



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:29 am BST

PDB ID : 3GYX
Title : Crystal structure of adenylylsulfate reductase from *Desulfovibrio gigas*
Authors : Chiang, Y.-L.; Hsieh, Y.-C.; Liu, E.-H.; Liu, M.-Y.; Chen, C.-J.
Deposited on : 2009-04-06
Resolution : 3.20 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

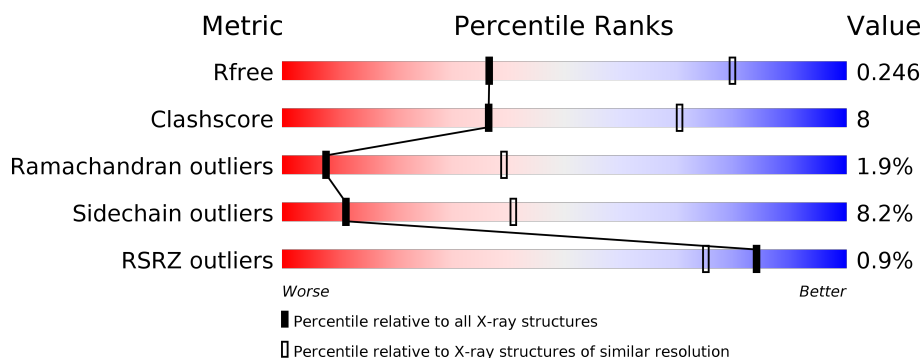
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	662	<div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	C	662	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	E	662	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	G	662	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	I	662	<div> <div>%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	K	662	<div> <div>74%</div> <div>23%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	166	<div><div></div><div>3%</div><div>82%</div><div>17%</div><div></div></div>
2	D	166	<div><div></div><div>%</div><div>85%</div><div>13%</div><div></div></div>
2	F	166	<div><div></div><div>4%</div><div>80%</div><div>17%</div><div></div></div>
2	H	166	<div><div></div><div>5%</div><div>83%</div><div>17%</div><div></div></div>
2	J	166	<div><div></div><div>2%</div><div>80%</div><div>17%</div><div></div></div>
2	L	166	<div><div></div><div>2%</div><div>79%</div><div>19%</div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39537 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 Adenylylsulfate Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5232	3320	914	957	41			
1	C	662	Total	C	N	O	S	0	0	0
			5232	3320	914	957	41			
1	E	662	Total	C	N	O	S	0	0	0
			5232	3320	914	957	41			
1	G	662	Total	C	N	O	S	0	0	0
			5232	3320	914	957	41			
1	I	662	Total	C	N	O	S	0	0	0
			5232	3320	914	957	41			
1	K	662	Total	C	N	O	S	0	0	0
			5232	3320	914	957	41			

- Molecule 2 is a protein called Adenylylsulfate Reductase.

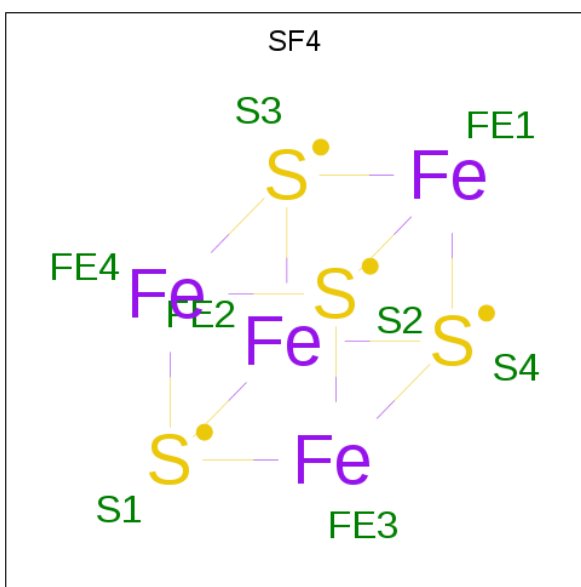
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1277	806	209	246	16			
2	D	166	Total	C	N	O	S	0	0	0
			1277	806	209	246	16			
2	F	166	Total	C	N	O	S	0	0	0
			1277	806	209	246	16			
2	H	166	Total	C	N	O	S	0	0	0
			1277	806	209	246	16			
2	J	166	Total	C	N	O	S	0	0	0
			1277	806	209	246	16			
2	L	166	Total	C	N	O	S	0	0	0
			1277	806	209	246	16			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	H	1	Total	Fe	S	0	0
			8	4	4		
4	H	1	Total	Fe	S	0	0
			8	4	4		
4	J	1	Total	Fe	S	0	0
			8	4	4		
4	J	1	Total	Fe	S	0	0
			8	4	4		
4	L	1	Total	Fe	S	0	0
			8	4	4		
4	L	1	Total	Fe	S	0	0
			8	4	4		

