



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:00 AM UTC

PDB ID : 2UX8 / pdb_00002ux8
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 ⓘ symbol.

The types of validation reports are described at

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

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

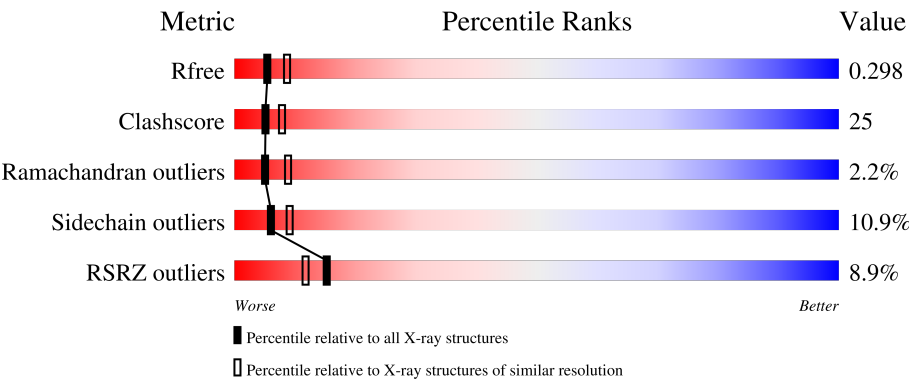
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	297	12% 48% 31% 6% 14%
1	B	297	7% 57% 28% 9% 6%
1	C	297	8% 53% 33% 8% 5%
1	D	297	10% 59% 28% 7% 5%

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Mol	Chain	Length	Quality of chain
1	E	297	7% 55% 32% • • 6%
1	F	297	8% 55% 32% 7% • 5%
1	G	297	7% 51% 38% 8% • •
1	H	297	7% 51% 23% 8% • 18%

2 Entry composition

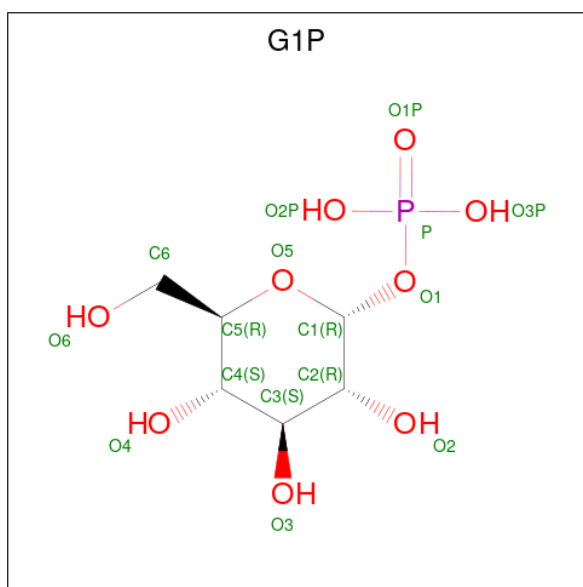
There are 3 unique types of molecules in this entry. The entry contains 16948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is 1-O-phosphono-alpha-D-glucopyranose (CCD ID: G1P) (formula: C₆H₁₃O₉P).



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

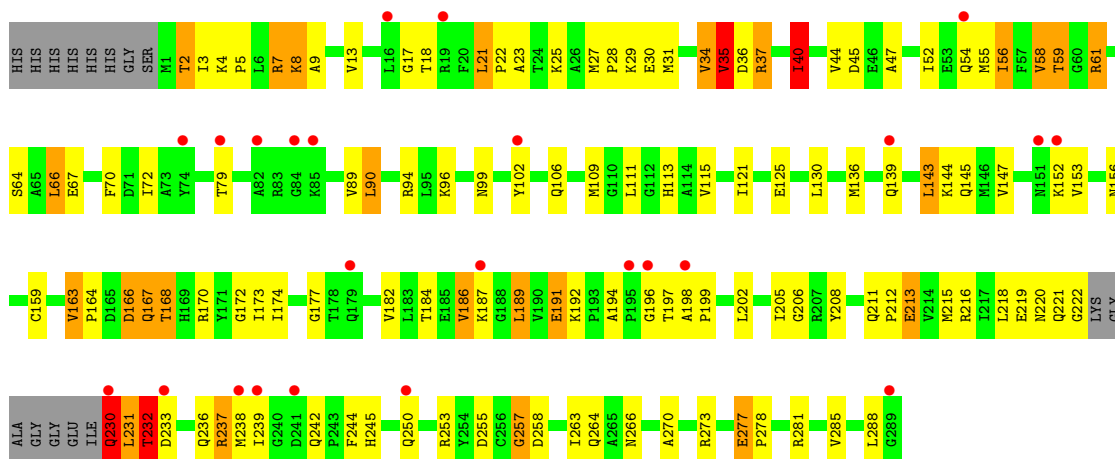
- Molecule 3 is water.

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

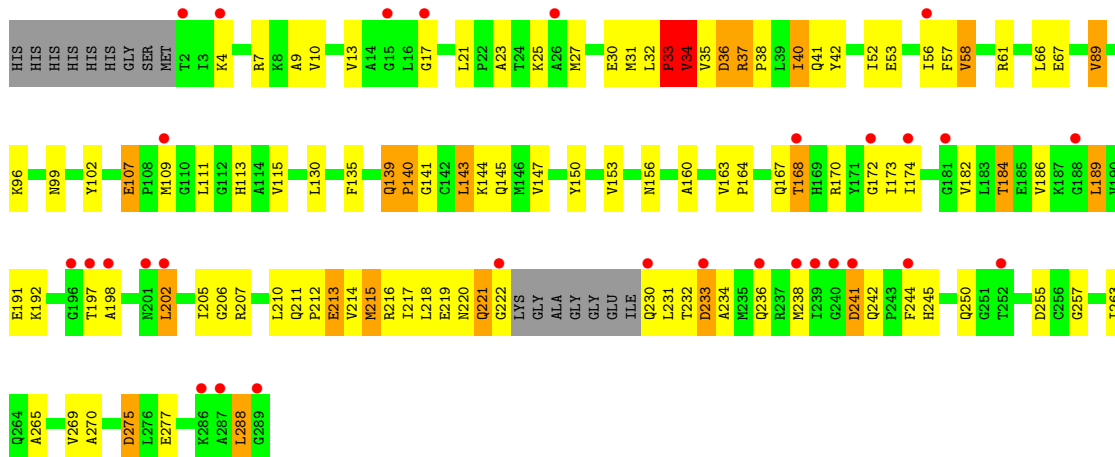
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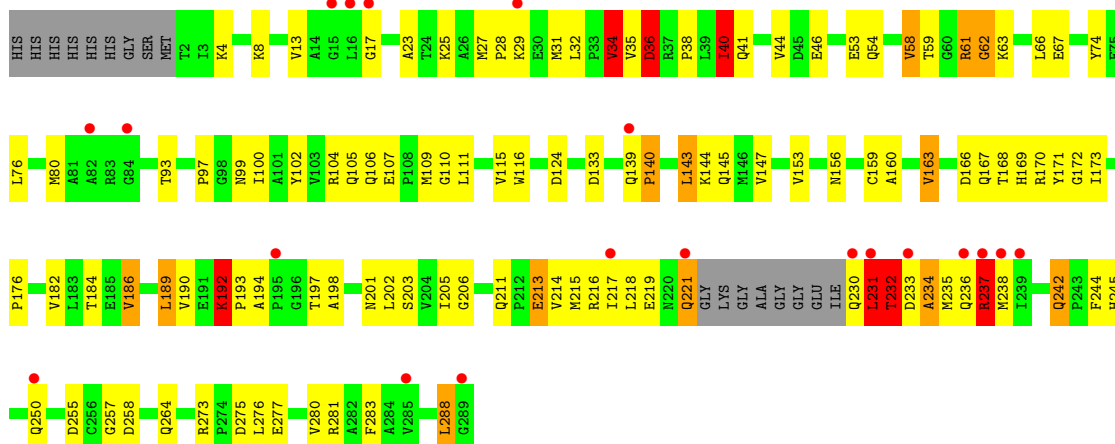
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	26	Total 26	O 26	0	0
3	F	12	Total 12	O 12	0	0
3	G	19	Total 19	O 19	0	0
3	H	20	Total 20	O 20	0	0



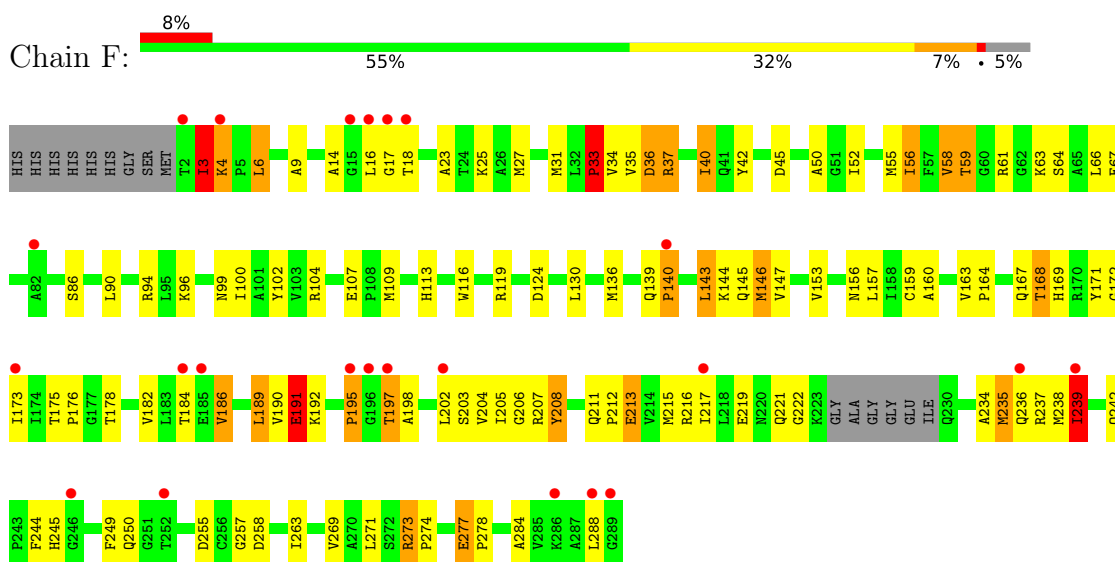
• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE



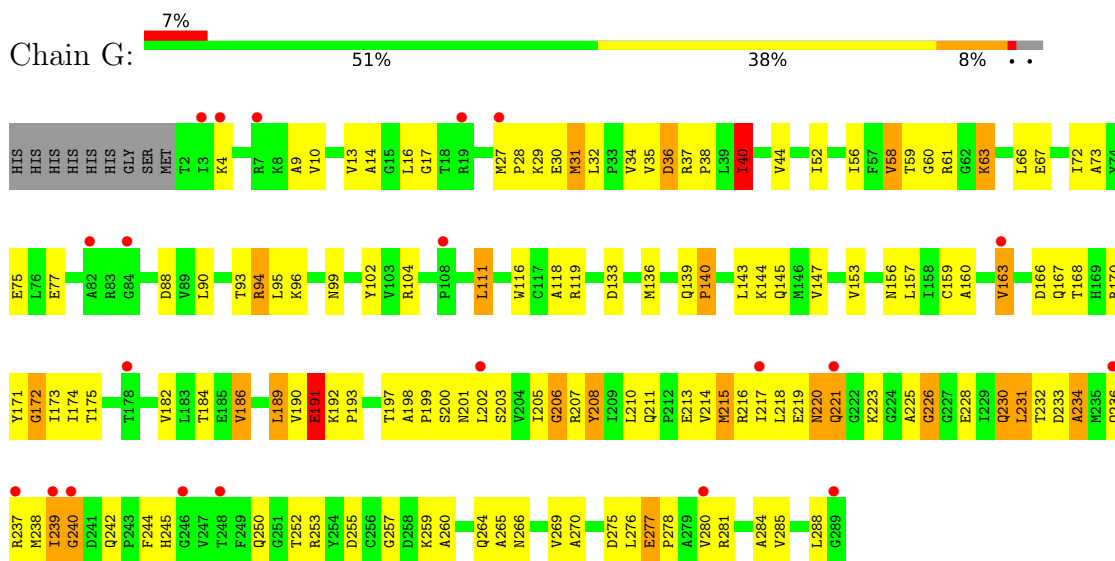
• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE



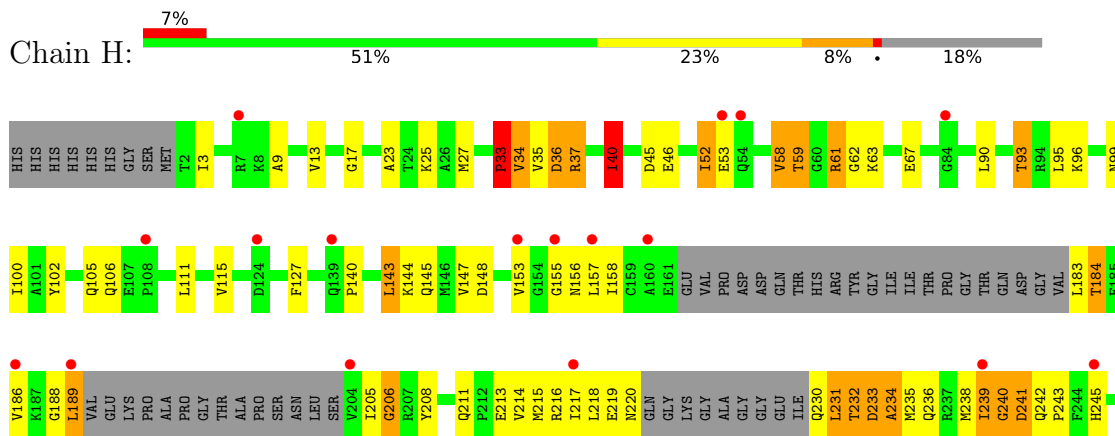
• Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE



- Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLYLTRANSFERASE



- Molecule 1: GLUCOSE-1-PHOSPHATE URIDYLTRANSFERASE





4 Data and refinement statistics

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 74.90 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.90-2.65) 99.7 (74.90-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.295 0.242 , 0.298	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)	0.35 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	2/1974 (0.1%)	1.07	11/2670 (0.4%)
1	B	0.55	0/2168	1.05	13/2939 (0.4%)
1	C	0.59	1/2187 (0.0%)	1.10	16/2964 (0.5%)
1	D	0.62	5/2177 (0.2%)	1.04	9/2951 (0.3%)
1	E	0.78	10/2173 (0.5%)	1.14	17/2946 (0.6%)
1	F	0.71	6/2186 (0.3%)	1.14	19/2962 (0.6%)
1	G	0.59	2/2217 (0.1%)	1.11	15/3005 (0.5%)
1	H	0.73	6/1899 (0.3%)	1.11	17/2565 (0.7%)
All	All	0.65	32/16981 (0.2%)	1.09	117/23002 (0.5%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	VAL	CA-CB	10.19	1.68	1.54
1	H	240	GLY	C-O	-9.02	1.11	1.23
1	F	36	ASP	CA-C	7.98	1.62	1.52
1	E	99	ASN	C-O	-7.62	1.14	1.24
1	C	34	VAL	C-O	-7.39	1.15	1.24
1	H	61	ARG	C-O	-7.16	1.16	1.23
1	G	191	GLU	C-O	-6.47	1.15	1.24
1	E	234	ALA	CA-C	-6.42	1.46	1.52
1	E	231	LEU	C-O	6.30	1.31	1.24
1	D	35	VAL	CA-CB	6.27	1.62	1.54
1	H	35	VAL	CA-CB	6.22	1.62	1.54
1	H	34	VAL	C-O	-6.22	1.14	1.23
1	A	233	ASP	N-CA	-6.09	1.38	1.46
1	G	239	ILE	C-O	-6.08	1.16	1.24
1	E	232	THR	CA-CB	6.05	1.63	1.53
1	E	288	LEU	C-O	-6.04	1.16	1.24
1	F	195	PRO	C-O	-5.96	1.16	1.24
1	D	37	ARG	CA-C	-5.76	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	33	PRO	CB-CG	5.58	1.77	1.49
1	D	33	PRO	CB-CG	5.57	1.77	1.49
1	F	35	VAL	C-O	-5.53	1.17	1.24
1	E	221	GLN	CB-CG	-5.51	1.35	1.52
1	H	33	PRO	CB-CG	5.49	1.77	1.49
1	H	36	ASP	N-CA	5.39	1.53	1.46
1	F	191	GLU	C-O	-5.39	1.17	1.24
1	E	61	ARG	C-O	-5.25	1.17	1.24
1	A	233	ASP	CA-C	5.25	1.59	1.53
1	E	231	LEU	N-CA	5.09	1.52	1.46
1	D	34	VAL	C-O	-5.07	1.18	1.24
1	E	235	MET	SD-CE	-5.05	1.67	1.79
1	D	33	PRO	CA-C	5.05	1.57	1.52
1	E	230	GLN	C-O	5.04	1.33	1.23

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	THR	N-CA-C	-14.68	95.82	113.88
1	E	234	ALA	N-CA-C	-13.46	95.02	112.93
1	D	36	ASP	N-CA-C	12.93	130.07	114.04
1	C	231	LEU	N-CA-C	12.48	124.62	111.14
1	F	36	ASP	N-CA-C	11.56	128.12	113.55
1	H	36	ASP	N-CA-C	11.25	127.72	113.55
1	A	235	MET	N-CA-C	-10.96	99.11	111.82
1	F	36	ASP	N-CA-CB	-9.81	96.18	110.40
1	G	234	ALA	N-CA-C	-9.63	101.30	113.43
1	G	61	ARG	N-CA-C	9.40	121.47	111.03
1	A	232	THR	CA-C-N	-9.23	107.50	122.26
1	A	232	THR	C-N-CA	-9.23	107.50	122.26
1	F	3	ILE	N-CA-C	-9.13	90.34	109.34
1	B	124	ASP	N-CA-C	-8.97	94.57	109.46
1	A	233	ASP	CB-CA-C	8.65	125.68	111.83
1	A	61	ARG	N-CA-C	8.56	120.53	111.03
1	F	61	ARG	N-CA-C	7.84	119.73	111.03
1	F	36	ASP	CA-C-O	7.70	128.53	119.67
1	C	7	ARG	N-CA-C	-7.66	103.25	112.59
1	G	36	ASP	N-CA-CB	-7.54	99.26	111.18
1	B	61	ARG	N-CA-C	7.35	119.19	111.03
1	H	234	ALA	N-CA-C	-7.34	104.85	113.88
1	G	4	LYS	N-CA-C	-7.33	94.30	108.45
1	E	172	GLY	N-CA-C	-7.18	98.91	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	230	GLN	CA-C-N	6.93	134.78	121.54
1	E	230	GLN	C-N-CA	6.93	134.78	121.54
1	H	240	GLY	N-CA-C	-6.90	96.82	113.18
1	D	61	ARG	N-CA-C	6.84	120.07	111.24
1	C	59	THR	N-CA-C	6.81	120.46	110.17
1	H	241	ASP	N-CA-C	6.78	125.24	110.80
1	E	34	VAL	N-CA-C	-6.72	97.06	106.53
1	B	172	GLY	N-CA-C	-6.67	99.82	111.62
1	H	40	ILE	CB-CA-C	-6.60	103.23	112.14
1	B	257	GLY	N-CA-C	-6.59	106.49	114.66
1	E	237	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	D	34	VAL	CA-C-N	6.52	133.71	121.97
1	D	34	VAL	C-N-CA	6.52	133.71	121.97
1	C	61	ARG	N-CA-C	6.52	119.64	111.24
1	C	172	GLY	N-CA-C	-6.42	100.26	111.62
1	G	240	GLY	N-CA-C	-6.33	98.17	113.18
1	E	231	LEU	N-CA-C	6.25	124.11	110.80
1	F	172	GLY	N-CA-C	-6.24	99.15	111.31
1	E	36	ASP	N-CA-C	6.22	121.76	114.04
1	F	221	GLN	N-CA-C	-6.17	104.67	111.82
1	A	63	LYS	N-CA-C	6.13	120.07	111.30
1	G	172	GLY	N-CA-C	-6.09	99.43	111.31
1	D	172	GLY	N-CA-C	-6.06	99.50	111.31
1	G	259	LYS	N-CA-C	6.03	118.34	111.11
1	F	273	ARG	CA-C-N	6.02	125.50	119.24
1	F	273	ARG	C-N-CA	6.02	125.50	119.24
1	C	8	LYS	N-CA-C	6.00	119.27	109.06
1	F	35	VAL	CB-CA-C	-5.98	101.48	111.29
1	E	237	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	G	111	LEU	N-CA-C	5.94	117.76	111.28
1	A	174	ILE	N-CA-C	5.91	118.70	108.95
1	F	198	ALA	CA-C-N	5.90	125.77	119.28
1	F	198	ALA	C-N-CA	5.90	125.77	119.28
1	B	59	THR	N-CA-C	5.89	119.06	110.17
1	F	239	ILE	N-CA-C	5.87	117.40	111.00
1	F	59	THR	N-CA-C	5.86	119.02	110.17
1	H	231	LEU	N-CA-C	5.83	118.14	111.02
1	G	231	LEU	N-CA-C	5.80	118.07	111.11
1	C	35	VAL	N-CA-C	-5.80	97.28	109.34
1	F	4	LYS	N-CA-C	5.79	117.19	109.83
1	H	35	VAL	CA-C-O	5.74	127.95	120.78
1	B	236	GLN	N-CA-C	5.72	119.44	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	36	ASP	CA-C-O	5.72	126.25	119.67
1	G	63	LYS	N-CA-C	5.71	120.61	111.81
1	C	230	GLN	CA-C-N	5.69	128.18	120.44
1	C	230	GLN	C-N-CA	5.69	128.18	120.44
1	D	36	ASP	CA-C-O	5.67	126.14	119.06
1	E	231	LEU	O-C-N	-5.66	115.06	122.59
1	F	35	VAL	CA-C-O	5.61	127.79	120.78
1	C	111	LEU	N-CA-C	5.59	117.05	111.07
1	G	191	GLU	CA-C-N	-5.58	115.26	123.30
1	G	191	GLU	C-N-CA	-5.58	115.26	123.30
1	E	192	LYS	CB-CA-C	-5.58	107.24	111.20
1	E	40	ILE	CB-CA-C	-5.56	104.64	112.14
1	H	59	THR	N-CA-C	5.56	118.56	110.17
1	E	111	LEU	N-CA-C	5.55	117.01	111.07
1	E	232	THR	N-CA-CB	5.55	119.16	109.72
1	H	35	VAL	CB-CA-C	-5.53	102.22	111.29
1	G	40	ILE	CB-CA-C	-5.42	103.76	112.16
1	G	220	ASN	N-CA-CB	-5.42	107.99	114.17
1	H	288	LEU	N-CA-C	5.42	119.20	112.59
1	C	257	GLY	N-CA-C	-5.38	107.98	114.66
1	D	36	ASP	CB-CA-C	-5.34	99.64	109.15
1	B	198	ALA	CA-C-N	5.32	124.98	119.56
1	B	198	ALA	C-N-CA	5.32	124.98	119.56
1	A	259	LYS	N-CA-C	5.27	117.71	111.33
1	B	110	GLY	N-CA-C	5.27	119.55	112.17
1	A	40	ILE	CB-CA-C	-5.25	104.02	112.16
1	H	240	GLY	O-C-N	-5.23	115.90	122.70
1	B	176	PRO	N-CA-C	5.21	119.66	111.38
1	C	40	ILE	CB-CA-C	-5.20	104.10	112.16
1	F	176	PRO	N-CA-C	5.19	119.62	111.38
1	B	175	THR	CA-C-N	5.18	125.08	119.85
1	B	175	THR	C-N-CA	5.18	125.08	119.85
1	C	232	THR	CB-CA-C	-5.18	102.68	110.92
1	H	111	LEU	N-CA-C	5.18	116.61	111.07
1	D	168	THR	N-CA-C	5.18	117.66	111.71
1	C	168	THR	N-CA-C	5.16	118.36	111.75
1	E	110	GLY	N-CA-C	5.15	118.56	112.33
1	H	45	ASP	N-CA-C	-5.14	105.67	111.28
1	A	233	ASP	CA-C-O	5.13	128.62	122.41
1	H	287	ALA	CA-C-N	-5.13	114.52	122.67
1	H	287	ALA	C-N-CA	-5.13	114.52	122.67
1	E	176	PRO	N-CA-C	5.08	119.46	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	ARG	CA-C-N	5.06	126.16	119.84
1	C	273	ARG	C-N-CA	5.06	126.16	119.84
1	F	175	THR	CA-C-N	5.06	124.96	119.85
1	F	175	THR	C-N-CA	5.06	124.96	119.85
1	E	99	ASN	N-CA-C	5.05	119.29	113.18
1	H	259	LYS	N-CA-C	5.04	117.42	111.33
1	A	142	CYS	N-CA-C	5.03	119.61	111.37
1	G	175	THR	N-CA-C	-5.01	98.78	108.59
1	D	139	GLN	N-CA-C	5.00	112.72	108.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1940	0	1955	119	0
1	B	2126	0	2135	120	0
1	C	2145	0	2160	117	0
1	D	2135	0	2143	116	0
1	E	2131	0	2140	116	0
1	F	2144	0	2156	107	0
1	G	2174	0	2182	123	0
1	H	1866	0	1887	99	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	2	0
3	B	23	0	0	1	0
3	C	30	0	0	2	0
3	D	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	829	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 25.

