



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 03:29 AM UTC

PDB ID : 1QKI / pdb_00001qki
Title : X-RAY STRUCTURE OF HUMAN GLUCOSE 6-PHOSPHATE DEHYDROGENASE (VARIANT CANTON R459L) COMPLEXED WITH STRUCTURAL NADP+
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Deposited on : 1999-07-20
Resolution : 3.00 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

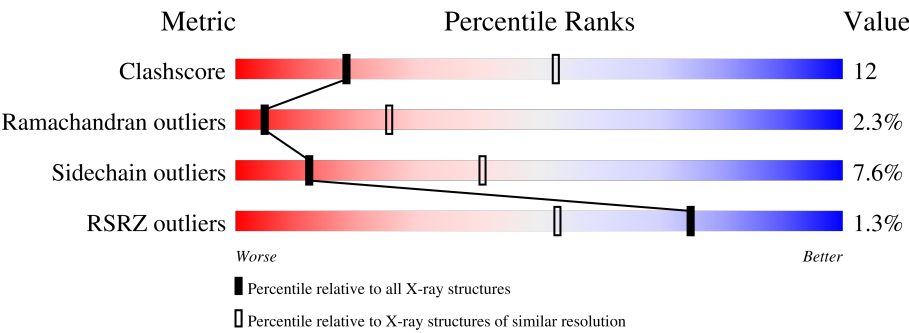
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	514	66% 25% • 5%
1	B	514	63% 28% • 5%
1	C	514	65% 27% • 5%
1	D	514	65% 26% • 5%
1	E	514	63% 27% • • 5%
1	F	514	68% 24% • •

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Mol	Chain	Length	Quality of chain
1	G	514	 % 64% 28% • 5%
1	H	514	 % 65% 27% • 5%

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
3	GOA	A	900	-	X	-	-
3	GOA	B	900	-	X	-	-
3	GOA	D	900	-	X	-	-
3	GOA	F	900	-	X	-	-
3	GOA	G	900	-	X	-	-
3	GOA	H	900	-	X	-	-
4	GOL	C	1103	-	-	X	-
4	GOL	E	1105	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31663 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-6-PHOSPHATE 1-DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3892	2484	674	714	20			
1	B	489	Total	C	N	O	S	0	0	0
			3892	2484	673	715	20			
1	C	489	Total	C	N	O	S	0	0	0
			3893	2484	673	715	21			
1	D	490	Total	C	N	O	S	0	0	0
			3898	2487	674	716	21			
1	E	487	Total	C	N	O	S	0	0	0
			3884	2479	671	713	21			
1	F	491	Total	C	N	O	S	0	0	0
			3903	2490	675	717	21			
1	G	489	Total	C	N	O	S	0	0	0
			3895	2486	674	715	20			
1	H	489	Total	C	N	O	S	0	0	0
			3897	2486	674	716	21			

There are 8 discrepancies between the modelled and reference sequences:

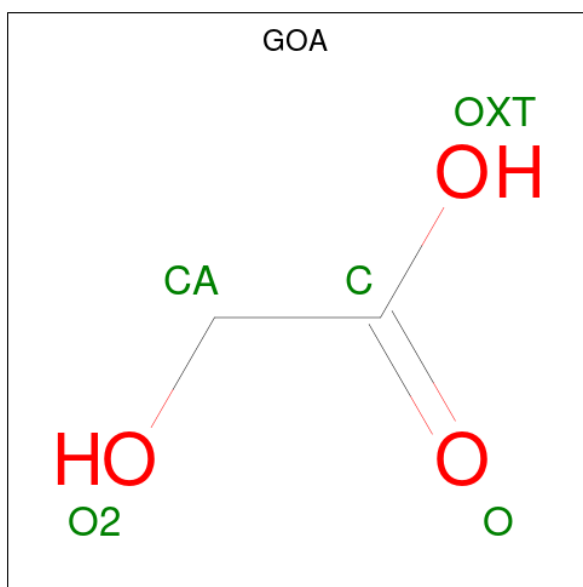
Chain	Residue	Modelled	Actual	Comment	Reference
A	459	LEU	ARG	variant	UNP P11413
B	459	LEU	ARG	variant	UNP P11413
C	459	LEU	ARG	variant	UNP P11413
D	459	LEU	ARG	variant	UNP P11413
E	459	LEU	ARG	variant	UNP P11413
F	459	LEU	ARG	variant	UNP P11413
G	459	LEU	ARG	variant	UNP P11413
H	459	LEU	ARG	variant	UNP P11413

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	H	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is GLYCOLIC ACID (CCD ID: GOA) (formula: $C_2H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	2	3		
3	B	1	Total	C	O	0	0
			5	2	3		
3	C	1	Total	C	O	0	0
			5	2	3		
3	D	1	Total	C	O	0	0
			5	2	3		
3	E	1	Total	C	O	0	0
			5	2	3		
3	F	1	Total	C	O	0	0
			5	2	3		
3	G	1	Total	C	O	0	0
			5	2	3		
3	H	1	Total	C	O	0	0
			5	2	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

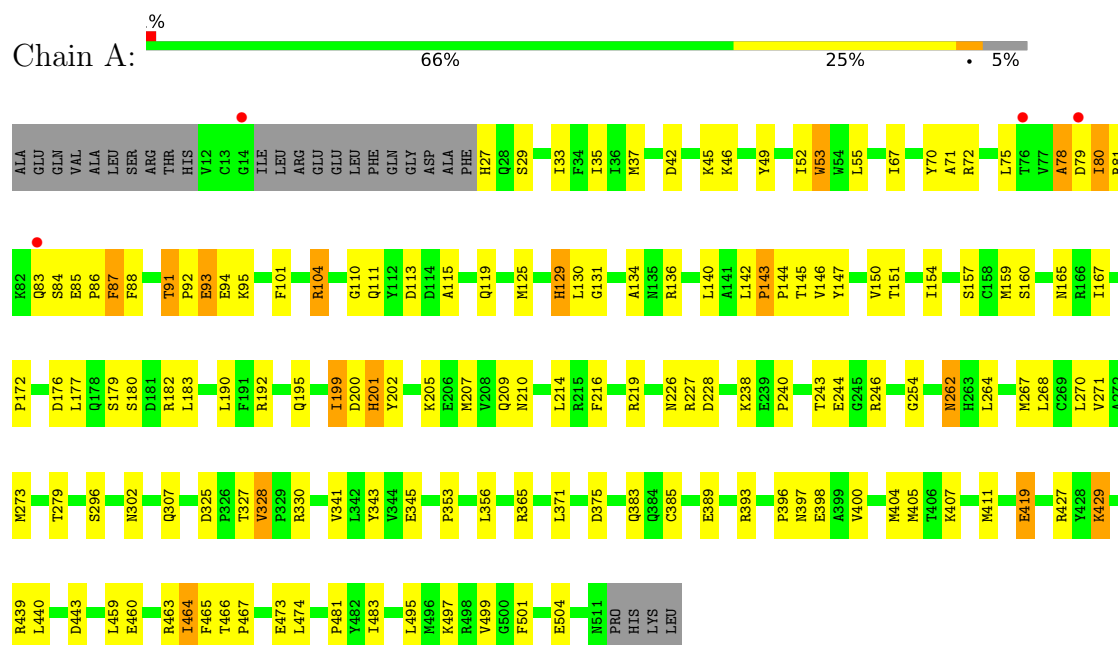
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	9	Total	O	0	0
			9	9		
5	C	3	Total	O	0	0
			3	3		
5	D	8	Total	O	0	0
			8	8		
5	E	11	Total	O	0	0
			11	11		
5	F	3	Total	O	0	0
			3	3		
5	H	8	Total	O	0	0
			8	8		

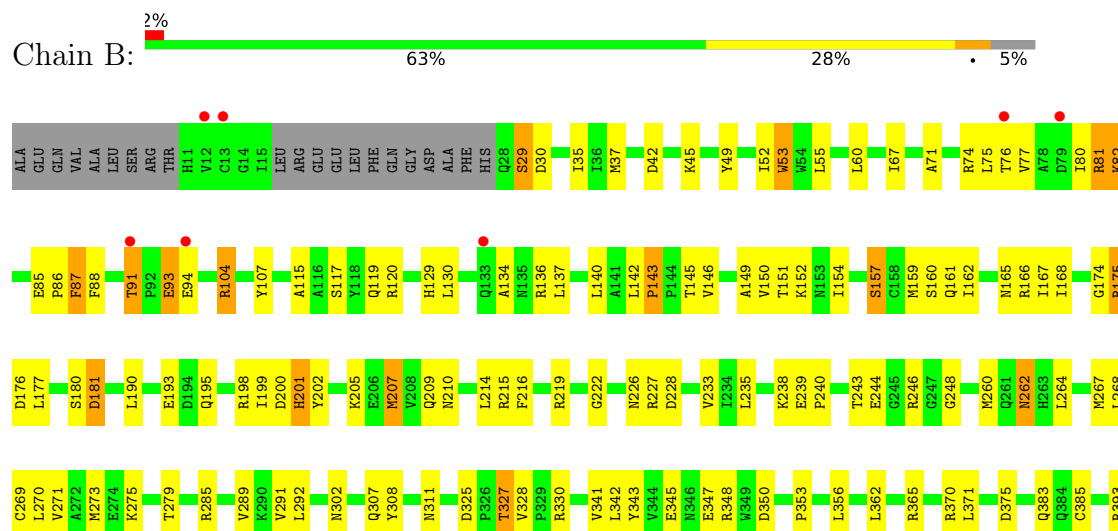
3 Residue-property plots

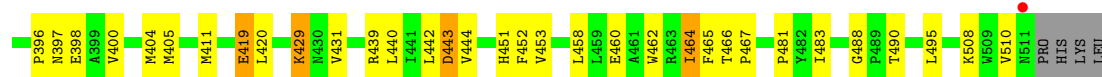
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE

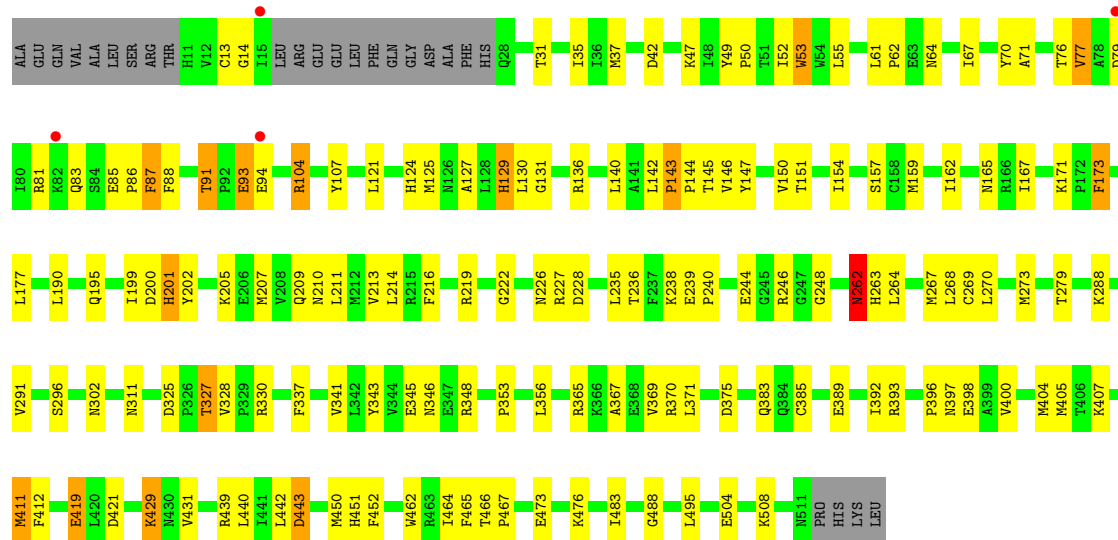


• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE

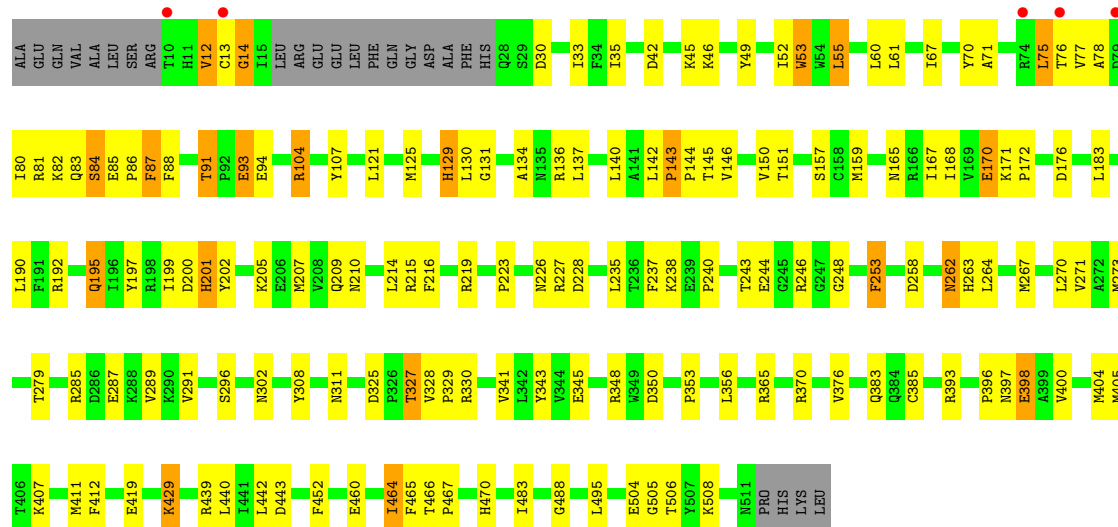




• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE

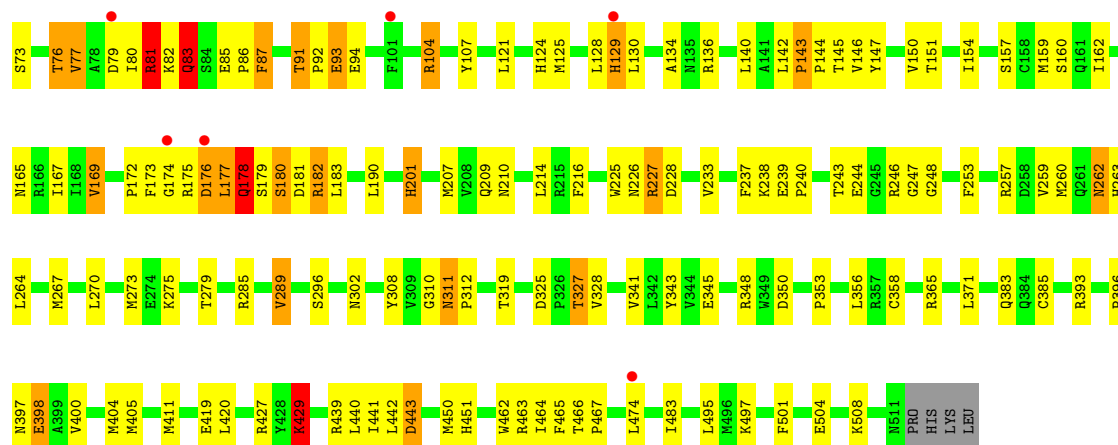


• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE

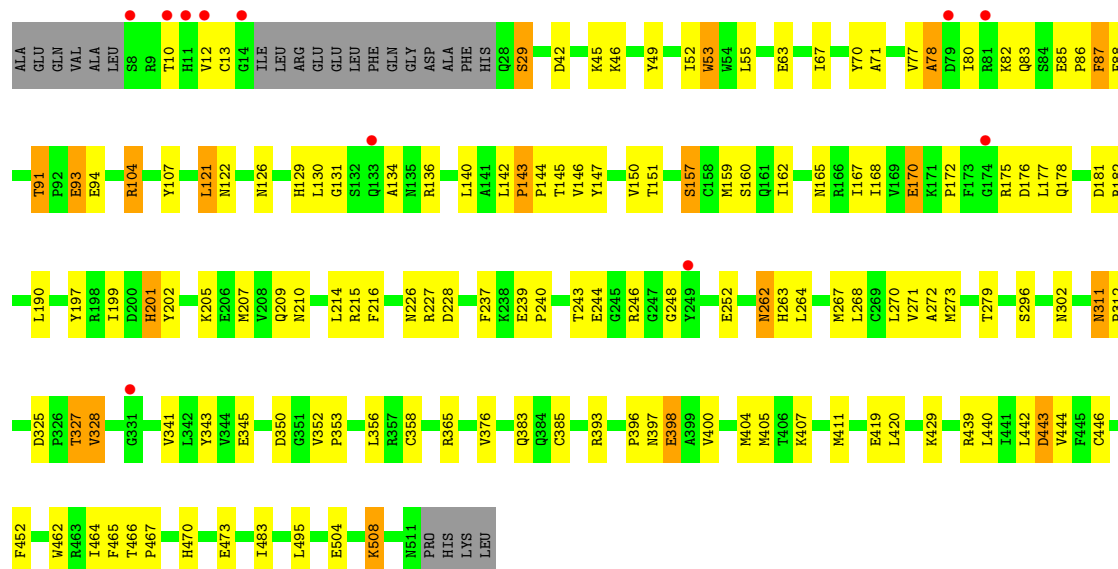


• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE

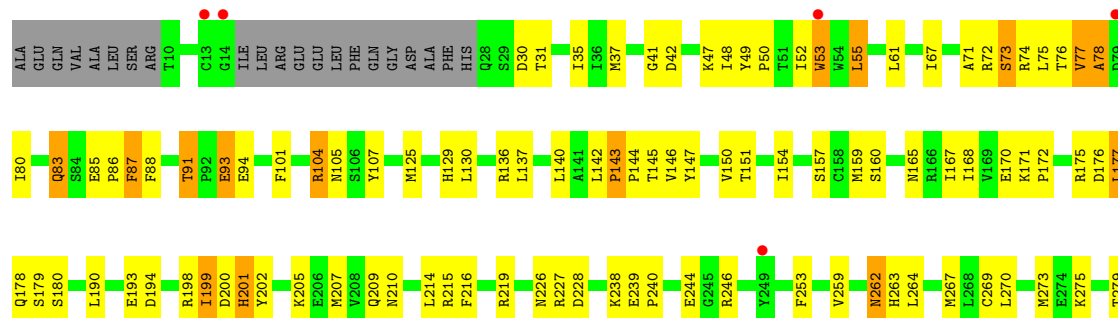


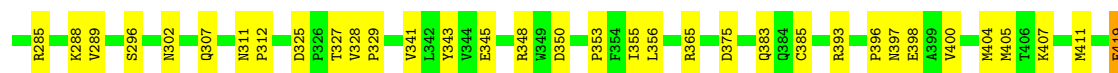


• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE

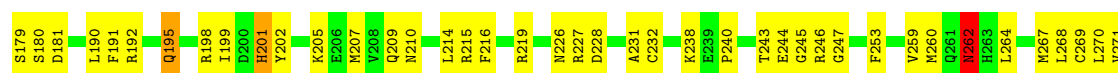


• Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE





● Molecule 1: GLUCOSE-6-PHOSPHATE 1-DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.90Å 208.70Å 214.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	85.3 (25.00-3.00) 85.2 (25.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.99Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.247 , 0.294 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31663	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: GOL, NAP, GOA

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	0.49	0/3985	0.98	14/5399 (0.3%)
1	B	0.49	0/3984	1.01	32/5398 (0.6%)
1	C	0.50	0/3985	1.01	22/5399 (0.4%)
1	D	0.49	0/3990	1.03	25/5406 (0.5%)
1	E	0.51	0/3976	1.03	21/5387 (0.4%)
1	F	0.49	0/3995	1.02	23/5413 (0.4%)
1	G	0.49	0/3987	1.04	23/5402 (0.4%)
1	H	0.51	0/3989	1.02	22/5404 (0.4%)
All	All	0.50	0/31891	1.02	182/43208 (0.4%)

There are no bond length outliers.