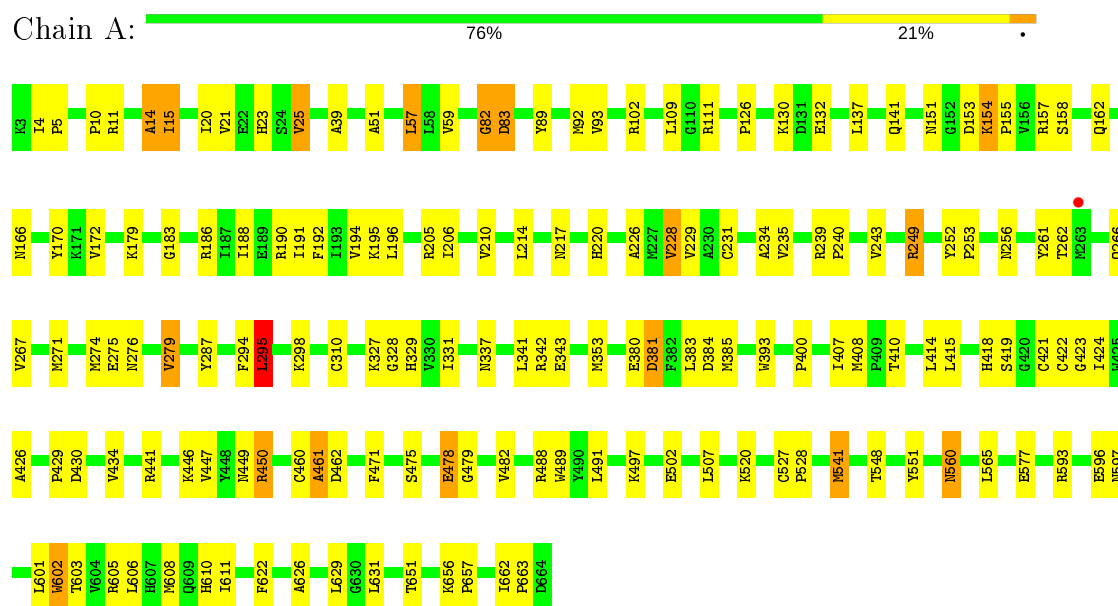
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	1	Total 1	O 1	0	0
5	C	14	Total 14	O 14	0	0
5	D	3	Total 3	O 3	0	0
5	E	12	Total 12	O 12	0	0
5	F	3	Total 3	O 3	0	0
5	G	6	Total 6	O 6	0	0
5	H	5	Total 5	O 5	0	0
5	I	2	Total 2	O 2	0	0
5	J	3	Total 3	O 3	0	0
5	K	7	Total 7	O 7	0	0
5	L	2	Total 2	O 2	0	0

