



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 06:12 am GMT

PDB ID : 2BO8
Title : DISSECTION OF MANNOSYLGLYCERATE SYNTHASE: AN ARCHETYPAL MANNOSYLTRANSFERASE
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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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

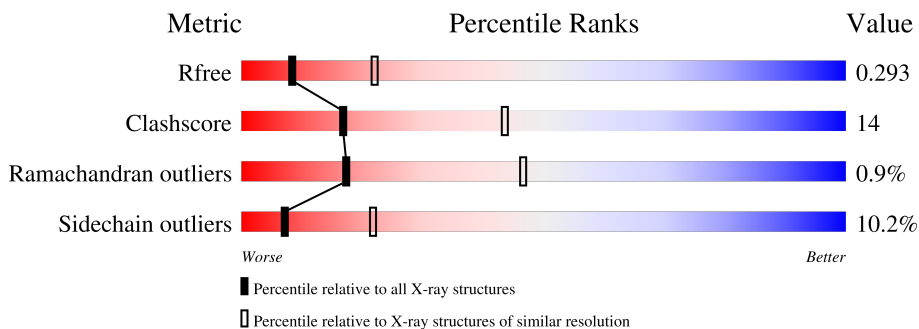
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	397	

2 Entry composition [i](#)

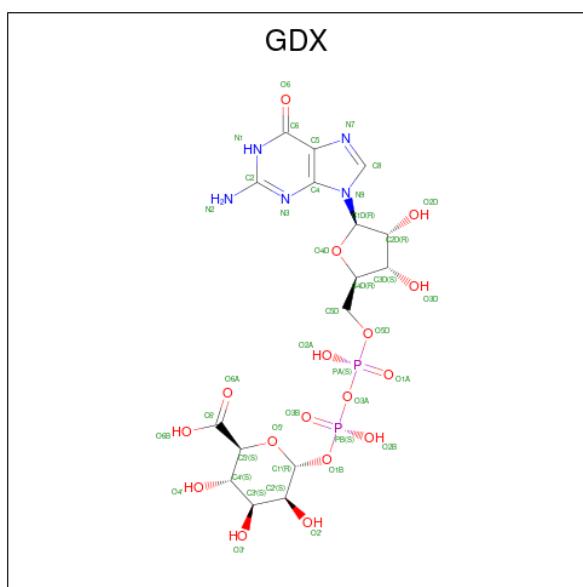
There are 5 unique types of molecules in this entry. The entry contains 32098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is GUANOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-D-MANNOPYRANOSYL ESTER (three-letter code: GDX) (formula: C₁₆H₂₃N₅O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
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 (three-letter code: 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 O 78 78	0	0
5	B	80	Total O 80 80	0	0
5	C	38	Total O 38 38	0	0
5	D	27	Total O 27 27	0	0
5	E	34	Total O 34 34	0	0
5	F	3	Total O 3 3	0	0
5	G	23	Total O 23 23	0	0
5	H	6	Total O 6 6	0	0
5	I	13	Total O 13 13	0	0
5	J	6	Total O 6 6	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 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 74.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (74.12-2.80) 97.4 (74.10-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.82Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.216 0.282 , 0.293	Depositor DCC
R_{free} test set	8687 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.151	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

4 Model quality i

4.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GDX, MN

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	1.51	24/3229 (0.7%)	1.24	28/4394 (0.6%)
1	B	1.50	28/3229 (0.9%)	1.22	29/4394 (0.7%)
1	C	1.09	7/3229 (0.2%)	0.97	13/4394 (0.3%)
1	D	1.16	9/3229 (0.3%)	0.95	10/4394 (0.2%)
1	E	1.00	4/3229 (0.1%)	0.92	7/4394 (0.2%)
1	F	0.75	3/3229 (0.1%)	0.77	4/4394 (0.1%)
1	G	1.17	15/3229 (0.5%)	0.97	8/4394 (0.2%)
1	H	0.80	2/3229 (0.1%)	0.82	4/4394 (0.1%)
1	I	0.90	5/3229 (0.2%)	0.88	9/4394 (0.2%)
1	J	1.14	24/3229 (0.7%)	0.98	7/4394 (0.2%)
All	All	1.13	121/32290 (0.4%)	0.98	119/43940 (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 (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	CYS	CB-SG	-17.09	1.53	1.82
1	A	209	CYS	CB-SG	-14.65	1.57	1.82
1	A	365	GLN	CB-CG	14.57	1.91	1.52
1	B	209	CYS	CB-SG	-14.55	1.57	1.82
1	I	209	CYS	CB-SG	-13.87	1.58	1.82
1	C	209	CYS	CB-SG	-13.41	1.59	1.82
1	H	209	CYS	CB-SG	-13.39	1.59	1.82
1	G	72	LEU	C-O	11.47	1.45	1.23
1	F	209	CYS	CB-SG	-10.43	1.64	1.82
1	J	338	GLU	CG-CD	9.86	1.66	1.51
1	J	347	ARG	C-O	9.78	1.42	1.23
1	G	169	MET	CG-SD	9.69	2.06	1.81
1	J	209	CYS	CB-SG	-9.18	1.66	1.82
1	C	365	GLN	CB-CG	8.99	1.76	1.52
1	G	188	ASP	CG-OD1	8.98	1.46	1.25
1	D	120	PHE	CE1-CZ	8.84	1.54	1.37
1	E	209	CYS	CB-SG	-8.82	1.67	1.82
1	J	341	PHE	C-O	8.77	1.40	1.23
1	B	316	MET	CG-SD	8.75	2.03	1.81
1	B	365	GLN	CB-CG	8.53	1.75	1.52
1	A	181	GLU	CD-OE2	8.31	1.34	1.25
1	D	120	PHE	CD1-CE1	8.31	1.55	1.39
1	B	181	GLU	CD-OE1	8.13	1.34	1.25
1	J	318	TRP	CE3-CZ3	8.09	1.52	1.38
1	D	365	GLN	CB-CG	7.90	1.73	1.52
1	D	120	PHE	CG-CD2	7.80	1.50	1.38
1	J	365	GLN	CB-CG	7.54	1.72	1.52
1	F	365	GLN	CB-CG	7.45	1.72	1.52
1	B	220	TYR	CD2-CE2	7.44	1.50	1.39
1	G	187	SER	CB-OG	7.39	1.51	1.42
1	J	230	LEU	CG-CD1	-7.36	1.24	1.51
1	D	304	CYS	CB-SG	-7.35	1.69	1.82
1	J	347	ARG	CZ-NH1	7.25	1.42	1.33
1	J	145	THR	C-N	7.19	1.46	1.33
1	A	373	ARG	CZ-NH1	7.17	1.42	1.33
1	A	306	ARG	CZ-NH1	7.11	1.42	1.33
1	J	348	VAL	C-O	7.09	1.36	1.23
1	D	120	PHE	CD2-CE2	7.07	1.53	1.39
1	G	186	ARG	C-O	7.01	1.36	1.23
1	J	368	TYR	N-CA	6.86	1.60	1.46
1	J	140	TRP	CB-CG	-6.61	1.38	1.50
1	A	131	ARG	CG-CD	6.59	1.68	1.51
1	J	231	VAL	CA-CB	6.58	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	ARG	CZ-NH1	6.55	1.41	1.33
1	B	172	GLU	CD-OE2	6.48	1.32	1.25
1	I	365	GLN	CB-CG	6.43	1.70	1.52
1	A	268	GLY	C-O	6.41	1.33	1.23
1	J	346	THR	CB-CG2	-6.41	1.31	1.52
1	I	338	GLU	CD-OE1	6.34	1.32	1.25
1	B	220	TYR	CD1-CE1	6.32	1.48	1.39
1	G	77	GLY	CA-C	6.25	1.61	1.51
1	B	299	GLU	CD-OE2	6.12	1.32	1.25
1	B	373	ARG	CZ-NH1	6.12	1.41	1.33
1	H	365	GLN	CB-CG	6.09	1.69	1.52
1	C	261	VAL	CB-CG1	-6.00	1.40	1.52
1	B	172	GLU	CD-OE1	5.99	1.32	1.25
1	B	269	TYR	C-O	-5.99	1.11	1.23
1	A	373	ARG	CZ-NH2	5.99	1.40	1.33
1	B	129	PHE	CB-CG	-5.90	1.41	1.51
1	A	218	ARG	CG-CD	5.88	1.66	1.51
1	G	209	CYS	CB-SG	-5.86	1.72	1.81
1	F	365	GLN	CG-CD	5.84	1.64	1.51
1	A	172	GLU	CD-OE1	5.81	1.32	1.25
1	A	362	TYR	CG-CD2	5.79	1.46	1.39
1	A	299	GLU	CG-CD	5.76	1.60	1.51
1	B	52	GLU	CD-OE2	5.76	1.31	1.25
1	B	181	GLU	CG-CD	5.75	1.60	1.51
1	A	288	GLU	CD-OE1	5.74	1.31	1.25
1	D	316	MET	CG-SD	5.74	1.96	1.81
1	A	299	GLU	CD-OE2	5.73	1.31	1.25
1	B	215	LYS	CE-NZ	5.72	1.63	1.49
1	G	192	ASP	C-O	5.71	1.34	1.23
1	J	317	ALA	C-O	5.71	1.34	1.23
1	G	85	ARG	CG-CD	-5.68	1.37	1.51
1	B	304	CYS	CB-SG	-5.68	1.72	1.81
1	G	70	GLY	C-O	5.68	1.32	1.23
1	J	366	TYR	CD1-CE1	5.67	1.47	1.39
1	E	59	THR	CB-CG2	5.66	1.71	1.52
1	C	94	GLU	CD-OE2	5.66	1.31	1.25
1	G	362	TYR	CE2-CZ	5.65	1.45	1.38
1	J	347	ARG	N-CA	-5.64	1.35	1.46
1	B	254	GLU	CB-CG	-5.63	1.41	1.52
1	B	180	ASP	C-O	-5.60	1.12	1.23
1	B	272	GLU	CB-CG	-5.58	1.41	1.52
1	A	360	TYR	CB-CG	-5.51	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	300	GLY	N-CA	5.51	1.54	1.46
1	J	366	TYR	CE2-CZ	5.50	1.45	1.38
1	A	272	GLU	CG-CD	5.47	1.60	1.51
1	A	14	GLU	CG-CD	5.45	1.60	1.51
1	B	351	TYR	CD2-CE2	-5.41	1.31	1.39
1	I	365	GLN	CG-CD	5.39	1.63	1.51
1	B	267	VAL	CB-CG2	5.38	1.64	1.52
1	C	181	GLU	CD-OE2	5.35	1.31	1.25
1	A	381	GLU	CB-CG	-5.33	1.42	1.52
1	J	362	TYR	CE1-CZ	5.30	1.45	1.38
1	B	312	PHE	CG-CD2	5.29	1.46	1.38
1	A	221	GLY	N-CA	5.28	1.53	1.46
1	B	185	ARG	CZ-NH2	5.26	1.39	1.33
1	G	94	GLU	CG-CD	5.24	1.59	1.51
1	A	208	GLU	CG-CD	-5.23	1.44	1.51
1	B	135	ASP	CG-OD2	5.23	1.37	1.25
1	B	327	GLU	CD-OE1	5.23	1.31	1.25
1	B	381	GLU	CD-OE1	5.20	1.31	1.25
1	J	304	CYS	CB-SG	5.19	1.91	1.82
1	B	352	THR	C-O	-5.18	1.13	1.23
1	G	82	THR	CA-CB	5.17	1.66	1.53
1	C	365	GLN	CG-CD	5.16	1.62	1.51
1	C	131	ARG	CG-CD	5.15	1.64	1.51
1	J	140	TRP	CE3-CZ3	-5.14	1.29	1.38
1	A	376	TYR	CE1-CZ	5.12	1.45	1.38
1	J	146	GLY	N-CA	5.10	1.53	1.46
1	E	360	TYR	CE2-CZ	5.10	1.45	1.38
1	J	142	ILE	CA-CB	-5.09	1.43	1.54
1	A	306	ARG	CZ-NH2	5.07	1.39	1.33
1	E	365	GLN	CB-CG	5.05	1.66	1.52
1	A	327	GLU	CG-CD	5.04	1.59	1.51
1	G	197	PHE	CE2-CZ	5.03	1.47	1.37
1	G	184	ARG	C-O	5.02	1.32	1.23
1	B	94	GLU	CG-CD	5.01	1.59	1.51
1	A	366	TYR	CG-CD2	-5.01	1.32	1.39
1	J	338	GLU	CD-OE2	5.01	1.31	1.25

