



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:30 pm BST

PDB ID : 5E7O
Title : Crystal structure of the perchlorate reductase PcrAB mutant W461E of PcrA from Azospira suillum PS
Authors : Tsai, C.-L.; Tainer, J.A.
Deposited on : 2015-10-12
Resolution : 2.40 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 : 2.11
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) : 2.11

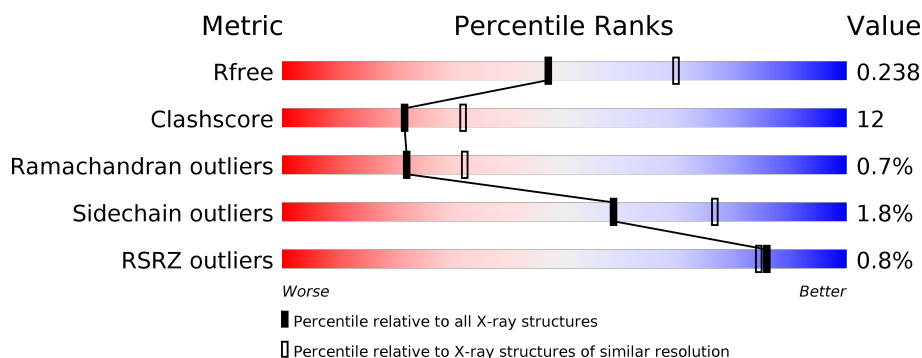
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	899	<div> <div>81%</div> <div>18%</div> </div>
1	C	899	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	E	899	<div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	G	899	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	I	899	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
1	K	899	<div> <div>2%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	333	
2	D	333	
2	F	333	
2	H	333	
2	J	333	
2	L	333	

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	SF4	I	1001	-	-	X	-
3	SF4	K	1001	-	-	X	-
7	EDO	F	401	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62374 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 DMSO reductase family type II enzyme, molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	C	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	E	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	G	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	I	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			
1	K	895	Total	C	N	O	S	0	3	0
			7180	4583	1246	1313	38			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	GLU	TRP	engineered mutation	UNP G8QM55
C	461	GLU	TRP	engineered mutation	UNP G8QM55
E	461	GLU	TRP	engineered mutation	UNP G8QM55
G	461	GLU	TRP	engineered mutation	UNP G8QM55
I	461	GLU	TRP	engineered mutation	UNP G8QM55
K	461	GLU	TRP	engineered mutation	UNP G8QM55

- Molecule 2 is a protein called DMSO reductase family type II enzyme, iron-sulfur subunit.

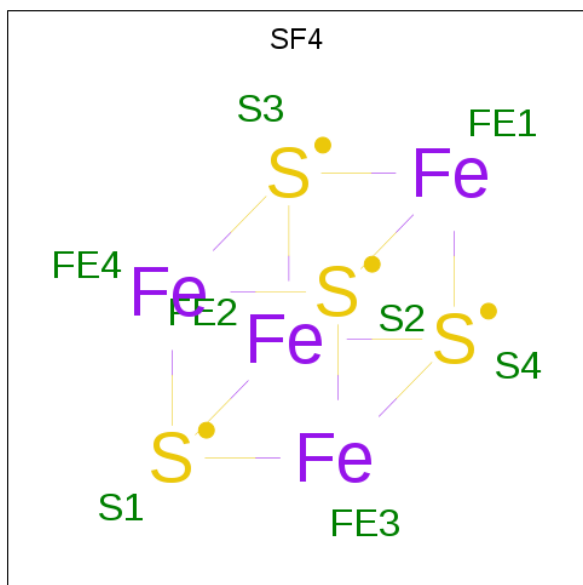
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	D	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	F	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	J	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			
2	L	329	Total	C	N	O	S	0	0	0
			2564	1627	447	465	25			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 8	Fe 4	S 4	0	0
3	F	1	Total 8	Fe 4	S 4	0	0
3	F	1	Total 8	Fe 4	S 4	0	0
3	F	1	Total 8	Fe 4	S 4	0	0
3	G	1	Total 8	Fe 4	S 4	0	0
3	H	1	Total 8	Fe 4	S 4	0	0
3	H	1	Total 8	Fe 4	S 4	0	0
3	H	1	Total 8	Fe 4	S 4	0	0
3	I	1	Total 8	Fe 4	S 4	0	0
3	J	1	Total 8	Fe 4	S 4	0	0
3	J	1	Total 8	Fe 4	S 4	0	0
3	J	1	Total 8	Fe 4	S 4	0	0
3	K	1	Total 8	Fe 4	S 4	0	0
3	L	1	Total 8	Fe 4	S 4	0	0
3	L	1	Total 8	Fe 4	S 4	0	0
3	L	1	Total 8	Fe 4	S 4	0	0

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

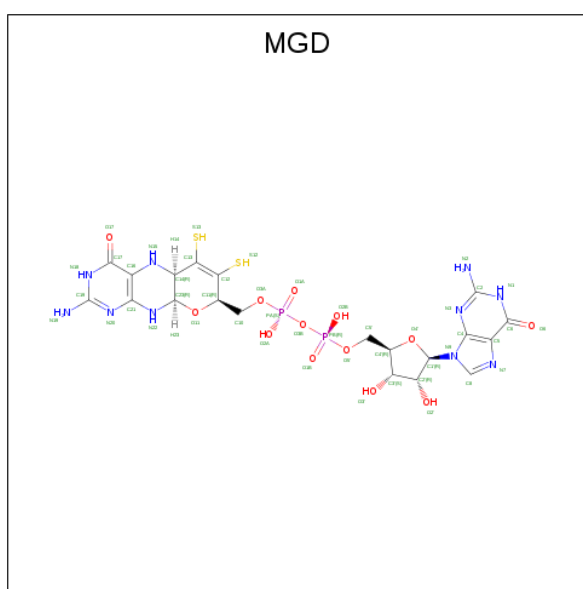
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mo 1	0	0
4	K	1	Total 1	Mo 1	0	0
4	E	1	Total 1	Mo 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Mo	0	0
			1	1		
4	C	1	Total	Mo	0	0
			1	1		
4	A	1	Total	Mo	0	0
			1	1		

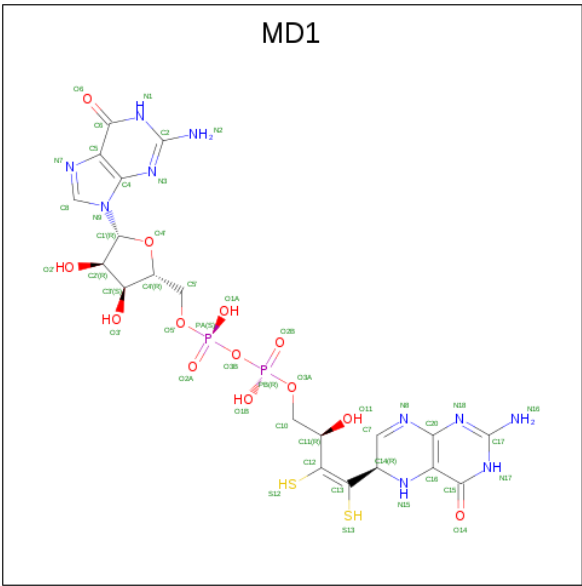
- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE

ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



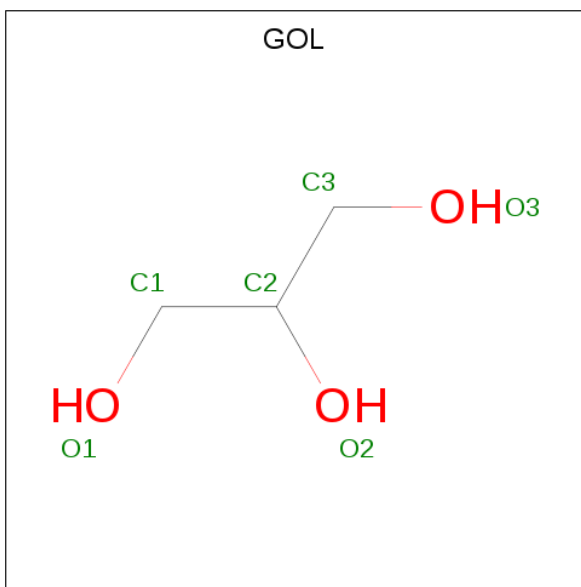
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		

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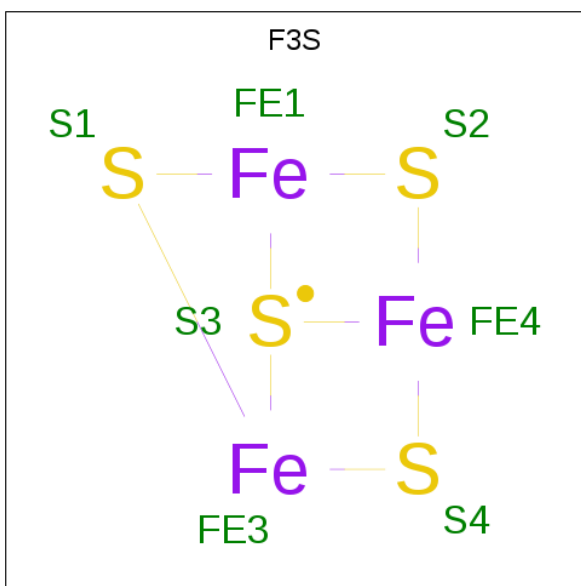
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	G	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	H	1	Total 4	C 2	O 2	0	0
7	I	1	Total 4	C 2	O 2	0	0
7	I	1	Total 4	C 2	O 2	0	0
7	J	1	Total 4	C 2	O 2	0	0
7	K	1	Total 4	C 2	O 2	0	0
7	K	1	Total 4	C 2	O 2	0	0
7	L	1	Total 4	C 2	O 2	0	0
7	L	1	Total 4	C 2	O 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	D	1	Total	Fe	S	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total 7	Fe 3	S 4	0	0
9	H	1	Total 7	Fe 3	S 4	0	0
9	J	1	Total 7	Fe 3	S 4	0	0
9	L	1	Total 7	Fe 3	S 4	0	0

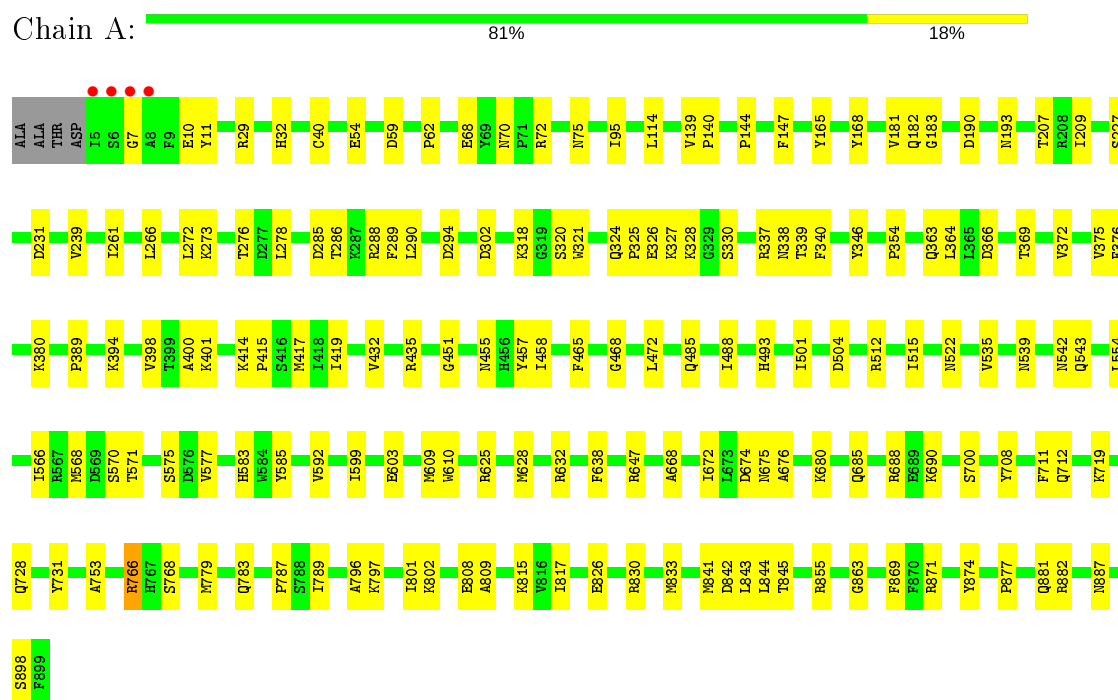
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	399	Total 399	O 399	0	0
10	B	179	Total 179	O 179	0	0
10	C	417	Total 417	O 417	0	0
10	D	176	Total 176	O 176	0	0
10	E	384	Total 384	O 384	0	0
10	F	148	Total 148	O 148	0	0
10	G	348	Total 348	O 348	0	0
10	H	116	Total 116	O 116	0	0
10	I	266	Total 266	O 266	0	0
10	J	127	Total 127	O 127	0	0
10	K	287	Total 287	O 287	0	0
10	L	131	Total 131	O 131	0	0

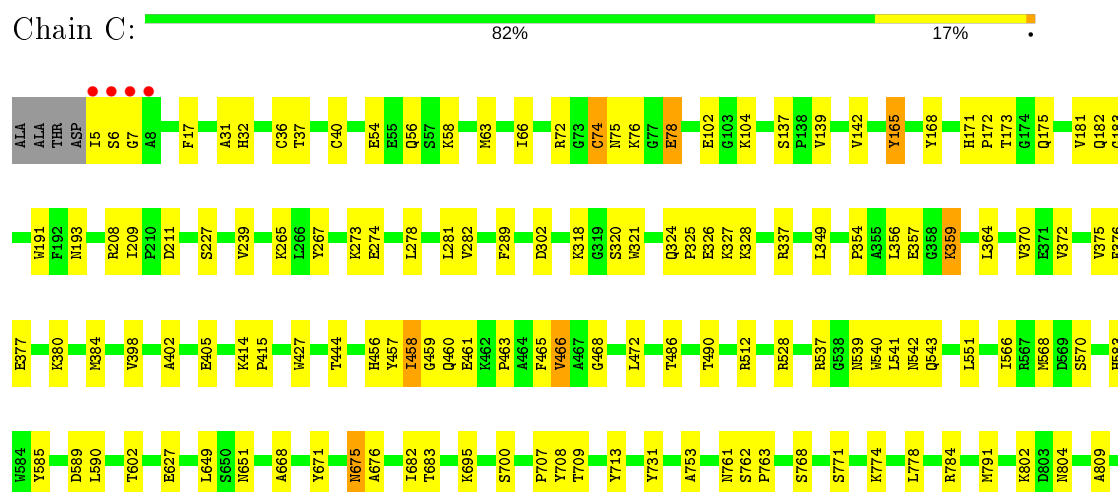
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DMSO reductase family type II enzyme, molybdopterin subunit



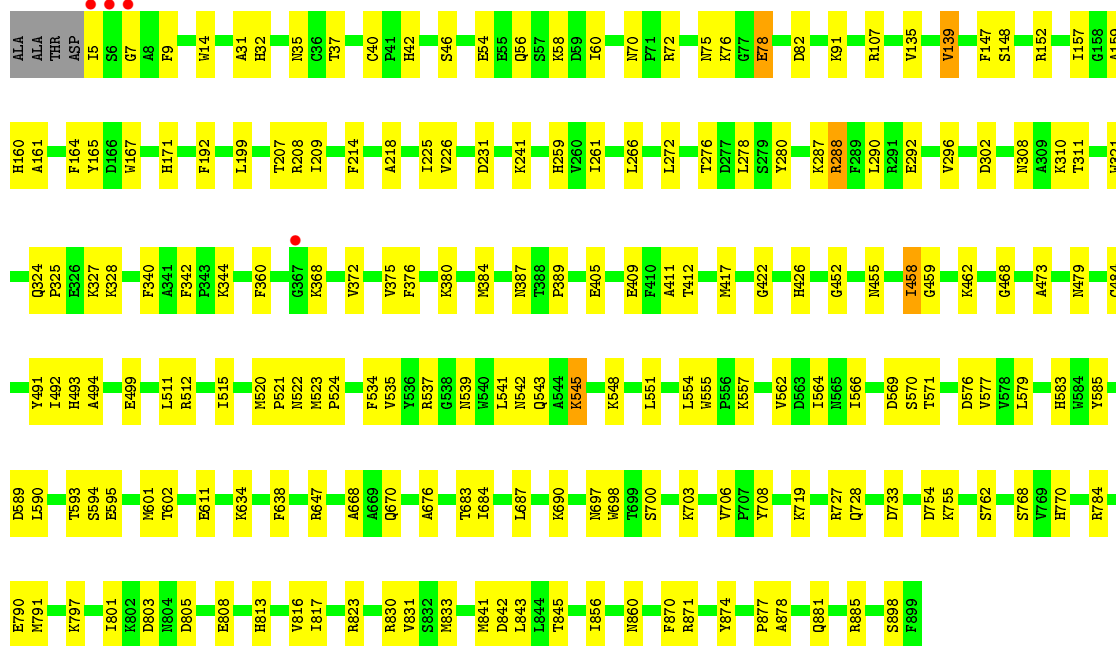
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit





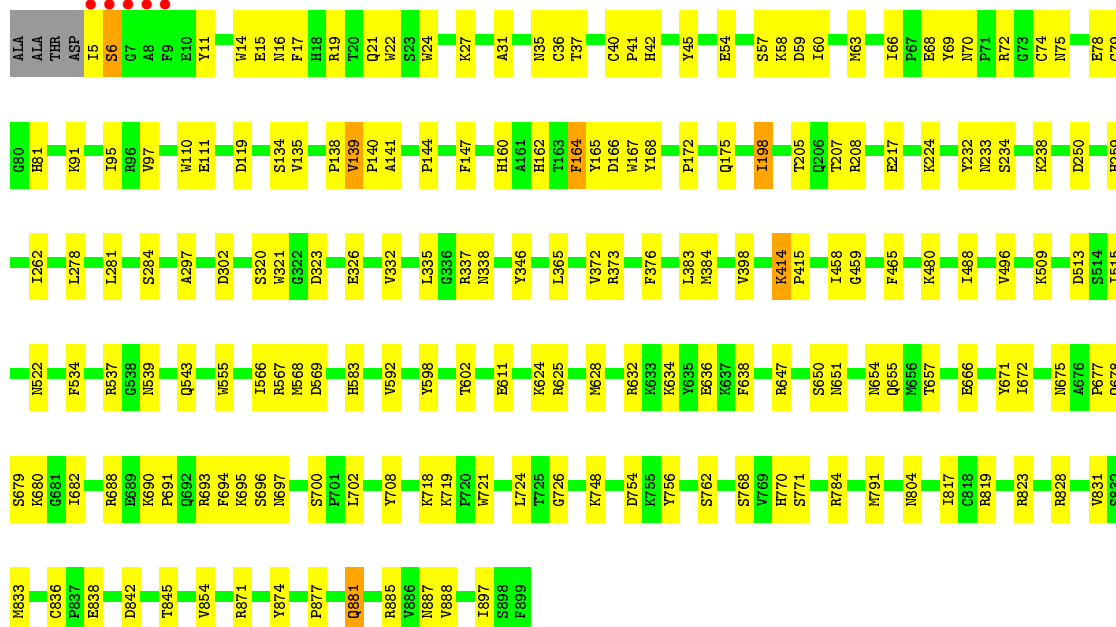
- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

Chain E: 78% 21%

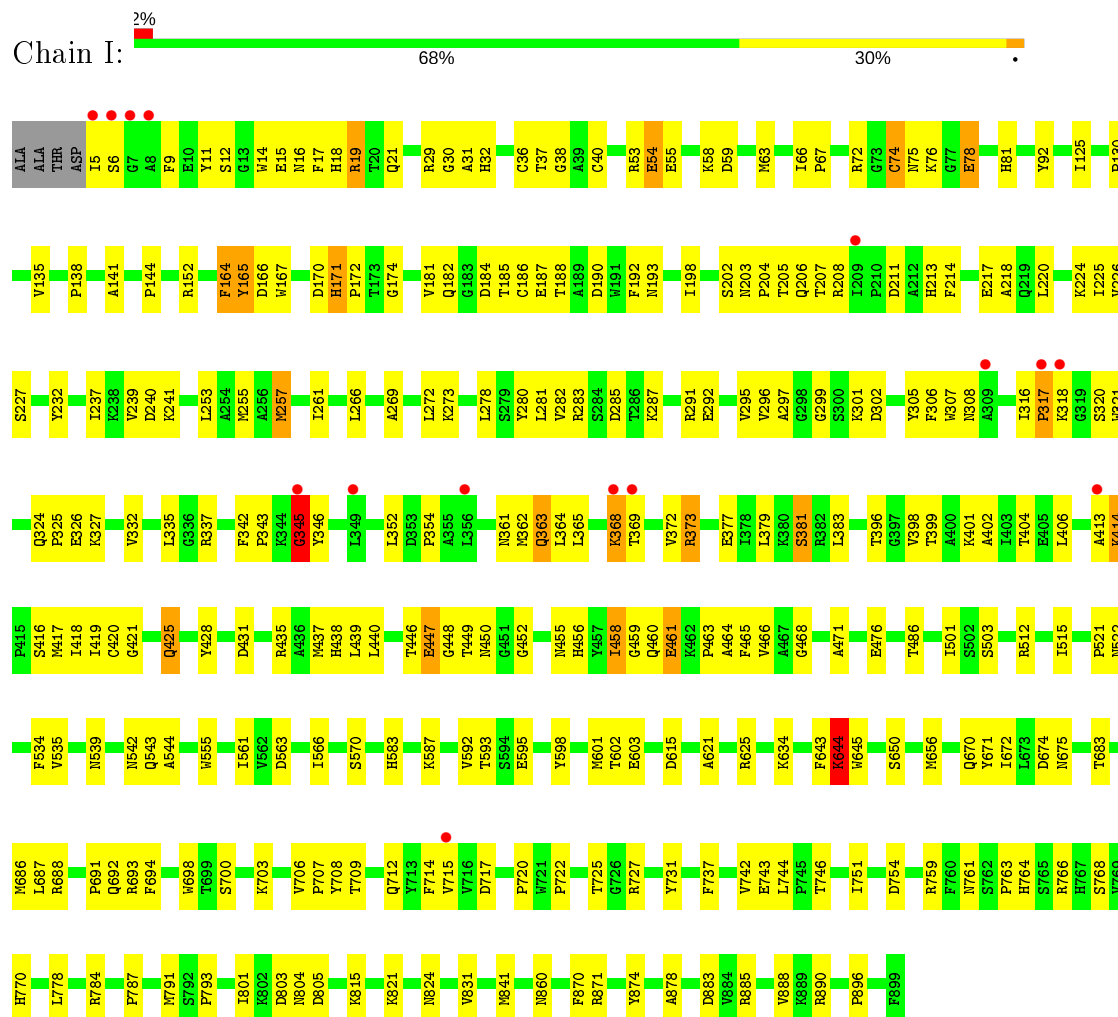


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

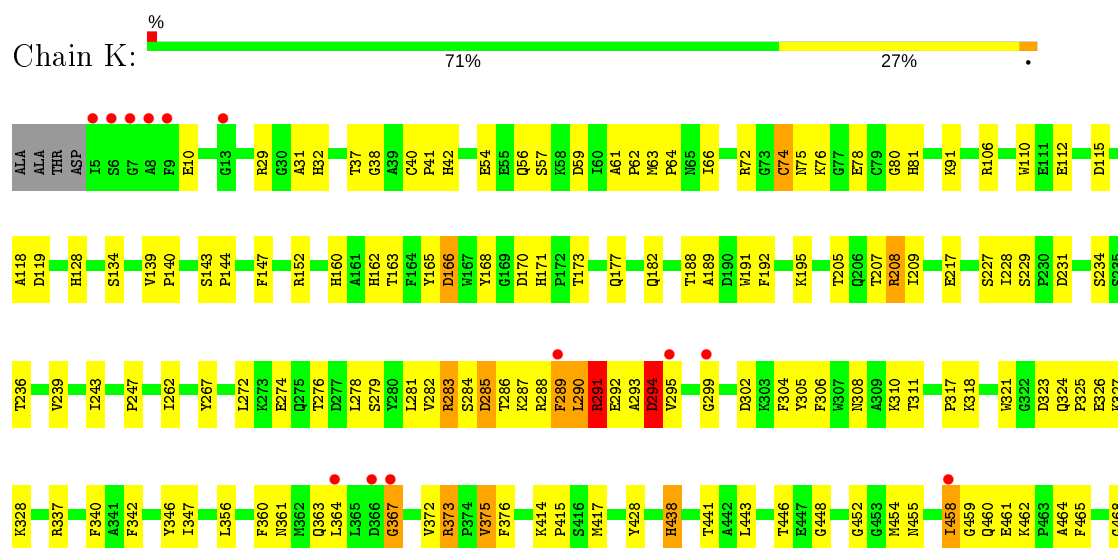
Chain G: 79% 20%

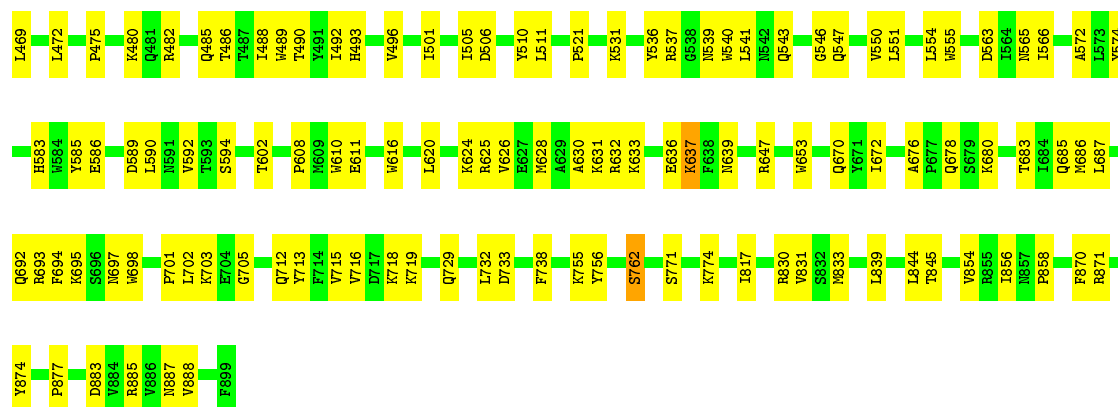


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

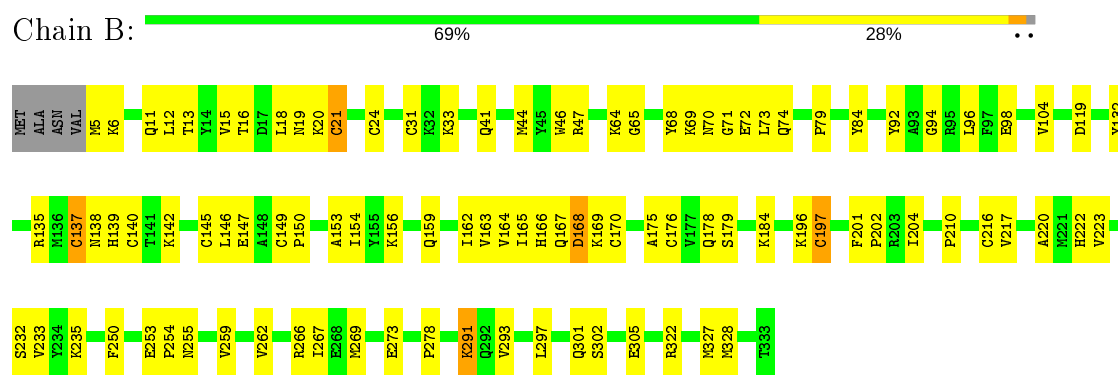


- Molecule 1: DMSO reductase family type II enzyme, molybdopterin subunit

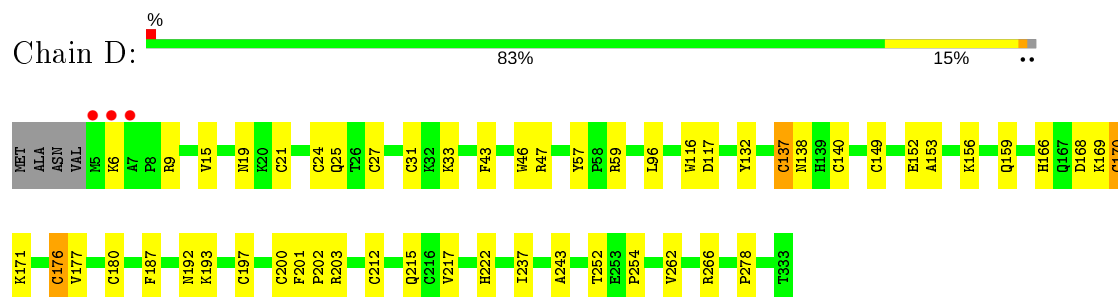




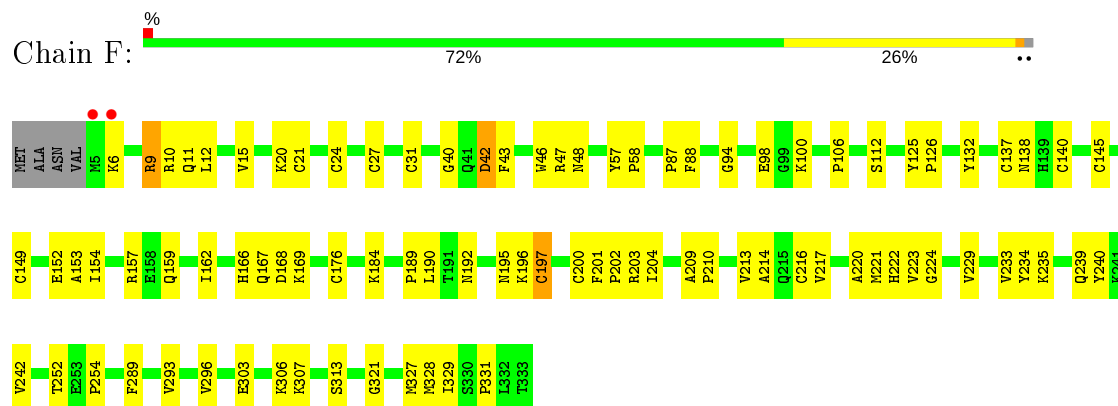
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



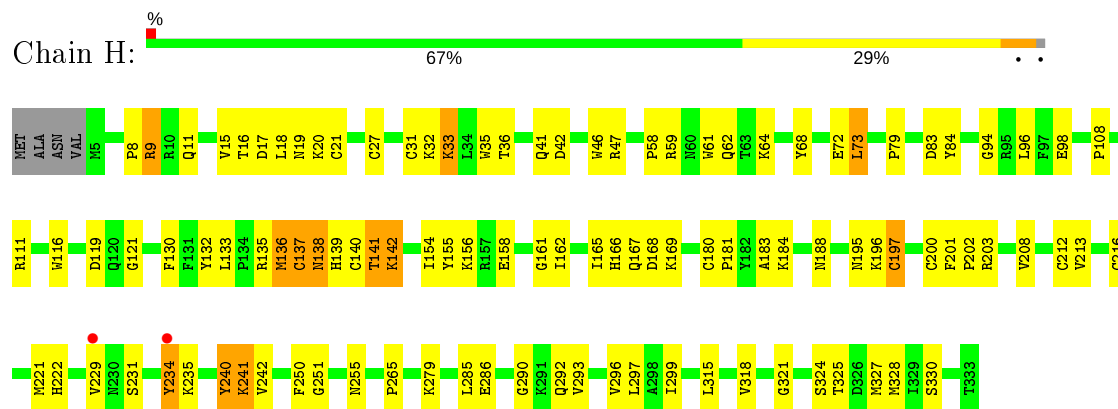
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



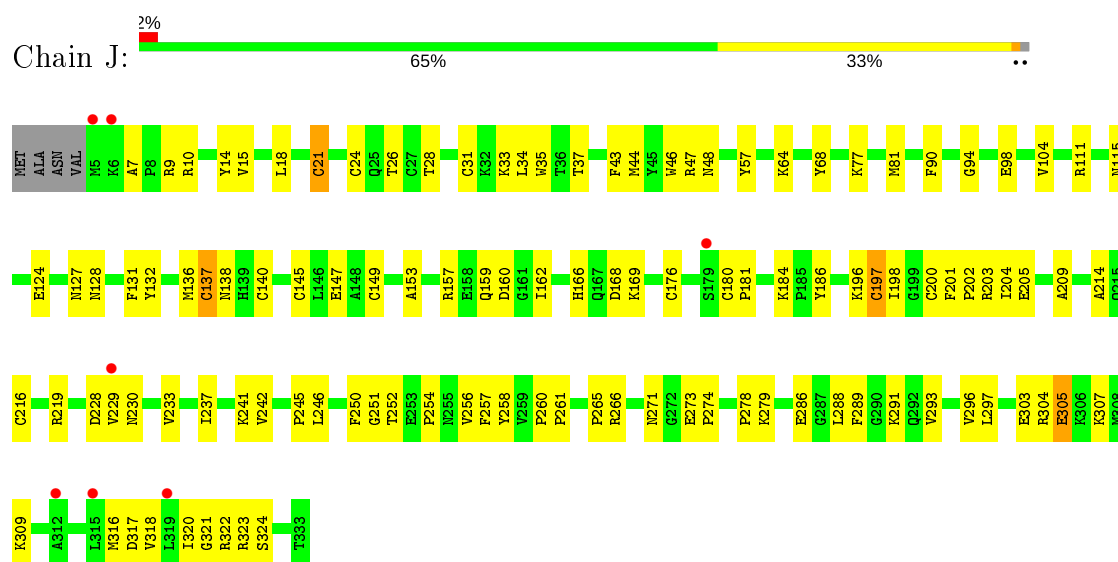
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



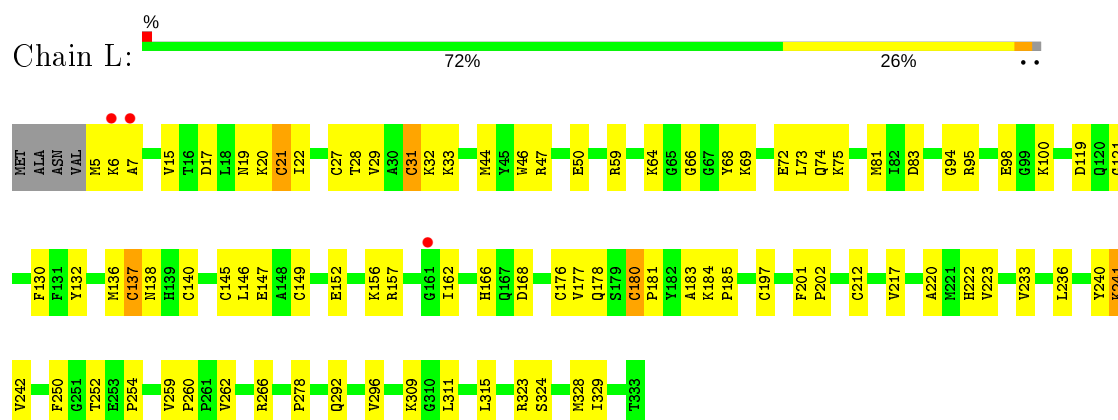
- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