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	GLN	N-CA-C	-9.74	101.75	114.31
1	E	143	PRO	CA-C-N	8.88	129.78	119.47
1	E	143	PRO	C-N-CA	8.88	129.78	119.47
1	B	181	ASP	N-CA-C	-8.73	101.07	112.68
1	F	157	SER	N-CA-C	8.10	123.34	113.38
1	G	77	VAL	N-CA-C	-8.06	99.08	109.80
1	G	30	ASP	N-CA-C	8.00	123.17	112.30
1	B	157	SER	N-CA-C	7.93	123.06	113.23
1	D	75	LEU	N-CA-C	7.80	121.24	110.24
1	G	216	PHE	N-CA-C	7.73	122.74	113.16
1	G	143	PRO	CA-C-N	7.65	128.34	119.47
1	G	143	PRO	C-N-CA	7.65	128.34	119.47
1	E	157	SER	N-CA-C	7.59	122.55	113.28
1	D	157	SER	N-CA-C	7.49	122.59	113.38
1	D	199	ILE	N-CA-C	7.47	119.36	109.21
1	H	157	SER	N-CA-C	7.32	122.31	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	PRO	CA-C-N	7.31	127.95	119.47
1	C	143	PRO	C-N-CA	7.31	127.95	119.47
1	C	216	PHE	N-CA-C	7.21	122.10	113.16
1	D	134	ALA	N-CA-C	7.21	119.61	110.24
1	A	157	SER	N-CA-C	7.19	122.14	113.23
1	C	157	SER	N-CA-C	7.16	122.10	113.23
1	F	504	GLU	N-CA-C	7.12	120.42	111.24
1	B	30	ASP	N-CA-C	-6.84	99.82	110.42
1	H	253	PHE	N-CA-C	6.83	121.76	112.68
1	B	143	PRO	CA-C-N	6.78	128.32	119.84
1	B	143	PRO	C-N-CA	6.78	128.32	119.84
1	E	216	PHE	N-CA-C	6.77	121.70	113.17
1	D	216	PHE	N-CA-C	6.75	121.53	113.16
1	H	216	PHE	N-CA-C	6.72	121.64	113.17
1	E	181	ASP	N-CA-C	-6.71	104.35	112.54
1	H	143	PRO	CA-C-N	6.68	128.19	119.84
1	H	143	PRO	C-N-CA	6.68	128.19	119.84
1	F	199	ILE	N-CA-C	6.64	118.71	109.55
1	A	216	PHE	N-CA-C	6.62	121.37	113.16
1	D	253	PHE	N-CA-C	6.59	119.79	111.69
1	G	239	GLU	CA-C-N	6.53	126.11	119.19
1	G	239	GLU	C-N-CA	6.53	126.11	119.19
1	B	216	PHE	N-CA-C	6.51	121.23	113.16
1	C	464	ILE	N-CA-C	6.50	116.64	110.53
1	G	465	PHE	N-CA-C	6.47	121.38	112.90
1	G	464	ILE	N-CA-C	6.47	116.61	110.53
1	F	311	ASN	CA-C-N	6.43	126.35	119.28
1	F	311	ASN	C-N-CA	6.43	126.35	119.28
1	A	143	PRO	CA-C-N	6.36	127.79	119.84
1	A	143	PRO	C-N-CA	6.36	127.79	119.84
1	D	465	PHE	N-CA-C	6.27	121.11	112.90
1	H	201	HIS	N-CA-C	6.27	120.49	112.34
1	D	195	GLN	N-CA-C	-6.25	106.62	114.56
1	D	201	HIS	N-CA-C	6.20	119.69	111.75
1	E	464	ILE	N-CA-C	6.15	116.93	110.72
1	E	239	GLU	CA-C-N	6.14	125.84	119.64
1	E	239	GLU	C-N-CA	6.14	125.84	119.64
1	G	199	ILE	N-CA-C	6.14	118.82	109.12
1	H	199	ILE	N-CA-C	6.12	118.00	109.55
1	B	134	ALA	N-CA-C	6.09	118.16	110.24
1	F	239	GLU	CA-C-N	6.09	125.64	119.19
1	F	239	GLU	C-N-CA	6.09	125.64	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	215	ARG	N-CA-C	6.02	117.64	111.14
1	B	464	ILE	N-CA-C	6.02	116.19	110.53
1	G	41	GLY	N-CA-C	5.99	118.92	112.33
1	G	157	SER	N-CA-C	5.98	120.65	113.23
1	C	465	PHE	N-CA-C	5.96	120.70	112.90
1	F	420	LEU	N-CA-C	-5.96	99.53	109.24
1	F	143	PRO	CA-C-N	5.95	126.38	119.47
1	F	143	PRO	C-N-CA	5.95	126.38	119.47
1	F	215	ARG	N-CA-C	5.92	117.54	111.14
1	G	31	THR	N-CA-C	-5.90	100.08	109.76
1	F	464	ILE	N-CA-C	5.89	116.67	110.72
1	D	488	GLY	CA-C-N	5.88	126.22	119.93
1	D	488	GLY	C-N-CA	5.88	126.22	119.93
1	G	488	GLY	CA-C-N	5.88	126.18	119.83
1	G	488	GLY	C-N-CA	5.88	126.18	119.83
1	F	216	PHE	N-CA-C	5.85	120.42	113.28
1	C	199	ILE	N-CA-C	5.84	117.15	109.21
1	E	143	PRO	N-CA-C	5.84	117.82	110.70
1	F	83	GLN	N-CA-C	-5.82	105.83	113.17
1	A	419	GLU	N-CA-C	5.81	117.36	108.52
1	H	262	ASN	N-CA-C	5.80	120.37	113.12
1	B	82	LYS	N-CA-C	5.79	119.48	111.55
1	D	200	ASP	N-CA-C	-5.79	98.47	110.80
1	A	143	PRO	N-CA-C	5.78	117.75	110.70
1	G	143	PRO	N-CA-C	5.75	117.72	110.70
1	E	81	ARG	N-CA-C	-5.75	104.70	110.97
1	A	134	ALA	N-CA-C	5.74	117.70	110.24
1	F	352	VAL	N-CA-C	5.74	113.56	108.63
1	D	311	ASN	CA-C-N	5.70	125.55	119.28
1	D	311	ASN	C-N-CA	5.70	125.55	119.28
1	F	143	PRO	N-CA-C	5.69	117.64	110.70
1	B	465	PHE	N-CA-C	5.68	120.34	112.90
1	C	419	GLU	N-CA-C	5.68	117.74	108.76
1	D	143	PRO	N-CA-C	5.67	117.61	110.70
1	F	134	ALA	N-CA-C	5.66	118.05	110.35
1	B	419	GLU	N-CA-C	5.64	117.09	108.52
1	D	171	LYS	CA-C-N	5.64	125.31	119.56
1	D	171	LYS	C-N-CA	5.64	125.31	119.56
1	G	83	GLN	N-CA-C	-5.63	98.81	110.80
1	C	173	PHE	N-CA-C	5.61	118.87	109.95
1	B	29	SER	N-CA-C	5.60	122.72	110.80
1	H	465	PHE	N-CA-C	5.59	120.22	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	ILE	N-CA-C	5.58	117.08	111.00
1	D	84	SER	N-CA-C	-5.58	104.60	111.40
1	F	13	CYS	N-CA-C	-5.58	101.19	109.11
1	H	31	THR	N-CA-C	5.58	122.68	110.80
1	A	201	HIS	N-CA-C	5.57	119.58	112.34
1	B	199	ILE	N-CA-C	5.56	116.77	109.21
1	E	420	LEU	N-CA-C	-5.56	100.18	109.24
1	C	488	GLY	CA-C-N	5.52	125.79	119.83
1	C	488	GLY	C-N-CA	5.52	125.79	119.83
1	H	420	LEU	N-CA-C	-5.51	100.26	109.24
1	F	170	GLU	N-CA-C	5.51	117.14	111.03
1	D	143	PRO	CA-C-N	5.47	126.68	119.84
1	D	143	PRO	C-N-CA	5.47	126.68	119.84
1	B	275	LYS	CA-C-N	5.46	125.44	120.03
1	B	275	LYS	C-N-CA	5.46	125.44	120.03
1	H	464	ILE	N-CA-C	5.44	116.09	110.82
1	B	420	LEU	N-CA-C	-5.43	99.88	108.73
1	E	429	LYS	N-CA-C	5.43	119.40	112.34
1	H	195	GLN	N-CA-C	-5.43	107.67	114.56
1	A	465	PHE	N-CA-C	5.42	119.95	113.23
1	B	200	ASP	N-CA-C	-5.42	99.27	110.80
1	E	134	ALA	N-CA-C	5.42	117.28	110.24
1	B	308	TYR	N-CA-C	5.41	118.75	110.20
1	A	254	GLY	N-CA-C	-5.41	105.94	112.48
1	C	311	ASN	CA-C-N	5.37	125.19	119.28
1	C	311	ASN	C-N-CA	5.37	125.19	119.28
1	E	308	TYR	N-CA-C	5.37	118.68	110.20
1	F	121	LEU	N-CA-C	-5.37	105.34	111.14
1	B	215	ARG	N-CA-C	5.36	116.93	111.14
1	H	275	LYS	CA-C-N	5.36	125.34	120.03
1	H	275	LYS	C-N-CA	5.36	125.34	120.03
1	B	174	GLY	N-CA-C	-5.36	100.48	113.18
1	A	199	ILE	N-CA-C	5.35	117.58	109.12
1	C	421	ASP	N-CA-C	5.34	118.27	109.72
1	C	143	PRO	N-CA-C	5.34	117.21	110.70
1	C	239	GLU	CA-C-N	5.33	124.84	119.19
1	C	239	GLU	C-N-CA	5.33	124.84	119.19
1	G	419	GLU	N-CA-C	5.33	117.18	108.76
1	H	158	CYS	N-CA-C	5.33	119.75	112.88
1	G	421	ASP	N-CA-C	5.31	118.22	109.72
1	C	77	VAL	N-CA-C	5.29	120.35	109.34
1	D	258	ASP	N-CA-C	5.28	116.72	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	464	ILE	N-CA-C	5.28	115.49	110.53
1	F	465	PHE	N-CA-C	5.26	119.78	112.90
1	D	170	GLU	N-CA-C	5.23	116.84	111.03
1	E	465	PHE	N-CA-C	5.22	119.74	112.90
1	B	207	MET	N-CA-C	5.21	117.71	111.71
1	A	84	SER	N-CA-C	-5.21	105.04	111.40
1	H	143	PRO	N-CA-C	5.20	117.05	110.70
1	B	195	GLN	N-CA-C	-5.20	107.96	114.56
1	E	275	LYS	CA-C-N	5.20	125.17	120.03
1	E	275	LYS	C-N-CA	5.20	125.17	120.03
1	G	215	ARG	N-CA-C	5.19	116.74	111.14
1	F	328	VAL	N-CA-C	5.18	114.17	108.05
1	E	260	MET	N-CA-C	5.18	116.61	110.97
1	E	311	ASN	CA-C-N	5.16	124.96	119.28
1	E	311	ASN	C-N-CA	5.16	124.96	119.28
1	C	195	GLN	N-CA-C	-5.16	107.66	114.31
1	E	83	GLN	N-CA-C	-5.16	99.81	110.80
1	H	121	LEU	N-CA-C	-5.14	105.36	110.97
1	B	239	GLU	CA-C-N	5.14	124.64	119.19
1	B	239	GLU	C-N-CA	5.14	124.64	119.19
1	A	328	VAL	N-CA-C	5.12	114.09	108.05
1	H	73	SER	N-CA-C	5.12	117.31	110.35
1	C	262	ASN	N-CA-C	5.11	119.13	112.13
1	D	14	GLY	N-CA-C	-5.11	101.07	113.18
1	F	272	ALA	N-CA-C	5.11	119.78	113.50
1	B	222	GLY	CA-C-N	5.11	126.22	119.84
1	B	222	GLY	C-N-CA	5.11	126.22	119.84
1	B	143	PRO	N-CA-C	5.09	116.91	110.70
1	B	488	GLY	CA-C-N	5.09	125.38	119.93
1	B	488	GLY	C-N-CA	5.09	125.38	119.93
1	H	181	ASP	N-CA-C	-5.09	106.17	112.38
1	B	311	ASN	CA-C-N	5.08	124.87	119.28
1	B	311	ASN	C-N-CA	5.08	124.87	119.28
1	D	215	ARG	N-CA-C	5.05	116.60	111.14
1	C	431	VAL	N-CA-C	5.05	115.92	109.30
1	G	48	ILE	N-CA-C	5.04	115.66	110.36
1	B	431	VAL	N-CA-C	5.04	116.17	109.37
1	C	200	ASP	N-CA-C	-5.03	100.09	110.80
1	G	275	LYS	CA-C-N	5.00	125.21	120.31
1	G	275	LYS	C-N-CA	5.00	125.21	120.31

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	3892	0	3770	88	0
1	B	3892	0	3767	99	0
1	C	3893	0	3768	96	0
1	D	3898	0	3770	92	0
1	E	3884	0	3763	110	0
1	F	3903	0	3772	77	0
1	G	3895	0	3770	108	0
1	H	3897	0	3774	97	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	0	0
2	H	48	0	25	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	B	12	0	16	3	0
4	C	6	0	8	4	0
4	E	6	0	8	4	0
4	G	6	0	8	3	0
5	A	13	0	0	0	0
5	B	9	0	0	1	0
5	C	3	0	0	1	0
5	D	8	0	0	0	0
5	E	11	0	0	0	0
5	F	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	8	0	0	2	0
All	All	31663	0	30394	747	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 12.