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	68	ARG	NE-CZ-NH2	12.44	126.52	120.30
1	J	347	ARG	NE-CZ-NH1	10.73	125.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASP	CB-CG-OD1	-10.67	108.69	118.30
1	J	347	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	A	347	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	85	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	B	68	ARG	NE-CZ-NH2	9.41	125.01	120.30
1	A	270	ASP	CB-CG-OD1	9.14	126.52	118.30
1	C	109	ASP	CB-CG-OD1	-8.66	110.50	118.30
1	J	307	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	D	68	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	E	68	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	C	68	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	D	109	ASP	CB-CG-OD1	-7.96	111.14	118.30
1	D	170	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	347	ARG	NH1-CZ-NH2	7.66	127.82	119.40
1	B	306	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	131	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	35	ILE	CG1-CB-CG2	-7.50	94.90	111.40
1	B	227	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	B	270	ASP	CB-CG-OD1	7.43	124.99	118.30
1	E	124	LEU	CA-CB-CG	7.35	132.21	115.30
1	G	124	LEU	CA-CB-CG	7.34	132.19	115.30
1	A	347	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	B	180	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	302	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	B	109	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	D	135	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	209	CYS	N-CA-CB	-6.90	98.18	110.60
1	C	170	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	259	VAL	CB-CA-C	-6.78	98.51	111.40
1	A	259	VAL	CB-CA-C	-6.78	98.52	111.40
1	C	184	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	306	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	211	ILE	CG1-CB-CG2	-6.62	96.83	111.40
1	C	209	CYS	N-CA-CB	-6.62	98.69	110.60
1	A	109	ASP	N-CA-CB	-6.54	98.82	110.60
1	C	211	ILE	CG1-CB-CG2	-6.44	97.24	111.40
1	A	343	LEU	CB-CG-CD1	6.43	121.94	111.00
1	I	68	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	B	306	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	170	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	F	307	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	I	131	ARG	NE-CZ-NH2	-6.27	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	211	ILE	CG1-CB-CG2	-6.22	97.71	111.40
1	B	302	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	B	347	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	E	68	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	A	357	LEU	CB-CG-CD2	-6.14	100.57	111.00
1	F	124	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	185	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	170	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	124	LEU	CA-CB-CG	6.09	129.31	115.30
1	D	370	MET	CG-SD-CE	6.09	109.94	100.20
1	A	21	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	I	304	CYS	CA-CB-SG	-6.08	103.05	114.00
1	G	188	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	109	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	I	109	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	A	131	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	346	THR	CA-C-O	-5.95	107.61	120.10
1	H	131	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	227	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	307	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	F	298	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	135	ASP	CB-CG-OD2	5.86	123.58	118.30
1	G	347	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	301	LEU	CB-CG-CD2	5.79	120.85	111.00
1	I	211	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	C	186	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	68	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	358	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	C	135	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	B	211	ILE	CG1-CB-CG2	-5.70	98.85	111.40
1	D	209	CYS	N-CA-CB	-5.70	100.34	110.60
1	J	227	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	124	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	211	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	H	109	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	B	209	CYS	N-CA-CB	-5.58	100.56	110.60
1	I	124	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	259	VAL	CB-CA-C	-5.54	100.87	111.40
1	A	370	MET	CG-SD-CE	5.52	109.04	100.20
1	C	252	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	E	302	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	E	131	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	185	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	198	VAL	CG1-CB-CG2	5.43	119.59	110.90
1	I	209	CYS	N-CA-CB	-5.43	100.83	110.60
1	I	270	ASP	CB-CG-OD2	5.42	123.18	118.30
1	G	180	ASP	CB-CG-OD2	5.42	123.17	118.30
1	J	343	LEU	CA-CB-CG	5.39	127.69	115.30
1	G	68	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	A	159	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	H	68	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	124	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	307	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	285	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	J	211	ILE	CG1-CB-CG2	-5.31	99.72	111.40
1	D	109	ASP	N-CA-CB	-5.30	101.05	110.60
1	B	277	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	G	109	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	272	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	I	68	ARG	NE-CZ-NH2	5.23	122.91	120.30
1	B	184	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	290	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	J	342	LYS	CD-CE-NZ	-5.18	99.79	111.70
1	B	182	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	285	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	H	209	CYS	N-CA-CB	-5.14	101.34	110.60
1	B	39	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	259	VAL	CB-CA-C	-5.07	101.77	111.40
1	B	159	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	E	209	CYS	N-CA-CB	-5.06	101.49	110.60
1	C	64	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	F	373	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	35	ILE	CG1-CB-CG2	-5.03	100.33	111.40
1	A	302	ARG	NH1-CZ-NH2	5.03	124.93	119.40

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

4.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3138	0	3037	102	2
1	B	3138	0	3037	91	1
1	C	3138	0	3037	96	0
1	D	3138	0	3037	101	0
1	E	3138	0	3037	70	0
1	F	3138	0	3037	81	0
1	G	3138	0	3037	106	1
1	H	3138	0	3037	79	0
1	I	3138	0	3037	78	0
1	J	3138	0	3036	100	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	880	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 14.