- Molecule 2: DMSO reductase family type II enzyme, iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.59Å 253.13Å 135.80Å 90.00° 119.77° 90.00°	Depositor
Resolution (Å)	48.32 – 2.40 48.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.32-2.40) 99.2 (48.32-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.195 , 0.249 0.189 , 0.238	Depositor DCC
R_{free} test set	14935 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.137 for -h-l,k,h 0.137 for l,k,-h-l 0.186 for h,-k,-h-l 0.135 for -h-l,-k,l 0.127 for l,-k,h	Xtriage
Reported twinning fraction	0.160 for l,k,-h-l	Depositor
Outliers	0 of 306123 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	62374	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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, MGD, SF4, EDO, F3S, MD1, MO

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	0.24	0/7396	0.43	0/10034
1	C	0.25	0/7396	0.44	0/10034
1	E	0.25	0/7396	0.45	0/10034
1	G	0.26	0/7396	0.45	0/10034
1	I	0.30	0/7396	0.50	3/10034 (0.0%)
1	K	0.29	1/7396 (0.0%)	0.48	1/10034 (0.0%)
2	B	0.26	0/2632	0.44	0/3567
2	D	0.26	0/2632	0.45	1/3567 (0.0%)
2	F	0.25	0/2632	0.43	0/3567
2	H	0.30	0/2632	0.50	1/3567 (0.0%)
2	J	0.28	0/2632	0.49	0/3567
2	L	0.28	0/2632	0.46	0/3567
All	All	0.27	1/60168 (0.0%)	0.46	6/81606 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	2
1	K	0	1
2	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	324	GLN	C-N	5.12	1.44	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	73	LEU	CA-CB-CG	-7.69	97.61	115.30
1	I	406	LEU	CA-CB-CG	6.90	131.18	115.30
1	K	294	ASP	CB-CG-OD1	-6.26	112.67	118.30
2	D	176	CYS	CA-CB-SG	-5.65	103.83	114.00
1	I	19	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	I	414	LYS	CD-CE-NZ	-5.34	99.41	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	240	TYR	Peptide
1	I	345	GLY	Peptide
1	I	644	LYS	Peptide
1	K	294	ASP	Peptide