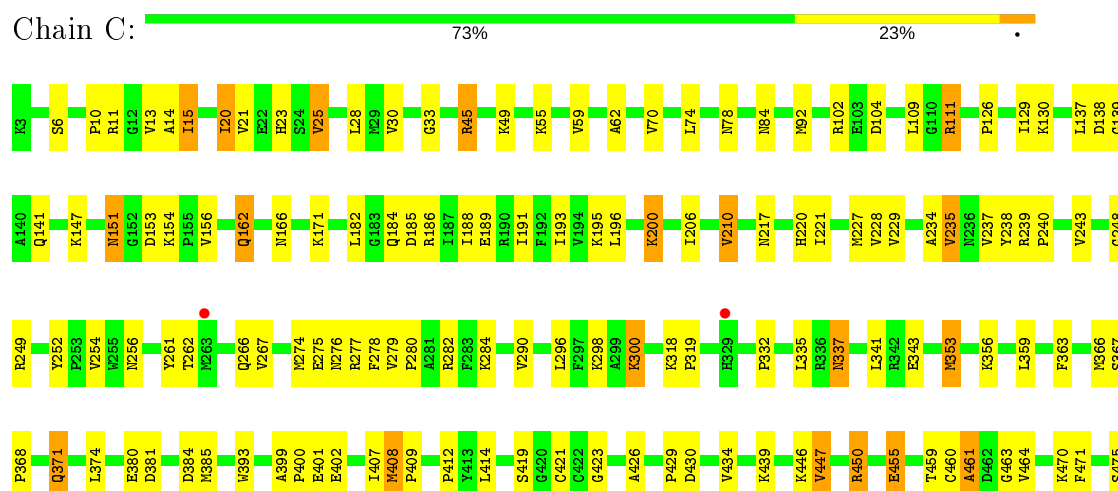
3 Residue-property plots [i](#)

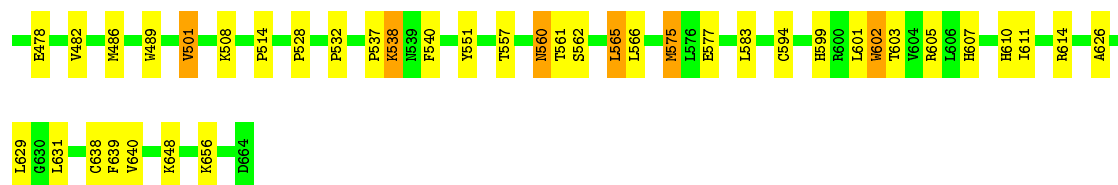
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Adenylylsulfate Reductase

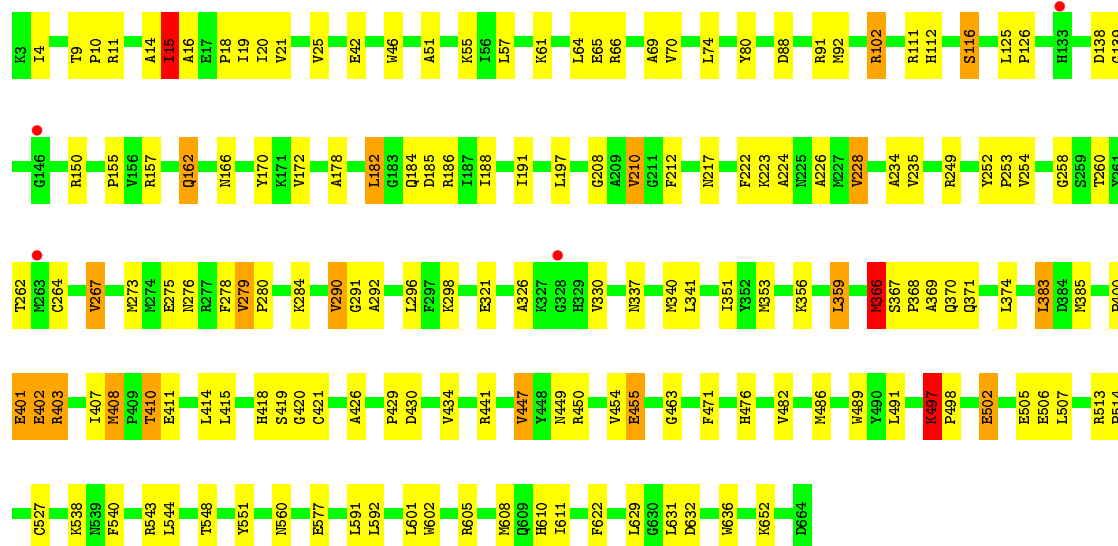
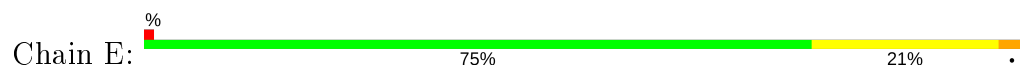