All (829) 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
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:E:27:MET:HE2	1:H:27:MET:HE3	1.39	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:H:238:MET:HE3	1:H:242:GLN:HE21	1.28	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: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: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:C:47:ALA:HB3	1:C:55:MET:HE1	1.52	0.90
1:G:94:ARG:HG2	1:G:94:ARG:NH1	1.82	0.90
1:B:213:GLU:HB2	1:B:238:MET:HE1	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:236:GLN:C	1:B:238:MET:H	1.77	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:139:GLN:HA	1:G:140:PRO:C	1.99	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:D:107:GLU:HG3	1:D:109:MET:HE2	1.56	0.87
1:E:231:LEU:O	1:E:232:THR:C	2.16	0.86
1:D:139:GLN:HA	1:D:140:PRO:C	1.99	0.86
1:E:139:GLN:HA	1:E:140:PRO:C	2.00	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
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:F:27:MET:HE1	1:G:31:MET:HB3	1.57	0.85
1:G:214:VAL:HG23	1:G:238:MET:HE2	1.59	0.84
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: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:A:221:GLN:CD	1:A:231:LEU:HD13	2.04	0.82
1:B:145:GLN:HE22	1:B:250:GLN:H	1.26	0.82
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:G:116:TRP:HA	1:G:215:MET:HE1	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:230:GLN:HG2	1:H:233:ASP:CG	2.07	0.79
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:B:116:TRP:HA	1:B:215:MET:HE1	1.62	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:F:139:GLN:HA	1:F:140:PRO:C	2.08	0.78
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: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: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:C:215:MET:HE2	1:C:215:MET:HA	1.65	0.77
1:B:6:LEU:O	1:B:7:ARG:HG2	1.85	0.76
1:A:93:THR:HG21	1:C:25:LYS:HZ2	1.49	0.76
1:F:236:GLN:C	1:F:238:MET:H	1.92	0.76
1:C:67:GLU:HG3	1:C:102:TYR:CZ	2.21	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:C:215:MET:HE2	1:C:218:LEU:HD12	1.66	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:D:115:VAL:HG12	1:D:215:MET:HE3	1.69	0.75
1:E:167:GLN:NE2	1:E:170:ARG:HH11	1.81	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:B:213:GLU:CB	1:B:238:MET:HE1	2.16	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:215:MET:HE2	1:D:218:LEU:HD12	1.70	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:E:25:LYS:HZ2	1:H:93:THR:HG23	1.56	0.71
1:G:29:LYS:HE2	1:G:133:ASP:OD1	1.91	0.71
1:D:115:VAL:HG12	1:D:215:MET:CE	2.21	0.71
1:H:215:MET:HE2	1:H:215:MET:HA	1.72	0.70
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
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:H:215:MET:HE2	1:H:218:LEU:HD12	1.73	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:F:27:MET:HE2	1:G:31:MET:HB3	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:236:GLN:C	1:B:238:MET:N	2.47	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: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:D:144:LYS:O	1:D:147:VAL:HG12	1.94	0.67
1:E:115:VAL:HG12	1:E:215:MET:HE3	1.77	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:A:236:GLN:C	1:A:238:MET:H	2.02	0.67
1:G:35:VAL:HG12	1:G:36:ASP:HB2	1.75	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:G:214:VAL:CG2	1:G:238:MET:HE2	2.24	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
1:C:56:ILE:HG13	1:C:56:ILE:O	1.95	0.66
1:H:115:VAL:HG12	1:H:215:MET:CE	2.25	0.65
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:B:238:MET:HE3	1:B:242:GLN:NE2	2.11	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:H:239:ILE:C	1:H:240:GLY:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:270:ALA:HB2	1:D:263:ILE:HD13	1.80	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:93:THR:CG2	1:D:25:LYS:HZ3	2.11	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:B:213:GLU:CG	1:B:238:MET:HE1	2.28	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:220:ASN:C	1:C:222:GLY:H	2.07	0.62
1:F:156:ASN:C	1:F:157:LEU:HD12	2.25	0.62
1:C:189:LEU:HD23	1:C:236:GLN:NE2	2.15	0.62
1:H:115:VAL:HG12	1:H:215:MET:HE1	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:ASP:C	1:H:257:GLY:H	2.08	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:A:112:GLY:C	1:A:231:LEU:HD23	2.26	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:F:236:GLN:C	1:F:238:MET:N	2.59	0.60
1:G:172:GLY:HA2	1:G:191:GLU:O	2.01	0.60
1:G:215:MET:HE3	1:G:218:LEU:HD12	1.83	0.60
1:E:104:ARG:HD3	3:F:2003:HOH:O	2.02	0.60
1:H:236:GLN:C	1:H:238:MET:H	2.09	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: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:G:236:GLN:C	1:G:238:MET:H	2.10	0.60
1:H:13:VAL:CG2	1:H:59:THR:HG22	2.31	0.60
1:A:215:MET:HE2	1:A:218:LEU:HD12	1.83	0.59
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:115:VAL:HG12	1:C:215:MET:HE3	1.84	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:E:25:LYS:HZ2	1:H:93:THR:CG2	2.15	0.59
1:E:215:MET:HE2	1:E:218:LEU:HD12	1.83	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:E:93:THR:HG22	1:H:25:LYS:HZ3	1.67	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
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:A:115:VAL:HG12	1:A:215:MET:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:TYR:HE2	1:F:235:MET:HE1	1.69	0.58
1:A:213:GLU:HB2	1:A:238:MET:HE1	1.83	0.58
1:B:31:MET:O	1:D:27:MET:HE1	2.03	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:93:THR:HG22	1:D:25:LYS:HZ3	1.68	0.58
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:139:GLN:HA	1:B:140:PRO:C	2.29	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:E:221:GLN:CD	1:E:237:ARG:HH12	2.11	0.57
1:E:97:PRO:O	1:F:119:ARG:NH2	2.37	0.57
1:F:27:MET:HE2	1:G:27:MET:SD	2.44	0.57
1:B:168:THR:HG23	1:B:173:ILE:HG13	1.85	0.57
1:H:238:MET:HE3	1:H:242:GLN:NE2	2.10	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:A:255:ASP:C	1:A:257:GLY:H	2.13	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:F:146:MET:HE1	1:F:207:ARG:O	2.05	0.56
1:A:211:GLN:NE2	1:A:212:PRO:HD2	2.20	0.56
1:B:27:MET:HE1	1:D:27:MET:HG3	1.86	0.56
1:D:255:ASP:C	1:D:257:GLY:H	2.13	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: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:93:THR:CG2	1:C:25:LYS:HZ2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLU:H	1:B:212:PRO:HB3	1.71	0.56
1:B:215:MET:HA	1:B:215:MET:HE2	1.88	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
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: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:E:107:GLU:OE2	1:E:109:MET:HE2	2.05	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:B:107:GLU:HB2	1:B:109:MET:HE2	1.89	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:80:MET:HE3	1:A:87:LEU:HD23	1.88	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:B:93:THR:HG21	1:D:25:LYS:HZ2	1.71	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: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:D:236:GLN:C	1:D:238:MET:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:THR:O	1:C:199:PRO:HD3	2.07	0.54
1:E:93:THR:CG2	1:H:25:LYS:HZ3	2.21	0.54
1:F:208:TYR:CE2	1:F:235:MET:HE1	2.43	0.54
1:G:58:VAL:HG22	1:G:58:VAL:O	2.08	0.54
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:F:109:MET:HE3	1:F:113:HIS:CE1	2.43	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:F:3:ILE:HG13	1:F:3:ILE:O	2.01	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: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: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: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:B:56:ILE:HD11	1:B:121:ILE:HD12	1.91	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:F:25:LYS:HZ3	1:G:93:THR:HG22	1.72	0.52
1:H:236:GLN:C	1:H:238:MET:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:MET:O	1:E:219:GLU:HG3	2.10	0.52
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:H:232:THR:C	1:H:234:ALA:H	2.18	0.52
1:F:255:ASP:C	1:F:257:GLY:H	2.17	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:C:47:ALA:CB	1:C:55:MET:HE1	2.35	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:34:VAL:O	1:G:35:VAL:HB	2.08	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: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:A:236:GLN:C	1:A:238:MET:N	2.64	0.51
1:C:13:VAL:HG12	1:C:30:GLU:HG2	1.93	0.51
1:E:25:LYS:HZ1	1:H:93:THR:CG2	2.22	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: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:E:238:MET:HE3	1:E:242:GLN:NE2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:238:MET:HE3	1:B:242:GLN:HE22	1.74	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:C:236:GLN:C	1:C:238:MET:H	2.19	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:E:236:GLN:C	1:E:238:MET:H	2.19	0.50
1:G:35:VAL:N	1:G:266:ASN:OD1	2.45	0.49
1:C:255:ASP:C	1:C:257:GLY:H	2.20	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: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:G:13:VAL:HG12	1:G:30:GLU:HG2	1.94	0.49
1:H:233:ASP:OD1	1:H:233:ASP:C	2.54	0.49
1:C:29:LYS:NZ	3:C:2007:HOH:O	2.45	0.49
1:F:116:TRP:HA	1:F:215:MET:HE2	1.93	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:C:109:MET:HE3	1:C:113:HIS:CE1	2.48	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: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:C:197:THR:O	1:C:197:THR:OG1	2.31	0.49
1:D:139:GLN:CA	1:D:140:PRO:C	2.78	0.48
1:D:220:ASN:C	1:D:222:GLY:H	2.20	0.48
1:D:238:MET:HE3	1:D:242:GLN:NE2	2.28	0.48
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: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: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:D:215:MET:HE2	1:D:215:MET:HA	1.95	0.48
1:E:36:ASP:HB2	1:E:273:ARG:NH2	2.28	0.48
1:E:255:ASP:C	1:E:257:GLY:H	2.21	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: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: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:H:255:ASP:C	1:H:257:GLY:N	2.72	0.48
1:C:27:MET:HE3	1:C:28:PRO:HD2	1.96	0.48
1:D:130:LEU:N	1:D:130:LEU:HD12	2.29	0.48
1:G:139:GLN:CA	1:G:140:PRO:C	2.81	0.48
1:H:115:VAL:HG12	1:H:215:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ASN:O	1:G:221:GLN:C	2.57	0.48
1:A:49:GLU:CD	1:A:140:PRO:O	2.57	0.48
1:B:90:LEU:O	1:B:93:THR:HB	2.13	0.48
1:G:236:GLN:C	1:G:238:MET:N	2.71	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:H:215:MET:CE	1:H:218:LEU:HD12	2.43	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:C:220:ASN:C	1:C:222:GLY:N	2.69	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:E:23:ALA:HB2	1:H:36:ASP:C	2.39	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:G:255:ASP:C	1:G:257:GLY:H	2.20	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: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:F:25:LYS:HZ2	1:G:93:THR:HG22	1.79	0.47
1:G:163:VAL:HG13	1:G:167:GLN:HB3	1.97	0.47
1:A:107:GLU:OE1	1:A:109:MET:HE2	2.15	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:H:156:ASN:C	1:H:157:LEU:HD12	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:36:ASP:CG	1:F:273:ARG:HH12	2.23	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
1:E:153:VAL:HG11	1:E:245:HIS:HE2	1.81	0.46
1:E:231:LEU:O	1:E:232:THR:O	2.32	0.46
1:F:107:GLU:HB2	1:F:109:MET:HE2	1.98	0.46
1:B:115:VAL:HG12	1:B:215:MET:HE3	1.98	0.46
1:A:19:ARG:O	1:A:259:LYS:HE3	2.16	0.46
1:B:215:MET:HE3	1:B:218:LEU:HD12	1.97	0.46
1:C:34:VAL:O	1:C:266:ASN:OD1	2.34	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:B:23:ALA:HB2	1:D:36:ASP:C	2.41	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:E:236:GLN:C	1:E:238:MET:N	2.75	0.45
1:C:115:VAL:HG12	1:C:215:MET:HE1	1.97	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:D:231:LEU:O	1:D:232:THR:C	2.59	0.45
1:F:25:LYS:HZ3	1:G:93:THR:CG2	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:D:255:ASP:C	1:D:257:GLY:N	2.74	0.45
1:E:115:VAL:HG12	1:E:215:MET:HE1	1.99	0.45
1:G:216:ARG:HD2	1:G:216:ARG:N	2.31	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:E:215:MET:HE2	1:E:215:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ASP:HA	1:H:236:GLN:HG2	1.96	0.45
1:A:255:ASP:C	1:A:257:GLY:N	2.75	0.45
1:B:22:PRO:HG3	1:D:89:VAL:O	2.16	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:A:23:ALA:O	1:A:27:MET:HE2	2.17	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
1:E:168:THR:CG2	1:E:198:ALA:HB2	2.37	0.45
1:G:225:ALA:HB3	1:G:228:GLU:CD	2.42	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:D:107:GLU:HG3	1:D:109:MET:CE	2.38	0.44
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:61:ARG:O	1:E:62:GLY:C	2.60	0.44
1:E:105:GLN:O	1:E:106:GLN:HB2	2.17	0.44
1:G:171:TYR:HB3	1:G:203:SER:HB2	2.00	0.44
1:G:238:MET:HE1	1:G:242:GLN:HE22	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:GLN:NE2	1:E:170:ARG:NH1	2.53	0.44
1:F:136:MET:HE3	1:F:249:PHE:CD2	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:E:213:GLU:HB2	1:E:238:MET:CE	2.48	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:D:115:VAL:HG12	1:D:215:MET:HE1	1.98	0.43
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: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
1:C:153:VAL:HG12	1:C:153:VAL:O	2.17	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:H:40:ILE:H	1:H:40:ILE:HG13	1.52	0.43
1:H:188:GLY:C	1:H:189:LEU:HD23	2.43	0.43
1:B:217:ILE:HD11	1:B:237:ARG:NH1	2.33	0.43
1:B:255:ASP:C	1:B:257:GLY:H	2.26	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:A:16:LEU:HD12	1:C:79:THR:HG21	2.01	0.43
1:C:191:GLU:O	1:C:192:LYS:C	2.61	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:231:LEU:C	1:A:231:LEU:HD12	2.43	0.43
1:C:40:ILE:H	1:C:40:ILE:HG13	1.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:PRO:CB	1:G:66:LEU:HD11	2.48	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:C:236:GLN:C	1:C:238:MET:N	2.76	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:H:232:THR:C	1:H:234:ALA:N	2.76	0.43
1:A:277:GLU:HB3	1:A:278:PRO:HD3	2.01	0.42
1:G:167:GLN:HG3	1:G:170:ARG:HD3	2.01	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:H:231:LEU:O	1:H:232:THR:C	2.60	0.42
1:D:109:MET:HE3	1:D:113:HIS:CE1	2.54	0.42
1:G:172:GLY:N	2:G:1290:G1P:H62	2.17	0.42
1:A:27:MET:HE3	1:A:32:LEU:HD21	2.01	0.42
1:A:183:LEU:C	1:A:184:THR:HG22	2.44	0.42
1:D:4:LYS:O	1:D:150:TYR:OH	2.34	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:183:LEU:C	1:H:184:THR:CG2	2.92	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: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:108:PRO:C	3:A:2011:HOH:O	2.62	0.42
1:A:115:VAL:HG12	1:A:215:MET:HE1	2.00	0.42
1:A:218:LEU:HB3	1:A:231:LEU:HD21	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:255:ASP:C	1:F:257:GLY:N	2.78	0.42
1:G:225:ALA:O	1:G:226:GLY:C	2.62	0.42
1:H:67:GLU:HG3	1:H:102:TYR:CE1	2.55	0.42
1:B:36:ASP:C	1:D:23:ALA:HB2	2.45	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
1:C:40:ILE:HD13	1:C:66:LEU:HG	2.02	0.41
1:E:27:MET:HE3	1:E:28:PRO:HD2	2.02	0.41
1:F:27:MET:HE1	1:G:31:MET:O	2.20	0.41
1:F:215:MET:HE3	1:F:215:MET:HA	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:E:29:LYS:HE2	1:E:133:ASP:CG	2.45	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:G:232:THR:C	1:G:234:ALA:H	2.27	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:156:ASN:C	1:G:157:LEU:HD12	2.45	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:D:191:GLU:O	1:D:192:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:ALA:HB2	1:C:36:ASP:C	2.46	0.41
1:A:34:VAL:O	1:A:35:VAL:HB	2.20	0.41
1:A:156:ASN:C	1:A:157:LEU:HD12	2.44	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: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:171:TYR:CB	1:B:203:SER:HB2	2.49	0.41
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:116:TRP:HA	1:E:215:MET:HE1	2.03	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:E:27:MET:CE	1:H:27:MET:HE3	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HH11	1:B:273:ARG:HG2	1.85	0.40
1:D:213:GLU:HG3	1:D:238:MET:HE1	2.03	0.40
1:H:127:PHE:CD2	1:H:127:PHE:N	2.89	0.40
1:A:72:ILE:HG12	1:A:94:ARG:CZ	2.52	0.40
1:A:180:ASP:O	1:A:180:ASP:CG	2.64	0.40
1:D:236:GLN:C	1:D:238:MET:N	2.75	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:HD12	1:G:157:LEU:N	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:A:232:THR:C	1:A:234:ALA:N	2.80	0.40
1:E:38:PRO:HG2	1:E:41:GLN:HB2	2.03	0.40
1:D:189:LEU:CD2	1:D:189:LEU:N	2.84	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
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: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%)	7	12
1	B	276/297 (93%)	252 (91%)	17 (6%)	7 (2%)	4	7
1	C	278/297 (94%)	252 (91%)	20 (7%)	6 (2%)	5	9
1	D	277/297 (93%)	251 (91%)	21 (8%)	5 (2%)	6	11