All (880) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:I:246:GLY:C	1:I:247:GLN:HG3	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:52:GLU:C	1:D:52:GLU:CD	2.33	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:I:246:GLY:C	1:I:247:GLN:CG	2.44	0.86
1:B:247:GLN:HB2	1:B:248:PRO:CB	2.05	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:52:GLU:C	1:D:52:GLU:OE2	2.30	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: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:A:52:GLU:C	1:A:52:GLU:OE2	2.30	0.69
1:E:218:ARG:HG2	1:E:218:ARG:HH11	1.57	0.69
1:D:52:GLU:O	1:D:52:GLU:CD	2.31	0.69
1:I:246:GLY:O	1:I:247:GLN:CD	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:GLN:O	1:J:287:VAL:C	2.32	0.68
1:A:262:HIS:HE1	5:A:2039:HOH:O	1.77	0.68
1:H:250:ILE:CD1	1:H:250:ILE:C	2.62	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:H:250:ILE:C	1:H:250:ILE:HD13	2.15	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
1:A:131:ARG:O	1:A:360:TYR:HE2	1.80	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:381:GLU:HG2	1:A:382:ASN:N	2.12	0.64
1:E:247:GLN:CB	1:E:248:PRO:HD3	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:53:ILE:C	1:D:55:ARG:H	2.01	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: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: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
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: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: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:D:246:GLY:O	1:D:247:GLN:HG2	2.01	0.60
1:E:277:ARG:CZ	1:E:281:HIS:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:168:LEU:HD23	1:A:168:LEU:C	2.23	0.59
1:G:247:GLN:O	1:G:248:PRO:C	2.41	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
1:E:245:VAL:HG12	1:E:246:GLY:H	1.68	0.58
1:I:201:GLN:CD	1:I:245:VAL:HG11	2.23	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:G:180:ASP:CG	1:G:182:ARG:HH11	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:177:LEU:C	1:G:179:GLU:H	2.06	0.57
1:I:182:ARG:NH2	1:I:201:GLN:OE1	2.34	0.57
1:B:168:LEU:C	1:B:168:LEU:HD23	2.25	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: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:A:270:ASP:OD2	1:A:270:ASP:C	2.42	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:D:50:ALA:O	1:D:51:PRO:C	2.43	0.56
1:B:177:LEU:HD23	1:B:198:VAL:HG22	1.86	0.56
1:I:168:LEU:C	1:I:168:LEU:HD23	2.25	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
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:H:168:LEU:HD23	1:H:168:LEU:C	2.27	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:C:109:ASP:CG	5:C:2008:HOH:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:G:177:LEU:C	1:G:179:GLU:N	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:52:GLU:CD	1:A:55:ARG:NH1	2.62	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:D:49:ALA:O	1:D:50:ALA:C	2.47	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:D:53:ILE:C	1:D:55:ARG:N	2.64	0.50
1:D:132:ALA:HB3	1:D:135:ASP:CG	2.32	0.50
1:E:257:HIS:N	1:E:257:HIS:CD2	2.79	0.50
1:H:123:GLY:HA2	1:H:170:ARG:CD	2.41	0.50
1:J:286:GLN:C	1:J:288:GLU:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:246:GLY:O	1:I:247:GLN:OE1	2.30	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: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:B:245:VAL:HG12	1:B:245:VAL:O	2.12	0.49
1:D:52:GLU:O	1:D:52:GLU:OE1	2.30	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:A:260:PRO:HG2	1:A:263:ILE:HD12	1.93	0.49
1:D:365:GLN:HG3	1:D:366:TYR:N	2.26	0.49
1:J:142:ILE:CD1	1:J:230:LEU:HD11	2.42	0.49
1:J:270:ASP:OD2	1:J:270:ASP:C	2.51	0.49
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:F:168:LEU:C	1:F:168:LEU:HD23	2.33	0.49
1:A:277:ARG:CZ	1:A:281:HIS:HD2	2.25	0.49
1:I:290:LEU:HB3	1:I:298:ARG:HG3	1.93	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:F:244:VAL:C	1:F:245:VAL:HG23	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:17:LEU:HD21	1:E:46:VAL:HA	1.96	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
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: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: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:A:14:GLU:CD	1:A:14:GLU:H	2.17	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:132:ALA:HB3	1:B:135:ASP:OD2	2.15	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
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: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:H:14:GLU:CD	1:H:14:GLU:H	2.19	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:D:168:LEU:C	1:D:168:LEU:HD23	2.36	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:C:168:LEU:HD23	1:C:168:LEU:C	2.36	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:J:180:ASP:OD2	1:J:182:ARG:NH1	2.48	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: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:A:181:GLU:HG3	1:A:182:ARG:N	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:66:GLN:HE21	2:H:400:GDX:HN21	1.64	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: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: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:J:168:LEU:C	1:J:168:LEU:HD23	2.37	0.45
1:J:283:THR:O	1:J:284:PRO:C	2.54	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:HE	1:C:258:ARG:HH21	1.63	0.45
1:G:14:GLU:H	1:G:14:GLU:CD	2.20	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:G:77:GLY:O	1:G:78:ASP:C	2.55	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: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:D:246:GLY:C	1:D:247:GLN:CG	2.85	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:I:14:GLU:CD	1:I:14:GLU:H	2.21	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:267:VAL:C	5:A:2053:HOH:O	2.56	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:G:168:LEU:C	1:G:168:LEU:HD23	2.38	0.43
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: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:J:277:ARG:CZ	1:J:281:HIS:HD2	2.31	0.43
1:A:17:LEU:HD21	1:A:46:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:178:TYR:CD2	1:G:178:TYR:C	2.88	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:J:313:MET:O	1:J:313:MET:HG3	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: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:14:GLU:CD	1:F:14:GLU:H	2.21	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:D:333:ASP:OD1	1:D:333:ASP:C	2.55	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:G:270:ASP:C	1:G:270:ASP:OD2	2.57	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:J:333:ASP:C	1:J:333:ASP:OD1	2.56	0.43
1:C:140:TRP:CZ3	1:C:367:LEU:HB3	2.54	0.43
1:C:244:VAL:C	1:C:245:VAL:HG12	2.39	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: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:F:100:ASP:O	1:F:103:ILE:HD12	2.19	0.42
1:F:270:ASP:OD2	1:F:270:ASP:C	2.57	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:A:258:ARG:HH22	1:A:361:ASP:CG	2.22	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: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: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:J:258:ARG:HH22	1:J:361:ASP:CG	2.23	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: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: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:D:14:GLU:CD	1:D:14:GLU:H	2.23	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
1:D:35:ILE:HD12	1:D:35:ILE:HG23	1.66	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:F:218:ARG:HH11	1:F:218:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:14:GLU:H	1:E:14:GLU:CD	2.23	0.41
1:E:362:TYR:O	1:E:365:GLN:HG3	2.20	0.41
1:H:333:ASP:C	1:H:333:ASP:OD1	2.59	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:J:366:TYR:CD1	1:J:366:TYR:C	2.93	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:A:364:GLN:O	1:A:365:GLN:C	2.59	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:J:14:GLU:H	1:J:14:GLU:CD	2.23	0.41
1:A:35:ILE:HD12	1:A:35:ILE:HG23	1.65	0.41
1:C:14:GLU:CD	1:C:14:GLU:H	2.24	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:A:52:GLU:O	1:A:53:ILE:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:333:ASP:OD1	1:I:333:ASP:C	2.59	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: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: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:G:177:LEU:O	1:G:178:TYR:C	2.60	0.40
1:C:194:LEU:O	1:C:198:VAL:HG13	2.22	0.40
1:E:70:GLY:HA2	1:E:185:ARG:HA	2.02	0.40
1:I:177:LEU:CD2	1:I:198:VAL:HG22	2.52	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:G:362:TYR:CD2	1:G:362:TYR:C	2.95	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:260:PRO:HG2	1:J:263:ILE:HD12	2.03	0.40
1:B:214:GLY:CA	5:B:2016:HOH:O	2.69	0.40
1:E:66:GLN:HE21	2:E:400:GDX:HN21	1.69	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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	379/397 (96%)	357 (94%)	16 (4%)	6 (2%)	9	31
1	B	379/397 (96%)	363 (96%)	13 (3%)	3 (1%)	19	49
1	C	379/397 (96%)	363 (96%)	13 (3%)	3 (1%)	19	49
1	D	379/397 (96%)	360 (95%)	14 (4%)	5 (1%)	12	36
1	E	379/397 (96%)	363 (96%)	14 (4%)	2 (0%)	29	61
1	F	379/397 (96%)	364 (96%)	13 (3%)	2 (0%)	29	61
1	G	379/397 (96%)	359 (95%)	15 (4%)	5 (1%)	12	36
1	H	379/397 (96%)	365 (96%)	12 (3%)	2 (0%)	29	61
1	I	379/397 (96%)	366 (97%)	11 (3%)	2 (0%)	29	61
1	J	379/397 (96%)	353 (93%)	22 (6%)	4 (1%)	14	41
All	All	3790/3970 (96%)	3613 (95%)	143 (4%)	34 (1%)	17	46

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

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Mol	Chain	Res	Type
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

4.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/338 (96%)	290 (89%)	36 (11%)	6	19
1	B	326/338 (96%)	290 (89%)	36 (11%)	6	19
1	C	326/338 (96%)	292 (90%)	34 (10%)	7	21
1	D	326/338 (96%)	289 (89%)	37 (11%)	6	18
1	E	326/338 (96%)	294 (90%)	32 (10%)	8	24
1	F	326/338 (96%)	294 (90%)	32 (10%)	8	24
1	G	326/338 (96%)	297 (91%)	29 (9%)	9	28
1	H	326/338 (96%)	293 (90%)	33 (10%)	7	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	326/338 (96%)	295 (90%)	31 (10%)	8	25
1	J	326/338 (96%)	292 (90%)	34 (10%)	7	21
All	All	3260/3380 (96%)	2926 (90%)	334 (10%)	7	22

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	GLU
1	A	41	GLN
1	A	44	GLU
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
1	A	124	LEU
1	A	131	ARG
1	A	159	ILE
1	A	167	LEU
1	A	181	GLU
1	A	182	ARG
1	A	186	ARG
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	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

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Mol	Chain	Res	Type
1	A	364	GLN
1	A	365	GLN
1	B	11	GLU
1	B	14	GLU
1	B	41	GLN
1	B	42	THR
1	B	44	GLU
1	B	48	ARG
1	B	54	SER
1	B	55	ARG
1	B	63	VAL
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	167	LEU
1	B	181	GLU
1	B	183	VAL
1	B	186	ARG
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	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	41	GLN
1	C	44	GLU

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Mol	Chain	Res	Type
1	C	48	ARG
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	159	ILE
1	C	167	LEU
1	C	181	GLU
1	C	182	ARG
1	C	209	CYS
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	48	ARG
1	D	52	GLU
1	D	54	SER
1	D	55	ARG
1	D	65	LEU
1	D	68	ARG
1	D	72	LEU

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Mol	Chain	Res	Type
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	209	CYS
1	D	218	ARG
1	D	223	LEU
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	364	GLN
1	D	365	GLN
1	E	11	GLU
1	E	14	GLU
1	E	41	GLN
1	E	44	GLU
1	E	48	ARG
1	E	54	SER
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	167	LEU
1	E	179	GLU
1	E	181	GLU
1	E	186	ARG

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Mol	Chain	Res	Type
1	E	209	CYS
1	E	218	ARG
1	E	223	LEU
1	E	237	ILE
1	E	247	GLN
1	E	258	ARG
1	E	266	ARG
1	E	283	THR
1	E	289	LEU
1	E	291	GLU
1	E	301	LEU
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	48	ARG
1	F	54	SER
1	F	63	VAL
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	167	LEU
1	F	181	GLU
1	F	182	ARG
1	F	183	VAL
1	F	186	ARG
1	F	218	ARG
1	F	223	LEU
1	F	237	ILE
1	F	258	ARG
1	F	266	ARG
1	F	283	THR
1	F	289	LEU
1	F	291	GLU

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Mol	Chain	Res	Type
1	F	301	LEU
1	F	316	MET
1	F	343	LEU
1	F	364	GLN
1	F	365	GLN
1	G	11	GLU
1	G	14	GLU
1	G	41	GLN
1	G	44	GLU
1	G	48	ARG
1	G	54	SER
1	G	63	VAL
1	G	65	LEU
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	218	ARG
1	G	223	LEU
1	G	247	GLN
1	G	258	ARG
1	G	266	ARG
1	G	283	THR
1	G	289	LEU
1	G	291	GLU
1	G	301	LEU
1	G	343	LEU
1	G	364	GLN
1	G	365	GLN
1	H	11	GLU
1	H	14	GLU
1	H	41	GLN
1	H	44	GLU
1	H	54	SER
1	H	63	VAL
1	H	68	ARG
1	H	72	LEU

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Mol	Chain	Res	Type
1	H	84	LEU
1	H	92	GLN
1	H	109	ASP
1	H	124	LEU
1	H	167	LEU
1	H	179	GLU
1	H	181	GLU
1	H	182	ARG
1	H	183	VAL
1	H	209	CYS
1	H	218	ARG
1	H	223	LEU
1	H	237	ILE
1	H	250	ILE
1	H	257	HIS
1	H	258	ARG
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
1	I	14	GLU
1	I	21	ARG
1	I	41	GLN
1	I	44	GLU
1	I	54	SER
1	I	63	VAL
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	167	LEU
1	I	181	GLU
1	I	182	ARG
1	I	218	ARG

