Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2023 – 03:14 pm GMT

PDB ID	:	2UX8
Title	:	Crystal Structure of Sphingomonas elodea ATCC 31461 Glucose-1- phosphate uridylyltransferase in Complex with glucose-1-phosphate.
Authors	:	Aragao, D.; Fialho, A.M.; Marques, A.R.; Frazao, C.; Sa-Correia, I.; Mitchell, E.P.
Deposited on	:	2007-03-27
Resolution	:	2.65 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 (i) 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 (i)) were used in the production of this report:

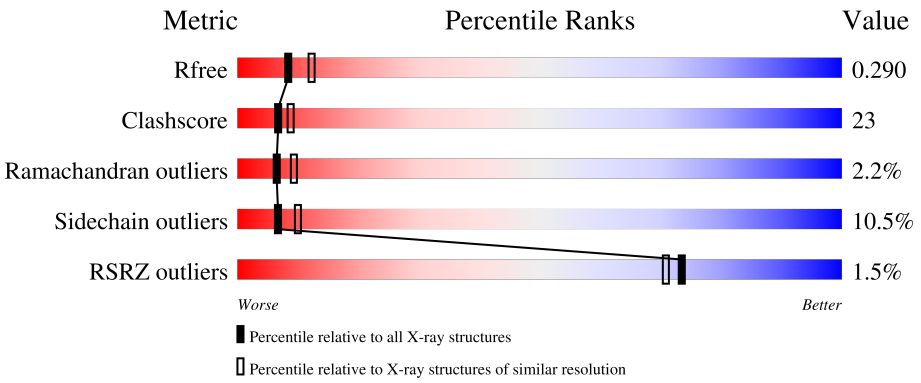
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	297	3%; 51%, 29%, 5%, 14%
1	B	297	.%; 61%, 26%, 8%, 6%
1	C	297	.%; 55%, 33%, 7%, 5%
1	D	297	.%; 61%, 27%, 6%, 5%

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Mol	Chain	Length	Quality of chain
1	E	297	%, 59%, 30%, 5%, 6%
1	F	297	3%, 57%, 31%, 6%, 5%
1	G	297	53%, 37%, 6%
1	H	297	53%, 23%, 6%, 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G1P	A	1290	-	-	-	X
2	G1P	H	1290	-	-	-	X

2 Entry composition (i)

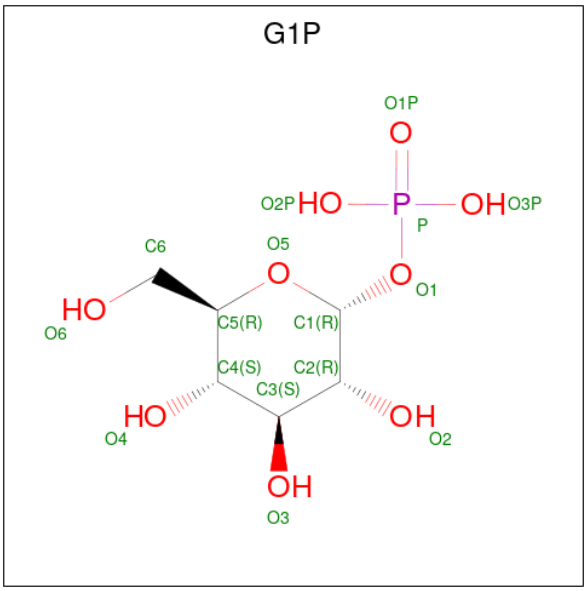
There are 3 unique types of molecules in this entry. The entry contains 16948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	1940	1235	334	357	14	0	0	0
1	B	280	2126	1350	367	395	14	0	0	0
1	C	282	2145	1361	370	399	15	0	0	0
1	D	281	2135	1355	369	397	14	0	0	0
1	E	280	2131	1353	368	396	14	0	0	0
1	F	282	2144	1361	371	398	14	0	0	0
1	G	288	2174	1379	376	405	14	0	0	0
1	H	244	1866	1191	322	339	14	0	0	0

- Molecule 2 is 1-O-phosphono-alpha-D-glucopyranose (three-letter code: G1P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	0	0
2	B	1	16	6	9	1	0	0
2	C	1	16	6	9	1	0	0
2	D	1	16	6	9	1	0	0
2	E	1	16	6	9	1	0	0
2	F	1	16	6	9	1	0	0
2	G	1	16	6	9	1	0	0
2	H	1	16	6	9	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	13	13	13	0	0
3	B	23	23	23	0	0
3	C	30	30	30	0	0
3	D	16	16	16	0	0

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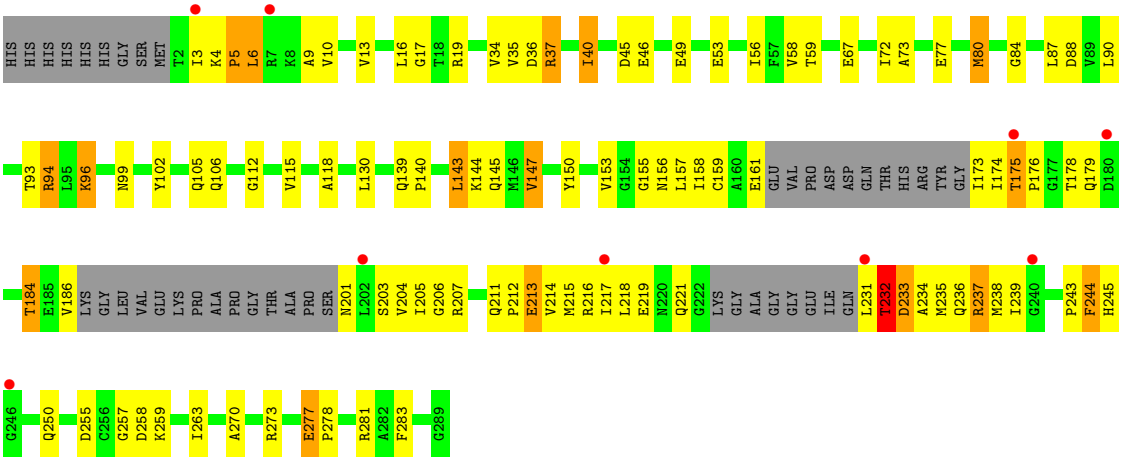
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	26	26	26	0	0
			Total	O		
3	F	12	12	12	0	0
			Total	O		
3	G	19	19	19	0	0
			Total	O		
3	H	20	20	20	0	0

3 Residue-property plots (i)

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

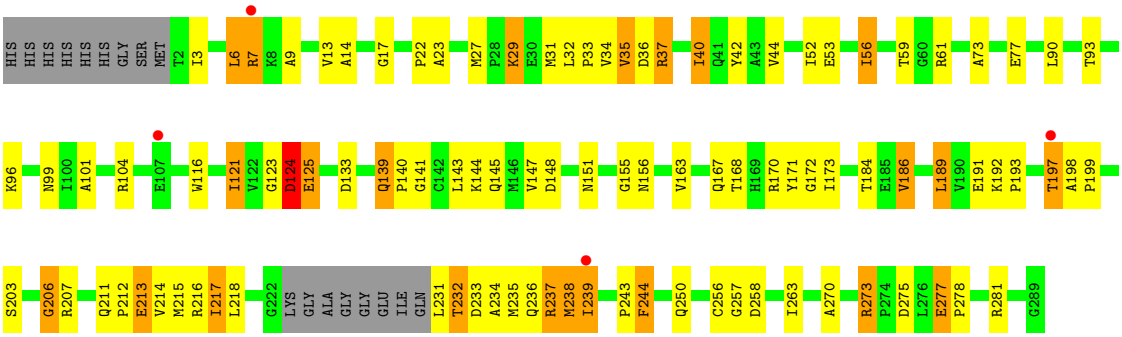
• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain A:



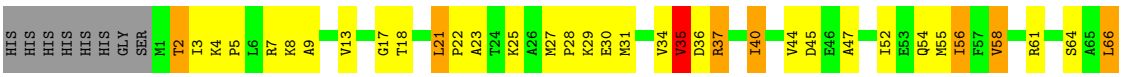
• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

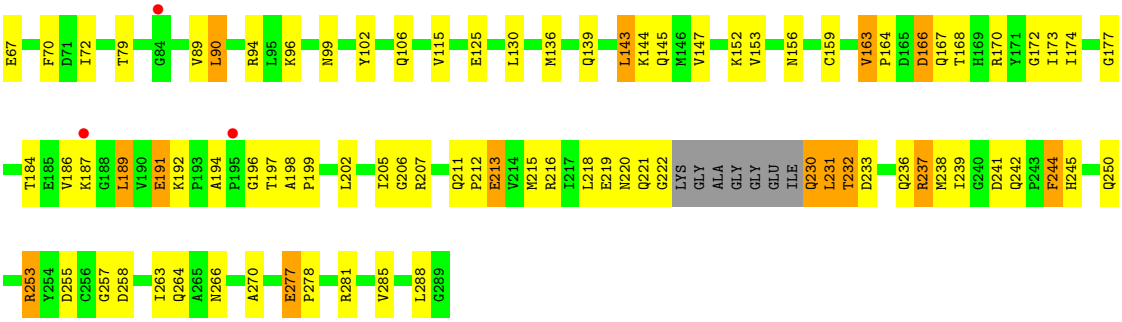
Chain B:



• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

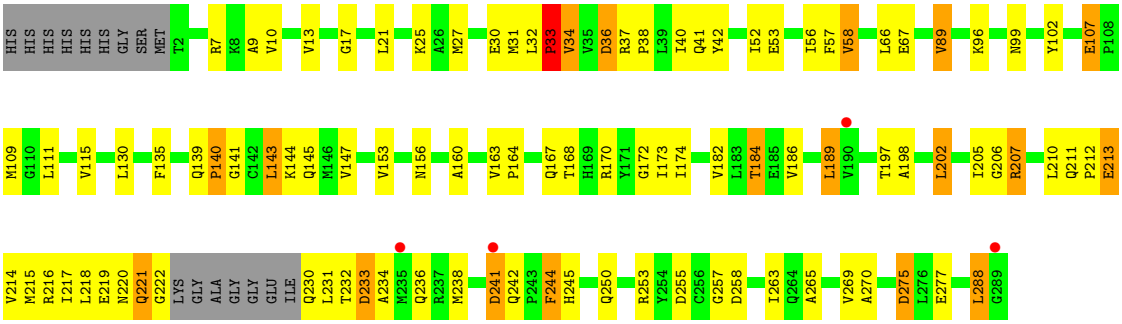
Chain C:





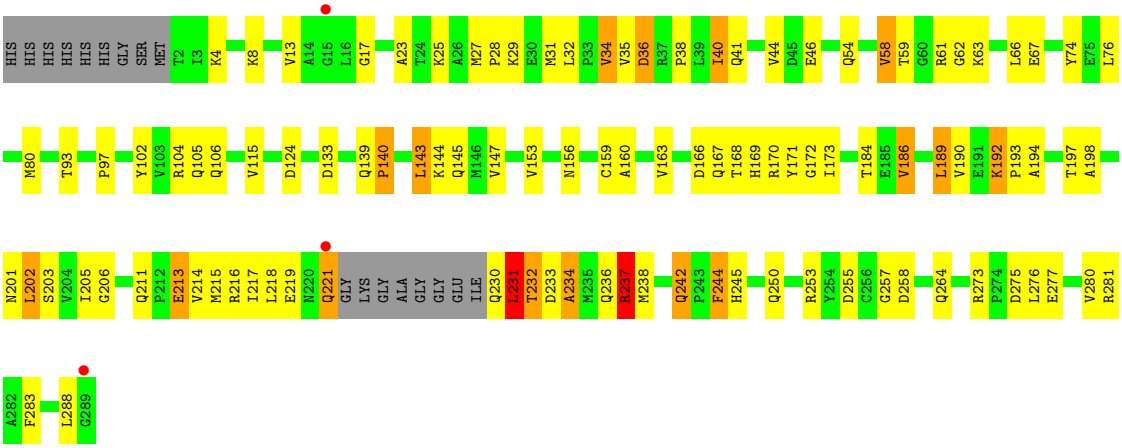
- Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain D:



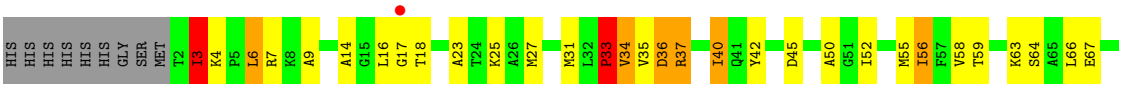
- Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

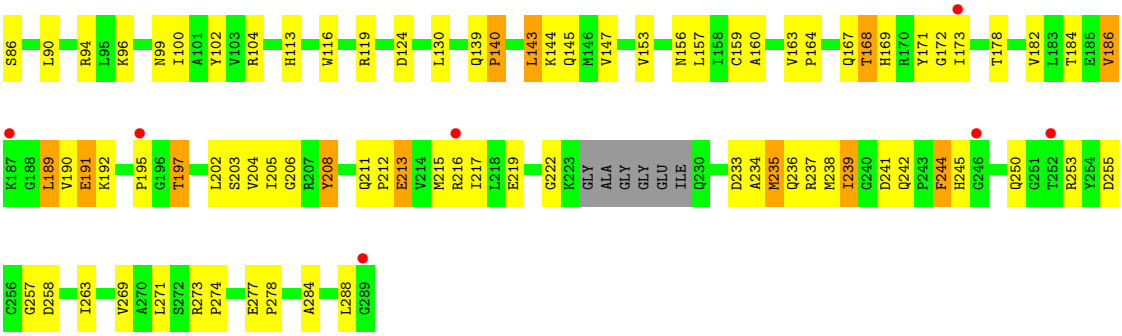
Chain E:



- Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

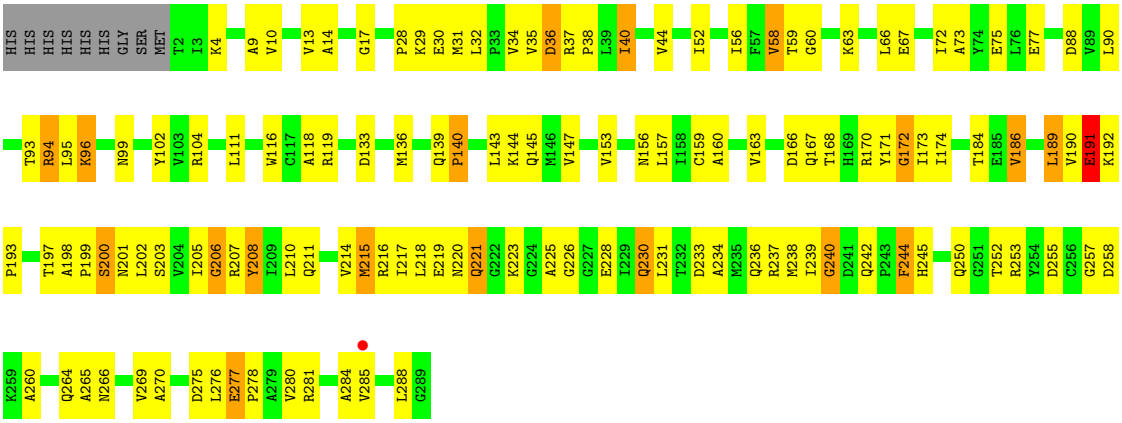
Chain F:





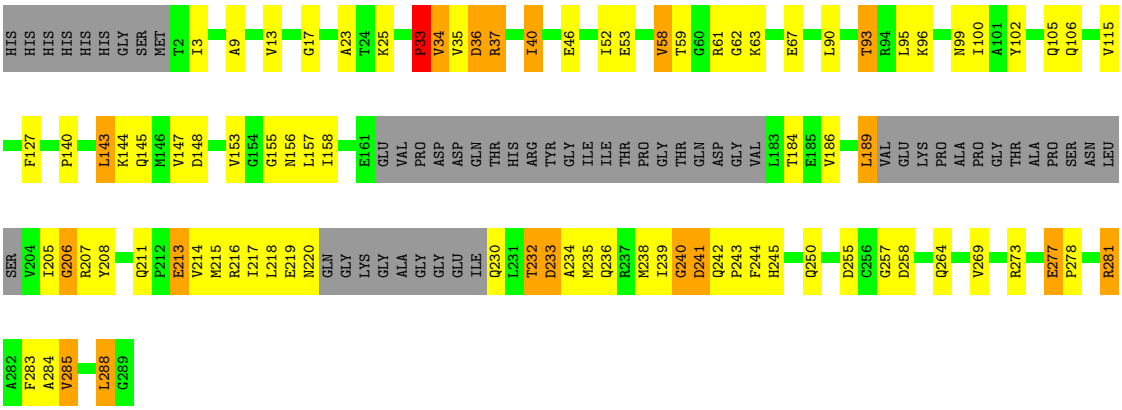
• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain G: 53% 37% 6%



• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain H: 53% 23% 6% 18%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.60Å 85.70Å 151.80Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	74.90 – 2.65 74.95 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.90-2.65) 99.7 (74.95-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.295 0.235 , 0.290	Depositor DCC
R_{free} test set	1992 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: G1P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.43	0/1974	0.78	4/2670 (0.1%)
1	B	0.44	0/2168	0.73	3/2939 (0.1%)
1	C	0.44	0/2187	0.76	3/2964 (0.1%)
1	D	0.49	1/2177 (0.0%)	0.75	4/2951 (0.1%)
1	E	0.59	2/2173 (0.1%)	0.86	8/2946 (0.3%)
1	F	0.55	4/2186 (0.2%)	0.82	7/2962 (0.2%)
1	G	0.46	0/2217	0.79	4/3005 (0.1%)
1	H	0.57	4/1899 (0.2%)	0.81	6/2565 (0.2%)
All	All	0.50	11/16981 (0.1%)	0.79	39/23002 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	240	GLY	C-O	-7.44	1.11	1.23
1	F	35	VAL	CB-CG1	7.16	1.67	1.52
1	F	35	VAL	CA-CB	6.46	1.68	1.54
1	E	221	GLN	CB-CG	-6.16	1.35	1.52
1	H	34	VAL	CB-CG1	5.55	1.64	1.52
1	F	33	PRO	CB-CG	5.52	1.77	1.50
1	D	33	PRO	CB-CG	5.51	1.77	1.50
1	H	33	PRO	CB-CG	5.43	1.77	1.50
1	E	230	GLN	C-O	5.41	1.33	1.23
1	F	34	VAL	CB-CG1	5.33	1.64	1.52
1	H	35	VAL	CB-CG1	5.24	1.63	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	237	ARG	NE-CZ-NH1	-10.70	114.95	120.30
1	A	233	ASP	CB-CG-OD2	10.02	127.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	237	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	A	233	ASP	CB-CG-OD1	-8.08	111.03	118.30
1	F	36	ASP	N-CA-CB	-8.01	96.18	110.60
1	F	3	ILE	N-CA-C	-7.65	90.34	111.00
1	A	233	ASP	CB-CA-C	7.64	125.68	110.40
1	H	288	LEU	CA-CB-CG	7.38	132.27	115.30
1	D	36	ASP	N-CA-C	7.06	130.07	111.00
1	F	36	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	H	240	GLY	N-CA-C	-6.51	96.82	113.10
1	F	36	ASP	N-CA-C	6.34	128.12	111.00
1	G	36	ASP	N-CA-CB	-6.30	99.26	110.60
1	E	231	LEU	CA-CB-CG	-6.29	100.83	115.30
1	H	36	ASP	N-CA-C	6.19	127.72	111.00
1	G	4	LYS	N-CA-C	-6.19	94.30	111.00
1	B	124	ASP	N-CA-C	-6.08	94.57	111.00
1	G	240	GLY	N-CA-C	-5.97	98.17	113.10
1	E	234	ALA	N-CA-C	-5.92	95.02	111.00
1	A	232	THR	C-N-CA	-5.68	107.50	121.70
1	E	172	GLY	N-CA-C	-5.68	98.91	113.10
1	B	232	THR	N-CA-C	-5.62	95.82	111.00
1	F	233	ASP	CB-CA-C	-5.59	99.22	110.40
1	F	172	GLY	N-CA-C	-5.58	99.15	113.10
1	H	240	GLY	CA-C-N	5.50	129.29	117.20
1	G	172	GLY	N-CA-C	-5.47	99.43	113.10
1	D	172	GLY	N-CA-C	-5.44	99.50	113.10
1	H	36	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	36	ASP	CB-CA-C	-5.38	99.64	110.40
1	B	172	GLY	N-CA-C	-5.31	99.82	113.10
1	H	241	ASP	N-CA-C	5.27	125.24	111.00
1	E	230	GLN	C-N-CA	5.23	134.78	121.70
1	D	36	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	F	35	VAL	CB-CA-C	-5.22	101.48	111.40
1	E	34	VAL	N-CA-C	-5.16	97.06	111.00
1	C	172	GLY	N-CA-C	-5.13	100.26	113.10
1	C	35	VAL	N-CA-C	-5.08	97.28	111.00
1	C	231	LEU	N-CA-C	5.04	124.62	111.00
1	E	202	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1940	0	1955	110	0
1	B	2126	0	2135	113	0
1	C	2145	0	2160	116	0
1	D	2135	0	2143	110	0
1	E	2131	0	2140	108	0
1	F	2144	0	2156	96	0
1	G	2174	0	2182	119	0
1	H	1866	0	1887	97	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0
2	E	16	0	11	0	0
2	F	16	0	11	2	0
2	G	16	0	11	3	0
2	H	16	0	11	0	0
3	A	13	0	0	1	0
3	B	23	0	0	1	0
3	C	30	0	0	2	0
3	D	16	0	0	2	0
3	E	26	0	0	0	0
3	F	12	0	0	3	0
3	G	19	0	0	4	0
3	H	20	0	0	1	0
All	All	16948	0	16846	787	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (787) 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:H:33:PRO:CG	1:H:33:PRO:CB	1.77	1.57
1:F:33:PRO:CB	1:F:33:PRO:CG	1.77	1.47
1:D:33:PRO:CB	1:D:33:PRO:CG	1.77	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:GLN:NE2	1:E:237:ARG:NH1	1.77	1.29
1:A:10:VAL:HG22	1:A:56:ILE:HD11	1.30	1.10
1:G:94:ARG:HH11	1:G:94:ARG:HG2	1.11	1.09
1:C:281:ARG:O	1:C:285:VAL:HG23	1.52	1.08
1:H:96:LYS:HB3	1:H:99:ASN:HD22	1.17	1.06
1:D:115:VAL:HG12	1:D:215:MET:HE3	1.37	1.04
1:F:27:MET:HE1	1:G:31:MET:HB3	1.42	1.01
1:D:221:GLN:OE1	1:D:230:GLN:N	1.94	1.01
1:F:27:MET:CE	1:G:31:MET:HB3	1.91	1.00
1:H:96:LYS:HB3	1:H:99:ASN:ND2	1.76	1.00
1:D:230:GLN:HG3	1:D:231:LEU:N	1.79	0.98
1:E:221:GLN:HE22	1:E:237:ARG:NH1	1.60	0.96
1:A:232:THR:O	1:A:235:MET:HG3	1.67	0.95
1:E:221:GLN:NE2	1:E:237:ARG:HH12	1.60	0.95
1:D:230:GLN:HG2	1:D:233:ASP:OD1	1.67	0.94
1:H:230:GLN:HG2	1:H:233:ASP:OD2	1.66	0.94
1:H:115:VAL:HG12	1:H:215:MET:HE3	1.50	0.94
1:E:221:GLN:NE2	1:E:237:ARG:HH11	1.53	0.93
1:A:218:LEU:HD22	1:A:231:LEU:HD11	1.47	0.93
1:H:284:ALA:O	1:H:288:LEU:HD23	1.67	0.93
1:H:145:GLN:HE22	1:H:250:GLN:H	1.13	0.92
1:E:167:GLN:HE21	1:E:170:ARG:HH11	0.97	0.92
1:E:115:VAL:HG12	1:E:215:MET:HE3	1.51	0.92
1:F:212:PRO:HB2	3:F:2007:HOH:O	1.70	0.91
1:C:2:THR:HG22	1:C:3:ILE:H	1.36	0.91
1:G:94:ARG:HG2	1:G:94:ARG:NH1	1.82	0.90
1:A:218:LEU:CD2	1:A:231:LEU:HD11	2.00	0.90
1:G:172:GLY:H	2:G:1290:G1P:H62	1.36	0.90
1:A:145:GLN:HE22	1:A:250:GLN:HB2	1.35	0.89
1:G:225:ALA:O	1:G:228:GLU:HG3	1.73	0.89
1:E:168:THR:HG21	1:E:198:ALA:HB2	1.54	0.89
1:B:56:ILE:HD11	1:B:121:ILE:HG21	1.55	0.89
1:H:90:LEU:O	1:H:93:THR:HB	1.73	0.88
1:D:167:GLN:HE21	1:D:170:ARG:HH11	1.20	0.88
1:F:25:LYS:HD2	1:G:93:THR:HG21	1.56	0.88
1:G:145:GLN:HE22	1:G:250:GLN:H	1.18	0.88
1:H:13:VAL:HG23	1:H:59:THR:HG22	1.55	0.87
1:E:145:GLN:HE22	1:E:250:GLN:H	1.22	0.87
1:B:236:GLN:C	1:B:238:MET:H	1.77	0.86
1:E:167:GLN:HE21	1:E:170:ARG:NH1	1.73	0.85
1:E:93:THR:HG21	1:H:25:LYS:HD2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ALA:HB2	1:B:52:ILE:HD13	1.57	0.85
1:D:174:ILE:HG23	1:D:186:VAL:HG23	1.56	0.85
1:E:139:GLN:HA	1:E:140:PRO:O	1.77	0.84
1:C:145:GLN:HE22	1:C:250:GLN:H	1.25	0.84
1:F:263:ILE:HD13	1:G:270:ALA:HB2	1.58	0.84
1:D:167:GLN:HE21	1:D:170:ARG:NH1	1.74	0.83
1:F:16:LEU:O	1:F:18:THR:N	2.12	0.83
1:G:139:GLN:HA	1:G:140:PRO:C	1.99	0.83
1:D:40:ILE:HD11	1:D:57:PHE:CE2	2.14	0.83
1:E:168:THR:HG21	1:E:198:ALA:CB	2.09	0.83
1:H:281:ARG:O	1:H:285:VAL:HG23	1.79	0.83
1:B:145:GLN:HE22	1:B:250:GLN:H	1.26	0.82
1:C:115:VAL:HG12	1:C:215:MET:HE1	1.61	0.82
1:H:238:MET:HE3	1:H:242:GLN:HE21	1.44	0.82
1:E:231:LEU:O	1:E:232:THR:C	2.16	0.82
1:D:139:GLN:HA	1:D:140:PRO:C	1.99	0.81
1:E:139:GLN:HA	1:E:140:PRO:C	2.00	0.81
1:B:124:ASP:O	1:B:125:GLU:CG	2.28	0.81
1:D:145:GLN:HE22	1:D:250:GLN:H	1.25	0.81
1:F:145:GLN:HE22	1:F:250:GLN:H	1.24	0.81
1:B:189:LEU:HD21	1:B:236:GLN:HB2	1.63	0.80
1:B:124:ASP:O	1:B:125:GLU:HG3	1.82	0.80
1:F:96:LYS:HB2	1:F:99:ASN:ND2	1.97	0.80
1:C:2:THR:HG22	1:C:3:ILE:N	1.97	0.80
1:A:235:MET:O	1:A:238:MET:HB2	1.82	0.80
1:C:37:ARG:NH1	1:C:45:ASP:OD2	2.16	0.79
1:D:168:THR:HG21	1:D:198:ALA:HB2	1.64	0.79
1:H:238:MET:CE	1:H:242:GLN:HE21	1.95	0.79
1:A:221:GLN:NE2	1:A:231:LEU:CD1	2.46	0.79
1:G:88:ASP:HB2	3:G:2004:HOH:O	1.82	0.78
1:A:214:VAL:O	1:A:218:LEU:HG	1.83	0.78
1:C:4:LYS:HD2	1:C:125:GLU:HG2	1.64	0.78
1:A:221:GLN:CD	1:A:231:LEU:HD13	2.04	0.78
1:A:263:ILE:HD13	1:C:270:ALA:HB2	1.65	0.77
1:B:167:GLN:HE21	1:B:170:ARG:NH1	1.83	0.77
1:A:115:VAL:HG12	1:A:215:MET:HE3	1.66	0.77
1:E:221:GLN:HE22	1:E:237:ARG:HH11	1.19	0.77
1:A:218:LEU:HD22	1:A:231:LEU:CD1	2.14	0.77
1:F:235:MET:O	1:F:238:MET:HB2	1.84	0.77
1:B:6:LEU:O	1:B:7:ARG:HG2	1.85	0.76
1:C:67:GLU:HG3	1:C:102:TYR:CZ	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:TRP:HA	1:F:215:MET:HE1	1.67	0.76
1:G:189:LEU:HD23	1:G:236:GLN:OE1	1.86	0.76
1:B:168:THR:HG21	1:B:198:ALA:CB	2.16	0.76
1:B:155:GLY:HA3	1:B:243:PRO:HG2	1.69	0.75
1:A:3:ILE:HD12	1:A:3:ILE:O	1.86	0.75
1:E:167:GLN:NE2	1:E:170:ARG:HH11	1.81	0.75
1:H:230:GLN:HG2	1:H:233:ASP:CG	2.07	0.75
1:G:191:GLU:HG2	1:G:230:GLN:NE2	2.01	0.74
1:B:163:VAL:CG1	1:B:167:GLN:HB3	2.17	0.74
1:D:163:VAL:CG1	1:D:167:GLN:HB3	2.17	0.74
1:H:153:VAL:HG11	1:H:245:HIS:NE2	2.02	0.74
1:B:168:THR:HG21	1:B:198:ALA:HB2	1.70	0.74
1:F:25:LYS:CD	1:G:93:THR:HG21	2.17	0.74
1:F:139:GLN:HA	1:F:140:PRO:C	2.08	0.73
1:A:10:VAL:HG22	1:A:56:ILE:CD1	2.14	0.73
1:B:167:GLN:HE21	1:B:170:ARG:HH11	1.35	0.73
1:C:215:MET:HE2	1:C:218:LEU:HD12	1.70	0.73
1:E:214:VAL:O	1:E:217:ILE:HG22	1.89	0.73
1:E:194:ALA:O	1:E:197:THR:HG22	1.89	0.73
1:B:236:GLN:O	1:B:239:ILE:HG12	1.88	0.73
1:F:236:GLN:C	1:F:238:MET:H	1.92	0.73
1:G:214:VAL:O	1:G:217:ILE:HG22	1.88	0.72
1:H:239:ILE:HG13	1:H:240:GLY:H	1.52	0.72
1:D:10:VAL:HG22	1:D:56:ILE:HD11	1.71	0.72
1:D:217:ILE:HG21	1:D:234:ALA:HB1	1.71	0.72
1:F:160:ALA:HB1	1:F:202:LEU:HD12	1.71	0.72
1:D:168:THR:HG21	1:D:198:ALA:CB	2.19	0.72
1:B:40:ILE:O	1:B:44:VAL:HG23	1.90	0.72
1:D:186:VAL:HG11	1:D:244:PHE:CD2	2.23	0.72
1:E:93:THR:HG21	1:H:25:LYS:CD	2.19	0.72
1:A:56:ILE:HD12	1:A:118:ALA:HB1	1.71	0.72
1:F:236:GLN:O	1:F:238:MET:N	2.22	0.72
1:B:217:ILE:CG2	1:B:234:ALA:HB1	2.20	0.71
1:A:93:THR:HG21	1:C:25:LYS:NZ	2.05	0.71
1:A:153:VAL:HG11	1:A:245:HIS:CE1	2.25	0.71
1:G:29:LYS:HE2	1:G:133:ASP:OD1	1.91	0.71
1:F:191:GLU:OE1	1:F:191:GLU:HA	1.91	0.70
1:A:5:PRO:O	1:A:6:LEU:HB2	1.90	0.70
1:A:53:GLU:O	1:A:99:ASN:ND2	2.24	0.70
1:A:214:VAL:O	1:A:217:ILE:HG22	1.91	0.70
1:C:277:GLU:HG3	1:C:278:PRO:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:THR:HG23	1:C:173:ILE:HG13	1.73	0.69
1:D:189:LEU:HD21	1:D:236:GLN:HG3	1.74	0.69
1:D:217:ILE:CG2	1:D:234:ALA:HB1	2.21	0.69
1:B:27:MET:SD	1:D:27:MET:HG3	2.33	0.69
1:B:93:THR:HG21	1:D:25:LYS:NZ	2.08	0.69
1:E:25:LYS:NZ	1:H:93:THR:CG2	2.56	0.69
1:H:214:VAL:O	1:H:217:ILE:HG22	1.93	0.69
1:A:139:GLN:HG2	1:A:140:PRO:HA	1.73	0.69
1:D:230:GLN:HG3	1:D:231:LEU:H	1.56	0.68
1:E:29:LYS:HE2	1:E:133:ASP:OD1	1.93	0.68
1:G:9:ALA:HB2	1:G:52:ILE:HD13	1.75	0.68
1:A:186:VAL:HG11	1:A:244:PHE:CD2	2.28	0.68
1:B:93:THR:CG2	1:D:25:LYS:NZ	2.57	0.68
1:C:9:ALA:HB2	1:C:52:ILE:HD13	1.74	0.68
1:H:236:GLN:O	1:H:239:ILE:HG23	1.93	0.68
1:B:93:THR:CG2	1:D:25:LYS:HZ3	2.05	0.68
1:E:115:VAL:HG12	1:E:215:MET:CE	2.23	0.68
1:B:217:ILE:HG21	1:B:234:ALA:HB1	1.75	0.68
1:D:9:ALA:O	1:D:56:ILE:HG12	1.94	0.68
1:G:10:VAL:HG22	1:G:56:ILE:HD11	1.76	0.68
1:D:115:VAL:HG12	1:D:215:MET:CE	2.21	0.68
1:F:31:MET:SD	1:F:40:ILE:HD11	2.34	0.68
1:A:218:LEU:HD22	1:A:231:LEU:HD21	1.74	0.67
1:B:7:ARG:HA	1:B:52:ILE:HA	1.75	0.67
1:E:25:LYS:HZ2	1:H:93:THR:CG2	2.07	0.67
1:D:144:LYS:O	1:D:147:VAL:HG12	1.94	0.67
1:F:263:ILE:HD13	1:G:270:ALA:CB	2.25	0.67
1:E:153:VAL:HG11	1:E:245:HIS:NE2	2.09	0.67
1:A:115:VAL:HG12	1:A:215:MET:CE	2.25	0.67
1:G:35:VAL:HG12	1:G:36:ASP:HB2	1.75	0.67
1:B:236:GLN:C	1:B:238:MET:N	2.47	0.67
1:F:190:VAL:O	1:F:191:GLU:O	2.12	0.67
1:A:218:LEU:HD22	1:A:231:LEU:CG	2.25	0.66
1:A:221:GLN:NE2	1:A:231:LEU:HD13	2.10	0.66
1:A:270:ALA:HB2	1:C:263:ILE:HD13	1.75	0.66
1:C:2:THR:CG2	1:C:3:ILE:H	2.09	0.66
1:F:216:ARG:CZ	3:F:2007:HOH:O	2.42	0.66
1:C:72:ILE:HG12	1:C:94:ARG:HH11	1.59	0.66
1:F:25:LYS:NZ	1:G:93:THR:HG22	2.11	0.66
1:A:84:GLY:HA2	3:A:2008:HOH:O	1.94	0.66
1:A:161:GLU:O	1:A:203:SER:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HG13	1:C:56:ILE:O	1.95	0.66
1:A:93:THR:HG21	1:C:25:LYS:HD3	1.78	0.65
1:A:263:ILE:HD13	1:C:270:ALA:CB	2.26	0.65
1:B:193:PRO:HB2	1:B:197:THR:HG22	1.78	0.65
1:E:36:ASP:HB2	1:E:273:ARG:HH22	1.60	0.65
1:G:14:ALA:HA	1:G:63:LYS:HE3	1.78	0.65
1:G:168:THR:HG21	1:G:198:ALA:CB	2.27	0.65
1:B:263:ILE:HD13	1:D:270:ALA:HB2	1.77	0.65
1:D:186:VAL:HG12	1:D:244:PHE:O	1.96	0.65
1:C:215:MET:CE	1:C:218:LEU:HD12	2.27	0.65
1:A:232:THR:O	1:A:234:ALA:N	2.30	0.65
1:F:9:ALA:HB2	1:F:52:ILE:HD13	1.76	0.65
1:A:10:VAL:CG2	1:A:56:ILE:HD11	2.19	0.65
1:F:144:LYS:O	1:F:147:VAL:HG12	1.97	0.64
1:F:239:ILE:H	1:F:239:ILE:HD13	1.62	0.64
1:H:67:GLU:HG3	1:H:102:TYR:CZ	2.33	0.64
1:B:281:ARG:NH1	1:D:288:LEU:HD12	2.13	0.64
1:G:94:ARG:HH11	1:G:94:ARG:CG	1.97	0.64
1:A:213:GLU:HB2	1:A:238:MET:CE	2.27	0.64
1:A:93:THR:HG21	1:C:25:LYS:HZ2	1.61	0.64
1:B:270:ALA:HB2	1:D:263:ILE:HD13	1.80	0.64
1:H:115:VAL:HG12	1:H:215:MET:CE	2.25	0.64
1:B:215:MET:CE	1:B:218:LEU:HD12	2.28	0.64
1:H:189:LEU:HD23	1:H:189:LEU:N	2.13	0.64
1:B:139:GLN:HG2	1:B:139:GLN:O	1.97	0.64
1:A:217:ILE:HD11	1:A:237:ARG:CZ	2.28	0.63
1:B:31:MET:HB3	1:D:27:MET:CE	2.28	0.63
1:H:216:ARG:O	1:H:220:ASN:ND2	2.27	0.63
1:E:156:ASN:ND2	1:E:211:GLN:H	1.97	0.63
1:D:153:VAL:HG11	1:D:245:HIS:CD2	2.33	0.63
1:A:155:GLY:HA3	1:A:243:PRO:HG2	1.81	0.62
1:G:191:GLU:HG2	1:G:230:GLN:HE21	1.62	0.62
1:A:236:GLN:C	1:A:238:MET:H	2.02	0.62
1:C:189:LEU:HD23	1:C:236:GLN:HE21	1.65	0.62
1:D:156:ASN:ND2	1:D:211:GLN:H	1.97	0.62
1:C:115:VAL:HG12	1:C:215:MET:CE	2.30	0.62
1:C:189:LEU:HD23	1:C:236:GLN:NE2	2.15	0.62
1:A:37:ARG:NH1	1:A:45:ASP:OD2	2.33	0.62
1:C:166:ASP:OD1	1:C:166:ASP:N	2.33	0.62
1:G:153:VAL:HG11	1:G:245:HIS:NE2	2.15	0.61
