



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:16 PM BST

PDB ID : 1UP6
Title : Structure of the 6-phospho-beta glucosidase from *Thermotoga maritima* at 2.55 Angstrom resolution in the tetragonal form with manganese, NAD⁺ and glucose-6-phosphate
Authors : Varrot, A.; Yip, V.L.; Withers, S.G.; Davies, G.J.
Deposited on : 2003-09-29
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

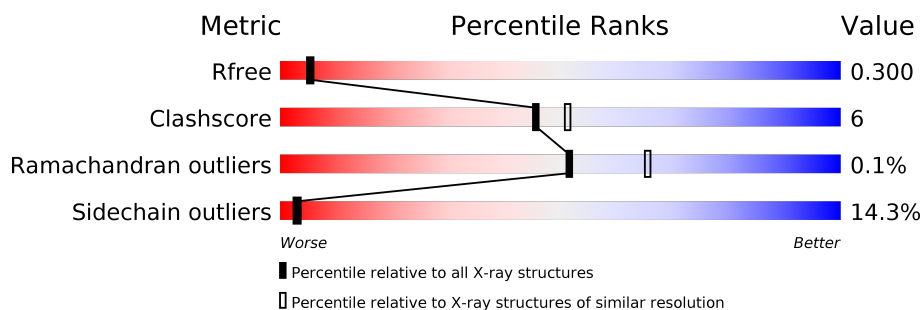
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	416	74% 22% . .
1	B	416	74% 21% . .
1	C	416	75% 19% . .
1	D	416	75% 19% . .
1	E	416	67% 22% 5% 6%
1	F	416	73% 20% . .
1	G	416	73% 21% . .

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Mol	Chain	Length	Quality of chain
1	H	416	

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
4	G6P	A	1418	X	-	-	-
4	G6P	C	1418	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26917 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 6-PHOSPHO-BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	Se	0	1	0
			3356	2164	560	623	2	7			
1	B	410	Total	C	N	O	S	Se	39	0	0
			3331	2150	552	620	2	7			
1	C	407	Total	C	N	O	S	Se	14	0	0
			3303	2129	548	617	2	7			
1	D	404	Total	C	N	O	S	Se	10	0	0
			3276	2113	543	611	2	7			
1	E	390	Total	C	N	O	S	Se	121	0	0
			3165	2041	525	591	2	6			
1	F	399	Total	C	N	O	S	Se	80	0	0
			3240	2091	539	602	2	6			
1	G	404	Total	C	N	O	S	Se	20	0	0
			3280	2117	544	610	2	7			
1	H	395	Total	C	N	O	S	Se	104	0	0
			3209	2072	533	596	2	6			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

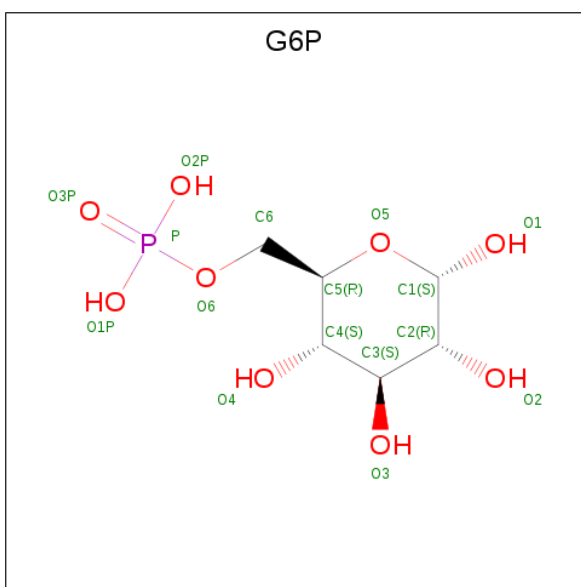


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	G	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: $\text{C}_6\text{H}_{13}\text{O}_9\text{P}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			16	6	9	1		
4	C	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		

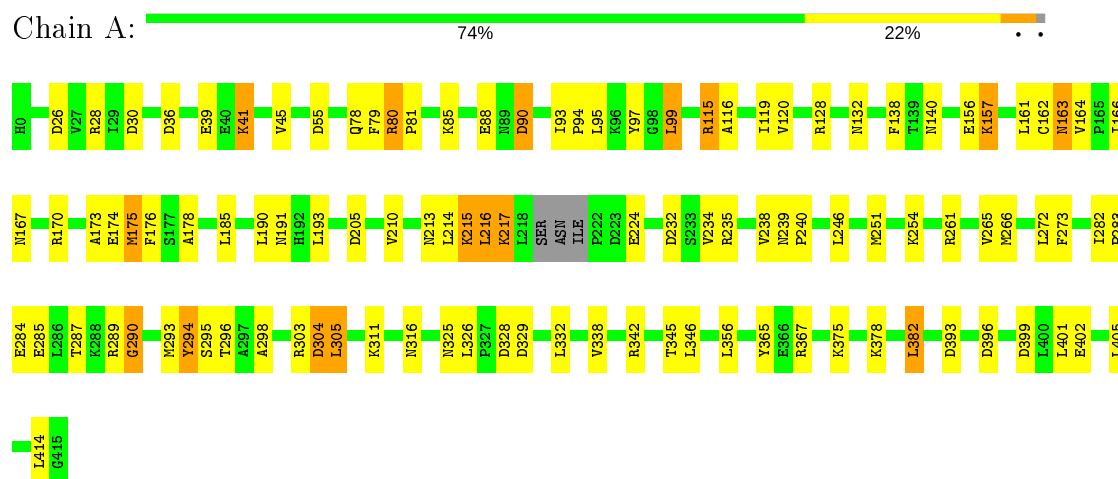
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	136	Total	O	0	0
			136	136		
6	B	83	Total	O	0	0
			83	83		
6	C	106	Total	O	0	0
			106	106		
6	D	95	Total	O	0	0
			95	95		
6	E	23	Total	O	0	0
			23	23		
6	F	36	Total	O	0	0
			36	36		
6	G	59	Total	O	0	0
			59	59		
6	H	30	Total	O	0	0
			30	30		

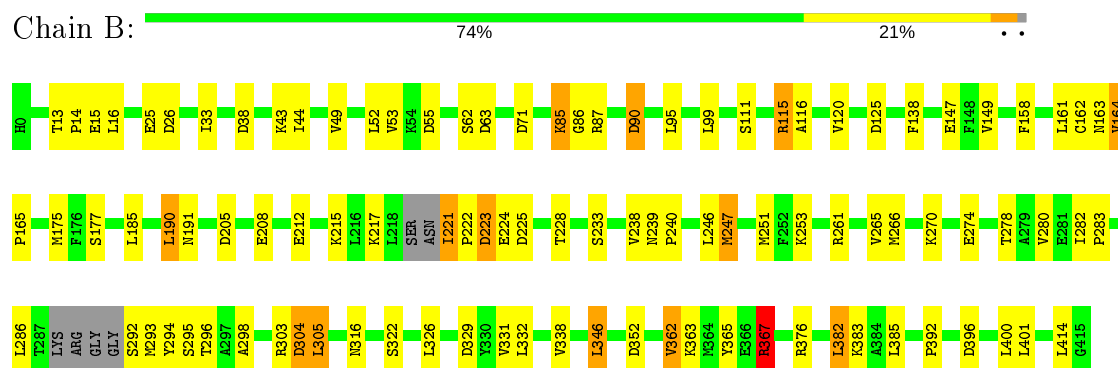
3 Residue-property plots

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. 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. 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.

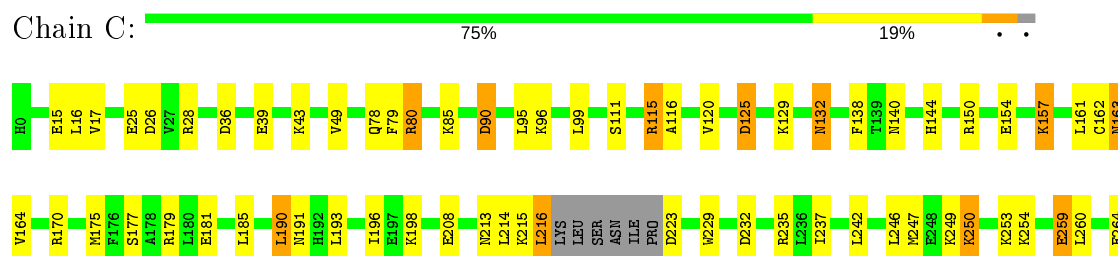
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE



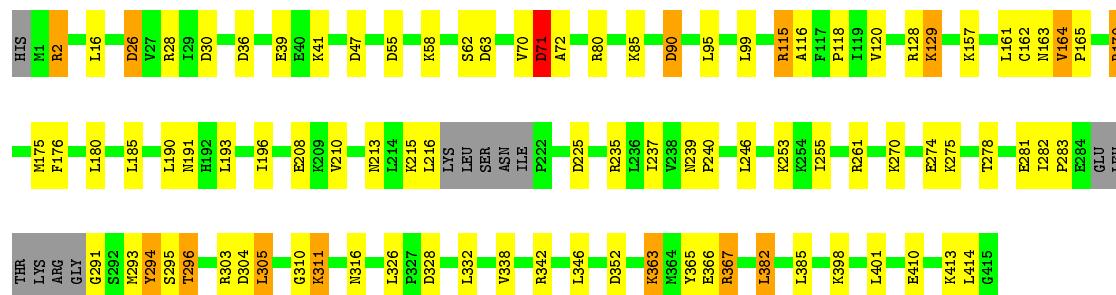
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE





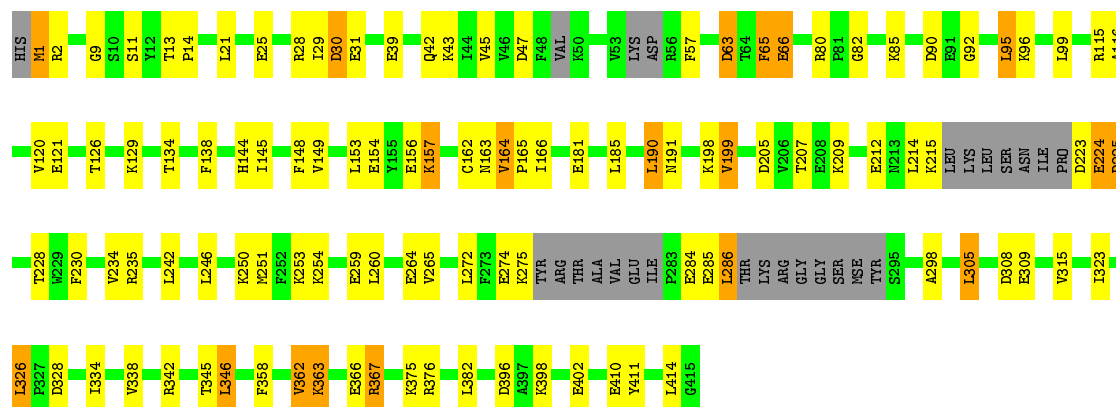
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain D: 75% 19%



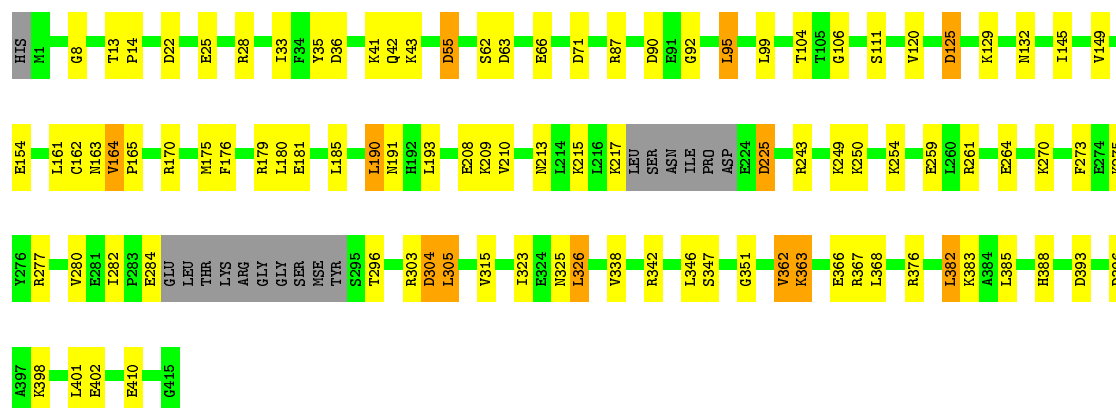
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain E: 67% 22% 5% 6%



