.40	84 (22%) 2 2	50, 57, 67, 83	0
All	All	3810/3970 (95%)	1.54	1072 (28%) 1 1	49, 57, 68, 83	0

All (1072) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	382	ASN	12.8
1	A	376	TYR	7.7
1	F	36	GLY	6.8
1	A	220	TYR	6.5
1	B	382	ASN	6.3
1	A	2	SER	5.5
1	G	223	LEU	5.5
1	B	364	GLN	5.3
1	A	222	GLY	5.0
1	B	185	ARG	5.0
1	A	247	GLN	4.9
1	A	224	ASP	4.9
1	F	216	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLU	4.8
1	F	65	LEU	4.8
1	F	86	TYR	4.7
1	A	380	LEU	4.7
1	B	92	GLN	4.7
1	F	32	VAL	4.7
1	B	247	GLN	4.6
1	F	8	PHE	4.6
1	A	253	GLN	4.6
1	E	376	TYR	4.5
1	F	43	TYR	4.5
1	C	184	ARG	4.5
1	F	219	LEU	4.5
1	A	214	GLY	4.5
1	B	377	GLN	4.5
1	B	183	VAL	4.4
1	B	220	TYR	4.4
1	F	7	PRO	4.4
1	F	165	GLY	4.3
1	F	38	GLU	4.3
1	A	133	SER	4.3
1	A	223	LEU	4.3
1	A	365	GLN	4.3
1	F	93	TRP	4.3
1	F	15	VAL	4.3
1	F	82	THR	4.3
1	F	81	ASN	4.2
1	J	2	SER	4.2
1	B	39	ARG	4.2
1	A	236	ALA	4.2
1	I	246	GLY	4.2
1	H	219	LEU	4.2
1	J	246	GLY	4.2
1	D	41	GLN	4.1
1	A	140	TRP	4.1
1	A	318	TRP	4.1
1	F	59	THR	4.1
1	G	219	LEU	4.1
1	F	63	VAL	4.1
1	J	221	GLY	4.1
1	B	165	GLY	4.0
1	F	79	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	373	ARG	4.0
1	F	46	VAL	4.0
1	F	83	ALA	4.0
1	B	99	TYR	4.0
1	C	135	ASP	4.0
1	A	268	GLY	4.0
1	B	223	LEU	4.0
1	F	84	LEU	4.0
1	A	221	GLY	3.9
1	B	179	GLU	3.9
1	A	267	VAL	3.9
1	G	2	SER	3.9
1	A	191	ILE	3.9
1	A	233	CYS	3.9
1	B	86	TYR	3.9
1	B	100	ASP	3.9
1	G	33	LEU	3.9
1	B	37	TYR	3.9
1	A	227	ARG	3.9
1	F	218	ARG	3.8
1	G	13	PRO	3.8
1	D	2	SER	3.8
1	F	44	GLU	3.8
1	J	93	TRP	3.8
1	E	381	GLU	3.8
1	B	78	ASP	3.8
1	F	33	LEU	3.8
1	B	139	THR	3.8
1	F	37	TYR	3.8
1	A	164	GLY	3.8
1	B	63	VAL	3.7
1	G	15	VAL	3.7
1	G	46	VAL	3.7
1	A	7	PRO	3.7
1	D	246	GLY	3.7
1	B	306	ARG	3.7
1	C	217	HIS	3.7
1	J	37	TYR	3.7
1	A	354	THR	3.7
1	B	138	ILE	3.7
1	B	236	ALA	3.7
1	B	233	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	76	LYS	3.7
1	A	326	LEU	3.7
1	E	10	HIS	3.7
1	I	219	LEU	3.7
1	A	218	ARG	3.7
1	G	98	PHE	3.7
1	J	33	LEU	3.6
1	A	165	GLY	3.6
1	G	221	GLY	3.6
1	B	380	LEU	3.6
1	J	13	PRO	3.6
1	A	147	PHE	3.6
1	G	43	TYR	3.6
1	G	267	VAL	3.6
1	E	59	THR	3.6
1	B	224	ASP	3.6
1	A	244	VAL	3.6
1	C	288	GLU	3.6
1	D	382	ASN	3.6
1	G	99	TYR	3.6
1	G	59	THR	3.6
1	B	79	GLY	3.6
1	C	380	LEU	3.6
1	A	331	PRO	3.6
1	F	87	PHE	3.5
1	F	99	TYR	3.5
1	J	59	THR	3.5
1	A	120	PHE	3.5
1	A	237	ILE	3.5
1	F	88	LEU	3.5
1	B	344	TRP	3.5
1	A	9	LYS	3.5
1	A	212	PRO	3.5
1	A	181	GLU	3.5
1	B	326	LEU	3.5
1	J	301	LEU	3.5
1	A	162	PRO	3.5
1	B	82	THR	3.5
1	J	382	ASN	3.5
1	B	378	ALA	3.5
1	B	268	GLY	3.5
1	F	246	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	12	HIS	3.5
1	F	30	HIS	3.5
1	B	142	ILE	3.4
1	B	36	GLY	3.4
1	G	77	GLY	3.4
1	D	219	LEU	3.4
1	A	160	GLU	3.4
1	J	334	PRO	3.4
1	A	129	PHE	3.4
1	A	215	LYS	3.4
1	A	316	MET	3.4
1	A	230	LEU	3.4
1	E	112	THR	3.4
1	D	300	GLY	3.4
1	B	381	GLU	3.4
1	B	152	PRO	3.4
1	B	331	PRO	3.4
1	A	255	HIS	3.4
1	F	62	SER	3.4
1	B	180	ASP	3.4
1	J	36	GLY	3.4
1	A	280	GLN	3.4
1	A	188	ASP	3.4
1	A	72	LEU	3.3
1	G	5	VAL	3.3
1	A	55	ARG	3.3
1	F	2	SER	3.3
1	J	57	THR	3.3
1	B	70	GLY	3.3
1	F	48	ARG	3.3
1	B	291	GLU	3.3
1	F	31	GLU	3.3
1	B	140	TRP	3.3
1	B	188	ASP	3.3
1	F	60	PRO	3.3
1	D	120	PHE	3.3
1	B	64	ARG	3.3
1	F	66	GLN	3.3
1	A	332	GLY	3.3
1	E	146	GLY	3.3
1	F	220	TYR	3.3
1	A	96	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	10	HIS	3.3
1	G	363	ALA	3.3
1	A	8	PHE	3.3
1	A	258	ARG	3.3
1	I	41	GLN	3.3
1	A	139	THR	3.3
1	A	344	TRP	3.3
1	A	148	ALA	3.2
1	F	255	HIS	3.2
1	G	10	HIS	3.2
1	A	269	TYR	3.2
1	B	210	TYR	3.2
1	G	382	ASN	3.2
1	A	168	LEU	3.2
1	A	379	ALA	3.2
1	F	49	ALA	3.2
1	B	302	ARG	3.2
1	J	41	GLN	3.2
1	B	75	GLY	3.2
1	B	300	GLY	3.2
1	F	42	THR	3.2
1	G	165	GLY	3.2
1	B	110	TRP	3.2
1	A	30	HIS	3.2
1	D	255	HIS	3.2
1	A	329	PHE	3.2
1	A	79	GLY	3.2
1	B	213	GLU	3.2
1	A	130	PRO	3.2
1	A	366	TYR	3.2
1	F	96	ILE	3.2
1	G	191	ILE	3.2
1	F	17	LEU	3.2
1	J	6	PHE	3.2
1	B	231	VAL	3.2
1	A	232	GLU	3.2
1	C	381	GLU	3.2
1	J	38	GLU	3.2
1	A	189	TRP	3.2
1	G	101	ALA	3.1
1	H	382	ASN	3.1
1	D	29	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	GLY	3.1
1	A	123	GLY	3.1
1	B	44	GLU	3.1
1	C	185	ARG	3.1
1	J	65	LEU	3.1
1	A	37	TYR	3.1
1	A	97	HIS	3.1
1	A	246	GLY	3.1
1	B	332	GLY	3.1
1	A	228	THR	3.1
1	B	35	ILE	3.1
1	A	351	TYR	3.1
1	B	351	TYR	3.1
1	H	220	TYR	3.1
1	B	109	ASP	3.1
1	A	41	GLN	3.1
1	J	70	GLY	3.1
1	C	250	ILE	3.1
1	F	184	ARG	3.1
1	G	282	TRP	3.1
1	A	312	PHE	3.1
1	G	125	VAL	3.1
1	B	221	GLY	3.1
1	B	358	ARG	3.1
1	J	249	ALA	3.0
1	D	8	PHE	3.0
1	E	255	HIS	3.0
1	B	90	GLU	3.0
1	B	181	GLU	3.0
1	C	181	GLU	3.0
1	G	94	GLU	3.0
1	G	249	ALA	3.0
1	A	135	ASP	3.0
1	A	70	GLY	3.0
1	D	286	GLN	3.0
1	D	365	GLN	3.0
1	A	304	CYS	3.0
1	B	186	ARG	3.0
1	B	290	LEU	3.0
1	H	301	LEU	3.0
1	A	381	GLU	3.0
1	B	235	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	137	MET	3.0
1	B	242	HIS	3.0
1	B	267	VAL	3.0
1	B	316	MET	3.0
1	F	106	PHE	3.0
1	G	279	MET	3.0
1	B	189	TRP	3.0
1	A	210	TYR	3.0
1	F	178	TYR	3.0
1	B	182	ARG	3.0
1	D	223	LEU	3.0
1	F	78	ASP	3.0
1	F	192	ASP	3.0
1	H	165	GLY	3.0
1	J	247	GLN	3.0
1	B	33	LEU	3.0
1	F	380	LEU	3.0
1	A	38	GLU	3.0
1	B	315	GLU	3.0
1	G	174	ALA	3.0
1	A	173	VAL	3.0
1	A	343	LEU	3.0
1	A	372	GLY	3.0
1	F	164	GLY	3.0
1	A	187	SER	3.0
1	E	172	GLU	3.0
1	H	212	PRO	3.0
1	A	283	THR	3.0
1	F	91	THR	3.0
1	A	245	VAL	3.0
1	B	147	PHE	3.0
1	F	5	VAL	3.0
1	F	22	VAL	3.0
1	B	257	HIS	3.0
1	A	144	ARG	2.9
1	A	306	ARG	2.9
1	A	358	ARG	2.9
1	B	375	ARG	2.9
1	E	373	ARG	2.9
1	I	218	ARG	2.9
1	G	168	LEU	2.9
1	G	339	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	376	TYR	2.9
1	A	229	MET	2.9
1	A	132	ALA	2.9
1	G	6	PHE	2.9
1	J	63	VAL	2.9
1	B	156	LEU	2.9
1	F	92	GLN	2.9
1	C	94	GLU	2.9
1	F	47	GLU	2.9
1	F	40	ASP	2.9
1	G	19	ASN	2.9
1	A	101	ALA	2.9
1	A	320	ALA	2.9
1	E	120	PHE	2.9
1	H	287	VAL	2.9
1	A	76	LYS	2.9
1	B	303	THR	2.9
1	F	97	HIS	2.9
1	G	354	THR	2.9
1	E	218	ARG	2.9
1	F	167	LEU	2.9
1	G	290	LEU	2.9
1	A	92	GLN	2.9
1	G	220	TYR	2.9
1	A	115	GLU	2.9
1	B	172	GLU	2.9
1	A	317	ALA	2.9
1	A	143	THR	2.9
1	A	242	HIS	2.9
1	D	298	ARG	2.9
1	F	104	THR	2.9
1	G	193	THR	2.9
1	G	301	LEU	2.9
1	A	300	GLY	2.9
1	A	282	TRP	2.9
1	G	81	ASN	2.9
1	A	355	VAL	2.9
1	F	100	ASP	2.9
1	G	24	ALA	2.9
1	A	186	ARG	2.9
1	G	39	ARG	2.9
1	B	42	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	380	LEU	2.9
1	A	161	GLN	2.8
1	B	130	PRO	2.8
1	B	160	GLU	2.8
1	B	269	TYR	2.8
1	B	322	TYR	2.8
1	B	376	TYR	2.8
1	D	376	TYR	2.8
1	A	4	VAL	2.8
1	B	287	VAL	2.8
1	F	19	ASN	2.8
1	G	216	ALA	2.8
1	A	87	PHE	2.8
1	G	120	PHE	2.8
1	H	266	ARG	2.8