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Mol	Chain	Res	Type
1	I	223	LEU
1	I	237	ILE
1	I	247	GLN
1	I	250	ILE
1	I	258	ARG
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	41	GLN
1	J	44	GLU
1	J	48	ARG
1	J	54	SER
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	167	LEU
1	J	181	GLU
1	J	182	ARG
1	J	186	ARG
1	J	218	ARG
1	J	223	LEU
1	J	230	LEU
1	J	244	VAL
1	J	245	VAL
1	J	247	GLN
1	J	258	ARG
1	J	266	ARG
1	J	283	THR
1	J	285	ARG
1	J	289	LEU

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Mol	Chain	Res	Type
1	J	291	GLU
1	J	301	LEU
1	J	343	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 (88) 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	257	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	127	HIS
1	B	257	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	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	202	GLN
1	D	255	HIS
1	D	257	HIS

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

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Mol	Chain	Res	Type
1	I	257	HIS
1	I	262	HIS
1	I	276	HIS
1	I	281	HIS
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	255	HIS
1	J	257	HIS
1	J	276	HIS
1	J	281	HIS

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

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	34,42,43	1.14	2 (5%)	42,65,67	1.35	6 (14%)
2	GDX	B	400	3	34,42,43	1.69	7 (20%)	42,65,67	1.77	10 (23%)
2	GDX	E	400	3	34,42,43	1.78	7 (20%)	42,65,67	1.73	9 (21%)
2	GDX	C	400	3	34,42,43	1.24	3 (8%)	42,65,67	1.64	9 (21%)
2	GDX	I	400	3	34,42,43	1.24	2 (5%)	42,65,67	1.47	7 (16%)
2	GDX	H	400	3	34,42,43	1.23	2 (5%)	42,65,67	1.62	8 (19%)
2	GDX	G	400	3	34,42,43	1.82	7 (20%)	42,65,67	1.41	6 (14%)
2	GDX	A	400	3	34,42,43	1.61	5 (14%)	42,65,67	1.51	10 (23%)
2	GDX	F	400	3	34,42,43	1.44	3 (8%)	42,65,67	1.62	7 (16%)
2	GDX	D	400	3	34,42,43	1.67	4 (11%)	42,65,67	1.60	8 (19%)

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	-	3/18/59/61	0/4/4/4
2	GDX	B	400	3	-	3/18/59/61	0/4/4/4
2	GDX	E	400	3	-	4/18/59/61	0/4/4/4
2	GDX	C	400	3	-	3/18/59/61	0/4/4/4
2	GDX	I	400	3	-	3/18/59/61	0/4/4/4
2	GDX	H	400	3	-	4/18/59/61	0/4/4/4
2	GDX	G	400	3	-	3/18/59/61	0/4/4/4
2	GDX	A	400	3	-	4/18/59/61	0/4/4/4
2	GDX	F	400	3	-	3/18/59/61	0/4/4/4
2	GDX	D	400	3	-	3/18/59/61	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GDX	O5'-C5'	6.07	1.53	1.43
2	D	400	GDX	C5-C6	-5.89	1.35	1.47
2	G	400	GDX	O5'-C5'	5.88	1.53	1.43
2	B	400	GDX	C5-C6	-5.70	1.35	1.47
2	E	400	GDX	O5'-C5'	5.19	1.52	1.43
2	G	400	GDX	C5-C6	-5.02	1.37	1.47
2	E	400	GDX	C5-C6	-4.50	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	GDX	O5'-C5'	4.43	1.51	1.43
2	F	400	GDX	C5-C6	-4.32	1.38	1.47
2	D	400	GDX	O5'-C5'	4.24	1.50	1.43
2	I	400	GDX	C5-C6	-4.16	1.39	1.47
2	J	400	GDX	C5-C6	-4.16	1.39	1.47
2	C	400	GDX	C5-C6	-4.09	1.39	1.47
2	H	400	GDX	C5-C6	-3.93	1.39	1.47
2	A	400	GDX	C5-C6	-3.62	1.40	1.47
2	B	400	GDX	PA-O5D	3.54	1.73	1.59
2	B	400	GDX	O5'-C5'	3.34	1.49	1.43
2	E	400	GDX	O5'-C1'	3.33	1.50	1.41
2	D	400	GDX	O4D-C1D	3.29	1.45	1.41
2	E	400	GDX	O4D-C1D	3.11	1.45	1.41
2	E	400	GDX	PB-O2B	-3.03	1.41	1.55
2	B	400	GDX	PB-O1B	2.83	1.67	1.60
2	E	400	GDX	O2'-C2'	2.72	1.49	1.43
2	D	400	GDX	O2'-C2'	2.68	1.49	1.43
2	C	400	GDX	O5'-C5'	2.66	1.48	1.43
2	A	400	GDX	PB-O1B	2.58	1.67	1.60
2	G	400	GDX	PB-O1B	2.56	1.67	1.60
2	I	400	GDX	O5'-C5'	2.48	1.47	1.43
2	G	400	GDX	C4'-C5'	2.43	1.56	1.52
2	G	400	GDX	O5'-C1'	2.31	1.47	1.41
2	G	400	GDX	O2'-C2'	2.28	1.48	1.43
2	F	400	GDX	O4D-C1D	2.27	1.44	1.41
2	B	400	GDX	PA-O2A	-2.23	1.44	1.55
2	E	400	GDX	C2D-C1D	-2.22	1.50	1.53
2	A	400	GDX	O5'-C1'	2.22	1.47	1.41
2	H	400	GDX	C2D-C1D	-2.19	1.50	1.53
2	B	400	GDX	O2'-C2'	2.14	1.48	1.43
2	C	400	GDX	PA-O2A	-2.13	1.45	1.55
2	J	400	GDX	O5'-C5'	2.12	1.47	1.43
2	G	400	GDX	O6A-C6'	2.10	1.28	1.19
2	B	400	GDX	C5-C4	-2.07	1.37	1.43
2	A	400	GDX	C4'-C5'	2.01	1.56	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	GDX	O5'-C1'-O1B	-5.94	103.61	111.36
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	GDX	O1B-C1'-C2'	5.20	117.91	108.38
2	C	400	GDX	O1B-C1'-C2'	4.83	117.23	108.38
2	F	400	GDX	O1B-C1'-C2'	4.52	116.66	108.38
2	E	400	GDX	O5'-C1'-C2'	-4.33	101.19	110.35
2	C	400	GDX	O4D-C1D-C2D	-4.15	100.86	106.93
2	I	400	GDX	O5'-C1'-C2'	-4.11	101.64	110.35
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	D	400	GDX	O5'-C1'-C2'	-3.65	102.62	110.35
2	J	400	GDX	O1B-C1'-C2'	3.62	115.01	108.38
2	A	400	GDX	O4D-C1D-C2D	-3.51	101.79	106.93
2	E	400	GDX	O4D-C1D-C2D	-3.44	101.90	106.93
2	I	400	GDX	O1B-C1'-C2'	3.44	114.67	108.38
2	A	400	GDX	O6-C6-N1	-3.36	116.68	120.65
2	H	400	GDX	O4D-C1D-C2D	-3.35	102.03	106.93
2	B	400	GDX	O1B-PB-O3B	-3.32	96.99	109.47
2	H	400	GDX	O5'-C1'-C2'	-3.30	103.36	110.35
2	I	400	GDX	O4D-C1D-C2D	-3.26	102.17	106.93
2	J	400	GDX	O5'-C1'-C2'	-3.25	103.48	110.35
2	H	400	GDX	C2-N1-C6	-3.22	119.17	125.10
2	I	400	GDX	C2-N1-C6	-3.19	119.22	125.10
2	H	400	GDX	C5-C6-N1	3.13	119.48	113.95
2	C	400	GDX	O5'-C1'-C2'	-3.10	103.79	110.35
2	B	400	GDX	O2B-PB-O3B	3.06	127.39	112.24
2	A	400	GDX	O4'-C4'-C3'	-3.02	103.36	110.35
2	F	400	GDX	C2-N1-C6	-3.01	119.55	125.10
2	D	400	GDX	O5'-C1'-O1B	-2.94	107.52	111.36
2	G	400	GDX	O5'-C1'-C2'	-2.86	104.29	110.35
2	B	400	GDX	O4D-C1D-C2D	-2.78	102.86	106.93
2	E	400	GDX	C5-C6-N1	2.69	118.70	113.95
2	E	400	GDX	C3'-C4'-C5'	-2.68	106.94	110.22
2	E	400	GDX	PB-O1B-C1'	2.65	129.97	119.74
2	A	400	GDX	C5-C6-N1	2.64	118.62	113.95
2	F	400	GDX	O4D-C1D-C2D	-2.62	103.09	106.93
2	B	400	GDX	O2A-PA-O5D	-2.61	95.62	107.75
2	B	400	GDX	C4'-C3'-C2'	-2.58	106.32	110.82
2	D	400	GDX	C8-N7-C5	2.58	107.90	102.99
2	A	400	GDX	O1B-PB-O3B	-2.54	99.94	109.47
2	I	400	GDX	C8-N7-C5	2.54	107.83	102.99
2	J	400	GDX	C2-N1-C6	-2.54	120.43	125.10
2	E	400	GDX	O6-C6-N1	-2.51	117.68	120.65
2	A	400	GDX	O5'-C1'-C2'	-2.51	105.04	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	GDX	C8-N7-C5	2.51	107.77	102.99
2	B	400	GDX	O5'-C1'-O1B	-2.50	108.09	111.36
2	I	400	GDX	C5-C6-N1	2.50	118.36	113.95
2	A	400	GDX	N1-C2-N3	-2.48	118.69	123.32
2	B	400	GDX	O3A-PB-O1B	2.45	107.44	102.48
2	J	400	GDX	C5-C6-N1	2.44	118.26	113.95
2	D	400	GDX	O4D-C1D-C2D	-2.43	103.37	106.93
2	H	400	GDX	O5'-C1'-O1B	-2.43	108.19	111.36
2	G	400	GDX	PB-O3A-PA	-2.42	124.53	132.83
2	F	400	GDX	C5-C6-N1	2.37	118.13	113.95
2	F	400	GDX	O6-C6-C5	-2.33	119.82	124.37
2	H	400	GDX	C8-N7-C5	2.31	107.39	102.99
2	C	400	GDX	C4'-C5'-C6'	-2.31	108.70	112.55
2	B	400	GDX	PB-O1B-C1'	2.29	128.59	119.74
2	C	400	GDX	O5'-C1'-O1B	-2.27	108.40	111.36
2	J	400	GDX	O5'-C1'-O1B	-2.24	108.43	111.36
2	E	400	GDX	C4'-C5'-C6'	-2.24	108.82	112.55
2	G	400	GDX	O3A-PB-O1B	-2.23	97.99	102.48
2	A	400	GDX	O1B-C1'-C2'	2.20	112.41	108.38
2	D	400	GDX	PB-O3A-PA	-2.18	125.35	132.83
2	F	400	GDX	C8-N7-C5	2.17	107.13	102.99
2	C	400	GDX	O4D-C4D-C5D	-2.16	102.26	109.37
2	C	400	GDX	N2-C2-N1	2.14	121.26	116.71
2	C	400	GDX	C2-N1-C6	-2.13	121.17	125.10
2	G	400	GDX	O4'-C4'-C5'	2.13	114.94	110.51
2	D	400	GDX	C2-N1-C6	-2.12	121.19	125.10
2	A	400	GDX	PB-O1B-C1'	2.11	127.88	119.74
2	E	400	GDX	O4D-C4D-C5D	-2.09	102.48	109.37
2	A	400	GDX	C8-N7-C5	2.07	106.94	102.99
2	B	400	GDX	O6-C6-N1	2.07	123.09	120.65
2	D	400	GDX	C5-C6-N1	2.06	117.58	113.95
2	H	400	GDX	O6-C6-C5	-2.04	120.39	124.37
2	G	400	GDX	C5-C6-N1	2.03	117.54	113.95
2	J	400	GDX	PB-O3A-PA	-2.02	125.90	132.83
2	I	400	GDX	PB-O3A-PA	-2.01	125.94	132.83