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	7180	0	7012	108	0
1	C	7180	0	7013	113	0
1	E	7180	0	7013	158	0
1	G	7180	0	7014	144	0
1	I	7180	0	7014	265	0
1	K	7180	0	7013	209	0
2	B	2564	0	2545	75	0
2	D	2564	0	2547	39	0
2	F	2564	0	2546	66	0
2	H	2564	0	2549	99	0
2	J	2564	0	2548	98	0
2	L	2564	0	2547	78	0
3	A	8	0	0	0	0
3	B	24	0	0	1	0
3	C	8	0	0	0	0
3	D	24	0	0	1	0
3	E	8	0	0	0	0
3	F	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	8	0	0	0	0
3	H	24	0	0	0	0
3	I	8	0	0	2	0
3	J	24	0	0	0	0
3	K	8	0	0	2	0
3	L	24	0	0	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	47	0	22	2	0
5	C	47	0	22	1	0
5	E	47	0	22	4	0
5	G	47	0	22	3	0
5	I	47	0	22	7	0
5	K	47	0	22	1	0
6	A	47	0	21	1	0
6	C	47	0	21	2	0
6	E	47	0	21	1	0
6	G	47	0	22	6	0
6	I	47	0	23	2	0
6	K	47	0	21	3	0
7	A	20	0	30	1	0
7	B	8	0	12	0	0
7	C	12	0	18	2	0
7	D	4	0	6	0	0
7	E	8	0	12	2	0
7	F	8	0	12	1	0
7	G	16	0	24	3	0
7	H	12	0	18	3	0
7	I	8	0	12	3	0
7	J	4	0	6	0	0
7	K	8	0	12	0	0
7	L	8	0	12	0	0
8	A	6	0	8	1	0
8	E	6	0	8	1	0
9	B	7	0	0	0	0
9	D	7	0	0	0	0
9	F	7	0	0	0	0
9	H	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	7	0	0	0	0
9	L	7	0	0	0	0
10	A	399	0	0	19	0
10	B	179	0	0	23	0
10	C	417	0	0	25	0
10	D	176	0	0	5	0
10	E	384	0	0	39	0
10	F	148	0	0	13	0
10	G	348	0	0	23	0
10	H	116	0	0	13	0
10	I	266	0	0	41	0
10	J	127	0	0	18	0
10	K	287	0	0	24	0
10	L	131	0	0	13	0
All	All	62374	0	57812	1396	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 (1396) 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:K:294:ASP:HB3	1:K:364:LEU:HD12	1.48	0.94
1:I:53:ARG:NH2	1:I:55:GLU:OE1	2.04	0.90
1:A:628:MET:SD	1:A:632:ARG:NH1	2.45	0.90
2:J:245:PRO:HB2	2:J:254:PRO:HG2	1.54	0.87
1:A:830:ARG:NH1	10:A:1101:HOH:O	2.08	0.87
2:J:157:ARG:NH2	2:J:160:ASP:OD2	2.08	0.86
1:K:81:HIS:NE2	2:L:33:LYS:HE3	1.92	0.83
1:E:225:ILE:O	10:E:1101:HOH:O	1.96	0.82
2:H:195:ASN:ND2	10:H:501:HOH:O	2.12	0.82
1:I:416:SER:H	1:I:446:THR:HG21	1.43	0.82
1:E:60:ILE:H	1:E:70:ASN:HD21	1.28	0.81
1:I:186:CYS:SG	10:I:1142:HOH:O	2.39	0.80
2:J:137:CYS:SG	2:J:196:LYS:NZ	2.55	0.79
1:A:278:LEU:HA	1:A:375:VAL:HB	1.64	0.79
1:G:284:SER:OG	1:G:373:ARG:NH1	2.14	0.79
1:I:399:THR:HG23	1:I:402:ALA:H	1.48	0.79
2:F:210:PRO:O	10:F:501:HOH:O	2.02	0.77
1:G:95:ILE:O	10:G:1101:HOH:O	2.03	0.77
1:K:170:ASP:HB3	1:K:458:ILE:HD13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:GLU:O	10:I:1102:HOH:O	2.04	0.76
1:K:278:LEU:HA	1:K:375:VAL:HG23	1.67	0.76
1:I:282:VAL:O	10:I:1101:HOH:O	2.03	0.76
1:A:324:GLN:OE1	1:A:328:LYS:NZ	2.19	0.76
2:H:240:TYR:O	2:H:242:VAL:N	2.19	0.75
2:L:73:LEU:HD22	2:L:147:GLU:HG2	1.67	0.75
1:A:766:ARG:NH2	2:B:119:ASP:OD2	2.19	0.75
2:L:47:ARG:NH1	10:L:501:HOH:O	2.19	0.75
1:I:202:SER:OG	10:I:1103:HOH:O	2.04	0.75
2:B:253:GLU:O	10:B:502:HOH:O	2.04	0.75
1:C:302:ASP:HB3	1:C:321:TRP:HB3	1.69	0.75
1:I:19:ARG:NH2	2:J:205:GLU:OE2	2.20	0.74
2:B:137:CYS:SG	2:B:196:LYS:NZ	2.58	0.74
1:I:461:GLU:HG2	1:I:463:PRO:HD3	1.67	0.74
2:J:44:MET:SD	10:J:504:HOH:O	2.45	0.74
1:G:804:ASN:HB3	7:G:1008:EDO:H21	1.70	0.74
2:F:303:GLU:OE1	10:F:502:HOH:O	2.05	0.73
2:D:193:LYS:NZ	10:D:501:HOH:O	2.09	0.73
1:I:693:ARG:NH2	10:I:1107:HOH:O	2.20	0.73
2:J:138:ASN:HD21	2:J:256:VAL:HG22	1.53	0.73
1:K:294:ASP:HB2	1:K:295:VAL:HG23	1.70	0.73
1:K:284:SER:HB2	1:K:373:ARG:HH12	1.53	0.73
2:L:137:CYS:HB3	2:L:197:CYS:HB3	1.68	0.73
2:H:196:LYS:NZ	10:H:504:HOH:O	2.20	0.72
1:I:447:GLU:OE1	1:I:715:VAL:HG21	1.88	0.72
1:I:208:ARG:NH2	5:I:1003:MGD:N22	2.37	0.72
2:B:175:ALA:HA	2:B:178:GLN:HE21	1.53	0.72
1:I:165:TYR:HE2	1:I:458:ILE:HD12	1.54	0.72
1:I:165:TYR:HE2	1:I:458:ILE:CD1	2.01	0.72
1:K:143:SER:OG	1:K:537:ARG:NH1	2.22	0.72
2:D:47:ARG:HB2	3:D:404:SF4:S4	2.30	0.72
1:G:651:ASN:HD21	1:G:654:ASN:HD22	1.38	0.72
2:B:267:ILE:O	10:B:504:HOH:O	2.07	0.72
2:B:16:THR:O	10:B:503:HOH:O	2.07	0.72
2:H:197:CYS:SG	10:H:504:HOH:O	2.47	0.72
1:C:583:HIS:ND1	10:C:1110:HOH:O	2.23	0.71
2:L:47:ARG:HB2	3:L:404:SF4:S4	2.29	0.71
1:C:874:TYR:O	10:C:1101:HOH:O	2.06	0.71
2:F:112:SER:O	10:F:503:HOH:O	2.08	0.71
2:L:136:MET:SD	10:L:501:HOH:O	2.48	0.71
1:G:45:TYR:OH	10:G:1102:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:342:PHE:HD2	1:I:720:PRO:HG2	1.54	0.71
1:E:520:MET:SD	10:E:1424:HOH:O	2.48	0.71
1:A:272:LEU:O	1:A:276:THR:OG1	2.07	0.71
1:G:36:CYS:SG	10:G:1232:HOH:O	2.48	0.71
1:K:311:THR:OG1	10:K:1101:HOH:O	2.08	0.71
1:G:509:LYS:NZ	1:G:513:ASP:OD1	2.19	0.71
2:J:318:VAL:O	10:J:501:HOH:O	2.08	0.71
1:G:657:THR:OG1	10:G:1103:HOH:O	2.09	0.70
1:I:420:CYS:HB2	1:I:456:HIS:HA	1.73	0.70
1:E:426:HIS:CG	1:E:881:GLN:HE21	2.09	0.70
2:J:286:GLU:HG2	2:J:291:LYS:HA	1.73	0.70
1:K:42:HIS:CE1	1:K:56:GLN:HG3	2.27	0.70
1:A:40:CYS:SG	1:A:72:ARG:HB3	2.31	0.70
1:I:674:ASP:OD2	10:I:1105:HOH:O	2.10	0.70
2:J:115:ASN:ND2	10:J:511:HOH:O	2.24	0.70
1:K:325:PRO:O	1:K:327:LYS:N	2.24	0.70
1:E:871:ARG:HB3	1:E:874:TYR:HB3	1.74	0.70
2:H:140:CYS:O	2:H:156:LYS:NZ	2.25	0.70
2:J:136:MET:HG3	10:J:512:HOH:O	1.90	0.70
1:E:148:SER:O	10:E:1102:HOH:O	2.09	0.69
2:J:46:TRP:NE1	10:J:504:HOH:O	2.22	0.69
2:J:138:ASN:ND2	2:J:256:VAL:HG22	2.06	0.69
2:J:145:CYS:HB2	2:J:176:CYS:HB2	1.74	0.69
2:J:64:LYS:NZ	2:J:77:LYS:O	2.26	0.69
1:K:461:GLU:OE1	10:K:1102:HOH:O	2.09	0.69
1:I:59:ASP:OD2	10:I:1104:HOH:O	2.09	0.69
1:I:283:ARG:HA	1:I:372:VAL:HG23	1.73	0.69
1:K:163:THR:H	1:K:486:THR:HG23	1.56	0.69
2:B:169:LYS:NZ	10:B:512:HOH:O	2.26	0.69
1:E:214:PHE:O	10:E:1103:HOH:O	2.11	0.69
2:H:137:CYS:HB2	2:H:184:LYS:HD2	1.74	0.69
1:I:670:GLN:HE22	1:I:683:THR:HA	1.57	0.69
1:I:896:PRO:HG2	7:I:1006:EDO:H12	1.73	0.69
1:G:768:SER:O	5:G:1003:MGD:N18	2.25	0.69
1:I:9:PHE:HB2	1:I:12:SER:HB2	1.75	0.69
1:E:684:ILE:HA	1:E:687:LEU:HD23	1.75	0.68
1:I:30:GLY:O	10:I:1106:HOH:O	2.11	0.68
1:G:634:LYS:NZ	10:G:1117:HOH:O	2.25	0.68
2:B:222:HIS:ND1	10:B:501:HOH:O	2.19	0.68
2:B:69:LYS:O	2:B:72:GLU:N	2.25	0.68
2:L:59:ARG:HD3	2:L:83:ASP:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:295:VAL:HG13	1:I:296:VAL:HG22	1.76	0.68
1:G:567:ARG:NH1	1:G:838:GLU:OE1	2.25	0.68
1:K:693:ARG:HH21	1:K:702:LEU:HD11	1.59	0.68
1:G:232:TYR:O	1:G:823:ARG:NH2	2.27	0.68
1:I:29:ARG:N	1:I:603:GLU:OE1	2.23	0.68
2:J:138:ASN:ND2	10:J:512:HOH:O	2.26	0.68
2:B:145:CYS:HB2	2:B:176:CYS:HB2	1.76	0.68
1:E:161:ALA:O	10:E:1104:HOH:O	2.12	0.68
1:G:166:ASP:OD2	10:G:1104:HOH:O	2.11	0.68
1:A:898:SER:O	1:C:512:ARG:NH1	2.27	0.67
2:H:17:ASP:OD2	10:H:502:HOH:O	2.12	0.67
1:I:165:TYR:CE2	1:I:458:ILE:CD1	2.77	0.67
1:I:198:ILE:HD13	1:I:226:VAL:CG1	2.24	0.67
1:I:16:ASN:ND2	1:I:19:ARG:HH11	1.92	0.67
1:I:332:VAL:HG13	1:I:335:LEU:HB2	1.76	0.67
1:I:815:LYS:NZ	10:I:1118:HOH:O	2.24	0.67
2:L:157:ARG:N	10:L:506:HOH:O	2.27	0.67
1:E:152:ARG:N	10:E:1102:HOH:O	2.15	0.67
1:K:460:GLN:NE2	1:K:592:VAL:O	2.26	0.67
1:A:380:LYS:NZ	10:A:1114:HOH:O	2.28	0.66
1:I:16:ASN:HD22	1:I:19:ARG:HH11	1.43	0.66
1:K:325:PRO:HB3	1:K:342:PHE:CE2	2.30	0.66
2:J:196:LYS:NZ	2:J:197:CYS:O	2.25	0.66
1:I:226:VAL:HG23	1:I:241:LYS:O	1.94	0.66
1:C:753:ALA:HB3	1:C:855:ARG:HH21	1.59	0.66
2:F:137:CYS:HB3	2:F:197:CYS:SG	2.36	0.66
1:G:680:LYS:O	1:G:695:LYS:NZ	2.28	0.66
2:H:11:GLN:NE2	2:H:255:ASN:OD1	2.29	0.66
1:I:706:VAL:O	10:I:1107:HOH:O	2.13	0.66
1:C:324:GLN:HE21	1:C:328:LYS:NZ	1.93	0.66
2:D:176:CYS:SG	2:D:177:VAL:N	2.69	0.66
1:I:688:ARG:NH2	10:I:1121:HOH:O	2.26	0.66
2:J:127:ASN:ND2	10:J:515:HOH:O	2.29	0.66
2:J:14:TYR:CD2	2:J:256:VAL:HG12	2.31	0.66
1:I:778:LEU:HD22	2:J:33:LYS:HE2	1.78	0.66
1:A:288:ARG:NH1	10:A:1113:HOH:O	2.28	0.66
1:A:609:MET:SD	10:A:1119:HOH:O	2.53	0.66
1:E:494:ALA:N	10:E:1125:HOH:O	2.27	0.66
2:F:224:GLY:O	10:F:504:HOH:O	2.13	0.66
1:G:24:TRP:NE1	10:G:1126:HOH:O	2.29	0.66
1:A:779:MET:O	10:A:1102:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:149:CYS:SG	2:J:153:ALA:N	2.69	0.65
1:A:675:ASN:ND2	10:A:1112:HOH:O	2.28	0.65
1:C:318:LYS:NZ	10:C:1121:HOH:O	2.28	0.65
2:F:149:CYS:SG	2:F:153:ALA:N	2.69	0.65
1:K:119:ASP:OD1	1:K:632:ARG:NH2	2.26	0.65
1:A:493:HIS:HB2	1:A:554:LEU:HD12	1.79	0.65
1:A:674:ASP:HA	1:A:680:LYS:HD3	1.78	0.65
1:C:274:GLU:HB2	1:C:349:LEU:HG	1.79	0.65
1:I:671:TYR:O	1:I:675:ASN:ND2	2.29	0.65
1:K:468:GLY:H	1:K:676:ALA:HB2	1.62	0.65
1:G:57:SER:OG	1:G:59:ASP:OD1	2.14	0.65
2:L:19:ASN:ND2	2:L:260:PRO:O	2.30	0.65
1:C:337:ARG:NH1	10:C:1130:HOH:O	2.30	0.65
1:I:170:ASP:HB3	1:I:458:ILE:HD12	1.79	0.65
1:I:36:CYS:O	1:I:37:THR:OG1	2.15	0.65
2:J:323:ARG:O	10:J:502:HOH:O	2.14	0.65
1:K:281:LEU:HD11	1:K:360:PHE:HD2	1.61	0.64
2:B:69:LYS:O	2:B:71:GLY:N	2.30	0.64
1:E:479:ASN:ND2	10:E:1138:HOH:O	2.31	0.64
2:H:292:GLN:OE1	10:H:503:HOH:O	2.15	0.64
1:I:332:VAL:HG11	1:I:335:LEU:HD12	1.78	0.64
1:C:804:ASN:HB3	7:C:1007:EDO:H11	1.78	0.64
1:E:241:LYS:N	10:E:1101:HOH:O	2.13	0.64
1:G:278:LEU:HB3	1:G:376:PHE:HB2	1.79	0.64
2:L:242:VAL:HG11	2:L:315:LEU:HD21	1.79	0.64
1:A:512:ARG:NH1	1:E:898:SER:O	2.31	0.64
2:F:145:CYS:HB2	2:F:176:CYS:HB2	1.80	0.64
1:K:281:LEU:HD23	1:K:306:PHE:HA	1.80	0.64
2:F:214:ALA:N	10:F:501:HOH:O	2.29	0.64
1:I:743:GLU:OE1	10:I:1108:HOH:O	2.15	0.64
1:C:325:PRO:O	1:C:327:LYS:N	2.31	0.64
1:I:377:GLU:O	1:I:381:SER:OG	2.16	0.63
1:K:29:ARG:HH21	1:K:41:PRO:HB3	1.60	0.63
1:E:82:ASP:OD2	10:E:1105:HOH:O	2.15	0.63
1:A:285:ASP:OD1	1:A:286:THR:N	2.31	0.63
2:B:170:CYS:O	10:B:505:HOH:O	2.14	0.63
1:K:152:ARG:NH1	10:K:1132:HOH:O	2.31	0.63
1:I:459:GLY:HA2	5:I:1003:MGD:S13	2.38	0.63
1:I:5:ILE:HG22	1:I:6:SER:H	1.64	0.63
1:K:294:ASP:HB3	1:K:364:LEU:CD1	2.28	0.63
2:B:149:CYS:SG	2:B:153:ALA:N	2.72	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:304:ARG:NH1	10:J:506:HOH:O	2.22	0.62
2:H:46:TRP:CE3	2:H:197:CYS:HA	2.35	0.62
1:C:768:SER:O	5:C:1003:MGD:N18	2.32	0.62
1:I:261:ILE:HG23	1:I:266:LEU:HB2	1.82	0.62
2:L:242:VAL:HA	2:L:296:VAL:HG13	1.81	0.62
1:K:205:THR:HG23	2:L:22:ILE:HB	1.81	0.62
1:I:227:SER:H	1:I:239:VAL:HG11	1.65	0.62
2:L:20:LYS:HB2	2:L:220:ALA:HB2	1.80	0.62
1:C:359:LYS:NZ	10:C:1112:HOH:O	2.26	0.62
1:E:499:GLU:O	10:E:1106:HOH:O	2.16	0.62
1:I:141:ALA:HB1	1:I:592:VAL:HG23	1.80	0.62
1:I:754:ASP:HB2	1:I:885[A]:ARG:HB2	1.80	0.62
2:B:140:CYS:O	2:B:156:LYS:NZ	2.33	0.62
1:K:492:ILE:HD11	1:K:511:LEU:HD21	1.80	0.62
2:B:232:SER:OG	10:B:501:HOH:O	1.98	0.62
1:E:40:CYS:SG	1:E:72:ARG:HB3	2.40	0.62
1:G:320:SER:O	1:G:337:ARG:NH2	2.32	0.62
1:I:831:VAL:HG11	1:I:888:VAL:HG21	1.81	0.62
2:B:68:TYR:N	2:B:250:PHE:O	2.33	0.62
2:H:8:PRO:HB3	2:H:158:GLU:HA	1.81	0.62
1:G:31:ALA:HB3	1:G:602:THR:HB	1.81	0.61
1:I:754:ASP:HB2	1:I:885[B]:ARG:HB2	1.80	0.61
2:B:15:VAL:HG23	2:B:233:VAL:HG22	1.81	0.61
1:I:282:VAL:N	10:I:1101:HOH:O	2.34	0.61
1:K:182:GLN:NE2	10:K:1126:HOH:O	2.32	0.61
1:A:753:ALA:HB3	1:A:855:ARG:HH21	1.65	0.61
2:B:15:VAL:HB	2:B:222:HIS:HB2	1.80	0.61
1:K:555:TRP:CZ3	1:K:574:TYR:HB3	2.35	0.61
1:K:458:ILE:HD12	1:K:459:GLY:N	2.16	0.61
2:L:64:LYS:NZ	10:L:502:HOH:O	2.20	0.61
1:C:181:VAL:HG12	1:C:183:GLY:H	1.64	0.61
1:E:160:HIS:HB2	1:E:523:MET:HE1	1.82	0.61
2:J:157:ARG:NH2	2:J:201:PHE:HB2	2.15	0.61
2:J:18:LEU:HD12	2:J:261:PRO:HD3	1.82	0.61
1:A:261:ILE:HG23	1:A:266:LEU:HB2	1.83	0.61
1:A:826:GLU:OE2	10:A:1101:HOH:O	2.16	0.61
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.40	0.61
1:E:548:LYS:HD2	1:E:813:HIS:O	2.01	0.61
2:H:154:ILE:HG12	2:H:165:ILE:HG12	1.82	0.61
1:I:398:VAL:HA	7:I:1005:EDO:H21	1.82	0.61
1:I:187:GLU:HG2	1:I:708:TYR:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:NZ	10:A:1126:HOH:O	2.33	0.61
2:D:171:LYS:NZ	10:D:520:HOH:O	2.34	0.61
1:I:203:ASN:C	1:I:207:THR:HG22	2.20	0.61
10:K:1119:HOH:O	2:L:266:ARG:NH1	2.33	0.60
1:G:27:LYS:HD3	1:G:45:TYR:HE1	1.64	0.60
2:L:5:MET:N	10:L:516:HOH:O	2.33	0.60
1:C:671:TYR:O	1:C:675:ASN:ND2	2.33	0.60
1:E:302:ASP:HB3	1:E:321:TRP:HB3	1.83	0.60
1:E:808:GLU:HB2	1:E:817:ILE:HG12	1.82	0.60
1:I:208:ARG:NH2	5:I:1003:MGD:H22	2.00	0.60
1:I:188:THR:HG22	1:I:595:GLU:O	1.99	0.60
1:K:871:ARG:HB3	1:K:874:TYR:HB3	1.81	0.60
2:L:69:LYS:HG2	2:L:74:GLN:NE2	2.16	0.60
1:E:668:ALA:O	10:E:1107:HOH:O	2.16	0.60
1:E:784:ARG:NH2	10:E:1147:HOH:O	2.34	0.60
2:H:72:GLU:HA	1:K:703:LYS:HE2	1.82	0.60
1:I:305:TYR:HA	1:I:317:PRO:HD2	1.84	0.60
1:I:324:GLN:OE1	1:I:324:GLN:N	2.34	0.60
1:E:9:PHE:HB2	7:E:1007:EDO:H22	1.83	0.60
1:E:387:ASN:ND2	10:E:1132:HOH:O	2.29	0.60
1:E:535:VAL:HG11	1:E:571:THR:HG21	1.82	0.60
1:G:60:ILE:HG21	1:G:69:TYR:HB2	1.83	0.60
1:I:207:THR:OG1	1:I:208:ARG:NH2	2.34	0.60
2:J:127:ASN:OD1	2:J:279:LYS:NZ	2.34	0.60
1:A:685:GLN:OE1	1:A:688:ARG:NH1	2.34	0.60
1:C:265:LYS:NZ	1:C:267:TYR:OH	2.34	0.60
2:F:209:ALA:HB2	2:F:329:ILE:HB	1.83	0.60
1:G:321:TRP:HB2	1:G:724:LEU:HA	1.82	0.60
2:B:145:CYS:SG	2:B:146:LEU:N	2.75	0.60
2:D:15:VAL:HB	2:D:222:HIS:HB2	1.84	0.60
1:G:651:ASN:HD21	1:G:654:ASN:ND2	1.99	0.60
1:I:172:PRO:HA	1:I:425:GLN:NE2	2.17	0.60
1:I:431:ASP:O	1:I:435:ARG:HG3	2.02	0.60
1:G:480:LYS:NZ	10:G:1143:HOH:O	2.33	0.60
2:J:14:TYR:HD2	2:J:256:VAL:HG12	1.67	0.60
2:D:176:CYS:SG	2:D:177:VAL:HG23	2.41	0.60
2:J:228:ASP:OD1	2:J:230:ASN:N	2.25	0.60
1:C:566[B]:ILE:HG21	1:C:583:HIS:HD2	1.67	0.59
1:I:74:CYS:SG	1:I:76:LYS:N	2.71	0.59
1:K:414:LYS:NZ	10:K:1109:HOH:O	2.34	0.59
1:A:302:ASP:HB3	1:A:321:TRP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:GLN:OE1	10:A:1103:HOH:O	2.16	0.59
1:C:74:CYS:SG	1:C:76:LYS:N	2.75	0.59
1:K:762:SER:HB2	6:K:1004:MD1:H17	1.67	0.59
2:D:138:ASN:HB3	2:D:254:PRO:HB3	1.84	0.59
1:E:462:LYS:NZ	1:E:697:ASN:HD21	2.01	0.59
1:E:46:SER:OG	10:E:1108:HOH:O	2.16	0.59
1:E:562:VAL:HG12	1:E:577:VAL:HB	1.85	0.59
2:L:66:GLY:HA2	2:L:74:GLN:HB2	1.85	0.59
2:F:94:GLY:HA2	2:F:98:GLU:HB2	1.85	0.59
2:J:33:LYS:HA	2:J:37:THR:HG23	1.84	0.59
1:A:802:LYS:NZ	8:A:1008:GOL:O2	2.32	0.59
1:A:592:VAL:HG12	1:A:599:ILE:HA	1.84	0.59
2:B:138:ASN:HB3	2:B:254:PRO:HB3	1.85	0.59
2:D:19:ASN:OD1	2:D:262:VAL:N	2.35	0.59
1:G:42:HIS:NE2	1:G:78:GLU:OE2	2.29	0.59
1:G:823:ARG:NH1	10:G:1148:HOH:O	2.35	0.59
2:H:188:ASN:ND2	10:H:501:HOH:O	2.22	0.59
1:I:295:VAL:HG11	1:I:305:TYR:OH	2.02	0.59
1:I:593:THR:OG1	1:I:595:GLU:OE2	2.21	0.59
1:C:193:ASN:HD21	1:C:707:PRO:HG2	1.68	0.59
1:I:16:ASN:HA	1:I:19:ARG:HD2	1.83	0.59
1:I:687:LEU:HD23	1:I:692:GLN:HB2	1.85	0.59
1:K:229:SER:OG	1:K:231:ASP:O	2.20	0.59
2:L:29:VAL:O	2:L:33:LYS:HB2	2.03	0.59
2:F:11:GLN:NE2	10:F:509:HOH:O	2.35	0.59
2:F:204:ILE:HD11	2:F:210:PRO:HD3	1.85	0.59
1:A:278:LEU:HB3	1:A:376:PHE:HB2	1.85	0.59
1:G:871:ARG:HB3	1:G:874:TYR:HB3	1.85	0.58
1:I:446:THR:HG22	1:I:452:GLY:HA3	1.84	0.58
1:K:287:LYS:HE3	1:K:738:PHE:CG	2.38	0.58
2:D:187:PHE:HE1	2:D:192:ASN:HD22	1.51	0.58
1:E:768:SER:O	5:E:1003:MGD:N18	2.33	0.58
1:G:671:TYR:O	1:G:675:ASN:ND2	2.36	0.58
1:I:791:MET:HG2	1:I:831:VAL:HG12	1.85	0.58
1:K:290:LEU:HD23	1:K:305:TYR:CD1	2.37	0.58
2:L:69:LYS:HE3	2:L:74:GLN:HE22	1.66	0.58
2:B:301:GLN:O	2:B:305:GLU:HG2	2.03	0.58
2:H:184:LYS:NZ	2:H:197:CYS:H	2.01	0.58
2:B:153:ALA:HA	2:B:169:LYS:HE2	1.85	0.58
1:C:273:LYS:HB2	1:C:349:LEU:HD11	1.85	0.58
1:G:60:ILE:HD11	1:G:598:TYR:CG	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LYS:NZ	10:I:1150:HOH:O	2.36	0.58
1:I:31:ALA:HB3	1:I:602:THR:HB	1.86	0.58
2:J:15:VAL:HG12	2:J:233:VAL:HG22	1.85	0.58
1:E:727:ARG:HH21	8:E:1006:GOL:H11	1.69	0.58
1:C:463:PRO:HG2	1:C:466:VAL:HG13	1.86	0.58
1:G:828:ARG:NH2	10:G:1138:HOH:O	2.31	0.58
1:K:81:HIS:NE2	2:L:33:LYS:CE	2.66	0.58
2:B:204:ILE:HD11	2:B:210:PRO:HG3	1.84	0.58
1:C:405:GLU:N	1:C:405:GLU:OE1	2.36	0.58
1:I:793:PRO:HG3	1:I:824:ASN:ND2	2.18	0.58
1:K:192:PHE:HE1	1:K:217:GLU:HB3	1.68	0.58
2:H:47:ARG:HE	2:H:212:CYS:HB2	1.68	0.58
2:J:14:TYR:HB2	2:J:256:VAL:HG12	1.85	0.58
1:C:56:GLN:NE2	10:C:1103:HOH:O	2.20	0.57
1:G:207:THR:O	5:G:1003:MGD:N22	2.29	0.57
1:G:625:ARG:HD2	1:G:628:MET:SD	2.44	0.57
1:G:718:LYS:O	10:G:1106:HOH:O	2.17	0.57
2:J:9:ARG:HD2	2:J:10:ARG:HG3	1.86	0.57
1:E:473:ALA:HA	10:E:1102:HOH:O	2.04	0.57
1:C:566[B]:ILE:HD13	1:C:583:HIS:HA	1.87	0.57
1:I:437:MET:O	10:I:1109:HOH:O	2.17	0.57
2:J:241:LYS:NZ	10:J:521:HOH:O	2.37	0.57
1:E:207:THR:O	5:E:1003:MGD:N22	2.26	0.57
2:H:32:LYS:HA	2:H:36:THR:OG1	2.04	0.57
1:I:804:ASN:ND2	7:I:1006:EDO:O2	2.33	0.57
1:E:324:GLN:OE1	1:E:328:LYS:NZ	2.26	0.57
1:I:182:GLN:HG2	1:I:874:TYR:HA	1.84	0.57
2:J:293:VAL:O	2:J:296:VAL:HG12	2.04	0.57
1:K:166:ASP:N	1:K:166:ASP:OD1	2.21	0.57
2:D:159:GLN:OE1	10:D:502:HOH:O	2.17	0.57
1:E:308:ASN:HD21	1:E:310:LYS:HE3	1.68	0.57
1:E:791:MET:HG2	1:E:831:VAL:HG12	1.85	0.57
1:G:881:GLN:OE1	6:G:1004:MD1:N17	2.37	0.57
2:H:184:LYS:HZ2	2:H:197:CYS:H	1.52	0.57
1:I:192:PHE:HA	1:I:218:ALA:HB2	1.85	0.57
1:K:340:PHE:HA	1:K:719:LYS:HD3	1.86	0.57
2:L:47:ARG:NH1	10:L:522:HOH:O	2.37	0.57
1:A:535:VAL:HG11	1:A:571:THR:HG21	1.87	0.57
2:F:27:CYS:SG	2:F:47:ARG:NE	2.69	0.57
2:J:46:TRP:HB3	2:J:197:CYS:HB2	1.86	0.57
1:K:32:HIS:NE2	1:K:585:TYR:OH	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:LYS:HD3	1:K:610:TRP:CE2	2.40	0.57
2:B:13:THR:HB	2:B:233:VAL:HG11	1.87	0.57
1:G:68:GLU:OE1	10:G:1105:HOH:O	2.17	0.57
1:I:38:GLY:HA3	3:I:1001:SF4:S3	2.45	0.57
1:K:464:ALA:HA	1:K:698:TRP:HE1	1.70	0.57
2:B:19:ASN:OD1	2:B:262:VAL:N	2.33	0.57
1:C:364:LEU:HD21	1:C:370:VAL:HG13	1.87	0.57
2:F:306:LYS:NZ	10:F:518:HOH:O	2.36	0.57
1:K:308:ASN:HB3	10:K:1101:HOH:O	2.04	0.57
1:A:871:ARG:HB3	1:A:874:TYR:HB3	1.87	0.56
1:I:18:HIS:HA	1:I:21:GLN:HG3	1.87	0.56
1:K:40:CYS:SG	1:K:72:ARG:HB3	2.44	0.56
2:L:145:CYS:HB2	2:L:176:CYS:HB2	1.87	0.56
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.38	0.56
2:L:240:TYR:O	2:L:241:LYS:HB3	2.03	0.56
1:E:241:LYS:HG3	7:F:401:EDO:H11	1.86	0.56
2:H:41:GLN:HG2	10:H:501:HOH:O	2.05	0.56
1:I:172:PRO:HA	1:I:425:GLN:HE22	1.70	0.56
1:K:74:CYS:SG	1:K:76:LYS:N	2.78	0.56
1:E:135:VAL:HA	1:E:534:PHE:HB2	1.87	0.56
1:I:373:ARG:O	10:I:1101:HOH:O	2.17	0.56
1:I:885[B]:ARG:NH2	10:I:1158:HOH:O	2.38	0.56
2:L:69:LYS:CE	2:L:74:GLN:HE22	2.19	0.56
1:E:411:ALA:N	10:E:1148:HOH:O	2.39	0.56
1:K:166:ASP:OD2	1:K:485:GLN:NE2	2.38	0.56
1:K:288:ARG:HD2	1:K:733:ASP:HB2	1.86	0.56
2:L:181:PRO:HB2	2:L:250:PHE:CD1	2.40	0.56
2:B:159:GLN:O	10:B:506:HOH:O	2.18	0.56
2:B:163:VAL:HG12	2:B:196:LYS:HE2	1.88	0.56
1:C:63:MET:HE2	1:C:66:ILE:HD11	1.87	0.56
1:I:188:THR:OG1	1:I:211:ASP:OD1	2.11	0.56
2:J:168:ASP:N	10:J:509:HOH:O	2.23	0.56
2:L:33:LYS:HD3	2:L:33:LYS:O	2.06	0.56
1:E:690[A]:LYS:NZ	10:E:1165:HOH:O	2.38	0.56
1:E:805:ASP:OD2	10:E:1109:HOH:O	2.18	0.56
2:F:43:PHE:O	2:F:57:TYR:OH	2.20	0.56
2:H:292:GLN:N	2:H:292:GLN:OE1	2.38	0.56
1:A:207:THR:O	5:A:1003:MGD:N22	2.30	0.56
1:I:743:GLU:N	10:I:1108:HOH:O	2.39	0.56
2:J:24:CYS:HG	2:J:26:THR:HG1	1.50	0.56
1:K:337:ARG:NH1	10:K:1113:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:486:THR:HA	1:K:489:TRP:HB3	1.87	0.56
2:L:149:CYS:SG	2:L:152:GLU:N	2.79	0.56
1:I:539:ASN:N	6:I:1004:MD1:O2B	2.39	0.56
1:I:186:CYS:HB3	1:I:709:THR:HA	1.89	0.56
1:I:345:GLY:N	1:I:717:ASP:O	2.38	0.56
1:E:458:ILE:CD1	1:E:459:GLY:N	2.69	0.55
2:F:152:GLU:O	2:F:169:LYS:NZ	2.39	0.55
2:H:141:THR:HG23	2:H:255:ASN:OD1	2.06	0.55
1:I:19:ARG:HH21	2:J:205:GLU:CD	2.08	0.55
1:K:683:THR:H	1:K:686:MET:HE3	1.71	0.55
1:C:414:LYS:NZ	1:C:444:THR:O	2.39	0.55
1:C:468:GLY:H	1:C:676:ALA:HB2	1.70	0.55
2:F:166:HIS:CE1	2:F:168:ASP:HB2	2.42	0.55
1:I:742:VAL:N	10:I:1108:HOH:O	2.39	0.55
1:K:228:ILE:HG12	1:K:243:ILE:HB	1.88	0.55
1:A:209:ILE:HD13	2:B:24:CYS:HB2	1.87	0.55
2:B:44:MET:HE3	2:B:46:TRP:HE1	1.70	0.55
1:E:14:TRP:HZ2	2:F:167:GLN:HG2	1.70	0.55
1:G:332:VAL:HG13	1:G:335:LEU:HB3	1.87	0.55
1:G:40:CYS:SG	1:G:72:ARG:HB3	2.46	0.55
1:A:231:ASP:HB3	10:A:1101:HOH:O	2.06	0.55
2:B:255:ASN:ND2	10:B:502:HOH:O	2.39	0.55
1:A:340:PHE:HA	1:A:719:LYS:HD3	1.89	0.55
1:A:278:LEU:HB2	10:A:1186:HOH:O	2.07	0.55
1:E:272:LEU:O	1:E:276:THR:OG1	2.19	0.55
1:I:190:ASP:N	10:I:1141:HOH:O	2.33	0.55
1:I:208:ARG:NE	1:I:208:ARG:HA	2.22	0.55
1:I:727:ARG:NH1	10:I:1166:HOH:O	2.40	0.55
1:K:302:ASP:HB3	1:K:321:TRP:HB3	1.88	0.55
2:H:68:TYR:CE2	2:H:73:LEU:HD21	2.41	0.55
1:K:163:THR:HB	1:K:486:THR:H	1.71	0.55
1:E:290:LEU:HD22	1:E:372:VAL:HG11	1.89	0.55
1:K:566[B]:ILE:HD13	1:K:583:HIS:HA	1.89	0.55
2:D:166:HIS:HE1	2:D:168:ASP:HB2	1.71	0.55
1:E:325:PRO:HD2	1:E:328:LYS:HZ3	1.70	0.55
2:F:223:VAL:HG12	2:F:328:MET:HB2	1.88	0.55
1:G:302:ASP:HB3	1:G:321:TRP:HB3	1.88	0.55
2:B:291:LYS:HD3	2:B:291:LYS:H	1.72	0.54
1:E:426:HIS:HB3	1:E:881:GLN:HE21	1.72	0.54
1:G:75:ASN:N	1:G:75:ASN:OD1	2.40	0.54
2:H:229:VAL:HA	2:H:234:TYR:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:GLU:OE2	1:A:815:LYS:NZ	2.35	0.54
2:F:15:VAL:HB	2:F:222:HIS:HB2	1.90	0.54
1:G:134:SER:HB3	1:G:160:HIS:NE2	2.22	0.54
1:G:60:ILE:HD11	1:G:598:TYR:CD1	2.41	0.54
1:K:325:PRO:HG2	1:K:328:LYS:HA	1.89	0.54
1:K:856:ILE:HG23	1:K:877:PRO:HB3	1.89	0.54
1:K:81:HIS:CE1	2:L:33:LYS:CE	2.90	0.54
2:H:11:GLN:HA	2:H:161:GLY:HA3	1.89	0.54
1:I:292:GLU:HG2	1:I:299:GLY:HA3	1.87	0.54
1:K:712:GLN:HA	1:K:715:VAL:HG22	1.89	0.54
1:A:417:MET:HG3	1:A:455:ASN:HD22	1.73	0.54
1:G:881:GLN:NE2	10:G:1169:HOH:O	2.40	0.54
2:H:235:LYS:O	2:H:240:TYR:N	2.35	0.54
1:K:285:ASP:OD2	1:K:285:ASP:N	2.28	0.54
1:A:330:SER:O	1:A:338:ASN:ND2	2.34	0.54
2:F:40:GLY:HA2	2:F:190:LEU:HD23	1.88	0.54
1:A:32:HIS:NE2	1:A:585:TYR:OH	2.40	0.54
1:C:324:GLN:HE21	1:C:328:LYS:HZ1	1.55	0.54
1:I:700:SER:HB2	1:I:708:TYR:CE1	2.43	0.54
1:I:793:PRO:HG3	1:I:824:ASN:HD22	1.71	0.54
2:L:46:TRP:CE3	2:L:197:CYS:HA	2.42	0.54
1:C:74:CYS:SG	1:C:75:ASN:N	2.81	0.54
1:G:79:CYS:HB2	2:H:33:LYS:HE2	1.88	0.54
1:G:791:MET:HG2	1:G:831:VAL:HG12	1.90	0.54
1:I:364:LEU:HD23	1:I:368:LYS:HB2	1.89	0.54
1:I:458:ILE:HG13	1:I:459:GLY:N	2.23	0.54
1:I:871:ARG:HB3	1:I:874:TYR:HB3	1.89	0.54
1:K:291:ARG:O	1:K:294:ASP:OD1	2.25	0.54
1:E:564:ILE:HG12	1:E:579:LEU:HD12	1.89	0.54
2:F:137:CYS:SG	2:F:196:LYS:NZ	2.71	0.54
1:I:416:SER:N	1:I:446:THR:HG21	2.20	0.54
1:I:74:CYS:SG	1:I:75:ASN:N	2.81	0.54
1:E:157:ILE:HG13	1:E:159:ALA:H	1.72	0.54
1:I:512:ARG:NH2	10:I:1172:HOH:O	2.41	0.54
1:K:195:LYS:HG3	1:K:415:PRO:HD2	1.90	0.54
1:A:363:GLN:HG3	1:A:369:THR:HG22	1.90	0.54
1:E:492:ILE:HD11	1:E:511:LEU:HD21	1.88	0.54
1:G:168:TYR:HB3	6:G:1004:MD1:S13	2.47	0.54
2:H:200:CYS:SG	2:H:203:ARG:HD3	2.48	0.54
1:I:768:SER:O	5:I:1003:MGD:N18	2.39	0.54
2:J:157:ARG:NH1	2:J:205:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:SER:O	1:E:512:ARG:NH1	2.41	0.53
1:K:205:THR:O	10:K:1104:HOH:O	2.18	0.53
1:K:32:HIS:HB2	3:K:1001:SF4:S1	2.47	0.53
2:L:241:LYS:HG3	10:L:614:HOH:O	2.08	0.53
1:A:398:VAL:HG13	7:A:1005:EDO:H22	1.90	0.53
1:A:566[B]:ILE:HD13	1:A:583:HIS:HA	1.90	0.53
2:B:47:ARG:HB2	3:B:405:SF4:S4	2.49	0.53
2:D:166:HIS:CE1	2:D:168:ASP:HB2	2.43	0.53
1:G:119:ASP:OD1	1:G:632:ARG:NH2	2.41	0.53
1:I:182:GLN:HG3	1:I:874:TYR:HD2	1.73	0.53
1:K:286:THR:O	1:K:287:LYS:HG2	2.07	0.53
2:L:15:VAL:HG23	2:L:233:VAL:HG23	1.90	0.53
1:C:528:ARG:NH2	10:C:1151:HOH:O	2.37	0.53
1:G:566[B]:ILE:HD13	1:G:583:HIS:HA	1.90	0.53
2:D:171:LYS:NZ	10:D:501:HOH:O	2.15	0.53
1:K:441:THR:HG21	1:K:454:MET:HB2	1.91	0.53
2:L:266:ARG:HH21	2:L:278:PRO:HB3	1.74	0.53
1:E:484:CYS:N	10:E:1104:HOH:O	2.34	0.53
2:H:11:GLN:NE2	2:H:139:HIS:O	2.42	0.53
1:C:209:ILE:HG22	2:D:217:VAL:HG11	1.90	0.53
2:F:166:HIS:HE1	2:F:168:ASP:HB2	1.74	0.53
1:G:819:ARG:NH2	1:G:842:ASP:OD2	2.40	0.53
1:I:703:LYS:HD2	1:I:706:VAL:HG11	1.90	0.53
1:K:262:ILE:HG13	10:K:1208:HOH:O	2.08	0.53
1:K:363:GLN:HE21	1:K:367:GLY:C	2.11	0.53
1:K:536:TYR:CD2	1:K:537:ARG:HG3	2.44	0.53
1:A:29:ARG:NH2	1:A:59:ASP:OD2	2.39	0.53
1:G:5:ILE:HG22	1:G:6:SER:H	1.73	0.53
2:H:68:TYR:N	2:H:250:PHE:O	2.39	0.53
1:E:278:LEU:HA	1:E:375:VAL:HB	1.90	0.53
1:E:462:LYS:HZ2	7:E:1005:EDO:H12	1.73	0.53
2:F:242:VAL:HA	2:F:296:VAL:HG13	1.90	0.53
2:L:156:LYS:HG3	10:L:506:HOH:O	2.08	0.53
1:E:566[B]:ILE:HD13	1:E:583:HIS:HA	1.91	0.53
1:E:542:ASN:HB2	1:E:570:SER:HB2	1.91	0.53
1:G:59:ASP:OD2	1:G:691:PRO:HD3	2.09	0.53
1:K:291:ARG:NH1	1:K:294:ASP:OD2	2.42	0.53
2:B:167:GLN:N	10:B:507:HOH:O	2.42	0.53
1:G:11:TYR:OH	2:H:169:LYS:NZ	2.31	0.53
1:G:693:ARG:HH21	1:G:702:LEU:HG	1.73	0.53
1:A:227:SER:HB2	1:A:239:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:140:CYS:C	2:H:142:LYS:H	2.12	0.52
2:H:73:LEU:HD12	1:K:703:LYS:HZ2	1.75	0.52
1:I:207:THR:HG23	1:I:208:ARG:H	1.75	0.52
1:G:198:ILE:HG12	10:G:1246:HOH:O	2.10	0.52
2:J:128:ASN:ND2	10:J:529:HOH:O	2.41	0.52
1:E:340:PHE:O	1:E:719:LYS:NZ	2.34	0.52
1:E:412:THR:N	10:E:1148:HOH:O	2.34	0.52
1:E:817:ILE:HG13	1:E:845:THR:HG22	1.90	0.52
2:F:209:ALA:N	10:F:527:HOH:O	2.43	0.52
2:F:21:CYS:SG	2:F:132:TYR:HB2	2.50	0.52
1:G:398:VAL:HG13	7:G:1005:EDO:H11	1.90	0.52
1:C:182:GLN:HA	10:C:1101:HOH:O	2.09	0.52
1:E:42:HIS:NE2	1:E:78:GLU:OE2	2.37	0.52
2:F:157:ARG:HD3	2:F:162:ILE:HB	1.91	0.52
2:H:61:TRP:CZ2	2:H:135:ARG:NH1	2.77	0.52
1:I:253:LEU:O	1:I:257:MET:HG2	2.09	0.52
1:I:285:ASP:N	1:I:285:ASP:OD1	2.36	0.52
1:I:373:ARG:N	10:I:1101:HOH:O	2.32	0.52
1:I:280:TYR:CE2	1:I:725:THR:HB	2.45	0.52
1:I:40:CYS:SG	1:I:72:ARG:HB3	2.50	0.52
1:I:255:MET:HE1	1:I:746:THR:HA	1.91	0.52
2:B:164:VAL:N	10:B:531:HOH:O	2.43	0.52
1:E:164:PHE:HA	1:E:167:TRP:HB3	1.90	0.52
1:E:417:MET:HG3	1:E:455:ASN:HD22	1.74	0.52
1:E:805:ASP:OD1	10:E:1110:HOH:O	2.19	0.52
2:F:189:PRO:HG2	2:F:190:LEU:HD22	1.90	0.52
1:I:325:PRO:HA	1:I:342:PHE:HE1	1.74	0.52
1:C:168:TYR:HB3	6:C:1004:MD1:S13	2.50	0.52
1:C:881:GLN:NE2	1:C:882:ARG:HE	2.07	0.52
1:E:325:PRO:O	1:E:327:LYS:N	2.42	0.52
1:I:220:LEU:HB3	2:J:316:MET:HE3	1.90	0.52
1:I:308:ASN:HD21	1:I:352:LEU:HD22	1.74	0.52
2:J:138:ASN:HD21	2:J:256:VAL:CG2	2.21	0.52
2:J:242:VAL:HA	2:J:296:VAL:HG23	1.90	0.52
1:G:690[B]:LYS:NZ	10:G:1125:HOH:O	2.28	0.52
1:I:217:GLU:HB3	2:J:320:ILE:HG23	1.91	0.52
1:A:11:TYR:OH	2:B:169:LYS:NZ	2.38	0.52
1:A:168:TYR:HB3	6:A:1004:MD1:S13	2.50	0.52
2:B:11:GLN:NE2	2:B:12:LEU:O	2.33	0.52
2:B:327:MET:SD	10:B:523:HOH:O	2.59	0.52
1:E:261:ILE:HA	1:E:266:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:ARG:NH1	1:E:733:ASP:O	2.43	0.52
2:F:47:ARG:HB2	3:F:405:SF4:S4	2.49	0.52
1:I:363:GLN:NE2	1:I:364:LEU:O	2.43	0.52
2:J:68:TYR:HB2	2:J:251:GLY:HA3	1.92	0.52
1:K:670:GLN:HE22	1:K:683:THR:HA	1.74	0.52
1:A:675:ASN:ND2	10:A:1169:HOH:O	2.43	0.52
1:C:456:HIS:ND1	10:C:1141:HOH:O	2.33	0.52
1:G:346:TYR:HB3	10:G:1106:HOH:O	2.09	0.52
1:I:272:LEU:HD22	1:I:278:LEU:HD12	1.92	0.52
2:J:200:CYS:SG	2:J:203:ARG:HD3	2.50	0.52
2:D:200:CYS:SG	2:D:203:ARG:HD3	2.50	0.52
1:I:542:ASN:HB2	1:I:570:SER:HB2	1.92	0.52
1:I:860:ASN:HD22	1:I:878:ALA:H	1.58	0.52
1:C:56:GLN:HE22	2:D:215:GLN:HB3	1.75	0.51
1:I:198:ILE:HB	1:I:418:ILE:HD13	1.92	0.51
1:K:140:PRO:HB3	1:K:147:PHE:CG	2.44	0.51
1:K:281:LEU:HD12	1:K:372:VAL:HG23	1.92	0.51
2:B:64:LYS:NZ	2:B:65:GLY:O	2.43	0.51
2:H:188:ASN:HB2	2:H:195:ASN:ND2	2.25	0.51
1:I:598:TYR:HA	1:I:693:ARG:HA	1.91	0.51
1:C:31:ALA:HB3	1:C:602:THR:HB	1.90	0.51
1:I:455:ASN:HB2	10:I:1177:HOH:O	2.10	0.51
1:K:496:VAL:HG11	1:K:854:VAL:H	1.75	0.51
2:B:259:VAL:N	10:B:503:HOH:O	2.44	0.51
1:G:677:PRO:HA	1:G:680:LYS:HG2	1.92	0.51
2:J:307:LYS:NZ	2:J:317:ASP:OD1	2.44	0.51
1:K:168:TYR:HB3	6:K:1004:MD1:S13	2.50	0.51
1:K:589:ASP:OD1	1:K:590:LEU:N	2.42	0.51
2:L:17:ASP:HA	2:L:259:VAL:HB	1.92	0.51
1:E:37:THR:HG21	1:E:208:ARG:HH12	1.75	0.51
1:E:426:HIS:CG	1:E:881:GLN:NE2	2.78	0.51
2:H:58:PRO:HB2	2:H:83:ASP:HB3	1.91	0.51
2:F:222:HIS:O	10:F:505:HOH:O	2.18	0.51
1:G:97:VAL:N	10:G:1101:HOH:O	2.44	0.51
1:I:138:PRO:HA	1:I:164:PHE:CD1	2.45	0.51
1:I:458:ILE:CG1	1:I:459:GLY:N	2.73	0.51
2:J:21:CYS:SG	2:J:132:TYR:HB2	2.51	0.51
1:K:81:HIS:HB3	1:K:585:TYR:HE1	1.75	0.51
2:F:46:TRP:HZ2	2:F:195:ASN:HB3	1.75	0.51
1:G:567:ARG:HH21	6:G:1004:MD1:H3'	1.75	0.51
1:I:447:GLU:OE2	1:I:715:VAL:HG11	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:124:GLU:OE1	10:J:503:HOH:O	2.19	0.51
2:J:46:TRP:CE3	2:J:197:CYS:HA	2.46	0.51
1:K:464:ALA:HB3	1:K:694:PHE:CE2	2.44	0.51
2:L:223:VAL:HG13	2:L:329:ILE:HG13	1.93	0.51
2:B:168:ASP:OD1	10:B:507:HOH:O	2.18	0.51
1:C:589:ASP:OD2	1:C:590:LEU:N	2.42	0.51
1:E:841:MET:O	1:E:843:LEU:N	2.42	0.51
2:J:153:ALA:HA	2:J:169:LYS:HE2	1.92	0.51
1:K:541:LEU:HD11	1:K:551:LEU:CD2	2.41	0.51
2:L:94:GLY:HA2	2:L:98:GLU:HB2	1.93	0.51
2:B:46:TRP:CE3	2:B:197:CYS:HA	2.46	0.51
2:H:94:GLY:HA2	2:H:98:GLU:HB2	1.93	0.51
2:J:246:LEU:HB2	2:J:258:TYR:CE2	2.46	0.51
1:A:325:PRO:O	1:A:327:LYS:N	2.44	0.51
2:D:137:CYS:HB3	2:D:197:CYS:HB3	1.92	0.51
1:E:218:ALA:N	10:E:1103:HOH:O	2.43	0.51
1:I:342:PHE:CD2	1:I:720:PRO:HG2	2.42	0.51
1:K:91:LYS:NZ	10:K:1168:HOH:O	2.43	0.51
1:G:234:SER:OG	2:H:119:ASP:OD2	2.29	0.50
1:I:566[B]:ILE:HD13	1:I:583:HIS:HA	1.92	0.50
2:L:81:MET:SD	10:L:545:HOH:O	2.59	0.50
1:A:568:MET:HG2	2:B:96:LEU:HB3	1.94	0.50
1:C:357:GLU:HA	1:C:377:GLU:HB2	1.93	0.50
1:C:72:ARG:O	10:C:1103:HOH:O	2.19	0.50
1:K:289:PHE:HB2	1:K:733:ASP:OD2	2.11	0.50
1:K:38:GLY:HA3	3:K:1001:SF4:S3	2.51	0.50
1:E:35:ASN:HB2	1:E:139:VAL:HG21	1.92	0.50
1:I:335:LEU:CD2	1:I:722:PRO:HG3	2.42	0.50
1:E:287:LYS:NZ	10:E:1174:HOH:O	2.44	0.50
1:E:91:LYS:NZ	10:E:1127:HOH:O	2.28	0.50
1:I:751:ILE:HB	1:I:883:ASP:HB3	1.92	0.50
1:I:240:ASP:O	2:J:265:PRO:HA	2.11	0.50
2:J:293:VAL:O	2:J:297:LEU:HG	2.10	0.50
1:K:274:GLU:OE2	1:K:718:LYS:HD2	2.12	0.50
1:A:190:ASP:OD1	1:A:193:ASN:ND2	2.30	0.50
2:B:21:CYS:SG	2:B:132:TYR:HB2	2.52	0.50
1:C:364:LEU:HD21	1:C:370:VAL:HG22	1.93	0.50
1:C:897:ILE:HD11	1:E:491:TYR:HE1	1.75	0.50
1:E:462:LYS:HZ1	1:E:697:ASN:HD21	1.58	0.50
1:K:292:GLU:HG2	1:K:299:GLY:HA3	1.91	0.50
1:K:281:LEU:HB3	1:K:372:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:679:SER:HA	1:G:682:ILE:HD13	1.92	0.50
1:I:29:ARG:NH2	10:I:1104:HOH:O	2.44	0.50
1:I:461:GLU:OE1	10:I:1110:HOH:O	2.19	0.50
1:K:115:ASP:CG	1:K:625:ARG:HH21	2.14	0.50
1:C:278:LEU:HB3	1:C:376:PHE:HB2	1.93	0.50
1:C:753:ALA:HB3	1:C:855:ARG:NH2	2.25	0.50
2:F:209:ALA:HB1	2:F:223:VAL:HG11	1.92	0.50
2:H:18:LEU:O	10:H:505:HOH:O	2.20	0.50
1:K:74:CYS:SG	1:K:75:ASN:N	2.85	0.50
2:H:133:LEU:O	2:H:135:ARG:HG3	2.12	0.50
2:H:8:PRO:HA	2:H:158:GLU:HB3	1.93	0.50
6:K:1004:MD1:H7	6:K:1004:MD1:H11	1.92	0.50
1:K:290:LEU:HD23	1:K:305:TYR:HD1	1.75	0.50
1:A:841:MET:O	1:A:843:LEU:N	2.44	0.50
2:B:73:LEU:HD11	2:B:179:SER:HB3	1.93	0.50
2:H:15:VAL:HG12	2:H:222:HIS:HB2	1.92	0.50
1:K:80:GLY:O	1:K:583:HIS:NE2	2.37	0.50
2:F:331:PRO:HA	10:F:527:HOH:O	2.11	0.49
1:G:636:GLU:HB3	1:G:650:SER:HB3	1.93	0.49
1:G:887:ASN:OD1	10:G:1107:HOH:O	2.20	0.49
1:I:515:ILE:HD13	1:I:522:ASN:HB2	1.93	0.49
2:J:219:ARG:NH1	2:J:321:GLY:O	2.42	0.49
2:L:309:LYS:HB2	2:L:311:LEU:HD13	1.93	0.49
1:C:142:VAL:HG12	1:C:460:GLN:CD	2.32	0.49
1:C:791:MET:HG2	1:C:831:VAL:HG12	1.94	0.49
2:J:219:ARG:NH2	2:J:324:SER:OG	2.45	0.49
1:K:192:PHE:CE1	1:K:217:GLU:HB3	2.47	0.49
1:K:287:LYS:HE3	1:K:738:PHE:CD2	2.47	0.49
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.47	0.49
2:B:266:ARG:HA	2:B:278:PRO:HA	1.93	0.49
1:C:762:SER:HA	1:C:833:MET:O	2.13	0.49
1:I:291:ARG:NH2	10:I:1154:HOH:O	2.42	0.49
1:E:700:SER:HB2	1:E:708:TYR:CE1	2.47	0.49
2:H:27:CYS:HB2	2:H:212:CYS:HB2	1.95	0.49
2:H:61:TRP:CZ2	2:H:62:GLN:HG3	2.48	0.49
1:K:510:TYR:CD1	1:K:858:PRO:HB3	2.47	0.49
2:L:64:LYS:HD2	2:L:183:ALA:HB2	1.93	0.49
1:E:226:VAL:HA	10:E:1101:HOH:O	2.12	0.49
1:E:259:HIS:CE1	1:E:384:MET:HA	2.47	0.49
1:I:135:VAL:HG22	1:I:534:PHE:HB2	1.94	0.49
1:I:372:VAL:HG22	10:I:1101:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:ARG:NH1	1:K:112:GLU:OE2	2.43	0.49
1:K:207:THR:O	5:K:1003:MGD:N22	2.30	0.49
1:K:446:THR:HB	1:K:452:GLY:HA3	1.93	0.49
1:K:152:ARG:NH1	1:K:472:LEU:O	2.44	0.49
1:K:771:SER:HA	1:K:774:LYS:HG3	1.94	0.49
1:K:81:HIS:CE1	2:L:33:LYS:HE3	2.47	0.49
1:C:490:THR:HG22	1:C:540:TRP:HZ2	1.75	0.49
2:L:241:LYS:HD2	2:L:241:LYS:O	2.13	0.49
2:B:20:LYS:HB2	2:B:220:ALA:HB2	1.94	0.49
2:J:209:ALA:HB3	2:J:214:ALA:HB2	1.95	0.49
2:J:48:ASN:ND2	10:J:534:HOH:O	2.45	0.49
1:C:841:MET:O	1:C:843:LEU:N	2.44	0.49
1:K:163:THR:H	1:K:486:THR:CG2	2.25	0.49