• Molecule 1: Adenylylsulfate Reductase

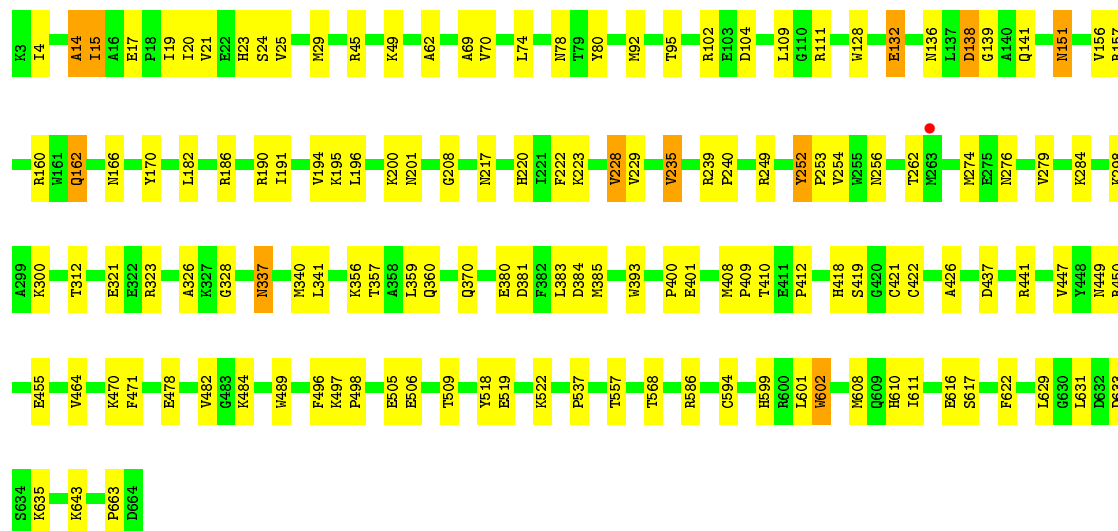




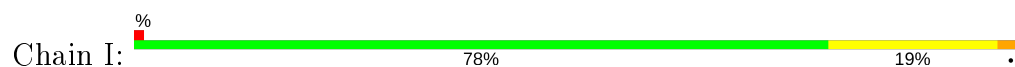
• Molecule 1: Adenylylsulfate Reductase

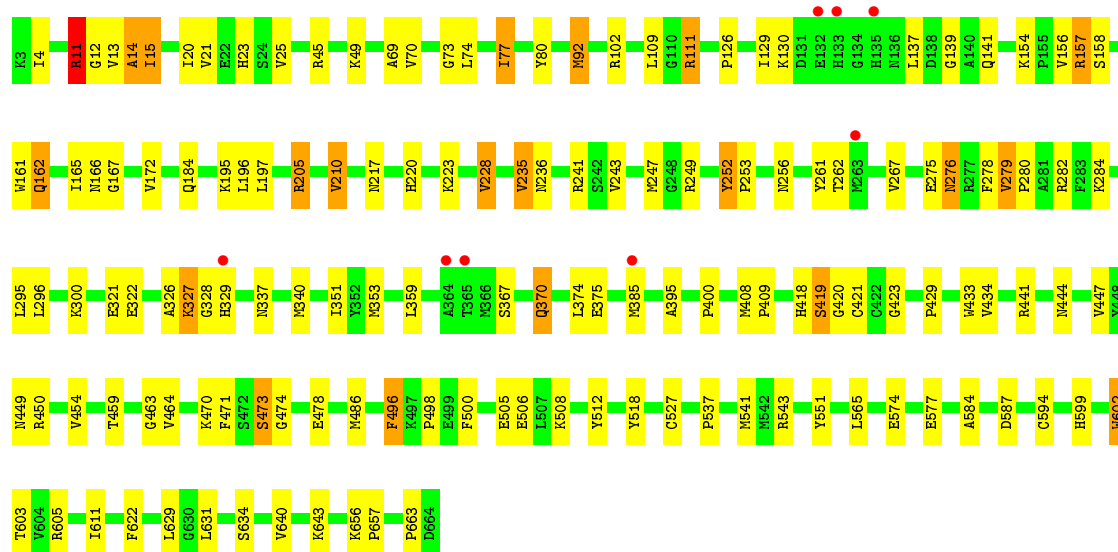


• Molecule 1: Adenylylsulfate Reductase



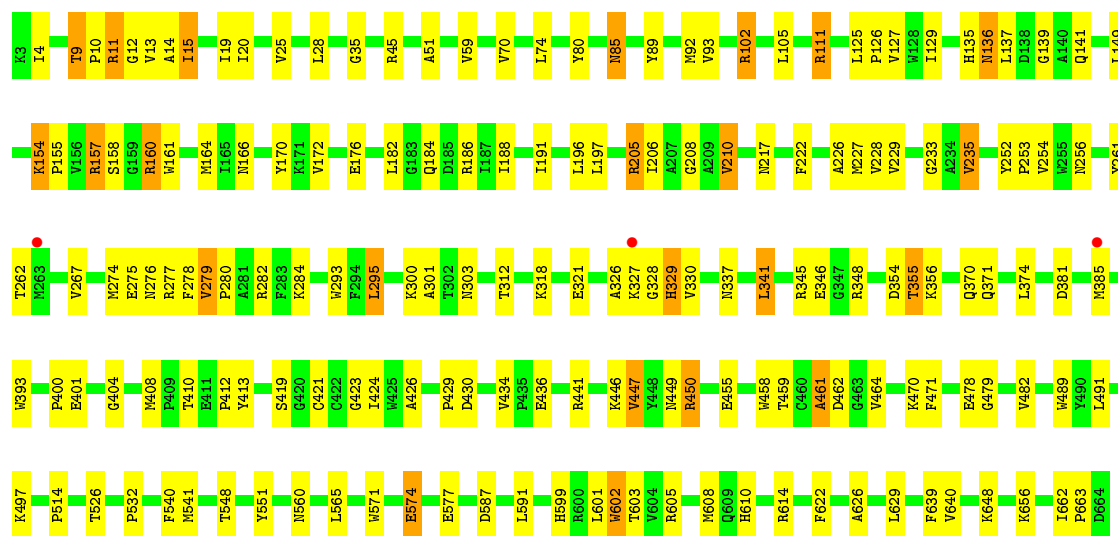
• Molecule 1: Adenylylsulfate Reductase





• Molecule 1: Adenylylsulfate Reductase