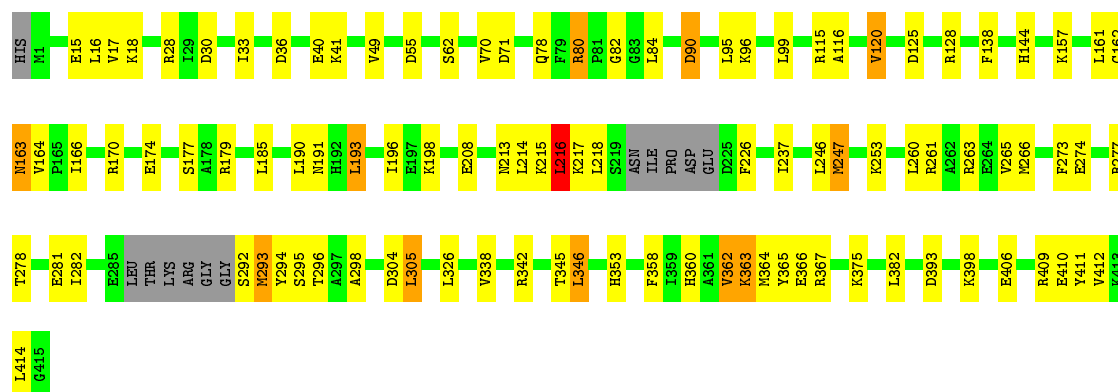
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain F: 73% 20%



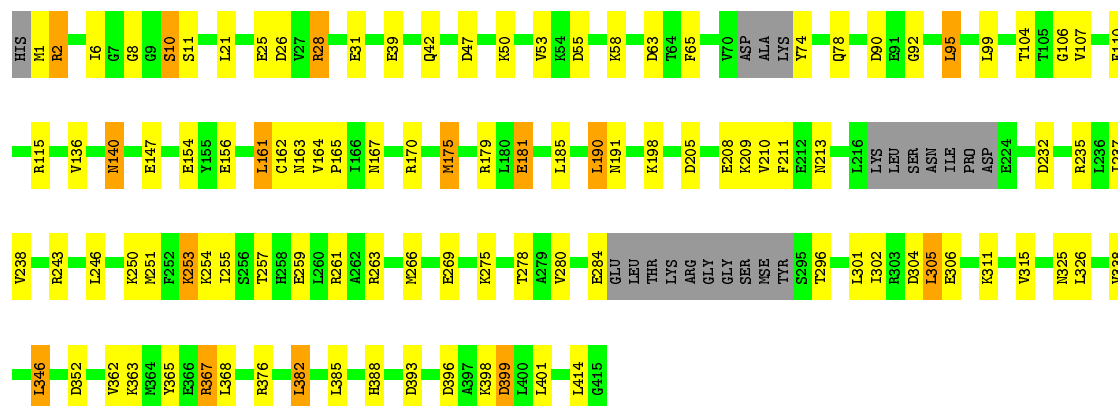
• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain G:  73% 21%



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain H:  70% 22% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.44Å 179.44Å 282.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.55 19.98 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.55) 99.8 (19.98-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.200 , 0.250 0.268 , 0.300	Depositor DCC
R_{free} test set	14357 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	26917	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% 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: G6P, MN, SO4, NAD

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	0.75	1/3420 (0.0%)	0.88	15/4595 (0.3%)
1	B	0.67	0/3390	0.89	13/4558 (0.3%)
1	C	0.72	0/3361	0.88	10/4518 (0.2%)
1	D	0.70	0/3335	0.89	12/4484 (0.3%)
1	E	0.51	0/3219	0.77	8/4323 (0.2%)
1	F	0.51	0/3298	0.78	9/4435 (0.2%)
1	G	0.59	0/3338	0.81	8/4487 (0.2%)
1	H	0.49	0/3266	0.77	11/4392 (0.3%)
All	All	0.63	1/26627 (0.0%)	0.84	86/35792 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ASN	CG-OD1	5.05	1.35	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	B	90	ASP	CB-CG-OD2	8.03	125.53	118.30
1	D	115	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	367	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	304	ASP	CB-CG-OD2	7.44	125.00	118.30
1	B	125	ASP	CB-CG-OD2	7.09	124.68	118.30
1	C	125	ASP	CB-CG-OD2	7.04	124.64	118.30
1	B	304	ASP	CB-CG-OD2	6.84	124.46	118.30
1	D	55	ASP	CB-CG-OD2	6.69	124.32	118.30
1	H	399	ASP	CB-CG-OD2	6.67	124.31	118.30
1	C	304	ASP	CB-CG-OD2	6.65	124.28	118.30
1	D	90	ASP	CB-CG-OD2	6.60	124.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	329	ASP	CB-CG-OD1	6.43	124.09	118.30
1	D	367	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	308	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	30	ASP	CB-CG-OD2	6.17	123.85	118.30
1	G	55	ASP	CB-CG-OD2	6.11	123.80	118.30
1	E	328	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	115	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	205	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	115	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	F	36	ASP	CB-CG-OD2	5.98	123.68	118.30
1	H	232	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	36	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	223	ASP	CB-CG-OD2	5.89	123.60	118.30
1	H	63	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	329	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	396	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	223	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	36	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	205	ASP	CB-CG-OD2	5.73	123.46	118.30
1	F	63	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	328	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	63	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	90	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	30	ASP	CB-CG-OD2	5.66	123.39	118.30
1	H	304	ASP	CB-CG-OD2	5.63	123.37	118.30
1	G	304	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	26	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	71	ASP	CB-CG-OD2	5.55	123.29	118.30
1	G	30	ASP	CB-CG-OD2	5.53	123.28	118.30
1	H	205	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	393	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	38	ASP	CB-CG-OD2	5.46	123.22	118.30
1	F	304	ASP	CB-CG-OD2	5.46	123.22	118.30
1	E	225	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	36	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	396	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	329	ASP	CB-CG-OD1	5.40	123.16	118.30
1	H	55	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	205	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	352	ASP	CB-CG-OD2	5.37	123.14	118.30
1	G	36	ASP	CB-CG-OD2	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	26	ASP	CB-CG-OD2	5.36	123.12	118.30
1	H	396	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	115	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	H	47	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	63	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	399	ASP	CB-CG-OD2	5.27	123.05	118.30
1	F	396	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	47	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	71	ASP	CB-CG-OD2	5.25	123.02	118.30
1	H	393	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	128	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	H	352	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	125	ASP	CB-CG-OD2	5.20	122.97	118.30
1	D	352	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	150	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	328	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	71	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	71	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	55	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	232	ASP	CB-CG-OD2	5.13	122.92	118.30
1	G	393	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	367	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	90	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	55	ASP	CB-CG-OD2	5.09	122.88	118.30
1	E	47	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	26	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	308	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	232	ASP	CB-CG-OD2	5.05	122.85	118.30
1	F	22	ASP	CB-CG-OD2	5.05	122.85	118.30
1	F	393	ASP	CB-CG-OD2	5.05	122.84	118.30
1	F	125	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	396	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3356	0	3393	54	0
1	B	3331	0	3362	46	0
1	C	3303	0	3322	47	0
1	D	3276	0	3300	36	0
1	E	3165	0	3184	43	0
1	F	3240	0	3275	38	0
1	G	3280	0	3313	45	0
1	H	3209	0	3239	37	0
2	A	44	0	26	5	0
2	C	44	0	26	2	0
2	G	44	0	26	3	0
3	A	3	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
4	A	16	0	9	1	0
4	C	16	0	10	1	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0
6	A	136	0	0	1	0
6	B	83	0	0	1	0
6	C	106	0	0	2	0
6	D	95	0	0	2	0
6	E	23	0	0	0	0
6	F	36	0	0	0	0
6	G	59	0	0	0	0
6	H	30	0	0	0	0
All	All	26917	0	26485	334	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 6.