1	A	239	SER	2.8
1	B	222	GLY	2.8
1	G	334	PRO	2.8
1	B	43	TYR	2.8
1	I	210	TYR	2.8
1	A	231	VAL	2.8
1	B	136	ALA	2.8
1	B	310	PHE	2.8
1	A	134	THR	2.8
1	A	274	THR	2.8
1	A	346	THR	2.8
1	E	193	THR	2.8
1	E	107	GLY	2.8
1	E	372	GLY	2.8
1	B	330	GLN	2.8
1	G	66	GLN	2.8
1	D	179	GLU	2.8
1	A	183	VAL	2.8
1	B	128	TYR	2.8
1	B	148	ALA	2.8
1	F	6	PHE	2.8
1	J	24	ALA	2.8
1	A	301	LEU	2.8
1	B	367	LEU	2.8
1	D	211	ILE	2.8
1	G	292	LEU	2.8
1	D	135	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	192	ASP	2.8
1	B	187	SER	2.8
1	B	229	MET	2.8
1	C	304	CYS	2.8
1	A	315	GLU	2.8
1	E	158	TRP	2.8
1	A	324	VAL	2.8
1	F	20	VAL	2.8
1	F	29	VAL	2.8
1	A	368	TYR	2.8
1	B	83	ALA	2.8
1	F	23	ALA	2.8
1	A	367	LEU	2.8
1	A	276	HIS	2.8
1	A	314	ASP	2.8
1	A	152	PRO	2.8
1	I	92	GLN	2.7
1	E	258	ARG	2.7
1	F	21	ARG	2.7
1	A	216	ALA	2.7
1	A	374	TYR	2.7
1	B	226	LEU	2.7
1	B	374	TYR	2.7
1	D	217	HIS	2.7
1	E	164	GLY	2.7
1	F	123	GLY	2.7
1	E	256	PRO	2.7
1	A	330	GLN	2.7
1	A	273	ALA	2.7
1	A	93	TRP	2.7
1	A	156	LEU	2.7
1	D	216	ALA	2.7
1	F	101	ALA	2.7
1	F	110	TRP	2.7
1	G	106	PHE	2.7
1	B	144	ARG	2.7
1	B	184	ARG	2.7
1	B	266	ARG	2.7
1	D	92	GLN	2.7
1	D	288	GLU	2.7
1	B	4	VAL	2.7
1	B	15	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	245	VAL	2.7
1	A	142	ILE	2.7
1	A	163	LEU	2.7
1	A	340	LEU	2.7
1	B	379	ALA	2.7
1	F	24	ALA	2.7
1	B	207	TYR	2.7
1	B	360	TYR	2.7
1	G	190	GLY	2.7
1	G	306	ARG	2.7
1	G	335	ASP	2.7
1	A	364	GLN	2.7
1	B	198	VAL	2.7
1	J	31	GLU	2.7
1	A	219	LEU	2.7
1	A	234	PHE	2.7
1	B	211	ILE	2.7
1	B	237	ILE	2.7
1	D	17	LEU	2.7
1	F	35	ILE	2.7
1	G	8	PHE	2.7
1	A	141	MET	2.7
1	J	12	HIS	2.7
1	D	210	TYR	2.7
1	J	178	TYR	2.7
1	A	73	ARG	2.7
1	G	186	ARG	2.7
1	B	81	ASN	2.7
1	I	152	PRO	2.7
1	A	270	ASP	2.7
1	A	200	VAL	2.7
1	A	339	LEU	2.7
1	A	349	LEU	2.7
1	G	275	LEU	2.7
1	A	25	ALA	2.6
1	B	129	PHE	2.6
1	A	151	TRP	2.6
1	B	318	TRP	2.6
1	H	360	TYR	2.6
1	A	277	ARG	2.6
1	G	131	ARG	2.6
1	F	248	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	42	THR	2.6
1	B	19	ASN	2.6
1	A	225	ASP	2.6
1	B	324	VAL	2.6
1	C	52	GLU	2.6
1	C	219	LEU	2.6
1	F	61	VAL	2.6
1	F	365	GLN	2.6
1	G	65	LEU	2.6
1	G	89	GLU	2.6
1	G	245	VAL	2.6
1	J	377	GLN	2.6
1	A	159	ILE	2.6
1	G	147	PHE	2.6
1	H	257	HIS	2.6
1	D	185	ARG	2.6
1	B	7	PRO	2.6
1	B	190	GLY	2.6
1	B	260	PRO	2.6
1	E	123	GLY	2.6
1	E	248	PRO	2.6
1	H	152	PRO	2.6
1	A	145	THR	2.6
1	A	5	VAL	2.6
1	B	301	LEU	2.6
1	A	179	GLU	2.6
1	B	201	GLN	2.6
1	B	244	VAL	2.6
1	D	63	VAL	2.6
1	G	156	LEU	2.6
1	E	148	ALA	2.6
1	B	153	HIS	2.6
1	B	48	ARG	2.6
1	E	266	ARG	2.6
1	G	195	TYR	2.6
1	G	360	TYR	2.6
1	F	13	PRO	2.6
1	F	74	PRO	2.6
1	F	221	GLY	2.6
1	B	304	CYS	2.6
1	B	173	VAL	2.6
1	G	103	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	29	VAL	2.6
1	A	172	GLU	2.6
1	C	179	GLU	2.6
1	H	299	GLU	2.6
1	A	100	ASP	2.6
1	A	319	ALA	2.6
1	A	126	ARG	2.6
1	G	218	ARG	2.6
1	A	122	TYR	2.6
1	F	77	GLY	2.6
1	J	122	TYR	2.6
1	A	371	LEU	2.6
1	B	72	LEU	2.6
1	G	69	LEU	2.6
1	J	340	LEU	2.6
1	B	5	VAL	2.6
1	B	259	VAL	2.6
1	B	297	VAL	2.6
1	F	53	ILE	2.6
1	F	111	ILE	2.6
1	B	249	ALA	2.6
1	A	192	ASP	2.6
1	A	323	HIS	2.5
1	D	266	ARG	2.5
1	G	215	LYS	2.5
1	B	77	GLY	2.5
1	B	212	PRO	2.5
1	B	214	GLY	2.5
1	A	128	TYR	2.5
1	A	240	LEU	2.5
1	A	357	LEU	2.5
1	J	69	LEU	2.5
1	G	199	THR	2.5
1	A	309	ALA	2.5
1	H	216	ALA	2.5
1	B	157	SER	2.5
1	G	9	LYS	2.5
1	J	54	SER	2.5
1	A	124	LEU	2.5
1	B	17	LEU	2.5
1	G	51	PRO	2.5
1	G	162	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	164	GLY	2.5
1	G	36	GLY	2.5
1	J	380	LEU	2.5
1	B	111	ILE	2.5
1	F	316	MET	2.5
1	A	207	TYR	2.5
1	A	362	TYR	2.5
1	F	11	GLU	2.5
1	G	253	GLN	2.5
1	F	25	ALA	2.5
1	B	85	ARG	2.5
1	B	131	ARG	2.5
1	G	227	ARG	2.5
1	B	127	HIS	2.5
1	B	262	HIS	2.5
1	F	10	HIS	2.5
1	A	137	MET	2.5
1	A	296	PRO	2.5
1	B	163	LEU	2.5
1	B	191	ILE	2.5
1	F	58	GLY	2.5
1	D	267	VAL	2.5
1	F	4	VAL	2.5
1	G	140	TRP	2.5
1	A	99	TYR	2.5
1	B	354	THR	2.5
1	C	42	THR	2.5
1	G	71	THR	2.5
1	G	293	PHE	2.5
1	H	293	PHE	2.5
1	I	309	ALA	2.5
1	G	76	LYS	2.5
1	D	30	HIS	2.5
1	F	109	ASP	2.5
1	B	230	LEU	2.5
1	G	137	MET	2.5
1	A	250	ILE	2.5
1	B	58	GLY	2.5
1	D	36	GLY	2.5
1	H	164	GLY	2.5
1	A	15	VAL	2.5
1	A	271	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	46	VAL	2.5
1	B	125	VAL	2.5
1	G	32	VAL	2.5
1	D	282	TRP	2.5
1	A	178	TYR	2.5
1	B	368	TYR	2.5
1	G	232	GLU	2.5
1	B	218	ARG	2.5
1	F	85	ARG	2.5
1	G	91	THR	2.5
1	G	294	THR	2.5
1	B	217	HIS	2.5
1	B	371	LEU	2.4
1	J	3	LEU	2.4
1	J	219	LEU	2.4
1	J	7	PRO	2.4
1	B	265	GLU	2.4
1	F	67	GLU	2.4
1	F	94	GLU	2.4
1	G	55	ARG	2.4
1	A	241	GLN	2.4
1	A	377	GLN	2.4
1	B	215	LYS	2.4
1	B	309	ALA	2.4
1	E	207	TYR	2.4
1	B	143	THR	2.4
1	B	251	HIS	2.4
1	F	26	HIS	2.4
1	B	350	ASN	2.4
1	A	278	LEU	2.4
1	F	16	LEU	2.4
1	F	69	LEU	2.4
1	G	340	LEU	2.4
1	A	108	PRO	2.4
1	A	256	PRO	2.4
1	A	333	ASP	2.4
1	E	142	ILE	2.4
1	G	111	ILE	2.4
1	H	248	PRO	2.4
1	J	248	PRO	2.4
1	G	63	VAL	2.4
1	G	231	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	2.4
1	A	157	SER	2.4
1	G	133	SER	2.4
1	A	98	PHE	2.4
1	B	6	PHE	2.4
1	D	181	GLU	2.4
1	G	93	TRP	2.4
1	G	272	GLU	2.4
1	A	136	ALA	2.4
1	B	216	ALA	2.4
1	G	344	TRP	2.4
1	H	247	GLN	2.4
1	J	23	ALA	2.4
1	D	86	TYR	2.4
1	E	57	THR	2.4
1	H	316	MET	2.4
1	I	380	LEU	2.4
1	B	74	PRO	2.4
1	B	204	VAL	2.4
1	D	121	GLY	2.4
1	E	221	GLY	2.4
1	B	14	GLU	2.4
1	G	208	GLU	2.4
1	A	356	ALA	2.4
1	E	216	ALA	2.4
1	I	220	TYR	2.4
1	H	294	THR	2.4
1	G	169	MET	2.4
1	J	80	MET	2.4
1	A	226	LEU	2.4
1	A	325	LEU	2.4
1	B	150	LEU	2.4
1	I	223	LEU	2.4
1	B	250	ILE	2.4
1	G	123	GLY	2.4
1	J	5	VAL	2.4
1	G	224	ASP	2.4
1	B	8	PHE	2.4
1	B	98	PHE	2.4
1	B	293	PHE	2.4
1	F	288	GLU	2.4
1	H	365	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	247	GLN	2.4
1	B	362	TYR	2.4
1	C	143	THR	2.4
1	J	91	THR	2.4
1	A	33	LEU	2.4
1	B	88	LEU	2.4
1	F	72	LEU	2.4
1	A	211	ILE	2.4
1	I	248	PRO	2.4
1	C	214	GLY	2.3
1	E	79	GLY	2.3
1	J	85	ARG	2.3
1	A	341	PHE	2.3
1	A	361	ASP	2.3
1	C	192	ASP	2.3
1	C	335	ASP	2.3
1	F	102	ASP	2.3
1	B	47	GLU	2.3
1	B	232	GLU	2.3
1	B	319	ALA	2.3
1	F	264	ALA	2.3
1	G	166	GLU	2.3
1	A	286	GLN	2.3
1	B	66	GLN	2.3
1	B	305	GLN	2.3
1	G	305	GLN	2.3
1	E	133	SER	2.3
1	F	187	SER	2.3
1	J	62	SER	2.3
1	B	228	THR	2.3
1	B	255	HIS	2.3
1	B	346	THR	2.3
1	E	37	TYR	2.3
1	G	269	TYR	2.3
1	B	55	ARG	2.3
1	J	185	ARG	2.3
1	B	135	ASP	2.3
1	G	38	GLU	2.3
1	G	273	ALA	2.3
1	A	202	GLN	2.3
1	A	313	MET	2.3
1	B	365	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	80	MET	2.3
1	G	229	MET	2.3
1	B	124	LEU	2.3
1	B	167	LEU	2.3
1	B	289	LEU	2.3
1	A	158	TRP	2.3
1	D	133	SER	2.3
1	D	289	LEU	2.3
1	E	292	LEU	2.3