1:H:238:MET:CE	1:H:242:GLN:NE2	2.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ALA:HB2	1:D:52:ILE:HD13	1.82	0.61
1:E:76:LEU:O	1:E:80:MET:HG3	2.01	0.61
1:E:186:VAL:HG11	1:E:244:PHE:CD2	2.35	0.61
1:C:144:LYS:O	1:C:147:VAL:HG12	2.01	0.61
1:C:153:VAL:HG11	1:C:245:HIS:NE2	2.15	0.61
1:C:186:VAL:HG12	1:C:244:PHE:O	2.00	0.61
1:B:96:LYS:HB2	1:B:99:ASN:ND2	2.15	0.61
1:D:7:ARG:HD3	1:D:53:GLU:OE2	2.00	0.61
1:H:96:LYS:CB	1:H:99:ASN:HD22	2.04	0.61
1:F:236:GLN:O	1:F:239:ILE:HD13	2.00	0.61
1:C:191:GLU:HG2	1:C:232:THR:OG1	2.00	0.61
1:D:13:VAL:HG12	1:D:30:GLU:HG2	1.82	0.61
1:A:93:THR:CG2	1:C:25:LYS:NZ	2.64	0.60
1:A:112:GLY:HA3	1:A:231:LEU:HB3	1.83	0.60
1:B:93:THR:HG22	1:D:25:LYS:HZ3	1.64	0.60
1:A:13:VAL:HG23	1:A:59:THR:HG22	1.81	0.60
1:B:235:MET:O	1:B:238:MET:HB3	2.00	0.60
1:C:213:GLU:HB2	1:C:238:MET:SD	2.42	0.60
1:C:236:GLN:O	1:C:239:ILE:HG13	2.00	0.60
1:G:172:GLY:HA2	1:G:191:GLU:O	2.01	0.60
1:E:104:ARG:HD3	3:F:2003:HOH:O	2.02	0.60
1:G:215:MET:HE3	1:G:215:MET:HA	1.83	0.60
1:H:239:ILE:C	1:H:240:GLY:O	2.34	0.60
1:A:49:GLU:OE1	1:A:140:PRO:O	2.19	0.60
1:D:160:ALA:HB1	1:D:202:LEU:HD12	1.84	0.60
1:E:189:LEU:HD23	1:E:189:LEU:N	2.17	0.60
1:G:214:VAL:HG23	1:G:238:MET:HE2	1.82	0.60
1:H:284:ALA:O	1:H:288:LEU:CD2	2.44	0.60
1:E:218:LEU:HD21	1:E:231:LEU:H	1.67	0.60
1:H:13:VAL:CG2	1:H:59:THR:HG22	2.31	0.60
1:B:32:LEU:HD22	1:D:33:PRO:HG3	1.84	0.59
1:D:10:VAL:HG22	1:D:56:ILE:CD1	2.32	0.59
1:E:74:TYR:CD1	1:G:75:GLU:HG3	2.36	0.59
1:C:189:LEU:HD23	1:C:189:LEU:N	2.18	0.59
1:E:163:VAL:CG1	1:E:167:GLN:HB3	2.31	0.59
1:F:163:VAL:HG13	1:F:164:PRO:HD2	1.85	0.59
1:F:217:ILE:CG2	1:F:234:ALA:HB1	2.32	0.59
1:B:3:ILE:O	1:B:3:ILE:HG13	2.03	0.59
1:D:156:ASN:HD21	1:D:211:GLN:H	1.51	0.59
1:H:153:VAL:HG11	1:H:245:HIS:CD2	2.38	0.58
1:C:89:VAL:HG13	1:C:90:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LYS:HZ3	1:H:93:THR:HG23	1.68	0.58
1:B:7:ARG:HB2	1:B:53:GLU:HG2	1.84	0.58
1:H:59:THR:HG21	3:H:2008:HOH:O	2.02	0.58
1:B:215:MET:HE3	1:B:218:LEU:HD12	1.86	0.58
1:F:33:PRO:HG3	1:G:32:LEU:HD22	1.85	0.58
1:F:189:LEU:N	1:F:189:LEU:HD23	2.19	0.58
1:D:197:THR:HG22	1:D:197:THR:O	2.03	0.58
1:B:116:TRP:HA	1:B:215:MET:HE1	1.86	0.57
1:H:34:VAL:HG11	1:H:269:VAL:HG21	1.86	0.57
1:A:211:GLN:HE21	1:A:212:PRO:HD2	1.69	0.57
1:B:214:VAL:O	1:B:217:ILE:HG22	2.04	0.57
1:F:168:THR:HG22	1:F:173:ILE:HG13	1.86	0.57
1:A:218:LEU:HD22	1:A:231:LEU:CD2	2.33	0.57
1:E:193:PRO:HB2	1:E:197:THR:HG23	1.85	0.57
1:C:220:ASN:C	1:C:222:GLY:H	2.07	0.57
1:E:97:PRO:O	1:F:119:ARG:NH2	2.37	0.57
1:B:168:THR:HG23	1:B:173:ILE:HG13	1.85	0.57
1:H:3:ILE:HG13	1:H:3:ILE:O	2.04	0.57
1:A:96:LYS:HB3	1:A:99:ASN:OD1	2.05	0.57
1:E:163:VAL:HG13	1:E:167:GLN:HB3	1.85	0.57
1:G:281:ARG:O	1:G:285:VAL:HG23	2.04	0.57
1:D:40:ILE:HD11	1:D:57:PHE:CZ	2.40	0.57
1:D:67:GLU:HG3	1:D:102:TYR:CZ	2.39	0.57
1:H:236:GLN:C	1:H:238:MET:H	2.09	0.56
1:A:281:ARG:NH1	1:C:288:LEU:O	2.36	0.56
1:D:163:VAL:HG13	1:D:164:PRO:HD2	1.87	0.56
1:H:255:ASP:C	1:H:257:GLY:H	2.08	0.56
1:A:211:GLN:NE2	1:A:212:PRO:HD2	2.20	0.56
1:E:34:VAL:O	1:E:34:VAL:HG22	2.04	0.56
1:F:96:LYS:CB	1:F:99:ASN:ND2	2.66	0.56
1:F:156:ASN:C	1:F:157:LEU:HD12	2.25	0.56
1:F:159:CYS:HB3	1:F:205:ILE:HB	1.86	0.56
1:C:156:ASN:ND2	1:C:211:GLN:H	2.03	0.56
1:G:197:THR:O	1:G:197:THR:HG22	2.04	0.56
1:A:140:PRO:HD2	1:A:145:GLN:HE21	1.71	0.56
1:F:284:ALA:O	1:F:288:LEU:HD13	2.05	0.56
1:A:112:GLY:CA	1:A:231:LEU:HD23	2.36	0.56
1:B:125:GLU:H	1:B:212:PRO:HB3	1.71	0.56
1:E:8:LYS:HG2	1:E:54:GLN:HB3	1.87	0.56
1:F:169:HIS:O	1:F:192:LYS:HB3	2.05	0.56
1:E:40:ILE:O	1:E:44:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:C	1:A:231:LEU:HD23	2.26	0.56
1:D:230:GLN:CG	1:D:233:ASP:OD1	2.49	0.56
1:F:153:VAL:HG11	1:F:245:HIS:CD2	2.41	0.56
1:F:236:GLN:C	1:F:238:MET:N	2.59	0.56
1:G:111:LEU:HD22	2:G:1290:G1P:O2	2.06	0.55
1:C:194:ALA:HB3	1:C:197:THR:HG22	1.87	0.55
1:F:189:LEU:O	1:F:236:GLN:NE2	2.38	0.55
1:G:236:GLN:C	1:G:238:MET:H	2.10	0.55
1:D:189:LEU:CD2	1:D:236:GLN:HG3	2.36	0.55
1:B:93:THR:HG21	1:D:25:LYS:CD	2.37	0.55
1:C:8:LYS:HG2	1:C:54:GLN:HB3	1.88	0.55
1:D:156:ASN:HD22	1:D:210:LEU:HA	1.70	0.55
1:E:13:VAL:HG23	1:E:59:THR:HG22	1.88	0.55
1:E:93:THR:CG2	1:H:25:LYS:NZ	2.70	0.55
1:E:231:LEU:O	1:E:234:ALA:N	2.35	0.55
1:B:56:ILE:HG22	1:B:56:ILE:O	2.06	0.55
1:C:230:GLN:HG2	1:C:231:LEU:N	2.22	0.55
1:F:163:VAL:CG1	1:F:167:GLN:HB3	2.37	0.55
1:C:61:ARG:NH2	1:C:106:GLN:O	2.40	0.55
1:G:116:TRP:HA	1:G:215:MET:HE1	1.87	0.55
1:B:6:LEU:O	1:B:7:ARG:CG	2.54	0.54
1:C:152:LYS:HG3	1:C:153:VAL:HG23	1.89	0.54
1:A:179:GLN:HG3	1:A:184:THR:HB	1.88	0.54
1:C:168:THR:HG21	1:C:198:ALA:CB	2.38	0.54
1:A:218:LEU:HD23	1:A:231:LEU:HD11	1.85	0.54
1:C:4:LYS:HB3	1:C:5:PRO:HD2	1.90	0.54
1:D:168:THR:HG23	1:D:173:ILE:HG13	1.90	0.54
1:F:124:ASP:OD2	1:F:216:ARG:NH2	2.40	0.54
1:G:34:VAL:O	1:G:35:VAL:HB	2.08	0.54
1:H:144:LYS:O	1:H:147:VAL:HG12	2.07	0.54
1:B:14:ALA:HB3	3:B:2001:HOH:O	2.07	0.54
1:E:31:MET:SD	1:E:40:ILE:HD11	2.47	0.54
1:B:144:LYS:O	1:B:147:VAL:HG12	2.07	0.54
1:B:281:ARG:HG3	1:D:288:LEU:HD11	1.89	0.54
1:E:213:GLU:HB2	1:E:238:MET:HE2	1.90	0.54
1:A:145:GLN:NE2	1:A:250:GLN:HB2	2.13	0.54
1:B:189:LEU:N	1:B:189:LEU:CD2	2.70	0.54
1:B:213:GLU:CG	1:B:238:MET:HE3	2.38	0.54
1:C:197:THR:O	1:C:199:PRO:HD3	2.07	0.54
1:F:3:ILE:HG13	1:F:3:ILE:O	2.01	0.54
1:G:58:VAL:HG22	1:G:58:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:VAL:HG11	1:G:245:HIS:CD2	2.43	0.54
1:D:197:THR:O	1:D:197:THR:CG2	2.56	0.53
1:A:9:ALA:O	1:A:56:ILE:HG12	2.07	0.53
1:B:124:ASP:O	1:B:125:GLU:CB	2.57	0.53
1:F:36:ASP:HB2	1:F:273:ARG:HH12	1.74	0.53
1:H:155:GLY:HA3	1:H:243:PRO:HG2	1.89	0.53
1:D:96:LYS:HB3	1:D:99:ASN:OD1	2.07	0.53
1:G:173:ILE:O	1:G:189:LEU:HA	2.08	0.53
1:B:31:MET:SD	1:B:40:ILE:HD11	2.49	0.53
1:F:213:GLU:HG3	1:F:242:GLN:OE1	2.09	0.53
1:H:53:GLU:O	1:H:99:ASN:OD1	2.26	0.53
1:B:270:ALA:CB	1:D:263:ILE:HD13	2.37	0.53
1:F:25:LYS:NZ	1:G:93:THR:CG2	2.70	0.53
1:A:174:ILE:CG2	1:A:175:THR:N	2.72	0.53
1:A:213:GLU:HB2	1:A:238:MET:HE3	1.90	0.53
1:C:170:ARG:O	1:C:192:LYS:HE2	2.09	0.53
1:G:168:THR:HG21	1:G:198:ALA:HB1	1.90	0.53
1:B:139:GLN:HA	1:B:140:PRO:C	2.29	0.53
1:B:236:GLN:O	1:B:238:MET:N	2.42	0.53
1:B:277:GLU:HB3	1:B:278:PRO:HD3	1.90	0.53
1:D:10:VAL:CG2	1:D:56:ILE:HD11	2.38	0.53
1:D:107:GLU:HG3	1:D:109:MET:CE	2.38	0.53
1:E:232:THR:HG22	1:E:233:ASP:N	2.23	0.53
1:G:168:THR:HG23	1:G:173:ILE:CD1	2.39	0.53
1:C:189:LEU:N	1:C:189:LEU:CD2	2.72	0.52
1:D:238:MET:CE	1:D:242:GLN:NE2	2.72	0.52
1:E:25:LYS:NZ	1:H:93:THR:HG23	2.24	0.52
1:B:56:ILE:HD11	1:B:121:ILE:HD12	1.91	0.52
1:E:221:GLN:CD	1:E:237:ARG:HH12	2.11	0.52
1:G:214:VAL:CG2	1:G:238:MET:HE2	2.39	0.52
1:G:168:THR:HG21	1:G:198:ALA:HB2	1.90	0.52
1:A:221:GLN:HE22	1:A:231:LEU:CD1	2.21	0.52
1:B:186:VAL:HG11	1:B:244:PHE:CD2	2.44	0.52
1:H:239:ILE:HG13	1:H:240:GLY:N	2.21	0.52
1:A:67:GLU:HG3	1:A:102:TYR:CZ	2.45	0.52
1:A:93:THR:HG21	1:C:25:LYS:CD	2.40	0.52
1:D:186:VAL:HG13	1:D:186:VAL:O	2.09	0.52
1:E:23:ALA:HB2	1:H:36:ASP:O	2.09	0.52
1:E:58:VAL:HG22	1:E:58:VAL:O	2.09	0.52
1:E:215:MET:O	1:E:219:GLU:HG3	2.10	0.52
1:G:215:MET:HE3	1:G:218:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:ASP:HB2	1:H:273:ARG:HH22	1.74	0.52
1:C:173:ILE:O	1:C:189:LEU:HA	2.09	0.52
1:E:61:ARG:O	1:E:63:LYS:N	2.42	0.52
1:A:144:LYS:O	1:A:147:VAL:HG12	2.09	0.52
1:B:6:LEU:HD12	1:B:147:VAL:HG23	1.92	0.52
1:E:27:MET:HE3	1:E:28:PRO:HD2	1.91	0.52
1:D:255:ASP:C	1:D:257:GLY:H	2.13	0.52
1:A:153:VAL:CG1	1:A:245:HIS:CE1	2.93	0.52
1:A:215:MET:O	1:A:219:GLU:HG3	2.10	0.52
1:F:277:GLU:HB3	1:F:278:PRO:HD3	1.92	0.52
1:C:96:LYS:HB2	1:C:99:ASN:ND2	2.26	0.51
1:G:60:GLY:H	1:G:63:LYS:HD2	1.75	0.51
1:G:277:GLU:HB3	1:G:278:PRO:HD3	1.92	0.51
1:H:239:ILE:CG1	1:H:240:GLY:H	2.23	0.51
1:B:33:PRO:HG3	1:D:32:LEU:HD22	1.92	0.51
1:G:219:GLU:O	1:G:220:ASN:CB	2.57	0.51
1:A:5:PRO:O	1:A:6:LEU:CB	2.59	0.51
1:A:93:THR:CG2	1:C:25:LYS:HZ3	2.24	0.51
1:A:236:GLN:C	1:A:238:MET:N	2.64	0.51
1:D:189:LEU:CD2	1:D:236:GLN:CG	2.88	0.51
1:E:169:HIS:O	1:E:192:LYS:HG3	2.11	0.51
1:G:13:VAL:HG23	1:G:59:THR:HG22	1.92	0.51
1:C:13:VAL:HG12	1:C:30:GLU:HG2	1.93	0.51
1:E:67:GLU:HB3	1:F:104:ARG:NH1	2.26	0.51
1:F:197:THR:HG23	1:F:197:THR:O	2.10	0.51
1:A:158:ILE:HG21	1:A:204:VAL:HG13	1.93	0.51
1:D:67:GLU:HG3	1:D:102:TYR:CE2	2.46	0.51
1:D:215:MET:HE1	1:D:218:LEU:HD12	1.93	0.51
1:E:36:ASP:CB	1:E:273:ARG:HH22	2.23	0.51
1:G:56:ILE:CD1	1:G:118:ALA:HB1	2.40	0.51
1:A:36:ASP:HB2	1:A:273:ARG:HH22	1.76	0.51
1:C:189:LEU:HD21	1:C:236:GLN:HA	1.92	0.51
1:A:156:ASN:ND2	1:A:211:GLN:H	2.08	0.51
1:B:61:ARG:HG3	1:B:61:ARG:HH11	1.75	0.51
1:C:221:GLN:OE1	1:C:230:GLN:N	2.44	0.51
1:G:186:VAL:HG13	1:G:244:PHE:HB3	1.93	0.51
1:A:90:LEU:HD22	1:C:25:LYS:HD2	1.91	0.51
1:A:221:GLN:OE1	1:A:231:LEU:HD13	2.11	0.51
1:C:31:MET:SD	1:C:40:ILE:HD11	2.51	0.51
1:E:67:GLU:HG2	1:E:102:TYR:CE2	2.46	0.51
1:C:27:MET:HE3	1:C:28:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:LEU:O	1:D:189:LEU:HD23	2.12	0.50
1:F:116:TRP:HA	1:F:215:MET:CE	2.41	0.50
1:A:255:ASP:C	1:A:257:GLY:H	2.13	0.50
1:B:27:MET:HE1	1:D:27:MET:HG3	1.94	0.50
1:A:159:CYS:HB3	1:A:205:ILE:HB	1.94	0.50
1:A:270:ALA:CB	1:C:263:ILE:HD13	2.41	0.50
1:C:174:ILE:HB	1:C:202:LEU:HG	1.92	0.50
1:E:13:VAL:CG2	1:E:59:THR:HG22	2.41	0.50
1:E:217:ILE:HG13	1:E:221:GLN:NE2	2.26	0.50
1:C:168:THR:HG21	1:C:198:ALA:HB1	1.94	0.50
1:E:189:LEU:N	1:E:189:LEU:CD2	2.74	0.50
1:F:14:ALA:HA	1:F:63:LYS:HE2	1.91	0.50
1:C:168:THR:HG23	1:C:173:ILE:CG1	2.40	0.50
1:B:29:LYS:NZ	1:B:256:CYS:O	2.45	0.50
1:B:123:GLY:O	1:B:216:ARG:NH2	2.42	0.50
1:B:263:ILE:HD13	1:D:270:ALA:CB	2.41	0.50
1:F:139:GLN:HA	1:F:140:PRO:O	2.11	0.50
1:A:5:PRO:O	1:A:150:TYR:HE2	1.95	0.50
1:C:191:GLU:OE1	1:C:192:LYS:HG3	2.12	0.50
1:D:218:LEU:HA	1:D:221:GLN:HG2	1.93	0.50
1:A:158:ILE:HD11	1:A:244:PHE:CZ	2.47	0.50
1:H:215:MET:HE1	1:H:218:LEU:HD12	1.93	0.50
1:B:37:ARG:HG3	1:B:42:TYR:CZ	2.47	0.50
1:C:30:GLU:HG3	3:C:2018:HOH:O	2.12	0.50
1:C:186:VAL:HG11	1:C:244:PHE:CD2	2.47	0.50
1:F:25:LYS:HZ2	1:G:93:THR:HG22	1.77	0.49
1:G:35:VAL:N	1:G:266:ASN:OD1	2.45	0.49
1:D:215:MET:O	1:D:219:GLU:HG3	2.12	0.49
1:E:159:CYS:HB3	1:E:205:ILE:HB	1.94	0.49
1:F:25:LYS:HZ3	1:G:93:THR:HG22	1.75	0.49
1:B:213:GLU:HB2	1:B:238:MET:HE1	1.95	0.49
1:B:191:GLU:HA	1:B:191:GLU:OE2	2.13	0.49
1:C:136:MET:SD	1:C:253:ARG:HG3	2.52	0.49
1:C:212:PRO:O	1:C:216:ARG:HD3	2.12	0.49
1:D:107:GLU:HG3	1:D:109:MET:HE2	1.93	0.49
1:D:236:GLN:C	1:D:238:MET:H	2.15	0.49
1:G:13:VAL:HG12	1:G:30:GLU:HG2	1.94	0.49
1:C:29:LYS:NZ	3:C:2007:HOH:O	2.45	0.49
1:B:61:ARG:HG3	1:B:61:ARG:NH1	2.27	0.49
1:G:156:ASN:ND2	1:G:211:GLN:H	2.10	0.49
1:G:217:ILE:CG2	1:G:234:ALA:HB1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:O	1:B:35:VAL:HB	2.13	0.49
1:D:173:ILE:O	1:D:189:LEU:HA	2.13	0.49
1:B:93:THR:HG22	1:D:25:LYS:NZ	2.26	0.49
1:D:189:LEU:O	1:D:236:GLN:NE2	2.45	0.49
1:A:236:GLN:O	1:A:239:ILE:HG13	2.13	0.49
1:A:243:PRO:HB2	1:A:245:HIS:HE1	1.78	0.49
1:B:93:THR:HG21	1:D:25:LYS:HZ2	1.77	0.49
1:C:186:VAL:HG13	1:C:244:PHE:HB3	1.95	0.49
1:D:139:GLN:HA	1:D:141:GLY:N	2.28	0.49
1:H:238:MET:HE3	1:H:242:GLN:NE2	2.21	0.49
1:H:215:MET:HE2	1:H:215:MET:HA	1.95	0.49
1:F:34:VAL:HG11	1:F:269:VAL:HG21	1.94	0.48
1:G:190:VAL:HG23	1:G:193:PRO:HD3	1.95	0.48
1:B:104:ARG:NH1	1:C:67:GLU:HG2	2.28	0.48
1:C:47:ALA:HB3	1:C:55:MET:HE1	1.95	0.48
1:E:173:ILE:O	1:E:189:LEU:HA	2.12	0.48
1:F:113:HIS:O	1:F:116:TRP:HB3	2.13	0.48
1:B:213:GLU:HB2	1:B:238:MET:CE	2.44	0.48
1:D:139:GLN:CA	1:D:140:PRO:C	2.78	0.48
1:E:186:VAL:HG12	1:E:244:PHE:O	2.13	0.48
1:G:191:GLU:OE1	1:G:191:GLU:HA	2.13	0.48
1:E:36:ASP:HB2	1:E:273:ARG:NH2	2.28	0.48
1:G:208:TYR:CD1	1:G:208:TYR:N	2.82	0.48
1:G:252:THR:HA	3:G:2016:HOH:O	2.13	0.48
1:B:189:LEU:HD21	1:B:236:GLN:CB	2.40	0.48
1:A:105:GLN:O	1:A:106:GLN:HB2	2.14	0.48
1:B:27:MET:CE	1:D:27:MET:HG3	2.42	0.48
1:H:215:MET:CE	1:H:218:LEU:HD12	2.43	0.48
1:H:236:GLN:C	1:H:238:MET:N	2.67	0.48
1:A:67:GLU:HG3	1:A:102:TYR:CE2	2.49	0.48
1:B:163:VAL:HG13	1:B:167:GLN:HB3	1.93	0.48
1:C:215:MET:HE2	1:C:215:MET:HA	1.96	0.48
1:D:111:LEU:HG	1:D:231:LEU:HD22	1.94	0.48
1:E:153:VAL:HG11	1:E:245:HIS:CD2	2.48	0.48
1:E:160:ALA:HB1	1:E:202:LEU:CD1	2.43	0.48
1:D:130:LEU:N	1:D:130:LEU:HD12	2.29	0.48
1:G:214:VAL:HG23	1:G:238:MET:CE	2.44	0.48
1:A:186:VAL:HG12	1:A:244:PHE:O	2.13	0.48
1:D:275:ASP:OD2	1:D:275:ASP:N	2.47	0.48
1:G:186:VAL:HG11	1:G:244:PHE:CD2	2.49	0.48
1:B:90:LEU:O	1:B:93:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:GLU:HB2	1:H:238:MET:HE2	1.96	0.48
1:D:38:PRO:HG2	1:D:41:GLN:HB2	1.96	0.47
1:D:163:VAL:HG12	1:D:167:GLN:HB3	1.96	0.47
1:F:157:LEU:HD12	1:F:157:LEU:N	2.29	0.47
1:F:217:ILE:HG21	1:F:234:ALA:HB1	1.95	0.47
1:B:73:ALA:O	1:B:77:GLU:HG3	2.13	0.47
1:B:273:ARG:HH11	1:B:273:ARG:CG	2.27	0.47