All (334) 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:G:41:LYS:HE2	1:G:273:PHE:CZ	1.75	1.22
1:F:175:MSE:HE3	1:F:213:ASN:ND2	1.62	1.15
1:F:175:MSE:HE3	1:F:213:ASN:HD22	1.05	1.15
1:G:41:LYS:HE2	1:G:273:PHE:CE2	1.85	1.11
1:D:175:MSE:HE3	1:D:213:ASN:HD22	0.92	1.07
1:D:175:MSE:HE3	1:D:213:ASN:ND2	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:GLY:HA3	1:F:42:GLN:HE21	1.27	0.99
1:G:41:LYS:CE	1:G:273:PHE:CZ	2.46	0.98
1:G:41:LYS:CE	1:G:273:PHE:CE2	2.55	0.90
1:F:175:MSE:CE	1:F:213:ASN:HD22	1.87	0.88
1:C:190:LEU:HD23	1:C:362:VAL:HG22	1.56	0.88
1:D:175:MSE:CE	1:D:213:ASN:HD22	1.84	0.87
1:D:175:MSE:HE1	1:D:210:VAL:HA	1.59	0.85
1:G:41:LYS:NZ	1:G:273:PHE:HZ	1.76	0.82
1:E:190:LEU:HD23	1:E:362:VAL:HG22	1.60	0.82
1:B:346:LEU:HD12	1:C:346:LEU:HD12	1.62	0.81
1:F:382:LEU:HD13	1:F:401:LEU:HD22	1.62	0.79
1:D:2:ARG:HG3	1:D:72:ALA:HA	1.64	0.77
1:C:125:ASP:OD1	1:C:129:LYS:HE3	1.87	0.75
1:H:190:LEU:HD23	1:H:362:VAL:HG22	1.70	0.73
1:A:162:CYS:HB2	1:A:191:ASN:ND2	2.02	0.73
1:D:170:ARG:HH22	1:D:293:MSE:HB2	1.52	0.73
1:G:41:LYS:NZ	1:G:273:PHE:CZ	2.56	0.73
1:G:80:ARG:HB2	2:G:1416:NAD:H3D	1.71	0.72
1:A:162:CYS:HB2	1:A:191:ASN:HD21	1.52	0.71
1:C:190:LEU:CD2	1:C:362:VAL:HG22	2.19	0.71
1:G:305:LEU:HD13	1:G:338:VAL:HG13	1.72	0.71
1:A:224:GLU:OE2	1:A:254:LYS:HE3	1.91	0.70
1:F:162:CYS:SG	1:F:163:ASN:N	2.65	0.69
1:H:162:CYS:SG	1:H:163:ASN:N	2.65	0.69
1:D:175:MSE:HE2	1:D:176:PHE:CE2	2.28	0.69
1:F:190:LEU:HD23	1:F:362:VAL:HG22	1.75	0.69
1:A:289:ARG:HG3	1:A:290:GLY:H	1.58	0.68
1:B:33:ILE:HD11	1:B:62:SER:HB2	1.76	0.67
1:G:15:GLU:OE1	1:G:18:LYS:NZ	2.26	0.67
1:B:346:LEU:CD1	1:C:346:LEU:HD12	2.23	0.67
1:B:138:PHE:CE1	1:B:294:TYR:HD2	2.13	0.67
1:E:1:MSE:HG3	1:E:1:MSE:O	1.94	0.66
1:E:9:GLY:HA2	1:E:45:VAL:HG21	1.78	0.66
1:A:224:GLU:HG2	1:A:251:MSE:HE1	1.78	0.66
1:E:162:CYS:HB2	1:E:191:ASN:ND2	2.10	0.66
1:E:162:CYS:HB2	1:E:191:ASN:HD21	1.60	0.65
1:G:41:LYS:HZ1	1:G:273:PHE:HZ	1.41	0.65
1:G:163:ASN:HD22	1:G:163:ASN:H	1.45	0.65
1:A:163:ASN:ND2	4:A:1418:G6P:O2	2.29	0.64
1:A:162:CYS:CB	1:A:191:ASN:HD21	2.10	0.64
1:H:162:CYS:HB2	1:H:191:ASN:HD21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:CYS:HB2	1:H:191:ASN:ND2	2.12	0.64
1:D:170:ARG:NH2	1:D:293:MSE:HB2	2.13	0.64
1:E:1:MSE:HE3	1:E:29:ILE:HG12	1.80	0.63
1:D:163:ASN:ND2	1:D:291:GLY:HA2	2.14	0.63
1:C:190:LEU:HD23	1:C:362:VAL:CG2	2.27	0.63
1:H:175:MSE:HE1	1:H:210:VAL:HA	1.81	0.63
1:C:345:THR:HG22	6:C:2081:HOH:O	1.97	0.63
1:B:190:LEU:HD23	1:B:362:VAL:HG22	1.79	0.62
1:E:164:VAL:HG22	1:E:165:PRO:HD3	1.81	0.62
1:G:116:ALA:O	1:G:120:VAL:HG13	2.00	0.62
1:F:259:GLU:OE1	1:F:264:GLU:HG3	2.00	0.62
1:E:346:LEU:HD12	1:H:346:LEU:HD12	1.81	0.61
1:A:138:PHE:O	2:A:1416:NAD:H2N	2.00	0.61
1:C:90:ASP:CG	1:C:115:ARG:HH22	2.03	0.61
1:F:346:LEU:HD23	1:G:346:LEU:CD1	2.31	0.61
1:C:162:CYS:SG	1:C:164:VAL:HG13	2.41	0.61
1:C:80:ARG:HB2	2:C:1416:NAD:H3D	1.82	0.60
1:C:179:ARG:NH1	1:C:181:GLU:OE2	2.35	0.60
1:G:162:CYS:SG	1:G:164:VAL:HG13	2.42	0.60
1:E:162:CYS:SG	1:E:164:VAL:HG13	2.41	0.59
1:B:224:GLU:HG2	1:B:251:MSE:HE1	1.83	0.59
1:F:175:MSE:HE2	1:F:176:PHE:CE2	2.38	0.59
1:B:138:PHE:CZ	1:B:298:ALA:HB2	2.38	0.59
1:A:261:ARG:HH22	1:A:289:ARG:HE	1.51	0.59
1:E:149:VAL:HG22	1:E:153:LEU:HD12	1.84	0.59
1:F:363:LYS:HE3	1:F:366:GLU:OE1	2.03	0.58
1:B:303:ARG:NH1	1:B:304:ASP:OD1	2.35	0.58
1:C:90:ASP:OD1	1:C:115:ARG:NH2	2.36	0.58
1:C:163:ASN:ND2	4:C:1418:G6P:O2	2.36	0.58
1:B:305:LEU:HD13	1:B:338:VAL:HG13	1.83	0.58
1:H:251:MSE:O	1:H:255:ILE:HG13	2.04	0.58
1:G:193:LEU:HD11	1:G:358:PHE:HB3	1.86	0.58
1:C:116:ALA:O	1:C:120:VAL:HG13	2.04	0.57
1:C:144:HIS:CD2	1:C:366:GLU:HB2	2.38	0.57
1:A:305:LEU:HD13	1:A:338:VAL:HG13	1.86	0.57
1:E:190:LEU:CD2	1:E:362:VAL:HG22	2.32	0.57
1:H:305:LEU:HD13	1:H:338:VAL:HG13	1.87	0.57
1:H:104:THR:OG1	1:H:140:ASN:ND2	2.38	0.57
1:G:406:GLU:OE1	1:G:406:GLU:HA	2.05	0.56
1:D:303:ARG:HD2	1:D:304:ASP:OD1	2.06	0.56
1:D:310:GLY:O	1:D:311:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:TYR:OH	1:H:306:GLU:HG2	2.06	0.56
1:H:382:LEU:HD13	1:H:401:LEU:HD22	1.88	0.55
1:G:16:LEU:HD22	1:G:78:GLN:OE1	2.07	0.55
1:A:41:LYS:HD3	1:A:273:PHE:CZ	2.41	0.55
1:B:215:LYS:HG2	1:B:228:THR:HG23	1.87	0.55
1:C:259:GLU:OE2	1:C:264:GLU:HG3	2.07	0.55
1:E:30:ASP:OD1	1:E:30:ASP:N	2.40	0.55
1:E:362:VAL:O	1:E:366:GLU:HG3	2.07	0.55
1:F:125:ASP:O	1:F:129:LYS:HG2	2.07	0.55
1:C:175:MSE:HE3	1:C:213:ASN:ND2	2.22	0.55
1:H:162:CYS:CB	1:H:191:ASN:HD21	2.20	0.55
1:H:253:LYS:O	1:H:257:THR:HG23	2.06	0.55
1:A:116:ALA:O	1:A:120:VAL:HG13	2.06	0.55
1:E:144:HIS:CD2	1:E:366:GLU:HB3	2.41	0.55
1:A:294:TYR:CD1	1:A:295:SER:N	2.75	0.55
1:C:163:ASN:H	1:C:163:ASN:HD22	1.55	0.55
1:H:21:LEU:HD11	1:H:53:VAL:HG12	1.88	0.55
1:A:90:ASP:CG	1:A:115:ARG:HH22	2.10	0.54
1:B:376:ARG:NH2	6:B:2066:HOH:O	2.39	0.54
1:A:261:ARG:HH12	1:A:289:ARG:NH2	2.05	0.54
1:E:346:LEU:CD1	1:H:346:LEU:HD12	2.37	0.54
1:A:305:LEU:HD13	1:A:338:VAL:CG1	2.38	0.54
1:A:162:CYS:CB	1:A:191:ASN:ND2	2.69	0.54
1:C:229:TRP:CD1	1:D:398:LYS:HD2	2.42	0.54
1:G:90:ASP:OD1	1:G:115:ARG:NH2	2.41	0.54
1:C:144:HIS:NE2	1:C:366:GLU:HB2	2.23	0.54
1:A:80:ARG:HB2	2:A:1416:NAD:H3D	1.89	0.53
1:G:80:ARG:HB2	2:G:1416:NAD:C3D	2.37	0.53
1:C:305:LEU:HD13	1:C:338:VAL:HG13	1.91	0.53
1:D:162:CYS:HB2	1:D:191:ASN:ND2	2.24	0.53
1:C:140:ASN:HB3	6:C:2026:HOH:O	2.08	0.53
1:F:175:MSE:HE1	1:F:210:VAL:HA	1.89	0.53
1:B:164:VAL:HG22	1:B:165:PRO:HD3	1.91	0.53
1:C:79:PHE:HB2	2:C:1416:NAD:C4A	2.39	0.53
1:D:162:CYS:SG	1:D:163:ASN:N	2.81	0.52
1:A:132:ASN:O	1:A:157:LYS:NZ	2.42	0.52
1:E:284:GLU:C	1:E:286:LEU:H	2.13	0.52
1:G:33:ILE:HD11	1:G:62:SER:HB2	1.92	0.52
1:C:162:CYS:HB2	1:C:191:ASN:ND2	2.24	0.52
1:D:305:LEU:HD13	1:D:338:VAL:HG13	1.92	0.52
1:E:134:THR:HA	1:E:157:LYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HA	1:B:295:SER:HB2	1.92	0.52
1:C:138:PHE:CZ	1:C:298:ALA:HB2	2.43	0.52
1:E:199:VAL:HG13	1:E:207:THR:HA	1.92	0.52
1:A:234:VAL:HA	1:B:383:LYS:HD2	1.92	0.52
1:D:80:ARG:HD3	6:D:2020:HOH:O	2.09	0.52
1:G:305:LEU:HD13	1:G:338:VAL:CG1	2.38	0.52
1:G:409:ARG:HB2	1:G:409:ARG:NH1	2.24	0.52
1:C:247:MSE:CE	1:C:250:LYS:HD2	2.39	0.51
1:H:90:ASP:CG	1:H:115:ARG:HH22	2.14	0.51
1:C:162:CYS:HB2	1:C:191:ASN:HD21	1.75	0.51
1:D:382:LEU:HD13	1:D:401:LEU:HD22	1.92	0.51
1:A:295:SER:OG	1:A:296:THR:N	2.42	0.51
1:F:90:ASP:OD1	1:F:111:SER:OG	2.29	0.51
1:A:81:PRO:HB3	1:A:119:ILE:HD12	1.93	0.51
1:E:65:PHE:HD1	1:E:66:GLU:H	1.58	0.51
1:B:138:PHE:HZ	1:B:298:ALA:HB2	1.76	0.50
1:A:138:PHE:CZ	1:A:298:ALA:HB2	2.46	0.50
1:B:90:ASP:CG	1:B:115:ARG:HH22	2.13	0.50
1:E:363:LYS:HA	1:E:366:GLU:HG3	1.93	0.50
1:D:90:ASP:CG	1:D:115:ARG:HH22	2.15	0.50
1:B:90:ASP:OD1	1:B:111:SER:OG	2.24	0.50
1:G:144:HIS:CD2	1:G:366:GLU:HB2	2.46	0.50
1:B:294:TYR:CG	1:B:295:SER:N	2.80	0.50
1:B:382:LEU:HD13	1:B:401:LEU:HD22	1.94	0.50
1:G:17:VAL:HG11	1:G:49:VAL:HG13	1.94	0.50
1:B:90:ASP:OD1	1:B:115:ARG:NH2	2.42	0.50
1:A:303:ARG:HD2	1:A:304:ASP:OD1	2.12	0.49
1:A:166:ILE:CD1	1:A:296:THR:HG22	2.42	0.49
1:B:164:VAL:N	1:B:165:PRO:CD	2.76	0.49
1:E:116:ALA:O	1:E:120:VAL:HG13	2.12	0.49
1:E:82:GLY:HA2	1:E:411:TYR:CZ	2.47	0.49
1:C:405:LEU:HD21	1:C:414:LEU:HD22	1.95	0.49
1:D:164:VAL:N	1:D:165:PRO:CD	2.76	0.49
1:E:21:LEU:HD23	1:E:57:PHE:CE2	2.48	0.49
1:E:230:PHE:CE1	1:E:234:VAL:HG21	2.48	0.49
1:H:2:ARG:HB2	1:H:31:GLU:HG2	1.95	0.48
1:C:132:ASN:O	1:C:157:LYS:NZ	2.46	0.48
1:C:247:MSE:HE2	1:C:250:LYS:HD2	1.95	0.48
1:A:289:ARG:HG3	1:A:290:GLY:N	2.26	0.48
1:F:368:LEU:HD22	1:F:383:LYS:HD3	1.95	0.48
1:F:41:LYS:HD3	1:F:273:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ARG:HG3	1:E:31:GLU:HG3	1.95	0.48