All (747) 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:B:177:LEU:HB2	1:B:466:THR:HG21	1.42	0.98
1:E:227:ARG:NH2	4:E:1105:GOL:H2	1.80	0.96
1:B:262:ASN:H	1:B:262:ASN:HD22	1.15	0.94
1:G:140:LEU:HD11	1:G:167:ILE:HD11	1.50	0.94
1:A:262:ASN:HD22	1:A:262:ASN:H	1.18	0.89
1:H:262:ASN:H	1:H:262:ASN:HD22	1.25	0.85
1:B:151:THR:HG22	1:B:190:LEU:HD12	1.62	0.82
1:H:140:LEU:HD11	1:H:167:ILE:HD11	1.59	0.82
1:E:177:LEU:HB2	1:E:462:TRP:HB3	1.60	0.81
1:A:240:PRO:HD3	1:A:365:ARG:HB2	1.61	0.81
1:A:463:ARG:HG2	1:E:474:LEU:HD21	1.61	0.81
1:D:264:LEU:HD23	1:D:356:LEU:HB3	1.62	0.80
1:G:264:LEU:HD23	1:G:356:LEU:HB3	1.63	0.79
1:D:240:PRO:HD3	1:D:365:ARG:HB2	1.62	0.79
1:F:264:LEU:HD23	1:F:356:LEU:HB3	1.65	0.78
1:H:240:PRO:HD3	1:H:365:ARG:HB2	1.64	0.78
1:B:264:LEU:HD23	1:B:356:LEU:HB3	1.65	0.78
1:E:227:ARG:HH22	4:E:1105:GOL:H2	1.44	0.78
1:H:175:ARG:H	1:H:175:ARG:HD3	1.47	0.78
1:C:76:THR:CB	1:C:81:ARG:HG2	2.13	0.78
1:H:508:LYS:HE2	1:H:508:LYS:H	1.49	0.78
1:B:146:VAL:HG12	1:B:150:VAL:HG23	1.66	0.77
1:C:227:ARG:HH22	4:C:1103:GOL:H2	1.49	0.77
1:B:140:LEU:HD11	1:B:167:ILE:HD11	1.65	0.77
1:E:146:VAL:HG12	1:E:150:VAL:HG23	1.67	0.76
1:C:240:PRO:HD3	1:C:365:ARG:HB2	1.67	0.76
1:C:146:VAL:HG12	1:C:150:VAL:HG23	1.68	0.75
1:F:82:LYS:O	1:F:86:PRO:HD2	1.86	0.75
1:H:264:LEU:HD23	1:H:356:LEU:HB3	1.69	0.75
1:D:140:LEU:HD11	1:D:167:ILE:HD11	1.69	0.74
1:G:262:ASN:H	1:G:262:ASN:HD22	1.36	0.74
1:C:264:LEU:HD23	1:C:356:LEU:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:PRO:HD3	1:E:365:ARG:HB2	1.70	0.73
1:G:177:LEU:HB2	1:G:466:THR:HG21	1.69	0.73
1:B:226:ASN:HD21	1:B:228:ASP:HB2	1.53	0.73
1:B:240:PRO:HD3	1:B:365:ARG:HB2	1.70	0.73
1:E:264:LEU:HD23	1:E:356:LEU:HB3	1.69	0.72
1:G:240:PRO:HD3	1:G:365:ARG:HB2	1.71	0.72
1:D:142:LEU:HB2	1:D:143:PRO:HD2	1.70	0.72
1:F:146:VAL:HG12	1:F:150:VAL:HG23	1.72	0.72
4:B:1101:GOL:H2	1:D:227:ARG:NH2	2.05	0.72
1:G:146:VAL:HG12	1:G:150:VAL:HG23	1.71	0.71
1:F:142:LEU:HB2	1:F:143:PRO:HD2	1.71	0.71
1:C:177:LEU:HB2	1:C:466:THR:HG21	1.72	0.71
1:F:140:LEU:HD11	1:F:167:ILE:HD11	1.71	0.71
1:D:146:VAL:HG12	1:D:150:VAL:HG23	1.73	0.71
1:A:140:LEU:HD11	1:A:167:ILE:HD11	1.72	0.69
1:E:35:ILE:HD12	1:E:35:ILE:H	1.57	0.69
1:E:136:ARG:HB2	1:E:165:ASN:HD22	1.57	0.69
1:A:146:VAL:HG12	1:A:150:VAL:HG23	1.73	0.69
1:E:262:ASN:H	1:E:262:ASN:HD22	1.39	0.69
1:B:75:LEU:HB2	1:B:107:TYR:CE2	2.29	0.68
1:C:140:LEU:HD11	1:C:167:ILE:HD11	1.74	0.68
1:E:151:THR:HG22	1:E:190:LEU:HD12	1.73	0.68
1:G:177:LEU:HD13	1:G:462:TRP:HB3	1.76	0.68
1:A:37:MET:HE2	1:A:154:ILE:HD11	1.74	0.68
1:H:270:LEU:HA	1:H:273:MET:HE3	1.74	0.68
1:G:226:ASN:HD21	1:G:228:ASP:HB2	1.59	0.67
1:B:177:LEU:HD13	1:B:462:TRP:HB3	1.76	0.67
1:G:170:GLU:HG3	1:G:171:LYS:HD3	1.77	0.67
1:G:227:ARG:HH21	4:G:1104:GOL:H11	1.60	0.66
1:A:325:ASP:O	1:A:328:VAL:HG12	1.96	0.66
1:B:180:SER:HB3	1:B:462:TRP:CH2	2.29	0.66
1:C:226:ASN:HD21	1:C:228:ASP:HB2	1.61	0.66
1:F:325:ASP:O	1:F:328:VAL:HG12	1.95	0.66
1:G:71:ALA:HB3	1:G:107:TYR:OH	1.96	0.66
1:C:325:ASP:O	1:C:328:VAL:HG12	1.96	0.66
1:D:226:ASN:HD21	1:D:228:ASP:HB2	1.60	0.66
1:B:76:THR:CB	1:B:81:ARG:HB2	2.26	0.65
1:C:270:LEU:HA	1:C:273:MET:CE	2.26	0.65
1:C:262:ASN:H	1:C:262:ASN:HD22	1.44	0.65
1:F:240:PRO:HD3	1:F:365:ARG:HB2	1.77	0.65
1:D:78:ALA:O	1:D:82:LYS:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:THR:HG22	1:H:190:LEU:HD12	1.77	0.65
1:A:226:ASN:HD21	1:A:228:ASP:HB2	1.61	0.65
1:D:35:ILE:HD12	1:D:35:ILE:H	1.61	0.65
1:B:91:THR:HG23	1:B:94:GLU:CB	2.27	0.64
1:F:262:ASN:H	1:F:262:ASN:ND2	1.95	0.64
1:C:142:LEU:HB2	1:C:143:PRO:HD2	1.79	0.64
1:G:35:ILE:HD12	1:G:35:ILE:H	1.62	0.64
1:G:262:ASN:H	1:G:262:ASN:ND2	1.95	0.64
1:F:170:GLU:O	1:F:172:PRO:HD3	1.97	0.63
1:F:385:CYS:HA	1:F:405:MET:HE2	1.80	0.63
1:E:182:ARG:HD2	1:E:182:ARG:N	2.13	0.63
1:B:136:ARG:HB2	1:B:165:ASN:HD22	1.64	0.62
1:G:227:ARG:NH2	4:G:1104:GOL:H11	2.14	0.62
1:A:35:ILE:HD12	1:A:35:ILE:H	1.64	0.62
1:C:151:THR:HG22	1:C:190:LEU:HD12	1.82	0.62
1:C:91:THR:HG23	1:C:94:GLU:CB	2.29	0.62
1:H:146:VAL:HG12	1:H:150:VAL:HG23	1.82	0.62
1:B:49:TYR:O	1:B:52:ILE:HG22	2.00	0.61
1:G:142:LEU:HB2	1:G:143:PRO:HD2	1.82	0.61
1:D:12:VAL:C	1:D:14:GLY:H	2.08	0.61
1:A:270:LEU:HA	1:A:273:MET:CE	2.30	0.61
1:E:76:THR:CB	1:E:81:ARG:HB2	2.30	0.61
1:H:302:ASN:HB3	1:H:341:VAL:HB	1.82	0.61
1:B:325:ASP:O	1:B:328:VAL:HG12	1.99	0.61
4:B:1101:GOL:H2	1:D:227:ARG:HH22	1.65	0.61
1:F:177:LEU:HB2	1:F:466:THR:HG21	1.82	0.61
1:H:88:PHE:H	1:H:88:PHE:HD1	1.45	0.61
1:E:262:ASN:H	1:E:262:ASN:ND2	1.99	0.61
1:F:71:ALA:HB3	1:F:107:TYR:OH	2.01	0.61
1:B:88:PHE:HD1	1:B:88:PHE:H	1.46	0.61
1:D:170:GLU:O	1:D:172:PRO:HD3	2.00	0.60
1:H:136:ARG:HB2	1:H:165:ASN:ND2	2.16	0.60
1:B:142:LEU:HB2	1:B:143:PRO:HD2	1.83	0.60
1:B:226:ASN:ND2	1:B:228:ASP:HB2	2.15	0.60
1:A:262:ASN:HD22	1:A:262:ASN:N	1.89	0.60
1:D:83:GLN:H	1:D:86:PRO:HD2	1.67	0.60
1:A:264:LEU:HD23	1:A:356:LEU:HB3	1.84	0.60
1:G:325:ASP:O	1:G:328:VAL:HG12	2.01	0.59
1:F:226:ASN:HD21	1:F:228:ASP:HB2	1.66	0.59
1:F:85:GLU:CB	1:F:86:PRO:HD3	2.32	0.59
1:E:227:ARG:NH2	4:E:1105:GOL:C2	2.62	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ASN:HB3	1:C:341:VAL:HB	1.85	0.59
1:H:49:TYR:O	1:H:52:ILE:HG22	2.02	0.59
1:A:151:THR:HG22	1:A:190:LEU:HD12	1.83	0.59
1:G:270:LEU:HA	1:G:273:MET:CE	2.32	0.59
1:A:429:LYS:HE2	1:A:429:LYS:N	2.17	0.59
1:A:473:GLU:OE1	1:E:178:GLN:HA	2.03	0.59
1:H:226:ASN:HD21	1:H:228:ASP:HB2	1.67	0.59
1:D:137:LEU:HD21	1:D:168:ILE:HD11	1.85	0.59
1:G:385:CYS:HA	1:G:405:MET:HE2	1.84	0.59
1:H:325:ASP:O	1:H:328:VAL:HG12	2.03	0.59
1:E:104:ARG:HG3	1:E:104:ARG:HH11	1.66	0.59
1:H:85:GLU:CB	1:H:86:PRO:HD3	2.33	0.59
1:G:343:TYR:HE1	1:G:353:PRO:HB3	1.69	0.58
1:H:270:LEU:HA	1:H:273:MET:CE	2.31	0.58
1:C:227:ARG:NH2	4:C:1103:GOL:H2	2.16	0.58
1:D:262:ASN:H	1:D:262:ASN:ND2	2.01	0.58
1:H:342:LEU:O	1:H:343:TYR:HD1	1.85	0.58
1:H:479:PRO:HG3	5:H:2004:HOH:O	2.02	0.58
1:G:137:LEU:HD21	1:G:168:ILE:HD11	1.85	0.58
1:H:142:LEU:HB2	1:H:143:PRO:HD2	1.85	0.58
1:C:104:ARG:HG3	1:C:104:ARG:HH11	1.69	0.58
1:G:466:THR:OG1	1:G:467:PRO:HD3	2.04	0.58
1:H:170:GLU:O	1:H:172:PRO:HD3	2.03	0.58
1:F:177:LEU:O	1:F:181:ASP:HB2	2.04	0.58
1:E:129:HIS:O	1:E:130:LEU:HB2	2.03	0.57
1:G:226:ASN:ND2	1:G:228:ASP:HB2	2.18	0.57
1:H:104:ARG:HG3	1:H:104:ARG:HH11	1.68	0.57
1:B:270:LEU:HA	1:B:273:MET:HE3	1.86	0.57
1:B:93:GLU:CD	1:B:93:GLU:H	2.13	0.57
1:B:227:ARG:HH22	4:B:1102:GOL:H11	1.68	0.57
1:D:49:TYR:O	1:D:52:ILE:HG22	2.05	0.57
1:A:104:ARG:HG3	1:A:104:ARG:HH11	1.69	0.57
1:F:136:ARG:HB2	1:F:165:ASN:HD22	1.70	0.57
1:G:72:ARG:HG3	1:G:73:SER:H	1.69	0.57
1:H:136:ARG:HB2	1:H:165:ASN:HD22	1.70	0.57
1:C:88:PHE:H	1:C:88:PHE:HD1	1.53	0.56
1:E:262:ASN:ND2	1:E:263:HIS:H	2.03	0.56
1:H:192:ARG:HG2	1:H:195:GLN:OE1	2.05	0.56
1:C:67:ILE:HD12	1:C:67:ILE:N	2.21	0.56
1:C:466:THR:OG1	1:C:467:PRO:HD3	2.05	0.56
1:D:67:ILE:N	1:D:67:ILE:HD12	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:GLN:HE22	1:E:439:ARG:HD3	1.69	0.56
1:E:270:LEU:HA	1:E:273:MET:CE	2.35	0.56
1:E:343:TYR:CE1	1:E:353:PRO:HA	2.39	0.56
1:G:72:ARG:HG3	1:G:73:SER:N	2.20	0.56
1:G:146:VAL:HG12	1:G:150:VAL:CG2	2.35	0.56
1:G:270:LEU:HA	1:G:273:MET:HE3	1.88	0.56
1:H:259:VAL:HA	1:H:262:ASN:HD21	1.71	0.56
1:E:325:ASP:O	1:E:328:VAL:HG12	2.05	0.56
1:D:226:ASN:ND2	1:D:228:ASP:HB2	2.20	0.56
1:H:175:ARG:HG2	1:H:176:ASP:H	1.69	0.56
1:E:67:ILE:HD12	1:E:67:ILE:N	2.21	0.56
1:F:262:ASN:H	1:F:262:ASN:HD22	1.54	0.56
1:B:302:ASN:HB3	1:B:341:VAL:HB	1.88	0.56
1:D:33:ILE:HG21	1:D:125:MET:HE3	1.88	0.56
1:H:209:GLN:HE22	1:H:439:ARG:HD3	1.71	0.56
1:A:67:ILE:HD12	1:A:67:ILE:N	2.21	0.56
1:A:210:ASN:OD1	1:A:214:LEU:HG	2.05	0.56
1:G:150:VAL:O	1:G:154:ILE:HG13	2.05	0.56
1:B:262:ASN:HD22	1:B:262:ASN:N	1.89	0.55
1:D:76:THR:CB	1:D:81:ARG:HD3	2.37	0.55
1:E:33:ILE:HG21	1:E:125:MET:HE3	1.88	0.55
1:G:104:ARG:HG3	1:G:104:ARG:HH11	1.71	0.55
1:B:75:LEU:HB2	1:B:107:TYR:CZ	2.41	0.55
1:G:151:THR:HG22	1:G:190:LEU:HD12	1.86	0.55
1:G:209:GLN:HE22	1:G:439:ARG:HD3	1.71	0.55
1:A:85:GLU:CB	1:A:86:PRO:HD3	2.36	0.55
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.72	0.55
1:E:45:LYS:HB3	1:E:82:LYS:HZ1	1.71	0.55
1:G:67:ILE:N	1:G:67:ILE:HD12	2.22	0.55
1:G:85:GLU:CB	1:G:86:PRO:HD3	2.37	0.55
1:G:343:TYR:CE1	1:G:353:PRO:HA	2.42	0.55
1:B:137:LEU:HD21	1:B:168:ILE:HD11	1.89	0.55
1:B:201:HIS:HA	1:B:440:LEU:HD11	1.88	0.55
1:D:136:ARG:HB2	1:D:165:ASN:HD22	1.72	0.55
1:F:88:PHE:HD1	1:F:88:PHE:H	1.53	0.55
1:H:75:LEU:HD23	1:H:81:ARG:HH11	1.71	0.55
1:D:93:GLU:CD	1:D:93:GLU:H	2.15	0.55
1:D:325:ASP:O	1:D:328:VAL:HG12	2.06	0.55
1:B:85:GLU:CB	1:B:86:PRO:HD3	2.37	0.55
1:E:264:LEU:HD12	1:E:267:MET:HE2	1.88	0.55
1:E:343:TYR:HE1	1:E:353:PRO:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:O	1:C:52:ILE:HG22	2.08	0.54
1:B:136:ARG:HB2	1:B:165:ASN:ND2	2.22	0.54
1:B:267:MET:O	1:B:271:VAL:HG23	2.07	0.54
1:E:49:TYR:O	1:E:52:ILE:HG22	2.06	0.54
1:A:136:ARG:HD2	1:A:160:SER:HB2	1.90	0.54
1:A:226:ASN:ND2	1:A:228:ASP:HB2	2.21	0.54
1:D:35:ILE:HD12	1:D:35:ILE:N	2.23	0.54
1:G:49:TYR:O	1:G:52:ILE:HG22	2.06	0.54
1:F:104:ARG:HG3	1:F:104:ARG:HH11	1.71	0.54
1:F:136:ARG:HB2	1:F:165:ASN:ND2	2.23	0.54
1:A:192:ARG:HG2	1:A:195:GLN:OE1	2.08	0.54
1:B:71:ALA:HB3	1:B:107:TYR:OH	2.08	0.54
1:C:504:GLU:O	1:C:504:GLU:HG2	2.08	0.54
1:D:82:LYS:C	1:D:84:SER:H	2.16	0.54
1:H:226:ASN:ND2	1:H:228:ASP:HB2	2.23	0.54
1:A:93:GLU:CD	1:A:93:GLU:H	2.15	0.54
1:B:175:ARG:HD3	1:B:176:ASP:H	1.73	0.54
1:D:91:THR:HG23	1:D:94:GLU:CB	2.38	0.54
1:G:407:LYS:HB3	1:H:210:ASN:ND2	2.23	0.54
1:A:270:LEU:HA	1:A:273:MET:HE3	1.90	0.53
1:B:150:VAL:O	1:B:154:ILE:HG13	2.09	0.53
1:A:91:THR:HG23	1:A:94:GLU:CB	2.38	0.53
1:D:407:LYS:HE2	1:D:412:PHE:O	2.08	0.53
1:D:466:THR:OG1	1:D:467:PRO:HD3	2.08	0.53
1:G:101:PHE:O	1:G:104:ARG:HB2	2.08	0.53
1:H:262:ASN:HD22	1:H:262:ASN:N	1.98	0.53
1:A:343:TYR:CE1	1:A:353:PRO:HA	2.43	0.53
1:A:393:ARG:HD2	1:A:396:PRO:O	2.08	0.53
1:E:136:ARG:HB2	1:E:165:ASN:ND2	2.22	0.53
1:C:227:ARG:NH2	4:C:1103:GOL:C2	2.71	0.53
1:E:51:THR:HG21	1:E:441:ILE:HD12	1.89	0.53
1:G:91:THR:HG23	1:G:94:GLU:CB	2.39	0.53
1:G:262:ASN:HD22	1:G:262:ASN:N	2.00	0.53
1:C:47:LYS:C	1:C:50:PRO:HD2	2.34	0.53
1:F:343:TYR:CE1	1:F:353:PRO:HA	2.43	0.53
1:G:144:PRO:HA	1:G:147:TYR:CD2	2.44	0.53
1:B:270:LEU:HA	1:B:273:MET:CE	2.38	0.53
1:F:175:ARG:HD3	1:F:252:GLU:HB3	1.91	0.53
1:F:151:THR:HG22	1:F:190:LEU:HD12	1.89	0.53
1:B:209:GLN:HE22	1:B:439:ARG:HD3	1.74	0.53
1:C:429:LYS:N	1:C:429:LYS:HE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:LEU:HA	1:E:273:MET:HE2	1.91	0.53
1:F:226:ASN:ND2	1:F:228:ASP:HB2	2.24	0.53
1:C:71:ALA:HB3	1:C:107:TYR:OH	2.09	0.53
1:D:393:ARG:NH1	1:D:397:ASN:O	2.42	0.53
1:F:175:ARG:HG2	1:F:175:ARG:O	2.08	0.53
1:E:140:LEU:HD11	1:E:167:ILE:HD11	1.89	0.52
1:F:49:TYR:O	1:F:52:ILE:HG22	2.09	0.52
1:F:136:ARG:HD2	1:F:160:SER:HB2	1.90	0.52
1:G:73:SER:O	1:G:75:LEU:N	2.42	0.52
1:A:33:ILE:HG21	1:A:125:MET:HE3	1.91	0.52
1:C:136:ARG:HB2	1:C:165:ASN:HD22	1.74	0.52
1:A:176:ASP:HB2	1:A:179:SER:OG	2.09	0.52
1:C:85:GLU:CB	1:C:86:PRO:HD3	2.39	0.52
1:F:227:ARG:NH1	1:F:350:ASP:O	2.43	0.52
1:A:182:ARG:HH11	1:A:182:ARG:HB2	1.74	0.52
1:H:71:ALA:HB3	1:H:107:TYR:OH	2.09	0.52
1:E:85:GLU:CB	1:E:86:PRO:HD3	2.40	0.52
1:F:53:TRP:CD1	1:F:53:TRP:C	2.88	0.52
1:C:270:LEU:HA	1:C:273:MET:HE2	1.90	0.52
1:D:385:CYS:HA	1:D:405:MET:HE2	1.91	0.52
1:G:177:LEU:HD22	1:G:466:THR:HG21	1.92	0.52
1:E:262:ASN:HD22	1:E:262:ASN:N	2.01	0.51
1:C:264:LEU:HD12	1:C:267:MET:HE2	1.91	0.51
1:E:53:TRP:CD1	1:E:53:TRP:C	2.88	0.51
1:A:427:ARG:NH1	1:B:510:VAL:HG22	2.26	0.51
1:B:88:PHE:CD1	1:B:88:PHE:N	2.78	0.51
1:D:70:TYR:HD2	1:D:121:LEU:HD13	1.73	0.51
1:G:238:LYS:O	1:G:365:ARG:HA	2.11	0.51
1:D:209:GLN:HE22	1:D:439:ARG:HD3	1.75	0.51
1:B:385:CYS:HA	1:B:405:MET:HE2	1.92	0.51
1:C:264:LEU:HB3	1:C:356:LEU:HD13	1.91	0.51
1:E:35:ILE:HD12	1:E:35:ILE:N	2.25	0.51
1:E:56:PHE:HB2	1:E:61:LEU:HD12	1.91	0.51
1:G:137:LEU:HD21	1:G:168:ILE:CD1	2.40	0.51
1:A:343:TYR:HE1	1:A:353:PRO:HB3	1.76	0.51
1:B:466:THR:OG1	1:B:467:PRO:HD3	2.11	0.51
1:C:144:PRO:HA	1:C:147:TYR:CD2	2.46	0.51
1:B:453:VAL:HG11	1:B:458:LEU:CD2	2.41	0.51
1:G:175:ARG:HG2	1:G:253:PHE:CE1	2.45	0.51
1:H:393:ARG:HD2	1:H:396:PRO:O	2.11	0.51
1:A:466:THR:OG1	1:A:467:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:HB2	1:C:165:ASN:ND2	2.26	0.51
1:E:182:ARG:HA	1:E:182:ARG:HH11	1.75	0.51
1:E:238:LYS:O	1:E:365:ARG:HA	2.11	0.51
1:G:47:LYS:C	1:G:50:PRO:HD2	2.36	0.51
1:H:35:ILE:H	1:H:35:ILE:HD12	1.75	0.51
1:H:91:THR:HG23	1:H:94:GLU:CB	2.41	0.51
1:H:129:HIS:O	1:H:130:LEU:HB2	2.10	0.51
1:B:136:ARG:HD2	1:B:160:SER:HB2	1.93	0.50
1:B:161:GLN:HA	1:B:161:GLN:NE2	2.25	0.50
1:B:177:LEU:HD13	1:B:462:TRP:CB	2.40	0.50
1:H:67:ILE:HD12	1:H:67:ILE:N	2.26	0.50
1:D:210:ASN:OD1	1:D:214:LEU:HG	2.11	0.50
1:E:91:THR:HG23	1:E:94:GLU:CB	2.40	0.50
1:H:393:ARG:NH1	1:H:397:ASN:O	2.45	0.50
1:B:429:LYS:N	1:B:429:LYS:HE2	2.26	0.50
1:C:35:ILE:H	1:C:35:ILE:HD12	1.77	0.50
1:C:248:GLY:H	1:C:327:THR:HB	1.77	0.50
1:D:136:ARG:HB2	1:D:165:ASN:ND2	2.26	0.50
1:E:227:ARG:HH22	4:E:1105:GOL:C2	2.20	0.50
1:H:175:ARG:H	1:H:175:ARG:CD	2.18	0.50
1:H:385:CYS:HA	1:H:405:MET:HE2	1.93	0.50
1:C:37:MET:HE2	1:C:154:ILE:HD11	1.92	0.50
1:B:342:LEU:O	1:B:343:TYR:HD1	1.94	0.50
1:E:285:ARG:O	1:E:289:VAL:HG12	2.12	0.50
1:F:197:TYR:HB3	1:F:452:PHE:CD2	2.46	0.50
1:F:267:MET:O	1:F:271:VAL:HG23	2.12	0.50
1:G:88:PHE:HD1	1:G:88:PHE:H	1.59	0.50
1:C:226:ASN:ND2	1:C:228:ASP:HB2	2.25	0.50
1:A:49:TYR:O	1:A:52:ILE:HG22	2.11	0.50
1:D:12:VAL:C	1:D:14:GLY:N	2.70	0.50
1:E:169:VAL:HG22	1:E:173:PHE:HE1	1.76	0.50
1:A:129:HIS:O	1:A:130:LEU:HB2	2.11	0.50
1:A:238:LYS:O	1:A:365:ARG:HA	2.12	0.50
1:A:427:ARG:HH11	1:B:510:VAL:HG22	1.77	0.50
1:F:91:THR:HG23	1:F:94:GLU:CB	2.41	0.50
1:D:270:LEU:HA	1:D:273:MET:CE	2.41	0.49
1:H:45:LYS:HG3	1:H:46:LYS:HG3	1.94	0.49
1:B:343:TYR:CE1	1:B:353:PRO:HA	2.47	0.49
1:D:71:ALA:HB3	1:D:107:TYR:OH	2.11	0.49
1:D:504:GLU:C	1:D:506:THR:H	2.20	0.49
1:H:78:ALA:C	1:H:80:ILE:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:TYR:HE1	1:D:353:PRO:HB3	1.77	0.49
1:E:343:TYR:HE1	1:E:353:PRO:CA	2.24	0.49
1:F:78:ALA:O	1:F:82:LYS:HB2	2.13	0.49
1:F:87:PHE:CD1	1:F:87:PHE:C	2.89	0.49
1:G:129:HIS:O	1:G:130:LEU:HB2	2.12	0.49
1:G:227:ARG:NH2	4:G:1104:GOL:C1	2.73	0.49
1:H:307:GLN:O	1:H:481:PRO:HA	2.12	0.49
1:B:235:LEU:HD12	1:B:356:LEU:HD22	1.95	0.49
1:E:177:LEU:HD12	1:E:462:TRP:CB	2.42	0.49
1:H:177:LEU:HD22	1:H:466:THR:HG21	1.94	0.49
1:D:151:THR:HG22	1:D:190:LEU:HD12	1.93	0.49
1:C:270:LEU:HA	1:C:273:MET:HE3	1.95	0.49
1:F:393:ARG:HD2	1:F:396:PRO:O	2.13	0.49
1:H:325:ASP:HB3	1:H:328:VAL:HG12	1.94	0.49
1:A:142:LEU:HB2	1:A:143:PRO:HD2	1.95	0.49
1:F:508:LYS:O	1:F:508:LYS:HG2	2.13	0.49
1:A:53:TRP:CD1	1:A:53:TRP:C	2.90	0.49
1:D:302:ASN:HB3	1:D:341:VAL:HB	1.95	0.49
1:D:393:ARG:HD2	1:D:396:PRO:O	2.11	0.49
1:E:70:TYR:CD1	1:E:70:TYR:C	2.91	0.49
1:E:440:LEU:O	1:E:443:ASP:HB2	2.13	0.49
1:B:45:LYS:HB2	1:B:86:PRO:HG3	1.95	0.49
1:E:429:LYS:N	1:E:429:LYS:HE2	2.27	0.49
1:F:170:GLU:C	1:F:172:PRO:HD3	2.37	0.49
1:F:376:VAL:HG13	5:H:2007:HOH:O	2.12	0.49
1:G:407:LYS:HB3	1:H:210:ASN:HD22	1.76	0.49
1:A:302:ASN:HB3	1:A:341:VAL:HB	1.93	0.49
1:B:82:LYS:HZ2	1:B:85:GLU:CB	2.25	0.49
1:C:129:HIS:O	1:C:130:LEU:HB2	2.12	0.49
1:D:129:HIS:O	1:D:130:LEU:HB2	2.13	0.48
1:E:210:ASN:OD1	1:E:214:LEU:HG	2.12	0.48
1:F:209:GLN:OE1	1:F:439:ARG:HD2	2.12	0.48
1:F:440:LEU:O	1:F:443:ASP:HB2	2.12	0.48
1:A:101:PHE:O	1:A:104:ARG:HB2	2.13	0.48
1:A:136:ARG:HB2	1:A:165:ASN:HD22	1.79	0.48
1:B:209:GLN:OE1	1:B:439:ARG:HD2	2.13	0.48
1:C:53:TRP:CD1	1:C:53:TRP:C	2.90	0.48
1:D:85:GLU:CB	1:D:86:PRO:HD3	2.43	0.48
1:B:137:LEU:HD21	1:B:168:ILE:CD1	2.43	0.48
1:B:248:GLY:H	1:B:327:THR:HB	1.77	0.48
1:C:70:TYR:HD2	1:C:121:LEU:HD13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:ASN:OD1	1:G:214:LEU:HG	2.13	0.48
1:H:267:MET:O	1:H:271:VAL:HG23	2.13	0.48
1:D:248:GLY:H	1:D:327:THR:HB	1.78	0.48
1:F:466:THR:OG1	1:F:467:PRO:HD3	2.13	0.48
1:A:143:PRO:HA	1:A:144:PRO:HD3	1.81	0.48
1:B:53:TRP:CD1	1:B:53:TRP:C	2.91	0.48
1:E:302:ASN:HB3	1:E:341:VAL:HB	1.96	0.48
1:F:67:ILE:N	1:F:67:ILE:HD12	2.28	0.48
1:F:202:TYR:HA	1:F:205:LYS:HG3	1.94	0.48
1:G:504:GLU:HG3	1:G:506:THR:OG1	2.13	0.48
1:H:87:PHE:CD1	1:H:87:PHE:C	2.91	0.48
1:C:407:LYS:HB3	1:D:210:ASN:ND2	2.29	0.48
1:E:37:MET:HE2	1:E:154:ILE:HD11	1.96	0.48
1:G:176:ASP:HB2	1:G:179:SER:HB3	1.96	0.48
1:H:175:ARG:HG2	1:H:176:ASP:N	2.28	0.48
1:H:407:LYS:HE2	1:H:412:PHE:O	2.14	0.48
1:A:267:MET:O	1:A:271:VAL:HG23	2.13	0.48