1	E	380	LEU	2.3
1	G	380	LEU	2.3
1	J	88	LEU	2.3
1	A	328	HIS	2.3
1	H	30	HIS	2.3
1	C	71	THR	2.3
1	G	211	ILE	2.3
1	B	9	LYS	2.3
1	A	347	ARG	2.3
1	C	306	ARG	2.3
1	E	28	ARG	2.3
1	F	171	ARG	2.3
1	C	245	VAL	2.3
1	E	70	GLY	2.3
1	J	222	GLY	2.3
1	A	6	PHE	2.3
1	C	120	PHE	2.3
1	F	45	ALA	2.3
1	F	181	GLU	2.3
1	G	50	ALA	2.3
1	G	319	ALA	2.3
1	H	272	GLU	2.3
1	I	299	GLU	2.3
1	J	56	ALA	2.3
1	G	40	ASP	2.3
1	B	202	GLN	2.3
1	F	209	CYS	2.3
1	I	209	CYS	2.3
1	J	92	GLN	2.3
1	A	138	ILE	2.3
1	B	263	ILE	2.3
1	B	328	HIS	2.3
1	D	263	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	257	HIS	2.3
1	G	30	HIS	2.3
1	G	142	ILE	2.3
1	J	30	HIS	2.3
1	E	54	SER	2.3
1	F	193	THR	2.3
1	H	295	THR	2.3
1	A	185	ARG	2.3
1	B	195	TYR	2.3
1	C	360	TYR	2.3
1	F	195	TYR	2.3
1	H	131	ARG	2.3
1	B	256	PRO	2.3
1	F	27	PRO	2.3
1	H	259	VAL	2.3
1	I	20	VAL	2.3
1	J	51	PRO	2.3
1	A	190	GLY	2.3
1	A	310	PHE	2.3
1	C	81	ASN	2.3
1	G	129	PHE	2.3
1	J	81	ASN	2.3
1	A	44	GLU	2.3
1	B	161	GLN	2.3
1	B	357	LEU	2.3
1	C	289	LEU	2.3
1	H	78	ASP	2.3
1	A	26	HIS	2.3
1	G	97	HIS	2.3
1	A	82	THR	2.3
1	A	298	ARG	2.3
1	C	139	THR	2.3
1	D	354	THR	2.3
1	F	64	ARG	2.3
1	G	126	ARG	2.3
1	H	133	SER	2.3
1	H	218	ARG	2.3
1	A	348	VAL	2.3
1	B	261	VAL	2.3
1	E	244	VAL	2.3
1	I	245	VAL	2.3
1	H	221	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	293	PHE	2.2
1	D	293	PHE	2.2
1	G	316	MET	2.2
1	G	14	GLU	2.2
1	B	349	LEU	2.2
1	F	168	LEU	2.2
1	J	17	LEU	2.2
1	J	223	LEU	2.2
1	B	241	GLN	2.2
1	E	41	GLN	2.2
1	G	92	GLN	2.2
1	J	225	ASP	2.2
1	G	35	ILE	2.2
1	I	250	ILE	2.2
1	D	170	ARG	2.2
1	I	373	ARG	2.2
1	J	262	HIS	2.2
1	J	34	CYS	2.2
1	B	27	PRO	2.2
1	B	134	THR	2.2
1	J	71	THR	2.2
1	B	348	VAL	2.2
1	C	368	TYR	2.2
1	D	205	SER	2.2
1	J	4	VAL	2.2
1	G	366	TYR	2.2
1	B	94	GLU	2.2
1	A	342	LYS	2.2
1	B	177	LEU	2.2
1	B	327	GLU	2.2
1	E	56	ALA	2.2
1	F	223	LEU	2.2
1	H	65	LEU	2.2
1	J	94	GLU	2.2
1	A	35	ILE	2.2
1	I	365	GLN	2.2
1	B	68	ARG	2.2
1	B	126	ARG	2.2
1	A	57	THR	2.2
1	A	104	THR	2.2
1	B	20	VAL	2.2
1	B	193	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	60	PRO	2.2
1	G	198	VAL	2.2
1	B	239	SER	2.2
1	C	164	GLY	2.2
1	B	176	MET	2.2
1	F	215	LYS	2.2
1	I	163	LEU	2.2
1	B	103	ILE	2.2
1	G	358	ARG	2.2
1	H	253	GLN	2.2
1	B	192	ASP	2.2
1	B	225	ASP	2.2
1	A	297	VAL	2.2
1	G	20	VAL	2.2
1	J	82	THR	2.2
1	B	34	CYS	2.2
1	C	128	TYR	2.2
1	C	220	TYR	2.2
1	D	221	GLY	2.2
1	B	312	PHE	2.2
1	J	98	PHE	2.2
1	B	84	LEU	2.2
1	C	163	LEU	2.2
1	F	3	LEU	2.2
1	H	275	LEU	2.2
1	A	254	GLU	2.2
1	B	243	GLU	2.2
1	D	24	ALA	2.2
1	D	208	GLU	2.2
1	F	50	ALA	2.2
1	A	263	ILE	2.2
1	C	64	ARG	2.2
1	E	103	ILE	2.2
1	C	330	GLN	2.2
1	G	364	GLN	2.2
1	C	255	HIS	2.2
1	D	257	HIS	2.2
1	C	15	VAL	2.2
1	D	256	PRO	2.2
1	G	173	VAL	2.2
1	H	20	VAL	2.2
1	H	244	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	143	THR	2.2
1	F	107	GLY	2.2
1	H	336	TRP	2.2
1	J	58	GLY	2.2
1	A	360	TYR	2.2
1	F	122	TYR	2.2
1	A	69	LEU	2.2
1	C	223	LEU	2.2
1	F	124	LEU	2.2
1	G	226	LEU	2.2
1	A	235	ALA	2.2
1	A	378	ALA	2.2
1	E	181	GLU	2.2
1	G	175	ALA	2.2
1	G	378	ALA	2.2
1	A	375	ARG	2.1
1	G	138	ILE	2.1
1	J	305	GLN	2.1
1	B	61	VAL	2.1
1	D	130	PRO	2.1
1	E	200	VAL	2.1
1	F	256	PRO	2.1
1	G	261	VAL	2.1
1	H	297	VAL	2.1
1	I	244	VAL	2.1
1	J	46	VAL	2.1
1	D	78	ASP	2.1
1	J	316	MET	2.1
1	D	215	LYS	2.1
1	I	215	LYS	2.1
1	J	354	THR	2.1
1	A	167	LEU	2.1
1	B	65	LEU	2.1
1	C	293	PHE	2.1
1	D	69	LEU	2.1
1	H	312	PHE	2.1
1	B	209	CYS	2.1
1	E	62	SER	2.1
1	A	67	GLU	2.1
1	A	131	ARG	2.1
1	E	265	GLU	2.1
1	J	14	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	66	GLN	2.1
1	D	97	HIS	2.1
1	F	262	HIS	2.1
1	J	276	HIS	2.1
1	A	125	VAL	2.1
1	E	7	PRO	2.1
1	G	287	VAL	2.1
1	I	316	MET	2.1
1	J	215	LYS	2.1
1	G	104	THR	2.1
1	A	177	LEU	2.1
1	B	329	PHE	2.1
1	B	341	PHE	2.1
1	G	240	LEU	2.1
1	J	87	PHE	2.1
1	A	170	ARG	2.1
1	A	363	ALA	2.1
1	B	45	ALA	2.1
1	C	178	TYR	2.1
1	E	378	ALA	2.1
1	F	185	ARG	2.1
1	F	249	ALA	2.1
1	G	86	TYR	2.1
1	J	99	TYR	2.1
1	J	317	ALA	2.1
1	A	208	GLU	2.1
1	D	62	SER	2.1
1	D	327	GLU	2.1
1	H	38	GLU	2.1
1	I	54	SER	2.1
1	D	253	GLN	2.1
1	J	365	GLN	2.1
1	J	257	HIS	2.1
1	E	316	MET	2.1
1	H	4	VAL	2.1
1	B	248	PRO	2.1
1	J	9	LYS	2.1
1	A	146	GLY	2.1
1	B	343	LEU	2.1
1	C	72	LEU	2.1
1	C	109	ASP	2.1
1	C	224	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	112	THR	2.1
1	G	188	ASP	2.1
1	A	24	ALA	2.1
1	F	56	ALA	2.1
1	B	299	GLU	2.1
1	D	299	GLU	2.1
1	E	374	TYR	2.1
1	G	53	ILE	2.1
1	G	122	TYR	2.1
1	G	288	GLU	2.1
1	J	35	ILE	2.1
1	J	250	ILE	2.1
1	A	209	CYS	2.1
1	D	209	CYS	2.1
1	G	280	GLN	2.1
1	B	12	HIS	2.1
1	B	313	MET	2.1
1	B	334	PRO	2.1
1	J	60	PRO	2.1
1	A	311	ASN	2.1
1	B	278	LEU	2.1
1	C	17	LEU	2.1
1	G	87	PHE	2.1
1	I	36	GLY	2.1
1	A	154	THR	2.1
1	A	266	ARG	2.1
1	B	199	THR	2.1
1	F	55	ARG	2.1
1	F	266	ARG	2.1
1	A	117	ALA	2.1
1	C	216	ALA	2.1
1	D	237	ILE	2.1
1	D	264	ALA	2.1
1	E	250	ILE	2.1
1	G	23	ALA	2.1
1	A	116	GLU	2.1
1	F	90	GLU	2.1
1	J	179	GLU	2.1
1	G	37	TYR	2.1
1	J	86	TYR	2.1
1	B	133	SER	2.0
1	G	62	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	41	GLN	2.0
1	E	377	GLN	2.0
1	G	276	HIS	2.0
1	H	34	CYS	2.0
1	H	279	MET	2.0
1	G	12	HIS	2.0
1	J	281	HIS	2.0
1	I	32	VAL	2.0
1	H	284	PRO	2.0
1	A	275	LEU	2.0
1	B	339	LEU	2.0
1	D	301	LEU	2.0
1	G	124	LEU	2.0
1	G	194	LEU	2.0
1	G	343	LEU	2.0
1	F	39	ARG	2.0
1	G	341	PHE	2.0
1	H	300	GLY	2.0
1	F	361	ASP	2.0
1	G	237	ILE	2.0
1	G	45	ALA	2.0
1	G	117	ALA	2.0
1	B	93	TRP	2.0
1	F	381	GLU	2.0
1	G	181	GLU	2.0
1	J	90	GLU	2.0
1	B	178	TYR	2.0
1	A	66	GLN	2.0
1	C	286	GLN	2.0
1	G	108	PRO	2.0
1	G	331	PRO	2.0
1	B	240	LEU	2.0
1	E	194	LEU	2.0
1	G	17	LEU	2.0
1	H	223	LEU	2.0
1	H	302	ARG	2.0
1	B	87	PHE	2.0
1	C	70	GLY	2.0
1	D	222	GLY	2.0
1	C	35	ILE	2.0
1	G	235	ALA	2.0
1	H	303	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	216	ALA	2.0
1	A	90	GLU	2.0
1	D	38	GLU	2.0
1	D	89	GLU	2.0
1	G	47	GLU	2.0
1	A	169	MET	2.0
1	G	80	MET	2.0
1	B	122	TYR	2.0
1	J	198	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDX	G	400	39/40	0.77	0.17	60,63,65,66	0
4	CL	F	1382	1/1	0.80	0.32	102,102,102,102	0
4	CL	J	1382	1/1	0.81	0.17	82,82,82,82	0
2	GDX	F	400	39/40	0.85	0.14	59,63,64,66	0
3	MN	J	500	1/1	0.85	0.11	80,80,80,80	0
4	CL	H	1382	1/1	0.87	0.19	77,77,77,77	0
4	CL	G	1382	1/1	0.90	0.18	79,79,79,79	0
2	GDX	I	400	39/40	0.90	0.13	59,63,65,67	0
2	GDX	J	400	39/40	0.90	0.12	60,63,64,66	0
3	MN	F	500	1/1	0.91	0.08	80,80,80,80	0
3	MN	G	500	1/1	0.92	0.09	79,79,79,79	0
4	CL	I	1382	1/1	0.92	0.16	70,70,70,70	0
2	GDX	E	400	39/40	0.92	0.16	59,63,65,67	0
2	GDX	C	400	39/40	0.93	0.11	59,63,65,66	0