1:F:162:CYS:CB	1:F:191:ASN:HD21	2.27	0.48
1:F:33:ILE:HD11	1:F:62:SER:HB2	1.96	0.48
1:C:138:PHE:HZ	1:C:298:ALA:HB2	1.78	0.47
1:C:363:LYS:HE3	1:C:366:GLU:OE2	2.13	0.47
1:D:239:ASN:OD1	1:D:240:PRO:HD2	2.14	0.47
1:H:164:VAL:N	1:H:165:PRO:CD	2.77	0.47
1:H:92:GLY:O	1:H:95:LEU:HB2	2.14	0.47
1:B:346:LEU:CD1	1:C:346:LEU:CD1	2.92	0.47
1:C:382:LEU:HD13	1:C:401:LEU:HD22	1.95	0.47
1:E:212:GLU:HA	1:E:215:LYS:HE2	1.96	0.47
1:E:90:ASP:OD2	1:E:115:ARG:NH2	2.46	0.47
1:B:247:MSE:HE2	1:B:251:MSE:HE3	1.96	0.47
1:E:9:GLY:HA2	1:E:45:VAL:CG2	2.43	0.47
1:H:106:GLY:HA2	1:H:388:HIS:CE1	2.49	0.47
1:B:190:LEU:CD2	1:B:362:VAL:HG22	2.43	0.47
1:F:382:LEU:HD13	1:F:401:LEU:CD2	2.38	0.47
1:G:362:VAL:O	1:G:366:GLU:HG2	2.15	0.47
1:A:215:LYS:C	1:A:217:LYS:H	2.19	0.46
1:A:170:ARG:HH22	1:A:293:MSE:HB3	1.80	0.46
1:H:136:VAL:HG13	1:H:161:LEU:HD22	1.97	0.46
1:A:79:PHE:HB2	2:A:1416:NAD:C4A	2.45	0.46
1:C:17:VAL:HG11	1:C:49:VAL:HG13	1.97	0.46
1:D:90:ASP:OD1	1:D:115:ARG:NH2	2.47	0.46
1:E:358:PHE:O	1:E:362:VAL:HG13	2.15	0.46
1:F:190:LEU:CD2	1:F:362:VAL:HG22	2.42	0.46
1:B:13:THR:HB	1:B:14:PRO:HD3	1.98	0.46
1:B:49:VAL:O	1:B:53:VAL:HG23	2.15	0.46
1:F:175:MSE:HE2	1:F:176:PHE:CZ	2.50	0.46
1:D:282:ILE:HA	1:D:283:PRO:HD3	1.84	0.46
1:B:162:CYS:HB2	1:B:191:ASN:HD21	1.80	0.46
1:D:129:LYS:HB3	1:D:129:LYS:HE3	1.70	0.46
1:F:162:CYS:HB2	1:F:191:ASN:HD21	1.81	0.46
1:F:305:LEU:HD13	1:F:338:VAL:HG13	1.98	0.46
1:H:162:CYS:CB	1:H:191:ASN:ND2	2.79	0.46
1:A:175:MSE:HE2	1:A:176:PHE:CE2	2.51	0.45
1:E:145:ILE:O	1:E:148:PHE:HB3	2.16	0.45
1:F:35:TYR:C	1:F:42:GLN:HE22	2.19	0.45
1:D:162:CYS:HB2	1:D:191:ASN:HD21	1.82	0.45
1:E:284:GLU:O	1:E:286:LEU:N	2.49	0.45
1:F:303:ARG:HD2	1:F:304:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASN:HD22	1:A:163:ASN:H	1.64	0.45
1:C:111:SER:HB3	1:C:404:ILE:HG23	1.99	0.45
1:D:255:ILE:O	1:D:255:ILE:HG22	2.15	0.45
1:H:90:ASP:OD1	1:H:115:ARG:NH2	2.50	0.45
1:A:272:LEU:HD21	1:A:285:GLU:HG2	1.97	0.45
1:B:149:VAL:HG11	1:B:158:PHE:CD2	2.52	0.45
1:E:92:GLY:HA2	1:E:95:LEU:HD22	1.98	0.45
1:G:138:PHE:CE1	1:G:294:TYR:HD2	2.35	0.45
1:D:164:VAL:HG22	1:D:165:PRO:HD3	1.99	0.45
1:H:74:TYR:CD2	1:H:302:ILE:HG12	2.52	0.45
1:A:261:ARG:HH22	1:A:289:ARG:NE	2.14	0.45
1:E:13:THR:HB	1:E:14:PRO:CD	2.47	0.45
1:B:15:GLU:OE1	1:B:292:SER:O	2.35	0.45
1:D:175:MSE:HE2	1:D:176:PHE:CZ	2.52	0.45
1:H:235:ARG:HH11	1:H:235:ARG:HG2	1.82	0.45
1:A:239:ASN:OD1	1:A:240:PRO:HD2	2.16	0.44
1:B:147:GLU:HA	1:B:331:VAL:HG21	1.98	0.44
1:B:85:LYS:HG3	1:B:86:GLY:N	2.32	0.44
1:F:8:GLY:HA3	1:F:42:GLN:NE2	2.11	0.44
1:A:261:ARG:HH12	1:A:289:ARG:HH21	1.63	0.44
1:H:6:ILE:HD12	1:H:65:PHE:CE1	2.52	0.44
1:A:173:ALA:HB1	1:A:178:ALA:O	2.16	0.44
1:A:215:LYS:HE2	1:A:215:LYS:HB2	1.81	0.44
1:A:382:LEU:HD13	1:A:401:LEU:HD22	2.00	0.44
1:B:138:PHE:CZ	1:B:161:LEU:HD23	2.53	0.44
1:B:138:PHE:CZ	1:B:294:TYR:HD2	2.35	0.44
1:A:88:GLU:OE1	1:A:266:MSE:HE1	2.16	0.44
1:A:138:PHE:HZ	1:A:298:ALA:HB2	1.82	0.44
1:B:162:CYS:CB	1:B:191:ASN:HD21	2.30	0.44
1:E:224:GLU:HG2	1:E:251:MSE:HE1	2.00	0.44
1:A:78:GLN:O	2:A:1416:NAD:H52N	2.18	0.44
1:A:90:ASP:OD1	1:A:115:ARG:NH2	2.49	0.44
1:C:16:LEU:HD22	1:C:78:GLN:OE1	2.18	0.44
1:E:65:PHE:CD1	1:E:66:GLU:N	2.83	0.44
1:G:360:HIS:O	1:G:364:MSE:HG2	2.17	0.44
1:A:162:CYS:SG	1:A:164:VAL:HG13	2.58	0.44
1:A:405:LEU:HD21	1:A:414:LEU:HD22	1.98	0.44
1:G:196:ILE:HB	1:G:237:ILE:HB	2.00	0.44
1:A:140:ASN:HB3	6:A:2035:HOH:O	2.17	0.44
1:F:106:GLY:HA2	1:F:388:HIS:CE1	2.52	0.44
1:D:2:ARG:CG	1:D:72:ALA:HA	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ILE:O	1:F:149:VAL:HG23	2.18	0.44
1:B:346:LEU:HD11	1:C:346:LEU:CD1	2.48	0.43
1:E:305:LEU:HD13	1:E:338:VAL:HG13	1.99	0.43
1:F:87:ARG:O	1:F:90:ASP:HB2	2.19	0.43
1:G:170:ARG:HH12	1:G:293:MSE:SE	2.51	0.43
1:G:216:LEU:H	1:G:216:LEU:HG	1.64	0.43
1:B:87:ARG:NH1	1:B:265:VAL:HG21	2.33	0.43
1:E:323:ILE:HG21	1:E:326:LEU:HD22	1.99	0.43
1:B:294:TYR:CE1	1:B:295:SER:HB3	2.54	0.43
1:E:362:VAL:O	1:E:366:GLU:CG	2.66	0.43
1:G:363:LYS:HA	1:G:366:GLU:HG2	2.00	0.43
1:C:215:LYS:HG3	1:C:216:LEU:N	2.32	0.43
1:D:116:ALA:O	1:D:120:VAL:HG13	2.19	0.43
1:F:13:THR:N	1:F:14:PRO:CD	2.82	0.43
1:F:92:GLY:O	1:F:95:LEU:HB2	2.17	0.43
1:F:363:LYS:CE	1:F:366:GLU:OE1	2.66	0.43
1:G:363:LYS:CE	1:G:366:GLU:OE2	2.66	0.43
1:B:316:ASN:HA	1:B:332:LEU:O	2.18	0.43
1:D:294:TYR:C	1:D:296:THR:H	2.22	0.43
1:D:363:LYS:HE3	1:D:366:GLU:OE1	2.19	0.43
1:G:215:LYS:C	1:G:217:LYS:H	2.23	0.43
1:A:175:MSE:HE1	1:A:210:VAL:HA	2.01	0.43
1:E:1:MSE:HG2	1:E:28:ARG:O	2.19	0.43
1:E:259:GLU:OE2	1:E:264:GLU:HG2	2.18	0.43
1:F:346:LEU:HD23	1:G:346:LEU:HD13	2.00	0.43
1:H:107:VAL:O	1:H:110:PHE:HB3	2.18	0.43
1:H:8:GLY:HA3	1:H:42:GLN:OE1	2.19	0.43
1:A:316:ASN:HA	1:A:332:LEU:O	2.19	0.42
1:E:234:VAL:HA	1:F:383:LYS:HG3	2.00	0.42
1:G:294:TYR:CD1	1:G:295:SER:N	2.87	0.42
1:H:235:ARG:HG2	1:H:235:ARG:NH1	2.33	0.42
1:H:301:LEU:HG	1:H:305:LEU:HD22	2.01	0.42
1:A:93:ILE:N	1:A:94:PRO:CD	2.81	0.42
1:B:116:ALA:O	1:B:120:VAL:HG13	2.19	0.42
1:C:196:ILE:HB	1:C:237:ILE:HB	2.01	0.42
1:H:147:GLU:OE2	1:H:367:ARG:NH1	2.41	0.42
1:C:15:GLU:OE2	1:C:287:THR:HG23	2.19	0.42
1:B:239:ASN:OD1	1:B:240:PRO:HD2	2.20	0.42
1:A:45:VAL:CG2	1:A:273:PHE:HE1	2.32	0.42
1:C:144:HIS:CE1	1:C:366:GLU:HB2	2.54	0.42
1:D:196:ILE:HB	1:D:237:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ILE:HA	1:B:283:PRO:HD3	1.89	0.42
1:D:316:ASN:HA	1:D:332:LEU:O	2.19	0.42
1:B:147:GLU:OE2	1:B:367:ARG:HD3	2.20	0.42
1:B:392:PRO:HG3	1:B:400:LEU:HD23	2.02	0.42
1:G:90:ASP:CG	1:G:115:ARG:HH22	2.24	0.42
1:C:16:LEU:HA	1:C:295:SER:HB2	2.02	0.42
1:A:261:ARG:O	1:A:265:VAL:HG23	2.21	0.41
1:G:166:ILE:CD1	1:G:296:THR:HG22	2.50	0.41
1:E:284:GLU:C	1:E:286:LEU:N	2.74	0.41
1:G:226:PHE:CD1	1:G:247:MSE:HE3	2.55	0.41
1:F:325:ASN:ND2	1:F:351:GLY:O	2.53	0.41
1:B:162:CYS:SG	1:B:191:ASN:ND2	2.90	0.41
1:B:49:VAL:HA	1:B:52:LEU:HD12	2.03	0.41
1:C:323:ILE:HG21	1:C:326:LEU:HD22	2.02	0.41
1:D:2:ARG:HG2	1:D:71:ASP:O	2.21	0.41
1:F:164:VAL:HG22	1:F:165:PRO:HD3	2.03	0.41
1:G:353:HIS:HB2	1:H:368:LEU:HD21	2.03	0.41
1:H:181:GLU:H	1:H:181:GLU:HG3	1.65	0.41
1:C:80:ARG:O	1:C:80:ARG:HG3	2.19	0.41
1:C:162:CYS:CB	1:C:191:ASN:HD21	2.34	0.41
1:A:326:LEU:HD21	1:A:356:LEU:HG	2.02	0.41
1:B:221:ILE:HA	1:B:222:PRO:HD3	1.66	0.41
1:D:16:LEU:HA	1:D:295:SER:HB3	2.03	0.41
1:G:138:PHE:CE2	1:G:298:ALA:HB2	2.56	0.41
1:A:282:ILE:HA	1:A:283:PRO:HD3	1.95	0.41
1:A:97:TYR:HB2	1:A:99:LEU:HD22	2.03	0.41
1:G:84:LEU:HD13	1:G:266:MSE:HG3	2.02	0.41
1:H:243:ARG:HB3	1:H:251:MSE:HE3	2.03	0.41
1:G:162:CYS:HB2	1:G:191:ASN:ND2	2.36	0.41
1:E:138:PHE:HE2	1:E:298:ALA:HB2	1.85	0.41
1:H:1:MSE:HE3	1:H:28:ARG:O	2.21	0.41
1:C:249:LYS:HE3	1:C:249:LYS:HB2	1.96	0.40
1:F:225:ASP:OD1	1:F:225:ASP:N	2.54	0.40
1:F:323:ILE:HG21	1:F:326:LEU:HD22	2.02	0.40
1:G:80:ARG:NH2	2:G:1416:NAD:O1N	2.54	0.40
1:G:166:ILE:HD13	1:G:296:THR:HG22	2.03	0.40
1:G:82:GLY:HA2	1:G:411:TYR:CZ	2.56	0.40
1:H:211:PHE:CE1	1:H:237:ILE:HG13	2.56	0.40
1:A:79:PHE:HB2	2:A:1416:NAD:C5A	2.51	0.40
1:D:118:PRO:HG2	6:D:2023:HOH:O	2.21	0.40
1:H:10:SER:HB3	1:H:78:GLN:NE2	2.36	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	410/416 (99%)	398 (97%)	10 (2%)	2 (0%)	29	40
1	B	404/416 (97%)	393 (97%)	11 (3%)	0	100	100
1	C	401/416 (96%)	395 (98%)	6 (2%)	0	100	100
1	D	398/416 (96%)	387 (97%)	11 (3%)	0	100	100
1	E	378/416 (91%)	372 (98%)	5 (1%)	1 (0%)	41	51
1	F	393/416 (94%)	383 (98%)	10 (2%)	0	100	100
1	G	398/416 (96%)	386 (97%)	11 (3%)	1 (0%)	41	51
1	H	387/416 (93%)	379 (98%)	8 (2%)	0	100	100
All	All	3169/3328 (95%)	3093 (98%)	72 (2%)	4 (0%)	51	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	290	GLY
1	E	285	GLU
1	G	216	LEU