1:C:385:CYS:HA	1:C:405:MET:HE2	1.94	0.48
1:E:237:PHE:O	1:E:358:CYS:HA	2.14	0.48
1:G:199:ILE:CG2	1:G:200:ASP:N	2.77	0.48
1:A:136:ARG:CD	1:A:160:SER:HB2	2.44	0.48
1:A:262:ASN:H	1:A:262:ASN:ND2	1.98	0.48
1:D:253:PHE:CD1	1:D:253:PHE:N	2.81	0.48
1:E:253:PHE:O	1:E:257:ARG:HD2	2.14	0.48
1:H:53:TRP:CD1	1:H:53:TRP:C	2.92	0.48
1:A:407:LYS:HB3	1:B:210:ASN:ND2	2.29	0.48
1:C:343:TYR:CE1	1:C:353:PRO:HA	2.49	0.48
1:E:146:VAL:HG12	1:E:150:VAL:CG2	2.40	0.48
1:F:302:ASN:HB3	1:F:341:VAL:HB	1.96	0.48
1:B:370:ARG:CZ	2:B:800:NAP:H51A	2.44	0.47
1:D:227:ARG:HG2	1:D:348:ARG:O	2.14	0.47
1:E:177:LEU:CB	1:E:466:THR:HG21	2.44	0.47
1:H:88:PHE:CD1	1:H:88:PHE:N	2.81	0.47
1:C:407:LYS:HE2	1:C:412:PHE:O	2.14	0.47
1:D:270:LEU:HA	1:D:273:MET:HE3	1.95	0.47
1:E:177:LEU:HD12	1:E:462:TRP:HB2	1.96	0.47
1:E:393:ARG:HD2	1:E:396:PRO:O	2.14	0.47
1:H:82:LYS:C	1:H:86:PRO:HD2	2.39	0.47
1:H:143:PRO:HA	1:H:144:PRO:HD3	1.75	0.47
1:B:393:ARG:HD2	1:B:396:PRO:O	2.13	0.47
1:D:343:TYR:CE1	1:D:353:PRO:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:GLU:H	1:H:93:GLU:CD	2.22	0.47
1:B:87:PHE:H	1:B:88:PHE:HD1	1.63	0.47
1:B:268:LEU:C	1:B:268:LEU:HD23	2.39	0.47
1:F:93:GLU:CD	1:F:93:GLU:H	2.23	0.47
1:G:53:TRP:CD1	1:G:53:TRP:C	2.92	0.47
1:G:136:ARG:HB2	1:G:165:ASN:ND2	2.29	0.47
1:B:460:GLU:O	1:B:464:ILE:HG13	2.15	0.47
1:F:210:ASN:OD1	1:F:214:LEU:HG	2.15	0.47
1:A:307:GLN:O	1:A:481:PRO:HA	2.14	0.47
1:G:35:ILE:HD12	1:G:35:ILE:N	2.28	0.47
1:A:45:LYS:HG3	1:A:46:LYS:HG3	1.97	0.47
1:A:81:ARG:HD2	1:A:81:ARG:N	2.29	0.47
1:A:201:HIS:HA	1:A:440:LEU:HD11	1.95	0.47
1:C:343:TYR:HE1	1:C:353:PRO:HB3	1.80	0.47
1:C:371:LEU:O	1:C:389:GLU:HA	2.14	0.47
1:E:71:ALA:HB3	1:E:107:TYR:OH	2.14	0.47
1:E:136:ARG:HD2	1:E:160:SER:HB2	1.96	0.47
1:E:343:TYR:HE1	1:E:353:PRO:HA	1.77	0.47
1:G:269:CYS:HB3	1:G:288:LYS:HG2	1.97	0.47
1:G:343:TYR:HE1	1:G:353:PRO:CA	2.28	0.47
1:G:497:LYS:HA	1:G:501:PHE:O	2.15	0.47
1:H:466:THR:OG1	1:H:467:PRO:HD3	2.14	0.47
1:E:343:TYR:HE1	1:E:353:PRO:CB	2.28	0.47
1:G:302:ASN:HB3	1:G:341:VAL:HB	1.96	0.47
1:C:93:GLU:H	1:C:93:GLU:CD	2.23	0.47
1:C:227:ARG:HG2	1:C:348:ARG:O	2.15	0.47
1:D:226:ASN:HD22	1:D:228:ASP:H	1.62	0.47
1:G:72:ARG:CG	1:G:73:SER:H	2.28	0.47
1:C:88:PHE:CD1	1:C:88:PHE:N	2.83	0.47
1:D:262:ASN:HD22	1:D:263:HIS:H	1.61	0.47
1:B:210:ASN:OD1	1:B:214:LEU:HG	2.15	0.46
1:E:174:GLY:HA3	1:E:180:SER:OG	2.16	0.46
1:C:213:VAL:HG21	1:D:407:LYS:HB2	1.97	0.46
1:D:53:TRP:C	1:D:53:TRP:CD1	2.93	0.46
1:E:93:GLU:CD	1:E:93:GLU:H	2.23	0.46
1:E:177:LEU:H	1:E:466:THR:HG21	1.79	0.46
1:F:104:ARG:HH11	1:F:104:ARG:CG	2.27	0.46
1:C:370:ARG:CZ	2:C:800:NAP:H51A	2.46	0.46
1:D:70:TYR:CD1	1:D:70:TYR:C	2.93	0.46
1:D:262:ASN:ND2	1:D:263:HIS:H	2.14	0.46
1:G:393:ARG:NH1	1:G:397:ASN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:CD1	1:A:70:TYR:C	2.93	0.46
1:C:87:PHE:CD1	1:C:87:PHE:C	2.94	0.46
1:D:370:ARG:NH2	2:D:800:NAP:O2N	2.47	0.46
1:G:227:ARG:HG2	1:G:348:ARG:O	2.16	0.46
1:B:243:THR:HG23	1:B:243:THR:O	2.16	0.46
1:E:201:HIS:HA	1:E:440:LEU:HD11	1.97	0.46
1:B:87:PHE:CD1	1:B:87:PHE:C	2.94	0.46
1:F:129:HIS:O	1:F:130:LEU:HB2	2.16	0.46
1:G:343:TYR:HE1	1:G:353:PRO:CB	2.28	0.46
1:B:129:HIS:O	1:B:130:LEU:HB2	2.15	0.46
1:B:393:ARG:NH1	1:B:397:ASN:O	2.48	0.46
1:E:124:HIS:O	1:E:128:LEU:HD13	2.15	0.46
1:E:259:VAL:O	1:E:262:ASN:ND2	2.49	0.45
1:G:194:ASP:HA	1:G:449:GLN:OE1	2.15	0.45
1:G:227:ARG:NH1	1:G:350:ASP:O	2.48	0.45
1:C:375:ASP:O	1:D:219:ARG:NH1	2.49	0.45
1:D:440:LEU:O	1:D:443:ASP:HB2	2.16	0.45
1:F:311:ASN:HA	1:F:312:PRO:HD2	1.78	0.45
1:A:268:LEU:HD23	1:A:268:LEU:C	2.42	0.45
1:B:227:ARG:NH1	1:B:350:ASP:O	2.49	0.45
1:C:269:CYS:HB3	1:C:288:LYS:HG2	1.98	0.45
1:E:233:VAL:HG22	1:E:371:LEU:HD22	1.98	0.45
1:F:248:GLY:H	1:F:327:THR:HB	1.81	0.45
1:G:87:PHE:CD1	1:G:87:PHE:C	2.95	0.45
1:H:496:MET:O	1:H:499:VAL:HG12	2.15	0.45
1:G:201:HIS:HA	1:G:440:LEU:HD11	1.97	0.45
1:G:307:GLN:O	1:G:481:PRO:HA	2.17	0.45
1:H:243:THR:O	1:H:245:GLY:N	2.48	0.45
1:B:180:SER:HB3	1:B:462:TRP:CZ2	2.51	0.45
1:C:210:ASN:OD1	1:C:214:LEU:HG	2.16	0.45
1:C:346:ASN:ND2	5:C:2001:HOH:O	2.50	0.45
1:D:197:TYR:HB3	1:D:452:PHE:CD2	2.51	0.45
1:D:270:LEU:HD23	1:D:273:MET:CE	2.47	0.45
1:E:150:VAL:O	1:E:154:ILE:HG13	2.17	0.45
1:H:201:HIS:HA	1:H:440:LEU:HD11	1.97	0.45
1:D:202:TYR:HA	1:D:205:LYS:HG3	1.99	0.45
1:D:240:PRO:CD	1:D:365:ARG:HB2	2.42	0.45
1:A:385:CYS:HA	1:A:405:MET:HE2	1.99	0.45
1:B:440:LEU:O	1:B:443:ASP:HB2	2.17	0.45
1:C:393:ARG:NH1	1:C:397:ASN:O	2.49	0.45
1:F:262:ASN:ND2	1:F:263:HIS:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:LEU:HD23	1:F:268:LEU:C	2.42	0.45
1:F:270:LEU:HA	1:F:273:MET:CE	2.46	0.45
1:H:136:ARG:HD2	1:H:160:SER:HB2	1.98	0.45
1:A:111:GLN:HA	1:A:111:GLN:NE2	2.32	0.45
1:B:35:ILE:HD12	1:B:35:ILE:H	1.81	0.45
1:B:285:ARG:O	1:B:289:VAL:HG12	2.16	0.45
1:A:343:TYR:HE1	1:A:353:PRO:CB	2.30	0.45
1:A:411:MET:HE1	1:B:439:ARG:HG3	1.98	0.45
1:G:177:LEU:HB2	1:G:466:THR:CG2	2.45	0.45
1:A:270:LEU:HA	1:A:273:MET:HE2	1.97	0.44
1:C:146:VAL:HG12	1:C:150:VAL:CG2	2.43	0.44
1:C:450:MET:HE2	1:C:451:HIS:CE1	2.52	0.44
1:E:385:CYS:HA	1:E:405:MET:HE2	1.98	0.44
1:F:45:LYS:HG3	1:F:46:LYS:HG3	1.98	0.44
1:F:262:ASN:HD22	1:F:262:ASN:N	2.13	0.44
1:H:473:GLU:O	1:H:473:GLU:HG3	2.17	0.44
1:A:209:GLN:HE22	1:A:439:ARG:HD3	1.81	0.44
1:B:452:PHE:N	1:B:452:PHE:CD1	2.85	0.44
1:C:31:THR:HA	1:C:64:ASN:HB2	1.99	0.44
1:C:262:ASN:HD22	1:C:262:ASN:N	2.08	0.44
1:H:135:ASN:ND2	1:H:164:TRP:H	2.15	0.44
1:H:176:ASP:HB2	1:H:179:SER:OG	2.17	0.44
1:C:70:TYR:CD2	1:C:121:LEU:HD22	2.53	0.44
1:D:104:ARG:HG3	1:D:104:ARG:HH11	1.82	0.44
1:D:460:GLU:O	1:D:464:ILE:HG13	2.18	0.44
1:E:83:GLN:H	1:E:86:PRO:HD2	1.82	0.44
1:B:166:ARG:NH1	1:B:444:VAL:O	2.51	0.44
1:D:235:LEU:HD12	1:D:356:LEU:HD22	1.99	0.44
1:D:285:ARG:O	1:D:289:VAL:HG12	2.17	0.44
1:D:87:PHE:CD1	1:D:87:PHE:C	2.95	0.44
1:G:219:ARG:NH1	1:H:375:ASP:O	2.51	0.44
1:E:227:ARG:NH1	1:E:350:ASP:O	2.51	0.44
1:E:397:ASN:O	1:E:398:GLU:C	2.59	0.44
1:H:172:PRO:HB3	1:H:198:ARG:HD3	1.99	0.44
1:C:238:LYS:O	1:C:365:ARG:HA	2.18	0.44
1:D:227:ARG:NH1	1:D:350:ASP:O	2.51	0.44
1:H:231:ALA:O	1:H:232:CYS:HB3	2.16	0.44
1:A:78:ALA:C	1:A:80:ILE:H	2.25	0.44
1:C:393:ARG:HD2	1:C:396:PRO:O	2.16	0.44
1:C:411:MET:CE	1:D:439:ARG:HG3	2.48	0.44
1:F:88:PHE:CD1	1:F:88:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:TYR:CD1	1:H:70:TYR:C	2.96	0.44
1:H:202:TYR:HA	1:H:205:LYS:HG3	2.00	0.44
1:C:35:ILE:HD12	1:C:35:ILE:N	2.33	0.44
1:D:452:PHE:CD1	1:D:452:PHE:N	2.84	0.44
1:E:45:LYS:HG3	1:E:46:LYS:HG3	1.99	0.44
1:G:77:VAL:O	1:G:78:ALA:C	2.61	0.44
1:H:161:GLN:HA	1:H:161:GLN:NE2	2.33	0.44
1:A:87:PHE:CD1	1:A:87:PHE:C	2.96	0.43
1:A:243:THR:HG23	1:A:243:THR:O	2.18	0.43
1:B:117:SER:HA	1:B:120:ARG:NH1	2.33	0.43
1:B:193:GLU:HG3	5:B:2009:HOH:O	2.19	0.43
1:B:233:VAL:HG22	1:B:371:LEU:HD22	2.00	0.43
1:E:70:TYR:HD2	1:E:121:LEU:HD13	1.83	0.43
1:G:72:ARG:CG	1:G:73:SER:N	2.81	0.43
1:G:202:TYR:HA	1:G:205:LYS:HG3	1.99	0.43
1:G:262:ASN:ND2	1:G:262:ASN:N	2.58	0.43
1:G:393:ARG:HD2	1:G:396:PRO:O	2.17	0.43
1:C:209:GLN:HE22	1:C:439:ARG:HD3	1.83	0.43
1:E:177:LEU:H	1:E:466:THR:CG2	2.31	0.43
1:H:139:TYR:HA	1:H:168:ILE:HB	1.99	0.43
1:C:337:PHE:CD1	1:C:337:PHE:C	2.96	0.43
1:D:88:PHE:H	1:D:88:PHE:HD1	1.63	0.43
1:F:343:TYR:HE1	1:F:353:PRO:HB3	1.84	0.43
1:G:37:MET:HE2	1:G:154:ILE:HD11	2.00	0.43
1:C:47:LYS:O	1:C:50:PRO:HD2	2.17	0.43
1:C:70:TYR:CD1	1:C:70:TYR:C	2.97	0.43
1:C:262:ASN:H	1:C:262:ASN:ND2	2.14	0.43
1:D:55:LEU:HB3	1:D:61:LEU:HG	2.00	0.43
1:D:237:PHE:HB2	1:D:264:LEU:HD11	2.00	0.43
1:G:93:GLU:CD	1:G:93:GLU:H	2.26	0.43
1:H:226:ASN:HD22	1:H:228:ASP:H	1.66	0.43
1:B:451:HIS:C	1:B:452:PHE:CD1	2.96	0.43
1:C:173:PHE:CE2	1:C:262:ASN:HB3	2.53	0.43
1:C:209:GLN:OE1	1:C:439:ARG:HD2	2.19	0.43
1:E:262:ASN:ND2	1:E:262:ASN:N	2.61	0.43
1:F:237:PHE:O	1:F:358:CYS:HA	2.19	0.43
1:F:270:LEU:HA	1:F:273:MET:HE3	2.00	0.43
1:G:136:ARG:HD2	1:G:160:SER:HB2	1.99	0.43
1:G:343:TYR:HE1	1:G:353:PRO:HA	1.82	0.43
1:G:440:LEU:O	1:G:444:VAL:HG23	2.19	0.43
1:A:393:ARG:NH1	1:A:397:ASN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:ARG:CG	1:G:253:PHE:CE1	3.02	0.43
1:H:238:LYS:NZ	2:H:800:NAP:O3X	2.51	0.43
1:H:270:LEU:HD23	1:H:273:MET:CE	2.49	0.43
1:E:30:ASP:O	1:E:64:ASN:HB2	2.18	0.43
1:E:142:LEU:HB2	1:E:143:PRO:HD2	2.00	0.43
1:H:174:GLY:HA3	1:H:180:SER:OG	2.18	0.43
1:A:460:GLU:O	1:A:464:ILE:HG13	2.18	0.43
1:E:209:GLN:OE1	1:E:439:ARG:HD2	2.18	0.43
1:E:310:GLY:HA3	1:E:319:THR:O	2.19	0.43
1:A:202:TYR:HA	1:A:205:LYS:HG3	2.01	0.43
1:A:343:TYR:HE1	1:A:353:PRO:HA	1.83	0.43
1:C:262:ASN:ND2	1:C:263:HIS:H	2.16	0.43
1:F:393:ARG:NH1	1:F:397:ASN:O	2.51	0.43
1:H:269:CYS:HB3	1:H:288:LYS:HG2	2.00	0.43
1:A:115:ALA:O	1:A:119:GLN:HB2	2.18	0.43
1:A:144:PRO:HA	1:A:147:TYR:CD2	2.53	0.43
1:B:117:SER:HA	1:B:120:ARG:CZ	2.49	0.43
1:C:219:ARG:NH1	1:D:376:VAL:HA	2.34	0.43
1:C:236:THR:O	1:C:367:ALA:HA	2.19	0.43
1:D:243:THR:HG22	1:D:308:TYR:OH	2.18	0.43
1:B:307:GLN:O	1:B:481:PRO:HA	2.19	0.42
1:C:124:HIS:O	1:C:127:ALA:HB3	2.19	0.42
1:E:136:ARG:CD	1:E:160:SER:HB2	2.49	0.42
1:E:144:PRO:HG2	1:E:172:PRO:HD2	2.00	0.42
1:G:270:LEU:HD23	1:G:273:MET:CE	2.48	0.42
1:H:452:PHE:N	1:H:452:PHE:CD1	2.87	0.42
1:D:75:LEU:HD23	1:D:75:LEU:HA	1.82	0.42
1:D:137:LEU:HD21	1:D:168:ILE:CD1	2.46	0.42
1:D:328:VAL:HA	1:D:329:PRO:HD3	1.91	0.42
1:F:168:ILE:HD11	1:F:444:VAL:HG21	2.01	0.42
1:G:264:LEU:HD12	1:G:267:MET:HE2	2.00	0.42
2:H:800:NAP:O2X	2:H:800:NAP:H3B	2.20	0.42
1:C:235:LEU:CD2	1:C:369:VAL:HG13	2.50	0.42
1:C:452:PHE:CD1	1:C:452:PHE:N	2.87	0.42
1:E:176:ASP:O	1:E:178:GLN:N	2.53	0.42
1:E:210:ASN:ND2	1:F:407:LYS:HB3	2.34	0.42
1:A:70:TYR:CD1	1:A:71:ALA:N	2.87	0.42
1:A:88:PHE:H	1:A:88:PHE:HD1	1.65	0.42
1:C:273:MET:HA	1:C:291:VAL:CG2	2.49	0.42
1:G:172:PRO:HB3	1:G:198:ARG:HD3	2.00	0.42
1:E:87:PHE:CD1	1:E:87:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASN:ND2	1:F:157:SER:O	2.53	0.42
1:F:162:ILE:HD13	1:F:162:ILE:HA	1.88	0.42
1:G:177:LEU:HD13	1:G:462:TRP:CB	2.47	0.42
1:G:262:ASN:ND2	1:G:263:HIS:H	2.18	0.42
1:H:82:LYS:O	1:H:86:PRO:HD2	2.19	0.42
1:B:198:ARG:HD3	1:B:458:LEU:HD11	2.00	0.42
1:C:125:MET:O	1:C:131:GLY:HA3	2.20	0.42
1:F:177:LEU:HD13	1:F:462:TRP:CG	2.55	0.42
1:H:75:LEU:HB2	1:H:107:TYR:CE2	2.54	0.42
1:H:101:PHE:O	1:H:104:ARG:HB2	2.20	0.42
1:H:151:THR:HG23	1:H:191:PHE:CE1	2.54	0.42
1:H:162:ILE:HD13	1:H:162:ILE:HA	1.86	0.42
1:A:81:ARG:HA	1:A:81:ARG:NE	2.35	0.42
1:B:67:ILE:N	1:B:67:ILE:HD12	2.35	0.42
1:E:76:THR:O	1:E:77:VAL:C	2.63	0.42
1:E:82:LYS:HD2	1:E:82:LYS:HA	1.73	0.42
1:E:450:MET:HE2	1:E:451:HIS:CE1	2.55	0.42
1:F:70:TYR:HD2	1:F:121:LEU:HD13	1.85	0.42
1:G:35:ILE:HD11	1:G:125:MET:HE1	2.02	0.42
1:H:35:ILE:HD12	1:H:35:ILE:N	2.35	0.42
1:H:35:ILE:HD11	1:H:125:MET:HE1	2.00	0.42
1:A:86:PRO:O	1:A:87:PHE:HB3	2.20	0.42
1:A:375:ASP:O	1:B:219:ARG:NH1	2.53	0.42
1:A:459:LEU:HA	1:A:459:LEU:HD12	1.76	0.42
1:C:473:GLU:O	1:C:476:LYS:HE3	2.20	0.42
1:D:45:LYS:HG3	1:D:46:LYS:HG3	2.01	0.42
1:D:243:THR:O	1:D:243:THR:HG23	2.20	0.42
1:D:398:GLU:CD	1:D:398:GLU:H	2.27	0.42
1:E:47:LYS:C	1:E:50:PRO:HD2	2.45	0.42
1:F:144:PRO:O	1:F:147:TYR:HB2	2.20	0.42
1:G:311:ASN:HA	1:G:312:PRO:HD2	1.88	0.42
1:G:429:LYS:N	1:G:429:LYS:HE2	2.35	0.42
1:H:122:ASN:ND2	1:H:157:SER:O	2.53	0.42
1:H:243:THR:OG1	1:H:247:GLY:HA2	2.20	0.42
1:A:72:ARG:HA	1:A:110:GLY:O	2.20	0.42
1:A:219:ARG:NH1	1:B:375:ASP:O	2.52	0.42
1:B:115:ALA:O	1:B:119:GLN:HB2	2.20	0.42
1:C:202:TYR:HA	1:C:205:LYS:HG3	2.01	0.42
1:E:178:GLN:HB3	1:E:179:SER:H	1.76	0.42
1:E:226:ASN:HD21	1:E:228:ASP:HB2	1.85	0.42
1:C:162:ILE:HD13	1:C:162:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LYS:HE2	1:C:171:LYS:HB3	1.79	0.41
1:D:267:MET:O	1:D:271:VAL:HG23	2.19	0.41
1:D:429:LYS:N	1:D:429:LYS:HE2	2.34	0.41
1:E:225:TRP:O	1:E:348:ARG:NH1	2.51	0.41
1:F:45:LYS:HB2	1:F:86:PRO:HG3	2.01	0.41
1:H:342:LEU:O	1:H:343:TYR:CD1	2.71	0.41
1:A:104:ARG:HH11	1:A:104:ARG:CG	2.32	0.41
1:B:149:ALA:O	1:B:152:LYS:HB3	2.20	0.41
1:C:177:LEU:HD13	1:C:462:TRP:HB3	2.02	0.41
1:C:201:HIS:HA	1:C:440:LEU:HD11	2.01	0.41
1:D:287:GLU:O	1:D:291:VAL:HG23	2.20	0.41
2:D:800:NAP:H71N	2:D:800:NAP:H4N	1.52	0.41
1:F:201:HIS:HA	1:F:440:LEU:HD11	2.03	0.41
1:G:328:VAL:HA	1:G:329:PRO:HD3	1.94	0.41
1:A:78:ALA:O	1:A:80:ILE:N	2.53	0.41
1:B:35:ILE:HG22	1:B:37:MET:SD	2.60	0.41
1:B:240:PRO:HA	1:B:362:LEU:O	2.20	0.41
1:B:269:CYS:SG	1:B:292:LEU:HD21	2.60	0.41
1:C:61:LEU:HA	1:C:62:PRO:HD3	1.96	0.41
1:C:411:MET:HE1	1:D:439:ARG:HG3	2.02	0.41
1:E:270:LEU:HD23	1:E:273:MET:CE	2.50	0.41
1:D:201:HIS:HA	1:D:440:LEU:HD11	2.01	0.41
1:H:260:MET:HE3	1:H:260:MET:HB2	1.99	0.41
1:E:162:ILE:HD13	1:E:162:ILE:HA	1.84	0.41
1:G:270:LEU:HA	1:G:273:MET:HE2	2.01	0.41
1:A:35:ILE:HD12	1:A:35:ILE:N	2.33	0.41
1:A:199:ILE:CG2	1:A:200:ASP:N	2.84	0.41
1:C:227:ARG:HH22	4:C:1103:GOL:C2	2.23	0.41
1:D:192:ARG:HG2	1:D:195:GLN:OE1	2.20	0.41
1:E:311:ASN:HA	1:E:312:PRO:HD2	1.84	0.41
1:E:466:THR:OG1	1:E:467:PRO:HD3	2.20	0.41
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.85	0.41
1:B:273:MET:HA	1:B:291:VAL:CG2	2.51	0.41
1:C:270:LEU:HD23	1:C:273:MET:HE1	2.03	0.41
1:F:126:ASN:HA	1:F:131:GLY:HA3	2.02	0.41
1:G:78:ALA:HB1	1:G:105:ASN:HB3	2.03	0.41
1:G:172:PRO:CG	1:G:198:ARG:HB3	2.51	0.41
1:G:176:ASP:HB2	1:G:179:SER:CB	2.50	0.41
1:G:209:GLN:OE1	1:G:439:ARG:HD2	2.21	0.41
1:G:285:ARG:O	1:G:289:VAL:HG12	2.21	0.41
1:H:210:ASN:OD1	1:H:214:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:ASN:O	1:H:281:SER:C	2.63	0.41
1:A:499:VAL:HG22	1:A:499:VAL:O	2.21	0.41
1:E:104:ARG:HH11	1:E:104:ARG:CG	2.32	0.41
1:E:144:PRO:HA	1:E:147:TYR:CD2	2.55	0.41
1:E:248:GLY:H	1:E:327:THR:HB	1.85	0.41
1:E:270:LEU:HD23	1:E:273:MET:HE1	2.01	0.41
1:E:325:ASP:HB3	1:E:328:VAL:HG12	2.02	0.41
1:F:144:PRO:HA	1:F:147:TYR:CD2	2.56	0.41
1:F:397:ASN:O	1:F:398:GLU:C	2.64	0.41
1:G:47:LYS:O	1:G:50:PRO:HD2	2.20	0.41
1:G:142:LEU:CB	1:G:143:PRO:HD2	2.49	0.41
1:H:268:LEU:C	1:H:268:LEU:HD23	2.45	0.41
1:A:371:LEU:O	1:A:389:GLU:HA	2.21	0.41
1:B:226:ASN:ND2	1:B:228:ASP:H	2.19	0.41
1:B:238:LYS:O	1:B:365:ARG:HA	2.21	0.41
1:C:143:PRO:HA	1:C:144:PRO:HD3	1.78	0.41
1:C:440:LEU:O	1:C:443:ASP:HB2	2.21	0.41
1:D:143:PRO:HA	1:D:144:PRO:HD3	1.84	0.41
1:E:55:LEU:HD12	1:E:55:LEU:HA	1.91	0.41
1:E:91:THR:HA	1:E:92:PRO:HD3	1.99	0.41
1:E:497:LYS:HA	1:E:501:PHE:O	2.21	0.41
1:F:209:GLN:HE22	1:F:439:ARG:HD3	1.85	0.41
1:F:243:THR:HG23	1:F:243:THR:O	2.20	0.41
1:G:136:ARG:HB2	1:G:165:ASN:HD22	1.85	0.41
1:G:202:TYR:O	1:G:205:LYS:HG3	2.21	0.41
1:G:375:ASP:O	1:H:219:ARG:NH1	2.54	0.41
1:H:142:LEU:HD13	1:H:146:VAL:HB	2.03	0.41
1:H:151:THR:HG23	1:H:191:PHE:HE1	1.84	0.41
1:B:162:ILE:HD13	1:B:162:ILE:HA	1.94	0.41
1:B:198:ARG:CD	1:B:458:LEU:HD11	2.51	0.41
1:B:260:MET:HE3	1:B:260:MET:HB2	1.95	0.41
1:B:325:ASP:HB3	1:B:328:VAL:HG12	2.02	0.41
1:D:238:LYS:O	1:D:365:ARG:HA	2.20	0.41
1:E:259:VAL:HA	1:E:262:ASN:HD21	1.86	0.41
1:D:125:MET:O	1:D:131:GLY:HA3	2.20	0.40
1:E:243:THR:OG1	1:E:247:GLY:HA2	2.21	0.40
1:G:355:ILE:HD13	1:G:496:MET:HG2	2.03	0.40
1:A:125:MET:O	1:A:131:GLY:HA3	2.22	0.40
1:A:177:LEU:HD22	1:A:466:THR:HG21	2.03	0.40
1:A:497:LYS:HA	1:A:501:PHE:O	2.21	0.40
1:F:104:ARG:CG	1:F:104:ARG:NH1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:LYS:H	1:F:508:LYS:HE2	1.87	0.40
1:G:55:LEU:HB3	1:G:61:LEU:HG	2.03	0.40
1:G:259:VAL:O	1:G:262:ASN:ND2	2.54	0.40
1:H:87:PHE:H	1:H:88:PHE:HD1	1.69	0.40
1:H:421:ASP:OD1	2:H:800:NAP:N7N	2.54	0.40
1:B:202:TYR:HA	1:B:205:LYS:HG3	2.03	0.40
1:D:12:VAL:O	1:D:14:GLY:N	2.54	0.40
1:E:427:ARG:NH2	1:F:508:LYS:O	2.55	0.40
1:G:343:TYR:CD1	1:G:353:PRO:HA	2.56	0.40
1:H:177:LEU:HG	1:H:178:GLN:N	2.35	0.40
1:B:227:ARG:HG2	1:B:348:ARG:O	2.21	0.40
1:B:342:LEU:O	1:B:343:TYR:CD1	2.74	0.40
1:C:211:LEU:HD23	1:C:392:ILE:HD13	2.03	0.40
1:G:210:ASN:ND2	1:H:407:LYS:HB3	2.35	0.40
1:A:343:TYR:HE1	1:A:353:PRO:CA	2.35	0.40
1:A:474:LEU:HD11	1:E:463:ARG:HG2	2.04	0.40
1:C:268:LEU:C	1:C:268:LEU:HD23	2.46	0.40
1:G:341:VAL:HG11	1:G:499:VAL:HG21	2.04	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	484/514 (94%)	420 (87%)	50 (10%)	14 (3%)	3	20
1	B	485/514 (94%)	430 (89%)	45 (9%)	10 (2%)	5	27
1	C	485/514 (94%)	431 (89%)	42 (9%)	12 (2%)	4	23
1	D	486/514 (95%)	435 (90%)	39 (8%)	12 (2%)	4	23
1	E	483/514 (94%)	424 (88%)	46 (10%)	13 (3%)	4	22
1	F	487/514 (95%)	424 (87%)	52 (11%)	11 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	485/514 (94%)	430 (89%)	45 (9%)	10 (2%)	5	27
1	H	485/514 (94%)	430 (89%)	48 (10%)	7 (1%)	9	36
All	All	3880/4112 (94%)	3424 (88%)	367 (10%)	89 (2%)	5	25