1:K:490:THR:HG22	1:K:540:TRP:HZ2	1.77	0.49
1:C:542:ASN:HB2	1:C:570:SER:HB2	1.95	0.49
2:H:241:LYS:HD2	2:H:299:ILE:HG21	1.95	0.49
1:I:399:THR:HG22	10:I:1248:HOH:O	2.11	0.49
1:I:471:ALA:O	10:I:1111:HOH:O	2.20	0.49
1:I:707:PRO:HB3	10:I:1141:HOH:O	2.12	0.49
1:C:281:LEU:HB3	1:C:372:VAL:HB	1.95	0.48
10:C:1102:HOH:O	2:D:117:ASP:HA	2.11	0.48
2:J:233:VAL:HG13	2:J:237:ILE:HD12	1.95	0.48
2:J:43:PHE:O	2:J:57:TYR:OH	2.26	0.48
1:K:173:THR:O	1:K:177:GLN:HG3	2.13	0.48
1:K:227:SER:HB2	1:K:239:VAL:HG11	1.94	0.48
1:A:62:PRO:HB3	1:A:68:GLU:HB3	1.94	0.48
2:D:25:GLN:NE2	10:D:510:HOH:O	2.29	0.48
1:E:231:ASP:OD2	10:E:1111:HOH:O	2.19	0.48
1:E:31:ALA:HB3	1:E:602:THR:HB	1.95	0.48
2:F:200:CYS:SG	2:F:203:ARG:HD3	2.52	0.48
1:E:209:ILE:HD13	2:F:24:CYS:HB2	1.95	0.48
1:G:651:ASN:O	1:G:655:GLN:HG3	2.13	0.48
1:I:225:ILE:O	10:I:1112:HOH:O	2.20	0.48
1:G:16:ASN:HA	1:G:19:ARG:HD2	1.95	0.48
1:I:321:TRP:CZ3	1:I:337:ARG:HG3	2.48	0.48
1:I:193:ASN:ND2	1:I:450:ASN:OD1	2.37	0.48
1:K:695:LYS:N	10:K:1111:HOH:O	2.46	0.48
1:E:192:PHE:HD1	10:E:1103:HOH:O	1.96	0.48
2:H:16:THR:HG22	2:H:221:MET:SD	2.54	0.48
2:H:203:ARG:HB3	2:H:208:VAL:HG23	1.95	0.48
2:H:68:TYR:HB2	2:H:251:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:LYS:HD2	2:H:183:ALA:HB2	1.95	0.48
1:I:455:ASN:ND2	10:I:1145:HOH:O	2.35	0.48
2:J:137:CYS:HB3	2:J:197:CYS:HB3	1.94	0.48
1:K:505:ILE:HG21	10:K:1103:HOH:O	2.13	0.48
1:K:565:ASN:ND2	10:K:1174:HOH:O	2.47	0.48
1:I:187:GLU:HG3	10:I:1141:HOH:O	2.13	0.48
1:I:227:SER:N	1:I:239:VAL:HG11	2.29	0.48
2:J:181:PRO:HB2	2:J:250:PHE:CD2	2.48	0.48
2:J:293:VAL:HA	2:J:296:VAL:HG12	1.96	0.48
1:C:585:TYR:N	10:C:1110:HOH:O	2.30	0.48
1:G:224:LYS:NZ	10:G:1190:HOH:O	2.46	0.48
1:I:203:ASN:O	1:I:207:THR:HG22	2.13	0.48
1:I:204:PRO:HA	1:I:207:THR:CG2	2.44	0.48
1:I:167:TRP:HB2	1:I:486:THR:HB	1.96	0.48
1:I:761:ASN:ND2	1:I:763:PRO:HG3	2.29	0.48
2:J:14:TYR:HB2	2:J:256:VAL:CG1	2.44	0.48
2:J:317:ASP:OD1	2:J:322:ARG:NH1	2.39	0.48
1:K:304:PHE:O	1:K:317:PRO:HD2	2.13	0.48
1:K:54:GLU:OE1	1:K:585:TYR:OH	2.31	0.48
2:D:21:CYS:SG	2:D:132:TYR:HB2	2.53	0.48
2:H:188:ASN:ND2	10:H:510:HOH:O	2.46	0.48
1:I:206:GLN:HG2	1:I:766:ARG:NH2	2.28	0.48
1:I:435:ARG:NH1	10:I:1184:HOH:O	2.47	0.48
1:K:308:ASN:HD21	1:K:310:LYS:HE2	1.76	0.48
1:K:624:LYS:HG3	1:K:653:TRP:CD1	2.47	0.48
1:E:539:ASN:N	6:E:1004:MD1:O2B	2.42	0.48
1:E:830:ARG:NH1	10:E:1157:HOH:O	2.37	0.48
1:I:447:GLU:O	1:I:449:THR:N	2.47	0.48
1:I:67:PRO:HG2	1:I:214:PHE:HD1	1.78	0.48
1:A:451:GLY:N	10:A:1109:HOH:O	2.45	0.48
2:H:166:HIS:CE1	2:H:168:ASP:HB2	2.49	0.48
2:H:73:LEU:HD12	1:K:703:LYS:NZ	2.28	0.48
1:I:207:THR:HG23	1:I:208:ARG:N	2.29	0.48
2:J:271:ASN:ND2	2:J:273:GLU:HG2	2.29	0.48
1:K:541:LEU:HD11	1:K:551:LEU:HD21	1.96	0.48
1:E:171:HIS:NE2	1:E:874:TYR:O	2.46	0.47
1:G:14:TRP:HE1	2:H:168:ASP:CG	2.17	0.47
1:I:521:PRO:HG3	1:I:870:PHE:CZ	2.49	0.47
10:C:1102:HOH:O	2:D:116:TRP:O	2.20	0.47
2:L:292:GLN:O	2:L:296:VAL:HG23	2.14	0.47
1:A:488:ILE:HG13	1:A:877:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:ASP:OD1	1:E:590:LEU:N	2.48	0.47
1:G:897:ILE:O	2:H:111:ARG:NE	2.37	0.47
2:J:46:TRP:HA	2:J:186:TYR:HE2	1.79	0.47
1:K:31:ALA:HB3	1:K:602:THR:HB	1.96	0.47
1:G:459:GLY:HA2	5:G:1003:MGD:S13	2.55	0.47
1:G:567:ARG:NH2	1:G:771:SER:OG	2.45	0.47
1:I:15:GLU:HB2	1:I:19:ARG:NH1	2.28	0.47
1:I:737:PHE:O	10:I:1108:HOH:O	2.20	0.47
2:J:131:PHE:HZ	2:J:288:LEU:HD11	1.79	0.47
2:L:27:CYS:SG	2:L:28:THR:N	2.87	0.47
2:L:75:LYS:HG3	2:L:178:GLN:OE1	2.14	0.47
1:G:17:PHE:O	1:G:21:GLN:HG3	2.15	0.47
1:I:316:ILE:O	1:I:318:LYS:N	2.48	0.47
1:K:472:LEU:HB3	10:K:1121:HOH:O	2.14	0.47
1:A:320:SER:O	1:A:337:ARG:NH1	2.42	0.47
1:A:337:ARG:HG3	1:A:339:THR:HG23	1.95	0.47
2:B:269:MET:HG3	10:B:504:HOH:O	2.13	0.47
1:G:817:ILE:HG13	1:G:845:THR:HG22	1.97	0.47
1:G:754:ASP:HB2	1:G:885[A]:ARG:HB2	1.97	0.47
2:H:212:CYS:SG	2:H:213:VAL:N	2.86	0.47
1:I:539:ASN:O	1:I:543:GLN:HG2	2.14	0.47
2:L:145:CYS:SG	2:L:146:LEU:N	2.87	0.47
1:A:501:ILE:HG13	1:A:504:ASP:H	1.79	0.47
2:D:170:CYS:SG	2:D:193:LYS:HA	2.55	0.47
1:E:762:SER:HA	1:E:833:MET:O	2.15	0.47
1:G:666:GLU:OE1	1:G:688:ARG:NH2	2.46	0.47
1:I:67:PRO:HG2	1:I:214:PHE:CD1	2.50	0.47
1:I:751:ILE:O	1:I:759:ARG:NH1	2.44	0.47
1:I:801:ILE:HG12	1:I:890:ARG:HB2	1.96	0.47
1:K:283:ARG:HA	1:K:372:VAL:HG12	1.97	0.47
1:K:686:MET:HB3	1:K:692:GLN:HG3	1.97	0.47
1:K:817:ILE:HB	1:K:844:LEU:HB2	1.97	0.47
2:B:139:HIS:CE1	2:B:162:ILE:HG23	2.50	0.47
1:I:152:ARG:HD3	1:I:656:MET:HA	1.95	0.47
1:I:186:CYS:HB2	1:I:708:TYR:O	2.15	0.47
2:J:140:CYS:HB3	2:J:252:THR:O	2.15	0.47
1:K:227:SER:HB3	1:K:236:THR:HG23	1.96	0.47
1:K:294:ASP:HB2	1:K:295:VAL:CG2	2.43	0.47
2:F:12:LEU:N	10:F:509:HOH:O	2.44	0.47
2:F:42:ASP:OD2	2:F:87:PRO:HG2	2.15	0.47
1:I:269:ALA:HB1	1:I:273:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:ARG:HB3	1:I:285:ASP:OD1	2.14	0.47
1:K:291:ARG:HD3	1:K:294:ASP:OD2	2.14	0.47
1:K:291:ARG:O	1:K:305:TYR:HE1	1.97	0.47
1:K:685:GLN:O	1:K:685:GLN:NE2	2.42	0.47
1:A:95:ILE:HD13	1:A:577:VAL:HG22	1.96	0.47
1:E:670:GLN:HE22	1:E:683:THR:HA	1.79	0.47
1:G:172:PRO:HB2	1:G:175:GLN:HB3	1.96	0.47
1:I:184:ASP:OD2	1:I:185:THR:N	2.48	0.47
1:I:281:LEU:HG	1:I:372:VAL:HG22	1.97	0.47
1:K:282:VAL:N	1:K:373:ARG:O	2.46	0.47
2:L:162:ILE:N	10:L:506:HOH:O	2.48	0.47
1:E:452:GLY:N	10:E:1141:HOH:O	2.47	0.47
1:I:59:ASP:N	1:I:59:ASP:OD1	2.48	0.47
1:I:805:ASP:OD2	1:I:890:ARG:NH1	2.48	0.47
1:K:356:LEU:O	1:K:376:PHE:HB3	2.15	0.47
1:C:354:PRO:O	10:C:1104:HOH:O	2.21	0.46
1:C:651:ASN:ND2	10:C:1137:HOH:O	2.33	0.46
1:A:272:LEU:HB3	10:A:1186:HOH:O	2.13	0.46
1:A:768:SER:O	5:A:1003:MGD:N18	2.42	0.46
1:C:802:LYS:NZ	10:C:1122:HOH:O	2.29	0.46
1:C:838:GLU:HB2	1:C:841:MET:HG3	1.97	0.46
2:D:46:TRP:CE3	2:D:197:CYS:HA	2.50	0.46
1:E:310:LYS:HG3	1:E:311:THR:HG23	1.97	0.46
1:E:545:LYS:H	1:E:545:LYS:HD2	1.80	0.46
1:E:554:LEU:HD12	10:E:1125:HOH:O	2.14	0.46
1:E:426:HIS:CB	1:E:881:GLN:HE21	2.26	0.46
2:F:222:HIS:CE1	2:F:327:MET:HG2	2.50	0.46
1:G:335:LEU:O	1:G:871:ARG:NH1	2.47	0.46
2:H:138:ASN:ND2	2:H:138:ASN:H	2.13	0.46
2:H:181:PRO:HB2	2:H:250:PHE:CD2	2.50	0.46
1:I:261:ILE:HA	1:I:266:LEU:HD12	1.96	0.46
1:I:714:PHE:HB2	1:I:715:VAL:HG23	1.96	0.46
1:I:54:GLU:CD	1:I:81:HIS:HD1	2.18	0.46
1:K:37:THR:HG21	1:K:458:ILE:O	2.15	0.46
1:A:700:SER:HB2	1:A:708:TYR:CE1	2.50	0.46
1:E:493:HIS:O	1:E:557:LYS:NZ	2.41	0.46
1:K:323:ASP:OD2	1:K:346:TYR:OH	2.33	0.46
1:K:485:GLN:HB3	1:K:488:ILE:HD12	1.97	0.46
2:B:73:LEU:HD22	2:B:147:GLU:HG2	1.98	0.46
1:E:816:VAL:HG23	10:E:1156:HOH:O	2.16	0.46
2:F:98:GLU:OE2	2:F:100:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:GLY:CA	2:F:190:LEU:HD23	2.46	0.46
1:G:831:VAL:HG11	1:G:888:VAL:HG21	1.96	0.46
2:H:21:CYS:SG	2:H:132:TYR:HB2	2.54	0.46
1:I:185:THR:OG1	1:I:455:ASN:HB3	2.16	0.46
2:J:201:PHE:CG	2:J:202:PRO:HD3	2.51	0.46
1:K:134:SER:HB3	1:K:160:HIS:NE2	2.30	0.46
1:A:414:LYS:HA	1:A:415:PRO:HA	1.74	0.46
1:A:468:GLY:H	1:A:676:ALA:HB2	1.80	0.46
1:G:11:TYR:O	1:G:15:GLU:HG2	2.15	0.46
2:H:31:CYS:SG	2:H:46:TRP:HB2	2.56	0.46
1:K:262:ILE:HA	1:K:267:TYR:CE1	2.51	0.46
1:K:631:LYS:HD2	1:K:636:GLU:OE1	2.15	0.46
2:D:27:CYS:HB2	2:D:212:CYS:HB2	1.98	0.46
1:G:15:GLU:HG3	1:G:19:ARG:NH2	2.30	0.46
1:G:337:ARG:HG3	1:G:337:ARG:O	2.15	0.46
2:H:73:LEU:HB2	1:K:703:LYS:HZ1	1.79	0.46
1:K:762:SER:HA	1:K:833:MET:O	2.16	0.46
2:L:31:CYS:SG	2:L:46:TRP:HB2	2.56	0.46
1:G:696:SER:OG	1:G:697:ASN:N	2.49	0.46
1:K:755:LYS:HA	1:K:885[A]:ARG:HH21	1.79	0.46
2:L:27:CYS:HB2	2:L:212:CYS:HB2	1.97	0.46
1:C:860:ASN:HB2	10:C:1106:HOH:O	2.15	0.46
1:C:871:ARG:HB3	1:C:874:TYR:HB3	1.97	0.46
1:E:5:ILE:HD12	1:E:7:GLY:N	2.31	0.46
1:G:140:PRO:HB3	1:G:147:PHE:CD1	2.51	0.46
1:I:16:ASN:ND2	1:I:19:ARG:HD3	2.31	0.46
2:L:140:CYS:HB3	2:L:252:THR:O	2.16	0.46
2:L:44:MET:HE3	2:L:46:TRP:HE1	1.80	0.46
2:L:59:ARG:H	2:L:59:ARG:HG2	1.46	0.46
1:G:14:TRP:HZ2	2:H:167:GLN:H	1.64	0.46
1:I:413:ALA:C	1:I:414:LYS:HD3	2.36	0.46
2:B:201:PHE:CG	2:B:202:PRO:HD3	2.51	0.46
1:C:209:ILE:HD13	2:D:24:CYS:HB2	1.97	0.46
2:D:153:ALA:HA	2:D:169:LYS:HE3	1.97	0.46
1:E:808:GLU:CB	1:E:817:ILE:HG12	2.45	0.46
1:I:317:PRO:O	10:I:1113:HOH:O	2.20	0.46
1:K:140:PRO:HB3	1:K:147:PHE:CD1	2.51	0.46
1:K:488:ILE:O	1:K:492:ILE:HD12	2.16	0.46
2:L:64:LYS:NZ	2:L:177:VAL:O	2.31	0.46
2:L:33:LYS:HB3	10:L:533:HOH:O	2.16	0.46
1:E:360:PHE:HB2	1:E:372:VAL:HG23	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:790:GLU:OE2	1:E:823:ARG:NE	2.39	0.45
2:F:140:CYS:HB3	2:F:252:THR:O	2.17	0.45
1:K:290:LEU:HG	1:K:294:ASP:OD1	2.16	0.45
1:E:484:CYS:HB3	1:E:523:MET:HE2	1.98	0.45
1:G:488:ILE:HG13	1:G:877:PRO:HG2	1.98	0.45
1:G:754:ASP:HB2	1:G:885[B]:ARG:HB2	1.97	0.45
2:H:321:GLY:HA3	2:H:327:MET:SD	2.56	0.45
1:K:505:ILE:HD13	10:K:1103:HOH:O	2.16	0.45
1:K:594:SER:O	10:K:1106:HOH:O	2.21	0.45
2:D:140:CYS:HB3	2:D:252:THR:O	2.16	0.45
2:F:138:ASN:HB3	2:F:254:PRO:HB3	1.98	0.45
1:I:476:GLU:HG3	1:I:645:TRP:CH2	2.50	0.45
2:J:111:ARG:NH2	10:J:522:HOH:O	2.37	0.45
2:J:81:MET:HE2	2:J:81:MET:HA	1.98	0.45
1:K:278:LEU:HA	1:K:375:VAL:CG2	2.43	0.45
1:G:568:MET:HG2	2:H:96:LEU:HB3	1.98	0.45
1:I:21:GLN:NE2	2:J:35:TRP:HE3	2.14	0.45
1:K:493:HIS:HB3	1:K:554:LEU:HG	1.98	0.45
1:K:539:ASN:O	1:K:543:GLN:HG2	2.17	0.45
1:A:294:ASP:HB3	1:A:364:LEU:HD22	1.98	0.45
1:C:541:LEU:HD21	1:C:551:LEU:HD21	1.98	0.45
1:E:368:LYS:HD2	1:E:368:LYS:H	1.81	0.45
1:E:541:LEU:HD21	1:E:551:LEU:HD21	1.98	0.45
1:G:262:ILE:HD12	1:G:383:LEU:HD12	1.99	0.45
2:H:231:SER:O	2:H:235:LYS:HG3	2.17	0.45
2:H:9:ARG:HB3	2:H:158:GLU:O	2.17	0.45
1:I:587:LYS:NZ	1:I:615:ASP:OD2	2.49	0.45
1:I:18:HIS:CE1	2:J:198:ILE:HG21	2.51	0.45
1:C:539:ASN:O	1:C:543:GLN:HG2	2.17	0.45
1:E:292:GLU:HG2	1:E:296:VAL:HG22	1.98	0.45
2:F:88:PHE:CD1	2:F:106:PRO:HB2	2.51	0.45
1:I:40:CYS:SG	1:I:72:ARG:NE	2.79	0.45
1:I:435:ARG:HA	1:I:438:HIS:HB2	1.99	0.45
1:K:188:THR:HG22	1:K:191:TRP:CZ2	2.52	0.45
2:F:12:LEU:HD22	2:F:162:ILE:HD11	1.98	0.45
1:I:16:ASN:HD22	1:I:19:ARG:HD3	1.81	0.45
1:I:181:VAL:HG12	1:I:335:LEU:HD23	1.98	0.45
1:K:443:LEU:HD13	10:K:1208:HOH:O	2.15	0.45
1:A:289:PHE:CZ	1:A:731:TYR:HB3	2.51	0.45
1:A:809:ALA:HA	1:A:887:ASN:O	2.17	0.45
2:B:135:ARG:HG2	10:B:513:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:ILE:HD13	1:E:459:GLY:H	1.82	0.45
1:I:273:LYS:HB3	1:I:354:PRO:HD2	1.98	0.45
1:I:464:ALA:HB3	1:I:694:PHE:CE1	2.52	0.45
1:A:140:PRO:HB3	1:A:147:PHE:CG	2.52	0.45
1:E:160:HIS:CG	1:E:523:MET:HE3	2.52	0.45
1:E:325:PRO:HB3	1:E:342:PHE:CD2	2.52	0.45
2:H:136:MET:SD	10:H:576:HOH:O	2.61	0.45
1:G:22:TRP:CH2	2:H:208:VAL:HG21	2.52	0.45
1:I:198:ILE:HD13	1:I:226:VAL:HG13	1.98	0.45
1:I:208:ARG:HH21	5:I:1003:MGD:H22	1.65	0.45
1:I:803:ASP:O	10:I:1114:HOH:O	2.21	0.45
2:J:305:GLU:OE1	2:J:309:LYS:HE3	2.17	0.45
1:K:147:PHE:HB2	1:K:537:ARG:NH2	2.32	0.45
2:B:235:LYS:NZ	10:B:542:HOH:O	2.50	0.45
2:B:223:VAL:HG12	2:B:328:MET:HB2	1.98	0.45
1:C:486:THR:O	1:C:490:THR:HG23	2.17	0.45
1:K:281:LEU:HD11	1:K:360:PHE:CD2	2.47	0.45
1:C:320:SER:O	1:C:337:ARG:NH2	2.50	0.44
1:E:380:LYS:O	1:E:384:MET:HG2	2.17	0.44
1:G:297:ALA:N	1:G:365:LEU:HD11	2.32	0.44
2:J:90:PHE:HB3	2:J:104:VAL:HG12	1.99	0.44
1:A:114:LEU:HB3	1:A:625:ARG:HG3	1.99	0.44
1:A:817:ILE:HG13	1:A:845:THR:HG22	1.99	0.44
1:C:771:SER:HA	1:C:774:LYS:HG3	2.00	0.44
1:E:576:ASP:HB2	10:E:1120:HOH:O	2.17	0.44
1:G:139:VAL:O	1:G:537:ARG:NH2	2.47	0.44
2:H:201:PHE:CG	2:H:202:PRO:HD3	2.53	0.44
2:H:265:PRO:HG2	2:H:279:LYS:HD2	1.99	0.44
1:I:335:LEU:HD22	1:I:722:PRO:HG3	1.99	0.44
2:J:68:TYR:OH	2:J:147:GLU:OE1	2.22	0.44
1:K:152:ARG:CZ	1:K:475:PRO:HG3	2.47	0.44
1:I:11:TYR:O	1:I:15:GLU:HG3	2.17	0.44
1:I:241:LYS:NZ	2:J:274:PRO:HG3	2.31	0.44
1:K:234:SER:OG	2:L:119:ASP:OD2	2.36	0.44
2:L:180:CYS:SG	2:L:183:ALA:N	2.91	0.44
1:A:318:LYS:HD3	1:A:346:TYR:CE1	2.53	0.44
2:F:20:LYS:HB2	2:F:220:ALA:HB2	1.98	0.44
2:F:222:HIS:N	10:F:505:HOH:O	2.49	0.44
2:H:140:CYS:O	2:H:142:LYS:N	2.45	0.44
1:I:343:PRO:HG2	1:I:346:TYR:CE1	2.52	0.44
1:I:53:ARG:NH1	2:J:34:LEU:HD22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:177:VAL:HG12	2:L:185:PRO:HB2	1.98	0.44
1:C:898:SER:OG	7:C:1007:EDO:H22	2.17	0.44
1:E:32:HIS:NE2	1:E:585:TYR:OH	2.49	0.44
1:G:144:PRO:HB2	1:G:672:ILE:HD13	2.00	0.44
1:G:719:LYS:NZ	10:G:1167:HOH:O	2.40	0.44
1:I:15:GLU:HB3	2:J:201:PHE:CE1	2.53	0.44
1:I:257:MET:CB	1:I:440:LEU:HD21	2.48	0.44
1:I:419:ILE:HA	10:I:1177:HOH:O	2.18	0.44
1:I:634:LYS:HA	1:I:634:LYS:HD3	1.84	0.44
2:J:162:ILE:HD11	2:J:204:ILE:HG13	1.98	0.44
1:K:63:MET:O	2:L:323:ARG:NH2	2.49	0.44
1:C:172:PRO:HB2	1:C:175:GLN:HB3	2.00	0.44
1:C:349:LEU:HD23	1:C:349:LEU:HA	1.84	0.44
1:G:496:VAL:HG11	1:G:854:VAL:H	1.82	0.44
1:G:598:TYR:CD1	1:G:693:ARG:HB2	2.52	0.44
1:I:306:PHE:CD2	1:I:317:PRO:HD3	2.52	0.44
1:K:628:MET:O	1:K:632:ARG:HB2	2.17	0.44
1:A:318:LYS:HD2	1:A:346:TYR:O	2.18	0.44
1:A:797:LYS:HE3	1:A:797:LYS:HB2	1.82	0.44
1:C:32:HIS:NE2	1:C:585:TYR:OH	2.44	0.44
1:C:357:GLU:HB3	1:C:377:GLU:OE1	2.17	0.44
2:F:145:CYS:SG	2:F:154:ILE:HG21	2.58	0.44
1:I:368:LYS:N	1:I:368:LYS:HD2	2.32	0.44
1:I:368:LYS:HD2	1:I:368:LYS:H	1.82	0.44
1:C:168:TYR:CZ	6:C:1004:MD1:H101	2.52	0.44
1:E:577:VAL:N	10:E:1120:HOH:O	2.39	0.44
2:H:68:TYR:CZ	2:H:73:LEU:HD11	2.53	0.44
1:I:75:ASN:N	1:I:75:ASN:OD1	2.43	0.44
1:K:616:TRP:HH2	10:K:1132:HOH:O	2.00	0.44
2:L:121:GLY:HA3	2:L:130:PHE:HB3	2.00	0.44
2:L:166:HIS:HE1	2:L:168:ASP:HB2	1.82	0.44
1:C:227:SER:HB2	1:C:239:VAL:HG11	2.00	0.44
1:C:165:TYR:CD1	1:C:461:GLU:HG2	2.53	0.44
1:E:261:ILE:HG23	1:E:266:LEU:HB2	1.98	0.44
1:E:539:ASN:ND2	1:E:569:ASP:HB2	2.32	0.44
1:E:801:ILE:HA	10:E:1109:HOH:O	2.18	0.44
2:F:94:GLY:HA3	2:F:100:LYS:HD2	2.00	0.44
1:G:539:ASN:O	1:G:543:GLN:HG2	2.17	0.44
1:G:678:GLN:NE2	1:G:697:ASN:O	2.51	0.44
1:G:81:HIS:CE1	2:H:33:LYS:HG3	2.52	0.44
2:H:140:CYS:C	2:H:142:LYS:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:401:LYS:O	1:I:404:THR:OG1	2.31	0.44
1:I:643:PHE:O	1:I:644:LYS:HB2	2.17	0.44
1:I:464:ALA:HA	1:I:698:TRP:NE1	2.33	0.44
1:E:458:ILE:HD12	10:E:1192:HOH:O	2.17	0.43
1:E:754:ASP:HB2	1:E:885[B]:ARG:HB2	2.00	0.43
2:F:307:LYS:HE2	2:F:313:SER:HB3	2.00	0.43
1:K:279:SER:OG	10:K:1105:HOH:O	2.21	0.43
2:L:222:HIS:N	10:L:503:HOH:O	2.51	0.43
2:H:155:TYR:HB2	7:H:406:EDO:H21	1.99	0.43
2:H:19:ASN:HB2	10:H:502:HOH:O	2.17	0.43
1:I:204:PRO:HA	1:I:207:THR:HG22	2.00	0.43
1:I:55:GLU:OE2	1:I:58:LYS:NZ	2.36	0.43
1:K:291:ARG:CZ	1:K:294:ASP:OD2	2.66	0.43
1:C:427:TRP:CE2	1:C:882:ARG:HB3	2.53	0.43
1:E:548:LYS:HE2	10:E:1202:HOH:O	2.18	0.43
1:E:634:LYS:HD3	1:E:634:LYS:HA	1.77	0.43
1:G:140:PRO:HB3	1:G:147:PHE:CG	2.54	0.43
1:I:302:ASP:HB3	1:I:321:TRP:HB3	1.98	0.43
1:K:325:PRO:HB3	1:K:342:PHE:CD2	2.53	0.43
1:K:555:TRP:HZ3	1:K:574:TYR:HB3	1.82	0.43
1:K:639:ASN:ND2	10:K:1182:HOH:O	2.51	0.43
2:L:19:ASN:OD1	2:L:262:VAL:N	2.42	0.43
1:A:432:VAL:HA	1:A:435:ARG:HD3	2.00	0.43
1:E:422:GLY:O	1:E:426:HIS:HB2	2.18	0.43
1:E:601:MET:HG2	1:E:687:LEU:HB3	2.00	0.43
1:I:287:LYS:O	1:I:731:TYR:OH	2.25	0.43
1:I:292:GLU:HA	1:I:295:VAL:HG12	2.00	0.43
1:I:784:ARG:CZ	1:I:821:LYS:HE3	2.48	0.43
2:J:153:ALA:O	2:J:166:HIS:HB3	2.18	0.43
1:K:438:HIS:HA	1:K:441:THR:HG22	1.99	0.43
1:K:616:TRP:O	1:K:620:LEU:HG	2.18	0.43
2:L:15:VAL:HG11	2:L:236:LEU:HD12	2.00	0.43
2:L:296:VAL:HA	10:L:614:HOH:O	2.17	0.43
1:C:398:VAL:HG12	1:C:402:ALA:HB3	2.01	0.43
2:D:201:PHE:CG	2:D:202:PRO:HD3	2.53	0.43
1:E:209:ILE:HG22	2:F:217:VAL:HG11	1.99	0.43
2:F:201:PHE:CG	2:F:202:PRO:HD3	2.54	0.43
1:G:654:ASN:HA	10:G:1103:HOH:O	2.18	0.43
1:G:721:TRP:O	1:G:726:GLY:HA2	2.19	0.43
2:H:15:VAL:CG1	2:H:222:HIS:HB2	2.48	0.43
1:I:166:ASP:OD1	1:I:166:ASP:N	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:ALA:N	1:I:365:LEU:HD21	2.34	0.43
1:K:37:THR:OG1	1:K:208:ARG:NH1	2.52	0.43
1:A:515:ILE:HD13	1:A:522:ASN:HB2	2.00	0.43
1:C:137:SER:OG	1:C:537:ARG:NH1	2.45	0.43
1:E:539:ASN:O	1:E:543:GLN:HG2	2.18	0.43
1:G:515:ILE:HD13	1:G:522:ASN:HB2	2.00	0.43
2:H:121:GLY:HA3	2:H:130:PHE:HB3	2.01	0.43
2:H:196:LYS:HG2	10:H:504:HOH:O	2.18	0.43
1:I:165:TYR:CD2	1:I:170:ASP:HB2	2.53	0.43
1:I:213:HIS:CD2	1:I:214:PHE:N	2.87	0.43
1:I:379:LEU:HD13	1:I:744:LEU:HD22	2.01	0.43
1:K:171:HIS:O	1:K:173:THR:N	2.52	0.43
1:K:469:LEU:HD12	10:K:1121:HOH:O	2.18	0.43
1:K:756:TYR:CD1	1:K:887:ASN:HB2	2.54	0.43
2:L:166:HIS:CE1	2:L:168:ASP:HB2	2.53	0.43
1:A:273:LYS:HB3	1:A:354:PRO:HD2	2.00	0.43
1:C:627:GLU:HG2	1:C:649:LEU:O	2.19	0.43
1:C:778:LEU:HD22	2:D:33:LYS:HE2	2.01	0.43
2:F:235:LYS:O	2:F:240:TYR:N	2.45	0.43
1:G:111:GLU:HB3	1:G:625:ARG:NH2	2.33	0.43
1:G:638:PHE:CZ	1:G:647:ARG:HD2	2.54	0.43
2:H:68:TYR:CZ	2:H:73:LEU:HD21	2.53	0.43
1:I:63:MET:HB2	1:I:66:ILE:HD11	1.99	0.43
1:I:821:LYS:NZ	10:I:1153:HOH:O	2.37	0.43
2:J:15:VAL:HA	2:J:257:PHE:O	2.19	0.43
2:J:266:ARG:NH1	2:J:278:PRO:HB3	2.33	0.43
1:K:438:HIS:CE1	1:K:454:MET:HB3	2.53	0.43
1:K:831:VAL:HG11	1:K:888:VAL:HG21	2.01	0.43
2:L:242:VAL:HG21	2:L:315:LEU:HD11	2.01	0.43
1:E:325:PRO:C	1:E:327:LYS:H	2.21	0.43
2:F:235:LYS:HA	2:F:239:GLN:HB3	2.01	0.43
1:G:238:LYS:NZ	10:H:505:HOH:O	2.47	0.43
1:I:217:GLU:OE2	2:J:219:ARG:HD3	2.19	0.43
1:I:428:TYR:HB3	10:I:1122:HOH:O	2.19	0.43
1:I:501:ILE:HG12	1:I:503:SER:H	1.84	0.43
2:J:137:CYS:HA	2:J:184:LYS:HG3	2.01	0.43
2:B:73:LEU:HD12	2:B:74:GLN:N	2.33	0.43
1:C:36:CYS:O	1:C:37:THR:OG1	2.29	0.43
1:E:860:ASN:HD22	1:E:878:ALA:H	1.67	0.43
1:G:57:SER:HG	1:G:59:ASP:CG	2.19	0.43
1:G:624:LYS:HB3	1:G:624:LYS:HE2	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:647:ARG:NH2	10:G:1152:HOH:O	2.37	0.43
1:I:598:TYR:CD2	1:I:693:ARG:HB2	2.54	0.43
1:I:787:PRO:HG3	1:I:841:MET:HE2	2.01	0.43
2:J:265:PRO:HB2	2:J:279:LYS:HE2	2.00	0.43
1:K:110:TRP:NE1	1:K:611:GLU:O	2.42	0.43
1:K:637:LYS:HD2	1:K:637:LYS:H	1.83	0.43
1:A:753:ALA:HB3	1:A:855:ARG:NH2	2.31	0.43
1:A:815:LYS:HD3	1:A:845:THR:HG21	2.01	0.43
2:B:142:LYS:HB2	10:B:537:HOH:O	2.18	0.43
1:C:102:GLU:OE2	1:C:104:LYS:NZ	2.38	0.43
1:C:171:HIS:O	1:C:173:THR:N	2.52	0.43
2:D:170:CYS:O	2:D:171:LYS:HD3	2.18	0.43
1:E:160:HIS:CG	1:E:523:MET:CE	3.01	0.43
1:E:515:ILE:HD13	1:E:522:ASN:HB2	2.00	0.43
1:G:41:PRO:HB2	1:G:57:SER:OG	2.19	0.43
2:H:285:LEU:HD12	2:H:297:LEU:HD11	1.99	0.43
1:I:14:TRP:NE1	10:J:509:HOH:O	2.37	0.43
1:K:247:PRO:HG3	1:K:830:ARG:HD3	2.01	0.43
2:L:21:CYS:SG	2:L:132:TYR:HB2	2.59	0.43
1:A:401:LYS:HE2	2:B:273:GLU:OE2	2.19	0.42
2:B:168:ASP:N	10:B:507:HOH:O	2.31	0.42
1:C:700:SER:HB2	1:C:708:TYR:CE1	2.54	0.42
1:E:147:PHE:HB2	1:E:537:ARG:CZ	2.49	0.42
1:E:755:LYS:HA	1:E:755:LYS:HD3	1.81	0.42
1:G:281:LEU:HD22	1:G:372:VAL:HG23	2.02	0.42
2:H:208:VAL:HA	2:H:330:SER:O	2.19	0.42
1:I:307:TRP:HZ3	1:I:362:MET:HE2	1.84	0.42
2:J:140:CYS:SG	2:J:254:PRO:HA	2.59	0.42
2:J:260:PRO:HB3	2:J:289:PHE:CE2	2.54	0.42
1:K:42:HIS:HE1	1:K:78:GLU:OE1	2.03	0.42
1:C:683:THR:HG23	10:C:1263:HOH:O	2.19	0.42
1:E:75:ASN:N	1:E:75:ASN:OD1	2.48	0.42
2:H:285:LEU:HB3	2:H:293:VAL:HG11	2.01	0.42
1:I:203:ASN:O	1:I:205:THR:N	2.53	0.42
2:B:166:HIS:ND1	2:B:169:LYS:HG3	2.34	0.42
1:C:356:LEU:HG	10:C:1104:HOH:O	2.18	0.42
1:E:278:LEU:HB3	1:E:376:PHE:HB2	2.01	0.42
2:F:6:LYS:NZ	10:F:523:HOH:O	2.39	0.42
1:G:35:ASN:ND2	6:G:1004:MD1:S12	2.92	0.42
2:H:79:PRO:HB2	2:H:84:TYR:CE2	2.54	0.42
1:I:211:ASP:C	1:I:213:HIS:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:ILE:HD12	1:K:189:ALA:HB1	2.01	0.42
1:K:547:GLN:OE1	10:K:1107:HOH:O	2.21	0.42
1:K:209:ILE:HG22	2:L:217:VAL:HG11	2.01	0.42
2:B:154:ILE:HG12	2:B:165:ILE:HG12	2.01	0.42
2:B:41:GLN:HE21	2:B:44:MET:HE1	1.85	0.42
1:C:282:VAL:O	10:C:1108:HOH:O	2.22	0.42
1:C:713:TYR:OH	10:C:1105:HOH:O	2.21	0.42
1:C:76:LYS:HB2	1:C:76:LYS:HE2	1.91	0.42
2:D:266:ARG:NH2	2:D:278:PRO:HB3	2.34	0.42
2:D:43:PHE:O	2:D:57:TYR:OH	2.30	0.42
1:E:56:GLN:O	1:E:58:LYS:HG3	2.19	0.42
1:E:58:LYS:C	1:E:70:ASN:HD22	2.23	0.42
1:E:856:ILE:HG23	1:E:877:PRO:HB3	2.00	0.42
1:G:233:ASN:HA	1:G:823:ARG:HH22	1.84	0.42
1:I:764:HIS:ND1	5:I:1003:MGD:N15	2.64	0.42
1:K:482:ARG:NH2	10:K:1183:HOH:O	2.52	0.42
2:L:201:PHE:CG	2:L:202:PRO:HD3	2.54	0.42
1:A:290:LEU:HD22	1:A:372:VAL:HG11	2.01	0.42
2:B:196:LYS:HG2	2:B:197:CYS:O	2.19	0.42
2:B:293:VAL:O	2:B:297:LEU:HG	2.19	0.42
1:C:458:ILE:HD12	1:C:459:GLY:N	2.33	0.42
1:C:165:TYR:CG	1:C:461:GLU:HG2	2.54	0.42
1:C:836:CYS:HB2	10:C:1229:HOH:O	2.19	0.42
1:C:857:ASN:O	10:C:1106:HOH:O	2.21	0.42
1:E:523:MET:HA	1:E:524:PRO:C	2.39	0.42
1:G:91:LYS:N	10:G:1206:HOH:O	2.51	0.42
2:H:138:ASN:ND2	2:H:138:ASN:N	2.67	0.42
2:H:315:LEU:HA	2:H:318:VAL:HG12	2.02	0.42
6:I:1004:MD1:H8	6:I:1004:MD1:H2'	1.92	0.42
1:I:291:ARG:HD3	1:I:301:LYS:O	2.19	0.42
1:I:171:HIS:NE2	1:I:874:TYR:O	2.50	0.42
1:K:501:ILE:H	1:K:501:ILE:HD12	1.84	0.42
1:K:563:ASP:OD2	1:K:572:ALA:HB2	2.19	0.42
1:A:294:ASP:O	1:A:364:LEU:HB3	2.20	0.42
1:A:539:ASN:O	1:A:543:GLN:HG2	2.20	0.42
1:E:160:HIS:ND1	10:E:1104:HOH:O	2.23	0.42
1:E:521:PRO:HG3	1:E:870:PHE:CZ	2.55	0.42
1:E:14:TRP:HE1	2:F:167:GLN:HB2	1.83	0.42
1:G:323:ASP:OD2	1:G:346:TYR:OH	2.22	0.42
1:G:678:GLN:N	1:G:678:GLN:OE1	2.52	0.42
1:G:748:LYS:O	7:G:1007:EDO:H21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:762:SER:HA	1:G:833:MET:O	2.19	0.42
2:H:286:GLU:HA	2:H:290:GLY:O	2.20	0.42
1:I:32:HIS:HB2	3:I:1001:SF4:S1	2.59	0.42
2:J:94:GLY:HA2	2:J:98:GLU:HB2	2.01	0.42
1:A:542:ASN:HB2	1:A:570:SER:HB2	2.01	0.42
1:A:181:VAL:HG21	1:A:711:PHE:HE1	1.85	0.42
1:A:817:ILE:HB	1:A:844:LEU:HB2	2.02	0.42
1:G:21:GLN:NE2	2:H:35:TRP:HE3	2.17	0.42
2:H:42:ASP:OD1	2:H:42:ASP:N	2.53	0.42
1:I:468:GLY:HA2	1:I:675:ASN:HB2	2.01	0.42
1:I:686:MET:HB3	1:I:692:GLN:HG3	2.01	0.42
2:J:260:PRO:HB3	2:J:289:PHE:HE2	1.85	0.42
1:A:796:ALA:HB1	1:A:801:ILE:HB	2.01	0.42
2:B:33:LYS:HD3	2:B:33:LYS:HA	1.79	0.42
1:C:472:LEU:HD21	1:C:668:ALA:HB1	2.02	0.42
1:E:199:LEU:N	1:E:226:VAL:O	2.42	0.42
1:G:259:HIS:CE1	1:G:384:MET:HA	2.54	0.42
2:H:33:LYS:HA	2:H:33:LYS:HD2	1.73	0.42
1:I:174:GLY:O	1:I:435:ARG:HG2	2.19	0.42
1:I:700:SER:OG	1:I:712:GLN:HG2	2.20	0.42
1:K:76:LYS:HB2	1:K:76:LYS:HE2	1.77	0.42
1:A:472:LEU:HD21	1:A:668:ALA:HB1	2.01	0.42
2:B:73:LEU:HD13	10:B:595:HOH:O	2.20	0.42
1:C:809:ALA:HA	1:C:887:ASN:O	2.20	0.42
1:G:784:ARG:HG2	2:H:116:TRP:CE3	2.54	0.42
1:I:15:GLU:HB3	2:J:201:PHE:CZ	2.55	0.42
1:I:37:THR:N	1:I:460:GLN:HB2	2.34	0.42
2:L:138:ASN:HB3	2:L:254:PRO:HB3	2.01	0.42
1:A:144:PRO:HB2	1:A:672:ILE:HD13	2.02	0.42
2:B:167:GLN:O	10:B:505:HOH:O	2.21	0.42
1:C:771:SER:O	10:C:1107:HOH:O	2.22	0.42
2:D:237:ILE:HG12	2:D:243:ALA:HB3	2.01	0.42
1:E:208:ARG:NH2	5:E:1003:MGD:H11	2.35	0.42
1:G:37:THR:HG21	1:G:208:ARG:HH12	1.85	0.42
1:G:110:TRP:NE1	1:G:611:GLU:O	2.46	0.42
1:G:700:SER:HB2	1:G:708:TYR:CE1	2.55	0.42
1:K:272:LEU:O	1:K:276:THR:OG1	2.24	0.42
1:K:310:LYS:HB3	1:K:310:LYS:HE2	1.76	0.42
2:L:184:LYS:HA	2:L:184:LYS:HD3	1.82	0.42
1:C:819:ARG:NH2	1:C:842:ASP:OD1	2.52	0.41
1:E:308:ASN:HD21	1:E:310:LYS:CE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:GLU:O	1:E:409:GLU:HG3	2.19	0.41
2:F:9:ARG:HG3	2:F:10:ARG:N	2.35	0.41
1:I:167:TRP:HZ2	1:I:544:ALA:HA	1.84	0.41
2:J:228:ASP:OD1	2:J:229:VAL:N	2.53	0.41
2:L:32:LYS:HE2	2:L:32:LYS:HB2	1.95	0.41
2:L:6:LYS:HG3	2:L:7:ALA:N	2.34	0.41
1:A:182:GLN:HG3	1:A:874:TYR:HA	2.01	0.41
1:A:394:LYS:HB2	1:A:394:LYS:HE3	1.94	0.41
1:A:512:ARG:NH1	10:A:1201:HOH:O	2.53	0.41
1:A:690[A]:LYS:HA	1:A:690[A]:LYS:HD3	1.82	0.41
1:A:75:ASN:N	1:A:75:ASN:OD1	2.53	0.41
1:A:485:GLN:CD	1:A:877:PRO:HD2	2.40	0.41
1:E:594:SER:OG	10:E:1112:HOH:O	2.22	0.41
2:F:213:VAL:HG22	2:F:221:MET:HB3	2.02	0.41
1:G:770:HIS:CD2	6:G:1004:MD1:H102	2.55	0.41
2:H:108:PRO:HG2	7:H:405:EDO:H22	2.02	0.41
2:H:138:ASN:HD22	2:H:138:ASN:H	1.67	0.41
1:K:64:PRO:HD2	1:K:705:GLY:O	2.20	0.41
1:K:701:PRO:HD3	1:K:713:TYR:CE1	2.55	0.41
1:A:419:ILE:HG23	1:A:457:TYR:CD2	2.56	0.41
2:B:168:ASP:N	2:B:168:ASP:OD1	2.53	0.41
2:D:9:ARG:HG3	2:D:9:ARG:HH11	1.85	0.41
1:E:593:THR:OG1	1:E:595:GLU:OE1	2.28	0.41
2:F:289:PHE:HB2	2:F:293:VAL:HG23	2.02	0.41
6:G:1004:MD1:H8	6:G:1004:MD1:H2'	1.92	0.41
2:H:139:HIS:CE1	2:H:162:ILE:HG23	2.55	0.41
1:G:217:GLU:HG3	2:H:20:LYS:NZ	2.35	0.41
2:J:303:GLU:HB2	10:J:528:HOH:O	2.20	0.41
1:K:134:SER:HB2	1:K:162:HIS:HE2	1.85	0.41
1:K:462:LYS:HB3	1:K:594:SER:HB3	2.03	0.41
1:K:521:PRO:HG3	1:K:870:PHE:CZ	2.54	0.41
1:K:57:SER:OG	1:K:59:ASP:OD1	2.32	0.41
1:K:586:GLU:HB3	1:K:608:PRO:HA	2.03	0.41
2:L:59:ARG:CD	2:L:83:ASP:HA	2.47	0.41
1:A:728:GLN:NE2	10:A:1121:HOH:O	2.31	0.41
1:E:280:TYR:O	1:E:375:VAL:HG23	2.20	0.41
1:E:458:ILE:HD13	1:E:459:GLY:N	2.34	0.41
1:G:138:PRO:HA	1:G:164:PHE:CD2	2.55	0.41
1:G:414:LYS:HA	1:G:415:PRO:HA	1.83	0.41
1:I:63:MET:O	2:J:323:ARG:NH2	2.53	0.41
1:I:144:PRO:HB2	1:I:672:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:ASP:HA	1:K:633:LYS:HZ3	1.86	0.41
1:K:632:ARG:HH12	1:K:633:LYS:NZ	2.17	0.41
1:C:191:TRP:HE1	1:C:457:TYR:HH	1.66	0.41
1:E:259:HIS:CD2	1:E:389:PRO:HD3	2.56	0.41
1:E:638:PHE:CE2	1:E:647:ARG:HD2	2.55	0.41
2:F:229:VAL:HA	2:F:234:TYR:CD2	2.55	0.41
2:F:321:GLY:HA3	2:F:327:MET:SD	2.60	0.41
1:G:60:ILE:HG22	1:G:70:ASN:OD1	2.21	0.41
1:I:379:LEU:HG	1:I:383:LEU:HD21	2.03	0.41
1:I:703:LYS:HG3	1:I:703:LYS:H	1.67	0.41
2:J:28:THR:HG23	2:J:47:ARG:O	2.20	0.41
1:K:318:LYS:HE3	1:K:347:ILE:HA	2.03	0.41
1:K:144:PRO:HB2	1:K:672:ILE:HD13	2.02	0.41
1:A:389:PRO:HB2	1:A:400:ALA:HB1	2.03	0.41
1:A:610:TRP:NE1	10:A:1119:HOH:O	2.30	0.41
2:B:322:ARG:NH1	10:B:539:HOH:O	2.47	0.41
2:B:5:MET:HG3	2:B:146:LEU:HD21	2.02	0.41
2:D:140:CYS:O	2:D:156:LYS:NZ	2.45	0.41
2:D:149:CYS:SG	2:D:152:GLU:N	2.94	0.41
1:E:797:LYS:HE2	1:E:797:LYS:HB3	1.91	0.41
2:F:145:CYS:SG	2:F:154:ILE:HD13	2.61	0.41
2:H:200:CYS:HB3	2:H:203:ARG:HB2	2.02	0.41
2:H:111:ARG:HB2	7:H:405:EDO:H12	2.03	0.41
1:K:626:VAL:O	1:K:630:ALA:N	2.54	0.41
2:L:95:ARG:HD2	2:L:100:LYS:O	2.19	0.41
2:B:18:LEU:HG	10:B:503:HOH:O	2.20	0.41
1:G:15:GLU:OE2	1:G:19:ARG:NH2	2.53	0.41
1:G:164:PHE:HA	1:G:167:TRP:HB3	2.03	0.41
1:G:37:THR:OG1	1:G:208:ARG:NH1	2.54	0.41
1:I:770:HIS:NE2	5:I:1003:MGD:S13	2.94	0.41
1:I:17:PHE:O	1:I:21:GLN:HG3	2.21	0.41
1:I:325:PRO:O	1:I:327:LYS:N	2.53	0.41
1:I:468:GLY:HA3	1:I:672:ILE:O	2.21	0.41
1:I:555:TRP:CE2	1:I:561:ILE:HD13	2.55	0.41
1:K:347:ILE:HG12	1:K:718:LYS:O	2.20	0.41
1:K:74:CYS:O	1:K:78:GLU:HG2	2.20	0.41
1:A:261:ILE:HA	1:A:266:LEU:HD12	2.03	0.41
2:B:92:TYR:CD1	2:B:104:VAL:HG11	2.55	0.41
2:B:79:PRO:HB2	2:B:84:TYR:CE2	2.56	0.41
2:B:94:GLY:HA2	2:B:98:GLU:HB2	2.03	0.41
1:C:761:ASN:ND2	1:C:763:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:690[A]:LYS:HA	1:E:690[A]:LYS:HD3	1.84	0.41
2:F:184:LYS:HA	2:F:184:LYS:HD3	1.76	0.41
1:G:141:ALA:HB1	1:G:592:VAL:HG23	2.02	0.41
1:G:111:GLU:HB3	1:G:625:ARG:HH21	1.84	0.41
1:G:693:ARG:HG2	1:G:694:PHE:O	2.21	0.41
1:I:232:TYR:CE2	1:I:237:ILE:HG22	2.56	0.41
2:J:169:LYS:HE3	2:J:169:LYS:HB3	1.69	0.41
1:K:817:ILE:HG13	1:K:845:THR:HG22	2.03	0.41
1:K:547:GLN:NE2	1:K:839:LEU:HD11	2.35	0.41
2:L:68:TYR:HA	2:L:72:GLU:O	2.21	0.41
2:B:184:LYS:HA	2:B:184:LYS:HD3	1.82	0.41
1:C:568:MET:HG2	2:D:96:LEU:HB3	2.03	0.41
1:E:60:ILE:H	1:E:70:ASN:ND2	2.08	0.41
1:E:107:ARG:NH2	1:E:611:GLU:OE2	2.45	0.41
2:F:15:VAL:HG23	2:F:233:VAL:HG12	2.02	0.41
1:G:321:TRP:CZ3	1:G:337:ARG:HG2	2.56	0.41
2:H:324:SER:O	2:H:328:MET:HG2	2.21	0.41
1:I:141:ALA:HB2	1:I:463:PRO:HB3	2.03	0.41
1:K:278:LEU:HD23	1:K:375:VAL:HG23	2.02	0.41
1:K:506:ASP:O	1:K:510:TYR:HD2	2.04	0.41
1:A:183:GLY:O	10:A:1104:HOH:O	2.22	0.41
1:A:29:ARG:O	1:A:603:GLU:HG2	2.21	0.41
1:C:208:ARG:HA	1:C:208:ARG:HD3	1.95	0.41
1:C:356:LEU:O	1:C:376:PHE:HB3	2.20	0.41
1:C:414:LYS:HA	1:C:415:PRO:HA	1.76	0.41
1:C:5:ILE:O	1:C:7:GLY:N	2.53	0.41
1:E:458:ILE:CD1	1:E:459:GLY:H	2.34	0.41
1:E:76:LYS:HB2	1:E:76:LYS:HE2	1.88	0.41
1:E:784:ARG:NH2	1:E:803:ASP:OD1	2.51	0.41
2:H:137:CYS:CB	2:H:184:LYS:HD2	2.47	0.41
1:I:166:ASP:O	1:I:878:ALA:HA	2.20	0.41
1:I:16:ASN:HA	1:I:19:ARG:HB2	2.02	0.41
1:I:207:THR:C	1:I:208:ARG:NH2	2.74	0.41
1:I:361:ASN:HB3	1:I:369:THR:CG2	2.51	0.41
1:I:621:ALA:O	1:I:625:ARG:HG2	2.21	0.41
2:J:291:LYS:O	10:J:505:HOH:O	2.22	0.41
1:I:21:GLN:HE21	2:J:35:TRP:HE3	1.69	0.41
1:C:208:ARG:HG3	1:C:211:ASP:HB2	2.02	0.41
1:C:278:LEU:HA	1:C:375:VAL:HB	2.03	0.41
1:C:289:PHE:CZ	1:C:731:TYR:HB3	2.56	0.41
1:E:770:HIS:CE1	5:E:1003:MGD:S13	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:LYS:HB2	1:E:706:VAL:HB	2.03	0.41
2:F:57:TYR:HA	2:F:58:PRO:HA	1.97	0.41
1:G:539:ASN:ND2	1:G:569:ASP:HB2	2.36	0.41
1:G:63:MET:HB2	1:G:66:ILE:HD11	2.02	0.41
1:G:693:ARG:NH2	1:G:702:LEU:HG	2.36	0.41
2:H:188:ASN:HB2	2:H:195:ASN:HD21	1.86	0.41
1:I:255:MET:HE2	1:I:255:MET:HB2	1.76	0.41
1:I:754:ASP:O	1:I:885[A]:ARG:NE	2.54	0.41
1:K:464:ALA:HA	1:K:698:TRP:NE1	2.35	0.41
1:K:128:HIS:NE2	1:K:531:LYS:HE3	2.36	0.41
1:A:783:GLN:NE2	10:A:1102:HOH:O	2.49	0.40
1:A:209:ILE:HG22	2:B:217:VAL:HG11	2.02	0.40
1:C:78:GLU:HG3	2:D:215:GLN:NE2	2.36	0.40
1:C:826:GLU:OE1	1:C:830:ARG:NH1	2.50	0.40
1:E:468:GLY:H	1:E:676:ALA:HB2	1.86	0.40
1:G:60:ILE:HG22	1:G:70:ASN:CG	2.41	0.40
1:G:756:TYR:O	1:G:885[B]:ARG:HD3	2.22	0.40
1:I:125:ILE:HG12	1:I:130:PRO:HA	2.03	0.40
1:I:343:PRO:HG2	1:I:346:TYR:HE1	1.85	0.40
1:I:421:GLY:O	1:I:425:GLN:HB2	2.21	0.40
1:I:463:PRO:O	1:I:466:VAL:HG23	2.21	0.40
1:I:703:LYS:O	1:I:706:VAL:HG22	2.21	0.40
1:K:546:GLY:O	1:K:550:VAL:HG23	2.21	0.40
1:K:729:GLN:NE2	1:K:732:LEU:HD23	2.36	0.40
1:A:571:THR:O	1:A:575:SER:OG	2.30	0.40
1:A:59:ASP:N	1:A:59:ASP:OD1	2.54	0.40
1:A:789:ILE:HG13	1:A:833:MET:HB2	2.04	0.40
1:A:863:GLY:HA2	1:A:869:PHE:HA	2.04	0.40
1:C:380:LYS:O	1:C:384:MET:HG2	2.21	0.40
1:E:697:ASN:HD22	1:E:698:TRP:H	1.69	0.40
1:I:12:SER:HA	1:I:15:GLU:OE2	2.22	0.40
1:I:253:LEU:HB2	1:I:396:THR:HG21	2.03	0.40
1:K:207:THR:C	1:K:208:ARG:HG2	2.42	0.40
1:A:787:PRO:HD2	1:A:842:ASP:HB3	2.03	0.40
2:B:46:TRP:HB3	2:B:197:CYS:HB2	2.03	0.40
1:C:682:ILE:HG13	1:C:695:LYS:NZ	2.36	0.40
1:C:784:ARG:NH2	10:C:1102:HOH:O	2.12	0.40
1:G:543:GLN:HA	1:G:836:CYS:SG	2.61	0.40
1:G:6:SER:O	1:G:6:SER:OG	2.33	0.40
2:H:242:VAL:HA	2:H:296:VAL:HG13	2.04	0.40
1:I:414:LYS:N	1:I:414:LYS:HD3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:228:ILE:HA	1:K:243:ILE:O	2.22	0.40
1:K:417:MET:HG3	1:K:455:ASN:HD22	1.85	0.40
1:K:162:HIS:ND1	1:K:486:THR:HG22	2.36	0.40
1:K:61:ALA:HA	1:K:62:PRO:HD3	1.96	0.40
1:K:637:LYS:HA	1:K:647:ARG:O	2.22	0.40
1:K:687:LEU:HD23	1:K:692:GLN:HB2	2.03	0.40
1:K:678:GLN:NE2	1:K:697:ASN:O	2.54	0.40
1:K:715:VAL:HG23	1:K:716:VAL:HG23	2.03	0.40
2:L:324:SER:O	2:L:328:MET:HG2	2.22	0.40
2:L:5:MET:O	2:L:6:LYS:HB3	2.21	0.40
1:C:56:GLN:O	1:C:58:LYS:NZ	2.43	0.40
2:D:27:CYS:SG	2:D:47:ARG:NE	2.72	0.40
1:G:135:VAL:HA	1:G:534:PHE:HB2	2.01	0.40
1:I:417:MET:HE3	1:I:417:MET:HB3	1.90	0.40
1:I:535:VAL:O	1:I:563:ASP:HA	2.21	0.40
1:K:448:GLY:HA3	1:K:715:VAL:HG21	2.01	0.40
1:K:428:TYR:N	1:K:883:ASP:OD1	2.52	0.40
1:A:882:ARG:HA	1:A:882:ARG:HD3	1.99	0.40
2:F:125:TYR:HA	2:F:126:PRO:HA	1.92	0.40
2:F:159:GLN:OE1	2:F:159:GLN:N	2.51	0.40
1:G:134:SER:HB2	1:G:162:HIS:NE2	2.36	0.40
1:G:58:LYS:HA	1:G:70:ASN:ND2	2.36	0.40
1:K:288:ARG:HD2	1:K:288:ARG:HA	1.78	0.40
1:K:118:ALA:HB1	1:K:626:VAL:HA	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	896/899 (100%)	852 (95%)	40 (4%)	4 (0%)	34 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	896/899 (100%)	849 (95%)	42 (5%)	5 (1%)	25	36
1	E	896/899 (100%)	845 (94%)	47 (5%)	4 (0%)	34	48
1	G	896/899 (100%)	841 (94%)	49 (6%)	6 (1%)	22	32
1	I	896/899 (100%)	815 (91%)	71 (8%)	10 (1%)	14	20
1	K	896/899 (100%)	822 (92%)	64 (7%)	10 (1%)	14	20
2	B	327/333 (98%)	314 (96%)	11 (3%)	2 (1%)	25	36
2	D	327/333 (98%)	311 (95%)	15 (5%)	1 (0%)	41	55
2	F	327/333 (98%)	312 (95%)	15 (5%)	0	100	100
2	H	327/333 (98%)	306 (94%)	16 (5%)	5 (2%)	10	14
2	J	327/333 (98%)	313 (96%)	13 (4%)	1 (0%)	41	55
2	L	327/333 (98%)	311 (95%)	16 (5%)	0	100	100
All	All	7338/7392 (99%)	6891 (94%)	399 (5%)	48 (1%)	22	32