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	366/361 (101%)	327 (89%)	39 (11%)	6	7
1	B	364/361 (101%)	319 (88%)	45 (12%)	4	4
1	C	360/361 (100%)	312 (87%)	48 (13%)	4	3
1	D	357/361 (99%)	306 (86%)	51 (14%)	3	3
1	E	345/361 (96%)	280 (81%)	65 (19%)	1	1
1	F	353/361 (98%)	302 (86%)	51 (14%)	3	3
1	G	358/361 (99%)	305 (85%)	53 (15%)	3	2
1	H	350/361 (97%)	295 (84%)	55 (16%)	2	2
All	All	2853/2888 (99%)	2446 (86%)	407 (14%)	3	3

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	39	GLU
1	A	41	LYS
1	A	80	ARG
1	A	85	LYS
1	A	95	LEU
1	A	99	LEU
1	A	156	GLU
1	A	157	LYS
1	A	161	LEU
1	A	163	ASN
1	A	174	GLU
1	A	175	MSE
1	A	185	LEU
1	A	190	LEU
1	A	193	LEU
1	A	213	ASN
1	A	214	LEU
1	A	215	LYS
1	A	216	LEU
1	A	217	LYS
1	A	235	ARG
1	A	238	VAL
1	A	246	LEU
1	A	284	GLU
1	A	287	THR
1	A	294	TYR

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Mol	Chain	Res	Type
1	A	305	LEU
1	A	311	LYS
1	A	325	ASN
1	A	342	ARG
1	A	345	THR
1	A	346	LEU
1	A	365	TYR
1	A	367	ARG
1	A	375	LYS
1	A	378	LYS
1	A	382	LEU
1	A	402	GLU
1	B	25	GLU
1	B	26	ASP
1	B	43	LYS
1	B	44	ILE
1	B	55	ASP
1	B	85	LYS
1	B	95	LEU
1	B	99	LEU
1	B	163	ASN
1	B	164	VAL
1	B	175	MSE
1	B	177	SER
1	B	185	LEU
1	B	190	LEU
1	B	208	GLU
1	B	212	GLU
1	B	217	LYS
1	B	221	ILE
1	B	223	ASP
1	B	225	ASP
1	B	233	SER
1	B	238	VAL
1	B	246	LEU
1	B	247	MSE
1	B	253	LYS
1	B	261	ARG
1	B	266	MSE
1	B	270	LYS
1	B	274	GLU
1	B	278	THR

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Mol	Chain	Res	Type
1	B	280	VAL
1	B	286	LEU
1	B	293	MSE
1	B	296	THR
1	B	305	LEU
1	B	322	SER
1	B	326	LEU
1	B	346	LEU
1	B	362	VAL
1	B	363	LYS
1	B	365	TYR
1	B	367	ARG
1	B	382	LEU
1	B	385	LEU
1	B	414	LEU
1	C	25	GLU
1	C	26	ASP
1	C	28	ARG
1	C	39	GLU
1	C	43	LYS
1	C	80	ARG
1	C	85	LYS
1	C	95	LEU
1	C	96	LYS
1	C	99	LEU
1	C	132	ASN
1	C	154	GLU
1	C	157	LYS
1	C	161	LEU
1	C	163	ASN
1	C	170	ARG
1	C	177	SER
1	C	185	LEU
1	C	190	LEU
1	C	193	LEU
1	C	198	LYS
1	C	208	GLU
1	C	214	LEU
1	C	216	LEU
1	C	235	ARG
1	C	242	LEU
1	C	246	LEU

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Mol	Chain	Res	Type
1	C	250	LYS
1	C	253	LYS
1	C	254	LYS
1	C	259	GLU
1	C	260	LEU
1	C	266	MSE
1	C	271	GLU
1	C	274	GLU
1	C	285	GLU
1	C	286	LEU
1	C	287	THR
1	C	292	SER
1	C	305	LEU
1	C	326	LEU
1	C	345	THR
1	C	347	SER
1	C	363	LYS
1	C	365	TYR
1	C	382	LEU
1	C	409	ARG
1	C	414	LEU
1	D	2	ARG
1	D	26	ASP
1	D	28	ARG
1	D	39	GLU
1	D	41	LYS
1	D	58	LYS
1	D	62	SER
1	D	63	ASP
1	D	70	VAL
1	D	71	ASP
1	D	85	LYS
1	D	95	LEU
1	D	99	LEU
1	D	128	ARG
1	D	129	LYS
1	D	157	LYS
1	D	161	LEU
1	D	164	VAL
1	D	170	ARG
1	D	180	LEU
1	D	185	LEU

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Mol	Chain	Res	Type
1	D	190	LEU
1	D	193	LEU
1	D	208	GLU
1	D	215	LYS
1	D	216	LEU
1	D	225	ASP
1	D	235	ARG
1	D	246	LEU
1	D	253	LYS
1	D	261	ARG
1	D	270	LYS
1	D	274	GLU
1	D	275	LYS
1	D	278	THR
1	D	281	GLU
1	D	294	TYR
1	D	296	THR
1	D	305	LEU
1	D	311	LYS
1	D	326	LEU
1	D	342	ARG
1	D	346	LEU
1	D	363	LYS
1	D	365	TYR
1	D	367	ARG
1	D	382	LEU
1	D	385	LEU
1	D	410	GLU
1	D	413	LYS
1	D	414	LEU
1	E	1	MSE
1	E	11	SER
1	E	25	GLU
1	E	30	ASP
1	E	39	GLU
1	E	42	GLN
1	E	43	LYS
1	E	63	ASP
1	E	65	PHE
1	E	66	GLU
1	E	80	ARG
1	E	85	LYS

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Mol	Chain	Res	Type
1	E	95	LEU
1	E	96	LYS
1	E	99	LEU
1	E	121	GLU
1	E	126	THR
1	E	129	LYS
1	E	154	GLU
1	E	156	GLU
1	E	157	LYS
1	E	163	ASN
1	E	164	VAL
1	E	166	ILE
1	E	181	GLU
1	E	185	LEU
1	E	190	LEU
1	E	198	LYS
1	E	199	VAL
1	E	209	LYS
1	E	214	LEU
1	E	223	ASP
1	E	224	GLU
1	E	225	ASP
1	E	228	THR
1	E	235	ARG
1	E	242	LEU
1	E	246	LEU
1	E	250	LYS
1	E	253	LYS
1	E	254	LYS
1	E	260	LEU
1	E	265	VAL
1	E	272	LEU
1	E	274	GLU
1	E	275	LYS
1	E	286	LEU
1	E	305	LEU
1	E	309	GLU
1	E	315	VAL
1	E	326	LEU
1	E	334	ILE
1	E	342	ARG
1	E	345	THR

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Mol	Chain	Res	Type
1	E	346	LEU
1	E	362	VAL
1	E	363	LYS
1	E	367	ARG
1	E	375	LYS
1	E	376	ARG
1	E	382	LEU
1	E	398	LYS
1	E	402	GLU
1	E	410	GLU
1	E	414	LEU
1	F	25	GLU
1	F	28	ARG
1	F	43	LYS
1	F	55	ASP
1	F	66	GLU
1	F	95	LEU
1	F	99	LEU
1	F	104	THR
1	F	120	VAL
1	F	132	ASN
1	F	154	GLU
1	F	161	LEU
1	F	164	VAL
1	F	170	ARG
1	F	179	ARG
1	F	180	LEU
1	F	181	GLU
1	F	185	LEU
1	F	190	LEU
1	F	193	LEU
1	F	208	GLU
1	F	209	LYS
1	F	215	LYS
1	F	217	LYS
1	F	225	ASP
1	F	243	ARG
1	F	249	LYS
1	F	250	LYS
1	F	254	LYS
1	F	261	ARG
1	F	270	LYS

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Mol	Chain	Res	Type
1	F	275	LYS
1	F	277	ARG
1	F	280	VAL
1	F	282	ILE
1	F	284	GLU
1	F	296	THR
1	F	305	LEU
1	F	315	VAL
1	F	326	LEU
1	F	342	ARG
1	F	347	SER
1	F	362	VAL
1	F	363	LYS
1	F	367	ARG
1	F	376	ARG
1	F	382	LEU
1	F	385	LEU
1	F	398	LYS
1	F	402	GLU
1	F	410	GLU
1	G	28	ARG
1	G	40	GLU
1	G	70	VAL
1	G	80	ARG
1	G	95	LEU
1	G	96	LYS
1	G	99	LEU
1	G	120	VAL
1	G	128	ARG
1	G	157	LYS
1	G	161	LEU
1	G	163	ASN
1	G	174	GLU
1	G	177	SER
1	G	179	ARG
1	G	185	LEU
1	G	190	LEU
1	G	193	LEU
1	G	198	LYS
1	G	208	GLU
1	G	213	ASN
1	G	214	LEU

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Mol	Chain	Res	Type
1	G	216	LEU
1	G	218	LEU
1	G	246	LEU
1	G	247	MSE
1	G	253	LYS
1	G	260	LEU
1	G	261	ARG
1	G	263	ARG
1	G	265	VAL
1	G	274	GLU
1	G	277	ARG
1	G	278	THR
1	G	281	GLU
1	G	282	ILE
1	G	292	SER
1	G	293	MSE
1	G	305	LEU
1	G	326	LEU
1	G	342	ARG
1	G	345	THR
1	G	346	LEU
1	G	362	VAL
1	G	363	LYS
1	G	365	TYR
1	G	367	ARG
1	G	375	LYS
1	G	382	LEU
1	G	398	LYS
1	G	410	GLU
1	G	412	VAL
1	G	414	LEU
1	H	2	ARG
1	H	10	SER
1	H	11	SER
1	H	25	GLU
1	H	28	ARG
1	H	39	GLU
1	H	50	LYS
1	H	58	LYS
1	H	95	LEU
1	H	99	LEU
1	H	140	ASN