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	PHE
1	A	244	GLU
1	A	383	GLN
1	B	87	PHE
1	B	244	GLU
1	B	383	GLN
1	C	77	VAL
1	C	79	ASP
1	C	83	GLN
1	C	87	PHE
1	C	244	GLU
1	D	77	VAL
1	D	87	PHE
1	D	244	GLU
1	E	76	THR
1	E	79	ASP
1	E	87	PHE
1	E	178	GLN
1	E	244	GLU
1	F	77	VAL
1	F	80	ILE
1	F	87	PHE
1	F	178	GLN
1	F	244	GLU
1	G	83	GLN
1	G	87	PHE
1	G	244	GLU
1	H	87	PHE
1	H	244	GLU
1	A	78	ALA
1	A	79	ASP
1	B	29	SER
1	B	80	ILE
1	B	201	HIS

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Mol	Chain	Res	Type
1	B	330	ARG
1	C	14	GLY
1	C	201	HIS
1	C	383	GLN
1	D	12	VAL
1	E	83	GLN
1	E	177	LEU
1	E	383	GLN
1	F	201	HIS
1	F	383	GLN
1	G	74	ARG
1	G	76	THR
1	G	193	GLU
1	G	383	GLN
1	H	77	VAL
1	H	170	GLU
1	H	383	GLN
1	A	75	LEU
1	A	83	GLN
1	B	347	GLU
1	D	330	ARG
1	D	383	GLN
1	G	78	ALA
1	G	201	HIS
1	A	113	ASP
1	D	80	ILE
1	E	180	SER
1	E	201	HIS
1	F	29	SER
1	H	79	ASP
1	A	80	ILE
1	A	129	HIS
1	B	74	ARG
1	C	13	CYS
1	C	129	HIS
1	C	330	ARG
1	D	13	CYS
1	E	129	HIS
1	F	10	THR
1	F	78	ALA
1	G	80	ILE
1	H	80	ILE

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Mol	Chain	Res	Type
1	A	95	LYS
1	A	330	ARG
1	D	30	ASP
1	D	129	HIS
1	E	80	ILE
1	A	92	PRO
1	D	505	GLY
1	F	12	VAL
1	A	172	PRO
1	B	77	VAL
1	E	77	VAL
1	C	222	GLY
1	D	223	PRO

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	410/449 (91%)	381 (93%)	29 (7%)	13	43
1	B	409/449 (91%)	378 (92%)	31 (8%)	12	41
1	C	410/449 (91%)	384 (94%)	26 (6%)	16	48
1	D	410/449 (91%)	381 (93%)	29 (7%)	13	43
1	E	410/449 (91%)	371 (90%)	39 (10%)	8	31
1	F	410/449 (91%)	377 (92%)	33 (8%)	11	38
1	G	409/449 (91%)	379 (93%)	30 (7%)	13	42
1	H	411/449 (92%)	380 (92%)	31 (8%)	12	41
All	All	3279/3592 (91%)	3031 (92%)	248 (8%)	12	41

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	29	SER

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Mol	Chain	Res	Type
1	A	42	ASP
1	A	53	TRP
1	A	55	LEU
1	A	91	THR
1	A	93	GLU
1	A	104	ARG
1	A	145	THR
1	A	159	MET
1	A	180	SER
1	A	183	LEU
1	A	207	MET
1	A	227	ARG
1	A	246	ARG
1	A	262	ASN
1	A	279	THR
1	A	296	SER
1	A	327	THR
1	A	345	GLU
1	A	398	GLU
1	A	400	VAL
1	A	404	MET
1	A	419	GLU
1	A	429	LYS
1	A	443	ASP
1	A	483	ILE
1	A	495	LEU
1	A	504	GLU
1	B	42	ASP
1	B	53	TRP
1	B	55	LEU
1	B	60	LEU
1	B	81	ARG
1	B	91	THR
1	B	93	GLU
1	B	104	ARG
1	B	145	THR
1	B	157	SER
1	B	159	MET
1	B	175	ARG
1	B	181	ASP
1	B	207	MET
1	B	246	ARG

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Mol	Chain	Res	Type
1	B	262	ASN
1	B	279	THR
1	B	327	THR
1	B	345	GLU
1	B	398	GLU
1	B	400	VAL
1	B	404	MET
1	B	411	MET
1	B	419	GLU
1	B	429	LYS
1	B	442	LEU
1	B	443	ASP
1	B	483	ILE
1	B	490	THR
1	B	495	LEU
1	B	508	LYS
1	C	42	ASP
1	C	53	TRP
1	C	55	LEU
1	C	91	THR
1	C	93	GLU
1	C	104	ARG
1	C	145	THR
1	C	159	MET
1	C	207	MET
1	C	246	ARG
1	C	262	ASN
1	C	279	THR
1	C	296	SER
1	C	327	THR
1	C	345	GLU
1	C	398	GLU
1	C	400	VAL
1	C	404	MET
1	C	411	MET
1	C	419	GLU
1	C	429	LYS
1	C	442	LEU
1	C	443	ASP
1	C	483	ILE
1	C	495	LEU
1	C	508	LYS

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Mol	Chain	Res	Type
1	D	42	ASP
1	D	53	TRP
1	D	55	LEU
1	D	60	LEU
1	D	91	THR
1	D	93	GLU
1	D	104	ARG
1	D	145	THR
1	D	159	MET
1	D	176	ASP
1	D	183	LEU
1	D	207	MET
1	D	246	ARG
1	D	262	ASN
1	D	279	THR
1	D	296	SER
1	D	327	THR
1	D	345	GLU
1	D	398	GLU
1	D	400	VAL
1	D	404	MET
1	D	411	MET
1	D	419	GLU
1	D	429	LYS
1	D	442	LEU
1	D	470	HIS
1	D	483	ILE
1	D	495	LEU
1	D	508	LYS
1	E	13	CYS
1	E	42	ASP
1	E	53	TRP
1	E	55	LEU
1	E	60	LEU
1	E	73	SER
1	E	81	ARG
1	E	91	THR
1	E	93	GLU
1	E	104	ARG
1	E	145	THR
1	E	159	MET
1	E	169	VAL

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Mol	Chain	Res	Type
1	E	175	ARG
1	E	176	ASP
1	E	178	GLN
1	E	182	ARG
1	E	183	LEU
1	E	207	MET
1	E	227	ARG
1	E	246	ARG
1	E	262	ASN
1	E	279	THR
1	E	289	VAL
1	E	296	SER
1	E	327	THR
1	E	345	GLU
1	E	398	GLU
1	E	400	VAL
1	E	404	MET
1	E	411	MET
1	E	419	GLU
1	E	429	LYS
1	E	442	LEU
1	E	443	ASP
1	E	483	ILE
1	E	495	LEU
1	E	504	GLU
1	E	508	LYS
1	F	29	SER
1	F	42	ASP
1	F	53	TRP
1	F	55	LEU
1	F	63	GLU
1	F	91	THR
1	F	93	GLU
1	F	104	ARG
1	F	145	THR
1	F	159	MET
1	F	176	ASP
1	F	182	ARG
1	F	207	MET
1	F	246	ARG
1	F	262	ASN
1	F	279	THR

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Mol	Chain	Res	Type
1	F	296	SER
1	F	327	THR
1	F	345	GLU
1	F	398	GLU
1	F	400	VAL
1	F	404	MET
1	F	411	MET
1	F	419	GLU
1	F	429	LYS
1	F	442	LEU
1	F	443	ASP
1	F	446	CYS
1	F	470	HIS
1	F	473	GLU
1	F	483	ILE
1	F	495	LEU
1	F	508	LYS
1	G	42	ASP
1	G	53	TRP
1	G	55	LEU
1	G	73	SER
1	G	91	THR
1	G	93	GLU
1	G	104	ARG
1	G	145	THR
1	G	159	MET
1	G	177	LEU
1	G	178	GLN
1	G	180	SER
1	G	207	MET
1	G	246	ARG
1	G	262	ASN
1	G	279	THR
1	G	296	SER
1	G	327	THR
1	G	345	GLU
1	G	398	GLU
1	G	400	VAL
1	G	404	MET
1	G	411	MET
1	G	419	GLU
1	G	429	LYS

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Mol	Chain	Res	Type
1	G	442	LEU
1	G	443	ASP
1	G	483	ILE
1	G	495	LEU
1	G	508	LYS
1	H	42	ASP
1	H	53	TRP
1	H	60	LEU
1	H	88	PHE
1	H	91	THR
1	H	93	GLU
1	H	104	ARG
1	H	145	THR
1	H	157	SER
1	H	159	MET
1	H	175	ARG
1	H	177	LEU
1	H	207	MET
1	H	227	ARG
1	H	246	ARG
1	H	262	ASN
1	H	285	ARG
1	H	296	SER
1	H	327	THR
1	H	345	GLU
1	H	356	LEU
1	H	398	GLU
1	H	400	VAL
1	H	404	MET
1	H	419	GLU
1	H	429	LYS
1	H	442	LEU
1	H	483	ILE
1	H	495	LEU
1	H	504	GLU
1	H	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	111	GLN
1	A	135	ASN
1	A	161	GLN
1	A	226	ASN
1	A	262	ASN
1	A	451	HIS
1	A	470	HIS
1	A	471	GLN
1	B	32	HIS
1	B	83	GLN
1	B	105	ASN
1	B	111	GLN
1	B	135	ASN
1	B	161	GLN
1	B	210	ASN
1	B	226	ASN
1	B	262	ASN
1	B	397	ASN
1	B	451	HIS
1	C	32	HIS
1	C	105	ASN
1	C	111	GLN
1	C	135	ASN
1	C	161	GLN
1	C	226	ASN
1	C	262	ASN
1	C	307	GLN
1	C	374	HIS
1	C	451	HIS
1	D	32	HIS
1	D	105	ASN
1	D	111	GLN
1	D	135	ASN
1	D	165	ASN
1	D	210	ASN
1	D	226	ASN
1	D	262	ASN
1	D	307	GLN
1	D	451	HIS
1	E	32	HIS
1	E	83	GLN
1	E	111	GLN