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	70	ASN
1	G	6	SER
2	H	141	THR
2	H	241	LYS
1	I	317	PRO
1	I	644	LYS
2	J	7	ALA
1	A	326	GLU
1	A	458	ILE
1	C	6	SER
1	C	458	ILE
1	E	458	ILE
1	G	338	ASN
1	G	458	ILE
1	I	458	ILE
1	K	10	GLU
1	K	326	GLU
1	K	637	LYS
1	K	680	LYS
1	E	842	ASP
1	G	326	GLU
2	H	9	ARG

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Mol	Chain	Res	Type
2	H	136	MET
2	H	142	LYS
1	I	447	GLU
1	I	461	GLU
1	C	326	GLU
1	E	728	GLN
1	I	326	GLU
1	K	367	GLY
1	A	139	VAL
1	C	842	ASP
2	D	6	LYS
1	I	257	MET
1	I	691	PRO
1	K	291	ARG
1	K	458	ILE
1	A	7	GLY
2	B	6	LYS
1	G	881	GLN
1	K	139	VAL
1	K	293	ALA
1	K	361	ASN
1	C	139	VAL
1	E	139	VAL
1	I	345	GLY
1	I	448	GLY
1	G	139	VAL

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	769/768 (100%)	761 (99%)	8 (1%)	76	88
1	C	769/768 (100%)	759 (99%)	10 (1%)	69	84
1	E	769/768 (100%)	762 (99%)	7 (1%)	78	90
1	G	769/768 (100%)	759 (99%)	10 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	769/768 (100%)	752 (98%)	17 (2%)	52	71
1	K	769/768 (100%)	754 (98%)	15 (2%)	55	74
2	B	278/281 (99%)	269 (97%)	9 (3%)	39	59
2	D	278/281 (99%)	273 (98%)	5 (2%)	59	76
2	F	278/281 (99%)	271 (98%)	7 (2%)	47	67
2	H	278/281 (99%)	269 (97%)	9 (3%)	39	59
2	J	278/281 (99%)	270 (97%)	8 (3%)	42	62
2	L	278/281 (99%)	272 (98%)	6 (2%)	52	71
All	All	6282/6294 (100%)	6171 (98%)	111 (2%)	59	76

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	54	GLU
1	A	70	ASN
1	A	165	TYR
1	A	366	ASP
1	A	465	PHE
1	A	766	ARG
1	A	881	GLN
2	B	21	CYS
2	B	31	CYS
2	B	137	CYS
2	B	150	PRO
2	B	168	ASP
2	B	197	CYS
2	B	216	CYS
2	B	291	LYS
2	B	302	SER
1	C	17	PHE
1	C	54	GLU
1	C	74	CYS
1	C	78	GLU
1	C	165	TYR
1	C	359	LYS
1	C	465	PHE
1	C	466	VAL
1	C	675	ASN

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Mol	Chain	Res	Type
1	C	709	THR
2	D	31	CYS
2	D	59	ARG
2	D	137	CYS
2	D	170	CYS
2	D	180	CYS
1	E	54	GLU
1	E	78	GLU
1	E	165	TYR
1	E	288	ARG
1	E	344	LYS
1	E	545	LYS
1	E	555	TRP
2	F	9	ARG
2	F	31	CYS
2	F	42	ASP
2	F	48	ASN
2	F	192	ASN
2	F	197	CYS
2	F	216	CYS
1	G	54	GLU
1	G	74	CYS
1	G	164	PHE
1	G	165	TYR
1	G	198	ILE
1	G	205	THR
1	G	250	ASP
1	G	414	LYS
1	G	465	PHE
1	G	555	TRP
2	H	33	LYS
2	H	59	ARG
2	H	137	CYS
2	H	138	ASN
2	H	180	CYS
2	H	197	CYS
2	H	216	CYS
2	H	234	TYR
2	H	325	THR
1	I	54	GLU
1	I	74	CYS
1	I	78	GLU

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Mol	Chain	Res	Type
1	I	92	TYR
1	I	164	PHE
1	I	165	TYR
1	I	171	HIS
1	I	320	SER
1	I	363	GLN
1	I	368	LYS
1	I	373	ARG
1	I	381	SER
1	I	425	GLN
1	I	439	LEU
1	I	465	PHE
1	I	601	MET
1	I	650	SER
2	J	21	CYS
2	J	31	CYS
2	J	137	CYS
2	J	159	GLN
2	J	180	CYS
2	J	197	CYS
2	J	216	CYS
2	J	305	GLU
1	K	74	CYS
1	K	165	TYR
1	K	166	ASP
1	K	208	ARG
1	K	283	ARG
1	K	285	ASP
1	K	289	PHE
1	K	290	LEU
1	K	291	ARG
1	K	373	ARG
1	K	375	VAL
1	K	438	HIS
1	K	465	PHE
1	K	480	LYS
1	K	762	SER
2	L	21	CYS
2	L	31	CYS
2	L	50	GLU
2	L	137	CYS
2	L	180	CYS

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Mol	Chain	Res	Type
2	L	241	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	HIS
2	B	178	GLN
1	C	324	GLN
2	D	192	ASN
1	E	70	ASN
1	E	697	ASN
1	E	881	GLN
2	F	192	ASN
1	G	21	GLN
1	G	651	ASN
2	H	195	ASN
1	I	16	ASN
1	I	21	GLN
1	I	363	GLN
1	I	425	GLN
1	I	670	GLN
1	I	881	GLN
2	J	138	ASN
2	J	239	GLN
2	J	271	ASN
1	K	42	HIS
1	K	547	GLN
2	L	74	GLN
2	L	167	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 79 ligands modelled in this entry, 6 are monoatomic - leaving 73 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$
3	SF4	B	405	2	0,12,12	0.00	-	-		
3	SF4	F	405	-	0,12,12	0.00	-	-		
9	F3S	B	402	-	0,9,9	0.00	-	-		
9	F3S	F	402	-	0,9,9	0.00	-	-		
7	EDO	I	1005	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	C	1006	-	3,3,3	0.44	0	2,2,2	0.34	0
7	EDO	C	1007	-	3,3,3	0.45	0	2,2,2	0.32	0
3	SF4	D	404	2	0,12,12	0.00	-	-		
6	MD1	C	1004	4	38,51,51	4.43	15 (39%)	35,78,78	1.42	5 (14%)
3	SF4	B	403	2	0,12,12	0.00	-	-		
7	EDO	A	1007	-	3,3,3	0.46	0	2,2,2	0.35	0
6	MD1	A	1004	4	38,51,51	4.43	15 (39%)	35,78,78	1.41	5 (14%)
3	SF4	L	404	2	0,12,12	0.00	-	-		
5	MGD	E	1003	4	41,52,52	6.50	27 (65%)	43,81,81	2.40	17 (39%)
8	GOL	A	1008	-	5,5,5	0.36	0	5,5,5	0.27	0
3	SF4	H	403	-	0,12,12	0.00	-	-		
9	F3S	D	401	-	0,9,9	0.00	-	-		
7	EDO	I	1006	-	3,3,3	0.46	0	2,2,2	0.37	0
7	EDO	H	406	-	3,3,3	0.46	0	2,2,2	0.32	0
3	SF4	H	404	-	0,12,12	0.00	-	-		
5	MGD	C	1003	4	41,52,52	6.48	27 (65%)	43,81,81	2.41	16 (37%)
3	SF4	D	402	-	0,12,12	0.00	-	-		
7	EDO	G	1006	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	A	1006	-	3,3,3	0.45	0	2,2,2	0.33	0
7	EDO	G	1007	-	3,3,3	0.45	0	2,2,2	0.33	0
3	SF4	E	1001	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	L	402	-	0,12,12	0.00	-	-		
3	SF4	F	403	2	0,12,12	0.00	-	-		
6	MD1	K	1004	4	38,51,51	4.40	17 (44%)	35,78,78	1.42	5 (14%)
7	EDO	A	1010	-	3,3,3	0.46	0	2,2,2	0.36	0
7	EDO	J	405	-	3,3,3	0.46	0	2,2,2	0.36	0
7	EDO	A	1009	-	3,3,3	0.45	0	2,2,2	0.33	0
9	F3S	L	401	-	0,9,9	0.00	-	-		
7	EDO	F	406	-	3,3,3	0.46	0	2,2,2	0.34	0
6	MD1	G	1004	4	38,51,51	4.42	17 (44%)	35,78,78	1.41	5 (14%)
7	EDO	K	1005	-	3,3,3	0.45	0	2,2,2	0.30	0
3	SF4	K	1001	1	0,12,12	0.00	-	-		
7	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.31	0
3	SF4	J	402	-	0,12,12	0.00	-	-		
7	EDO	L	406	-	3,3,3	0.47	0	2,2,2	0.34	0
3	SF4	C	1001	1	0,12,12	0.00	-	-		
7	EDO	A	1005	-	3,3,3	0.46	0	2,2,2	0.35	0
8	GOL	E	1006	-	5,5,5	0.37	0	5,5,5	0.34	0
3	SF4	D	403	-	0,12,12	0.00	-	-		
7	EDO	G	1008	-	3,3,3	0.46	0	2,2,2	0.34	0
7	EDO	H	405	-	3,3,3	0.45	0	2,2,2	0.32	0
3	SF4	B	404	-	0,12,12	0.00	-	-		
5	MGD	A	1003	4	41,52,52	6.48	27 (65%)	43,81,81	2.49	17 (39%)
5	MGD	G	1003	4	41,52,52	6.51	27 (65%)	43,81,81	2.41	17 (39%)
7	EDO	E	1005	-	3,3,3	0.45	0	2,2,2	0.34	0
3	SF4	F	404	-	0,12,12	0.00	-	-		
3	SF4	J	404	-	0,12,12	0.00	-	-		
7	EDO	B	406	-	3,3,3	0.46	0	2,2,2	0.37	0
3	SF4	A	1001	1	0,12,12	0.00	-	-		
7	EDO	G	1005	-	3,3,3	0.46	0	2,2,2	0.32	0
7	EDO	H	407	-	3,3,3	0.44	0	2,2,2	0.39	0
7	EDO	C	1005	-	3,3,3	0.45	0	2,2,2	0.35	0
3	SF4	G	1001	1	0,12,12	0.00	-	-		
7	EDO	E	1007	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	D	405	-	3,3,3	0.45	0	2,2,2	0.32	0
9	F3S	J	401	-	0,9,9	0.00	-	-		
7	EDO	K	1006	-	3,3,3	0.45	0	2,2,2	0.32	0
5	MGD	K	1003	4	41,52,52	6.49	27 (65%)	43,81,81	2.49	17 (39%)
6	MD1	I	1004	4	38,51,51	4.39	17 (44%)	35,78,78	1.39	5 (14%)
7	EDO	L	405	-	3,3,3	0.47	0	2,2,2	0.31	0
3	SF4	H	402	-	0,12,12	0.00	-	-		
9	F3S	H	401	-	0,9,9	0.00	-	-		
3	SF4	I	1001	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	L	403	-	0,12,12	0.00	-	-		
6	MD1	E	1004	4	38,51,51	4.41	15 (39%)	35,78,78	1.41	4 (11%)
3	SF4	J	403	-	0,12,12	0.00	-	-		
7	EDO	F	401	-	3,3,3	0.45	0	2,2,2	0.33	0
5	MGD	I	1003	4	41,52,52	6.53	27 (65%)	43,81,81	2.46	17 (39%)

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
3	SF4	B	405	2	-	-	0/6/5/5
3	SF4	F	405	-	-	-	0/6/5/5
9	F3S	B	402	-	-	-	0/3/3/3
3	SF4	L	404	2	-	-	0/6/5/5
7	EDO	I	1005	-	-	0/1/1/1	-
7	EDO	C	1006	-	-	1/1/1/1	-
7	EDO	C	1007	-	-	1/1/1/1	-
3	SF4	D	404	2	-	-	0/6/5/5
7	EDO	E	1007	-	-	0/1/1/1	-
3	SF4	B	403	2	-	-	0/6/5/5
7	EDO	A	1007	-	-	0/1/1/1	-
6	MD1	A	1004	4	-	5/21/59/59	0/5/5/5
6	MD1	C	1004	4	-	8/21/59/59	0/5/5/5
5	MGD	E	1003	4	-	2/18/66/66	0/6/6/6
8	GOL	A	1008	-	-	0/4/4/4	-
3	SF4	H	403	-	-	-	0/6/5/5
9	F3S	D	401	-	-	-	0/3/3/3
7	EDO	I	1006	-	-	0/1/1/1	-
7	EDO	H	406	-	-	0/1/1/1	-
7	EDO	K	1006	-	-	0/1/1/1	-
5	MGD	C	1003	4	-	6/18/66/66	0/6/6/6
3	SF4	D	402	-	-	-	0/6/5/5
7	EDO	G	1006	-	-	0/1/1/1	-
7	EDO	A	1006	-	-	0/1/1/1	-
7	EDO	G	1007	-	-	0/1/1/1	-
3	SF4	E	1001	1	-	-	0/6/5/5
3	SF4	L	402	-	-	-	0/6/5/5
3	SF4	F	403	2	-	-	0/6/5/5
6	MD1	K	1004	4	-	8/21/59/59	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1010	-	-	0/1/1/1	-
7	EDO	J	405	-	-	0/1/1/1	-
7	EDO	A	1009	-	-	0/1/1/1	-
9	F3S	L	401	-	-	-	0/3/3/3
7	EDO	F	406	-	-	0/1/1/1	-
6	MD1	G	1004	4	-	5/21/59/59	0/5/5/5
7	EDO	K	1005	-	-	0/1/1/1	-
3	SF4	K	1001	1	-	-	0/6/5/5
7	EDO	B	401	-	-	0/1/1/1	-
3	SF4	J	402	-	-	-	0/6/5/5
7	EDO	L	406	-	-	0/1/1/1	-
3	SF4	C	1001	1	-	-	0/6/5/5
3	SF4	H	404	-	-	-	0/6/5/5
8	GOL	E	1006	-	-	0/4/4/4	-
3	SF4	D	403	-	-	-	0/6/5/5
7	EDO	G	1008	-	-	0/1/1/1	-
7	EDO	H	405	-	-	0/1/1/1	-
3	SF4	B	404	-	-	-	0/6/5/5
5	MGD	A	1003	4	-	2/18/66/66	0/6/6/6
5	MGD	G	1003	4	-	2/18/66/66	0/6/6/6
7	EDO	E	1005	-	-	0/1/1/1	-
3	SF4	F	404	-	-	-	0/6/5/5
3	SF4	J	404	-	-	-	0/6/5/5
7	EDO	B	406	-	-	0/1/1/1	-
3	SF4	A	1001	1	-	-	0/6/5/5
7	EDO	G	1005	-	-	0/1/1/1	-
7	EDO	H	407	-	-	0/1/1/1	-
3	SF4	J	403	-	-	-	0/6/5/5
3	SF4	G	1001	1	-	-	0/6/5/5
7	EDO	C	1005	-	-	1/1/1/1	-
9	F3S	F	402	-	-	-	0/3/3/3
7	EDO	D	405	-	-	0/1/1/1	-
9	F3S	J	401	-	-	-	0/3/3/3
5	MGD	K	1003	4	-	1/18/66/66	0/6/6/6
6	MD1	I	1004	4	-	7/21/59/59	0/5/5/5
7	EDO	L	405	-	-	0/1/1/1	-
3	SF4	H	402	-	-	-	0/6/5/5
9	F3S	H	401	-	-	-	0/3/3/3
3	SF4	I	1001	1	-	-	0/6/5/5
3	SF4	L	403	-	-	-	0/6/5/5
6	MD1	E	1004	4	-	3/21/59/59	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	1005	-	-	1/1/1/1	-
7	EDO	F	401	-	-	0/1/1/1	-
5	MGD	I	1003	4	-	1/18/66/66	0/6/6/6