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Mol	Chain	Res	Type
1	H	154	GLU
1	H	156	GLU
1	H	161	LEU
1	H	167	ASN
1	H	170	ARG
1	H	175	MSE
1	H	179	ARG
1	H	181	GLU
1	H	185	LEU
1	H	190	LEU
1	H	198	LYS
1	H	208	GLU
1	H	209	LYS
1	H	213	ASN
1	H	238	VAL
1	H	246	LEU
1	H	250	LYS
1	H	253	LYS
1	H	254	LYS
1	H	259	GLU
1	H	261	ARG
1	H	263	ARG
1	H	266	MSE
1	H	269	GLU
1	H	275	LYS
1	H	278	THR
1	H	280	VAL
1	H	284	GLU
1	H	296	THR
1	H	305	LEU
1	H	311	LYS
1	H	315	VAL
1	H	325	ASN
1	H	326	LEU
1	H	346	LEU
1	H	363	LYS
1	H	365	TYR
1	H	367	ARG
1	H	376	ARG
1	H	382	LEU
1	H	385	LEU
1	H	398	LYS

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Mol	Chain	Res	Type
1	H	399	ASP
1	H	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
1	A	320	ASN
1	B	132	ASN
1	B	191	ASN
1	C	191	ASN
1	C	320	ASN
1	D	89	ASN
1	D	163	ASN
1	D	167	ASN
1	D	213	ASN
1	D	320	ASN
1	E	191	ASN
1	E	320	ASN
1	F	42	GLN
1	F	213	ASN
1	F	320	ASN
1	F	353	HIS
1	G	163	ASN
1	G	320	ASN
1	H	140	ASN
1	H	167	ASN
1	H	191	ASN
1	H	213	ASN
1	H	300	HIS
1	H	320	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	1416	3	42,48,48	1.80	3 (7%)	50,73,73	1.21	2 (4%)
2	NAD	C	1416	3	42,48,48	1.79	3 (7%)	50,73,73	1.33	7 (14%)
4	G6P	A	1418	3	16,16,16	0.94	1 (6%)	24,24,24	1.16	3 (12%)
5	SO4	D	1416	-	4,4,4	0.78	0	6,6,6	0.35	0
5	SO4	E	1416	-	4,4,4	0.29	0	6,6,6	0.46	0
4	G6P	C	1418	3	16,16,16	0.53	0	24,24,24	1.02	1 (4%)
5	SO4	B	1416	-	4,4,4	0.70	0	6,6,6	0.43	0
2	NAD	G	1416	3	42,48,48	1.76	3 (7%)	50,73,73	1.27	2 (4%)
5	SO4	G	1418	-	4,4,4	0.26	0	6,6,6	0.30	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
4	G6P	C	1418	3	1/1/6/6	2/6/26/26	0/1/1/1
2	NAD	A	1416	3	-	7/26/62/62	0/5/5/5
4	G6P	A	1418	3	1/1/6/6	3/6/26/26	0/1/1/1
2	NAD	C	1416	3	-	10/26/62/62	0/5/5/5
2	NAD	G	1416	3	-	10/26/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1416	NAD	O7N-C7N	9.55	1.42	1.24
2	C	1416	NAD	O7N-C7N	9.19	1.41	1.24
2	G	1416	NAD	O7N-C7N	9.15	1.41	1.24
2	C	1416	NAD	C2A-N3A	4.00	1.38	1.32
2	G	1416	NAD	C2A-N3A	3.98	1.38	1.32
2	A	1416	NAD	C2A-N3A	3.94	1.38	1.32
2	C	1416	NAD	C2A-N1A	2.58	1.38	1.33
2	A	1416	NAD	C2A-N1A	2.54	1.38	1.33
2	G	1416	NAD	C2A-N1A	2.42	1.38	1.33
4	A	1418	G6P	P-O2P	-2.15	1.46	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1416	NAD	N3A-C2A-N1A	-5.82	119.59	128.68
2	A	1416	NAD	N3A-C2A-N1A	-4.72	121.30	128.68
2	C	1416	NAD	N3A-C2A-N1A	-4.63	121.45	128.68
2	G	1416	NAD	PN-O3-PA	-3.63	120.36	132.83
2	A	1416	NAD	O7N-C7N-C3N	-3.21	115.79	119.63
2	C	1416	NAD	O7N-C7N-C3N	-3.11	115.91	119.63
2	C	1416	NAD	PN-O3-PA	-3.06	122.34	132.83
4	A	1418	G6P	O2P-P-O6	2.75	114.05	106.73
2	C	1416	NAD	C2N-C3N-C4N	2.47	121.06	118.26
2	C	1416	NAD	O7N-C7N-N7N	2.32	125.87	122.58
4	C	1418	G6P	C4-C3-C2	-2.27	106.86	110.82
4	A	1418	G6P	O1P-P-O3P	-2.26	101.81	110.68
2	C	1416	NAD	O5B-C5B-C4B	2.24	116.70	108.99
2	C	1416	NAD	O4B-C1B-C2B	-2.17	103.75	106.93
4	A	1418	G6P	O6-P-O3P	2.14	112.47	106.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1418	G6P	C1
4	C	1418	G6P	C1

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1416	NAD	PN-O3-PA-O5B
2	A	1416	NAD	PA-O3-PN-O5D
2	A	1416	NAD	C5D-O5D-PN-O3
2	A	1416	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	C	1416	NAD	C5B-O5B-PA-O2A
2	C	1416	NAD	C5D-O5D-PN-O1N
2	C	1416	NAD	O4D-C1D-N1N-C6N
4	A	1418	G6P	C4-C5-C6-O6
4	A	1418	G6P	O5-C5-C6-O6
4	C	1418	G6P	C4-C5-C6-O6
4	C	1418	G6P	O5-C5-C6-O6
2	G	1416	NAD	C5B-O5B-PA-O1A
2	G	1416	NAD	C5B-O5B-PA-O2A
2	G	1416	NAD	C5D-O5D-PN-O3
2	A	1416	NAD	O4D-C4D-C5D-O5D
2	C	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	O4D-C4D-C5D-O5D
2	C	1416	NAD	C3D-C4D-C5D-O5D
2	A	1416	NAD	C3D-C4D-C5D-O5D
2	G	1416	NAD	C3D-C4D-C5D-O5D
2	C	1416	NAD	PN-O3-PA-O5B
2	G	1416	NAD	PN-O3-PA-O5B
2	C	1416	NAD	C5B-O5B-PA-O3
2	G	1416	NAD	C5B-O5B-PA-O3
2	A	1416	NAD	C5D-O5D-PN-O1N
2	C	1416	NAD	C5B-O5B-PA-O1A
2	G	1416	NAD	C5D-O5D-PN-O1N
2	G	1416	NAD	C4B-C5B-O5B-PA
2	C	1416	NAD	C4B-C5B-O5B-PA
2	G	1416	NAD	PA-O3-PN-O2N
4	A	1418	G6P	C6-O6-P-O1P
2	C	1416	NAD	C5D-O5D-PN-O3

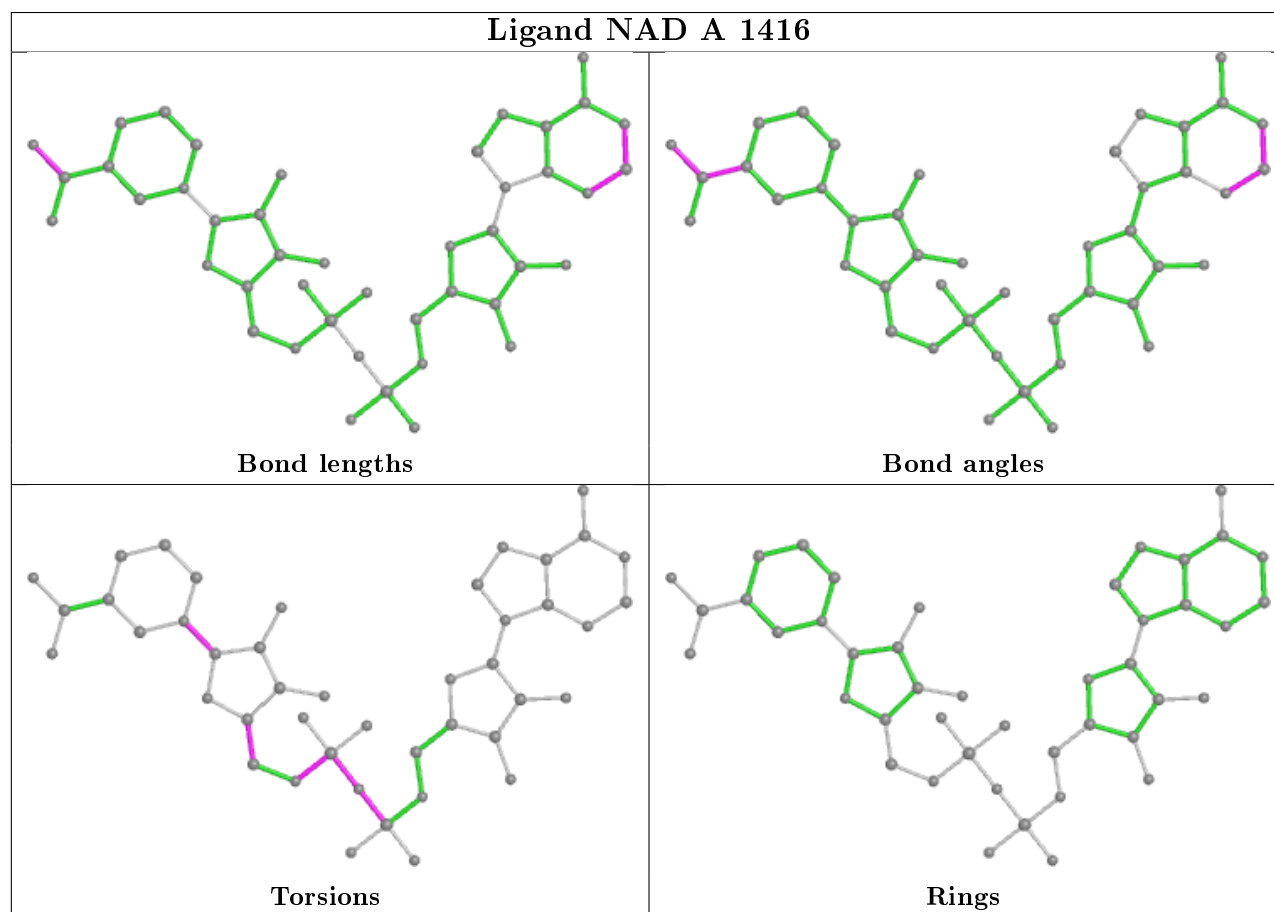
There are no ring outliers.