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Mol	Chain	Res	Type
1	E	124	HIS
1	E	126	ASN
1	E	135	ASN
1	E	161	GLN
1	E	165	ASN
1	E	178	GLN
1	E	210	ASN
1	E	226	ASN
1	E	262	ASN
1	E	307	GLN
1	E	451	HIS
1	F	83	GLN
1	F	111	GLN
1	F	161	GLN
1	F	178	GLN
1	F	201	HIS
1	F	210	ASN
1	F	226	ASN
1	F	262	ASN
1	G	32	HIS
1	G	105	ASN
1	G	111	GLN
1	G	135	ASN
1	G	161	GLN
1	G	185	ASN
1	G	201	HIS
1	G	226	ASN
1	G	262	ASN
1	G	307	GLN
1	G	397	ASN
1	G	451	HIS
1	H	32	HIS
1	H	83	GLN
1	H	111	GLN
1	H	126	ASN
1	H	135	ASN
1	H	161	GLN
1	H	226	ASN
1	H	262	ASN
1	H	307	GLN
1	H	451	HIS
1	H	511	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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	NAP	A	800	-	50,52,52	1.12	2 (4%)	71,80,80	1.44	12 (16%)
2	NAP	E	800	-	50,52,52	1.35	2 (4%)	71,80,80	1.45	7 (9%)
4	GOL	B	1102	-	5,5,5	0.37	0	5,5,5	0.17	0
2	NAP	B	800	-	50,52,52	1.03	3 (6%)	71,80,80	1.47	12 (16%)
2	NAP	D	800	-	50,52,52	1.22	3 (6%)	71,80,80	1.41	8 (11%)
2	NAP	F	800	-	50,52,52	1.01	1 (2%)	71,80,80	1.49	9 (12%)
3	GOA	F	900	-	4,4,4	0.93	0	4,4,4	2.13	2 (50%)
3	GOA	C	900	-	4,4,4	0.89	0	4,4,4	2.15	1 (25%)
3	GOA	G	900	-	4,4,4	0.85	0	4,4,4	2.28	2 (50%)
2	NAP	G	800	-	50,52,52	1.02	2 (4%)	71,80,80	1.38	10 (14%)
4	GOL	G	1104	-	5,5,5	0.75	0	5,5,5	0.36	0
2	NAP	C	800	-	50,52,52	1.05	3 (6%)	71,80,80	1.54	13 (18%)
4	GOL	B	1101	-	5,5,5	0.54	0	5,5,5	0.20	0
4	GOL	C	1103	-	5,5,5	0.40	0	5,5,5	0.21	0
3	GOA	A	900	-	4,4,4	0.86	0	4,4,4	2.13	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOA	B	900	-	4,4,4	0.96	0	4,4,4	2.11	2 (50%)
3	GOA	D	900	-	4,4,4	0.76	0	4,4,4	2.29	2 (50%)
2	NAP	H	800	-	50,52,52	0.99	1 (2%)	71,80,80	1.42	12 (16%)
3	GOA	E	900	-	4,4,4	0.87	0	4,4,4	2.32	2 (50%)
4	GOL	E	1105	-	5,5,5	0.27	0	5,5,5	0.50	0
3	GOA	H	900	-	4,4,4	0.90	0	4,4,4	2.41	3 (75%)

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	NAP	A	800	-	-	12/35/67/67	0/5/5/5
2	NAP	E	800	-	-	10/35/67/67	0/5/5/5
4	GOL	B	1102	-	-	2/4/4/4	-
2	NAP	B	800	-	-	9/35/67/67	0/5/5/5
2	NAP	D	800	-	-	9/35/67/67	0/5/5/5
2	NAP	F	800	-	-	10/35/67/67	0/5/5/5
3	GOA	F	900	-	-	2/2/2/2	-
3	GOA	C	900	-	-	2/2/2/2	-
3	GOA	G	900	-	-	2/2/2/2	-
2	NAP	G	800	-	-	7/35/67/67	0/5/5/5
4	GOL	G	1104	-	-	2/4/4/4	-
2	NAP	C	800	-	-	10/35/67/67	0/5/5/5
4	GOL	B	1101	-	-	2/4/4/4	-
4	GOL	C	1103	-	-	2/4/4/4	-
3	GOA	A	900	-	-	2/2/2/2	-
3	GOA	B	900	-	-	2/2/2/2	-
3	GOA	D	900	-	-	2/2/2/2	-
2	NAP	H	800	-	-	8/35/67/67	0/5/5/5
3	GOA	E	900	-	-	0/2/2/2	-
4	GOL	E	1105	-	-	2/4/4/4	-
3	GOA	H	900	-	-	2/2/2/2	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	NAP	PN-O3	-5.16	1.53	1.59
2	E	800	NAP	PA-O3	-4.90	1.54	1.59
2	D	800	NAP	PN-O3	-4.19	1.55	1.59
2	D	800	NAP	PA-O3	-3.70	1.55	1.59
2	A	800	NAP	PN-O3	-3.48	1.55	1.59
2	C	800	NAP	PA-O3	-3.03	1.56	1.59
2	A	800	NAP	C2N-N1N	-3.02	1.31	1.35
2	H	800	NAP	PN-O3	-2.90	1.56	1.59
2	G	800	NAP	C2N-N1N	-2.78	1.31	1.35
2	G	800	NAP	PN-O3	-2.63	1.56	1.59
2	F	800	NAP	C4A-N9A	2.47	1.42	1.37
2	B	800	NAP	PN-O3	-2.40	1.56	1.59
2	B	800	NAP	PA-O3	-2.36	1.57	1.59
2	B	800	NAP	C2N-N1N	-2.32	1.32	1.35
2	C	800	NAP	C2N-N1N	-2.13	1.32	1.35
2	C	800	NAP	C2B-C1B	-2.07	1.48	1.53
2	D	800	NAP	C2N-N1N	-2.02	1.32	1.35

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	800	NAP	O4B-C1B-C2B	-5.28	97.50	106.59
2	G	800	NAP	O4B-C1B-C2B	-4.91	98.13	106.59
2	B	800	NAP	O4B-C1B-C2B	-4.89	98.17	106.59
2	H	800	NAP	O4B-C1B-C2B	-4.60	98.68	106.59
2	F	800	NAP	C4D-O4D-C1D	-4.54	105.77	109.92
2	F	800	NAP	O4B-C1B-C2B	-4.46	98.90	106.59
2	D	800	NAP	C4D-O4D-C1D	-4.44	105.86	109.92
2	A	800	NAP	O4B-C1B-C2B	-4.42	98.97	106.59
2	C	800	NAP	C2N-C3N-C7N	4.38	132.10	119.46
2	D	800	NAP	C2N-C3N-C7N	4.23	131.68	119.46
2	H	800	NAP	C4D-O4D-C1D	-4.13	106.14	109.92
2	G	800	NAP	C4D-O4D-C1D	-4.04	106.22	109.92
2	B	800	NAP	C4D-O4D-C1D	-4.02	106.24	109.92
2	C	800	NAP	O4B-C1B-C2B	-4.01	99.69	106.59
2	C	800	NAP	C4N-C3N-C7N	-3.99	110.18	121.06
2	E	800	NAP	C6N-N1N-C2N	-3.99	118.48	121.88
2	E	800	NAP	P2B-O2B-C2B	3.97	134.03	123.43
2	D	800	NAP	C4N-C3N-C7N	-3.81	110.68	121.06
2	H	800	NAP	C3B-C2B-C1B	-3.65	95.82	102.81
2	B	800	NAP	C2N-C3N-C7N	3.61	129.89	119.46
2	F	800	NAP	C2N-C3N-C7N	3.56	129.73	119.46
2	D	800	NAP	O4B-C1B-C2B	-3.55	100.47	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	NAP	C4D-O4D-C1D	-3.55	106.67	109.92
2	A	800	NAP	C4D-O4D-C1D	-3.50	106.72	109.92
2	G	800	NAP	P2B-O2B-C2B	-3.41	114.32	123.43
2	E	800	NAP	C2N-C3N-C7N	3.32	129.05	119.46
2	B	800	NAP	C4N-C3N-C7N	-3.26	112.17	121.06
2	A	800	NAP	C2N-C3N-C7N	3.14	128.52	119.46
2	C	800	NAP	C6N-N1N-C2N	-3.11	119.23	121.88
2	D	800	NAP	O7N-C7N-N7N	3.09	127.08	122.62
3	H	900	GOA	OXT-C-O	-3.07	115.44	123.33
2	H	800	NAP	C2N-C3N-C7N	3.06	128.29	119.46
2	G	800	NAP	C3B-C2B-C1B	-3.05	96.97	102.81
2	H	800	NAP	C6N-N1N-C2N	-3.04	119.29	121.88
3	G	900	GOA	OXT-C-O	-3.04	115.51	123.33
3	E	900	GOA	OXT-C-O	-3.02	115.55	123.33
3	D	900	GOA	OXT-C-O	-3.01	115.58	123.33
2	F	800	NAP	C3B-C2B-C1B	-3.01	97.04	102.81
2	B	800	NAP	C6N-N1N-C2N	-2.91	119.40	121.88
2	D	800	NAP	C3B-C2B-C1B	-2.90	97.26	102.81
2	A	800	NAP	O7N-C7N-N7N	2.89	126.80	122.62
2	F	800	NAP	C4N-C3N-C7N	-2.89	113.19	121.06
2	G	800	NAP	O7N-C7N-N7N	2.87	126.77	122.62
2	A	800	NAP	C4N-C3N-C7N	-2.86	113.27	121.06
3	A	900	GOA	OXT-C-O	-2.84	116.02	123.33
2	A	800	NAP	C6N-N1N-C2N	-2.83	119.47	121.88
2	C	800	NAP	C3B-C2B-C1B	-2.83	97.39	102.81
3	C	900	GOA	OXT-C-O	-2.82	116.08	123.33
3	B	900	GOA	OXT-C-O	-2.76	116.22	123.33
3	F	900	GOA	OXT-C-O	-2.76	116.22	123.33
2	E	800	NAP	C4D-O4D-C1D	-2.75	107.41	109.92
2	E	800	NAP	C4N-C3N-C7N	-2.73	113.61	121.06
2	D	800	NAP	O2A-PA-O3	2.71	114.59	107.27
2	F	800	NAP	O7N-C7N-N7N	2.70	126.52	122.62
2	B	800	NAP	C2B-C1B-N9A	-2.67	109.36	113.75
2	D	800	NAP	C2B-C1B-N9A	-2.66	109.37	113.75
2	B	800	NAP	O4B-C1B-N9A	2.66	113.19	108.09
2	C	800	NAP	C4B-O4B-C1B	-2.63	103.66	109.47
2	A	800	NAP	C2B-C1B-N9A	-2.61	109.46	113.75
2	G	800	NAP	C2N-C3N-C7N	2.57	126.87	119.46
2	E	800	NAP	O2A-PA-O3	2.55	114.17	107.27
2	C	800	NAP	O7N-C7N-N7N	2.52	126.26	122.62
2	F	800	NAP	O4B-C1B-N9A	2.51	112.91	108.09
2	H	800	NAP	C4N-C3N-C7N	-2.51	114.23	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	900	GOA	OXT-C-CA	2.47	116.38	111.90
3	D	900	GOA	OXT-C-CA	2.45	116.36	111.90
2	F	800	NAP	C4B-O4B-C1B	-2.43	104.09	109.47
2	C	800	NAP	C2B-C1B-N9A	-2.43	109.76	113.75
3	H	900	GOA	OXT-C-CA	2.41	116.29	111.90
2	A	800	NAP	C4B-O4B-C1B	-2.41	104.14	109.47
2	C	800	NAP	C3N-C7N-N7N	-2.41	114.77	117.74
2	H	800	NAP	P2B-O2B-C2B	-2.40	117.03	123.43
2	B	800	NAP	C4B-O4B-C1B	-2.39	104.19	109.47
3	G	900	GOA	OXT-C-CA	2.39	116.24	111.90
2	A	800	NAP	O2N-PN-O3	2.35	113.64	107.27
2	H	800	NAP	O7N-C7N-N7N	2.34	126.00	122.62
2	F	800	NAP	C6N-N1N-C2N	-2.32	119.90	121.88
2	G	800	NAP	C4B-O4B-C1B	-2.29	104.42	109.47
2	A	800	NAP	O2A-PA-O3	2.28	113.44	107.27
3	H	900	GOA	O2-CA-C	2.27	118.00	112.37
2	C	800	NAP	O2N-PN-O3	2.26	113.39	107.27
2	C	800	NAP	O4B-C1B-N9A	2.26	112.43	108.09
3	A	900	GOA	OXT-C-CA	2.26	116.00	111.90
2	A	800	NAP	O7N-C7N-C3N	-2.23	116.87	119.60
2	H	800	NAP	C4B-O4B-C1B	-2.23	104.55	109.47
2	B	800	NAP	C3N-C7N-N7N	-2.22	115.00	117.74
2	B	800	NAP	C3B-C2B-C1B	-2.22	98.56	102.81
2	C	800	NAP	O2A-PA-O3	2.19	113.19	107.27
2	G	800	NAP	O7N-C7N-C3N	-2.18	116.94	119.60
2	H	800	NAP	O2A-PA-O3	2.17	113.15	107.27
2	G	800	NAP	C4N-C3N-C7N	-2.15	115.21	121.06
2	B	800	NAP	O2N-PN-O3	2.14	113.06	107.27
2	G	800	NAP	O2A-PA-O3	2.12	113.00	107.27
2	H	800	NAP	C5B-C4B-C3B	-2.08	107.71	115.21
3	B	900	GOA	OXT-C-CA	2.08	115.68	111.90
2	A	800	NAP	O4B-C1B-N9A	2.06	112.04	108.09
2	H	800	NAP	O2B-C2B-C1B	2.04	117.22	110.05
2	B	800	NAP	C4A-C5A-N7A	2.02	112.89	110.58
3	F	900	GOA	OXT-C-CA	2.00	115.54	111.90

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	NAP	C5B-O5B-PA-O2A
2	A	800	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	800	NAP	O4B-C4B-C5B-O5B
2	C	800	NAP	C5D-O5D-PN-O1N
2	D	800	NAP	C5B-O5B-PA-O2A
2	D	800	NAP	C5B-O5B-PA-O3
2	D	800	NAP	O4B-C4B-C5B-O5B
2	E	800	NAP	O4B-C4B-C5B-O5B
2	E	800	NAP	C5D-O5D-PN-O1N
2	F	800	NAP	O4B-C4B-C5B-O5B
2	F	800	NAP	O4D-C4D-C5D-O5D
2	F	800	NAP	O4D-C1D-N1N-C2N
2	G	800	NAP	C5B-O5B-PA-O1A
2	G	800	NAP	C5B-O5B-PA-O2A
2	G	800	NAP	O4B-C4B-C5B-O5B
2	H	800	NAP	O4D-C4D-C5D-O5D
3	A	900	GOA	O-C-CA-O2
3	A	900	GOA	OXT-C-CA-O2
3	B	900	GOA	O-C-CA-O2
3	B	900	GOA	OXT-C-CA-O2
3	C	900	GOA	O-C-CA-O2
3	C	900	GOA	OXT-C-CA-O2
3	F	900	GOA	O-C-CA-O2
3	F	900	GOA	OXT-C-CA-O2
3	G	900	GOA	O-C-CA-O2
3	G	900	GOA	OXT-C-CA-O2
3	H	900	GOA	O-C-CA-O2
3	H	900	GOA	OXT-C-CA-O2
4	B	1101	GOL	C1-C2-C3-O3
4	B	1101	GOL	O2-C2-C3-O3
4	B	1102	GOL	C1-C2-C3-O3
4	C	1103	GOL	O1-C1-C2-C3
4	E	1105	GOL	C1-C2-C3-O3
4	G	1104	GOL	O1-C1-C2-C3
2	B	800	NAP	C3B-C4B-C5B-O5B
2	C	800	NAP	O4B-C4B-C5B-O5B
2	C	800	NAP	C3B-C4B-C5B-O5B
2	D	800	NAP	C3B-C4B-C5B-O5B
2	F	800	NAP	C3B-C4B-C5B-O5B
2	G	800	NAP	C3B-C4B-C5B-O5B
2	H	800	NAP	C3B-C4B-C5B-O5B
2	B	800	NAP	C3B-C2B-O2B-P2B
2	H	800	NAP	C3B-C2B-O2B-P2B
2	B	800	NAP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	H	800	NAP	O4B-C4B-C5B-O5B
2	C	800	NAP	C2N-C3N-C7N-N7N
2	E	800	NAP	C1B-C2B-O2B-P2B
2	F	800	NAP	C1B-C2B-O2B-P2B
2	D	800	NAP	C3B-C2B-O2B-P2B
2	E	800	NAP	C3B-C2B-O2B-P2B
2	F	800	NAP	C3B-C2B-O2B-P2B
2	A	800	NAP	C3B-C4B-C5B-O5B
4	B	1102	GOL	O2-C2-C3-O3
4	G	1104	GOL	O1-C1-C2-O2
2	E	800	NAP	C3B-C4B-C5B-O5B
2	H	800	NAP	C3D-C4D-C5D-O5D
2	C	800	NAP	C1B-C2B-O2B-P2B
2	C	800	NAP	C4N-C3N-C7N-N7N
2	F	800	NAP	C3D-C4D-C5D-O5D
2	A	800	NAP	C1B-C2B-O2B-P2B
2	C	800	NAP	C3B-C2B-O2B-P2B
4	E	1105	GOL	O2-C2-C3-O3
2	D	800	NAP	C1B-C2B-O2B-P2B
2	B	800	NAP	PN-O3-PA-O1A
2	D	800	NAP	PN-O3-PA-O1A
2	G	800	NAP	PN-O3-PA-O1A
2	H	800	NAP	PN-O3-PA-O1A
2	E	800	NAP	O4D-C4D-C5D-O5D
4	C	1103	GOL	O1-C1-C2-O2
2	H	800	NAP	C2B-C1B-N9A-C8A
2	A	800	NAP	PN-O3-PA-O1A
2	E	800	NAP	PN-O3-PA-O2A
2	A	800	NAP	C5B-O5B-PA-O3
2	A	800	NAP	C5D-O5D-PN-O1N
2	C	800	NAP	C5D-O5D-PN-O3
2	E	800	NAP	C5D-O5D-PN-O3
2	G	800	NAP	C5B-O5B-PA-O3
2	D	800	NAP	O4D-C4D-C5D-O5D
2	D	800	NAP	PN-O3-PA-O2A
2	F	800	NAP	PN-O3-PA-O2A
2	H	800	NAP	PN-O3-PA-O2A
2	B	800	NAP	C2N-C3N-C7N-N7N
2	A	800	NAP	C3B-C2B-O2B-P2B
2	B	800	NAP	PN-O3-PA-O2A
2	F	800	NAP	PN-O3-PA-O1A
2	G	800	NAP	PN-O3-PA-O2A

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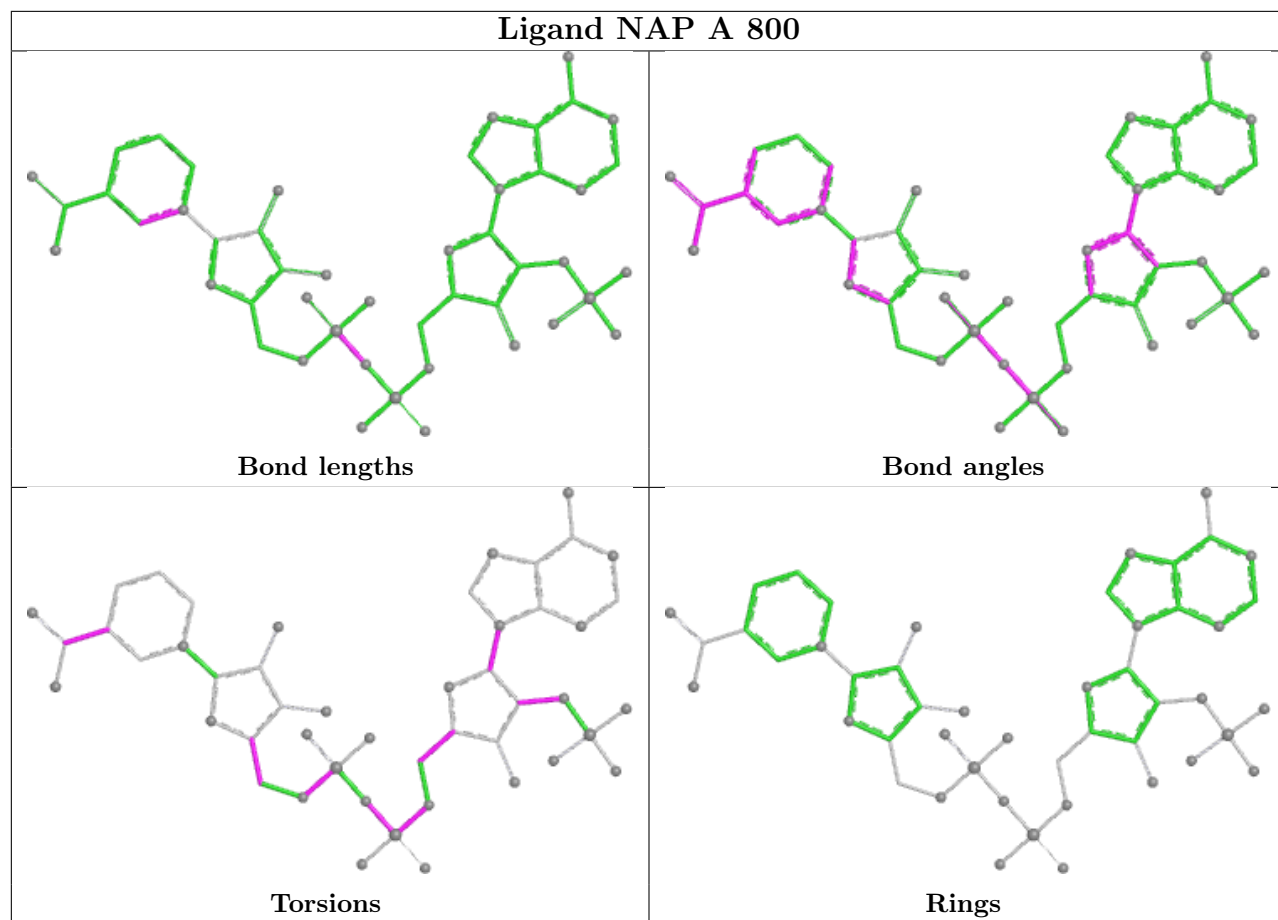
Mol	Chain	Res	Type	Atoms
2	A	800	NAP	O4D-C4D-C5D-O5D
2	E	800	NAP	C2B-C1B-N9A-C8A
2	A	800	NAP	C2B-C1B-N9A-C8A
2	F	800	NAP	C2B-C1B-N9A-C8A
2	C	800	NAP	C2N-C3N-C7N-O7N
2	A	800	NAP	PN-O3-PA-O2A
2	C	800	NAP	PA-O3-PN-O2N
2	E	800	NAP	PN-O3-PA-O1A
2	B	800	NAP	C4N-C3N-C7N-N7N
2	B	800	NAP	C2B-C1B-N9A-C8A
3	D	900	GOA	O-C-CA-O2
3	D	900	GOA	OXT-C-CA-O2
2	A	800	NAP	C2N-C3N-C7N-O7N