There are no chirality outliers.

All (33) 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

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Mol	Chain	Res	Type	Atoms
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	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
2	G	400	GDX	C1'-O1B-PB-O3A
2	A	400	GDX	C1'-O1B-PB-O3A
2	C	400	GDX	C1'-O1B-PB-O3A
2	H	400	GDX	C1'-O1B-PB-O3A
2	I	400	GDX	C1'-O1B-PB-O3A
2	D	400	GDX	C1'-O1B-PB-O3A
2	F	400	GDX	C1'-O1B-PB-O3A
2	J	400	GDX	C1'-O1B-PB-O3A
2	A	400	GDX	C5D-O5D-PA-O3A
2	E	400	GDX	C1'-O1B-PB-O3A
2	H	400	GDX	C1'-O1B-PB-O3B
2	B	400	GDX	C1'-O1B-PB-O3A

There are no ring outliers.

10 monomers are involved in 33 short contacts:

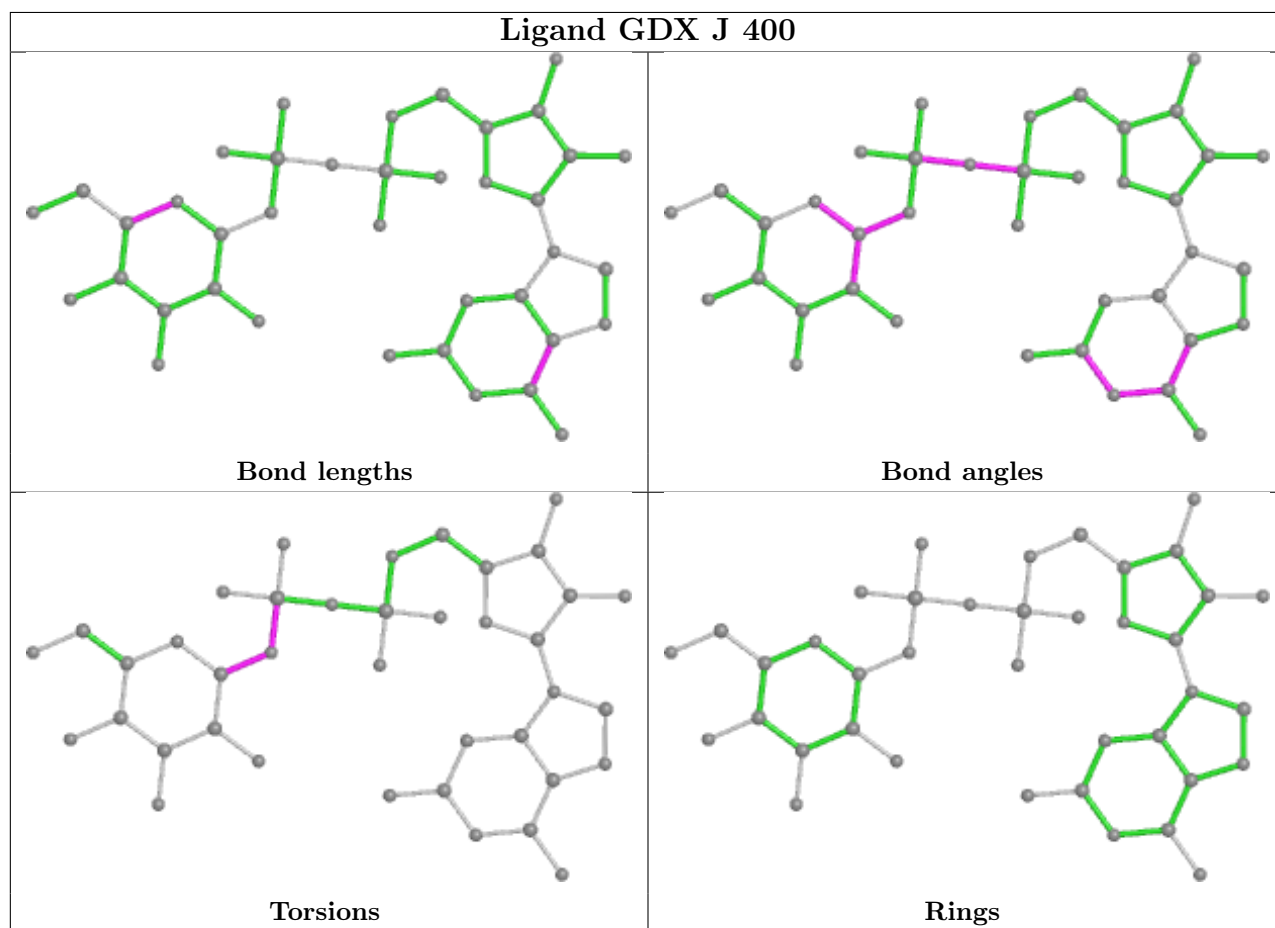
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	400	GDX	3	0
2	B	400	GDX	4	0
2	E	400	GDX	3	0
2	C	400	GDX	3	0
2	I	400	GDX	3	0
2	H	400	GDX	3	0