Chain K: 74% 23%



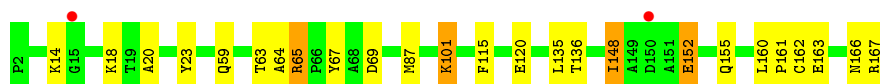
• Molecule 2: Adenylylsulfate Reductase

Chain B: 3% 82% 17%

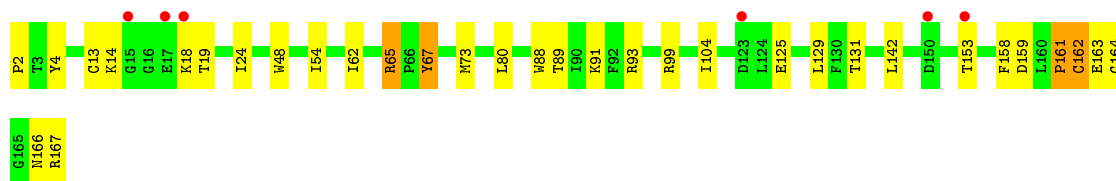
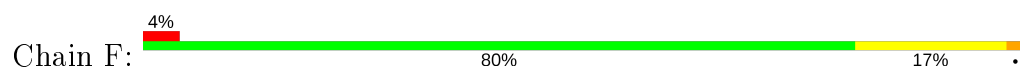


• Molecule 2: Adenylylsulfate Reductase

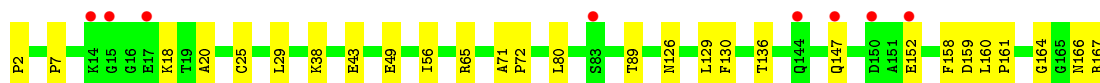
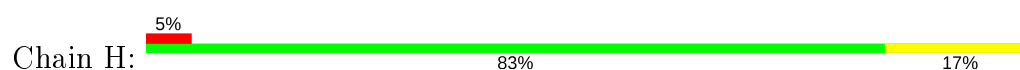
Chain D: 85% 13%