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1003	MGD	C2'-C1'	-17.21	1.27	1.53
5	G	1003	MGD	C2'-C1'	-17.20	1.27	1.53
5	C	1003	MGD	C2'-C1'	-17.18	1.27	1.53
5	K	1003	MGD	C2'-C1'	-17.16	1.27	1.53
5	A	1003	MGD	C2'-C1'	-17.15	1.27	1.53
5	I	1003	MGD	C2'-C1'	-17.11	1.27	1.53
6	E	1004	MD1	C7-N8	15.42	1.46	1.27
6	A	1004	MD1	C7-N8	15.41	1.46	1.27
6	G	1004	MD1	C7-N8	15.41	1.46	1.27
6	C	1004	MD1	C7-N8	15.35	1.45	1.27
6	K	1004	MD1	C7-N8	15.24	1.45	1.27
6	I	1004	MD1	C7-N8	15.14	1.45	1.27
5	I	1003	MGD	O11-C11	13.23	1.61	1.43
5	G	1003	MGD	O11-C11	12.67	1.60	1.43
5	K	1003	MGD	O11-C11	12.65	1.60	1.43
5	E	1003	MGD	O11-C11	12.61	1.60	1.43
5	A	1003	MGD	O11-C11	12.56	1.60	1.43
5	C	1003	MGD	O11-C11	12.48	1.60	1.43
6	C	1004	MD1	C4-N9	-11.89	1.31	1.47
6	A	1004	MD1	C4-N9	-11.76	1.32	1.47
6	G	1004	MD1	C4-N9	-11.74	1.32	1.47
6	I	1004	MD1	C4-N9	-11.63	1.32	1.47
6	K	1004	MD1	C4-N9	-11.57	1.32	1.47
6	E	1004	MD1	C4-N9	-11.46	1.32	1.47
5	I	1003	MGD	C19-N18	11.07	1.55	1.35
5	E	1003	MGD	C19-N18	10.94	1.54	1.35
5	A	1003	MGD	C19-N18	10.93	1.54	1.35
5	C	1003	MGD	C19-N18	10.91	1.54	1.35
5	G	1003	MGD	C19-N18	10.91	1.54	1.35
5	K	1003	MGD	C19-N18	10.87	1.54	1.35
5	C	1003	MGD	C16-C21	10.85	1.61	1.41
5	E	1003	MGD	C16-C21	10.85	1.61	1.41
5	G	1003	MGD	C16-C21	10.83	1.61	1.41
5	A	1003	MGD	C16-C21	10.81	1.61	1.41
5	K	1003	MGD	C16-C21	10.81	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	O4'-C1'	10.60	1.55	1.41
5	E	1003	MGD	O4'-C1'	10.55	1.55	1.41
5	K	1003	MGD	O4'-C1'	10.51	1.55	1.41
5	I	1003	MGD	O4'-C1'	10.51	1.55	1.41
5	G	1003	MGD	O4'-C1'	10.48	1.55	1.41
5	A	1003	MGD	O4'-C1'	10.45	1.55	1.41
5	G	1003	MGD	C14-N15	10.30	1.59	1.45
5	A	1003	MGD	C14-N15	10.29	1.59	1.45
5	E	1003	MGD	C14-N15	10.28	1.59	1.45
5	K	1003	MGD	C14-N15	10.26	1.59	1.45
5	C	1003	MGD	C14-N15	10.22	1.59	1.45
5	I	1003	MGD	C14-N15	10.22	1.59	1.45
5	I	1003	MGD	C16-C21	10.16	1.60	1.41
5	E	1003	MGD	C3'-C4'	-9.62	1.28	1.53
5	C	1003	MGD	C3'-C4'	-9.60	1.28	1.53
5	A	1003	MGD	C3'-C4'	-9.60	1.28	1.53
5	K	1003	MGD	C3'-C4'	-9.59	1.28	1.53
5	I	1003	MGD	C3'-C4'	-9.58	1.28	1.53
5	G	1003	MGD	C3'-C4'	-9.54	1.28	1.53
5	A	1003	MGD	C17-N18	9.26	1.49	1.33
5	I	1003	MGD	C17-N18	9.25	1.49	1.33
5	C	1003	MGD	C17-N18	9.23	1.49	1.33
5	E	1003	MGD	C17-N18	9.19	1.49	1.33
5	G	1003	MGD	C17-N18	9.18	1.49	1.33
5	K	1003	MGD	C17-N18	9.15	1.49	1.33
5	K	1003	MGD	C19-N20	9.03	1.51	1.35
5	E	1003	MGD	C19-N20	9.01	1.51	1.35
5	C	1003	MGD	C19-N20	9.01	1.51	1.35
5	K	1003	MGD	C4-N3	8.99	1.49	1.35
5	A	1003	MGD	C19-N20	8.95	1.51	1.35
5	C	1003	MGD	C4-N3	8.92	1.49	1.35
5	I	1003	MGD	C4-N3	8.92	1.49	1.35
5	G	1003	MGD	C19-N20	8.91	1.51	1.35
5	A	1003	MGD	C4-N3	8.89	1.49	1.35
5	E	1003	MGD	C4-N3	8.88	1.49	1.35
5	G	1003	MGD	C4-N3	8.86	1.49	1.35
6	I	1004	MD1	O4'-C1'	8.82	1.62	1.42
6	C	1004	MD1	O4'-C1'	8.81	1.62	1.42
6	A	1004	MD1	O4'-C1'	8.81	1.62	1.42
6	G	1004	MD1	O4'-C1'	8.80	1.62	1.42
6	K	1004	MD1	O4'-C1'	8.78	1.62	1.42
6	E	1004	MD1	O4'-C1'	8.75	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1003	MGD	C19-N20	8.64	1.50	1.35
6	E	1004	MD1	C5-C6	-8.59	1.38	1.52
6	G	1004	MD1	C5-C6	-8.53	1.38	1.52
6	A	1004	MD1	C5-C6	-8.51	1.38	1.52
6	K	1004	MD1	C5-C6	-8.50	1.38	1.52
6	C	1004	MD1	C5-C6	-8.48	1.38	1.52
6	I	1004	MD1	C5-C6	-8.46	1.38	1.52
5	I	1003	MGD	C23-C14	-8.37	1.47	1.53
5	K	1003	MGD	C23-N22	8.04	1.60	1.44
5	C	1003	MGD	C23-N22	7.97	1.60	1.44
5	A	1003	MGD	C23-N22	7.96	1.60	1.44
5	E	1003	MGD	C23-N22	7.92	1.60	1.44
5	G	1003	MGD	C23-N22	7.90	1.60	1.44
5	I	1003	MGD	C23-N22	7.43	1.59	1.44
5	G	1003	MGD	C6-C5	7.28	1.53	1.41
5	I	1003	MGD	C6-C5	7.27	1.53	1.41
5	C	1003	MGD	C6-C5	7.27	1.53	1.41
5	A	1003	MGD	C6-C5	7.20	1.53	1.41
5	E	1003	MGD	C6-C5	7.19	1.53	1.41
5	K	1003	MGD	C6-C5	7.18	1.53	1.41
5	G	1003	MGD	O11-C23	-7.04	1.33	1.43
5	A	1003	MGD	O11-C23	-6.98	1.33	1.43
5	E	1003	MGD	O11-C23	-6.91	1.33	1.43
5	K	1003	MGD	O11-C23	-6.90	1.33	1.43
5	C	1003	MGD	O11-C23	-6.84	1.34	1.43
5	G	1003	MGD	C23-C14	-6.24	1.48	1.53
6	G	1004	MD1	C2'-C1'	-6.09	1.34	1.53
6	K	1004	MD1	C2'-C1'	-6.08	1.34	1.53
6	A	1004	MD1	C2'-C1'	-6.07	1.34	1.53
5	I	1003	MGD	O11-C23	-6.06	1.35	1.43
6	C	1004	MD1	C2'-C1'	-6.05	1.34	1.53
5	A	1003	MGD	C6-N1	6.04	1.43	1.33
5	G	1003	MGD	C6-N1	6.03	1.43	1.33
6	E	1004	MD1	C2'-C1'	-6.02	1.34	1.53
5	E	1003	MGD	C6-N1	6.01	1.43	1.33
5	I	1003	MGD	C6-N1	5.99	1.43	1.33
5	C	1003	MGD	C6-N1	5.98	1.43	1.33
6	I	1004	MD1	C2'-C1'	-5.97	1.34	1.53
5	K	1003	MGD	C6-N1	5.97	1.43	1.33
6	K	1004	MD1	C16-N15	5.93	1.50	1.38
5	A	1003	MGD	C2-N2	5.90	1.45	1.33
6	A	1004	MD1	C16-N15	5.89	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1003	MGD	C2-N2	5.89	1.45	1.33
5	E	1003	MGD	C23-C14	-5.88	1.49	1.53
5	E	1003	MGD	C2-N2	5.87	1.45	1.33
5	K	1003	MGD	C2-N2	5.87	1.45	1.33
6	I	1004	MD1	C16-N15	5.86	1.50	1.38
5	I	1003	MGD	C2-N2	5.85	1.45	1.33
5	G	1003	MGD	C2-N2	5.85	1.45	1.33
6	E	1004	MD1	C16-N15	5.83	1.50	1.38
6	C	1004	MD1	C16-N15	5.80	1.49	1.38
5	A	1003	MGD	C17-C16	5.74	1.49	1.41
5	A	1003	MGD	C19-N19	5.73	1.45	1.33
5	K	1003	MGD	C17-C16	5.72	1.49	1.41
5	G	1003	MGD	C17-C16	5.72	1.49	1.41
5	E	1003	MGD	C19-N19	5.71	1.45	1.33
5	K	1003	MGD	C19-N19	5.70	1.45	1.33
5	I	1003	MGD	C19-N19	5.70	1.45	1.33
6	G	1004	MD1	C16-N15	5.70	1.49	1.38
5	C	1003	MGD	C17-C16	5.69	1.49	1.41
5	C	1003	MGD	C19-N19	5.69	1.45	1.33
5	G	1003	MGD	C19-N19	5.68	1.45	1.33
5	E	1003	MGD	C17-C16	5.66	1.49	1.41
6	C	1004	MD1	O4'-C4'	-5.57	1.32	1.45
6	A	1004	MD1	O4'-C4'	-5.55	1.32	1.45
6	I	1004	MD1	O4'-C4'	-5.52	1.32	1.45
6	E	1004	MD1	O4'-C4'	-5.52	1.32	1.45
6	G	1004	MD1	O4'-C4'	-5.49	1.32	1.45
6	K	1004	MD1	O4'-C4'	-5.46	1.32	1.45
5	K	1003	MGD	C23-C14	-5.44	1.49	1.53
5	I	1003	MGD	C17-C16	5.40	1.48	1.41
6	I	1004	MD1	C17-N16	5.38	1.44	1.33
6	G	1004	MD1	C17-N16	5.38	1.44	1.33
6	C	1004	MD1	C17-N16	5.38	1.44	1.33
6	K	1004	MD1	C17-N16	5.36	1.44	1.33
6	A	1004	MD1	C17-N16	5.32	1.44	1.33
6	E	1004	MD1	C17-N16	5.32	1.44	1.33
5	K	1003	MGD	C21-N20	5.31	1.44	1.34
5	A	1003	MGD	C23-C14	-5.29	1.49	1.53
5	C	1003	MGD	C23-C14	-5.24	1.49	1.53
5	C	1003	MGD	C21-N20	5.24	1.44	1.34
5	E	1003	MGD	C21-N20	5.23	1.44	1.34
5	A	1003	MGD	C21-N20	5.23	1.44	1.34
5	I	1003	MGD	C2-N1	5.21	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1003	MGD	C2-N1	5.19	1.44	1.35
5	A	1003	MGD	C2-N1	5.19	1.44	1.35
5	E	1003	MGD	C2-N1	5.18	1.44	1.35
5	G	1003	MGD	C21-N20	5.17	1.44	1.34
5	K	1003	MGD	C2-N1	5.17	1.44	1.35
5	C	1003	MGD	C2-N1	5.16	1.44	1.35
5	K	1003	MGD	O4'-C4'	5.07	1.56	1.45
5	I	1003	MGD	C21-N20	5.06	1.44	1.34
5	C	1003	MGD	O4'-C4'	5.04	1.56	1.45
5	E	1003	MGD	O4'-C4'	5.03	1.56	1.45
5	G	1003	MGD	O4'-C4'	5.03	1.56	1.45
5	A	1003	MGD	O4'-C4'	4.98	1.56	1.45
5	I	1003	MGD	O4'-C4'	4.96	1.56	1.45
5	I	1003	MGD	C2'-C3'	4.82	1.66	1.53
5	A	1003	MGD	C2'-C3'	4.80	1.66	1.53
5	E	1003	MGD	C2'-C3'	4.76	1.66	1.53
5	G	1003	MGD	C2'-C3'	4.75	1.66	1.53
5	K	1003	MGD	C2'-C3'	4.73	1.66	1.53
5	C	1003	MGD	C2'-C3'	4.71	1.66	1.53
5	I	1003	MGD	C10-C11	3.78	1.57	1.52
6	K	1004	MD1	O3'-C3'	-3.62	1.34	1.43
6	G	1004	MD1	O3'-C3'	-3.61	1.34	1.43
6	E	1004	MD1	O3'-C3'	-3.61	1.34	1.43
6	C	1004	MD1	O3'-C3'	-3.59	1.34	1.43
6	A	1004	MD1	O3'-C3'	-3.59	1.34	1.43
6	I	1004	MD1	O3'-C3'	-3.58	1.34	1.43
6	K	1004	MD1	C14-C13	3.48	1.55	1.51
6	A	1004	MD1	C14-C13	3.44	1.55	1.51
6	E	1004	MD1	C14-C13	3.38	1.55	1.51
6	C	1004	MD1	C14-C13	3.13	1.54	1.51
6	G	1004	MD1	C14-C13	3.03	1.54	1.51
6	I	1004	MD1	C14-C13	2.97	1.54	1.51
5	I	1003	MGD	C13-C12	2.96	1.54	1.35
6	E	1004	MD1	C8-N9	-2.87	1.35	1.45
5	G	1003	MGD	C13-C12	2.87	1.54	1.35
6	C	1004	MD1	C8-N9	-2.86	1.35	1.45
6	G	1004	MD1	C8-N9	-2.86	1.35	1.45
6	K	1004	MD1	C8-N9	-2.86	1.35	1.45
6	A	1004	MD1	C8-N9	-2.84	1.35	1.45
5	E	1003	MGD	C13-C12	2.84	1.53	1.35
6	I	1004	MD1	C8-N9	-2.84	1.35	1.45
5	A	1003	MGD	C13-C12	2.84	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1003	MGD	C13-C12	2.83	1.53	1.35
5	C	1003	MGD	C13-C12	2.82	1.53	1.35
6	C	1004	MD1	C5-C4	-2.80	1.35	1.53
6	G	1004	MD1	C5-C4	-2.79	1.35	1.53
6	A	1004	MD1	C5-C4	-2.79	1.35	1.53
6	K	1004	MD1	C5-C4	-2.77	1.35	1.53
6	E	1004	MD1	C5-C4	-2.77	1.35	1.53
6	I	1004	MD1	C5-C4	-2.77	1.36	1.53
5	G	1003	MGD	C10-C11	2.60	1.55	1.52
5	K	1003	MGD	C10-C11	2.59	1.55	1.52
5	E	1003	MGD	C2-N3	2.57	1.46	1.34
5	A	1003	MGD	C2-N3	2.55	1.46	1.34
5	K	1003	MGD	C2-N3	2.55	1.46	1.34
6	A	1004	MD1	PB-O3A	2.55	1.69	1.59
5	E	1003	MGD	C10-C11	2.54	1.55	1.52
5	I	1003	MGD	C2-N3	2.53	1.46	1.34
5	C	1003	MGD	C2-N3	2.53	1.46	1.34
6	E	1004	MD1	PB-O3A	2.51	1.69	1.59
5	G	1003	MGD	C2-N3	2.51	1.46	1.34
6	G	1004	MD1	PB-O3A	2.51	1.69	1.59
6	E	1004	MD1	C2-N2	2.49	1.49	1.36
6	G	1004	MD1	C2-N2	2.49	1.49	1.36
6	A	1004	MD1	C2-N2	2.48	1.49	1.36
6	K	1004	MD1	PB-O3A	2.48	1.69	1.59
6	I	1004	MD1	C2-N2	2.48	1.49	1.36
6	K	1004	MD1	C2-N2	2.48	1.49	1.36
6	C	1004	MD1	C2-N2	2.47	1.49	1.36
5	C	1003	MGD	C10-C11	2.47	1.55	1.52
5	A	1003	MGD	C10-C11	2.46	1.55	1.52
6	I	1004	MD1	PB-O3A	2.46	1.69	1.59
6	C	1004	MD1	PB-O3A	2.46	1.69	1.59
6	C	1004	MD1	O14-C15	-2.44	1.18	1.24
6	E	1004	MD1	O14-C15	-2.41	1.18	1.24
6	A	1004	MD1	O14-C15	-2.41	1.18	1.24
6	K	1004	MD1	O14-C15	-2.40	1.18	1.24
6	G	1004	MD1	O14-C15	-2.40	1.18	1.24
6	I	1004	MD1	O14-C15	-2.37	1.18	1.24
5	C	1003	MGD	O6-C6	-2.36	1.18	1.24
5	G	1003	MGD	O6-C6	-2.30	1.18	1.24
5	E	1003	MGD	O6-C6	-2.30	1.18	1.24
5	I	1003	MGD	O6-C6	-2.27	1.18	1.24
5	A	1003	MGD	O6-C6	-2.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1003	MGD	O6-C6	-2.25	1.18	1.24
5	K	1003	MGD	O17-C17	-2.24	1.18	1.24
5	I	1003	MGD	O17-C17	-2.24	1.18	1.24
5	A	1003	MGD	O17-C17	-2.23	1.18	1.24
6	G	1004	MD1	C15-C16	-2.22	1.38	1.41
5	E	1003	MGD	O17-C17	-2.22	1.19	1.24
5	G	1003	MGD	O17-C17	-2.21	1.19	1.24
5	C	1003	MGD	O17-C17	-2.20	1.19	1.24
6	I	1004	MD1	C15-C16	-2.14	1.38	1.41
6	I	1004	MD1	O11-C11	-2.12	1.38	1.42
6	K	1004	MD1	O11-C11	-2.03	1.38	1.42
6	K	1004	MD1	C15-C16	-2.02	1.38	1.41
6	G	1004	MD1	O11-C11	-2.00	1.38	1.42

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1003	MGD	O11-C23-N22	-7.00	101.38	108.57
5	K	1003	MGD	O11-C23-C14	6.00	112.96	108.96
5	A	1003	MGD	O11-C23-C14	5.86	112.87	108.96
5	K	1003	MGD	C17-C16-C21	5.83	119.75	114.57
5	G	1003	MGD	C17-C16-C21	5.76	119.68	114.57
5	C	1003	MGD	C17-C16-C21	5.71	119.64	114.57
5	E	1003	MGD	C17-C16-C21	5.69	119.62	114.57
5	A	1003	MGD	C17-C16-C21	5.66	119.60	114.57
5	E	1003	MGD	N3-C2-N1	-5.44	119.96	127.22
5	G	1003	MGD	N3-C2-N1	-5.43	119.98	127.22
5	K	1003	MGD	N3-C2-N1	-5.41	120.00	127.22
5	A	1003	MGD	N3-C2-N1	-5.41	120.00	127.22
5	I	1003	MGD	N3-C2-N1	-5.40	120.02	127.22
5	C	1003	MGD	N3-C2-N1	-5.40	120.02	127.22
5	I	1003	MGD	C17-C16-C21	5.16	119.15	114.57
5	G	1003	MGD	C21-N22-C23	-4.87	114.13	123.67
5	C	1003	MGD	O11-C23-C14	4.79	112.16	108.96
5	A	1003	MGD	O11-C23-N22	-4.76	103.68	108.57
5	C	1003	MGD	C21-N22-C23	-4.70	114.46	123.67
5	E	1003	MGD	C21-N22-C23	-4.65	114.56	123.67
5	A	1003	MGD	C21-N22-C23	-4.46	114.93	123.67
5	K	1003	MGD	O11-C23-N22	-4.42	104.03	108.57
5	K	1003	MGD	C21-N22-C23	-4.41	115.03	123.67
5	G	1003	MGD	C1'-N9-C4	-4.38	118.95	126.64
5	E	1003	MGD	O11-C23-C14	4.31	111.84	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1003	MGD	O11-C23-C14	4.23	111.78	108.96
5	E	1003	MGD	O11-C23-N22	-4.18	104.27	108.57
5	C	1003	MGD	C1'-N9-C4	-4.15	119.34	126.64
6	K	1004	MD1	C4-C5-N7	4.14	107.95	102.46
5	I	1003	MGD	C1'-N9-C4	-4.14	119.37	126.64
5	E	1003	MGD	C2-N3-C4	4.11	120.05	115.36
5	G	1003	MGD	C2-N3-C4	4.11	120.05	115.36
6	E	1004	MD1	C4-C5-N7	4.10	107.89	102.46
5	C	1003	MGD	C2-N3-C4	4.10	120.03	115.36
5	I	1003	MGD	C2-N3-C4	4.09	120.03	115.36
5	C	1003	MGD	C16-C21-N22	4.09	121.87	118.13
5	A	1003	MGD	C2-N3-C4	4.04	119.97	115.36
5	G	1003	MGD	C16-C21-N22	4.04	121.83	118.13
5	K	1003	MGD	C2-N3-C4	4.04	119.97	115.36
5	A	1003	MGD	C16-C21-N22	4.04	121.82	118.13
6	G	1004	MD1	C4-C5-N7	4.03	107.80	102.46
6	I	1004	MD1	C4-C5-N7	4.01	107.77	102.46
5	K	1003	MGD	C16-C21-N22	4.01	121.80	118.13
6	C	1004	MD1	C4-C5-N7	3.96	107.71	102.46
5	A	1003	MGD	C1'-N9-C4	-3.95	119.71	126.64
6	A	1004	MD1	C4-C5-N7	3.93	107.67	102.46
5	E	1003	MGD	C1'-N9-C4	-3.91	119.77	126.64
5	G	1003	MGD	O11-C23-N22	-3.81	104.65	108.57
5	E	1003	MGD	C16-C21-N22	3.79	121.60	118.13
5	G	1003	MGD	O11-C23-C14	3.74	111.46	108.96
5	K	1003	MGD	C1'-N9-C4	-3.69	120.16	126.64
5	C	1003	MGD	O11-C23-N22	-3.50	104.97	108.57
5	I	1003	MGD	C3'-C2'-C1'	3.38	106.07	100.98
6	K	1004	MD1	N17-C17-N18	-3.37	120.13	125.42
6	G	1004	MD1	N17-C17-N18	-3.31	120.23	125.42
6	I	1004	MD1	N17-C17-N18	-3.29	120.26	125.42
6	A	1004	MD1	N17-C17-N18	-3.28	120.27	125.42
6	E	1004	MD1	N17-C17-N18	-3.27	120.29	125.42
6	C	1004	MD1	N17-C17-N18	-3.21	120.38	125.42
6	C	1004	MD1	PA-O3B-PB	-3.14	122.05	132.83
5	I	1003	MGD	C21-N22-C23	-3.09	117.63	123.67
5	E	1003	MGD	N18-C19-N20	-3.05	120.63	125.42
5	C	1003	MGD	N18-C19-N20	-3.02	120.68	125.42
5	I	1003	MGD	N18-C19-N20	-3.01	120.69	125.42
5	A	1003	MGD	N18-C19-N20	-2.99	120.73	125.42
5	G	1003	MGD	N18-C19-N20	-2.98	120.74	125.42
6	K	1004	MD1	PA-O3B-PB	-2.93	122.78	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1003	MGD	N18-C19-N20	-2.92	120.84	125.42
6	G	1004	MD1	PA-O3B-PB	-2.84	123.08	132.83
5	I	1003	MGD	C17-N18-C19	2.84	120.44	115.93
6	E	1004	MD1	PA-O3B-PB	-2.78	123.28	132.83
5	K	1003	MGD	O4'-C1'-C2'	-2.75	102.91	106.93
6	I	1004	MD1	PA-O3B-PB	-2.75	123.39	132.83
6	G	1004	MD1	C15-N17-C17	2.72	120.26	115.93
6	K	1004	MD1	C15-N17-C17	2.71	120.24	115.93
5	I	1003	MGD	C2'-C3'-C4'	2.69	107.87	102.64
6	A	1004	MD1	PA-O3B-PB	-2.69	123.60	132.83
5	G	1003	MGD	C17-N18-C19	2.68	120.19	115.93
6	E	1004	MD1	C15-N17-C17	2.68	120.19	115.93
5	E	1003	MGD	C17-N18-C19	2.68	120.18	115.93
5	C	1003	MGD	C17-N18-C19	2.67	120.17	115.93
6	A	1004	MD1	C15-N17-C17	2.66	120.16	115.93
6	I	1004	MD1	C15-N17-C17	2.66	120.16	115.93
5	C	1003	MGD	PA-O3B-PB	-2.63	123.79	132.83
6	C	1004	MD1	C15-N17-C17	2.63	120.11	115.93
5	K	1003	MGD	C5-C6-N1	-2.62	119.84	123.43
5	A	1003	MGD	C17-N18-C19	2.62	120.09	115.93
5	K	1003	MGD	C17-N18-C19	2.59	120.04	115.93
5	E	1003	MGD	C19-N20-C21	2.57	120.30	114.54
5	A	1003	MGD	C19-N20-C21	2.56	120.28	114.54
5	C	1003	MGD	C19-N20-C21	2.56	120.28	114.54
5	A	1003	MGD	C5-C6-N1	-2.56	119.93	123.43
5	G	1003	MGD	C19-N20-C21	2.55	120.26	114.54
5	K	1003	MGD	C19-N20-C21	2.53	120.22	114.54
5	K	1003	MGD	PA-O3B-PB	-2.53	124.15	132.83
5	G	1003	MGD	PA-O3B-PB	-2.52	124.18	132.83
5	I	1003	MGD	C5-C6-N1	-2.51	120.00	123.43
5	I	1003	MGD	C17-C16-N15	2.48	121.20	119.12
5	E	1003	MGD	O4'-C1'-C2'	-2.48	103.31	106.93
5	A	1003	MGD	PA-O3B-PB	-2.48	124.33	132.83
5	G	1003	MGD	C5-C6-N1	-2.46	120.07	123.43
5	K	1003	MGD	C6-N1-C2	2.46	119.84	115.93
5	G	1003	MGD	C16-N15-C14	-2.46	111.09	120.00
5	E	1003	MGD	C5-C6-N1	-2.44	120.09	123.43
5	C	1003	MGD	C5-C6-N1	-2.44	120.10	123.43
5	A	1003	MGD	C6-N1-C2	2.40	119.74	115.93
5	I	1003	MGD	C6-N1-C2	2.36	119.68	115.93
5	E	1003	MGD	PA-O3B-PB	-2.36	124.72	132.83
5	G	1003	MGD	C6-N1-C2	2.36	119.68	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1003	MGD	C6-N1-C2	2.35	119.66	115.93
5	C	1003	MGD	C6-N1-C2	2.34	119.64	115.93
5	I	1003	MGD	C16-C21-N22	2.32	120.25	118.13
5	G	1003	MGD	O4'-C1'-C2'	-2.32	103.54	106.93
5	E	1003	MGD	C16-N15-C14	-2.31	111.60	120.00
5	C	1003	MGD	C16-N15-C14	-2.25	111.83	120.00
5	A	1003	MGD	C3'-C2'-C1'	2.24	104.35	100.98
5	I	1003	MGD	PA-O3B-PB	-2.24	125.14	132.83
5	A	1003	MGD	C2'-C3'-C4'	2.22	106.95	102.64
5	G	1003	MGD	C2'-C3'-C4'	2.17	106.86	102.64
5	A	1003	MGD	C16-N15-C14	-2.13	112.25	120.00
5	K	1003	MGD	C16-N15-C14	-2.13	112.26	120.00
5	K	1003	MGD	C2'-C3'-C4'	2.12	106.76	102.64
5	I	1003	MGD	C19-N20-C21	2.10	119.25	114.54
6	C	1004	MD1	O6-C6-N1	-2.09	119.88	122.69
6	A	1004	MD1	O6-C6-N1	-2.07	119.91	122.69
5	C	1003	MGD	O4'-C1'-C2'	-2.06	103.92	106.93
6	G	1004	MD1	O6-C6-N1	-2.03	119.97	122.69
6	I	1004	MD1	O6-C6-N1	-2.02	119.98	122.69
6	K	1004	MD1	O6-C6-N1	-2.00	120.00	122.69
5	E	1003	MGD	C2'-C3'-C4'	2.00	106.53	102.64

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1003	MGD	C5'-O5'-PB-O1B
5	E	1003	MGD	O3A-C10-C11-O11
6	C	1004	MD1	PB-O3B-PA-O5'
6	C	1004	MD1	C5'-O5'-PA-O1A
6	C	1004	MD1	O4'-C4'-C5'-O5'
6	A	1004	MD1	C10-O3A-PB-O1B
5	C	1003	MGD	C5'-O5'-PB-O3B
5	C	1003	MGD	O3A-C10-C11-O11
6	K	1004	MD1	C5'-O5'-PA-O1A
6	G	1004	MD1	C10-O3A-PB-O1B
6	G	1004	MD1	C10-O3A-PB-O2B
6	G	1004	MD1	C2'-C1'-N9-C8
6	I	1004	MD1	PB-O3B-PA-O5'
6	I	1004	MD1	C5'-O5'-PA-O1A
6	K	1004	MD1	O4'-C4'-C5'-O5'
6	K	1004	MD1	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	I	1004	MD1	O4'-C4'-C5'-O5'
6	I	1004	MD1	C3'-C4'-C5'-O5'
6	E	1004	MD1	O4'-C4'-C5'-O5'
6	C	1004	MD1	C3'-C4'-C5'-O5'
6	E	1004	MD1	C3'-C4'-C5'-O5'
7	C	1006	EDO	O1-C1-C2-O2
7	C	1007	EDO	O1-C1-C2-O2
5	C	1003	MGD	O4'-C4'-C5'-O5'
5	C	1003	MGD	C3'-C4'-C5'-O5'
5	A	1003	MGD	O3A-C10-C11-O11
5	G	1003	MGD	O3A-C10-C11-O11
5	K	1003	MGD	O3A-C10-C11-O11
6	K	1004	MD1	PB-O3B-PA-O5'
6	C	1004	MD1	C5'-O5'-PA-O3B
6	A	1004	MD1	C10-O3A-PB-O3B
6	K	1004	MD1	C5'-O5'-PA-O3B
6	G	1004	MD1	C10-O3A-PB-O3B
6	I	1004	MD1	C5'-O5'-PA-O3B
6	C	1004	MD1	PA-O3B-PB-O2B
6	K	1004	MD1	PA-O3B-PB-O2B
6	C	1004	MD1	C5'-O5'-PA-O2A
6	A	1004	MD1	C10-O3A-PB-O2B
5	C	1003	MGD	C5'-O5'-PB-O1B
5	C	1003	MGD	C5'-O5'-PB-O2B
6	K	1004	MD1	C5'-O5'-PA-O2A
6	I	1004	MD1	C5'-O5'-PA-O2A
7	A	1005	EDO	O1-C1-C2-O2
7	C	1005	EDO	O1-C1-C2-O2
6	A	1004	MD1	O4'-C4'-C5'-O5'
6	G	1004	MD1	O4'-C4'-C5'-O5'
5	I	1003	MGD	C11-C10-O3A-PA
5	A	1003	MGD	C5'-O5'-PB-O1B
6	C	1004	MD1	C2'-C1'-N9-C4
6	A	1004	MD1	C2'-C1'-N9-C4
6	K	1004	MD1	C2'-C1'-N9-C4
6	I	1004	MD1	C2'-C1'-N9-C4
6	E	1004	MD1	C2'-C1'-N9-C4
5	G	1003	MGD	C11-C10-O3A-PA

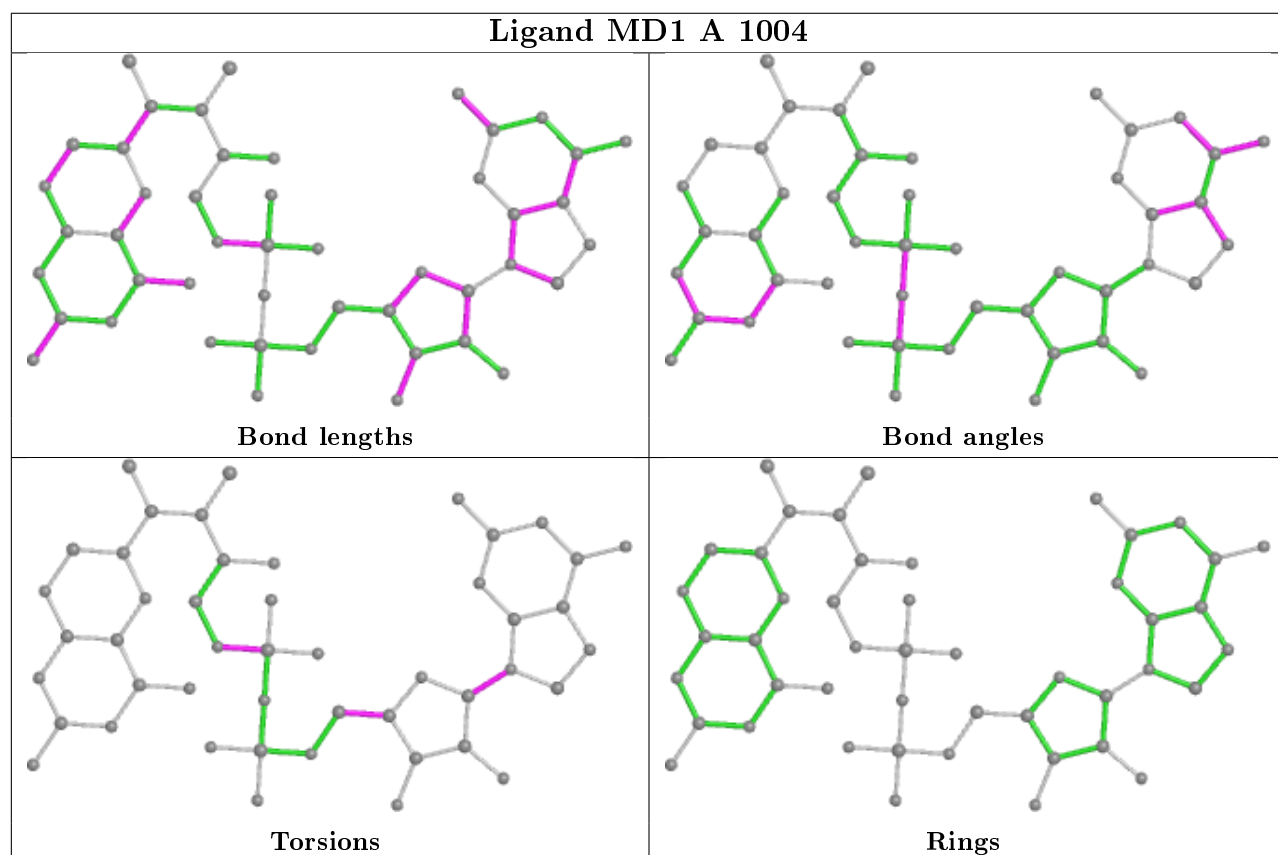
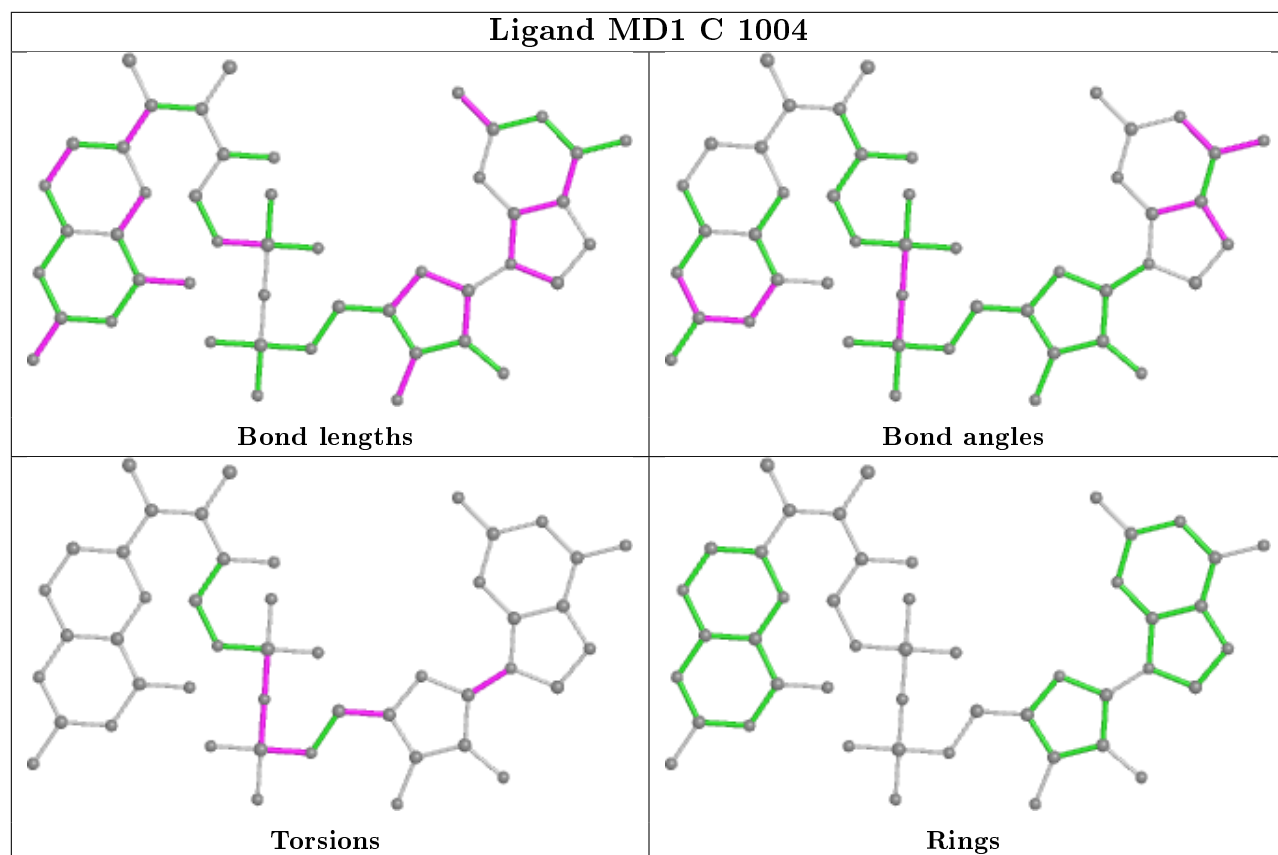
There are no ring outliers.