1:D:189:LEU:HD21	1:D:236:GLN:CG	2.43	0.47
1:F:67:GLU:HG3	1:F:102:TYR:CE2	2.49	0.47
1:B:173:ILE:O	1:B:189:LEU:HA	2.14	0.47
1:F:58:VAL:O	1:F:58:VAL:HG22	2.15	0.47
1:F:189:LEU:N	1:F:189:LEU:CD2	2.77	0.47
1:B:168:THR:HG21	1:B:198:ALA:HB1	1.95	0.47
1:C:7:ARG:NH2	1:C:125:GLU:OE2	2.35	0.47
1:C:215:MET:O	1:C:219:GLU:HG3	2.13	0.47
1:G:56:ILE:HD12	1:G:118:ALA:HB1	1.96	0.47
1:H:232:THR:C	1:H:234:ALA:H	2.18	0.47
1:B:6:LEU:O	1:B:7:ARG:CB	2.62	0.47
1:B:197:THR:HG23	1:B:197:THR:O	2.13	0.47
1:C:34:VAL:O	1:C:35:VAL:HG23	2.15	0.47
1:C:215:MET:CE	1:C:215:MET:HA	2.45	0.47
1:G:163:VAL:HG13	1:G:167:GLN:HB3	1.97	0.47
1:B:9:ALA:HB2	1:B:52:ILE:CD1	2.38	0.47
1:G:174:ILE:HB	1:G:202:LEU:HG	1.96	0.47
1:A:130:LEU:N	1:A:130:LEU:HD12	2.29	0.46
1:B:29:LYS:HE3	1:B:133:ASP:OD1	2.15	0.46
1:C:4:LYS:CD	1:C:125:GLU:HG2	2.41	0.46
1:D:143:LEU:HD22	1:D:143:LEU:HA	1.77	0.46
1:F:255:ASP:C	1:F:257:GLY:H	2.17	0.46
1:G:156:ASN:HD22	1:G:210:LEU:HA	1.80	0.46
1:H:9:ALA:HB2	1:H:52:ILE:HD12	1.97	0.46
1:D:184:THR:CG2	3:D:2012:HOH:O	2.63	0.46
1:A:36:ASP:O	1:C:22:PRO:HD2	2.16	0.46
1:B:156:ASN:ND2	1:B:211:GLN:H	2.13	0.46
1:C:58:VAL:HG22	1:C:58:VAL:O	2.15	0.46
1:E:40:ILE:H	1:E:40:ILE:HG13	1.42	0.46
1:G:28:PRO:O	1:G:31:MET:HB2	2.16	0.46
1:G:225:ALA:O	1:G:228:GLU:CG	2.56	0.46
1:A:40:ILE:H	1:A:40:ILE:HG13	1.40	0.46
1:A:158:ILE:HD11	1:A:244:PHE:HZ	1.81	0.46
1:B:198:ALA:HA	1:B:199:PRO:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:LEU:O	1:E:232:THR:O	2.32	0.46
1:H:233:ASP:OD1	1:H:233:ASP:C	2.54	0.46
1:A:19:ARG:O	1:A:259:LYS:HE3	2.16	0.46
1:D:215:MET:CE	1:D:218:LEU:HD12	2.46	0.46
1:C:34:VAL:O	1:C:266:ASN:OD1	2.34	0.46
1:D:238:MET:HE3	1:D:242:GLN:NE2	2.31	0.46
1:E:218:LEU:CD2	1:E:231:LEU:H	2.28	0.46
1:F:186:VAL:HG12	1:F:244:PHE:O	2.16	0.46
1:G:136:MET:SD	1:G:253:ARG:HG3	2.56	0.46
1:C:168:THR:CG2	1:C:173:ILE:HG13	2.43	0.46
1:B:36:ASP:OD1	1:B:273:ARG:NH2	2.47	0.45
1:B:273:ARG:NH1	1:B:273:ARG:HG2	2.30	0.45
1:A:213:GLU:HB2	1:A:238:MET:HE1	1.96	0.45
1:F:236:GLN:O	1:F:239:ILE:CD1	2.64	0.45
1:H:240:GLY:O	1:H:241:ASP:HB2	2.16	0.45
1:A:112:GLY:HA3	1:A:231:LEU:HD23	1.98	0.45
1:D:140:PRO:HB3	1:D:144:LYS:HG2	1.98	0.45
1:E:93:THR:CG2	1:H:25:LYS:HZ2	2.30	0.45
1:G:168:THR:CG2	1:G:173:ILE:HG13	2.46	0.45
1:H:36:ASP:HB3	1:H:37:ARG:HG3	1.98	0.45
1:B:217:ILE:HD11	1:B:237:ARG:HD2	1.97	0.45
1:D:163:VAL:HG11	1:D:167:GLN:HB3	1.97	0.45
1:C:236:GLN:C	1:C:238:MET:H	2.19	0.45
1:E:236:GLN:C	1:E:238:MET:H	2.19	0.45
1:G:216:ARG:HD2	1:G:216:ARG:N	2.31	0.45
1:H:115:VAL:CG1	1:H:215:MET:HE3	2.33	0.45
1:H:205:ILE:HG22	1:H:206:GLY:N	2.30	0.45
1:A:186:VAL:CG1	1:A:244:PHE:CD2	2.99	0.45
1:C:167:GLN:HE21	1:C:170:ARG:HD2	1.82	0.45
1:C:220:ASN:C	1:C:222:GLY:N	2.69	0.45
1:H:233:ASP:HA	1:H:236:GLN:HG2	1.96	0.45
1:B:22:PRO:HG3	1:D:89:VAL:O	2.16	0.45
1:C:255:ASP:C	1:C:257:GLY:H	2.20	0.45
1:E:145:GLN:NE2	1:E:250:GLN:HG2	2.32	0.45
1:F:263:ILE:CD1	1:G:270:ALA:HB2	2.40	0.45
1:B:23:ALA:HB2	1:D:36:ASP:O	2.16	0.45
1:C:163:VAL:HG22	1:C:164:PRO:HD2	1.99	0.45
1:D:31:MET:HG2	1:D:66:LEU:HD12	1.99	0.45
1:H:216:ARG:HD2	1:H:216:ARG:N	2.31	0.45
1:B:3:ILE:HD12	1:B:151:ASN:HA	1.98	0.45
1:D:265:ALA:O	1:D:269:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:THR:CG2	1:E:198:ALA:HB2	2.37	0.45
1:C:30:GLU:HB2	1:C:66:LEU:HD11	1.98	0.45
1:D:205:ILE:O	1:D:207:ARG:N	2.43	0.45
1:G:260:ALA:O	1:G:264:GLN:HG3	2.17	0.45
1:G:265:ALA:O	1:G:269:VAL:HG23	2.17	0.45
1:F:273:ARG:HA	1:F:274:PRO:HD3	1.84	0.44
1:F:23:ALA:HA	1:G:38:PRO:HD3	2.00	0.44
1:G:72:ILE:CG1	1:G:94:ARG:HE	2.30	0.44
1:A:216:ARG:HA	1:A:219:GLU:OE1	2.16	0.44
1:E:163:VAL:O	1:E:201:ASN:ND2	2.47	0.44
1:F:3:ILE:O	1:F:3:ILE:CG1	2.64	0.44
1:F:4:LYS:HB2	1:F:4:LYS:HE3	1.79	0.44
1:F:219:GLU:O	1:F:222:GLY:N	2.50	0.44
1:G:284:ALA:O	1:G:288:LEU:HG	2.17	0.44
1:F:36:ASP:CB	1:F:273:ARG:HH12	2.30	0.44
1:F:55:MET:HB2	1:F:100:ILE:HG12	1.99	0.44
1:H:189:LEU:N	1:H:189:LEU:CD2	2.81	0.44
1:E:105:GLN:O	1:E:106:GLN:HB2	2.17	0.44
1:E:238:MET:HE3	1:E:242:GLN:NE2	2.33	0.44
1:G:171:TYR:HB3	1:G:203:SER:HB2	2.00	0.44
1:F:96:LYS:HB2	1:F:99:ASN:HD21	1.80	0.44
1:H:105:GLN:O	1:H:106:GLN:HB2	2.17	0.44
1:D:214:VAL:O	1:D:217:ILE:HG22	2.18	0.44
1:D:220:ASN:C	1:D:222:GLY:H	2.20	0.44
1:E:34:VAL:O	1:E:34:VAL:CG2	2.65	0.44
1:C:189:LEU:H	1:C:236:GLN:HE21	1.66	0.44
1:E:36:ASP:O	1:H:23:ALA:HB2	2.18	0.44
1:E:167:GLN:NE2	1:E:170:ARG:NH1	2.53	0.44
1:F:208:TYR:CD1	1:F:208:TYR:N	2.85	0.44
1:C:143:LEU:HD22	1:C:143:LEU:HA	1.85	0.44
1:F:145:GLN:NE2	1:F:250:GLN:HG2	2.33	0.44
1:H:144:LYS:HE2	1:H:148:ASP:OD2	2.18	0.44
1:E:93:THR:HG21	1:H:25:LYS:NZ	2.33	0.43
1:E:189:LEU:O	1:E:236:GLN:NE2	2.50	0.43
1:E:264:GLN:HG2	1:H:283:PHE:CG	2.52	0.43
1:E:283:PHE:CG	1:H:264:GLN:HG2	2.52	0.43
1:G:139:GLN:CA	1:G:140:PRO:C	2.81	0.43
1:G:144:LYS:HA	1:G:147:VAL:HG12	2.00	0.43
1:G:206:GLY:O	1:G:207:ARG:HD2	2.17	0.43
1:H:140:PRO:HG2	1:H:145:GLN:CG	2.48	0.43
1:B:189:LEU:N	1:B:189:LEU:HD23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:VAL:HG12	1:C:153:VAL:O	2.17	0.43
1:E:93:THR:HG22	1:H:25:LYS:HZ3	1.82	0.43
1:E:144:LYS:O	1:E:147:VAL:HG12	2.18	0.43
1:F:34:VAL:HB	1:F:42:TYR:CE1	2.53	0.43
1:F:37:ARG:NH1	1:F:45:ASP:OD2	2.51	0.43
1:G:255:ASP:C	1:G:257:GLY:H	2.20	0.43
1:H:40:ILE:H	1:H:40:ILE:HG13	1.52	0.43
1:B:217:ILE:HD11	1:B:237:ARG:NH1	2.33	0.43
1:E:46:GLU:HG2	1:E:143:LEU:HB2	2.00	0.43
1:B:13:VAL:HG23	1:B:59:THR:HG22	2.01	0.43
1:C:67:GLU:HG3	1:C:102:TYR:CE2	2.52	0.43
1:H:255:ASP:C	1:H:257:GLY:N	2.72	0.43
1:A:16:LEU:HD12	1:C:79:THR:HG21	2.01	0.43
1:C:47:ALA:HB3	1:C:55:MET:CE	2.49	0.43
1:G:73:ALA:O	1:G:77:GLU:HG3	2.18	0.43
1:H:58:VAL:O	1:H:58:VAL:HG22	2.17	0.43
1:A:49:GLU:CD	1:A:140:PRO:O	2.57	0.43
1:C:40:ILE:H	1:C:40:ILE:HG13	1.46	0.43
1:E:213:GLU:HB2	1:E:238:MET:CE	2.48	0.43
1:G:220:ASN:O	1:G:221:GLN:C	2.57	0.43
1:H:239:ILE:CG1	1:H:240:GLY:N	2.82	0.43
1:C:216:ARG:N	1:C:216:ARG:CD	2.81	0.43
1:D:34:VAL:O	1:D:34:VAL:HG22	2.17	0.43
1:E:171:TYR:CB	1:E:203:SER:HB2	2.49	0.43
1:F:50:ALA:HB3	1:F:143:LEU:HD12	2.00	0.43
1:F:204:VAL:HB	2:F:1290:G1P:H62	2.00	0.43
1:G:236:GLN:C	1:G:238:MET:N	2.71	0.43
1:A:36:ASP:O	1:C:23:ALA:HB2	2.19	0.43
1:C:72:ILE:HG13	1:C:94:ARG:HD2	2.00	0.43
1:G:28:PRO:CB	1:G:66:LEU:HD11	2.48	0.43
1:C:44:VAL:HB	1:C:55:MET:HE2	2.00	0.43
1:C:216:ARG:N	1:C:216:ARG:HD2	2.33	0.43
1:G:104:ARG:NH1	1:H:67:GLU:HG2	2.33	0.43
1:H:95:LEU:HD22	1:H:100:ILE:HD11	2.01	0.43
1:E:23:ALA:HB2	1:H:36:ASP:C	2.39	0.43
1:E:93:THR:HG22	1:H:25:LYS:NZ	2.34	0.43
1:E:106:GLN:OE1	1:F:94:ARG:HD3	2.19	0.43
1:F:173:ILE:O	1:F:189:LEU:HA	2.19	0.43
1:G:159:CYS:HB3	1:G:205:ILE:HB	1.99	0.43
1:G:230:GLN:OE1	1:G:233:ASP:OD2	2.37	0.43
1:A:277:GLU:HB3	1:A:278:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ASP:C	1:E:257:GLY:H	2.21	0.42
1:G:167:GLN:HG3	1:G:170:ARG:HD3	2.01	0.42
1:G:238:MET:HE3	1:G:242:GLN:NE2	2.33	0.42
1:B:193:PRO:HB2	1:B:197:THR:CG2	2.46	0.42
1:C:36:ASP:N	1:C:36:ASP:OD1	2.52	0.42
1:C:194:ALA:HB3	1:C:197:THR:CG2	2.49	0.42
1:G:116:TRP:CD1	1:G:119:ARG:HD3	2.54	0.42
1:C:238:MET:HE3	1:C:238:MET:HB3	1.82	0.42
1:G:172:GLY:N	2:G:1290:G1P:H62	2.17	0.42
1:E:168:THR:HG23	1:E:173:ILE:HG13	2.00	0.42
1:G:96:LYS:HB3	1:G:99:ASN:ND2	2.34	0.42
1:H:216:ARG:HA	1:H:219:GLU:OE1	2.19	0.42
1:H:232:THR:O	1:H:234:ALA:N	2.52	0.42
1:A:157:LEU:N	1:A:157:LEU:HD12	2.34	0.42
1:B:56:ILE:HD13	1:B:101:ALA:HB3	2.02	0.42
1:B:206:GLY:O	1:B:207:ARG:HD2	2.18	0.42
1:B:40:ILE:H	1:B:40:ILE:HG13	1.56	0.42
1:C:197:THR:O	1:C:197:THR:OG1	2.31	0.42
1:E:160:ALA:HB1	1:E:202:LEU:HD11	2.01	0.42
1:F:143:LEU:HD22	1:F:143:LEU:HA	1.88	0.42
1:C:18:THR:O	1:C:21:LEU:HD22	2.19	0.42
1:G:200:SER:OG	1:G:201:ASN:N	2.52	0.42
1:H:46:GLU:HG2	1:H:143:LEU:HB2	2.02	0.42
1:A:93:THR:HG22	1:C:25:LYS:HZ3	1.83	0.42
1:A:218:LEU:HB3	1:A:231:LEU:HD21	2.02	0.42
1:B:29:LYS:HZ1	1:B:257:GLY:HA2	1.83	0.42
1:C:145:GLN:HE22	1:C:250:GLN:HG2	1.84	0.42
1:E:194:ALA:H	1:E:197:THR:CG2	2.33	0.42
1:F:145:GLN:OE1	1:F:250:GLN:HB2	2.20	0.42
1:G:40:ILE:O	1:G:44:VAL:HG13	2.19	0.42
1:G:167:GLN:HE21	1:G:170:ARG:CD	2.33	0.42
1:A:88:ASP:N	1:A:88:ASP:OD1	2.53	0.42
1:E:25:LYS:NZ	1:H:93:THR:HG21	2.35	0.42
1:E:281:ARG:NH1	1:H:288:LEU:HB2	2.35	0.42
1:H:67:GLU:HG3	1:H:102:TYR:CE1	2.55	0.42
1:H:156:ASN:C	1:H:157:LEU:HD12	2.40	0.42
1:E:156:ASN:HD22	1:E:211:GLN:H	1.67	0.42
1:E:194:ALA:N	1:E:197:THR:CG2	2.82	0.42
1:F:211:GLN:HE21	1:F:212:PRO:HD2	1.85	0.42
1:G:30:GLU:HG3	3:G:2010:HOH:O	2.20	0.42
1:B:61:ARG:HD3	1:C:72:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:HD13	1:C:66:LEU:HG	2.02	0.41
1:G:96:LYS:CB	1:G:99:ASN:ND2	2.83	0.41
1:H:34:VAL:CG1	1:H:269:VAL:HG21	2.50	0.41
1:B:168:THR:HG23	1:B:173:ILE:CD1	2.50	0.41
1:C:177:GLY:HA3	1:C:187:LYS:HE3	2.01	0.41
1:D:212:PRO:O	1:D:216:ARG:HD3	2.20	0.41
1:F:36:ASP:CG	1:F:273:ARG:HH12	2.23	0.41
1:H:215:MET:CE	1:H:215:MET:HA	2.50	0.41
1:C:159:CYS:HB3	1:C:205:ILE:HB	2.02	0.41
1:F:191:GLU:OE2	2:F:1290:G1P:H3	2.21	0.41
1:F:288:LEU:HD21	1:G:284:ALA:HB3	2.01	0.41
1:G:66:LEU:HD12	1:G:66:LEU:N	2.36	0.41
1:H:144:LYS:HA	1:H:147:VAL:HG12	2.01	0.41
1:B:29:LYS:NZ	1:B:257:GLY:HA2	2.35	0.41
1:G:116:TRP:HA	1:G:215:MET:CE	2.50	0.41
1:G:189:LEU:HD22	1:G:239:ILE:HD11	2.02	0.41
1:G:215:MET:O	1:G:219:GLU:HG3	2.20	0.41
1:A:46:GLU:HG2	1:A:143:LEU:HB2	2.03	0.41
1:A:93:THR:CG2	1:C:25:LYS:HD3	2.50	0.41
1:B:191:GLU:HG3	1:B:192:LYS:HG2	2.02	0.41
1:C:130:LEU:N	1:C:130:LEU:HD12	2.36	0.41
1:C:153:VAL:HG11	1:C:245:HIS:CD2	2.55	0.41
1:C:168:THR:HG21	1:C:198:ALA:HB2	2.03	0.41
1:E:238:MET:CE	1:E:242:GLN:NE2	2.83	0.41
1:G:168:THR:HG23	1:G:173:ILE:HD11	2.02	0.41
1:H:143:LEU:HD22	1:H:143:LEU:HA	1.79	0.41
1:A:13:VAL:HG23	1:A:59:THR:CG2	2.49	0.41
1:A:34:VAL:O	1:A:35:VAL:HB	2.20	0.41
1:B:141:GLY:O	1:B:145:GLN:HG3	2.20	0.41
1:D:58:VAL:O	1:D:58:VAL:HG22	2.20	0.41
1:E:186:VAL:HG13	1:E:244:PHE:HB3	2.03	0.41
1:E:216:ARG:HD2	1:E:216:ARG:N	2.34	0.41
1:F:25:LYS:HZ3	1:G:93:THR:CG2	2.33	0.41
1:F:34:VAL:CG1	1:F:269:VAL:HG21	2.50	0.41
1:A:73:ALA:O	1:A:77:GLU:HG3	2.21	0.41
1:B:144:LYS:HE2	1:B:148:ASP:OD2	2.21	0.41
1:D:40:ILE:CD1	1:D:57:PHE:CE2	2.96	0.41
1:H:61:ARG:O	1:H:63:LYS:N	2.54	0.41
1:H:235:MET:O	1:H:238:MET:HB2	2.21	0.41
1:B:23:ALA:HB2	1:D:36:ASP:C	2.41	0.41
1:B:171:TYR:CB	1:B:203:SER:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:VAL:HG12	1:B:244:PHE:O	2.21	0.41
1:E:4:LYS:NZ	1:E:124:ASP:OD1	2.54	0.41
1:E:190:VAL:O	1:E:190:VAL:HG23	2.20	0.41
1:F:56:ILE:O	1:F:56:ILE:HG13	2.20	0.41
1:G:111:LEU:HD23	1:G:231:LEU:HD23	2.03	0.41
1:H:277:GLU:HB3	1:H:278:PRO:HD3	2.03	0.41
1:A:283:PHE:CG	1:C:264:GLN:HG2	2.55	0.41
1:C:44:VAL:HG21	1:C:70:PHE:HE2	1.85	0.41
1:D:37:ARG:HD2	3:D:2003:HOH:O	2.21	0.41
1:D:42:TYR:CG	1:D:135:PHE:HE1	2.38	0.41
1:E:236:GLN:C	1:E:238:MET:N	2.75	0.41
1:F:40:ILE:H	1:F:40:ILE:HG13	1.35	0.41
1:F:271:LEU:O	1:F:277:GLU:HG3	2.21	0.41
1:G:67:GLU:HG3	1:G:102:TYR:CZ	2.56	0.41
1:G:276:LEU:O	1:G:280:VAL:HG23	2.21	0.41
1:G:281:ARG:NH1	3:G:2018:HOH:O	2.46	0.41
1:H:156:ASN:ND2	1:H:211:GLN:H	2.19	0.41
1:D:231:LEU:O	1:D:232:THR:C	2.59	0.41
1:F:34:VAL:O	1:F:34:VAL:HG12	2.19	0.41
1:F:130:LEU:HD12	1:F:130:LEU:N	2.36	0.41
1:F:171:TYR:CB	1:F:203:SER:HB2	2.51	0.41
1:G:13:VAL:O	1:G:63:LYS:HD3	2.21	0.41
1:B:186:VAL:HG13	1:B:244:PHE:HB3	2.01	0.40
1:B:273:ARG:HH11	1:B:273:ARG:HG2	1.85	0.40
1:D:255:ASP:C	1:D:257:GLY:N	2.74	0.40
1:H:127:PHE:CD2	1:H:127:PHE:N	2.89	0.40
1:H:238:MET:HE1	1:H:242:GLN:HE21	1.82	0.40
1:A:72:ILE:HG12	1:A:94:ARG:CZ	2.52	0.40
1:E:236:GLN:O	1:E:238:MET:N	2.54	0.40
1:E:276:LEU:O	1:E:280:VAL:HG23	2.21	0.40
1:G:157:LEU:N	1:G:157:LEU:HD12	2.37	0.40
1:G:160:ALA:HB1	1:G:202:LEU:HD12	2.02	0.40
1:A:4:LYS:HA	1:A:5:PRO:HD2	1.77	0.40
1:A:173:ILE:O	1:A:173:ILE:HG13	2.21	0.40
1:E:38:PRO:HG2	1:E:41:GLN:HB2	2.03	0.40
1:A:80:MET:HE3	1:A:87:LEU:HD23	2.04	0.40
1:A:255:ASP:C	1:A:257:GLY:N	2.75	0.40
1:D:189:LEU:CD2	1:D:189:LEU:N	2.84	0.40
1:D:236:GLN:C	1:D:238:MET:N	2.75	0.40
1:F:23:ALA:HB2	1:G:36:ASP:O	2.21	0.40
1:G:10:VAL:HG22	1:G:56:ILE:CD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:ALA:HA	1:G:199:PRO:HD2	1.98	0.40
1:A:5:PRO:O	1:A:150:TYR:CE2	2.73	0.40
1:D:212:PRO:HG2	1:D:213:GLU:OE2	2.22	0.40
1:D:238:MET:HE3	1:D:238:MET:HB3	1.96	0.40
1:G:104:ARG:HH11	1:H:67:GLU:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	247/297 (83%)	223 (90%)	20 (8%)	4 (2%)	9 14
1	B	276/297 (93%)	252 (91%)	17 (6%)	7 (2%)	5 7
1	C	278/297 (94%)	252 (91%)	20 (7%)	6 (2%)	6 9
1	D	277/297 (93%)	251 (91%)	21 (8%)	5 (2%)	8 12
1	E	276/297 (93%)	249 (90%)	19 (7%)	8 (3%)	4 6
1	F	278/297 (94%)	252 (91%)	20 (7%)	6 (2%)	6 9
1	G	286/297 (96%)	254 (89%)	24 (8%)	8 (3%)	5 6
1	H	236/297 (80%)	215 (91%)	17 (7%)	4 (2%)	9 13
All	All	2154/2376 (91%)	1948 (90%)	158 (7%)	48 (2%)	6 9