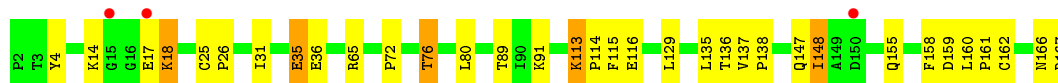
• Molecule 2: Adenylylsulfate Reductase



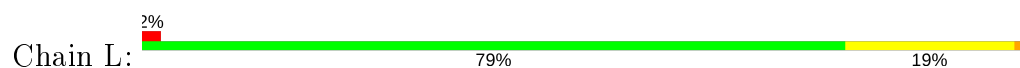
• Molecule 2: Adenylylsulfate Reductase



• Molecule 2: Adenylylsulfate Reductase



• Molecule 2: Adenylylsulfate Reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.63Å 199.63Å 317.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.00-3.20) 97.7 (29.85-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.245 0.199 , 0.246	Depositor DCC
R_{free} test set	6533 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	39537	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: SF4, FAD

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	0.34	0/5364	0.53	1/7254 (0.0%)
1	C	0.34	0/5364	0.51	0/7254
1	E	0.35	0/5364	0.51	0/7254
1	G	0.34	0/5364	0.52	0/7254
1	I	0.34	0/5364	0.53	0/7254
1	K	0.34	0/5364	0.52	0/7254
2	B	0.36	0/1309	0.54	0/1773
2	D	0.36	0/1309	0.57	0/1773
2	F	0.37	0/1309	0.54	0/1773
2	H	0.36	0/1309	0.53	0/1773
2	J	0.36	0/1309	0.53	0/1773
2	L	0.36	0/1309	0.52	0/1773
All	All	0.35	0/40038	0.52	1/54162 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	CA-CB-CG	5.86	128.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5232	0	5114	86	0
1	C	5232	0	5114	118	0
1	E	5232	0	5114	97	0
1	G	5232	0	5114	74	0
1	I	5232	0	5114	87	0
1	K	5232	0	5114	103	0
2	B	1277	0	1228	15	0
2	D	1277	0	1228	20	0
2	F	1277	0	1228	18	0
2	H	1277	0	1228	17	0
2	J	1277	0	1228	19	0
2	L	1277	0	1228	16	0
3	A	53	0	31	3	0
3	C	53	0	31	1	0
3	E	53	0	31	1	0
3	G	53	0	31	1	0
3	I	53	0	31	2	0
3	K	53	0	31	2	0
4	B	16	0	0	0	0
4	D	16	0	0	1	0
4	F	16	0	0	0	0
4	H	16	0	0	0	0
4	J	16	0	0	0	0
4	L	16	0	0	0	0
5	A	11	0	0	0	0
5	B	1	0	0	0	0
5	C	14	0	0	0	0
5	D	3	0	0	0	0
5	E	12	0	0	0	0
5	F	3	0	0	0	0
5	G	6	0	0	1	0
5	H	5	0	0	0	0
5	I	2	0	0	0	0
5	J	3	0	0	0	0
5	K	7	0	0	0	0
5	L	2	0	0	0	0
All	All	39537	0	38238	611	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 8.