32 monomers are involved in 58 short contacts:

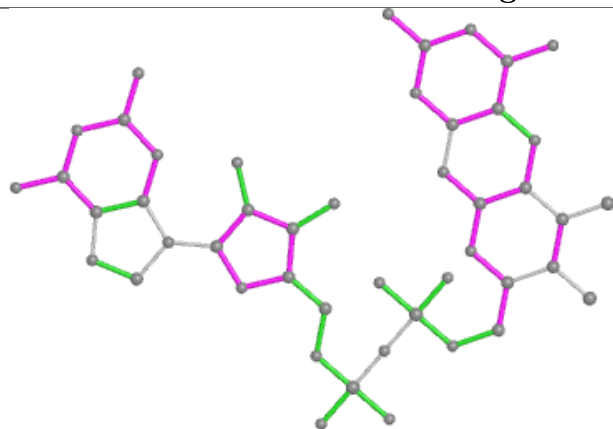
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	SF4	1	0
3	F	405	SF4	1	0
7	I	1005	EDO	1	0
7	C	1007	EDO	2	0
3	D	404	SF4	1	0
6	C	1004	MD1	2	0
6	A	1004	MD1	1	0
3	L	404	SF4	1	0
5	E	1003	MGD	4	0
8	A	1008	GOL	1	0
7	I	1006	EDO	2	0
7	H	406	EDO	1	0
5	C	1003	MGD	1	0
7	G	1007	EDO	1	0
6	K	1004	MD1	3	0
6	G	1004	MD1	6	0
3	K	1001	SF4	2	0
7	A	1005	EDO	1	0
8	E	1006	GOL	1	0
7	G	1008	EDO	1	0
7	H	405	EDO	2	0
5	A	1003	MGD	2	0
5	G	1003	MGD	3	0
7	E	1005	EDO	1	0
7	G	1005	EDO	1	0
7	E	1007	EDO	1	0
5	K	1003	MGD	1	0
6	I	1004	MD1	2	0
3	I	1001	SF4	2	0
6	E	1004	MD1	1	0
7	F	401	EDO	1	0
5	I	1003	MGD	7	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

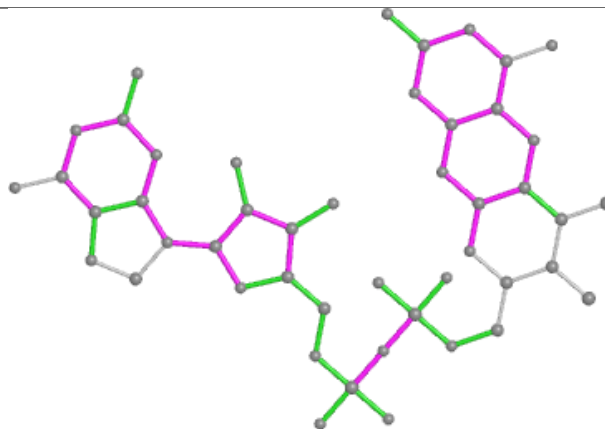
equivalents in the CSD to analyse the geometry.



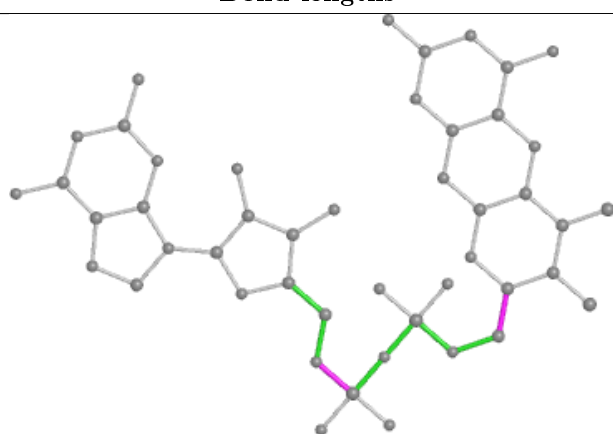
Ligand MGD E 1003



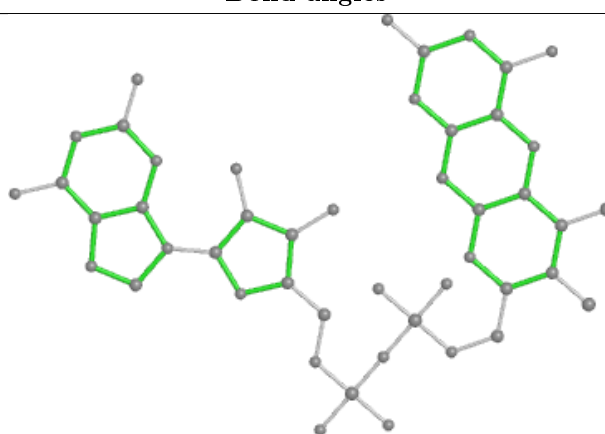
Bond lengths



Bond angles

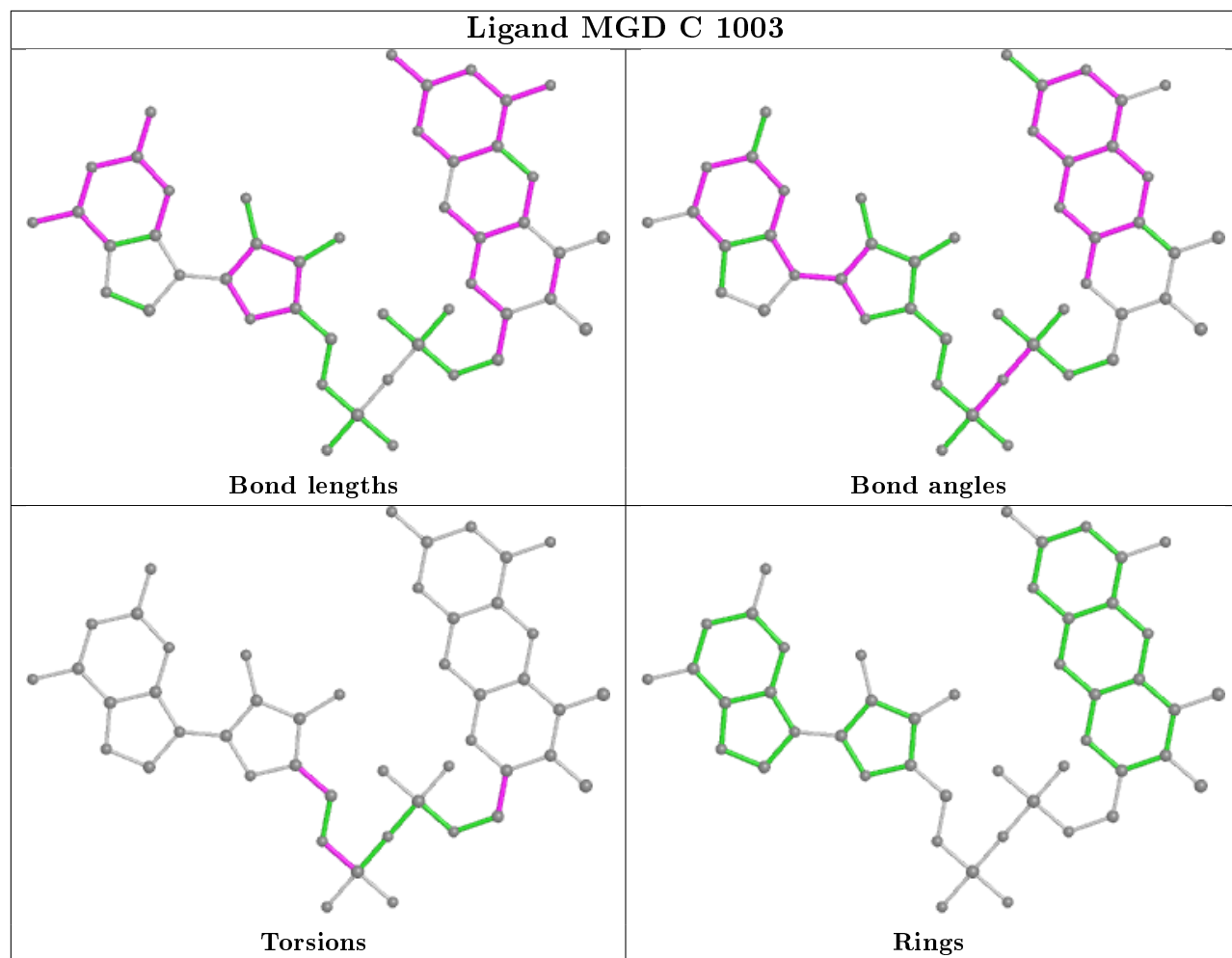


Torsions

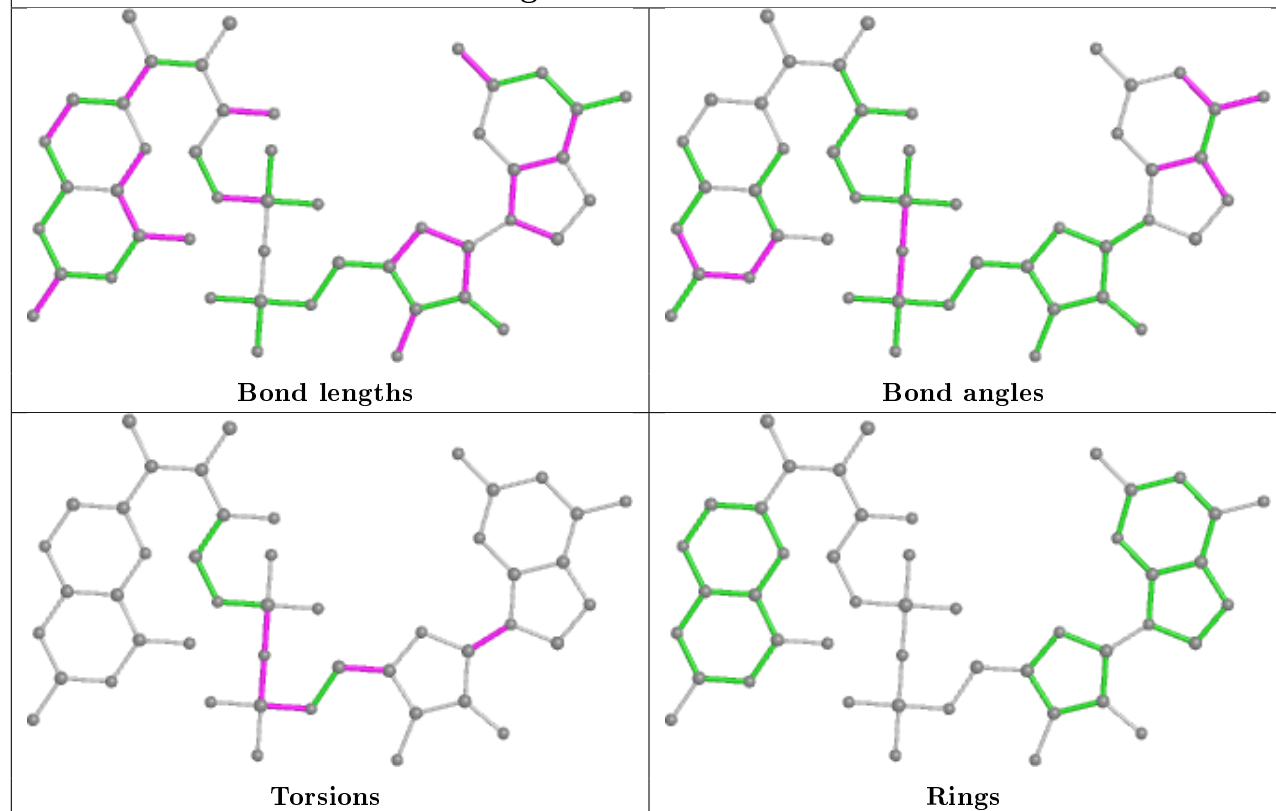


Rings

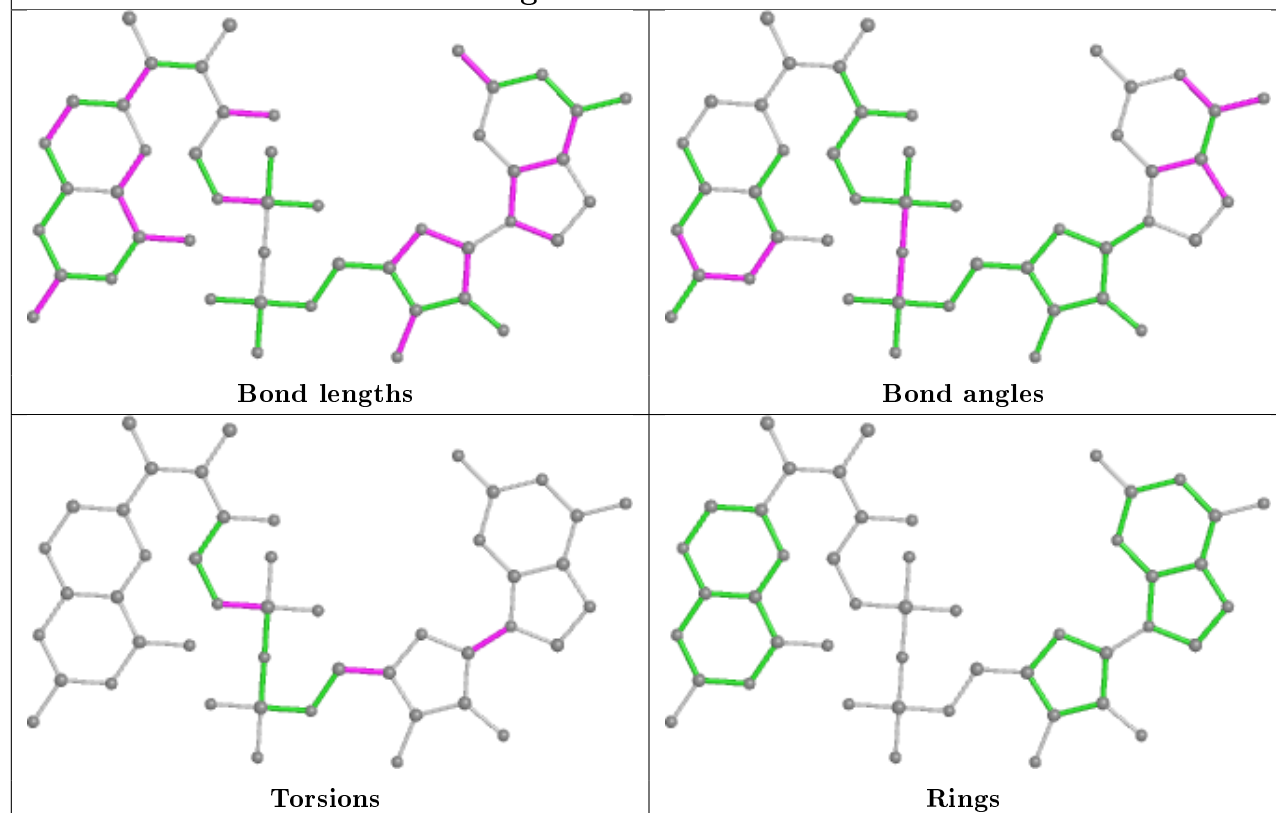
Ligand MGD C 1003



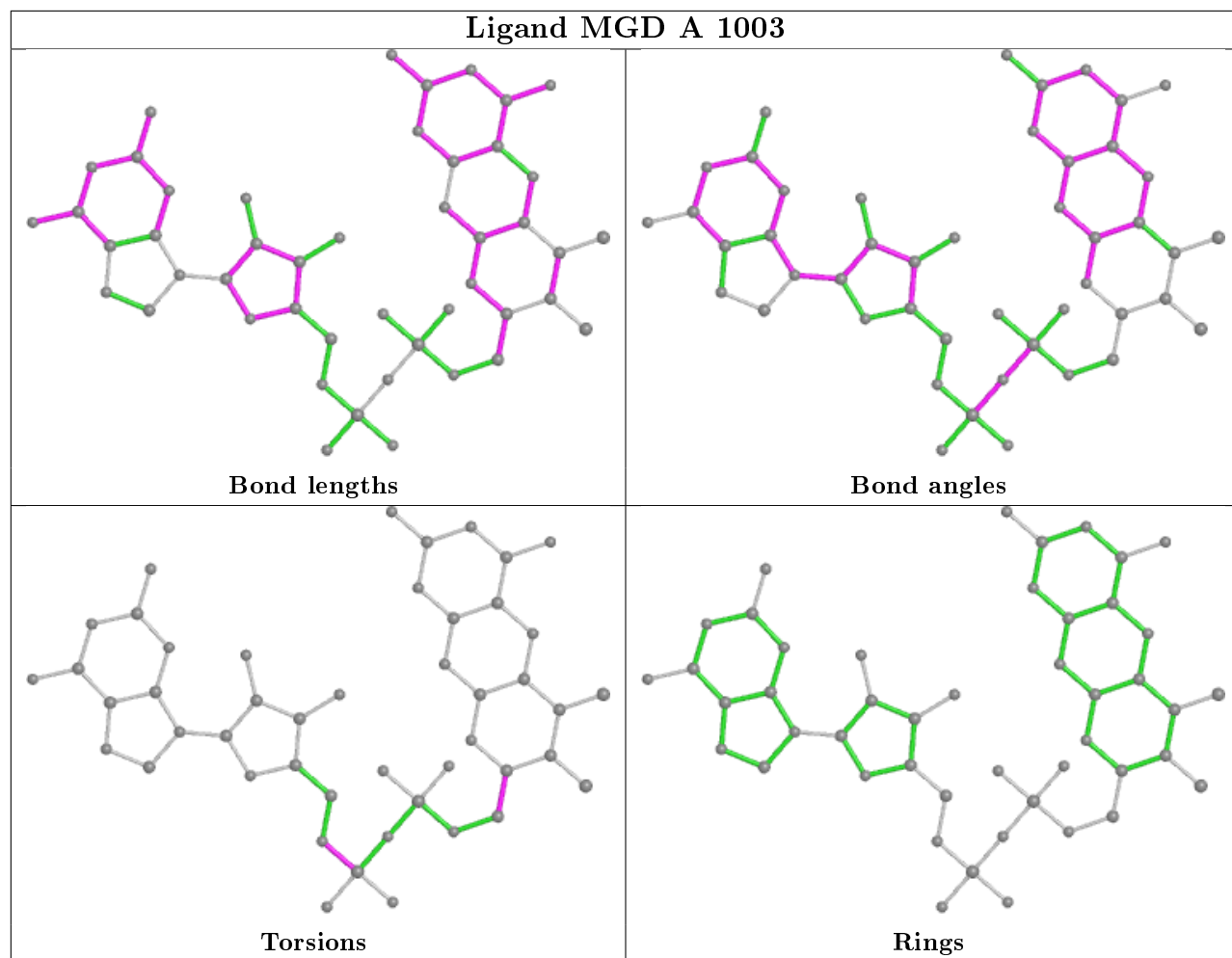
Ligand MD1 K 1004

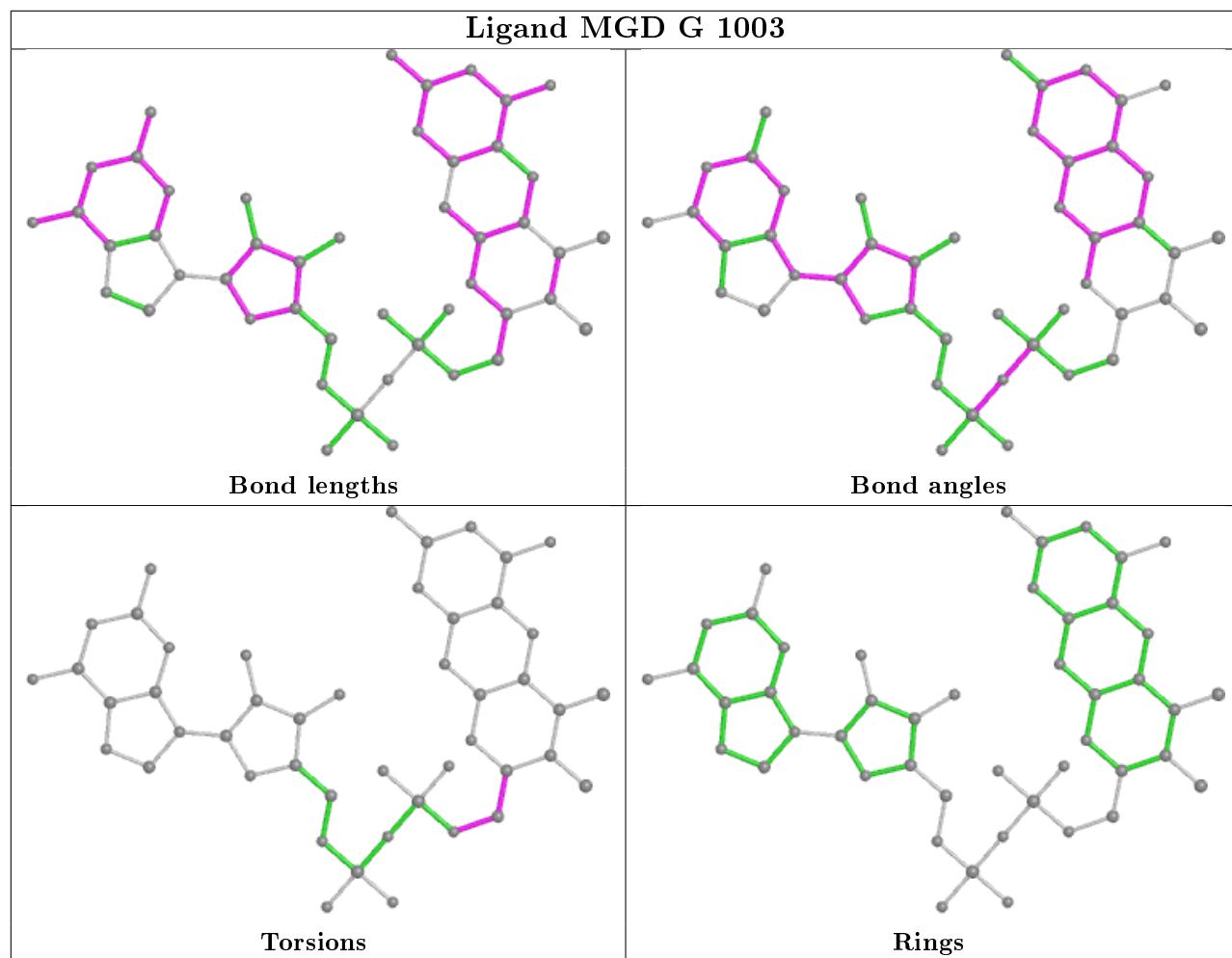


Ligand MD1 G 1004

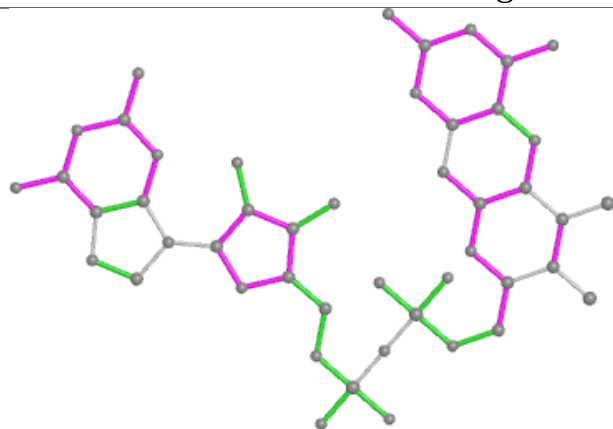


Ligand MGD A 1003

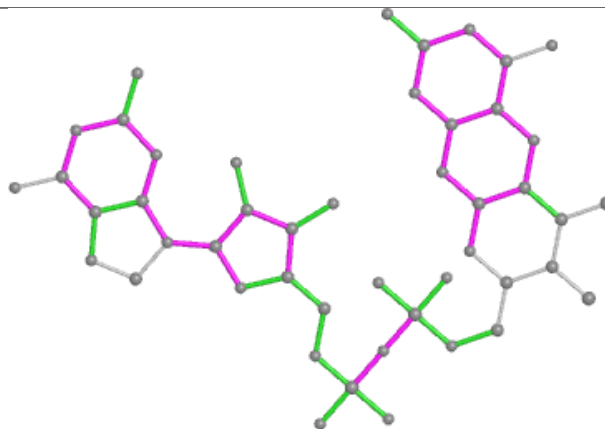




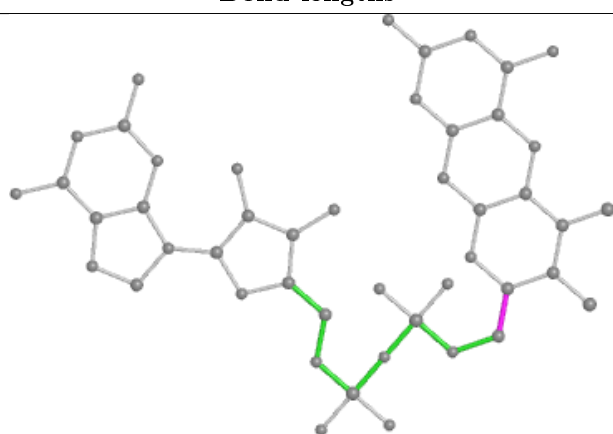
Ligand MGD K 1003



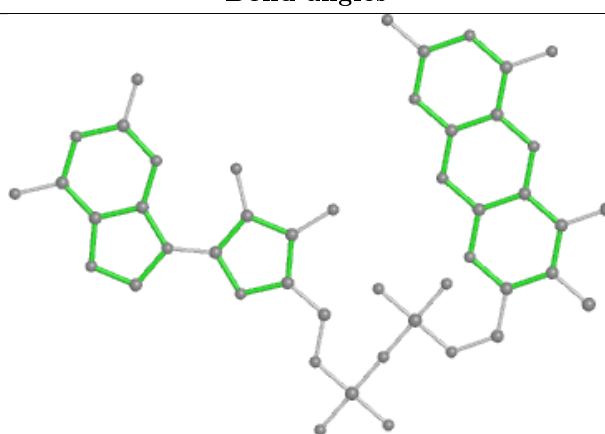
Bond lengths



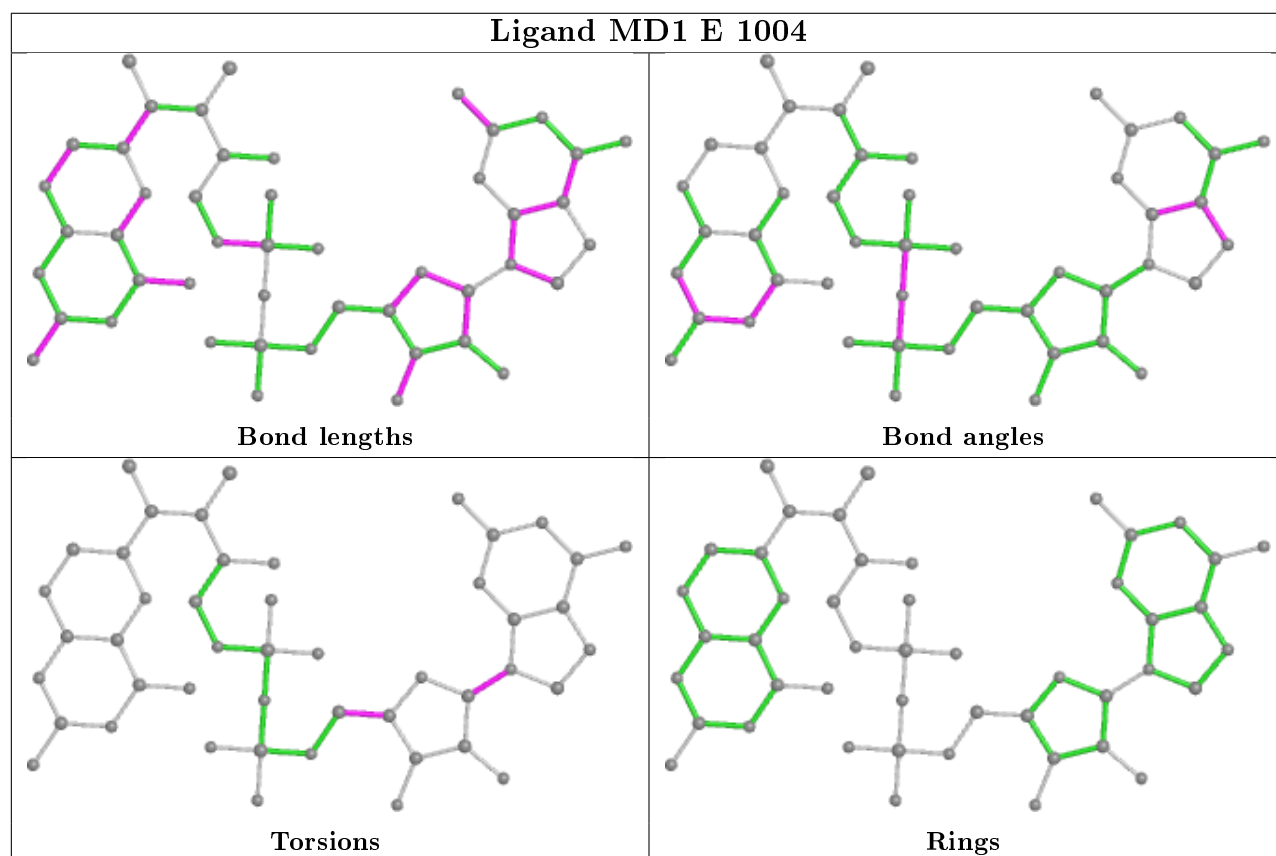
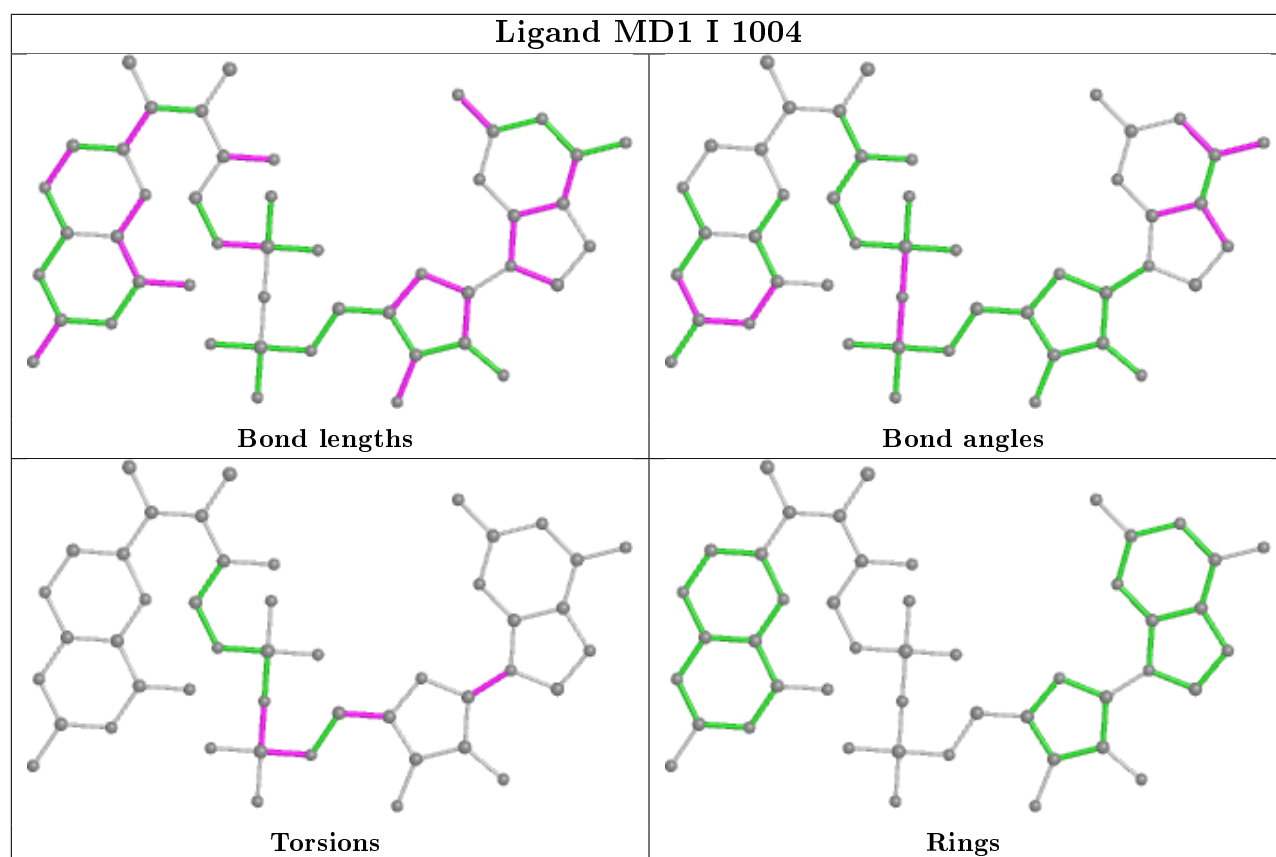
Bond angles