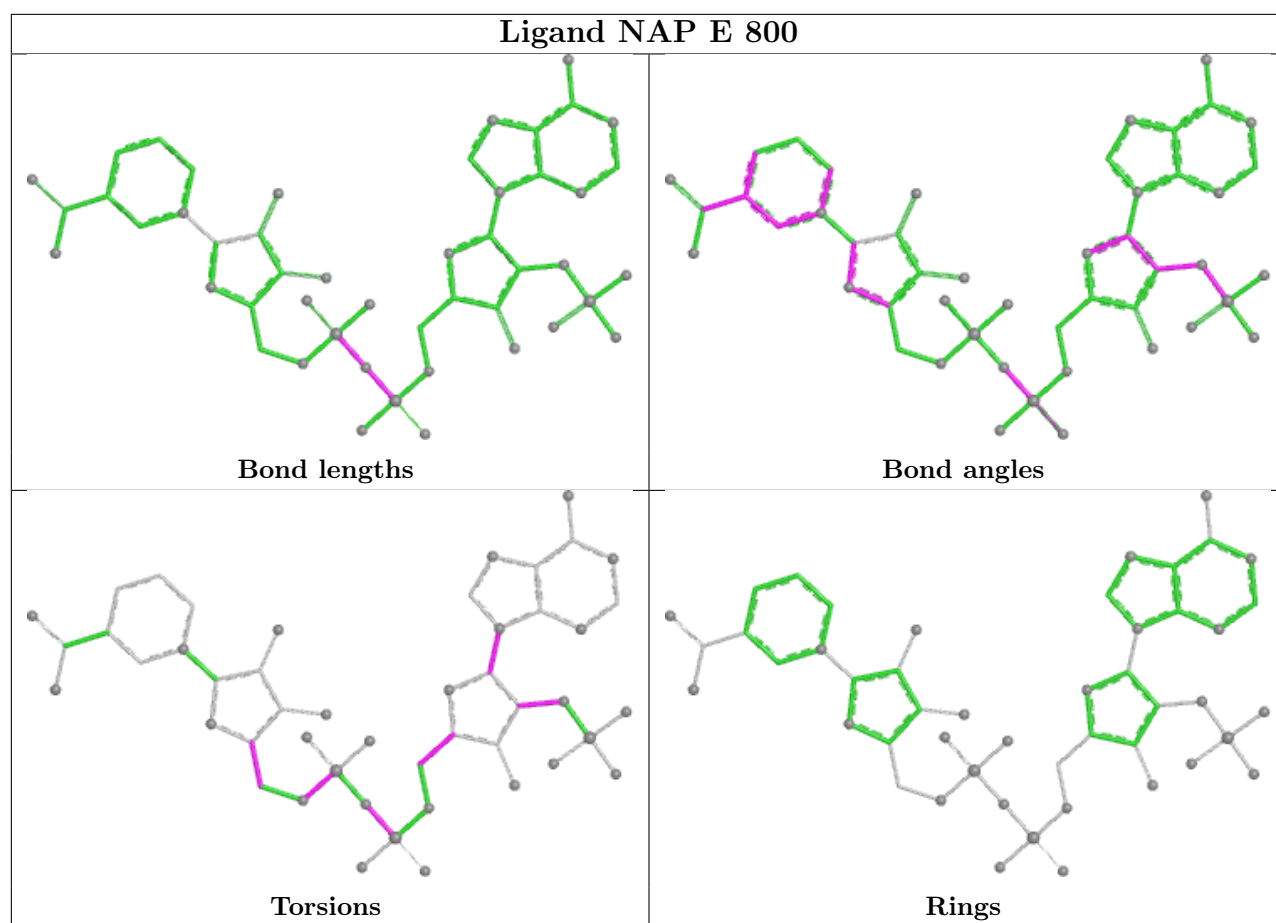
There are no ring outliers.

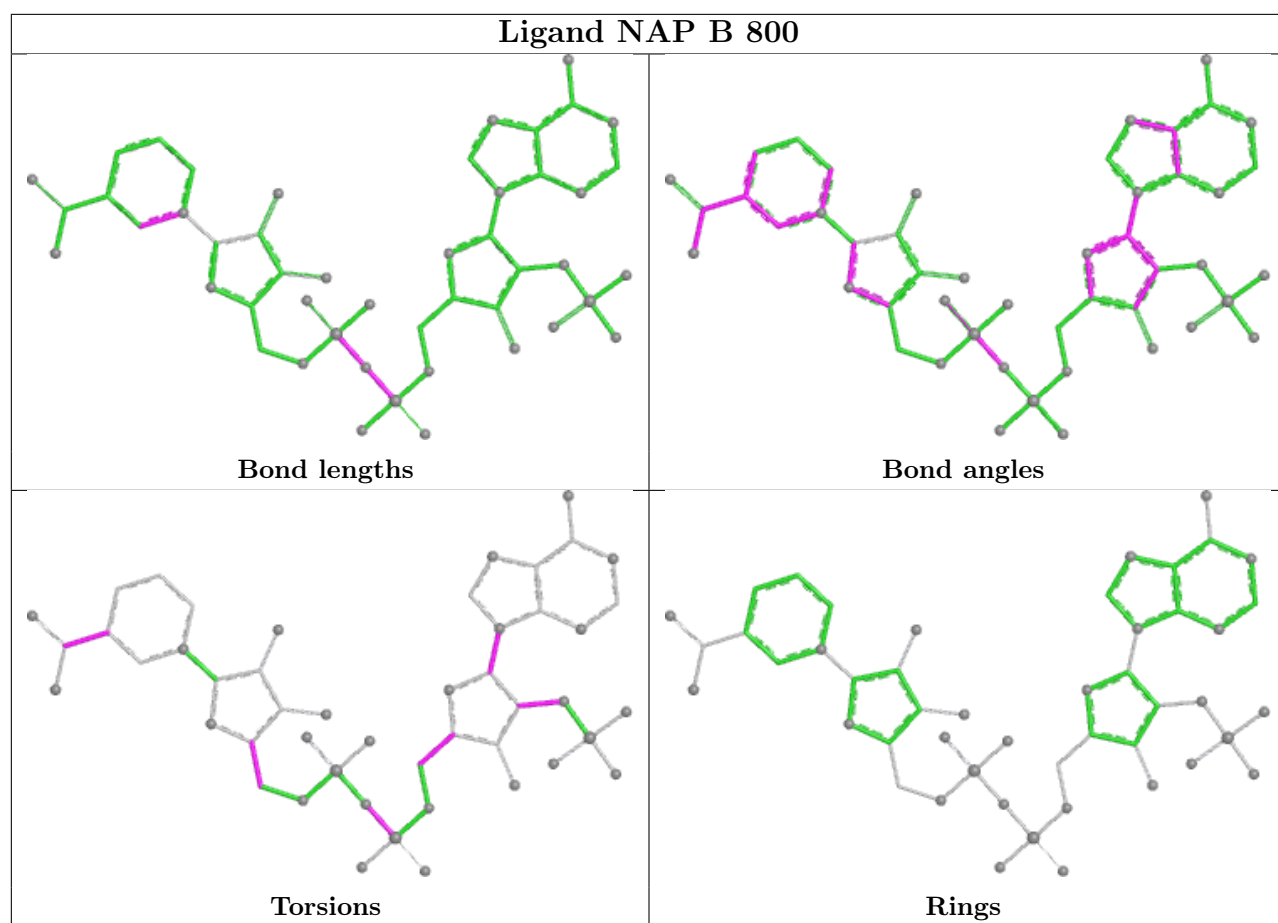
9 monomers are involved in 21 short contacts:

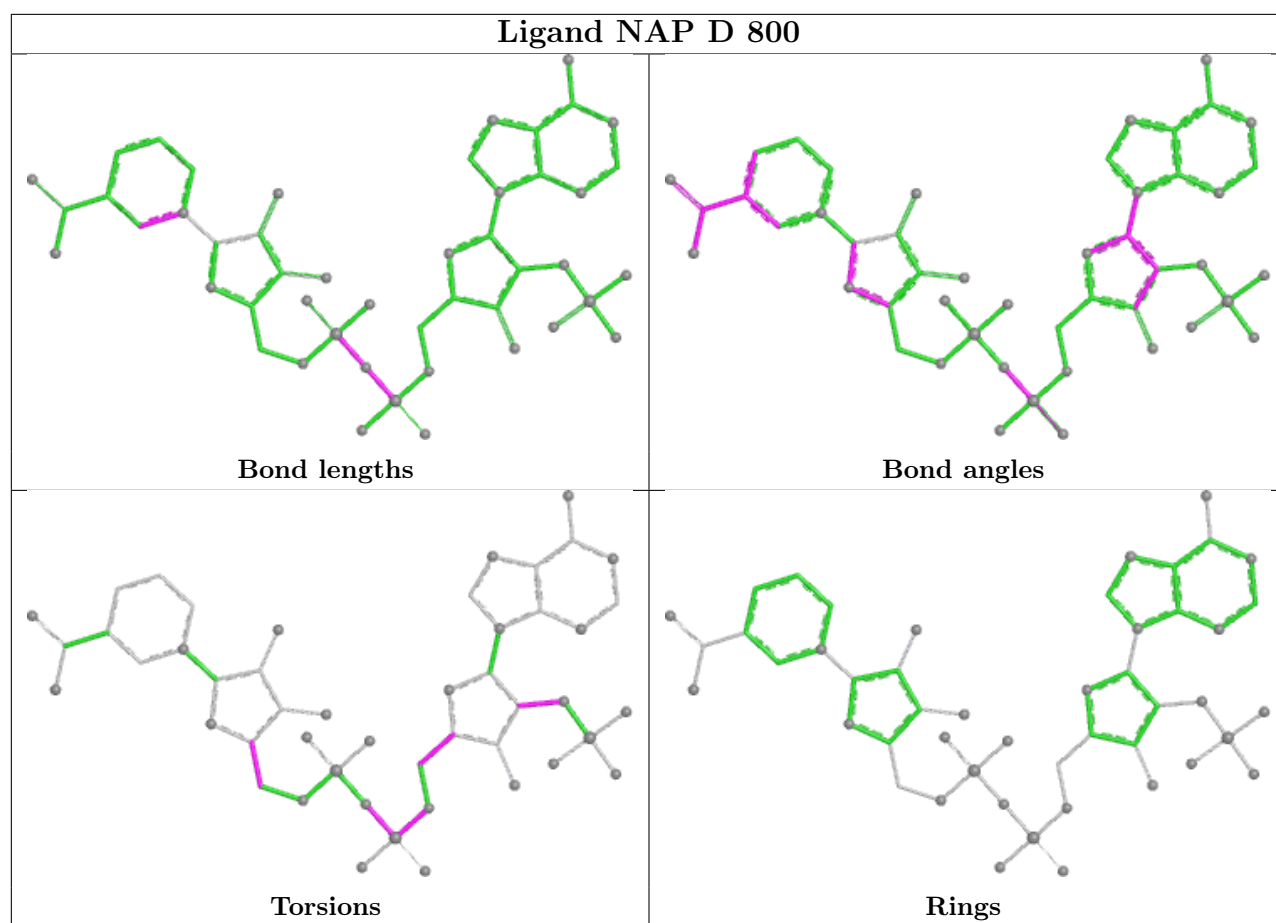
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1102	GOL	1	0
2	B	800	NAP	1	0
2	D	800	NAP	2	0
4	G	1104	GOL	3	0
2	C	800	NAP	1	0
4	B	1101	GOL	2	0
4	C	1103	GOL	4	0
2	H	800	NAP	3	0
4	E	1105	GOL	4	0

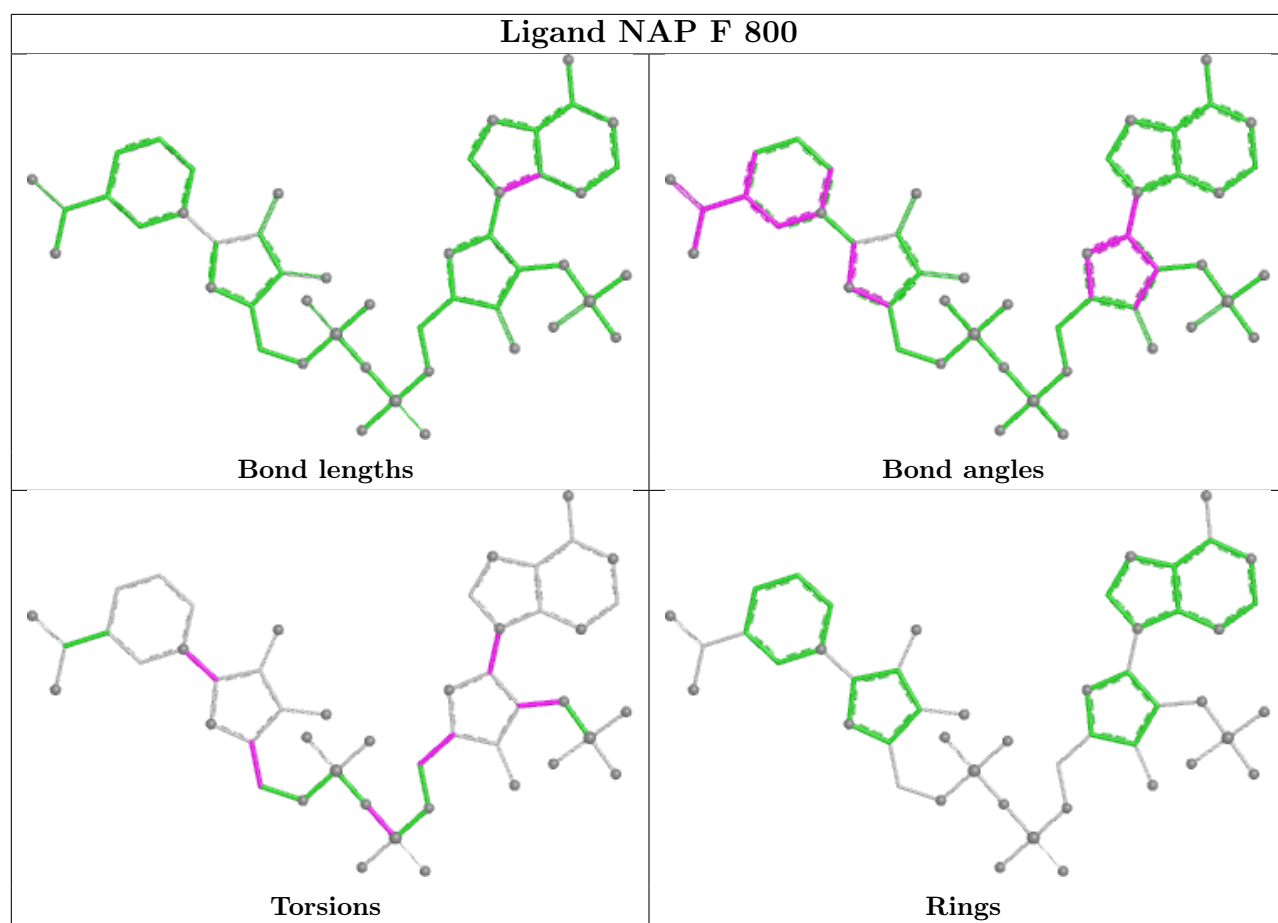
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