All (611) 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:205:ARG:HH21	1:K:205:ARG:HG3	1.26	0.98
2:D:65:ARG:HH21	2:D:65:ARG:HG2	1.26	0.97
1:I:205:ARG:HG3	1:I:205:ARG:HH21	1.28	0.96
1:G:102:ARG:NH1	1:G:426:ALA:O	1.99	0.95
2:F:65:ARG:HH21	2:F:65:ARG:HG2	1.32	0.95
2:J:167:ARG:HD3	1:K:158:SER:HB3	1.48	0.94
1:A:158:SER:HB3	2:D:167:ARG:HD3	1.50	0.93
1:I:23:HIS:HE1	1:I:220:HIS:HD2	1.12	0.92
1:K:228:VAL:HG11	1:K:482:VAL:HG11	1.52	0.92
1:E:577:GLU:HG3	1:E:605:ARG:HH22	1.37	0.90
2:H:65:ARG:HG2	2:H:65:ARG:HH21	1.35	0.90
1:I:111:ARG:HH21	1:I:433:TRP:HZ2	1.21	0.87
1:G:138:ASP:H	1:G:141:GLN:HE21	1.22	0.86
2:L:65:ARG:HH21	2:L:65:ARG:HG2	1.39	0.85
1:K:205:ARG:CG	1:K:205:ARG:HH21	1.90	0.85
1:I:464:VAL:HG23	1:I:470:LYS:HE3	1.59	0.84
1:E:429:PRO:HD2	1:E:434:VAL:HG21	1.58	0.83
1:C:235:VAL:HG13	1:C:256:ASN:HB2	1.61	0.82
1:I:23:HIS:HE1	1:I:220:HIS:CD2	1.96	0.82
1:E:4:ILE:HD11	2:L:38:LYS:HB2	1.62	0.82
1:I:23:HIS:CE1	1:I:220:HIS:HD2	1.97	0.82
1:C:15:ILE:HA	1:C:217:ASN:HD21	1.45	0.81
1:K:577:GLU:HG3	1:K:605:ARG:HH22	1.45	0.79
1:I:162:GLN:H	1:I:162:GLN:HE21	1.31	0.79
1:A:205:ARG:HG2	1:A:205:ARG:HH21	1.46	0.78
2:F:161:PRO:O	2:F:162:CYS:HB2	1.83	0.78
2:B:65:ARG:HH21	2:B:65:ARG:HG2	1.48	0.78
1:C:429:PRO:HD2	1:C:434:VAL:HG21	1.66	0.78
1:A:228:VAL:CG1	1:A:482:VAL:HG11	2.14	0.77
1:C:455:GLU:HG3	1:C:489:TRP:HH2	1.50	0.76
1:K:228:VAL:CG1	1:K:482:VAL:HG11	2.15	0.76
1:G:228:VAL:CG1	1:G:482:VAL:HG11	2.16	0.76
1:E:321:GLU:HB3	1:E:326:ALA:HB3	1.69	0.75
1:I:205:ARG:CG	1:I:205:ARG:HH21	1.99	0.75
1:G:23:HIS:HE1	1:G:220:HIS:HD2	1.34	0.75
2:J:155:GLN:HE22	1:K:301:ALA:H	1.33	0.74
1:I:15:ILE:HA	1:I:217:ASN:HD21	1.53	0.73
1:I:235:VAL:HG13	1:I:256:ASN:HB2	1.68	0.73
1:A:262:THR:CG2	1:A:602:TRP:HB3	2.18	0.73
1:C:262:THR:O	1:C:266:GLN:HB2	1.88	0.73
1:E:455:GLU:HG3	1:E:489:TRP:HH2	1.53	0.72
1:A:23:HIS:HE1	1:A:220:HIS:HD2	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLU:HG2	1:A:605:ARG:HH22	1.53	0.72
1:K:430:ASP:HB2	1:K:447:VAL:HG21	1.71	0.72
1:A:429:PRO:HD2	1:A:434:VAL:HG21	1.72	0.71
1:K:262:THR:CG2	1:K:602:TRP:HB3	2.20	0.71
2:D:65:ARG:CG	2:D:65:ARG:HH21	2.01	0.71
1:E:15:ILE:HA	1:E:217:ASN:HD21	1.55	0.71
1:I:577:GLU:HG3	1:I:605:ARG:HH22	1.56	0.71
1:I:408:MET:HG3	1:I:409:PRO:HD2	1.72	0.70
1:A:23:HIS:HE1	1:A:220:HIS:CD2	2.10	0.70
1:G:15:ILE:HA	1:G:217:ASN:HD21	1.56	0.70
1:E:74:LEU:HA	1:E:385:MET:HB3	1.74	0.70