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

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Mol	Chain	Res	Type
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
1	B	17	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/235 (86%)	182 (90%)	20 (10%)	7	11
1	B	222/235 (94%)	195 (88%)	27 (12%)	5	7
1	C	225/235 (96%)	196 (87%)	29 (13%)	4	6
1	D	223/235 (95%)	204 (92%)	19 (8%)	10	17
1	E	223/235 (95%)	201 (90%)	22 (10%)	7	11
1	F	224/235 (95%)	195 (87%)	29 (13%)	4	6
1	G	225/235 (96%)	201 (89%)	24 (11%)	6	9
1	H	193/235 (82%)	174 (90%)	19 (10%)	7	11
All	All	1737/1880 (92%)	1548 (89%)	189 (11%)	6	9

All (189) 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	139	GLN
1	A	143	LEU
1	A	147	VAL
1	A	175	THR
1	A	176	PRO
1	A	178	THR
1	A	179	GLN
1	A	184	THR
1	A	213	GLU
1	A	232	THR
1	A	233	ASP
1	A	237	ARG
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	66	LEU
1	B	67	GLU
1	B	94	ARG
1	B	121	ILE
1	B	124	ASP
1	B	139	GLN
1	B	143	LEU
1	B	182	VAL
1	B	184	THR
1	B	186	VAL
1	B	189	LEU
1	B	197	THR
1	B	213	GLU
1	B	215	MET
1	B	217	ILE
1	B	231	LEU
1	B	232	THR
1	B	233	ASP
1	B	239	ILE

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Mol	Chain	Res	Type
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	59	THR
1	C	64	SER
1	C	66	LEU
1	C	90	LEU
1	C	121	ILE
1	C	139	GLN
1	C	143	LEU
1	C	163	VAL
1	C	166	ASP
1	C	167	GLN
1	C	182	VAL
1	C	184	THR
1	C	186	VAL
1	C	189	LEU
1	C	191	GLU
1	C	208	TYR
1	C	213	GLU
1	C	230	GLN
1	C	232	THR
1	C	233	ASP
1	C	237	ARG
1	C	242	GLN
1	C	258	ASP
1	C	277	GLU
1	D	21	LEU
1	D	33	PRO
1	D	34	VAL
1	D	40	ILE
1	D	58	VAL
1	D	89	VAL
1	D	107	GLU
1	D	143	LEU
1	D	182	VAL

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Mol	Chain	Res	Type
1	D	184	THR
1	D	189	LEU
1	D	202	LEU
1	D	213	GLU
1	D	215	MET
1	D	233	ASP
1	D	241	ASP
1	D	275	ASP
1	D	277	GLU
1	D	288	LEU
1	E	32	LEU
1	E	34	VAL
1	E	36	ASP
1	E	40	ILE
1	E	53	GLU
1	E	58	VAL
1	E	66	LEU
1	E	100	ILE
1	E	143	LEU
1	E	163	VAL
1	E	166	ASP
1	E	182	VAL
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	258	ASP
1	E	275	ASP
1	E	277	GLU
1	F	3	ILE
1	F	6	LEU
1	F	33	PRO
1	F	37	ARG
1	F	40	ILE
1	F	56	ILE
1	F	58	VAL
1	F	59	THR
1	F	64	SER
1	F	66	LEU

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Mol	Chain	Res	Type
1	F	86	SER
1	F	90	LEU
1	F	143	LEU
1	F	146	MET
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	191	GLU
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	258	ASP
1	F	277	GLU
1	G	16	LEU
1	G	31	MET
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	143	LEU
1	G	163	VAL
1	G	166	ASP
1	G	182	VAL
1	G	184	THR
1	G	186	VAL
1	G	189	LEU
1	G	191	GLU
1	G	192	LYS
1	G	208	TYR
1	G	213	GLU
1	G	215	MET
1	G	223	LYS
1	G	230	GLN
1	G	275	ASP

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Mol	Chain	Res	Type
1	G	277	GLU
1	H	33	PRO
1	H	37	ARG
1	H	40	ILE
1	H	52	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	208	TYR
1	H	213	GLU
1	H	232	THR
1	H	239	ILE
1	H	258	ASP
1	H	277	GLU
1	H	281	ARG
1	H	285	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	145	GLN
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	169	HIS
1	B	211	GLN
1	B	220	ASN
1	B	242	GLN
1	B	245	HIS
1	C	113	HIS
1	C	145	GLN

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Mol	Chain	Res	Type
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	169	HIS
1	D	211	GLN
1	D	221	GLN
1	D	242	GLN
1	E	105	GLN
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	F	41	GLN
1	F	99	ASN
1	F	113	HIS
1	F	145	GLN
1	F	211	GLN
1	F	230	GLN
1	F	245	HIS
1	F	250	GLN
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	211	GLN
1	H	236	GLN
1	H	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	1290	-	15,16,16	1.31	2 (13%)	24,24,24	1.39	1 (4%)
2	G1P	D	1290	-	15,16,16	1.12	1 (6%)	24,24,24	1.29	1 (4%)
2	G1P	C	1290	-	15,16,16	1.05	0	24,24,24	1.24	1 (4%)
2	G1P	E	1290	-	15,16,16	1.15	1 (6%)	24,24,24	1.22	1 (4%)
2	G1P	F	1290	-	15,16,16	1.14	0	24,24,24	1.55	2 (8%)
2	G1P	B	1290	-	15,16,16	1.20	2 (13%)	24,24,24	1.27	1 (4%)
2	G1P	A	1290	-	15,16,16	1.13	1 (6%)	24,24,24	1.37	1 (4%)
2	G1P	H	1290	-	15,16,16	1.14	1 (6%)	24,24,24	1.44	1 (4%)

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	G	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	D	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	C	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	E	1290	-	-	1/7/27/27	0/1/1/1
2	G1P	F	1290	-	-	0/7/27/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G1P	B	1290	-	-	0/7/27/27	0/1/1/1
2	G1P	A	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	3.01	1.64	1.59
2	E	1290	G1P	P-O1	2.34	1.63	1.59
2	G	1290	G1P	P-O3P	2.20	1.63	1.54
2	B	1290	G1P	O5-C1	2.14	1.47	1.41
2	A	1290	G1P	O5-C1	2.12	1.47	1.41
2	B	1290	G1P	P-O3P	2.11	1.62	1.54
2	D	1290	G1P	P-O1	2.08	1.63	1.59
2	H	1290	G1P	P-O1	2.05	1.63	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1290	G1P	P-O1-C1	-6.23	106.84	123.54
2	H	1290	G1P	P-O1-C1	-5.79	108.00	123.54
2	A	1290	G1P	P-O1-C1	-5.62	108.46	123.54
2	G	1290	G1P	P-O1-C1	-5.50	108.78	123.54
2	D	1290	G1P	P-O1-C1	-5.12	109.81	123.54
2	B	1290	G1P	P-O1-C1	-4.98	110.19	123.54
2	C	1290	G1P	P-O1-C1	-4.90	110.40	123.54
2	E	1290	G1P	P-O1-C1	-4.77	110.76	123.54
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:

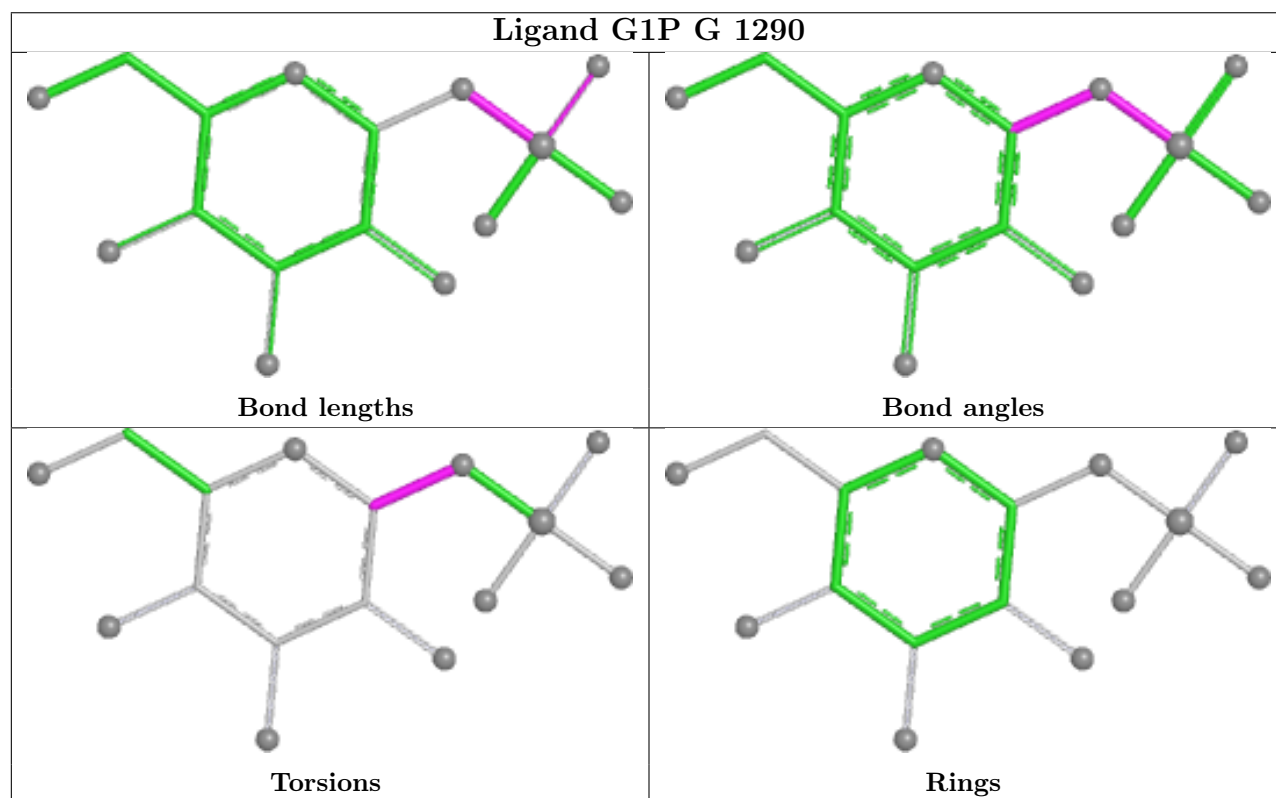
Mol	Chain	Res	Type	Atoms
2	C	1290	G1P	C2-C1-O1-P
2	E	1290	G1P	C2-C1-O1-P
2	G	1290	G1P	O5-C1-O1-P
2	D	1290	G1P	C2-C1-O1-P