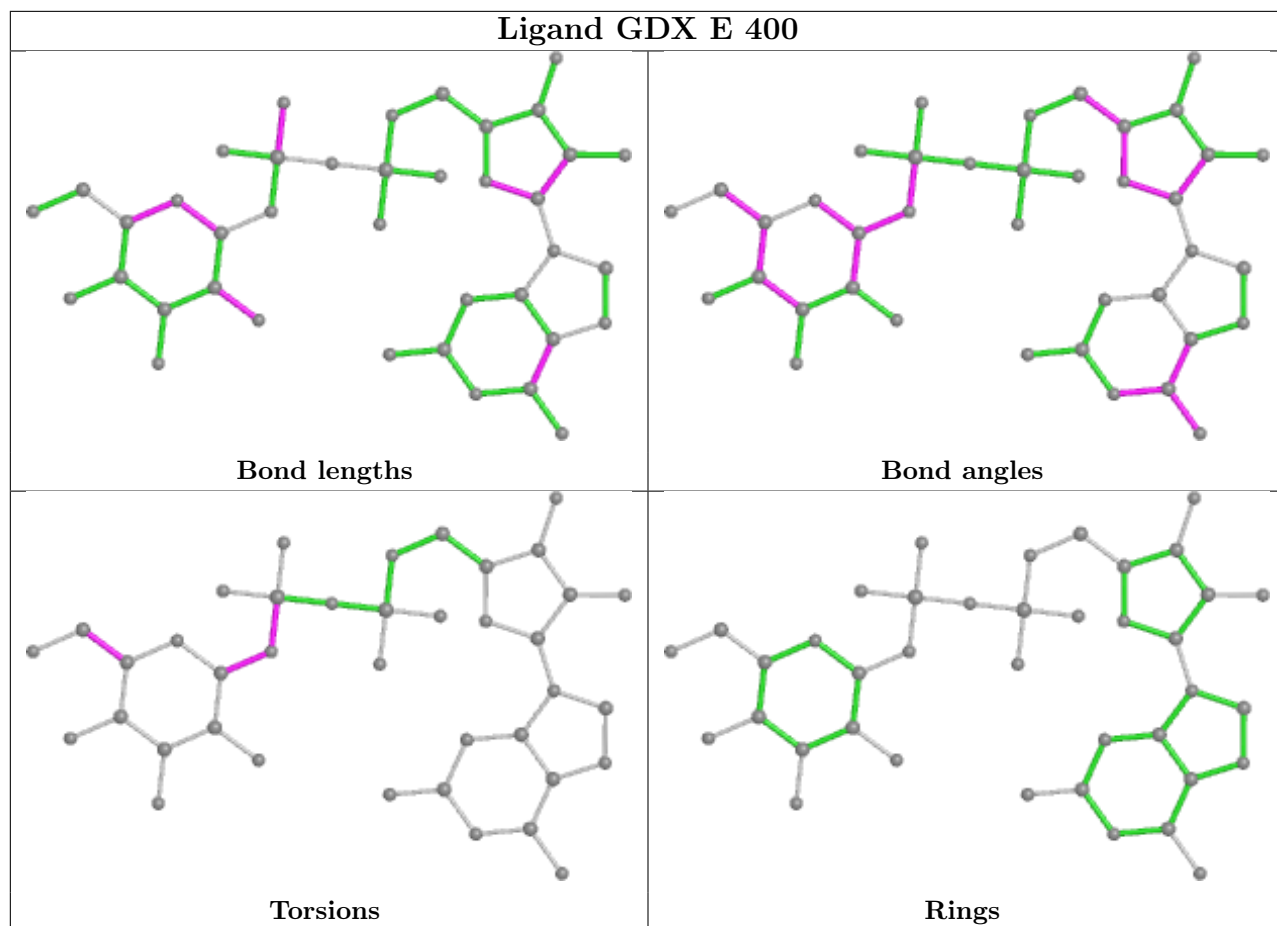
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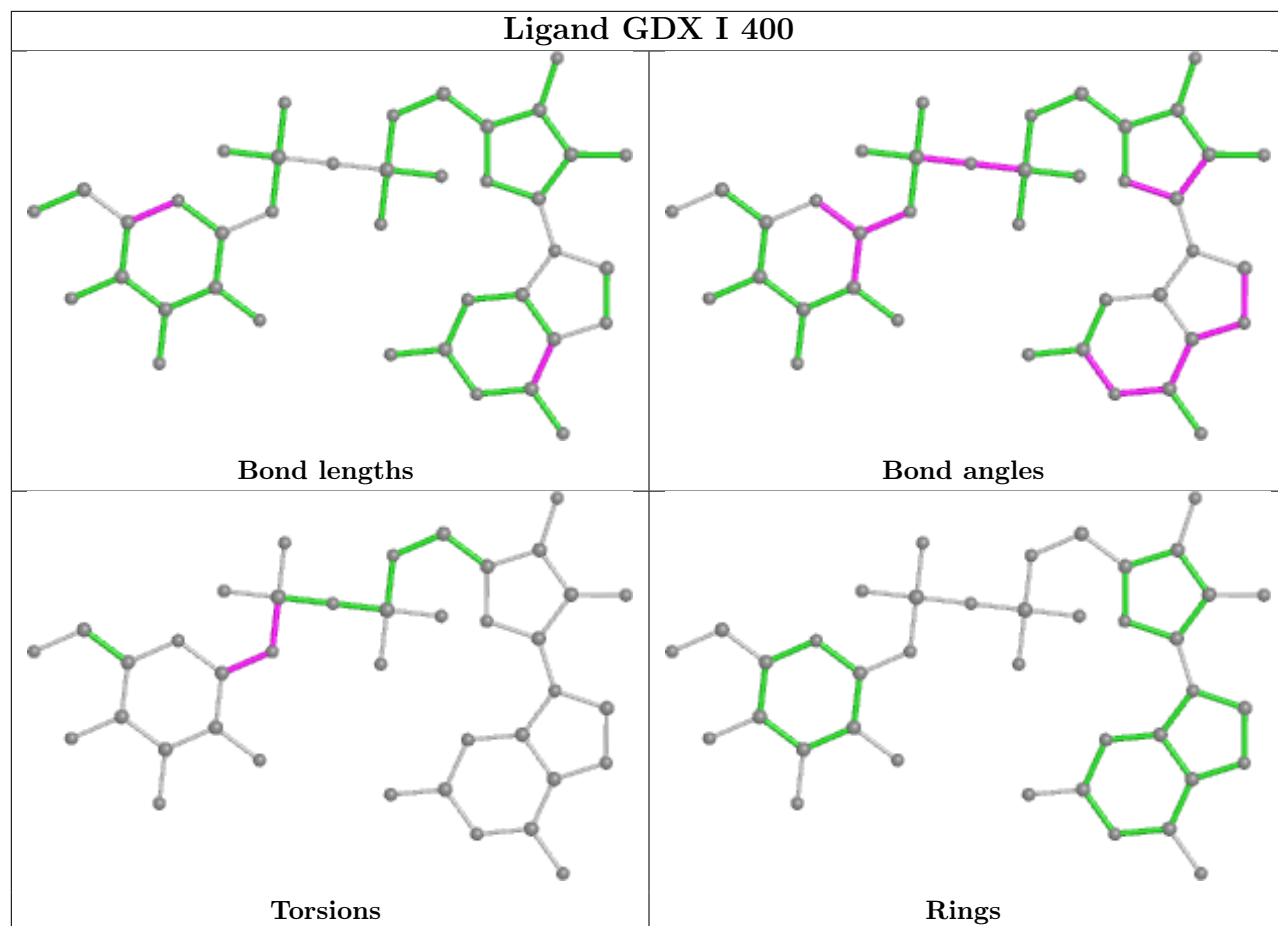
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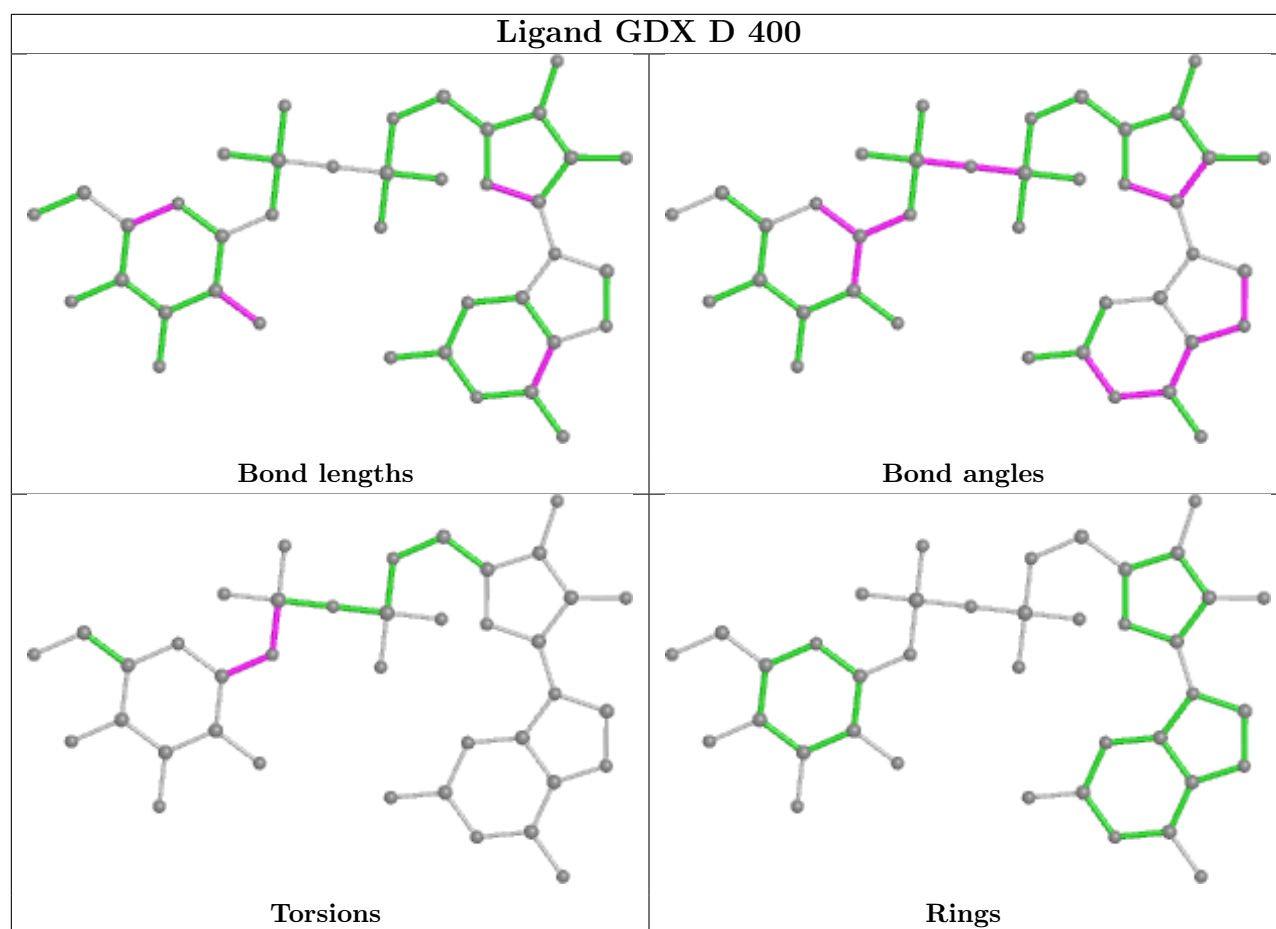
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	400	GDX	3	0
2	A	400	GDX	4	0
2	F	400	GDX	3	0
2	D	400	GDX	4	0

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









4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

5.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

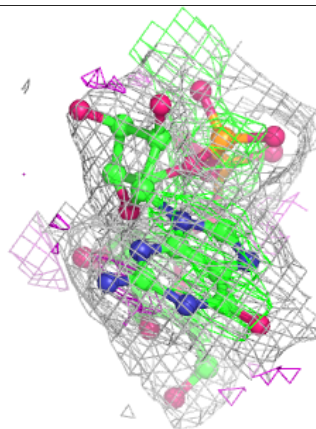
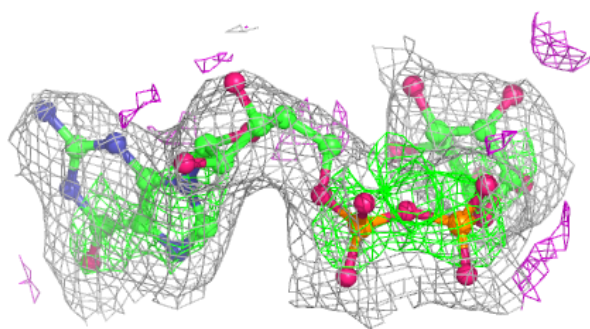
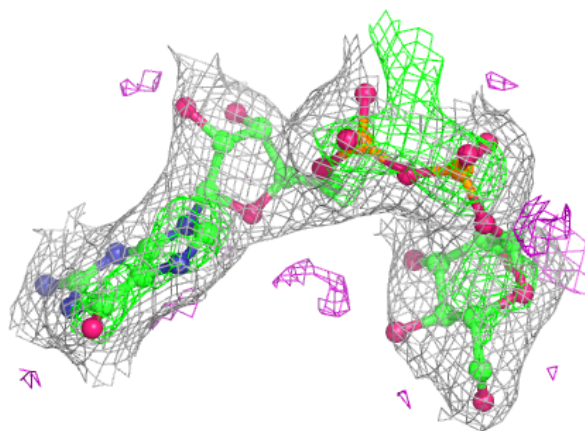
5.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