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	6	LEU
1	B	6	LEU
1	B	125	GLU
1	E	62	GLY

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Mol	Chain	Res	Type
1	E	140	PRO
1	F	6	LEU
1	F	17	GLY
1	F	140	PRO
1	F	191	GLU
1	F	237	ARG
1	G	140	PRO
1	G	191	GLU
1	C	35	VAL
1	D	206	GLY
1	D	241	ASP
1	E	17	GLY
1	E	231	LEU
1	F	206	GLY
1	G	206	GLY
1	G	221	GLN
1	H	62	GLY
1	B	237	ARG
1	C	17	GLY
1	C	237	ARG
1	D	17	GLY
1	E	206	GLY
1	E	237	ARG
1	E	288	LEU
1	H	206	GLY
1	H	233	ASP
1	A	17	GLY
1	B	7	ARG
1	C	196	GLY
1	D	140	PRO
1	D	221	GLN
1	G	237	ARG
1	A	206	GLY
1	C	2	THR
1	G	226	GLY
1	C	206	GLY
1	E	35	VAL
1	G	17	GLY
1	G	240	GLY
1	H	17	GLY
1	B	206	GLY
1	B	35	VAL

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Mol	Chain	Res	Type
1	B	17	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/235 (86%)	181 (90%)	21 (10%)	7 10
1	B	222/235 (94%)	198 (89%)	24 (11%)	6 9
1	C	225/235 (96%)	198 (88%)	27 (12%)	5 7
1	D	223/235 (95%)	202 (91%)	21 (9%)	8 13
1	E	223/235 (95%)	204 (92%)	19 (8%)	10 15
1	F	224/235 (95%)	195 (87%)	29 (13%)	4 5
1	G	225/235 (96%)	202 (90%)	23 (10%)	7 10
1	H	193/235 (82%)	174 (90%)	19 (10%)	8 11
All	All	1737/1880 (92%)	1554 (90%)	183 (10%)	7 10

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	40	ILE
1	A	58	VAL
1	A	80	MET
1	A	94	ARG
1	A	96	LYS
1	A	143	LEU
1	A	147	VAL
1	A	175	THR
1	A	176	PRO
1	A	178	THR
1	A	184	THR
1	A	201	ASN
1	A	207	ARG

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Mol	Chain	Res	Type
1	A	213	GLU
1	A	232	THR
1	A	233	ASP
1	A	237	ARG
1	A	244	PHE
1	A	258	ASP
1	A	277	GLU
1	B	29	LYS
1	B	37	ARG
1	B	40	ILE
1	B	56	ILE
1	B	121	ILE
1	B	124	ASP
1	B	139	GLN
1	B	143	LEU
1	B	184	THR
1	B	186	VAL
1	B	189	LEU
1	B	197	THR
1	B	213	GLU
1	B	217	ILE
1	B	231	LEU
1	B	232	THR
1	B	233	ASP
1	B	238	MET
1	B	239	ILE
1	B	244	PHE
1	B	258	ASP
1	B	273	ARG
1	B	275	ASP
1	B	277	GLU
1	C	21	LEU
1	C	37	ARG
1	C	40	ILE
1	C	56	ILE
1	C	58	VAL
1	C	64	SER
1	C	66	LEU
1	C	90	LEU
1	C	139	GLN
1	C	143	LEU
1	C	163	VAL

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Mol	Chain	Res	Type
1	C	166	ASP
1	C	184	THR
1	C	189	LEU
1	C	191	GLU
1	C	207	ARG
1	C	213	GLU
1	C	230	GLN
1	C	232	THR
1	C	233	ASP
1	C	237	ARG
1	C	241	ASP
1	C	242	GLN
1	C	244	PHE
1	C	253	ARG
1	C	258	ASP
1	C	277	GLU
1	D	21	LEU
1	D	33	PRO
1	D	34	VAL
1	D	58	VAL
1	D	89	VAL
1	D	107	GLU
1	D	143	LEU
1	D	182	VAL
1	D	184	THR
1	D	189	LEU
1	D	202	LEU
1	D	207	ARG
1	D	213	GLU
1	D	233	ASP
1	D	241	ASP
1	D	244	PHE
1	D	253	ARG
1	D	258	ASP
1	D	275	ASP
1	D	277	GLU
1	D	288	LEU
1	E	32	LEU
1	E	36	ASP
1	E	40	ILE
1	E	58	VAL
1	E	66	LEU