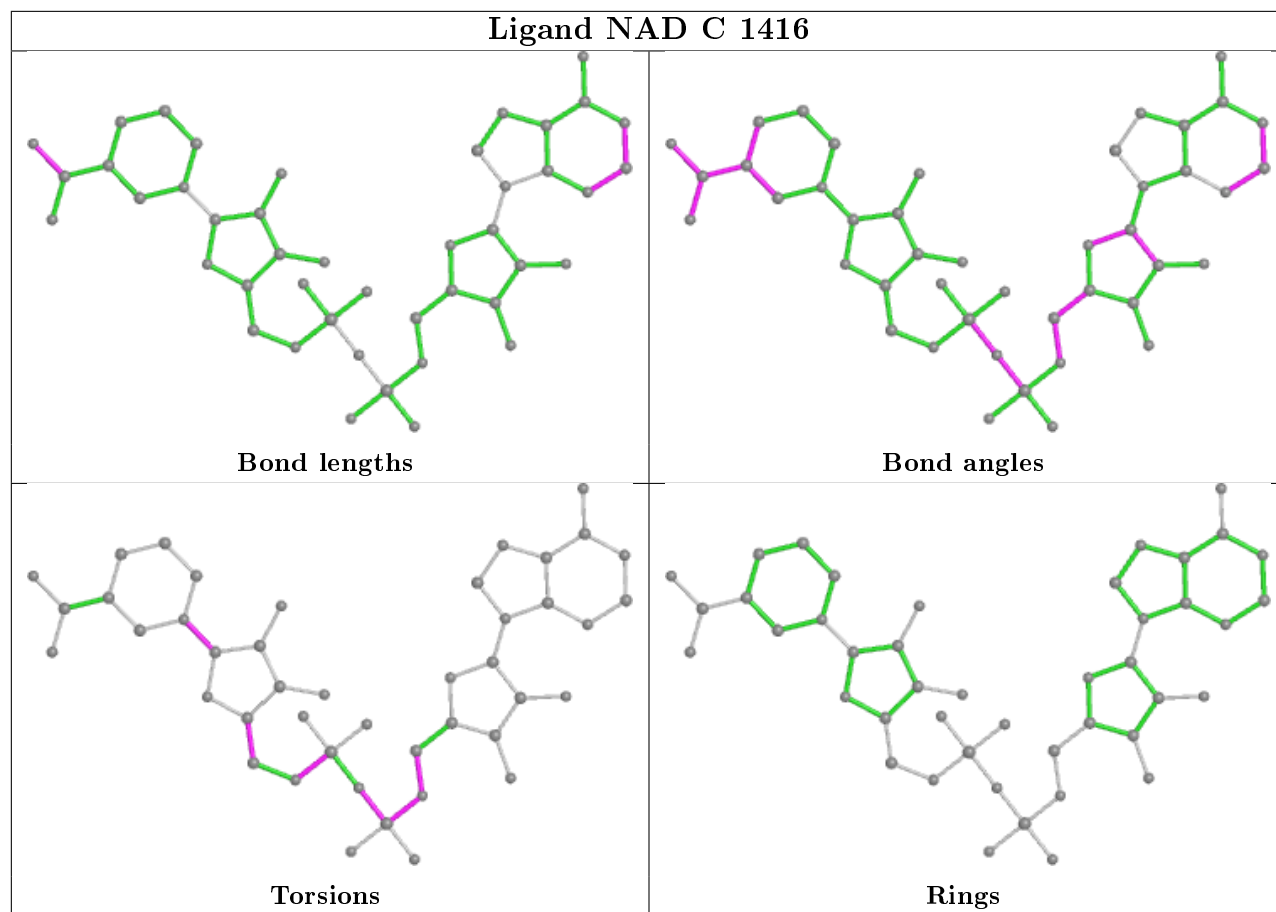
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1416	NAD	5	0
2	C	1416	NAD	2	0
4	A	1418	G6P	1	0
4	C	1418	G6P	1	0
2	G	1416	NAD	3	0

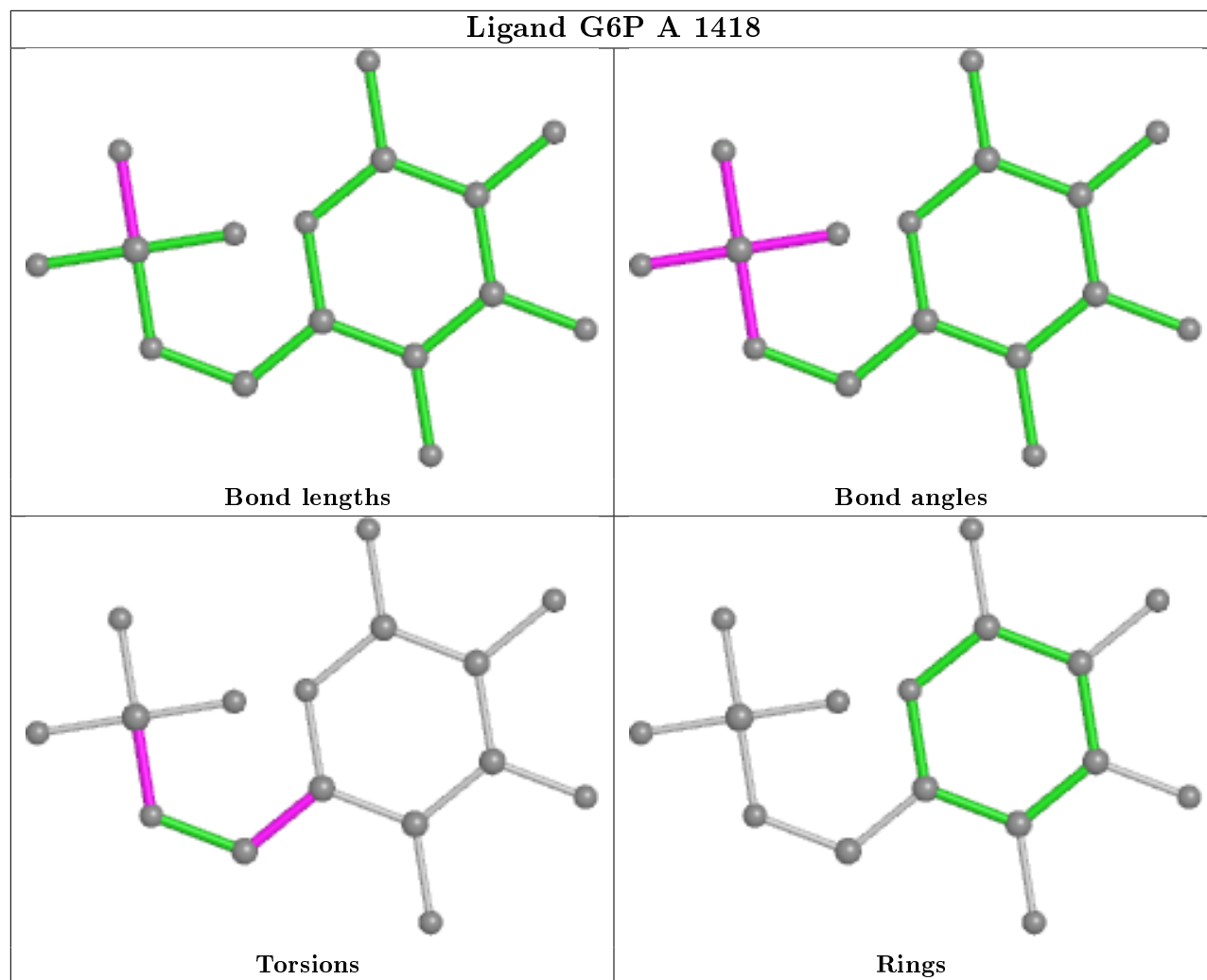
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

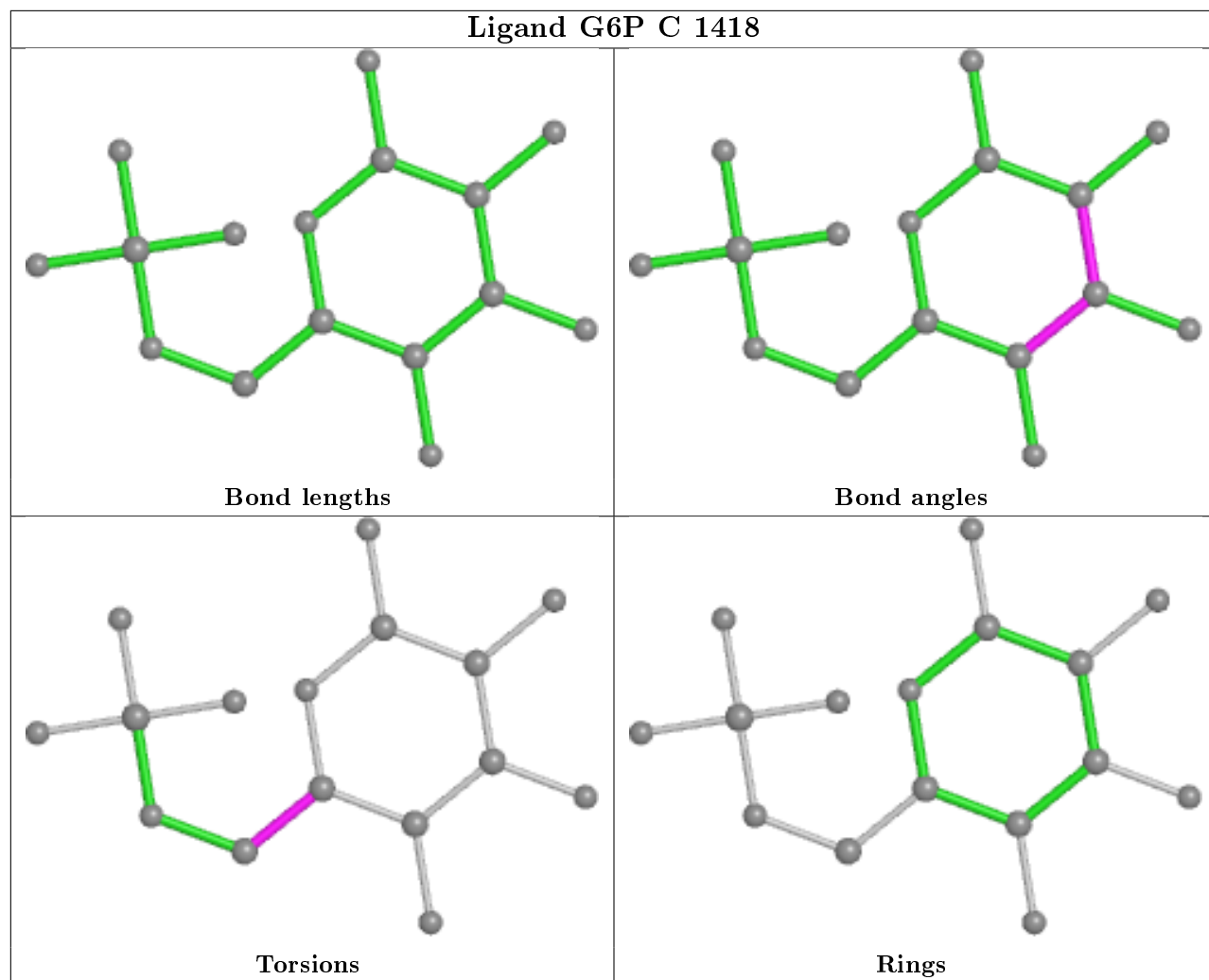
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