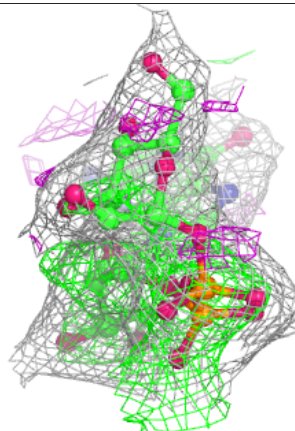
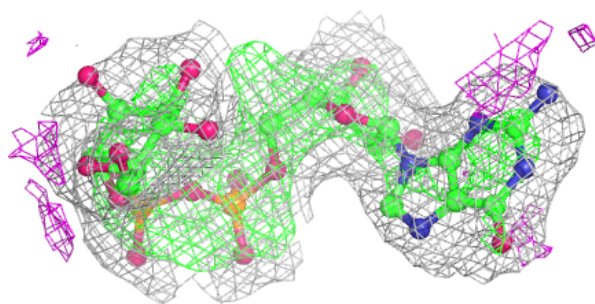
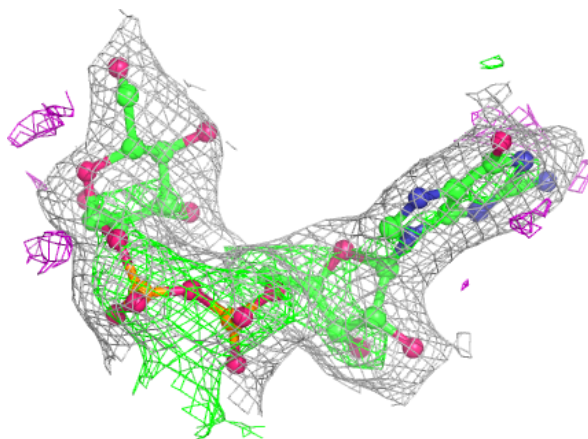
Electron density around GDX A 400:

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



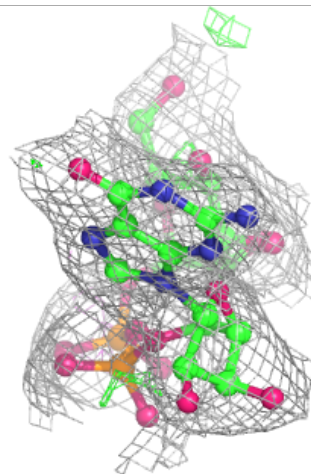
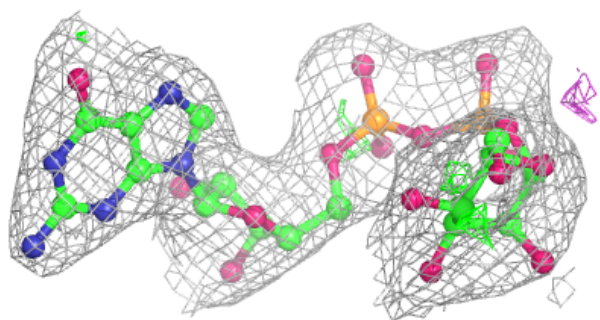
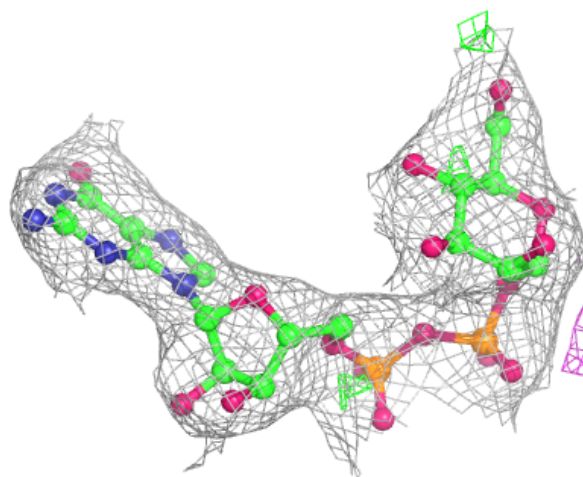
Electron density around GDX B 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



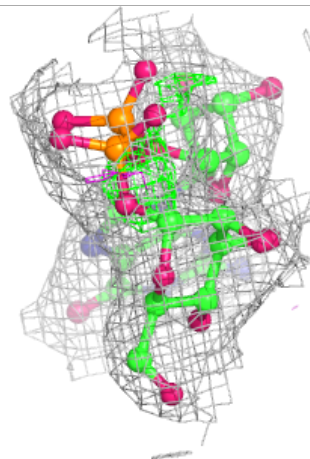
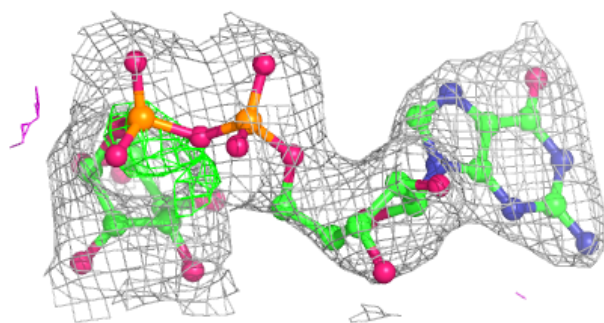
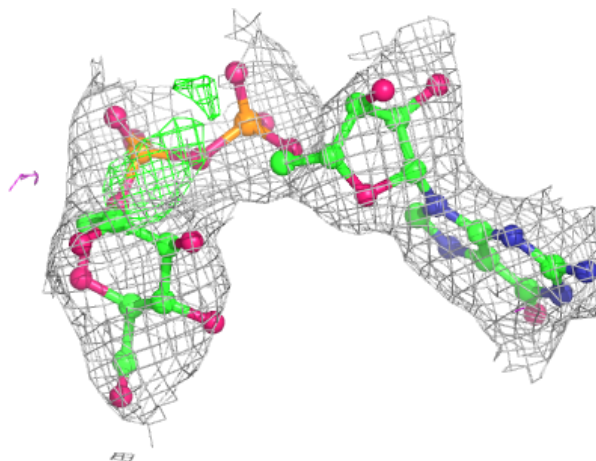
Electron density around GDX C 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



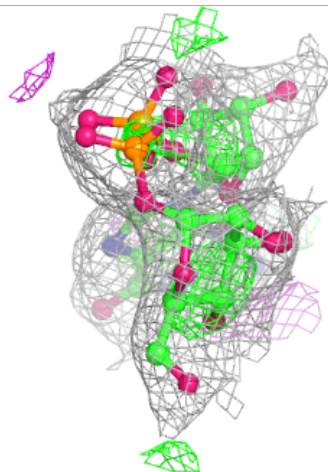
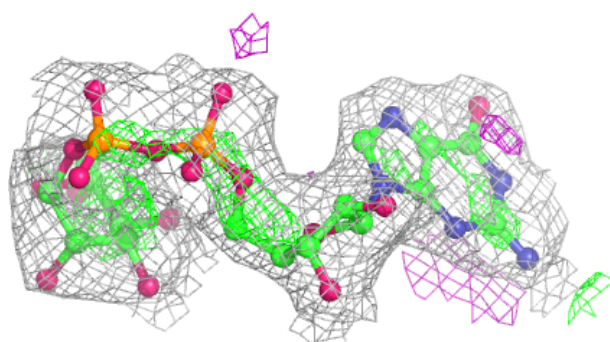
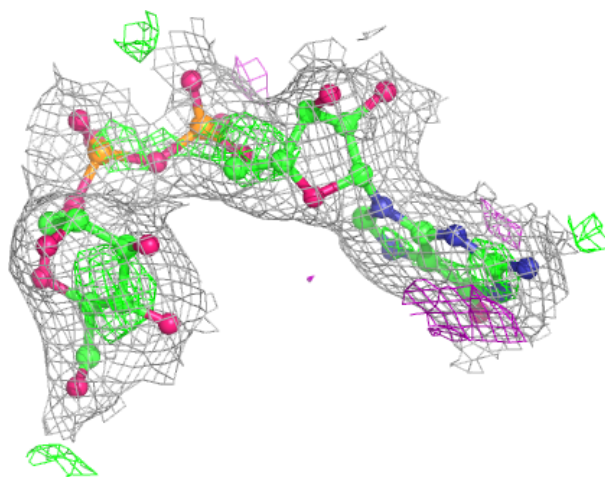
Electron density around GDX D 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



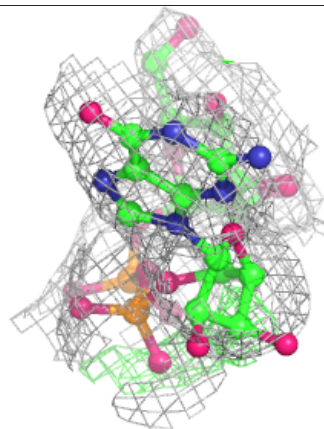
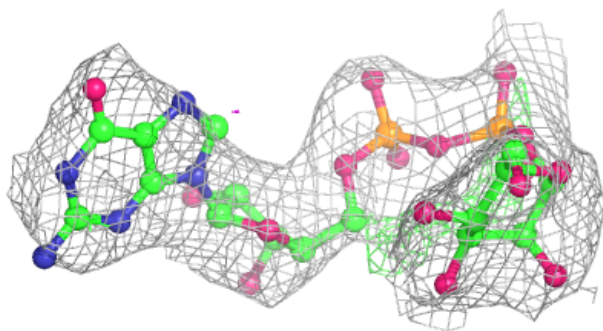
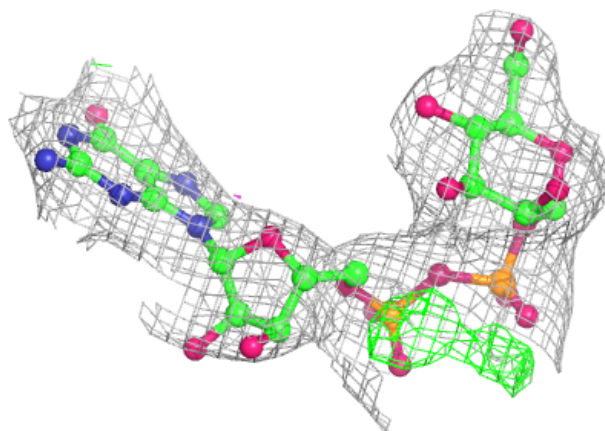
Electron density around GDX E 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