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Mol	Chain	Res	Type
1	E	143	LEU
1	E	166	ASP
1	E	184	THR
1	E	186	VAL
1	E	189	LEU
1	E	192	LYS
1	E	213	GLU
1	E	232	THR
1	E	242	GLN
1	E	244	PHE
1	E	253	ARG
1	E	258	ASP
1	E	275	ASP
1	E	277	GLU
1	F	3	ILE
1	F	6	LEU
1	F	7	ARG
1	F	33	PRO
1	F	37	ARG
1	F	40	ILE
1	F	56	ILE
1	F	59	THR
1	F	64	SER
1	F	66	LEU
1	F	86	SER
1	F	90	LEU
1	F	143	LEU
1	F	168	THR
1	F	178	THR
1	F	182	VAL
1	F	184	THR
1	F	186	VAL
1	F	189	LEU
1	F	195	PRO
1	F	197	THR
1	F	208	TYR
1	F	213	GLU
1	F	235	MET
1	F	239	ILE
1	F	241	ASP
1	F	244	PHE
1	F	253	ARG

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Mol	Chain	Res	Type
1	F	258	ASP
1	G	37	ARG
1	G	40	ILE
1	G	58	VAL
1	G	90	LEU
1	G	94	ARG
1	G	95	LEU
1	G	96	LYS
1	G	143	LEU
1	G	166	ASP
1	G	184	THR
1	G	186	VAL
1	G	189	LEU
1	G	191	GLU
1	G	192	LYS
1	G	200	SER
1	G	208	TYR
1	G	215	MET
1	G	223	LYS
1	G	230	GLN
1	G	244	PHE
1	G	258	ASP
1	G	275	ASP
1	G	277	GLU
1	H	33	PRO
1	H	37	ARG
1	H	40	ILE
1	H	58	VAL
1	H	93	THR
1	H	143	LEU
1	H	158	ILE
1	H	184	THR
1	H	186	VAL
1	H	189	LEU
1	H	207	ARG
1	H	208	TYR
1	H	213	GLU
1	H	232	THR
1	H	244	PHE
1	H	258	ASP
1	H	277	GLU
1	H	281	ARG

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Mol	Chain	Res	Type
1	H	285	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	156	ASN
1	A	211	GLN
1	A	221	GLN
1	A	242	GLN
1	A	245	HIS
1	B	113	HIS
1	B	145	GLN
1	B	156	ASN
1	B	167	GLN
1	B	211	GLN
1	B	242	GLN
1	B	245	HIS
1	C	113	HIS
1	C	145	GLN
1	C	156	ASN
1	C	167	GLN
1	C	211	GLN
1	C	236	GLN
1	C	242	GLN
1	D	145	GLN
1	D	156	ASN
1	D	167	GLN
1	D	211	GLN
1	D	221	GLN
1	D	242	GLN
1	E	113	HIS
1	E	145	GLN
1	E	156	ASN
1	E	167	GLN
1	E	211	GLN
1	E	221	GLN
1	E	242	GLN
1	E	250	GLN
1	F	41	GLN
1	F	99	ASN
1	F	113	HIS

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Mol	Chain	Res	Type
1	F	145	GLN
1	F	211	GLN
1	F	230	GLN
1	F	245	HIS
1	F	250	GLN
1	G	99	ASN
1	G	145	GLN
1	G	156	ASN
1	G	167	GLN
1	G	211	GLN
1	G	230	GLN
1	G	242	GLN
1	H	99	ASN
1	H	145	GLN
1	H	156	ASN
1	H	211	GLN
1	H	242	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	G1P	A	1290	-	15,16,16	1.12	1 (6%)	23,24,24	0.75	0
2	G1P	E	1290	-	15,16,16	1.13	1 (6%)	23,24,24	0.74	0
2	G1P	G	1290	-	15,16,16	1.29	2 (13%)	23,24,24	0.82	0
2	G1P	C	1290	-	15,16,16	1.03	0	23,24,24	0.73	0
2	G1P	D	1290	-	15,16,16	1.11	1 (6%)	23,24,24	0.77	0
2	G1P	B	1290	-	15,16,16	1.19	2 (13%)	23,24,24	0.76	0
2	G1P	F	1290	-	15,16,16	1.13	0	23,24,24	0.89	1 (4%)
2	G1P	H	1290	-	15,16,16	1.12	1 (6%)	23,24,24	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G1P	A	1290	-	-	0/7/27/27	0/1/1/1
2	G1P	E	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	G	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	C	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	D	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	B	1290	-	-	0/7/27/27	0/1/1/1
2	G1P	F	1290	-	-	0/7/27/27	0/1/1/1
2	G1P	H	1290	-	-	0/7/27/27	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1290	G1P	P-O1	2.91	1.64	1.59
2	E	1290	G1P	P-O1	2.29	1.63	1.59
2	B	1290	G1P	O5-C1	2.15	1.47	1.41
2	A	1290	G1P	O5-C1	2.13	1.47	1.41
2	G	1290	G1P	P-O3P	2.11	1.63	1.54
2	D	1290	G1P	P-O1	2.05	1.63	1.59
2	B	1290	G1P	P-O3P	2.03	1.62	1.54
2	H	1290	G1P	P-O1	2.02	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1290	G1P	O1-C1-C2	2.42	112.82	108.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1290	G1P	C2-C1-O1-P
2	E	1290	G1P	C2-C1-O1-P
2	G	1290	G1P	O5-C1-O1-P
2	D	1290	G1P	C2-C1-O1-P

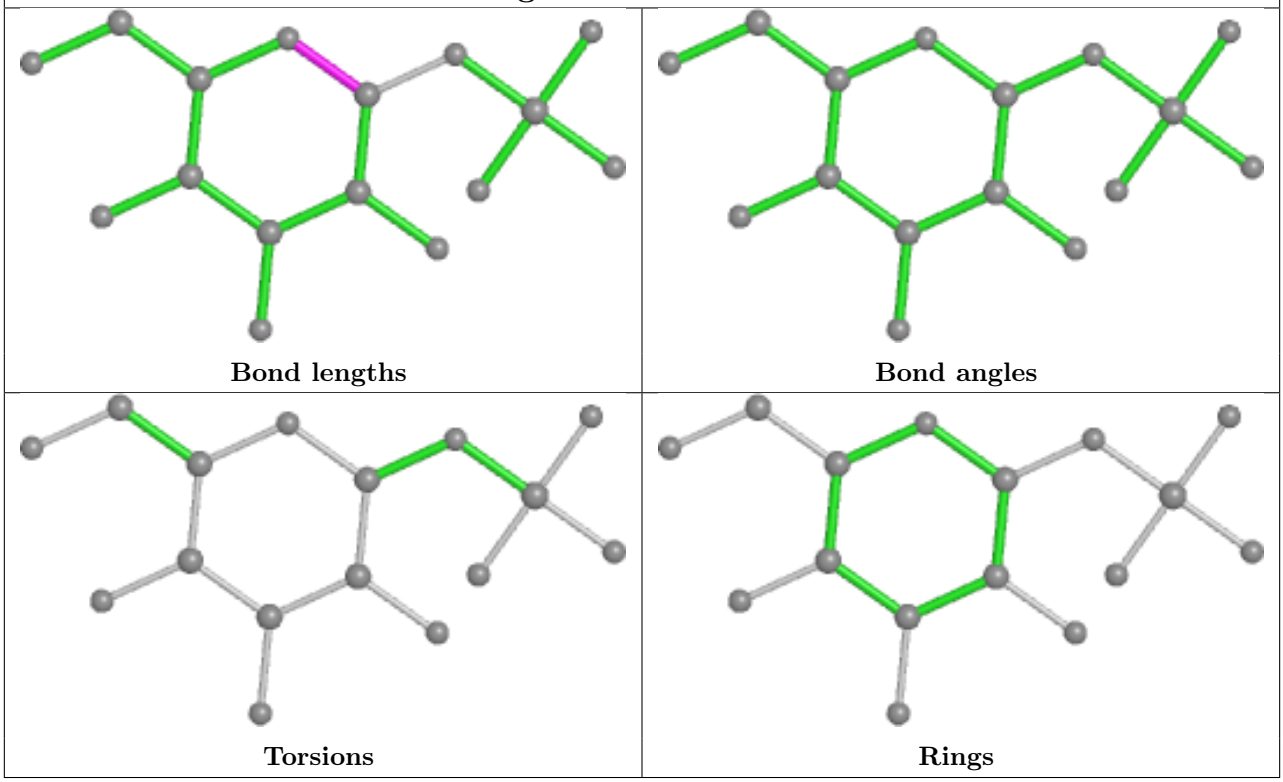
There are no ring outliers.

2 monomers are involved in 5 short contacts:

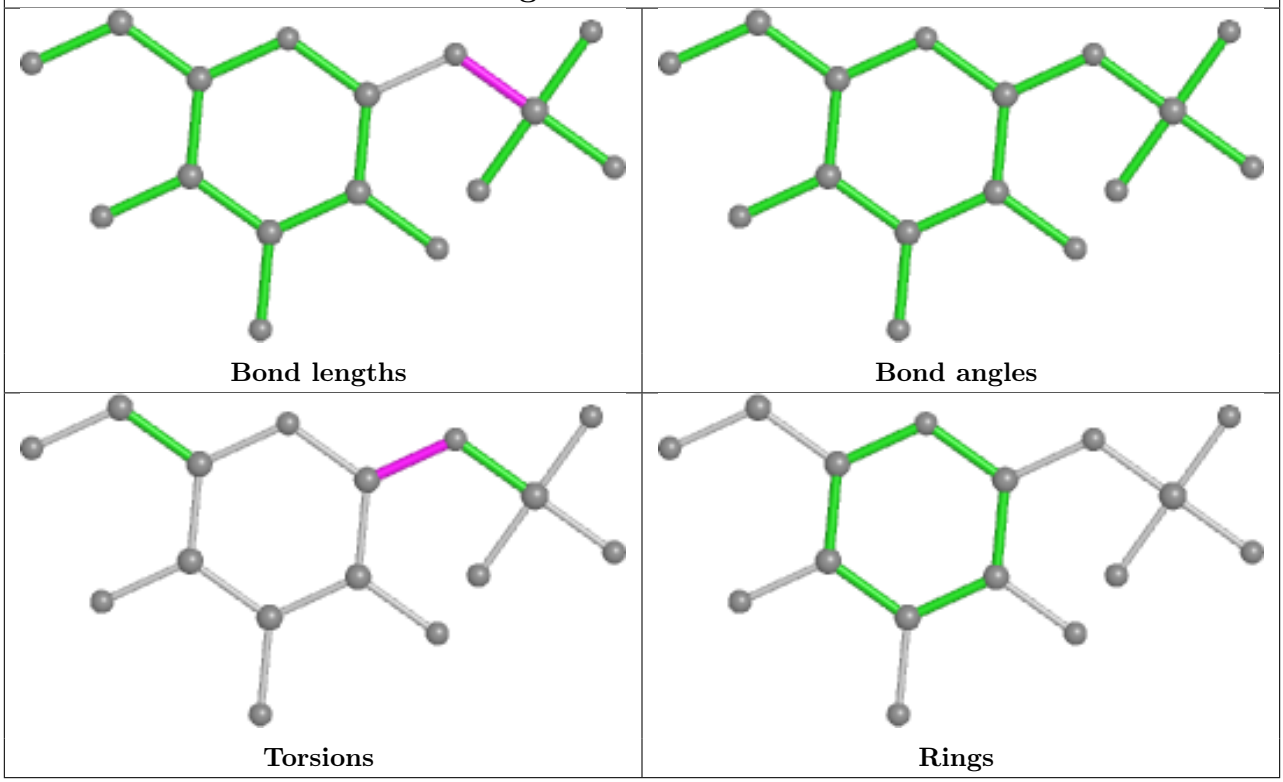
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1290	G1P	3	0
2	F	1290	G1P	2	0