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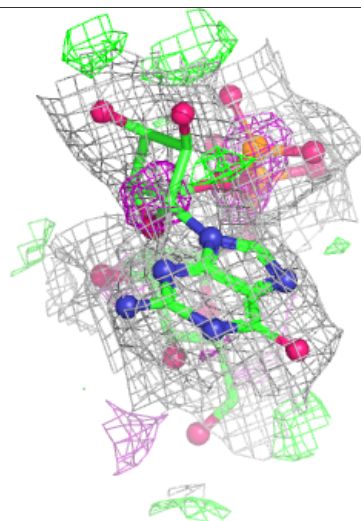
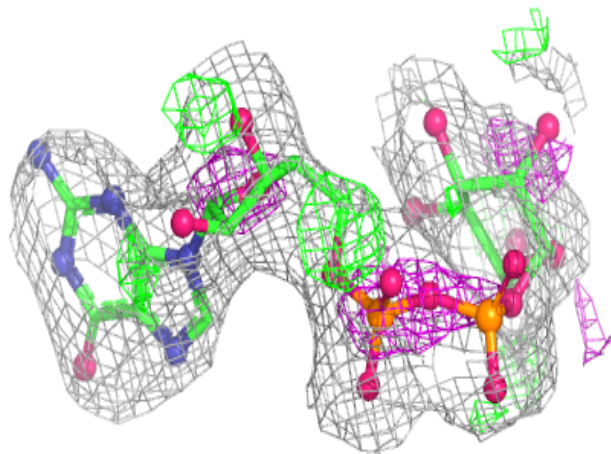
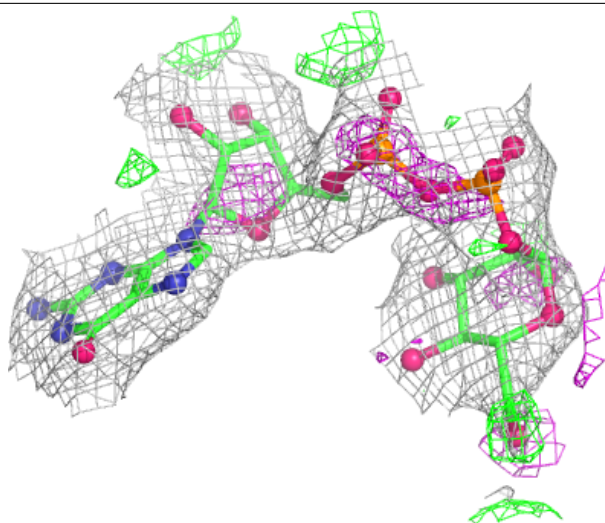
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	1382	1/1	0.93	0.14	38,38,38,38	0
4	CL	D	1382	1/1	0.93	0.11	55,55,55,55	0
2	GDX	H	400	39/40	0.93	0.12	60,63,64,66	0
3	MN	H	500	1/1	0.94	0.08	80,80,80,80	0
3	MN	B	500	1/1	0.94	0.12	82,82,82,82	0
4	CL	A	1382	1/1	0.94	0.08	38,38,38,38	0
2	GDX	B	400	39/40	0.94	0.19	59,63,65,66	0
2	GDX	A	400	39/40	0.94	0.19	60,63,65,67	0
3	MN	C	500	1/1	0.95	0.07	80,80,80,80	0
3	MN	I	500	1/1	0.96	0.06	80,80,80,80	0
4	CL	C	1382	1/1	0.96	0.10	58,58,58,58	0
3	MN	D	500	1/1	0.96	0.07	80,80,80,80	0
2	GDX	D	400	39/40	0.96	0.11	59,63,65,66	0
4	CL	E	1382	1/1	0.97	0.14	65,65,65,65	0
3	MN	E	500	1/1	0.97	0.06	79,79,79,79	0
3	MN	A	500	1/1	0.97	0.09	80,80,80,80	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.