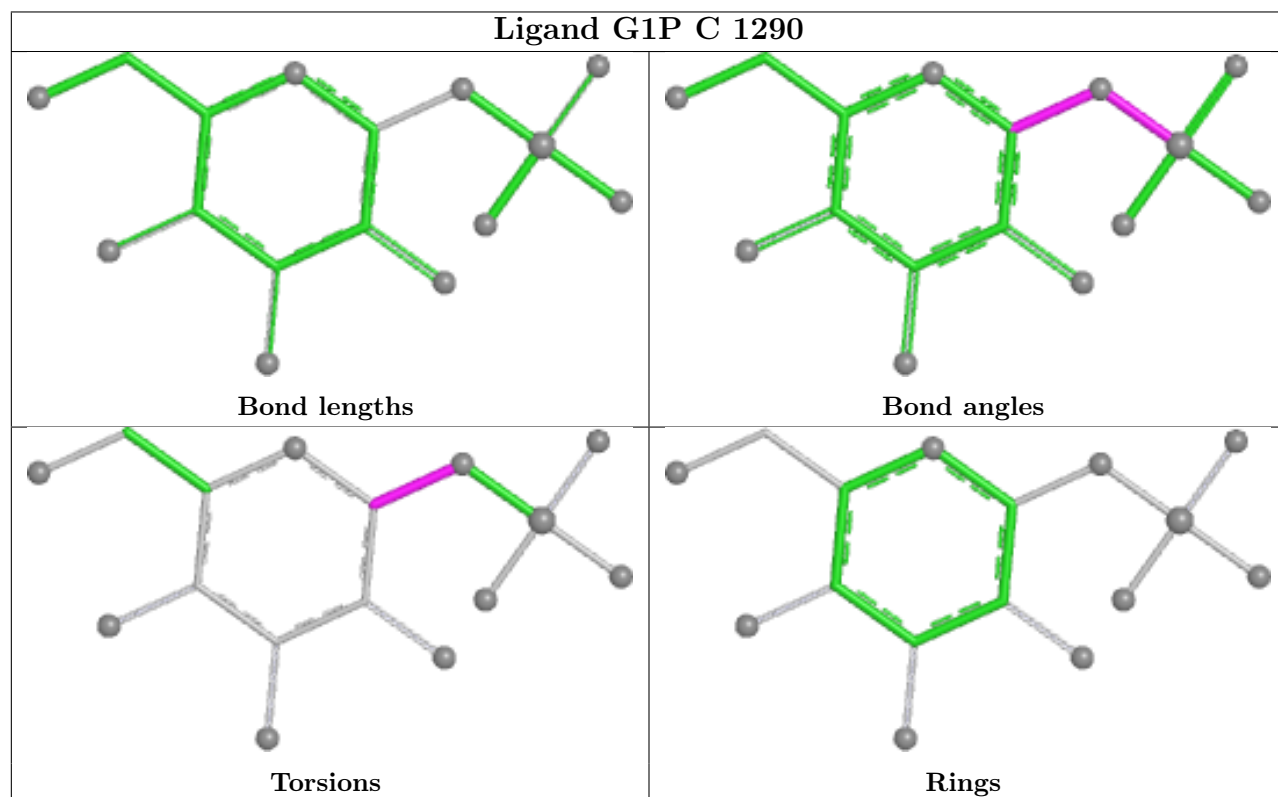
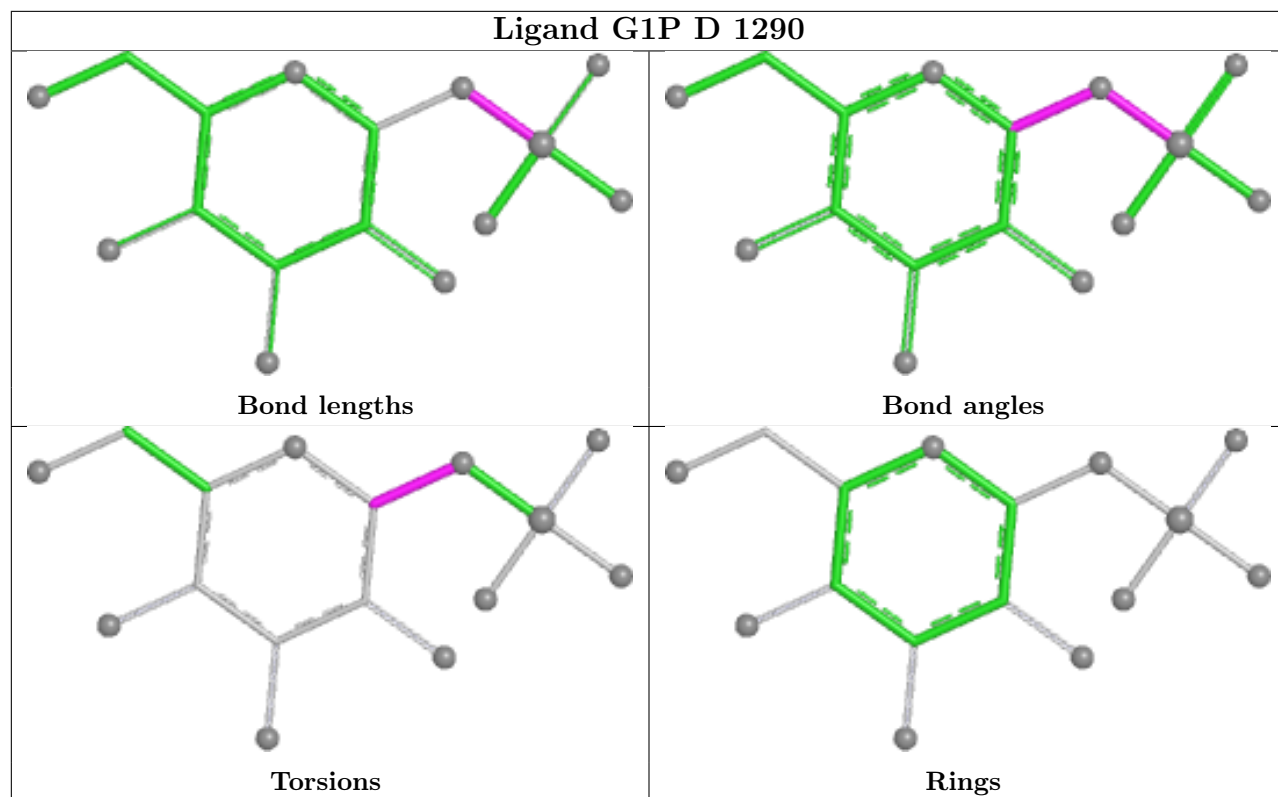
There are no ring outliers.

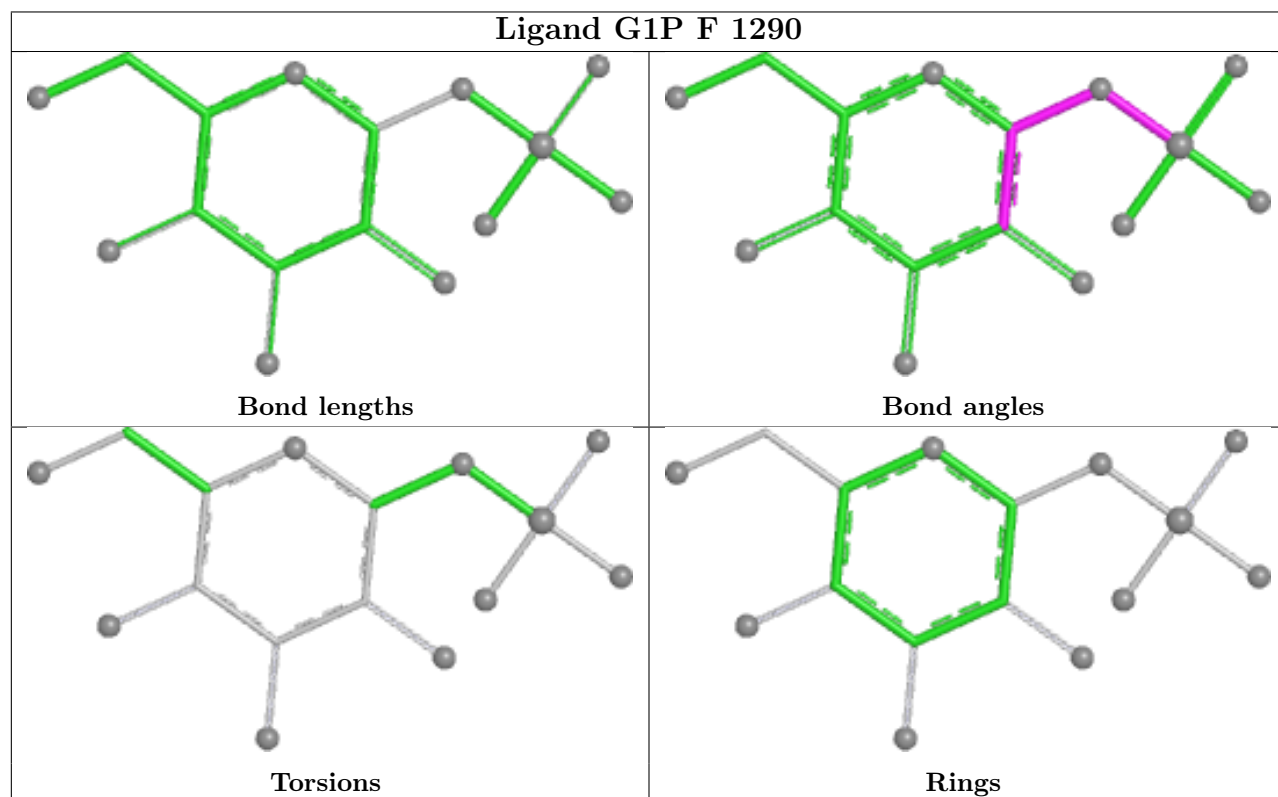
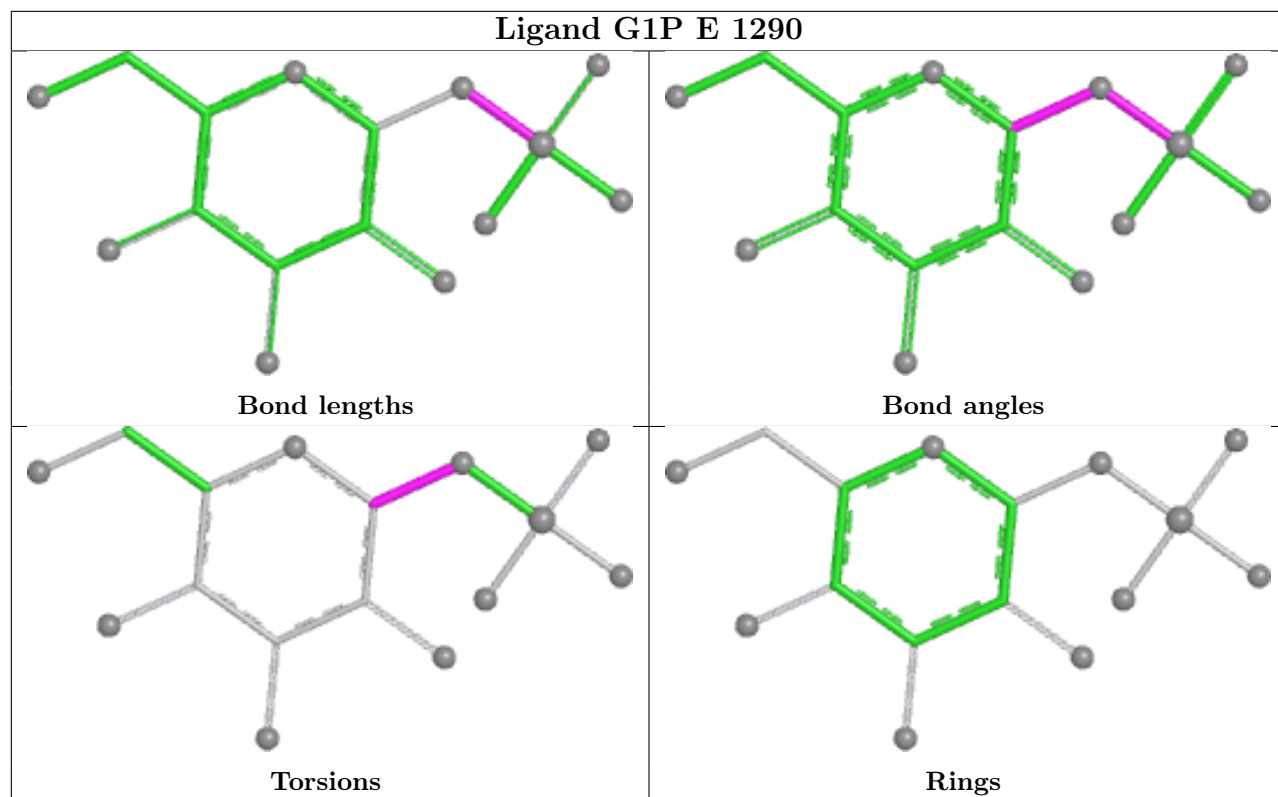
2 monomers are involved in 5 short contacts:

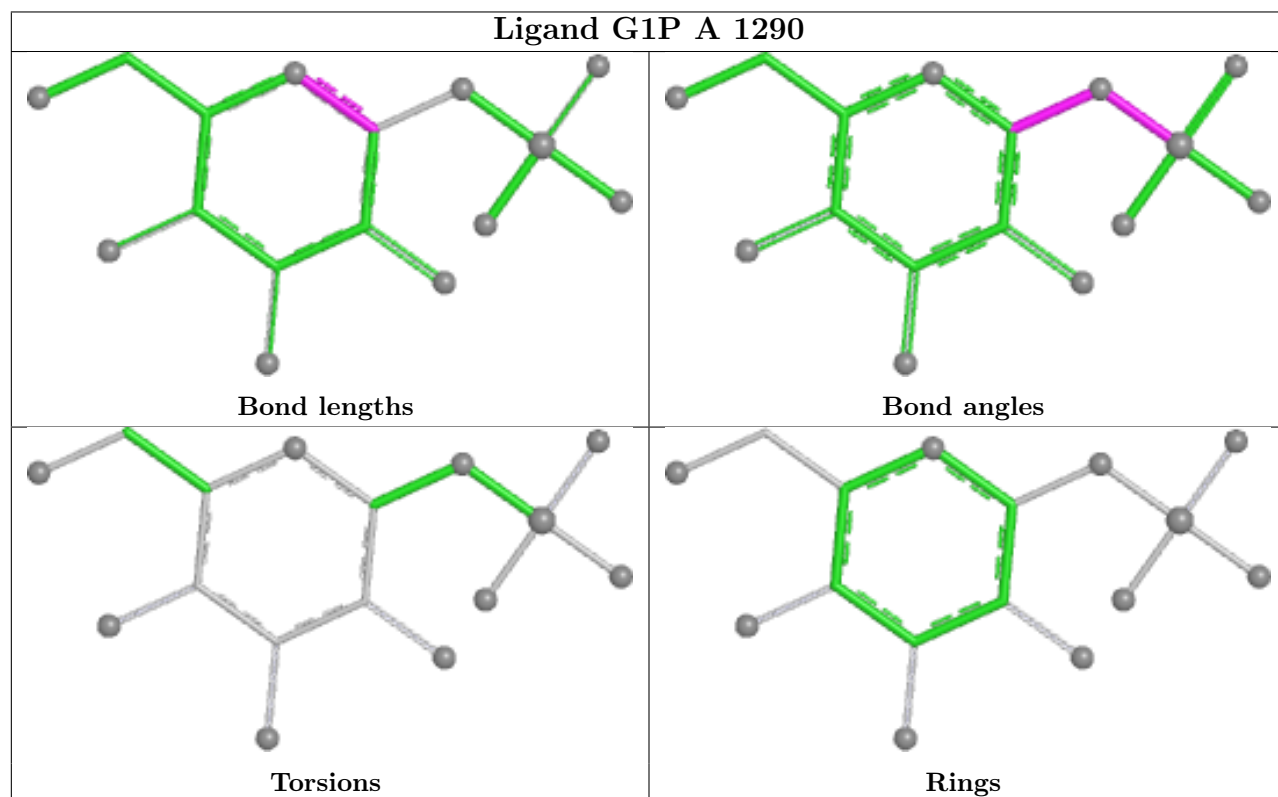
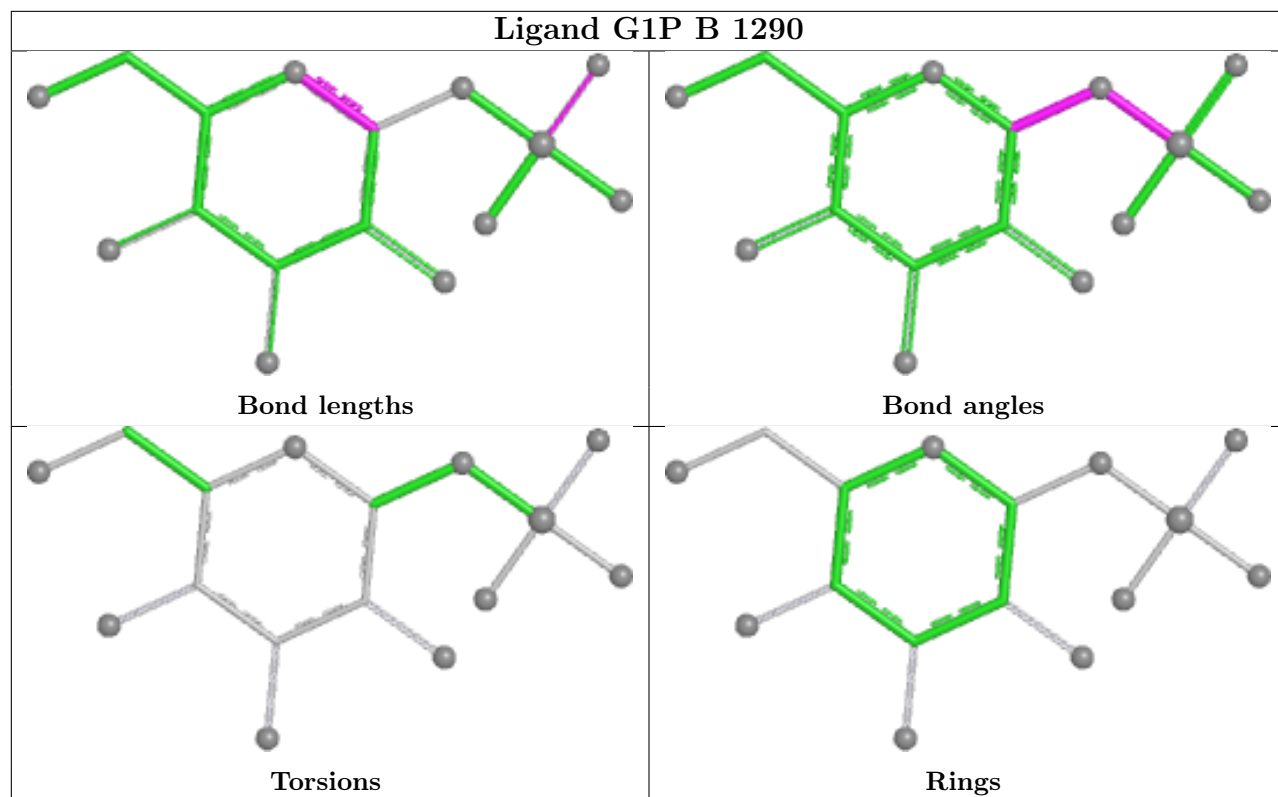
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1290	G1P	3	0
2	F	1290	G1P	2	0

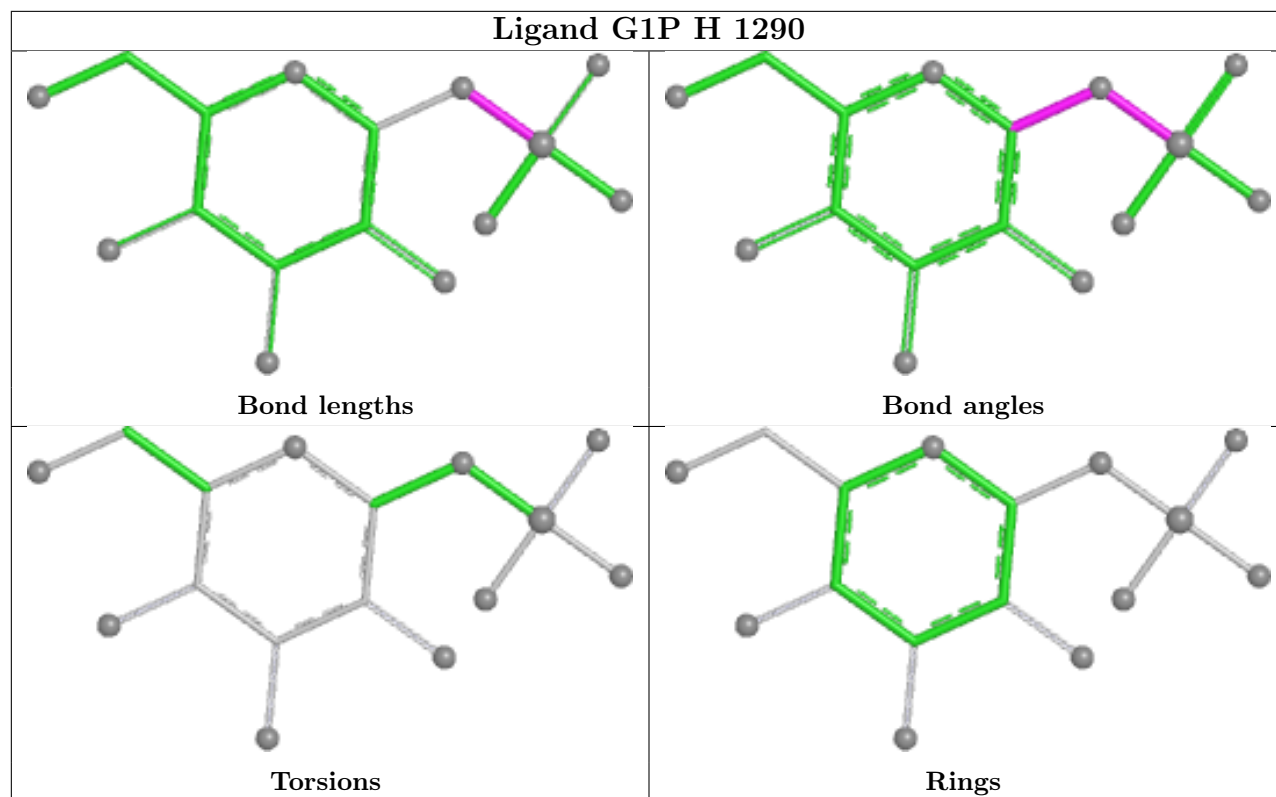
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	255/297 (85%)	0.86	36 (14%) 6 5	22, 55, 101, 150	0
1	B	280/297 (94%)	0.56	20 (7%) 22 16	23, 48, 80, 114	0
1	C	282/297 (94%)	0.65	24 (8%) 16 12	20, 46, 88, 116	0
1	D	281/297 (94%)	0.79	30 (10%) 11 9	27, 51, 83, 125	0
1	E	280/297 (94%)	0.39	20 (7%) 22 16	21, 44, 73, 120	0
1	F	282/297 (94%)	0.76	23 (8%) 17 13	27, 54, 88, 120	0
1	G	288/297 (96%)	0.57	21 (7%) 21 15	21, 48, 84, 110	0
1	H	244/297 (82%)	0.58	20 (8%) 17 13	18, 46, 89, 122	1 (0%)
All	All	2192/2376 (92%)	0.64	194 (8%) 15 12	18, 49, 89, 150	1 (0%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	GLY	4.9
1	A	173	ILE	4.9
1	A	186	VAL	4.8
1	F	289	GLY	4.7
1	A	231	LEU	4.6
1	C	289	GLY	4.4
1	D	289	GLY	4.4
1	E	221	GLN	4.4
1	C	151	ASN	4.4
1	H	54	GLN	4.2
1	A	202	LEU	4.2
1	F	2	THR	4.1
1	E	15	GLY	4.0
1	E	29	LYS	4.0
1	D	202	LEU	4.0
1	D	15	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	197	THR	3.9
1	H	7	ARG	3.9
1	B	239	ILE	3.9
1	F	239	ILE	3.8
1	H	239	ILE	3.7
1	H	289	GLY	3.7
1	A	217	ILE	3.7
1	D	238	MET	3.7
1	F	195	PRO	3.6
1	A	232	THR	3.6
1	B	17	GLY	3.6
1	F	17	GLY	3.6
1	G	240	GLY	3.6
1	G	217	ILE	3.5
1	A	54	GLN	3.5
1	D	26	ALA	3.4
1	C	195	PRO	3.4
1	B	107	GLU	3.4
1	C	239	ILE	3.4
1	B	27	MET	3.4
1	H	155	GLY	3.3
1	F	217	ILE	3.3
1	A	7	ARG	3.3
1	A	244	PHE	3.3
1	D	233	ASP	3.3
1	H	108	PRO	3.1
1	E	217	ILE	3.1
1	G	237	ARG	3.1
1	E	233	ASP	3.1
1	B	181	GLY	3.1
1	E	17	GLY	3.1
1	G	289	GLY	3.1
1	A	174	ILE	3.1
1	B	2	THR	3.1
1	C	179	GLN	3.1
1	D	17	GLY	3.1
1	C	233	ASP	3.0
1	H	250	GLN	3.0
1	B	56	ILE	3.0
1	D	239	ILE	3.0
1	C	250	GLN	3.0
1	D	222	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	245	HIS	3.0
1	A	240	GLY	3.0
1	E	230	GLN	3.0
1	E	231	LEU	2.9
1	B	289	GLY	2.9
1	F	140	PRO	2.9
1	C	238	MET	2.9
1	H	160	ALA	2.9
1	B	231	LEU	2.9
1	E	250	GLN	2.9
1	H	139	GLN	2.9
1	A	175	THR	2.8
1	A	257	GLY	2.8
1	F	185	GLU	2.8
1	H	245	HIS	2.8
1	H	248	THR	2.8
1	A	108	PRO	2.8
1	F	288	LEU	2.8
1	E	82	ALA	2.8
1	C	19	ARG	2.8
1	B	84	GLY	2.7
1	F	15	GLY	2.7
1	A	235	MET	2.7
1	F	246	GLY	2.7
1	D	2	THR	2.7
1	G	248	THR	2.7
1	E	16	LEU	2.7
1	D	287	ALA	2.7
1	B	62	GLY	2.7
1	F	196	GLY	2.7
1	H	84	GLY	2.7
1	C	187	LYS	2.7
1	B	217	ILE	2.6
1	A	289	GLY	2.6
1	E	285	VAL	2.6
1	D	230	GLN	2.6
1	A	239	ILE	2.6
1	C	152	LYS	2.6
1	C	230	GLN	2.6
1	C	241	ASP	2.5
1	A	3	ILE	2.5
1	H	53	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	82	ALA	2.5
1	D	168	THR	2.5
1	H	189	LEU	2.5
1	C	84	GLY	2.5
1	D	172	GLY	2.5
1	G	84	GLY	2.5
1	G	221	GLN	2.5
1	E	195	PRO	2.5
1	C	54	GLN	2.5
1	D	198	ALA	2.5
1	F	18	THR	2.5
1	F	202	LEU	2.5
1	G	82	ALA	2.5
1	A	201	ASN	2.4
1	C	16	LEU	2.4
1	A	150	TYR	2.4
1	C	74	TYR	2.4
1	D	286	LYS	2.4
1	F	82	ALA	2.4
1	H	217	ILE	2.4
1	E	84	GLY	2.4
1	E	236	GLN	2.4
1	G	4	LYS	2.4
1	G	246	GLY	2.4
1	H	153	VAL	2.4
1	B	237	ARG	2.4
1	G	3	ILE	2.4
1	B	124	ASP	2.4
1	C	85	LYS	2.4
1	A	15	GLY	2.4
1	E	139	GLN	2.4
1	A	218	LEU	2.3
1	B	275	ASP	2.3
1	G	202	LEU	2.3
1	E	239	ILE	2.3
1	C	102	TYR	2.3
1	D	241	ASP	2.3
1	H	204	VAL	2.3
1	G	239	ILE	2.3
1	A	180	ASP	2.3
1	A	181	GLY	2.3
1	A	251	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	196	GLY	2.3
1	H	186	VAL	2.3
1	D	236	GLN	2.2
1	D	181	GLY	2.2
1	D	188	GLY	2.2
1	G	7	ARG	2.2
1	D	4	LYS	2.2
1	D	244	PHE	2.2
1	A	160	ALA	2.2
1	F	252	THR	2.2
1	E	238	MET	2.2
1	A	158	ILE	2.2
1	F	173	ILE	2.2
1	A	178	THR	2.2
1	A	248	THR	2.2
1	D	252	THR	2.2
1	F	197	THR	2.2
1	G	27	MET	2.2
1	H	124	ASP	2.2
1	A	184	THR	2.1
1	B	4	LYS	2.1
1	F	236	GLN	2.1
1	A	246	GLY	2.1
1	A	233	ASP	2.1
1	D	56	ILE	2.1
1	G	280	VAL	2.1
1	C	198	ALA	2.1
1	C	79	THR	2.1
1	A	236	GLN	2.1
1	A	237	ARG	2.1
1	G	19	ARG	2.1
1	F	4	LYS	2.1
1	C	139	GLN	2.1
1	B	3	ILE	2.1
1	B	7	ARG	2.1
1	F	286	LYS	2.1
1	G	178	THR	2.1
1	B	108	PRO	2.1
1	F	16	LEU	2.1
1	C	196	GLY	2.1
1	A	204	VAL	2.1
1	G	163	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	109	MET	2.0
1	G	108	PRO	2.0
1	G	236	GLN	2.0
1	H	157	LEU	2.0
1	D	201	ASN	2.0
1	E	237	ARG	2.0
1	D	197	THR	2.0
1	F	184	THR	2.0
1	D	174	ILE	2.0
1	D	240	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