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

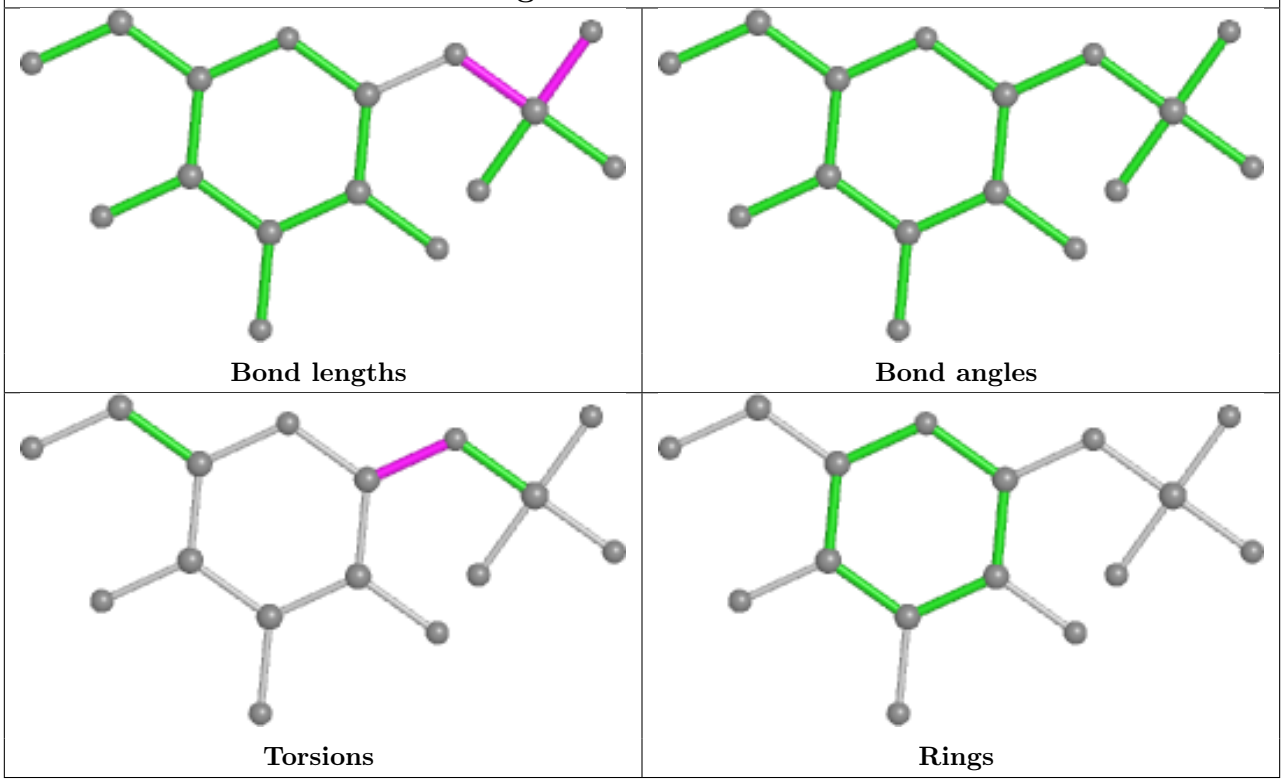
Ligand G1P A 1290



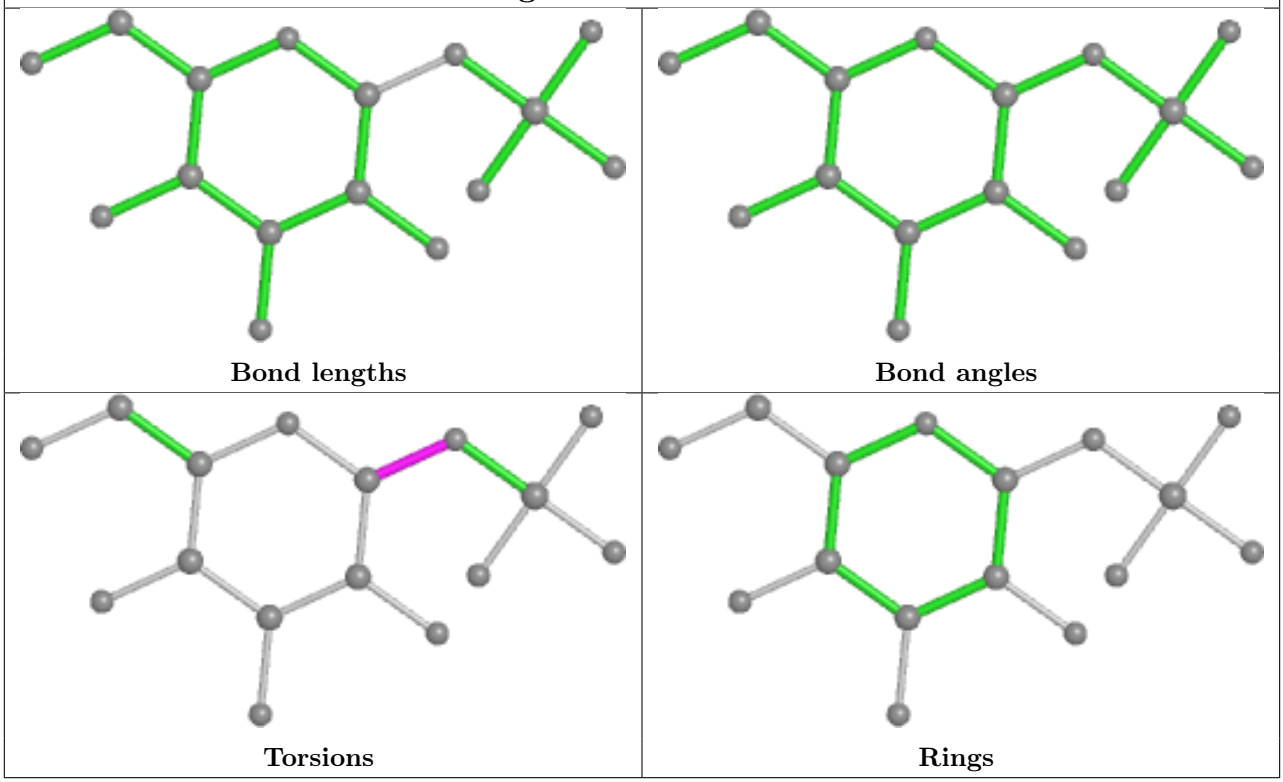
Ligand G1P E 1290



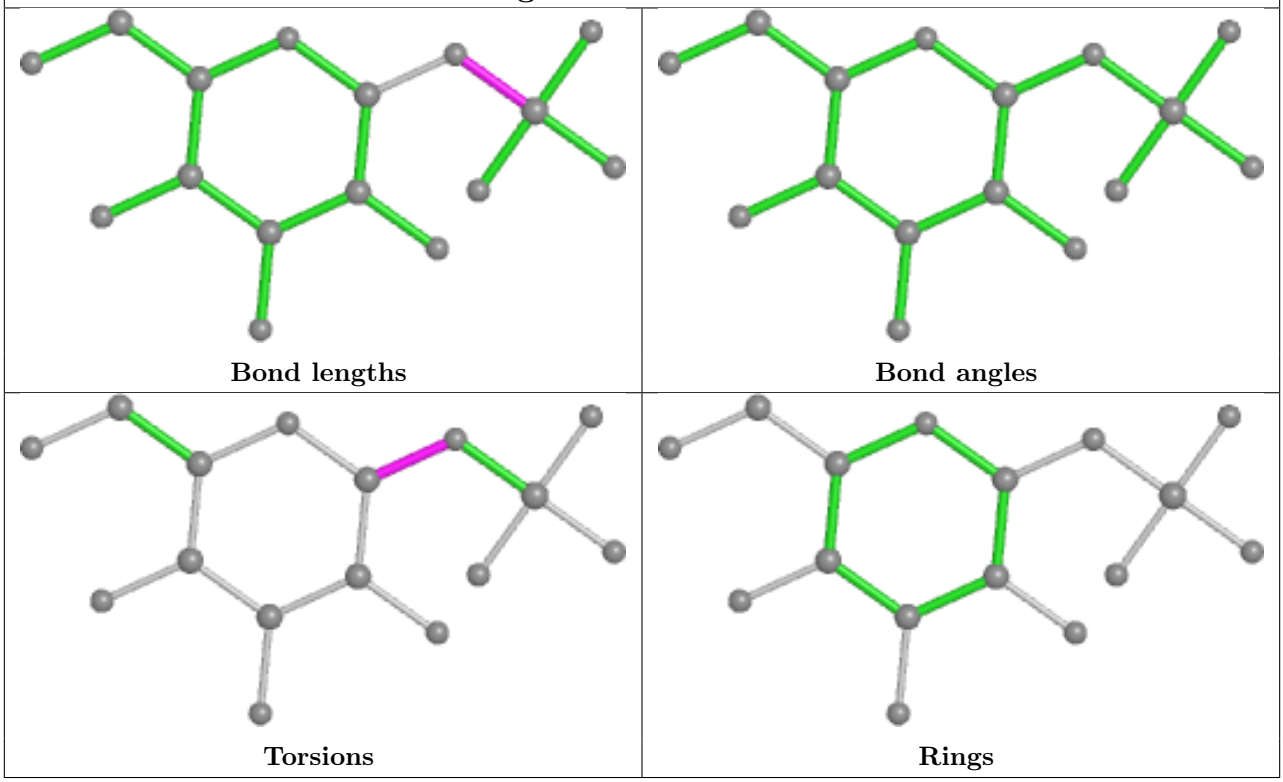
Ligand G1P G 1290



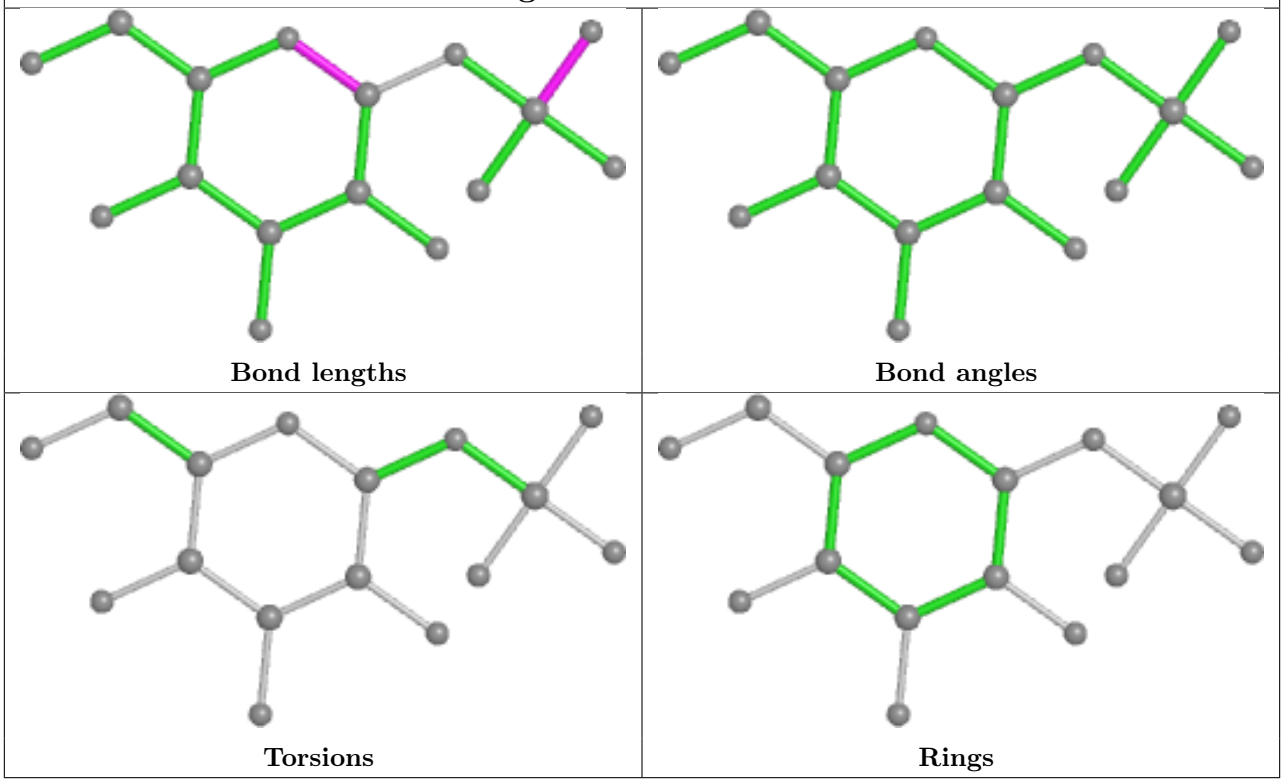
Ligand G1P C 1290



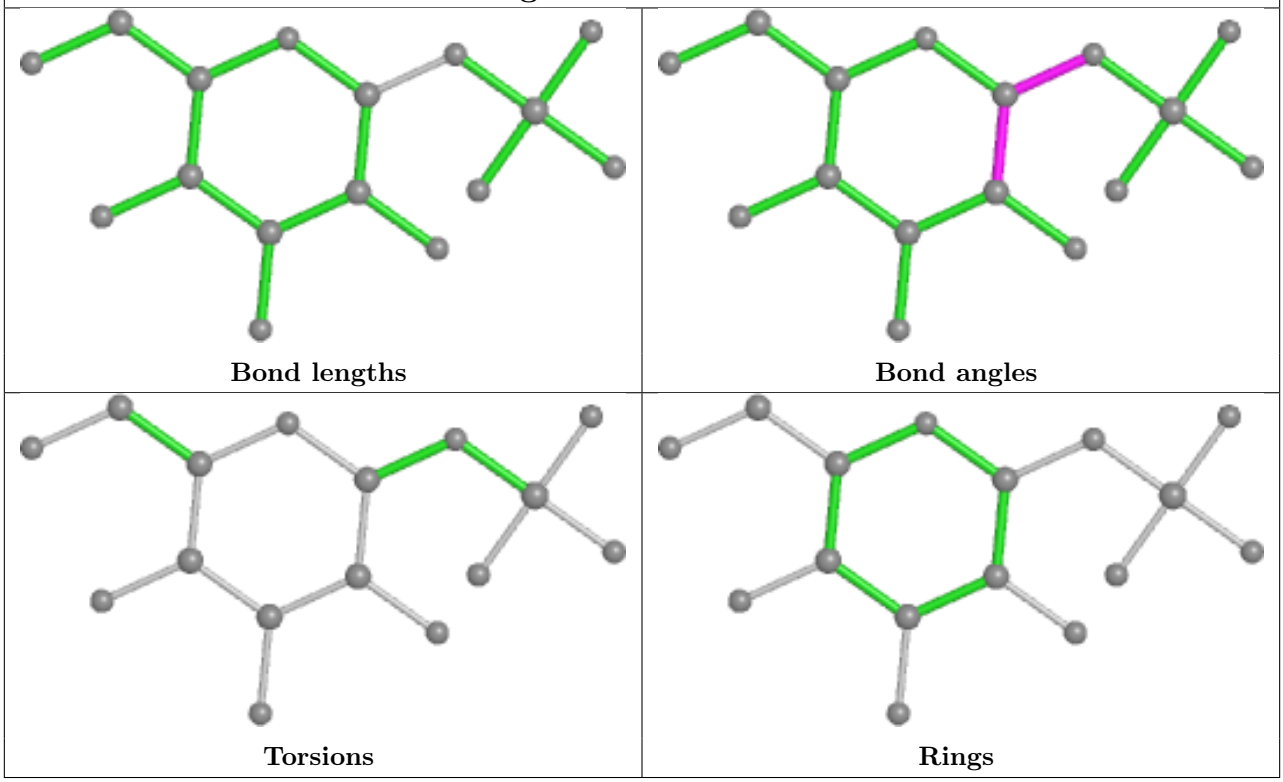
Ligand G1P D 1290



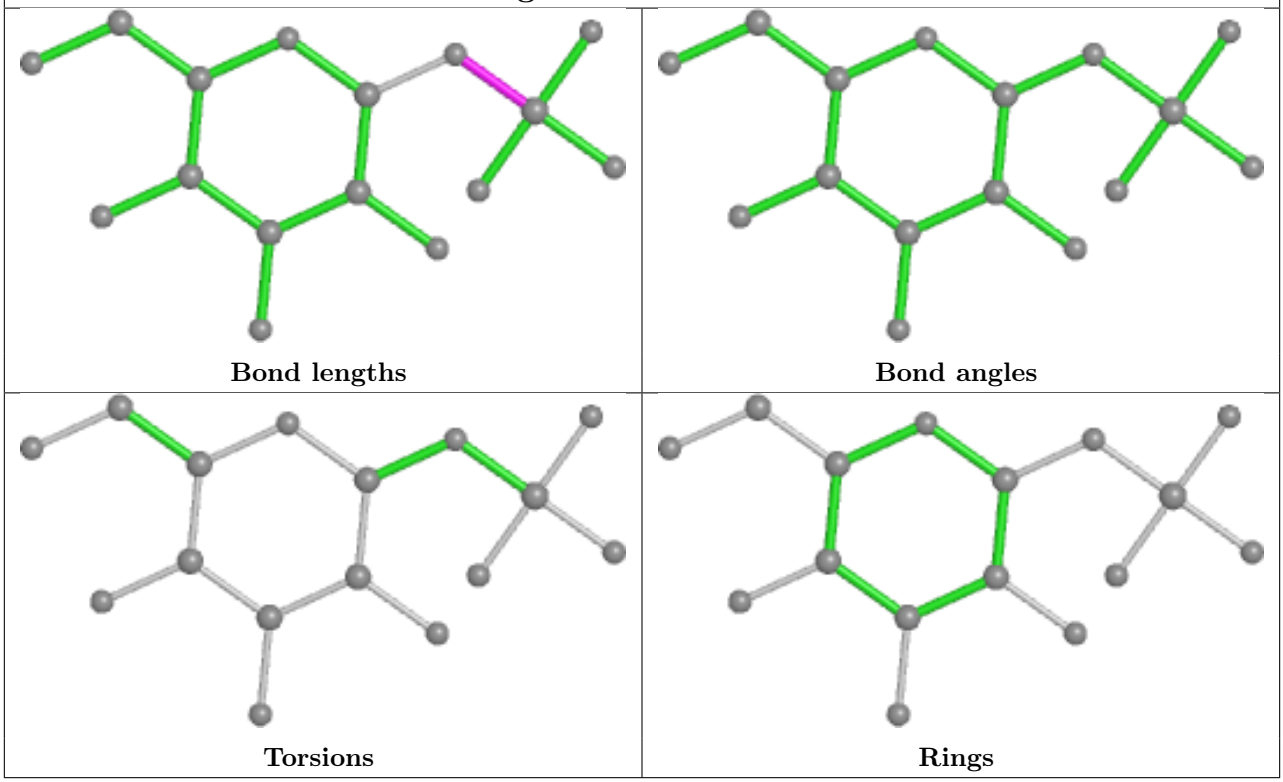
Ligand G1P B 1290



Ligand G1P F 1290



Ligand G1P H 1290



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	255/297 (85%)	0.31	9 (3%)	44	40	22, 55, 101, 150	0
1	B	280/297 (94%)	0.01	4 (1%)	75	73	23, 48, 80, 114	0
1	C	282/297 (94%)	0.14	3 (1%)	80	79	20, 46, 88, 116	0
1	D	281/297 (94%)	0.17	4 (1%)	75	73	27, 51, 83, 125	0
1	E	280/297 (94%)	0.02	3 (1%)	80	79	21, 44, 73, 120	0
1	F	282/297 (94%)	0.33	8 (2%)	53	49	27, 54, 88, 120	0
1	G	288/297 (96%)	0.09	1 (0%)	94	95	21, 48, 84, 110	0
1	H	244/297 (82%)	0.05	0	100	100	18, 46, 89, 122	1 (0%)
All	All	2192/2376 (92%)	0.14	32 (1%)	73	71	18, 49, 89, 150	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	GLY	4.1
1	A	231	LEU	3.9
1	D	289	GLY	3.8
1	A	240	GLY	3.4
1	E	221	GLN	3.2
1	F	173	ILE	2.9
1	A	202	LEU	2.7
1	B	239	ILE	2.6
1	B	107	GLU	2.5
1	F	252	THR	2.4
1	B	7	ARG	2.4
1	F	17	GLY	2.4
1	F	246	GLY	2.4
1	F	289	GLY	2.4
1	C	195	PRO	2.3
1	G	285	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	217	ILE	2.3
1	A	246	GLY	2.2
1	A	180	ASP	2.2
1	C	187	LYS	2.2
1	D	241	ASP	2.2
1	A	3	ILE	2.2
1	C	84	GLY	2.1
1	B	197	THR	2.1
1	A	7	ARG	2.1
1	D	235	MET	2.1
1	F	187	LYS	2.1
1	F	195	PRO	2.1
1	E	15	GLY	2.1
1	D	190	VAL	2.0
1	F	216	ARG	2.0
1	A	175	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å^2)	Q<0.9
2	G1P	H	1290	16/16	0.49	0.45	70,70,70,70	16
2	G1P	A	1290	16/16	0.55	0.46	104,106,106,106	16
2	G1P	C	1290	16/16	0.66	0.38	60,60,60,60	16
2	G1P	G	1290	16/16	0.72	0.37	60,60,60,60	16
2	G1P	F	1290	16/16	0.76	0.32	80,80,80,80	16
2	G1P	B	1290	16/16	0.79	0.33	60,60,60,60	16
2	G1P	D	1290	16/16	0.84	0.29	60,60,60,90	16

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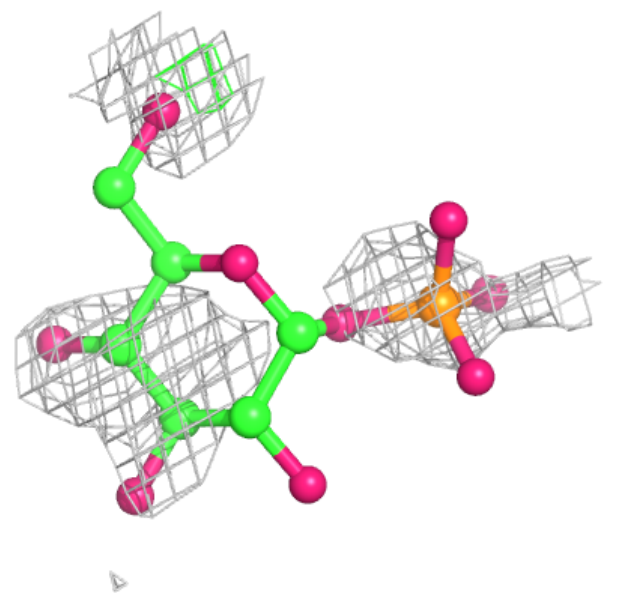
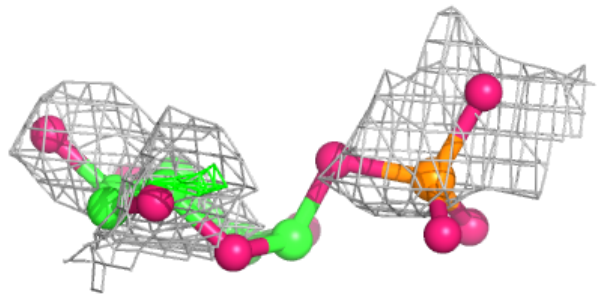
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G1P	E	1290	16/16	0.85	0.25	45,45,45,45	16

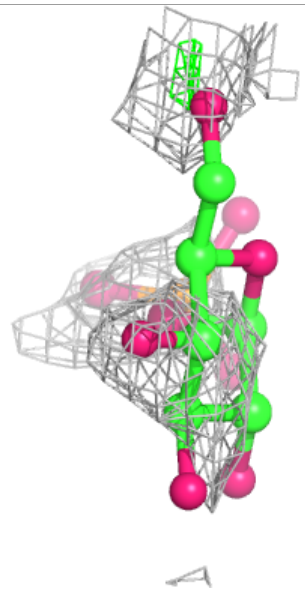
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G1P H 1290:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