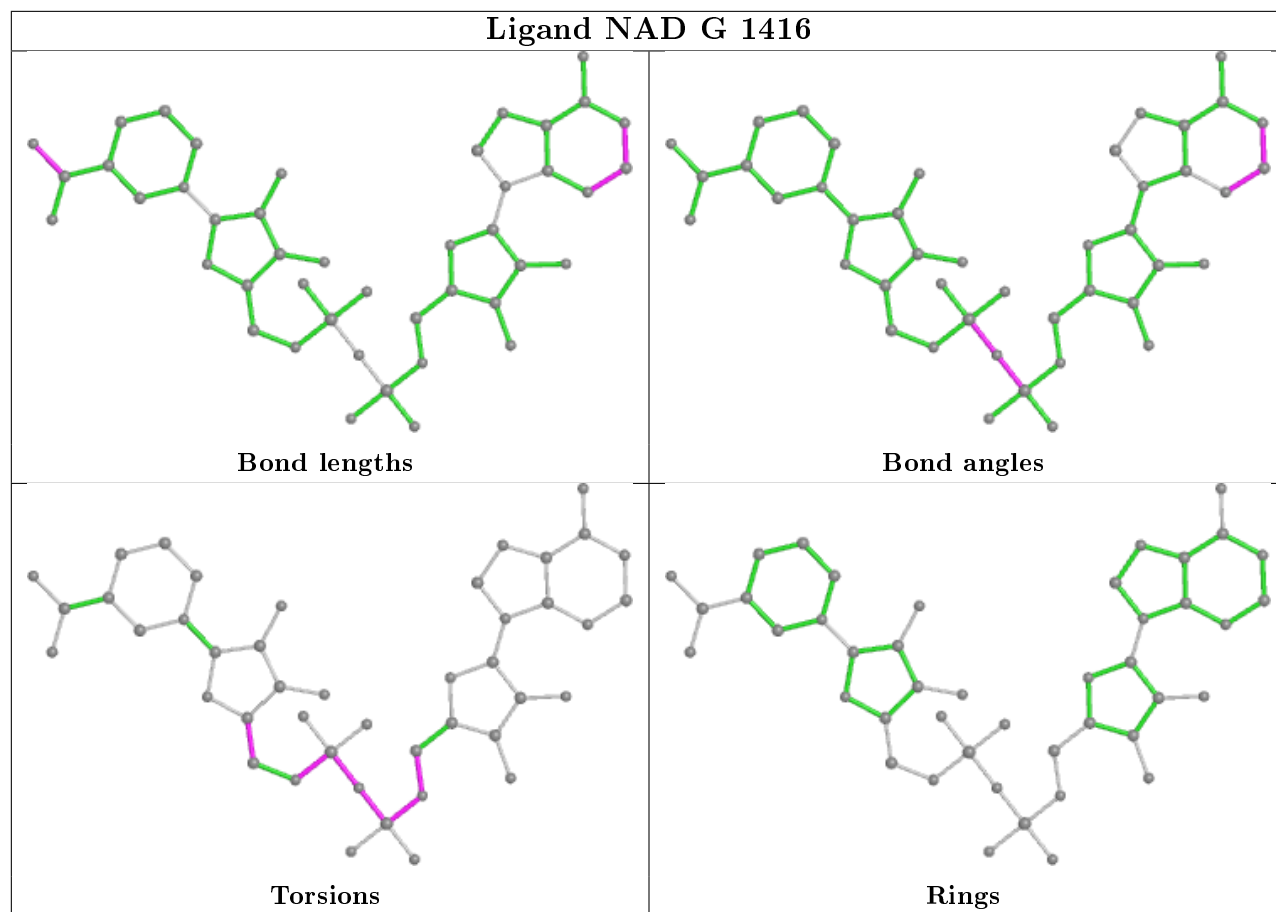




Ligand G6P A 1418







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 ⓘ

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

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

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

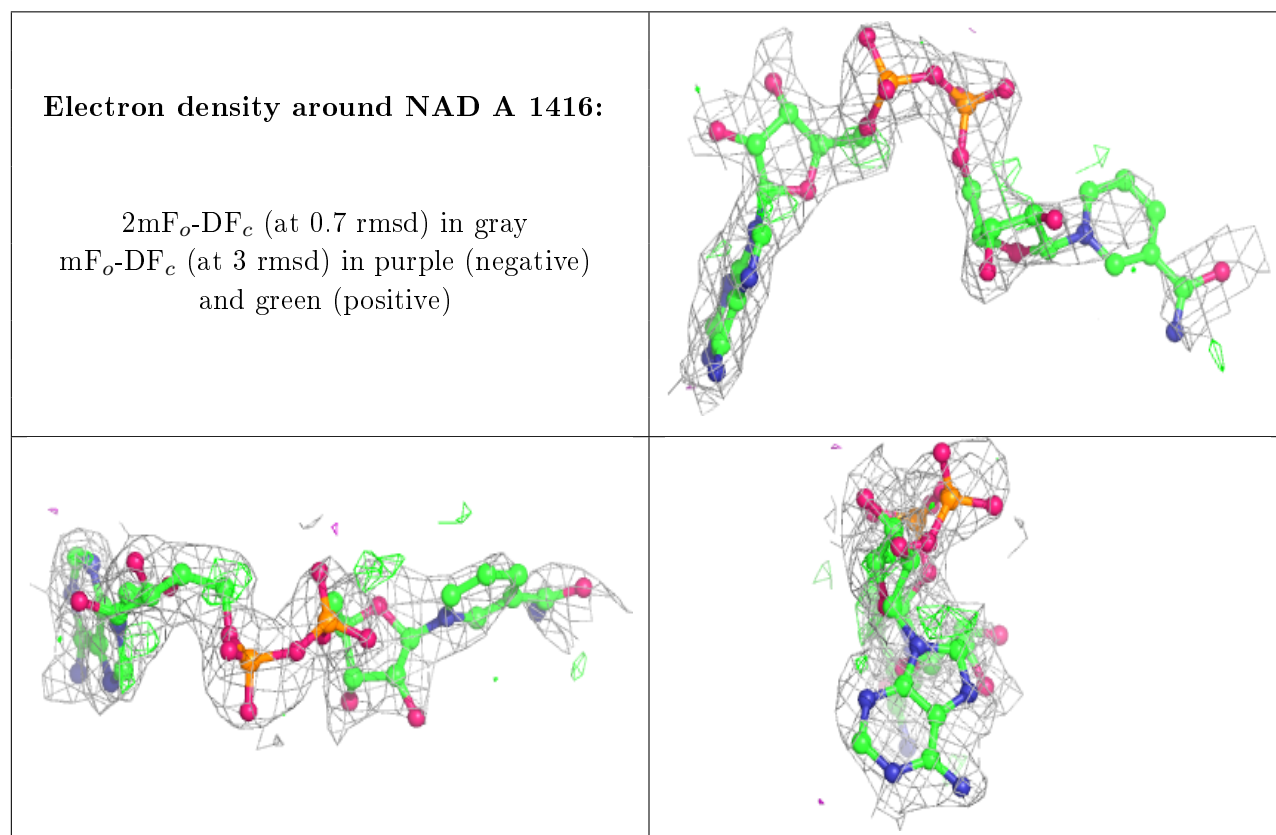
6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

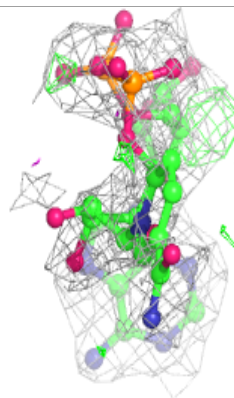
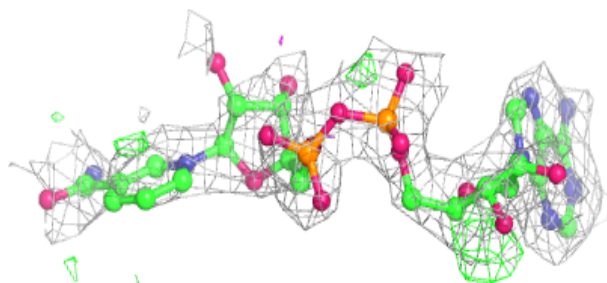
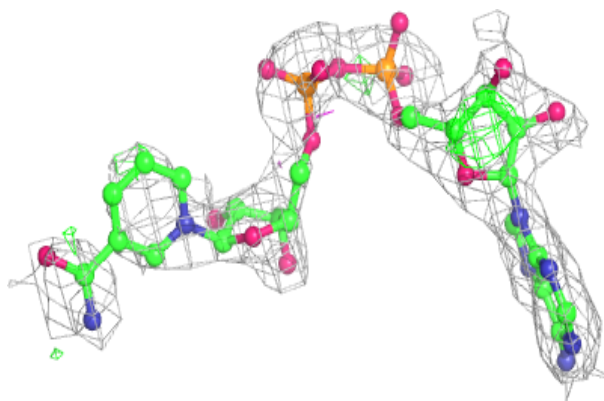
Unable to reproduce the depositors R factor - this section is therefore empty.

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

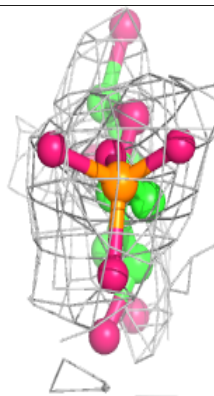
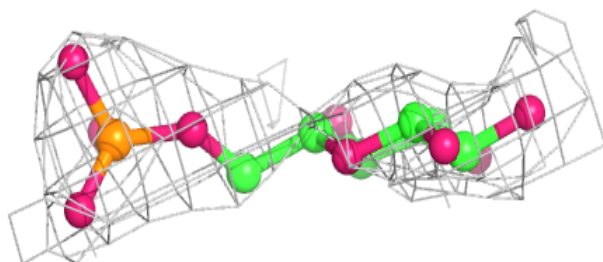
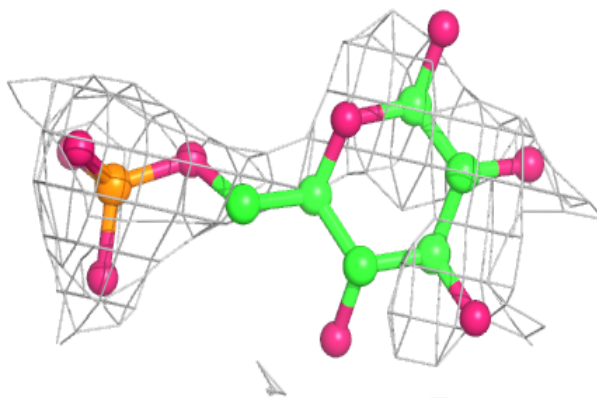


Electron density around NAD C 1416:

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

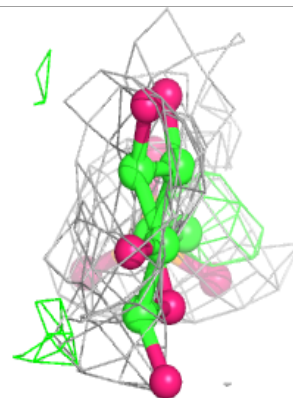
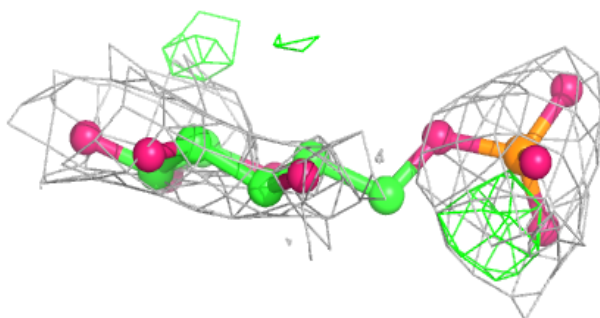
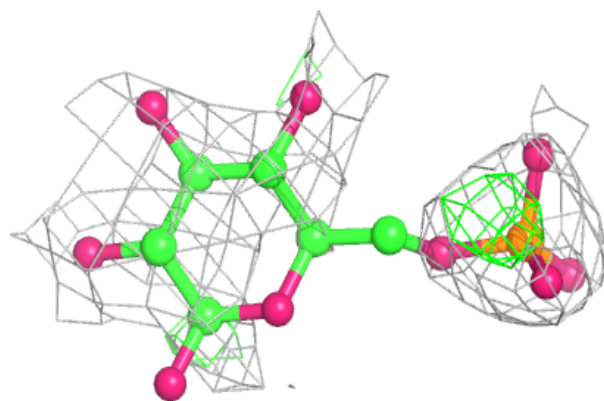
**Electron density around G6P A 1418:**

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

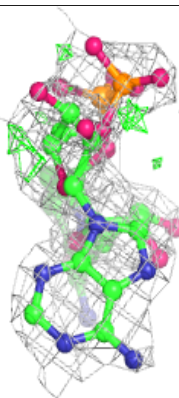
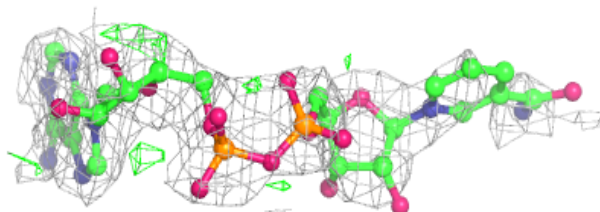
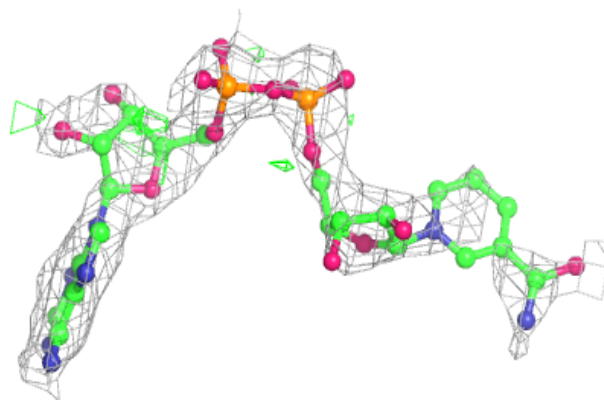


Electron density around G6P C 1418:

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

**Electron density around NAD G 1416:**

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



6.5 Other polymers

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