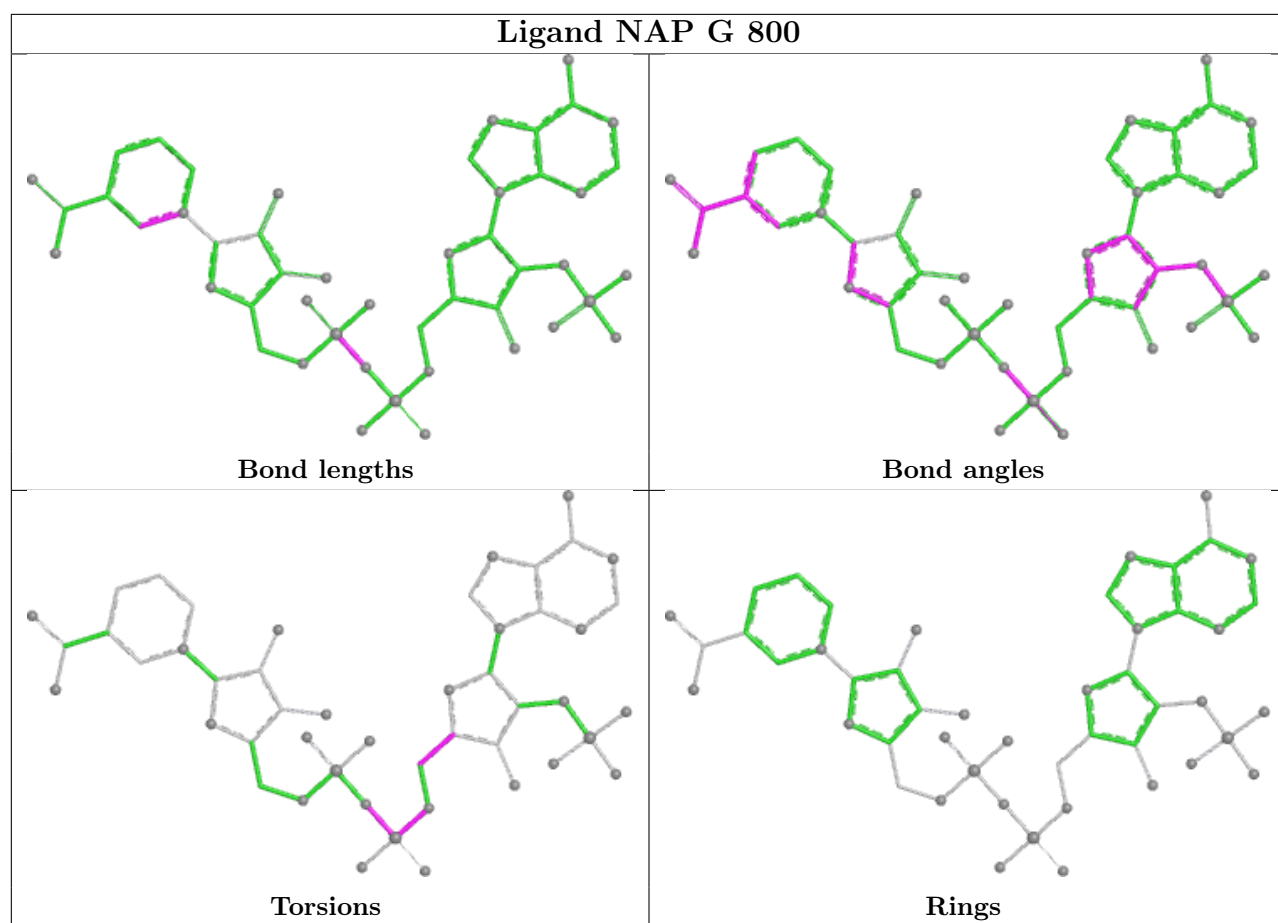


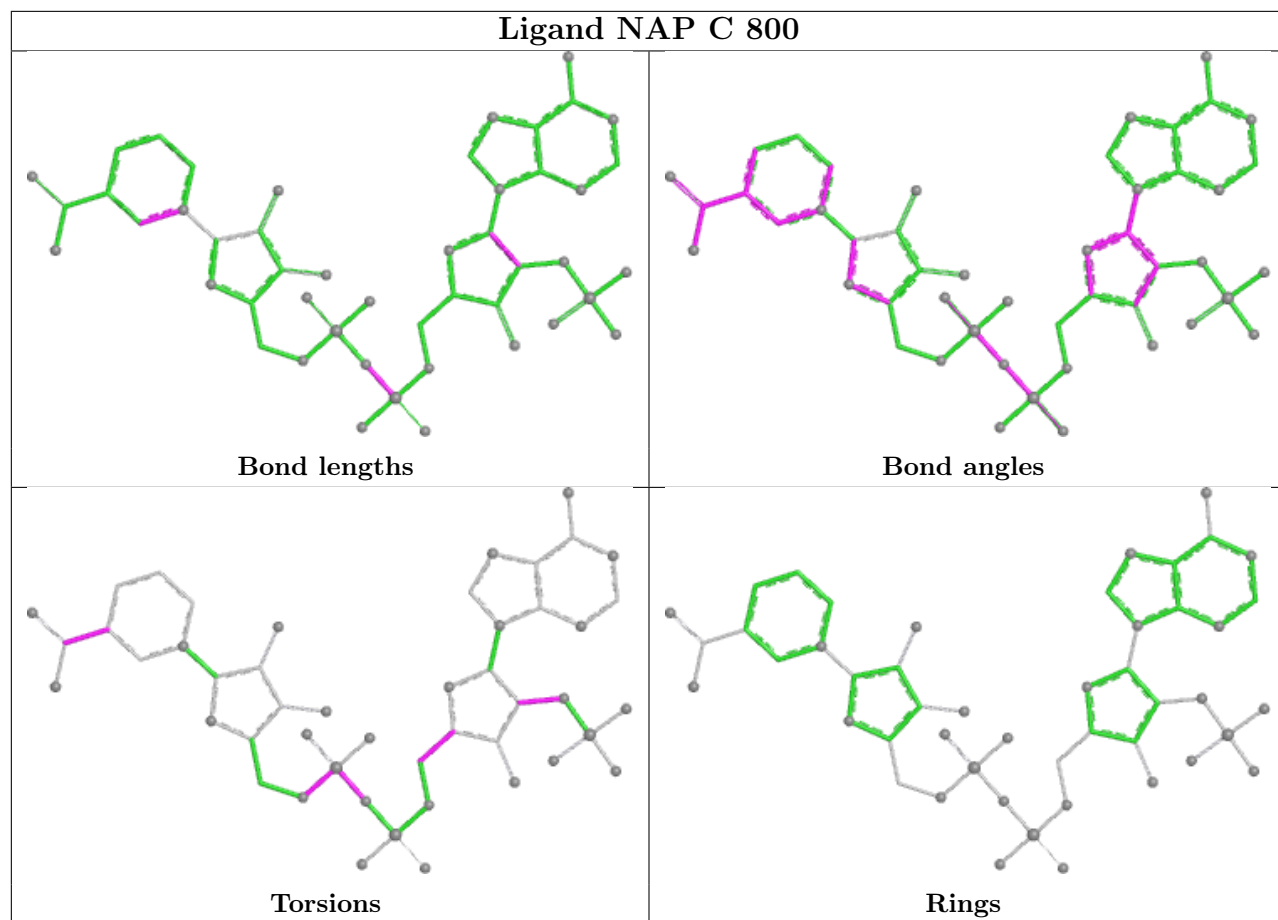


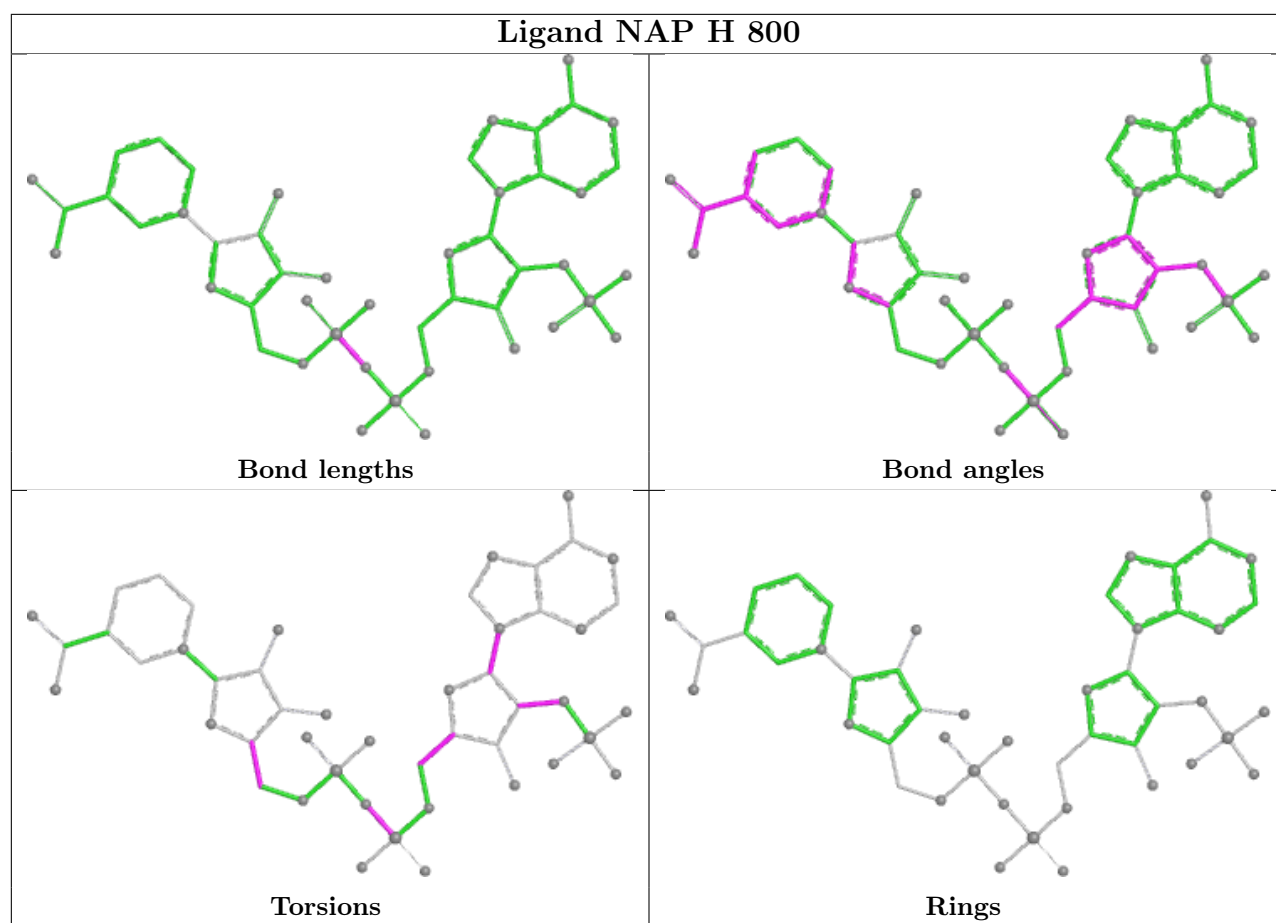












5.7 Other polymers [i](#)

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	488/514 (94%)	0.00	4 (0%) 82 64	17, 50, 69, 78	0
1	B	489/514 (95%)	0.03	8 (1%) 70 47	17, 52, 69, 81	0
1	C	489/514 (95%)	0.10	4 (0%) 82 64	19, 52, 70, 80	0
1	D	490/514 (95%)	0.00	5 (1%) 79 59	13, 49, 68, 81	0
1	E	487/514 (94%)	0.07	8 (1%) 70 47	18, 49, 69, 75	0
1	F	491/514 (95%)	0.08	11 (2%) 62 39	16, 50, 69, 81	0
1	G	489/514 (95%)	0.06	6 (1%) 76 55	17, 51, 69, 78	0
1	H	489/514 (95%)	0.14	3 (0%) 85 69	16, 51, 69, 78	0
All	All	3912/4112 (95%)	0.06	49 (1%) 75 53	13, 51, 69, 81	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	79	ASP	6.8
1	D	79	ASP	4.4
1	A	79	ASP	3.9
1	B	79	ASP	3.7
1	A	14	GLY	3.7
1	E	129	HIS	3.5
1	G	79	ASP	3.4
1	F	79	ASP	3.4
1	E	13	CYS	3.3
1	F	14	GLY	3.2
1	H	14	GLY	3.1
1	E	474	LEU	3.1
1	G	13	CYS	3.0
1	G	14	GLY	3.0
1	F	11	HIS	2.9
1	C	15	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	13	CYS	2.9
1	D	10	THR	2.8
1	B	13	CYS	2.8
1	B	76	THR	2.8
1	F	174	GLY	2.7
1	F	133	GLN	2.7
1	H	504	GLU	2.7
1	F	10	THR	2.7
1	C	94	GLU	2.6
1	C	79	ASP	2.5
1	G	53	TRP	2.5
1	F	249	TYR	2.5
1	D	76	THR	2.5
1	C	82	LYS	2.5
1	F	81	ARG	2.5
1	E	79	ASP	2.4
1	F	8	SER	2.4
1	B	511	ASN	2.3
1	B	12	VAL	2.3
1	E	71	ALA	2.3
1	E	101	PHE	2.3
1	E	176	ASP	2.3
1	F	12	VAL	2.3
1	A	76	THR	2.2
1	G	249	TYR	2.2
1	B	133	GLN	2.1
1	B	94	GLU	2.1
1	F	331	GLY	2.1
1	D	74	ARG	2.1
1	B	91	THR	2.1
1	E	174	GLY	2.0
1	A	83	GLN	2.0
1	G	504	GLU	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 ⓘ

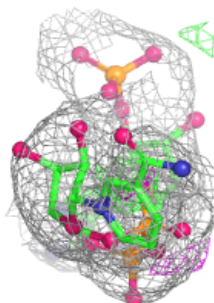
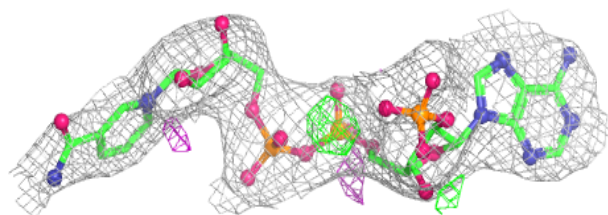
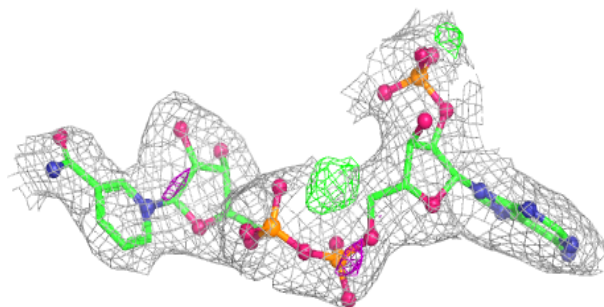
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOA	G	900	5/5	0.57	0.14	47,49,54,54	0
3	GOA	F	900	5/5	0.73	0.13	43,46,48,49	0
3	GOA	B	900	5/5	0.75	0.14	50,51,52,55	0
3	GOA	A	900	5/5	0.76	0.14	42,45,49,51	0
3	GOA	H	900	5/5	0.84	0.08	49,52,54,55	0
4	GOL	B	1102	6/6	0.84	0.12	54,55,58,61	0
4	GOL	B	1101	6/6	0.85	0.13	26,38,43,45	0
4	GOL	E	1105	6/6	0.85	0.11	4,21,24,27	0
3	GOA	C	900	5/5	0.87	0.08	44,46,53,56	0
3	GOA	E	900	5/5	0.87	0.11	33,45,49,49	0
3	GOA	D	900	5/5	0.89	0.10	25,27,29,31	0
2	NAP	H	800	48/48	0.89	0.10	39,45,60,67	0
4	GOL	C	1103	6/6	0.90	0.09	27,38,41,42	0
2	NAP	G	800	48/48	0.91	0.09	39,48,58,65	0
4	GOL	G	1104	6/6	0.91	0.11	8,17,23,27	0
2	NAP	A	800	48/48	0.92	0.08	34,44,58,67	0
2	NAP	D	800	48/48	0.92	0.09	32,48,58,61	0
2	NAP	F	800	48/48	0.92	0.09	35,46,55,58	0
2	NAP	E	800	48/48	0.93	0.10	35,45,55,61	0
2	NAP	C	800	48/48	0.94	0.08	33,48,54,56	0
2	NAP	B	800	48/48	0.95	0.07	36,48,56,60	0

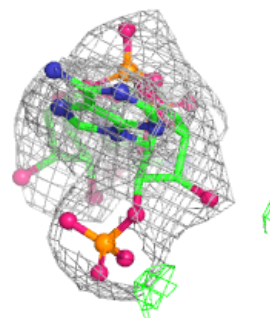
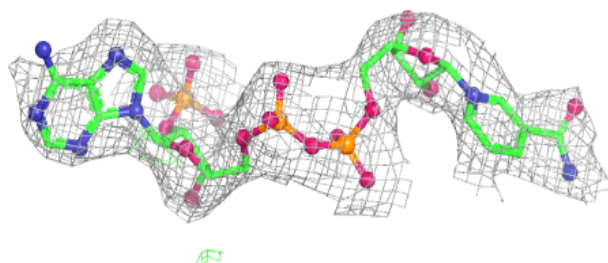
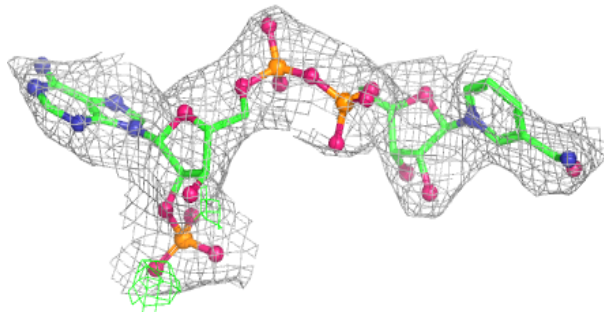
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP H 800:

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

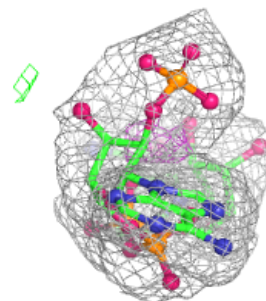
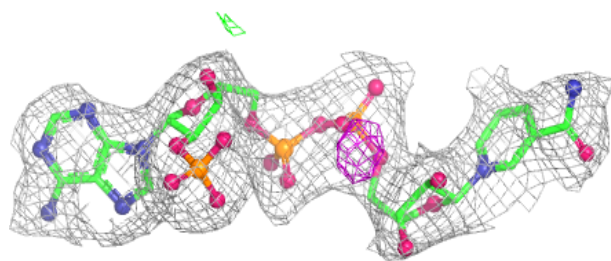
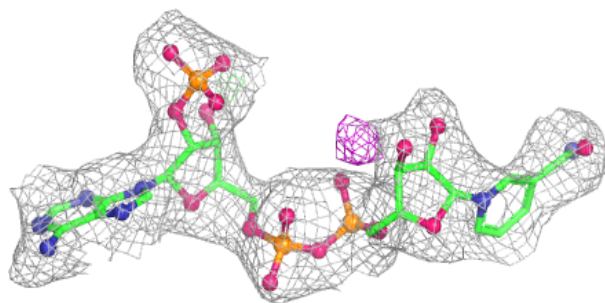
**Electron density around NAP G 800:**

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

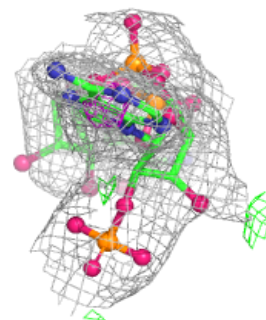
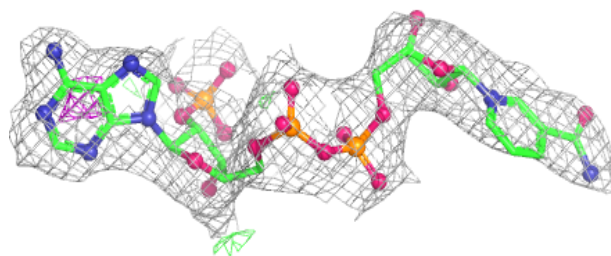
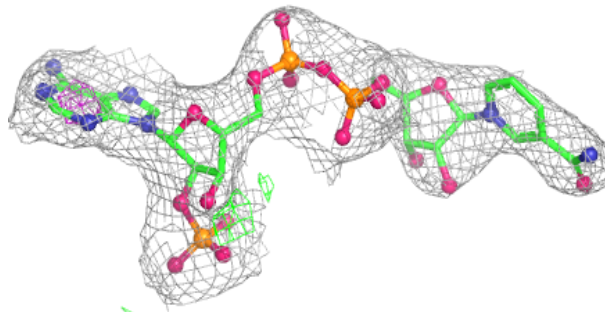


Electron density around NAP A 800:

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

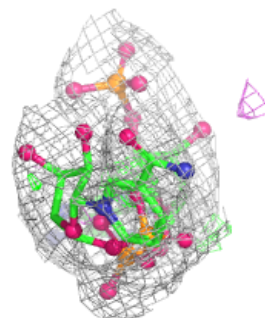
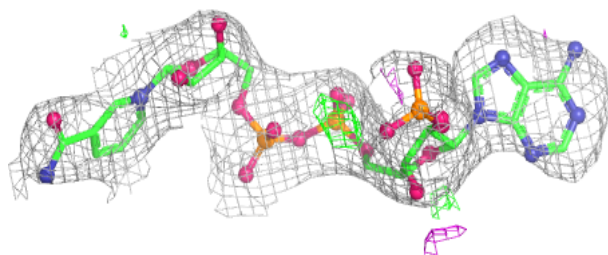
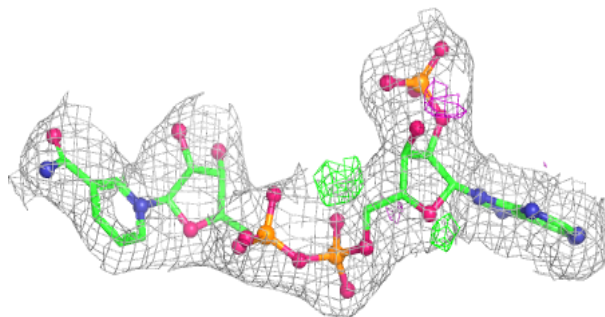
**Electron density around NAP D 800:**

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

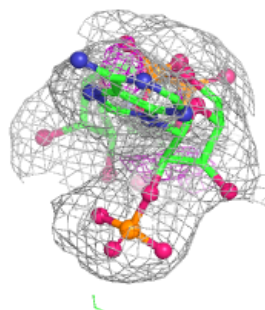
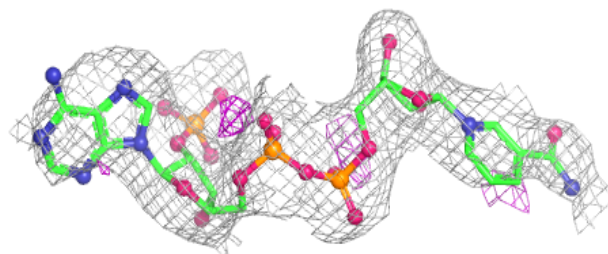
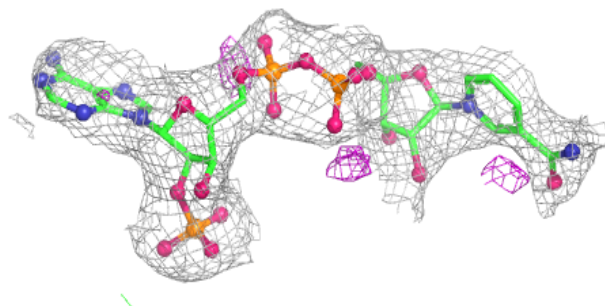


Electron density around NAP F 800:

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

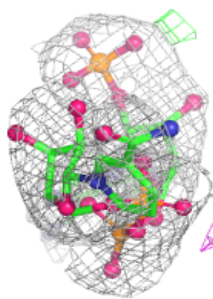
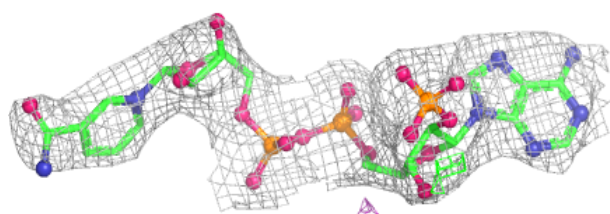
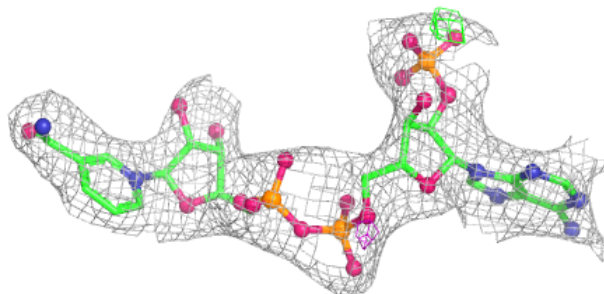
**Electron density around NAP E 800:**

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

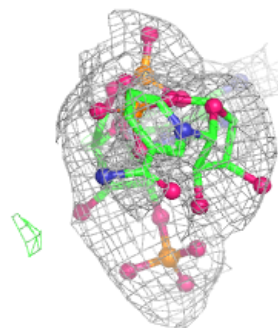
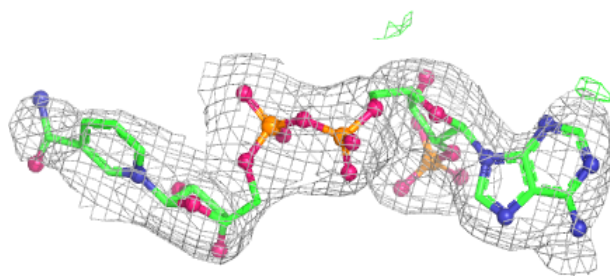
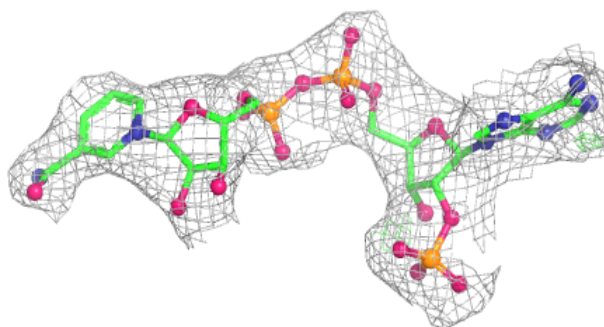


Electron density around NAP C 800:

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

**Electron density around NAP B 800:**

$2mF_o-DF_c$ (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.