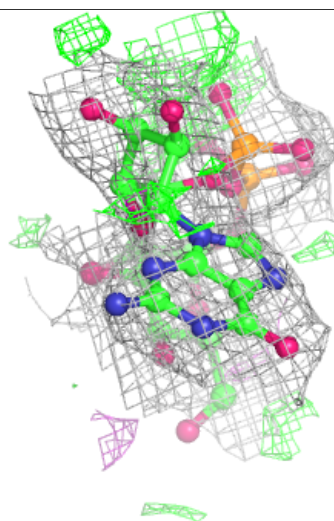
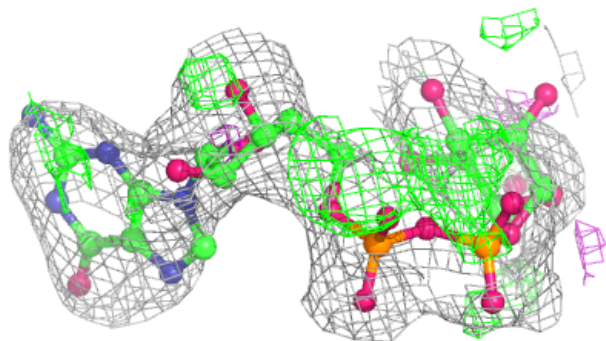
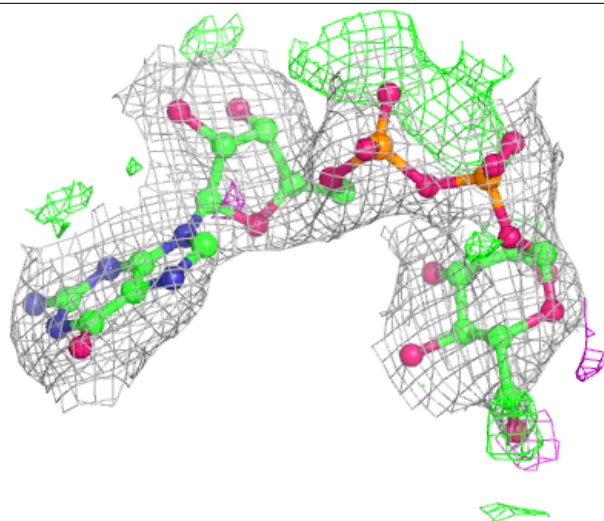
Electron density around GDX F 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



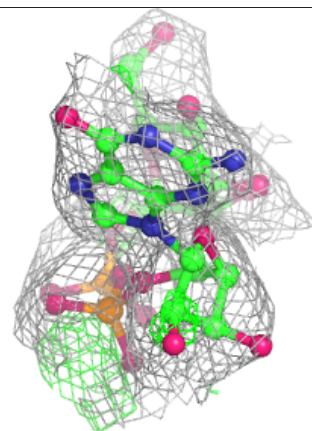
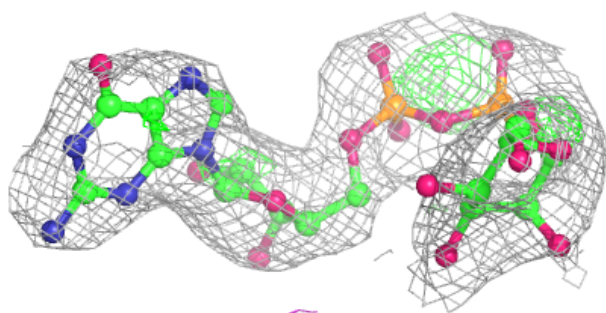
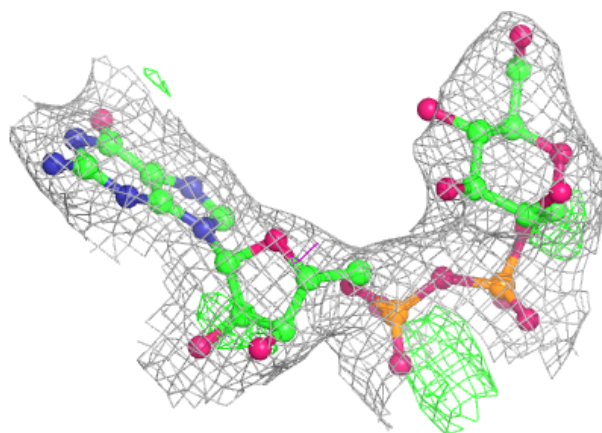
Electron density around GDX G 400:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



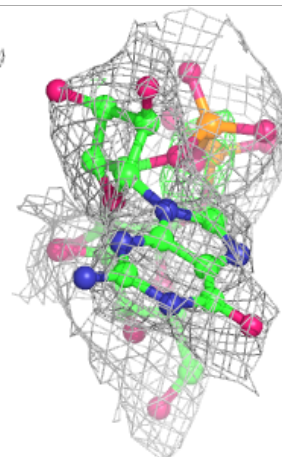
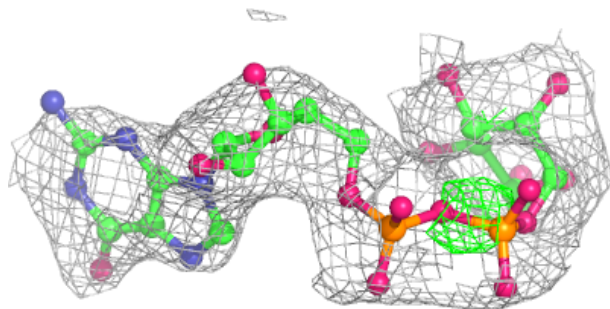
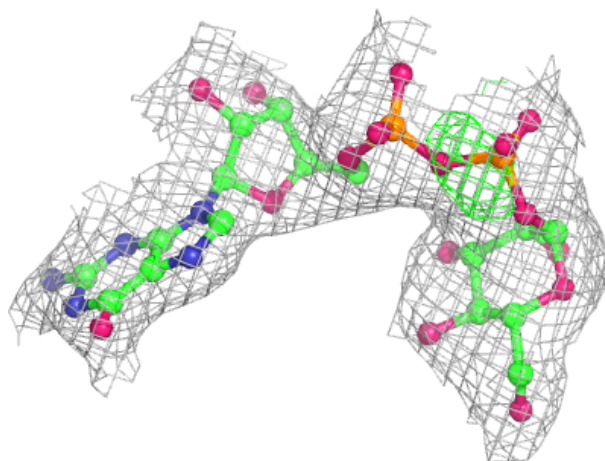
Electron density around GDX H 400:

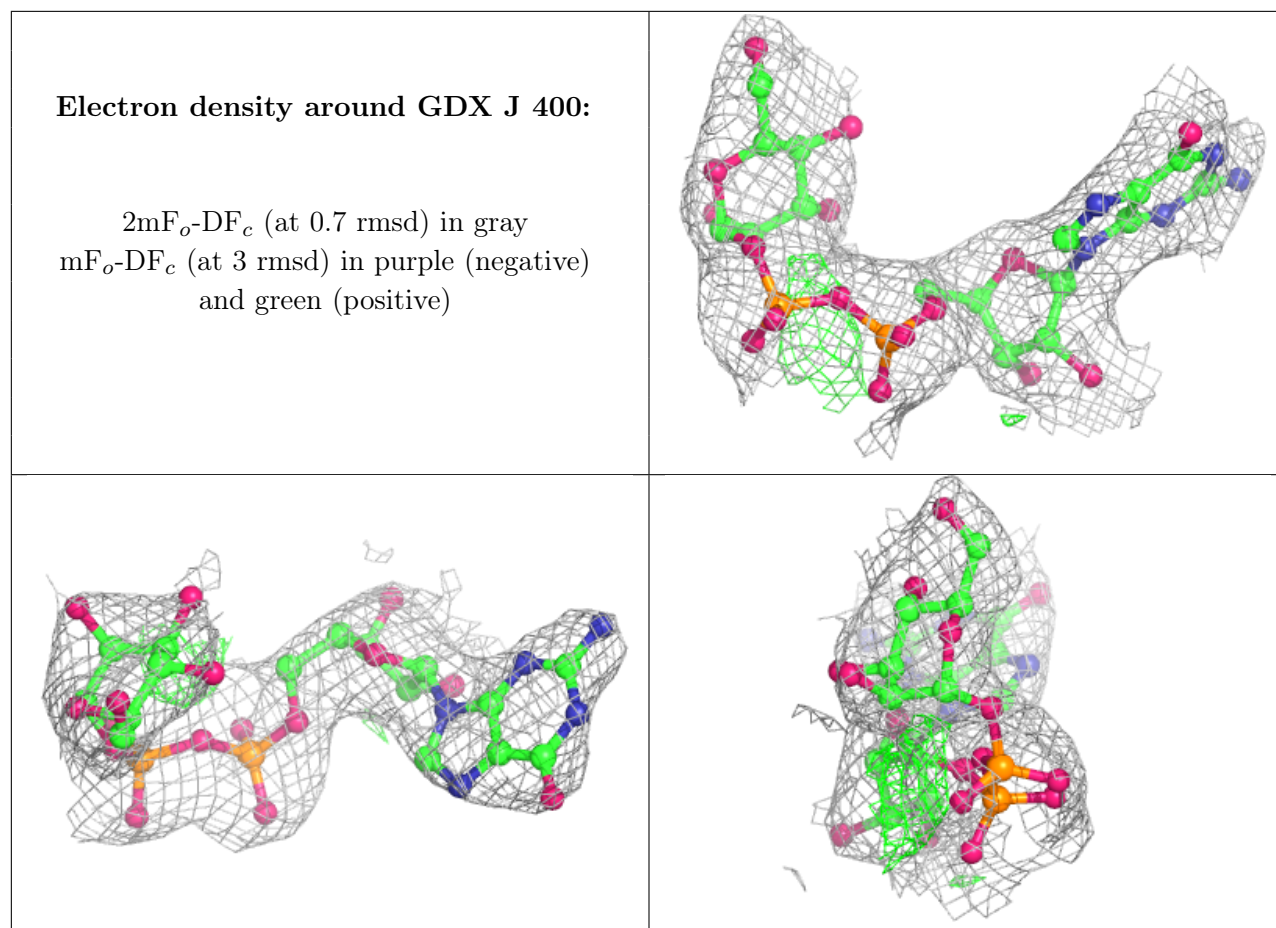
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDX 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)





5.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.