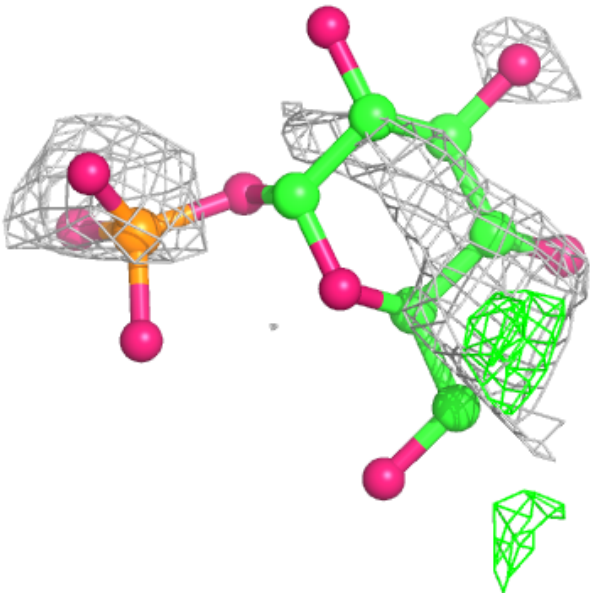


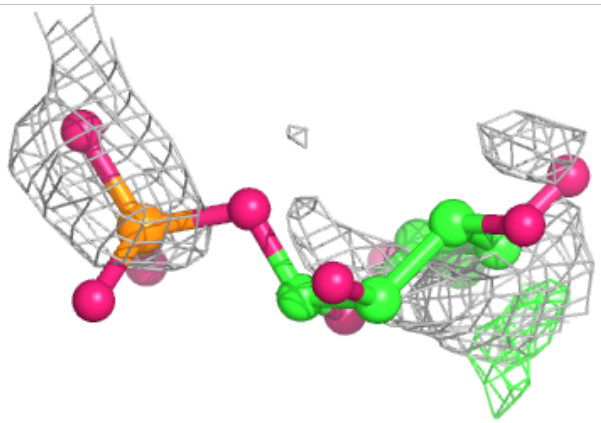


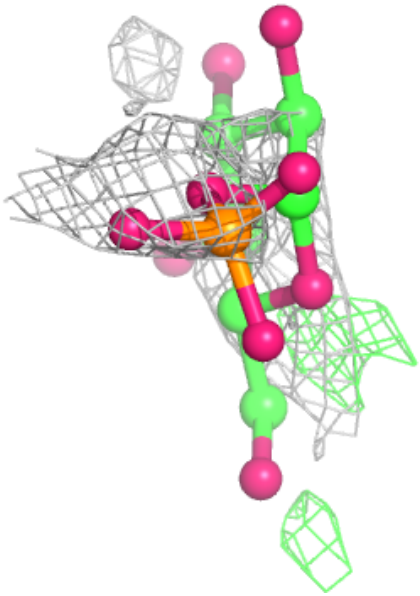


Electron density around G1P A 1290:

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

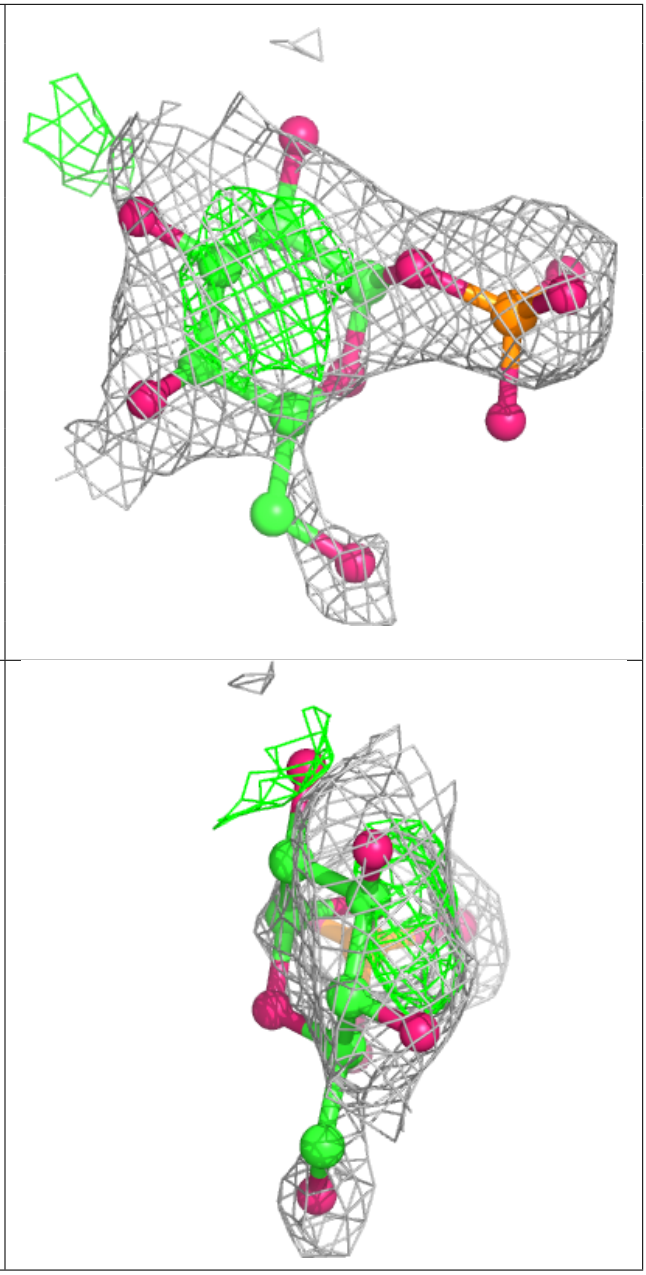


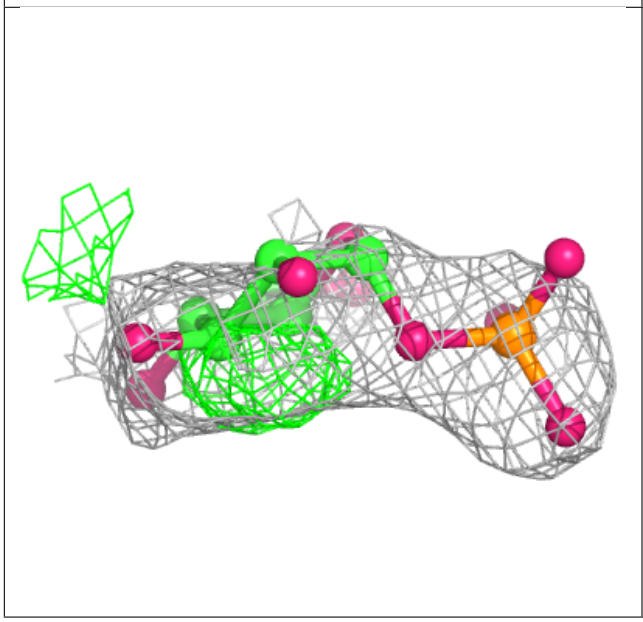




Electron density around G1P C 1290:

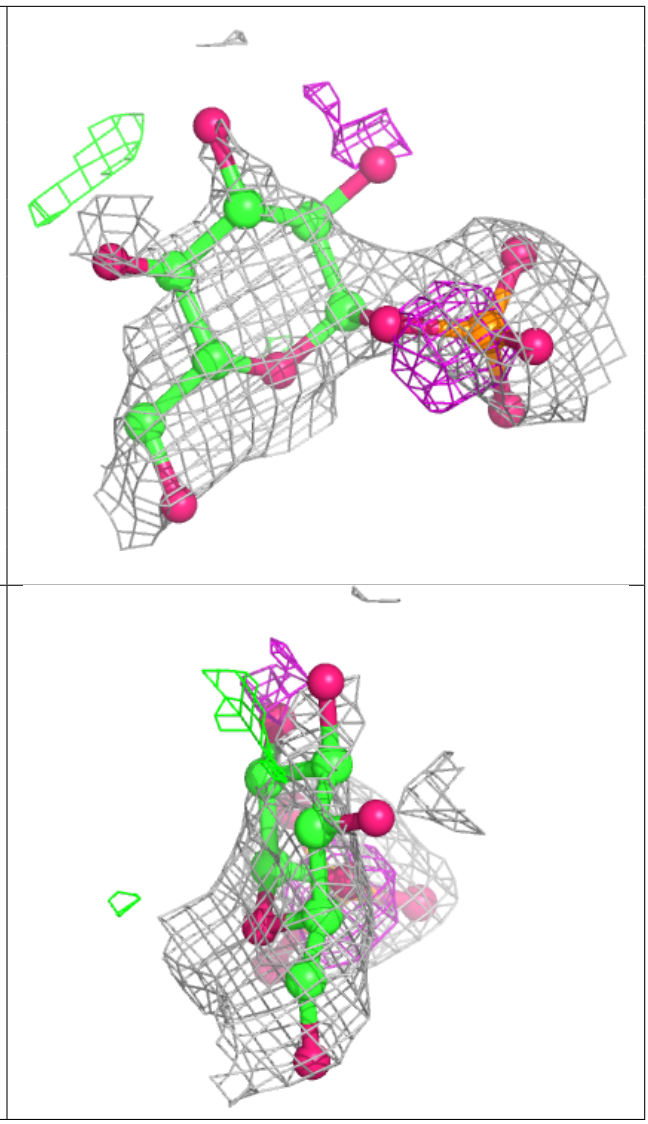
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





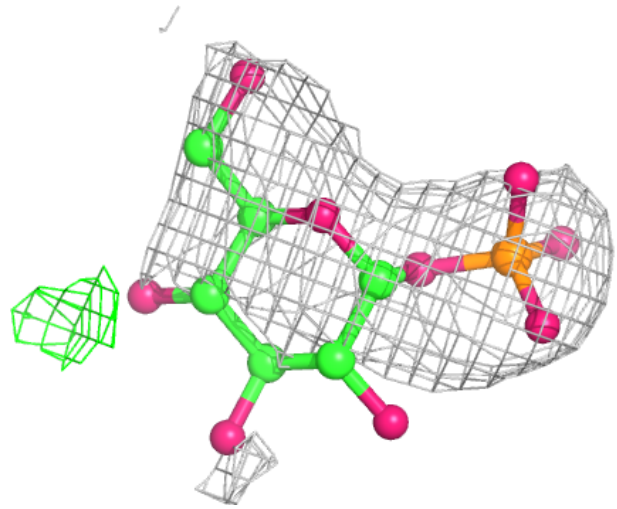
Electron density around G1P G 1290:

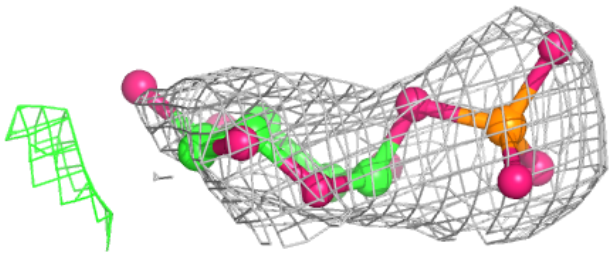
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

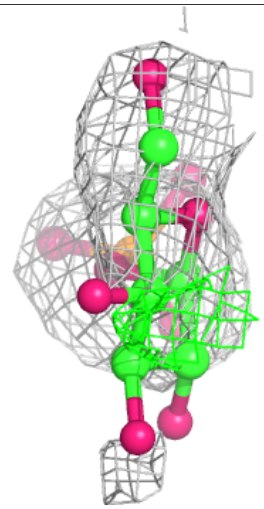


Electron density around G1P F 1290:

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

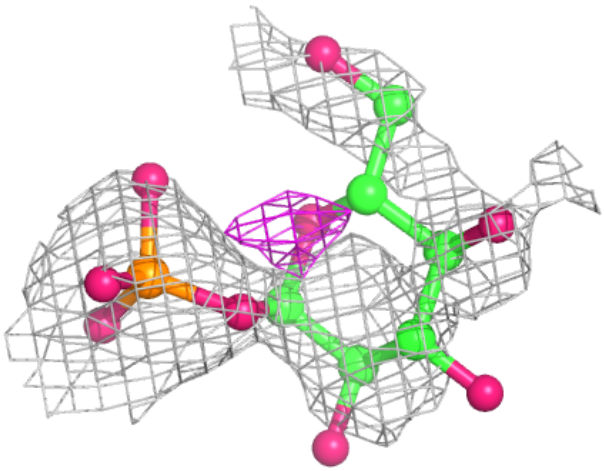


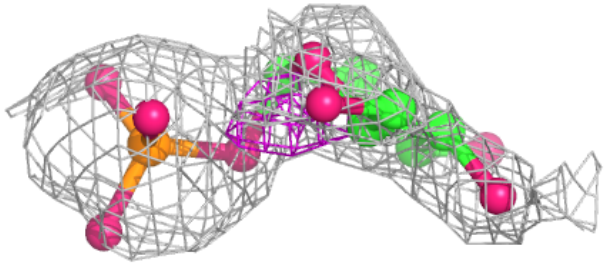


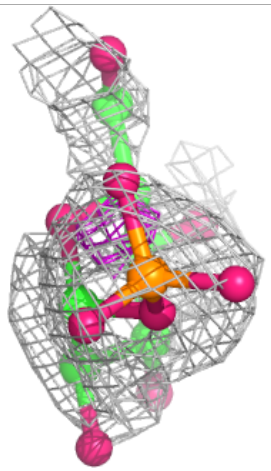


Electron density around G1P B 1290:

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

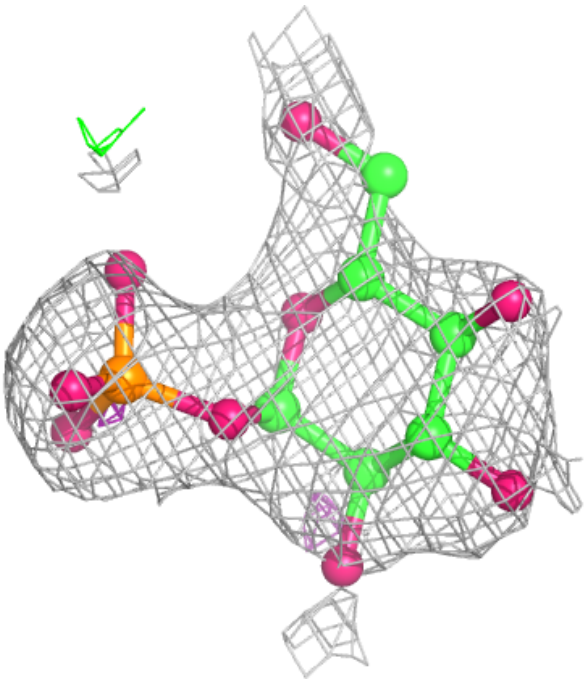


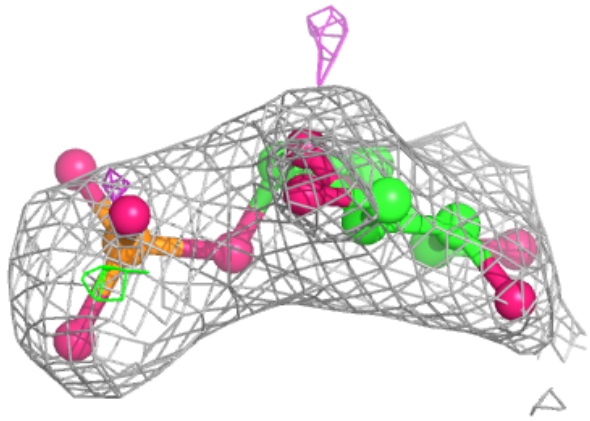


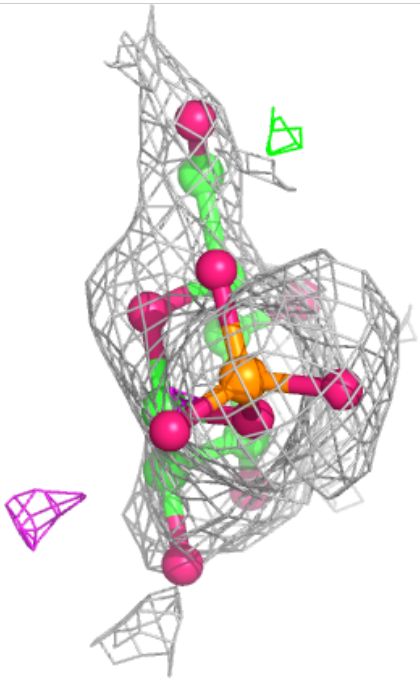


Electron density around G1P D 1290:

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

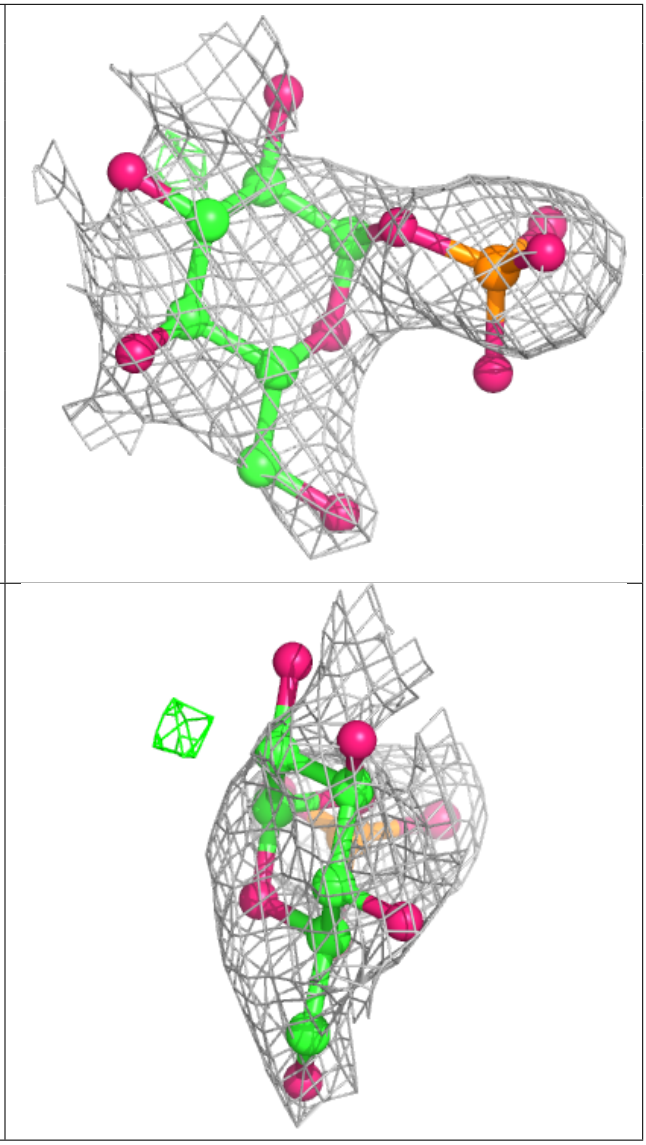






Electron density around G1P E 1290:

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



6.5 Other polymers (i)

There are no such residues in this entry.