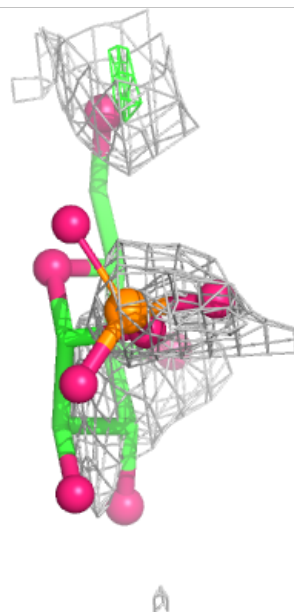
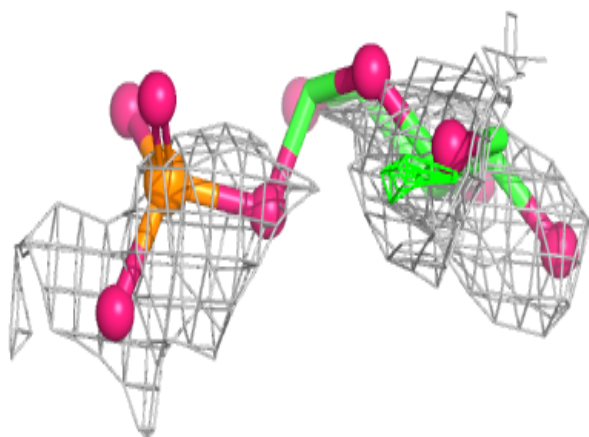
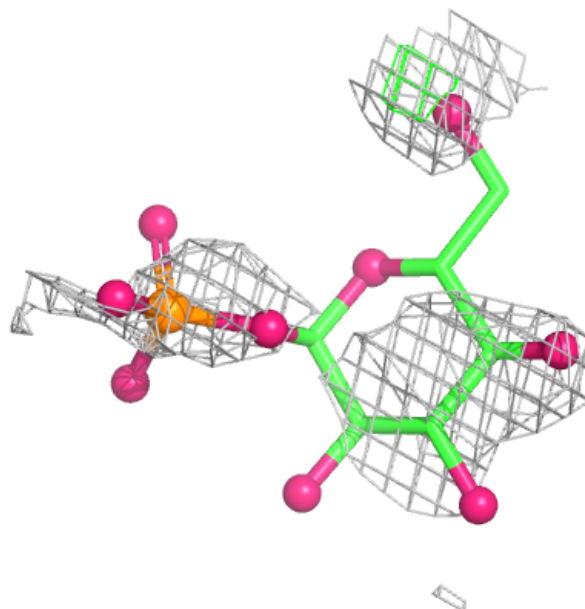
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G1P	H	1290	16/16	0.64	0.22	70,70,70,70	16
2	G1P	A	1290	16/16	0.66	0.26	104,106,106,106	16
2	G1P	C	1290	16/16	0.73	0.26	60,60,60,60	16
2	G1P	G	1290	16/16	0.75	0.17	60,60,60,60	16
2	G1P	B	1290	16/16	0.76	0.16	60,60,60,60	16
2	G1P	F	1290	16/16	0.77	0.17	80,80,80,80	16
2	G1P	D	1290	16/16	0.80	0.18	60,60,60,90	16
2	G1P	E	1290	16/16	0.83	0.17	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.

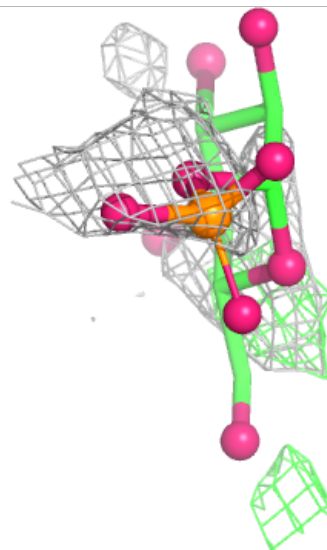
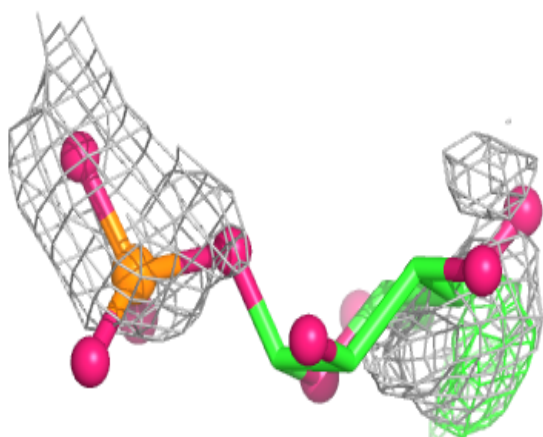
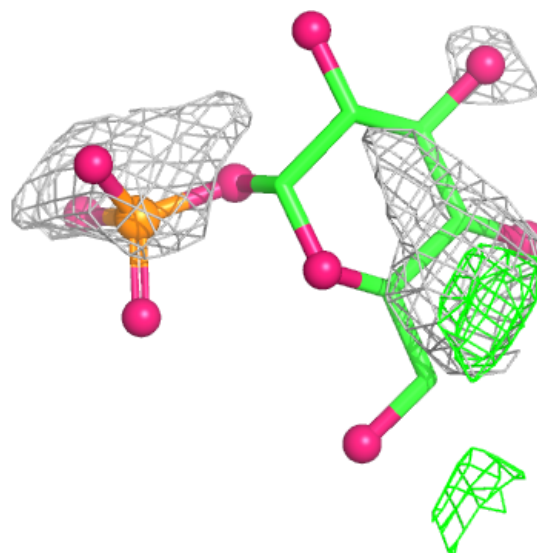
Electron density around G1P H 1290:

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



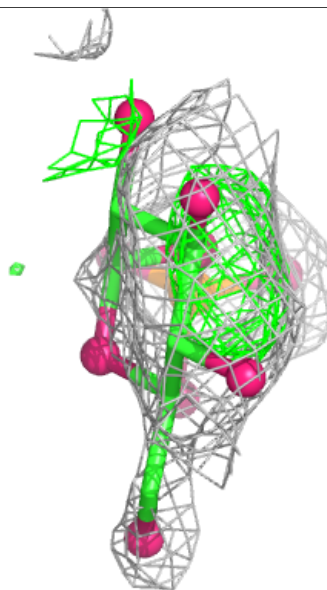
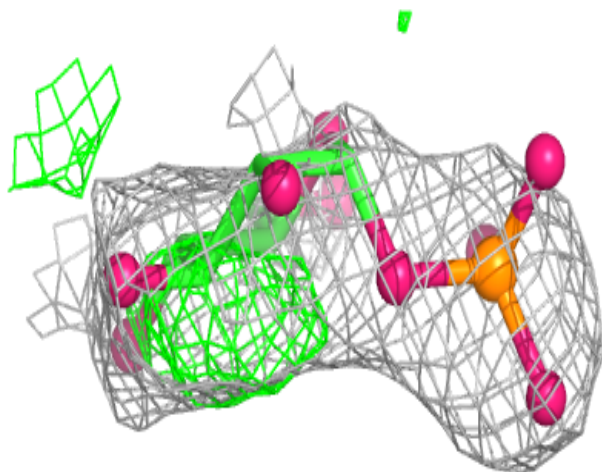
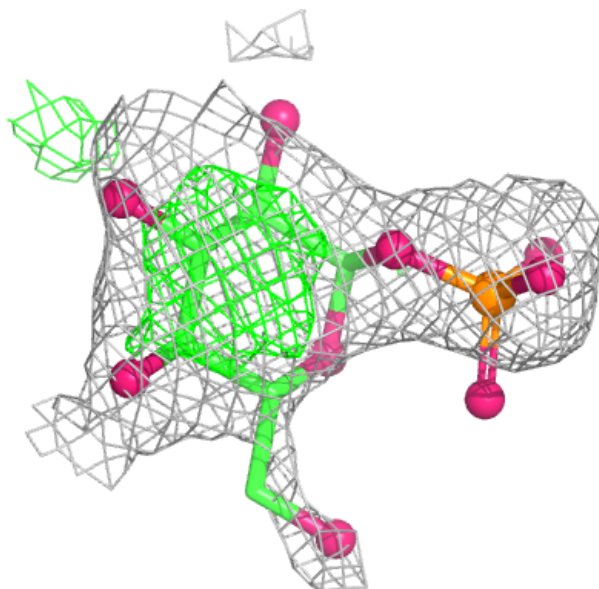
Electron density around G1P A 1290:

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



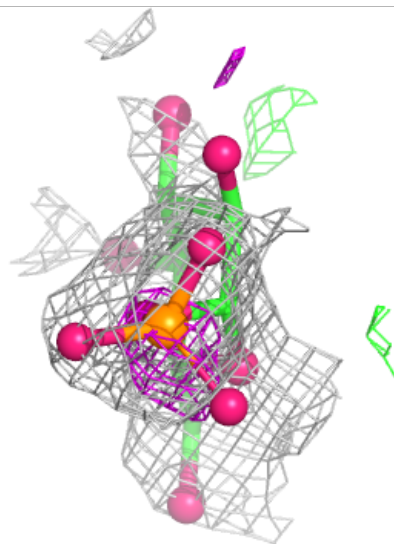
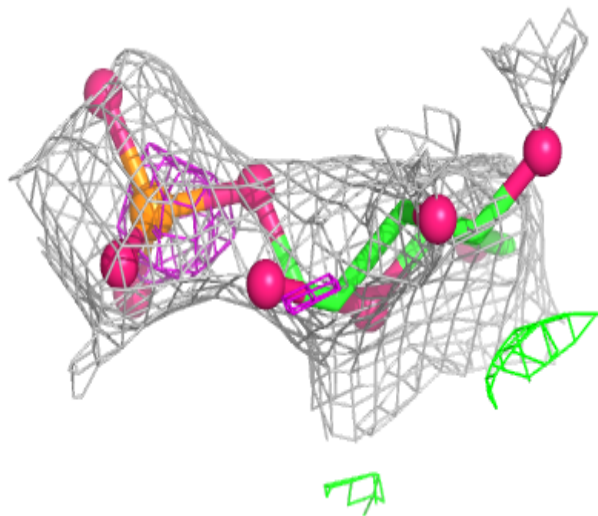
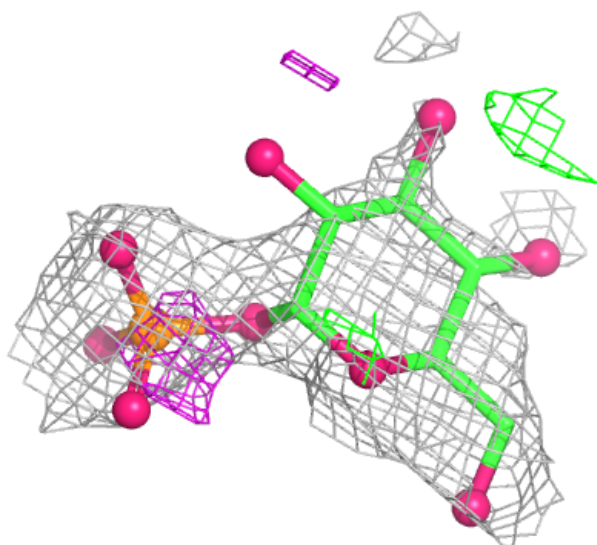
Electron density around G1P C 1290:

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



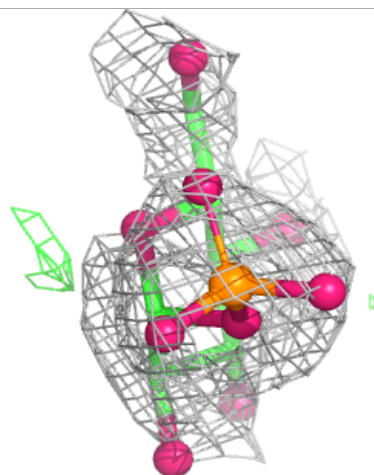
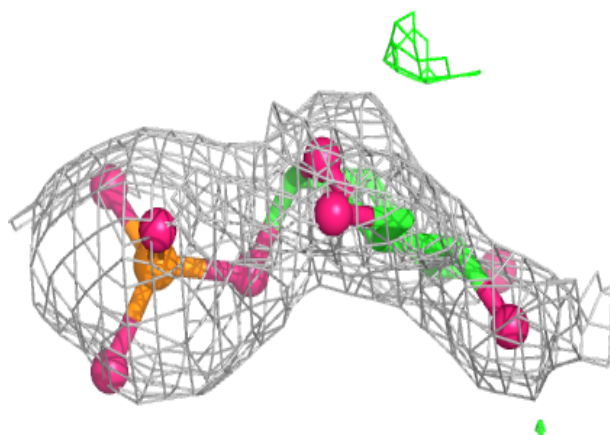
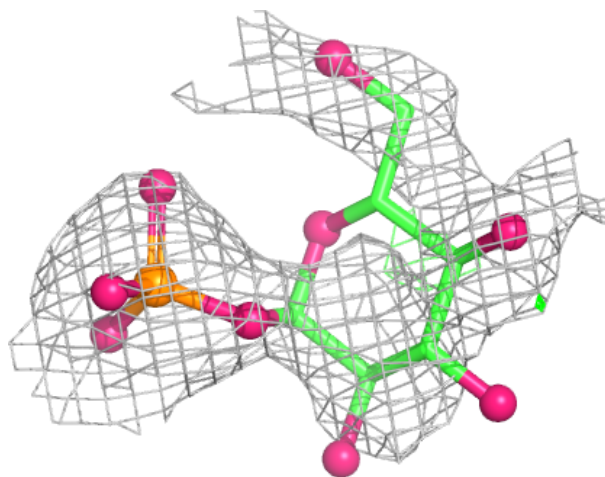
Electron density around G1P G 1290:

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



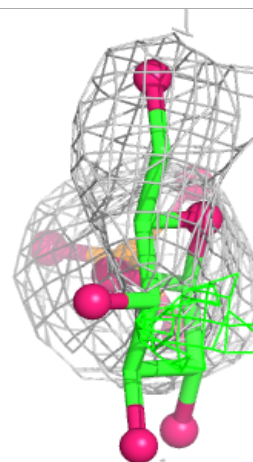
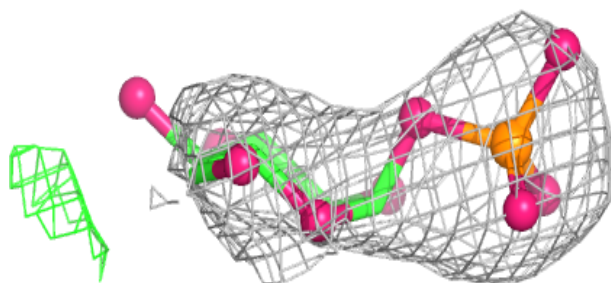
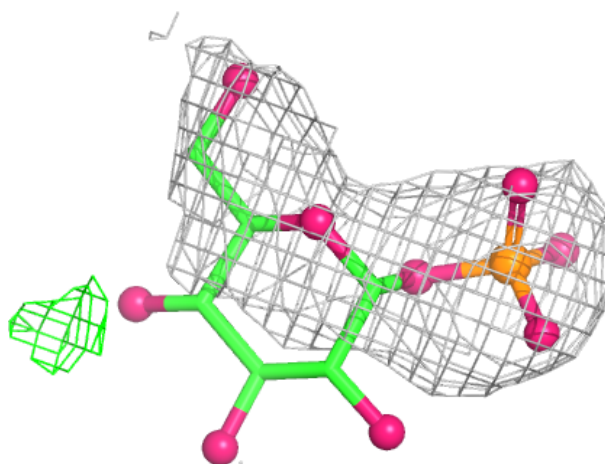
Electron density around G1P B 1290:

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



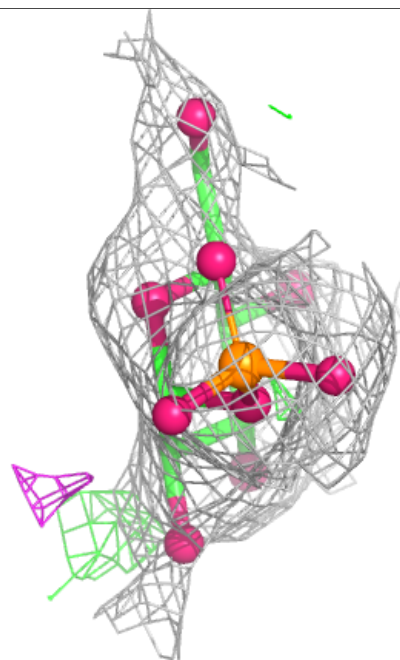
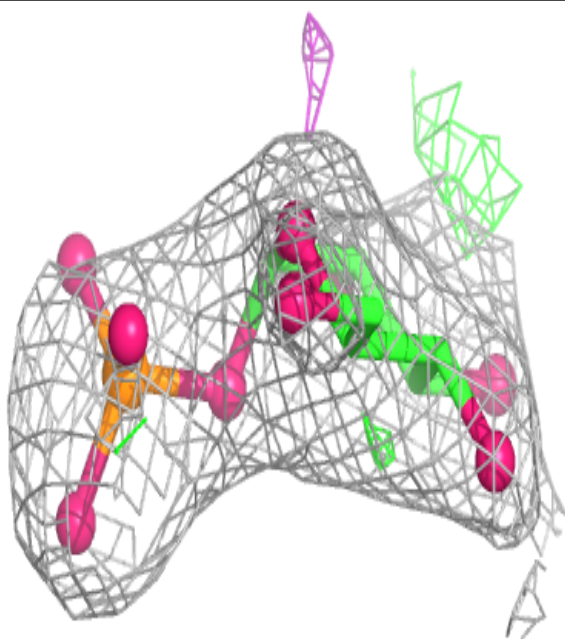
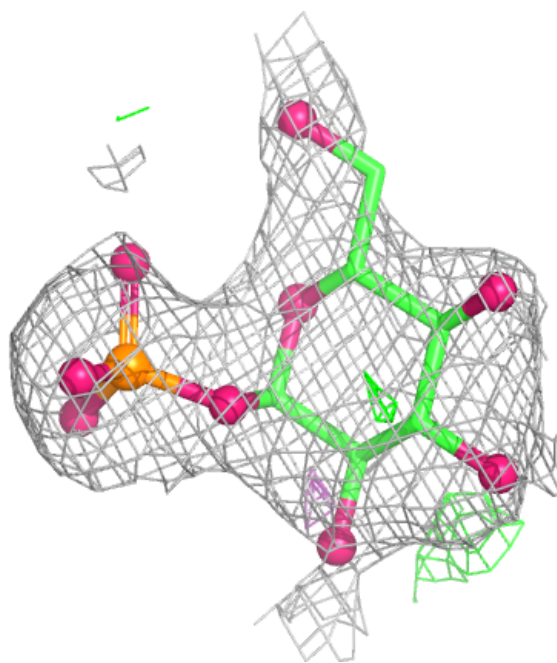
Electron density around G1P F 1290:

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



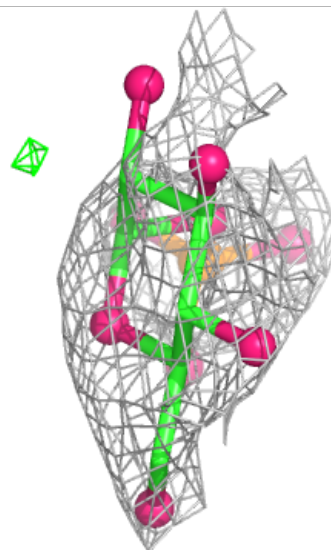
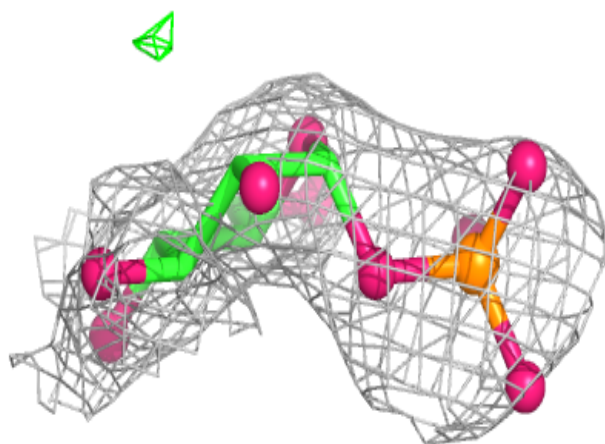
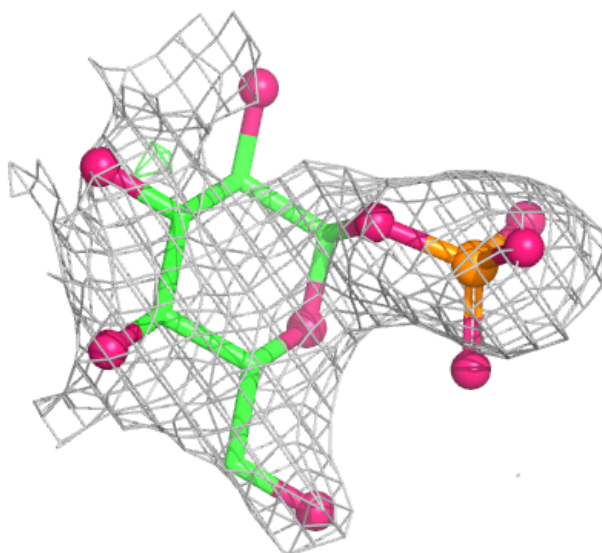
Electron density around G1P D 1290:

$2mF_o-DF_c$ (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.