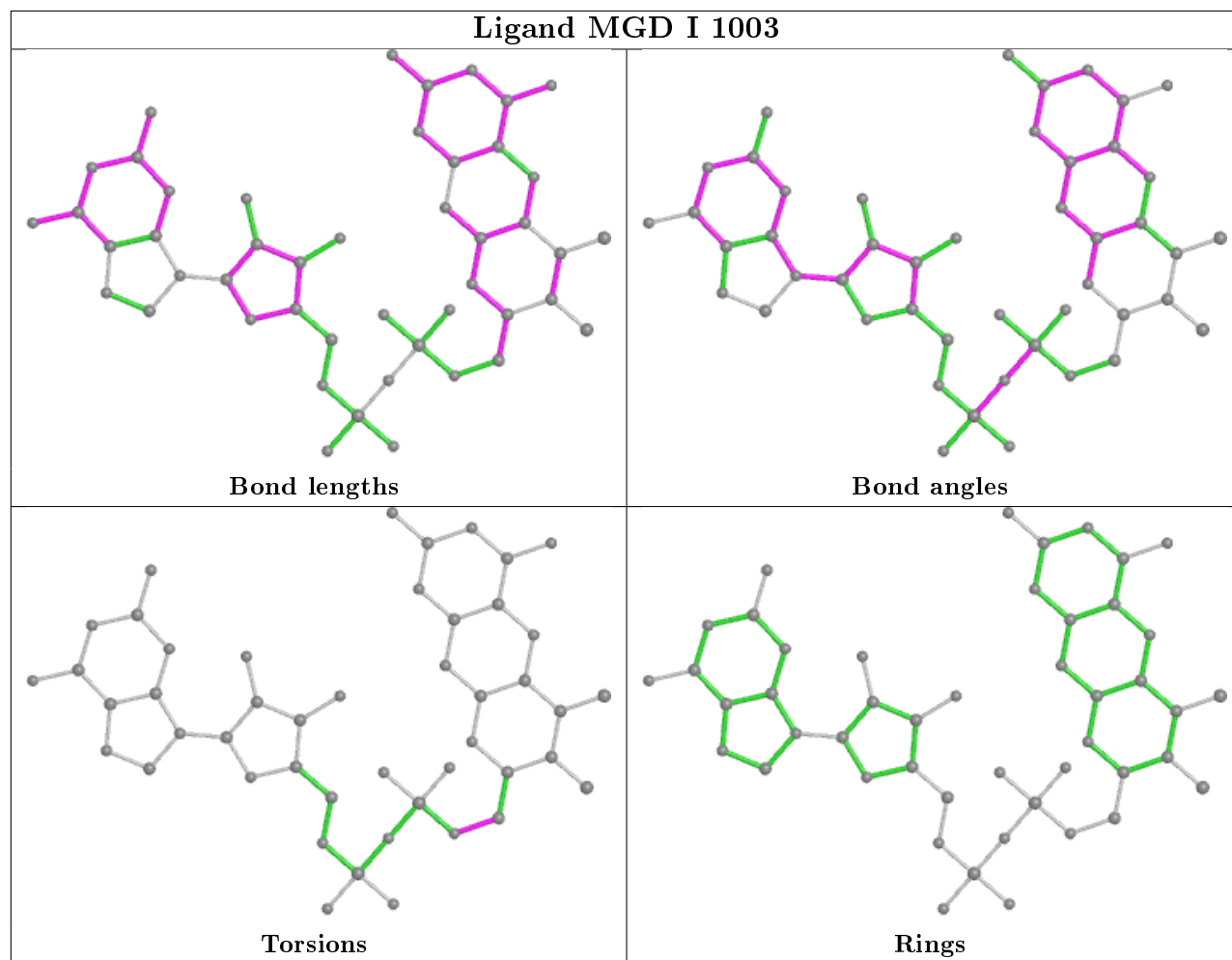


Torsions



Rings





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	895/899 (99%)	-0.58	4 (0%) 92 91	20, 32, 47, 80	0
1	C	895/899 (99%)	-0.62	4 (0%) 92 91	20, 30, 41, 76	0
1	E	895/899 (99%)	-0.57	4 (0%) 92 91	22, 32, 44, 81	0
1	G	895/899 (99%)	-0.44	5 (0%) 89 88	20, 37, 53, 76	0
1	I	895/899 (99%)	-0.16	15 (1%) 70 68	25, 46, 66, 90	0
1	K	895/899 (99%)	-0.28	13 (1%) 73 72	25, 43, 62, 91	0
2	B	329/333 (98%)	-0.51	0 100 100	21, 34, 47, 66	0
2	D	329/333 (98%)	-0.58	3 (0%) 84 82	22, 33, 44, 72	0
2	F	329/333 (98%)	-0.55	2 (0%) 89 88	23, 35, 49, 62	0
2	H	329/333 (98%)	-0.13	2 (0%) 89 88	27, 46, 63, 78	0
2	J	329/333 (98%)	0.02	7 (2%) 63 61	26, 53, 65, 79	0
2	L	329/333 (98%)	-0.33	3 (0%) 84 82	27, 44, 55, 72	0
All	All	7344/7392 (99%)	-0.41	62 (0%) 86 84	20, 36, 58, 91	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	6	SER	7.9
1	E	5	ILE	7.7
1	I	7	GLY	6.6
1	K	367	GLY	6.6
1	A	5	ILE	6.2
1	K	5	ILE	5.7
1	A	6	SER	5.4
1	I	8	ALA	5.3
1	K	7	GLY	5.3
2	D	6	LYS	5.0
1	G	7	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	K	8	ALA	4.6
1	C	5	ILE	4.6
2	F	6	LYS	4.5
1	I	317	PRO	4.3
2	J	5	MET	4.3
2	L	7	ALA	3.8
1	A	7	GLY	3.8
1	I	6	SER	3.6
1	I	413	ALA	3.6
1	E	7	GLY	3.6
2	D	5	MET	3.5
1	K	295	VAL	3.4
2	F	5	MET	3.4
2	J	312	ALA	3.4
2	H	229	VAL	3.4
1	E	6	SER	3.2
1	A	8	ALA	3.1
1	G	8	ALA	3.1
2	J	229	VAL	3.1
1	I	309	ALA	3.0
2	J	319	LEU	3.0
1	K	364	LEU	2.9
1	K	366	ASP	2.8
1	I	318	LYS	2.8
1	I	5	ILE	2.8
1	C	8	ALA	2.7
1	I	345	GLY	2.7
1	I	356	LEU	2.6
1	C	6	SER	2.6
1	G	6	SER	2.6
1	K	9	PHE	2.6
1	I	715	VAL	2.5
2	D	7	ALA	2.5
2	J	315	LEU	2.4
2	L	6	LYS	2.4
1	K	13	GLY	2.3
1	K	299	GLY	2.3
1	E	367	GLY	2.3
1	I	369	THR	2.2
1	I	349	LEU	2.2
1	K	458	ILE	2.2
1	I	368	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	209	ILE	2.2
1	G	9	PHE	2.1
2	J	6	LYS	2.1
1	C	7	GLY	2.1
2	H	234	TYR	2.1
1	G	5	ILE	2.1
2	J	179	SER	2.1
2	L	161	GLY	2.1
1	K	289	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	F	401	4/4	0.77	0.50	47,50,55,56	0
7	EDO	K	1005	4/4	0.78	0.25	36,41,42,45	0
7	EDO	H	406	4/4	0.81	0.31	56,57,59,67	0
7	EDO	C	1005	4/4	0.82	0.24	34,38,39,39	0
7	EDO	I	1005	4/4	0.84	0.24	46,50,60,60	0
7	EDO	G	1006	4/4	0.84	0.28	50,51,51,53	0
8	GOL	E	1006	6/6	0.85	0.22	35,36,41,41	0
3	SF4	H	402	8/8	0.87	0.14	47,55,63,69	0
7	EDO	L	406	4/4	0.88	0.17	30,32,33,36	0
7	EDO	G	1005	4/4	0.89	0.15	28,32,34,40	0
7	EDO	H	405	4/4	0.89	0.22	30,33,34,37	0
7	EDO	H	407	4/4	0.89	0.14	23,26,27,30	0
7	EDO	E	1005	4/4	0.90	0.16	36,36,36,39	0
7	EDO	A	1005	4/4	0.92	0.14	23,29,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SF4	F	405	8/8	0.92	0.15	20,38,44,44	0
7	EDO	G	1007	4/4	0.93	0.15	25,26,34,36	0
3	SF4	K	1001	8/8	0.93	0.13	39,45,53,58	0
7	EDO	E	1007	4/4	0.93	0.24	42,46,46,47	0
7	EDO	D	405	4/4	0.93	0.17	35,43,48,49	0
7	EDO	K	1006	4/4	0.93	0.20	33,33,36,38	0
7	EDO	I	1006	4/4	0.93	0.13	38,40,41,43	0
8	GOL	A	1008	6/6	0.93	0.14	29,35,36,36	0
3	SF4	J	402	8/8	0.93	0.11	52,58,65,65	0
5	MGD	I	1003	47/47	0.93	0.14	37,44,49,54	0
9	F3S	L	401	7/7	0.94	0.08	45,50,52,59	0
7	EDO	A	1007	4/4	0.94	0.17	40,40,44,47	0
3	SF4	L	404	8/8	0.94	0.14	43,48,57,60	0
3	SF4	B	405	8/8	0.94	0.14	25,33,37,38	0
3	SF4	J	403	8/8	0.94	0.14	38,51,56,65	0
3	SF4	G	1001	8/8	0.94	0.14	39,43,48,51	0
7	EDO	G	1008	4/4	0.94	0.27	32,32,36,41	0
7	EDO	A	1010	4/4	0.95	0.09	28,28,30,31	0
7	EDO	A	1009	4/4	0.95	0.11	27,28,30,32	0
9	F3S	J	401	7/7	0.95	0.10	47,52,56,62	0
7	EDO	A	1006	4/4	0.95	0.10	32,33,34,39	0
7	EDO	F	406	4/4	0.95	0.15	24,26,27,29	0
7	EDO	B	406	4/4	0.95	0.13	23,24,24,27	0
3	SF4	I	1001	8/8	0.95	0.13	42,53,54,66	0
3	SF4	L	403	8/8	0.95	0.11	38,45,51,55	0
3	SF4	A	1001	8/8	0.95	0.14	24,32,42,44	0
4	MO	I	1002	1/1	0.95	0.09	73,73,73,73	0
7	EDO	C	1007	4/4	0.95	0.12	28,29,30,30	0
3	SF4	F	403	8/8	0.96	0.13	25,34,41,46	0
7	EDO	B	401	4/4	0.96	0.12	25,28,28,31	0
6	MD1	K	1004	47/47	0.96	0.11	27,34,43,46	0
3	SF4	H	404	8/8	0.96	0.14	40,47,58,58	0
7	EDO	J	405	4/4	0.96	0.13	32,39,40,44	0
3	SF4	C	1001	8/8	0.96	0.14	28,36,50,59	0
5	MGD	C	1003	47/47	0.96	0.11	22,29,35,37	0
3	SF4	D	404	8/8	0.96	0.13	23,33,41,41	0
5	MGD	K	1003	47/47	0.96	0.12	27,37,41,42	0
6	MD1	I	1004	47/47	0.96	0.12	25,37,47,49	0
7	EDO	C	1006	4/4	0.96	0.11	21,25,26,28	0
6	MD1	G	1004	47/47	0.96	0.12	20,32,36,38	0
9	F3S	H	401	7/7	0.96	0.08	53,54,62,72	0
6	MD1	A	1004	47/47	0.96	0.12	19,28,35,37	0

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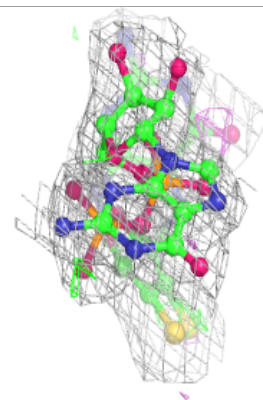
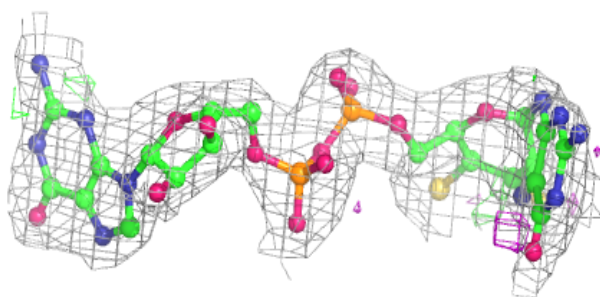
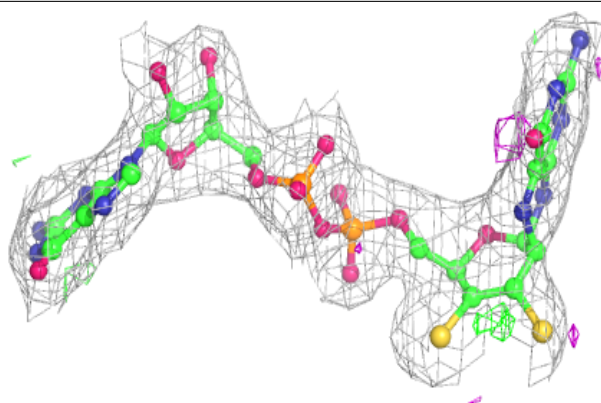
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MGD	A	1003	47/47	0.96	0.12	23,28,33,36	0
5	MGD	G	1003	47/47	0.96	0.12	23,30,34,37	0
3	SF4	L	402	8/8	0.96	0.11	36,44,55,58	0
3	SF4	J	404	8/8	0.96	0.12	47,53,60,63	0
9	F3S	F	402	7/7	0.97	0.11	37,44,50,54	0
3	SF4	D	402	8/8	0.97	0.13	26,30,38,40	0
3	SF4	H	403	8/8	0.97	0.15	39,45,47,53	0
3	SF4	D	403	8/8	0.97	0.14	24,31,35,47	0
9	F3S	D	401	7/7	0.97	0.10	31,34,39,42	0
6	MD1	C	1004	47/47	0.97	0.11	18,27,32,33	0
3	SF4	E	1001	8/8	0.97	0.12	31,33,42,49	0
6	MD1	E	1004	47/47	0.97	0.10	20,26,33,37	0
3	SF4	F	404	8/8	0.97	0.14	26,39,44,47	0
3	SF4	B	403	8/8	0.97	0.14	24,35,40,41	0
5	MGD	E	1003	47/47	0.97	0.13	23,29,35,37	0
4	MO	C	1002	1/1	0.98	0.07	52,52,52,52	0
4	MO	G	1002	1/1	0.98	0.06	50,50,50,50	0
9	F3S	B	402	7/7	0.98	0.12	31,39,45,48	0
7	EDO	L	405	4/4	0.98	0.10	30,32,32,35	0
3	SF4	B	404	8/8	0.98	0.15	29,37,40,43	0
4	MO	A	1002	1/1	0.98	0.07	49,49,49,49	0
4	MO	E	1002	1/1	0.99	0.06	51,51,51,51	0
4	MO	K	1002	1/1	0.99	0.08	53,53,53,53	0

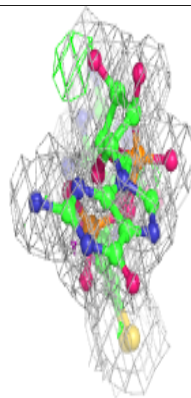
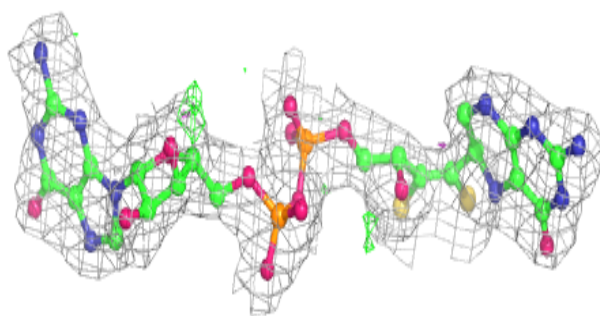
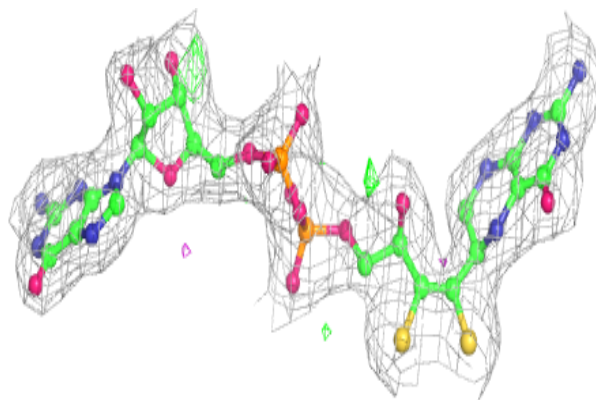
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD I 1003:

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

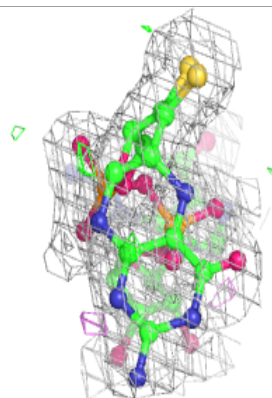
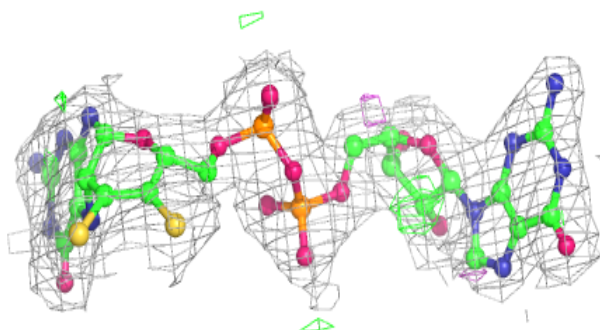
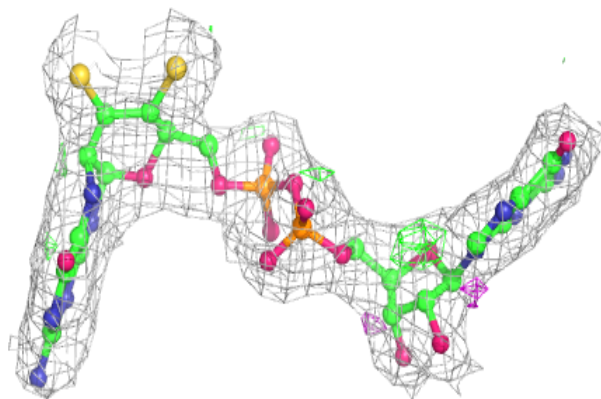
**Electron density around MD1 K 1004:**

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

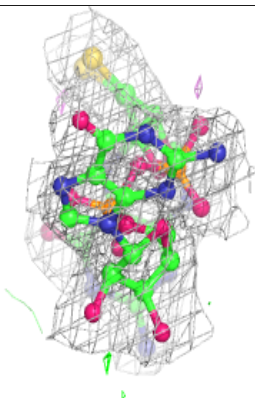
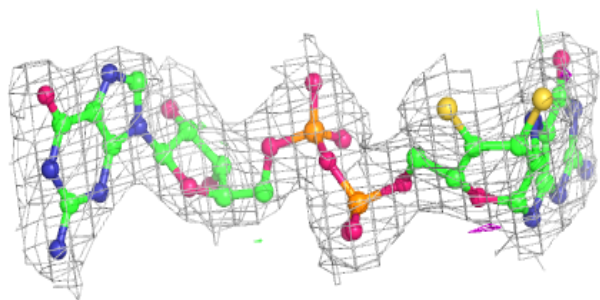
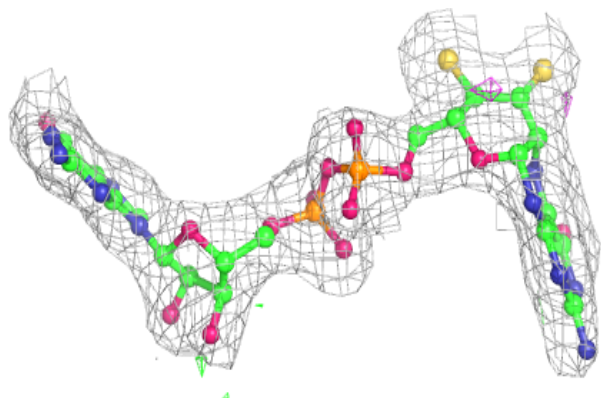


Electron density around MGD C 1003:

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

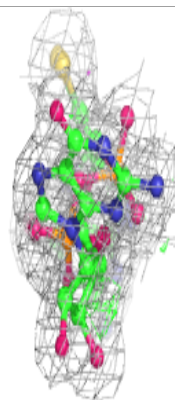
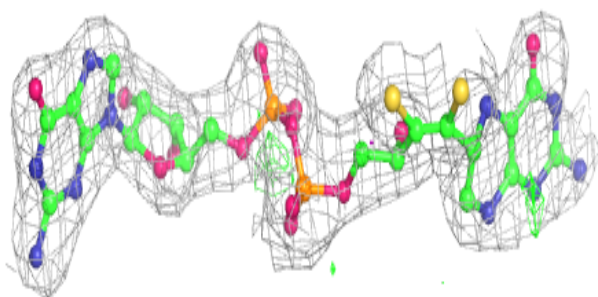
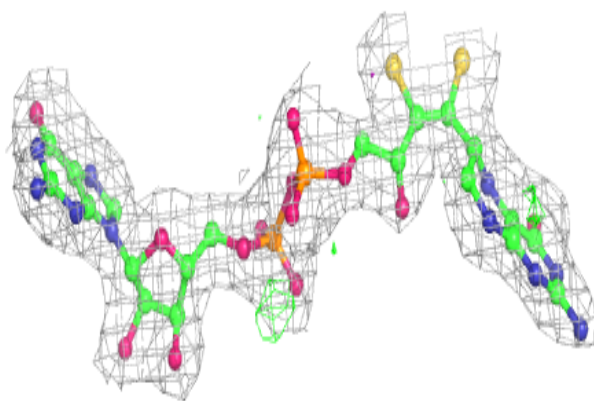
**Electron density around MGD K 1003:**

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

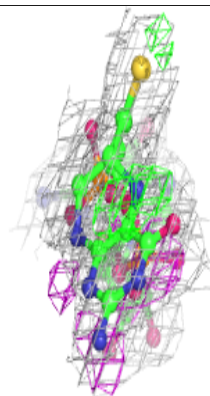
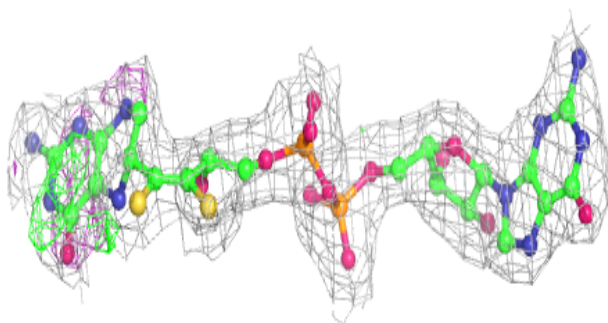
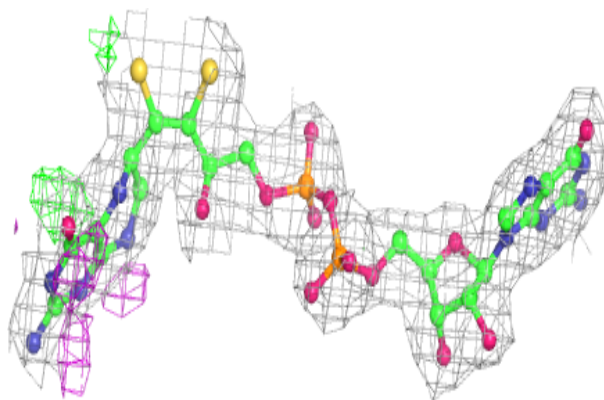


Electron density around MD1 I 1004:

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

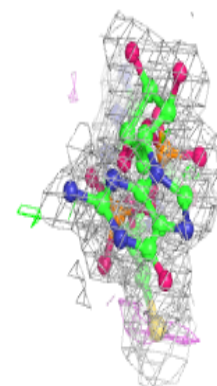
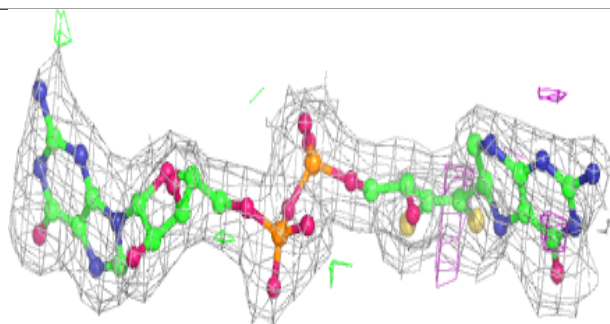
**Electron density around MD1 G 1004:**

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

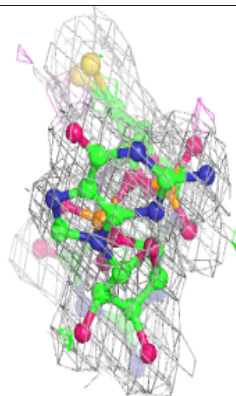
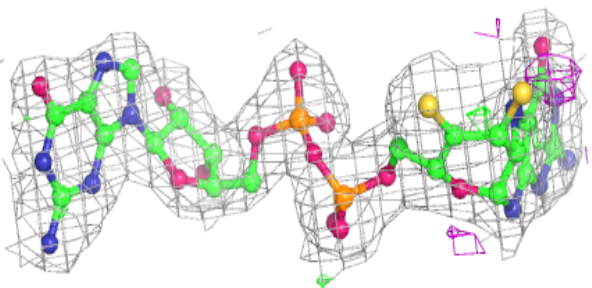
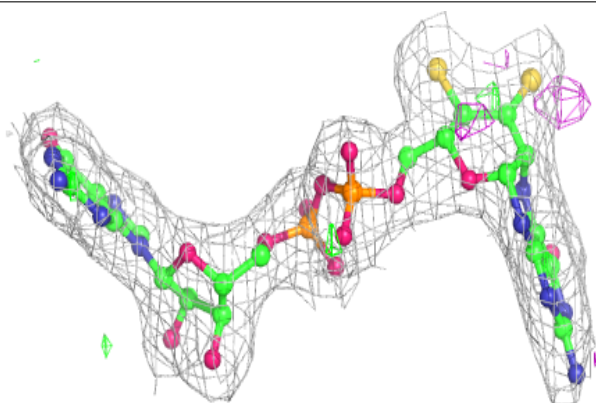


Electron density around MD1 A 1004:

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

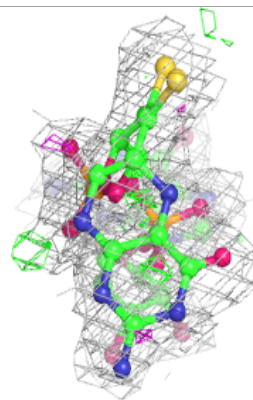
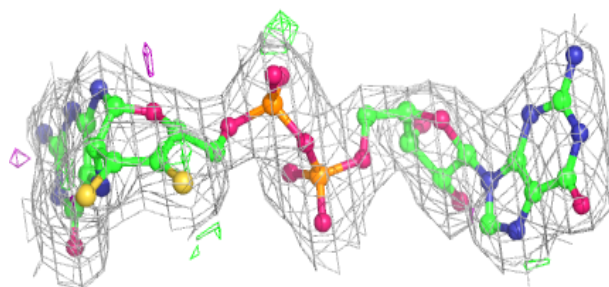
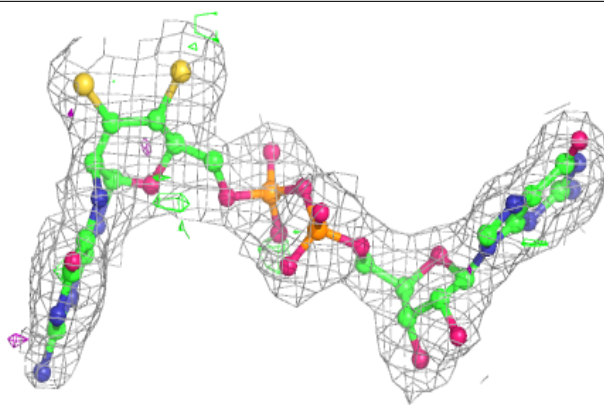
**Electron density around MGD A 1003:**

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

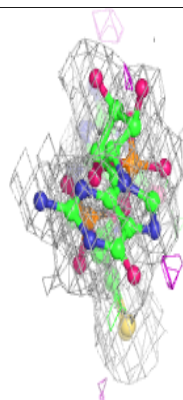
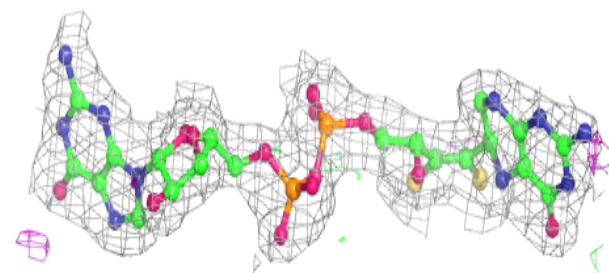
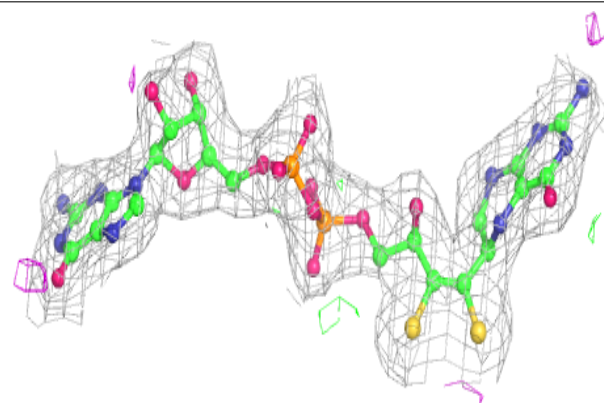


Electron density around MGD G 1003:

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

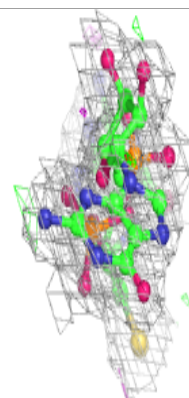
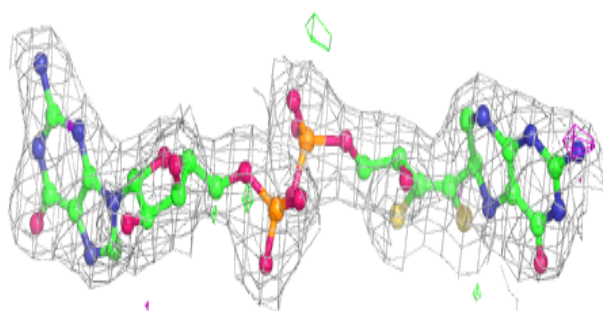
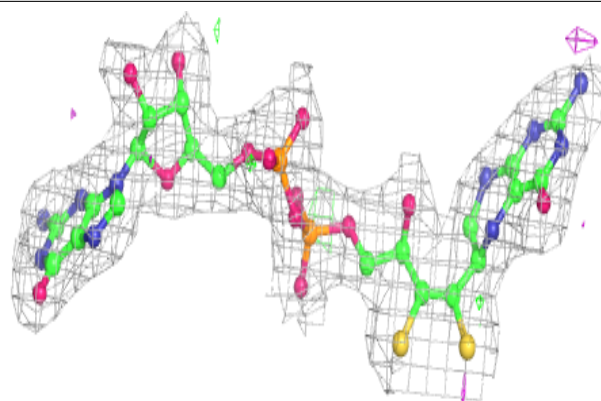
**Electron density around MD1 C 1004:**

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

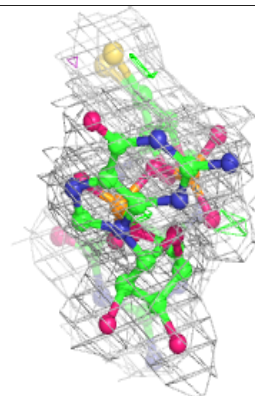
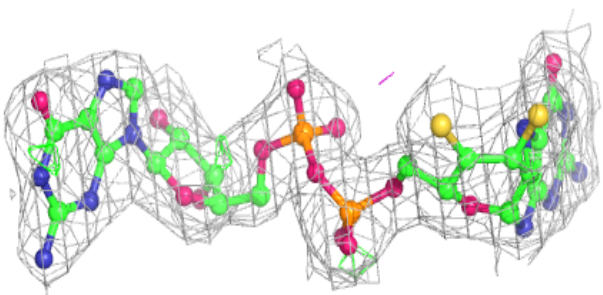
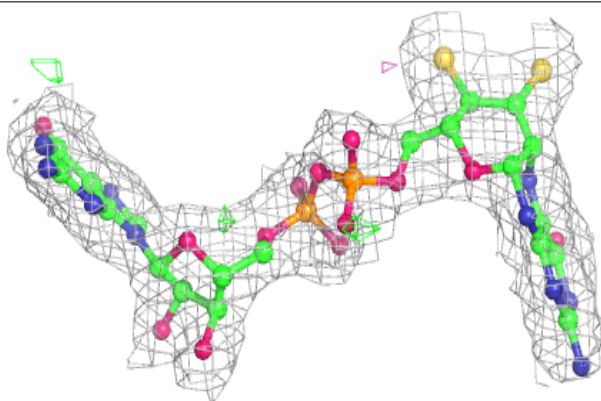


Electron density around MD1 E 1004:

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

**Electron density around MGD E 1003:**

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



6.5 Other polymers

There are no such residues in this entry.