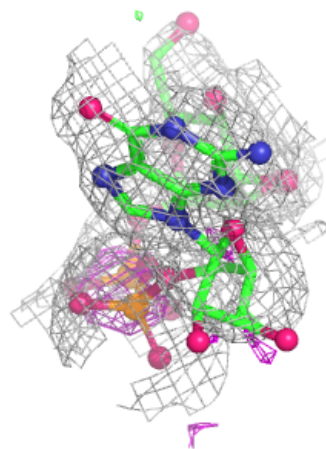
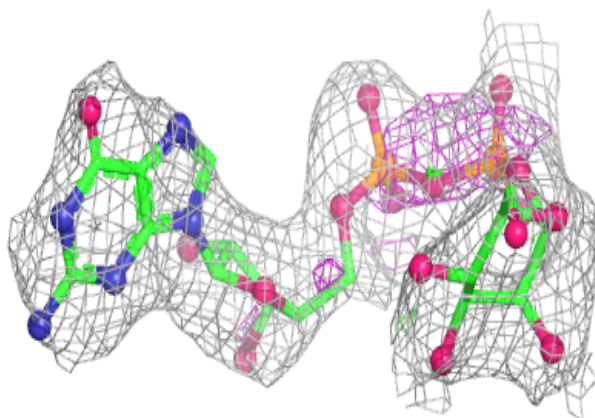
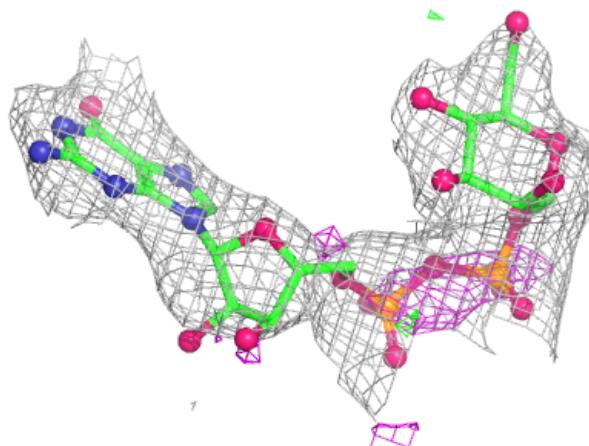
Electron density around GDX G 400:

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



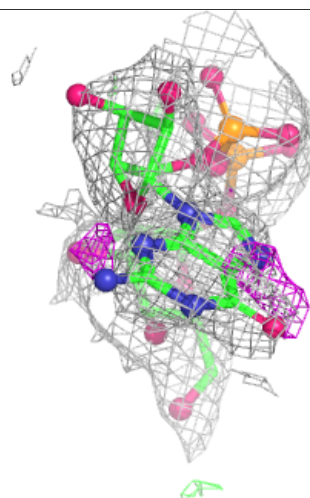
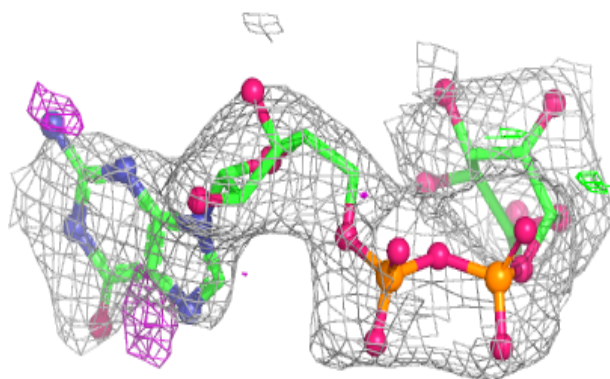
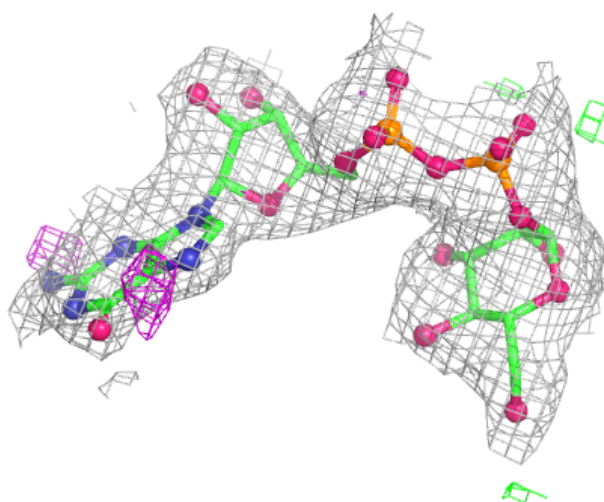
Electron density around GDX F 400:

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



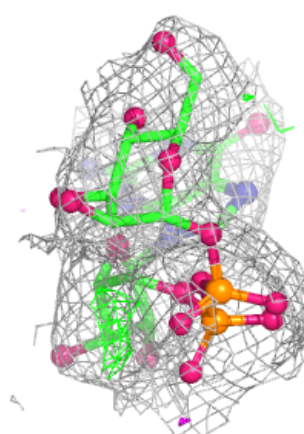
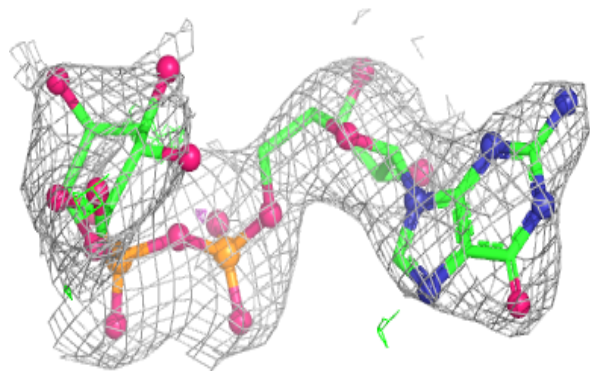
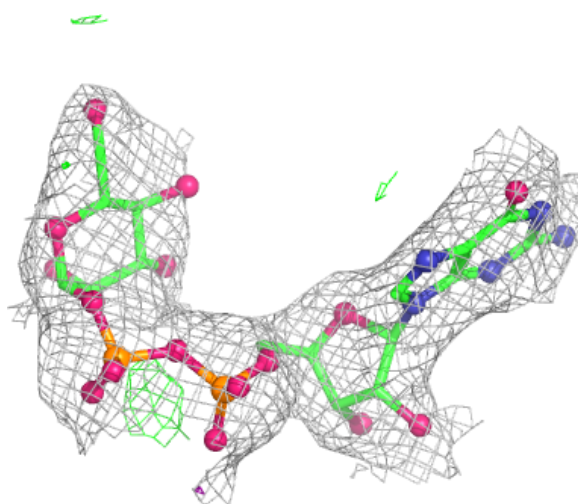
Electron density around GDX I 400:

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



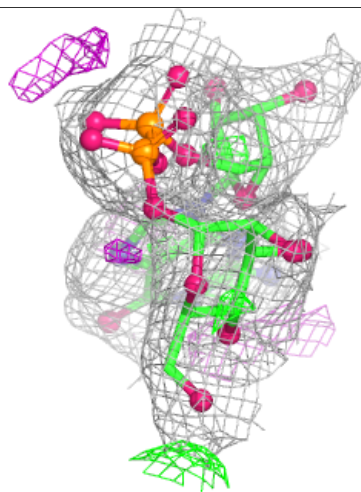
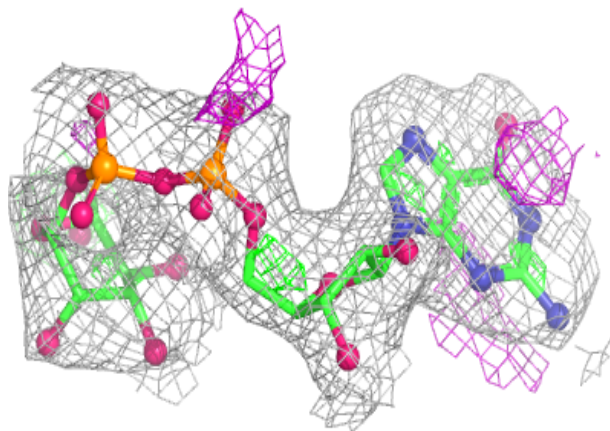
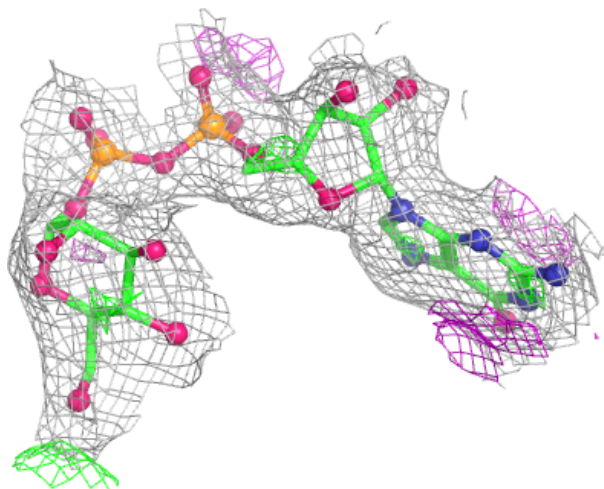
Electron density around GDX J 400:

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



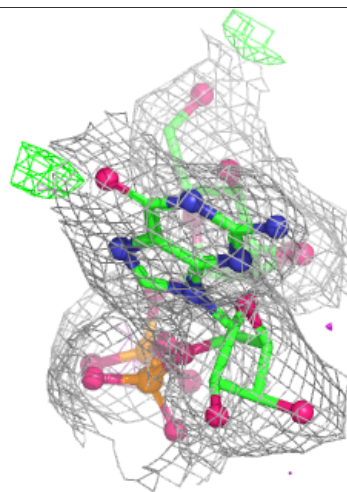
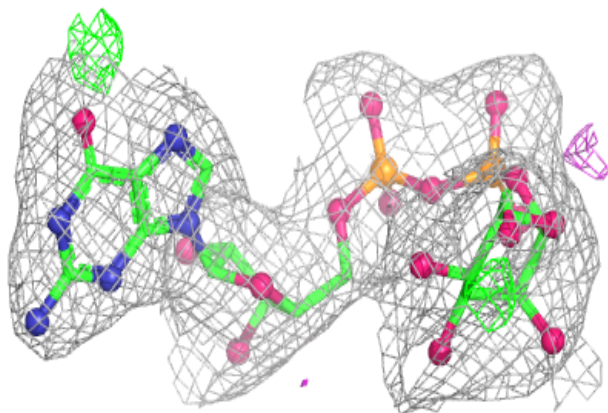
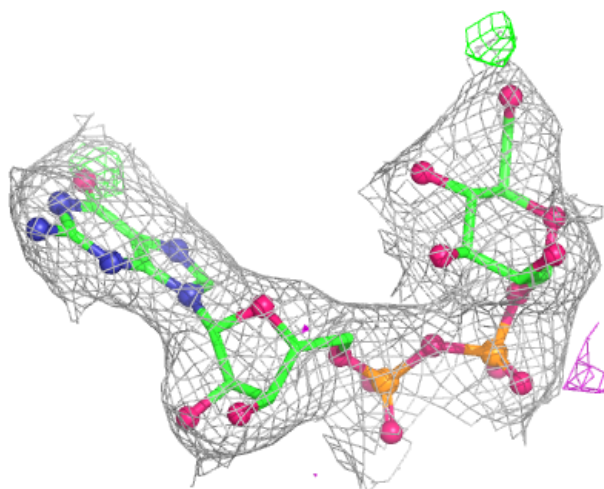
Electron density around GDX E 400:

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



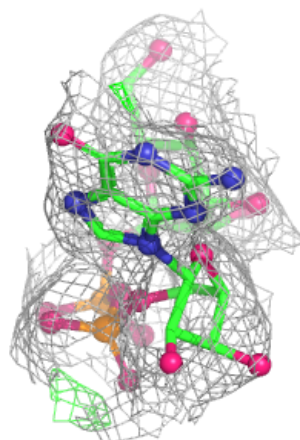
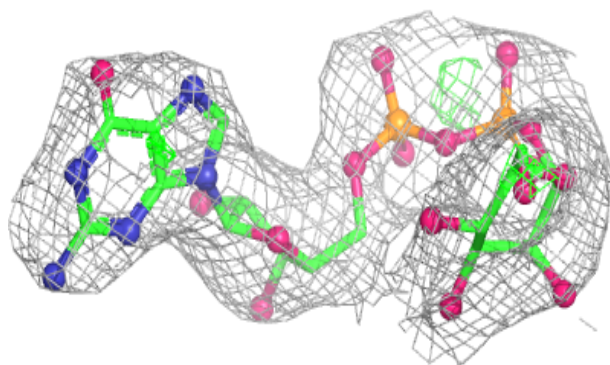
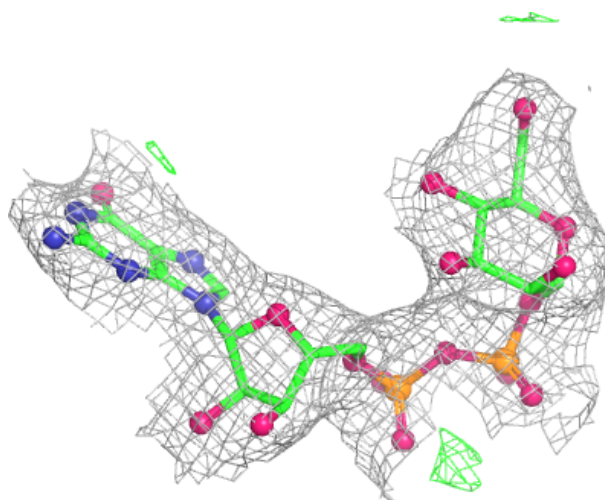
Electron density around GDX C 400:

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



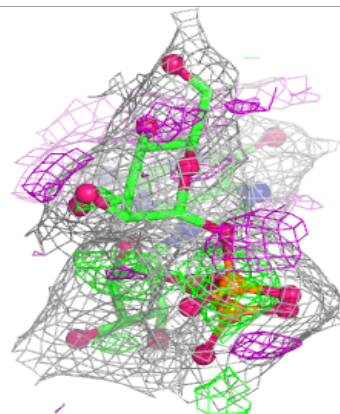
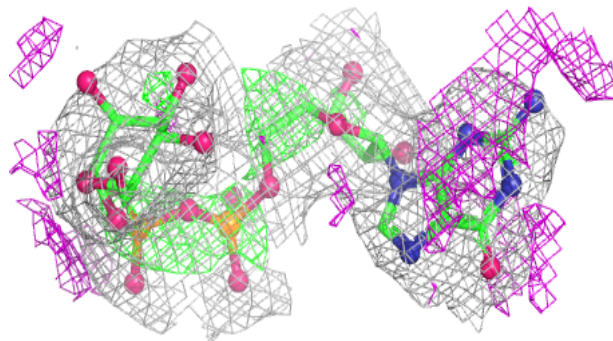
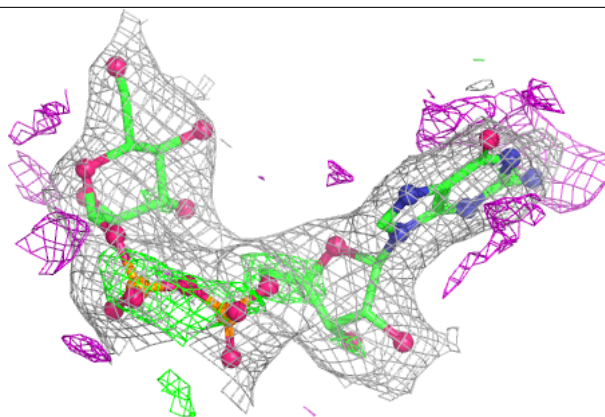
Electron density around GDX H 400:

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

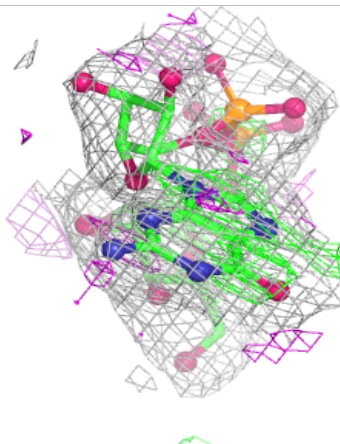
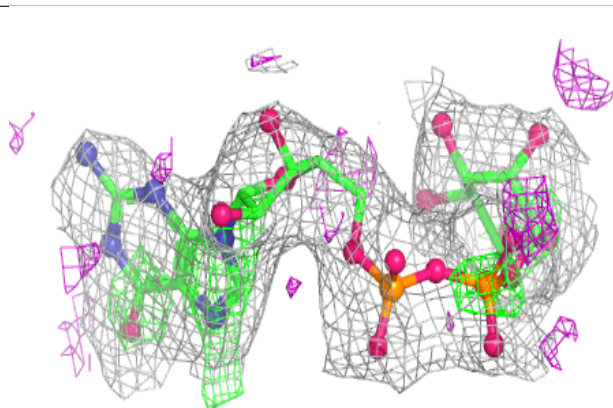
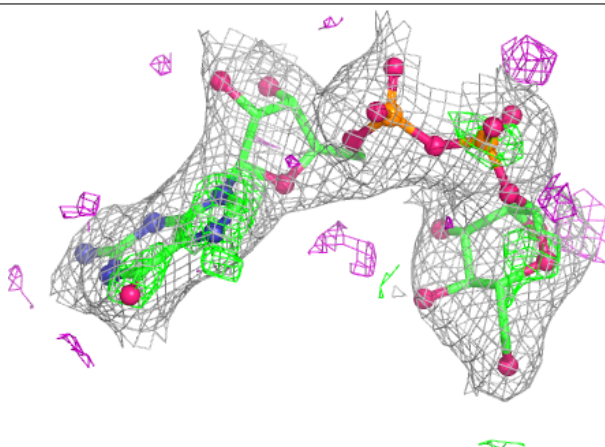


Electron density around GDX B 400:

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

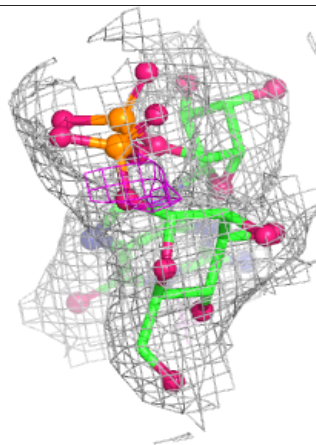
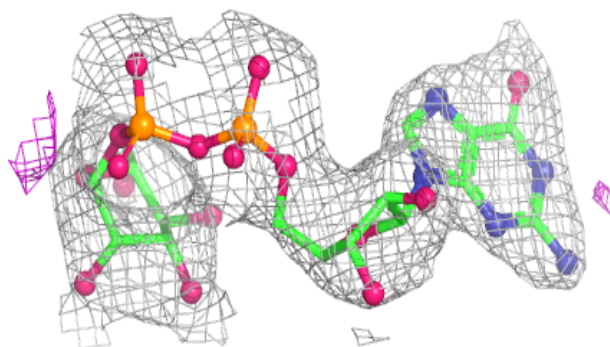
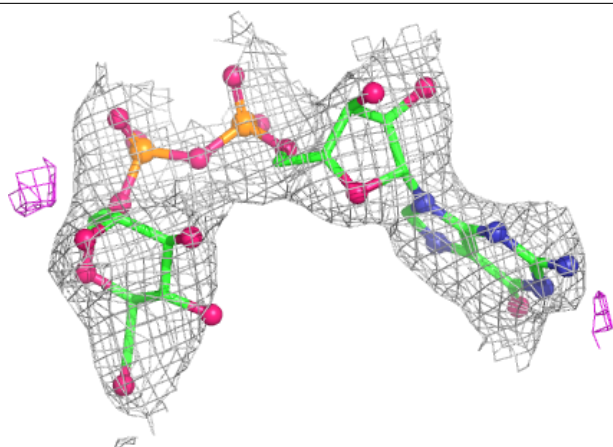
**Electron density around GDX A 400:**

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



Electron density around GDX D 400:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.