1:K:205:ARG:NH2	1:K:205:ARG:HG3	2.05	0.70
1:G:464:VAL:HG23	1:G:470:LYS:HE3	1.71	0.70
1:A:82:GLY:O	1:A:83:ASP:HB2	1.92	0.69
1:I:111:ARG:HH11	2:J:135:LEU:HD13	1.58	0.69
1:E:280:PRO:HD2	1:E:410:THR:HG23	1.74	0.68
1:A:560:ASN:HD21	1:A:626:ALA:HB2	1.58	0.68
2:L:161:PRO:O	2:L:162:CYS:HB2	1.93	0.68
1:I:321:GLU:HB3	1:I:326:ALA:HB3	1.76	0.68
1:A:461:ALA:O	1:A:462:ASP:HB2	1.93	0.67
1:C:353:MET:HG3	1:C:407:ILE:HD11	1.77	0.67
1:A:235:VAL:HG13	1:A:256:ASN:HB2	1.75	0.67
1:K:560:ASN:HD21	1:K:626:ALA:HB2	1.60	0.67
1:A:15:ILE:HA	1:A:217:ASN:HD21	1.60	0.67
1:K:430:ASP:HB2	1:K:447:VAL:CG2	2.25	0.66
2:B:158:PHE:O	2:B:159:ASP:HB2	1.95	0.66
2:J:113:LYS:HD3	2:J:116:GLU:HB2	1.78	0.66
1:C:102:ARG:NH1	1:C:426:ALA:O	2.28	0.66
1:C:23:HIS:HE1	1:C:220:HIS:CD2	2.12	0.66
1:C:284:LYS:HE2	1:I:551:TYR:OH	1.95	0.65
1:I:262:THR:CG2	1:I:602:TRP:HB3	2.27	0.65
1:K:429:PRO:HD2	1:K:434:VAL:HG21	1.79	0.65
1:E:577:GLU:CG	1:E:605:ARG:HH22	2.09	0.64
1:C:162:GLN:H	1:C:162:GLN:HE21	1.45	0.64
1:K:15:ILE:HA	1:K:217:ASN:HD21	1.62	0.64
2:J:76:THR:HG23	2:J:91:LYS:HB2	1.79	0.64
1:I:429:PRO:HD2	1:I:434:VAL:HG21	1.79	0.64
1:C:459:THR:HG23	1:C:464:VAL:HG12	1.79	0.64
1:G:228:VAL:HG13	1:G:482:VAL:HG11	1.80	0.64
1:A:23:HIS:CE1	1:A:220:HIS:HD2	2.15	0.64
2:F:54:ILE:HG12	2:F:62:ILE:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:ARG:NH1	1:K:426:ALA:O	2.30	0.64
1:E:16:ALA:H	1:E:217:ASN:ND2	1.97	0.63
1:K:276:ASN:ND2	1:K:421:CYS:H	1.96	0.63
1:E:278:PHE:CE2	1:E:280:PRO:HG3	2.33	0.63
1:C:577:GLU:HG3	1:C:605:ARG:HH22	1.64	0.63
1:A:418:HIS:CD2	1:A:419:SER:H	2.16	0.63
1:A:577:GLU:CG	1:A:605:ARG:HH22	2.12	0.63
1:C:210:VAL:HG12	1:C:221:ILE:HG13	1.80	0.63
1:E:197:LEU:HD11	1:E:210:VAL:HG22	1.80	0.63
1:C:408:MET:HG3	1:C:409:PRO:HD2	1.81	0.62
1:G:157:ARG:HB3	2:L:166:ASN:HD21	1.63	0.62
1:E:280:PRO:HD2	1:E:410:THR:CG2	2.28	0.62
1:E:228:VAL:CG1	1:E:482:VAL:HG11	2.29	0.62
1:C:275:GLU:HB3	1:C:610:HIS:HB3	1.82	0.62
1:E:367:SER:HB3	1:E:368:PRO:HD3	1.80	0.62
1:I:126:PRO:HB2	1:I:166:ASN:HD22	1.65	0.62
1:C:455:GLU:HG3	1:C:489:TRP:CH2	2.33	0.62
1:G:162:GLN:H	1:G:162:GLN:HE21	1.46	0.62
1:I:205:ARG:NH2	1:I:205:ARG:HG3	2.08	0.62
1:I:252:TYR:CG	1:I:253:PRO:HD2	2.35	0.61
1:G:418:HIS:CD2	1:G:419:SER:H	2.17	0.61
1:K:262:THR:HG21	1:K:602:TRP:HB3	1.83	0.61
1:K:74:LEU:HA	1:K:385:MET:HB3	1.81	0.61
1:I:111:ARG:NH2	1:I:433:TRP:HZ2	1.95	0.61
1:E:252:TYR:CG	1:E:253:PRO:HD2	2.35	0.61
1:K:436:GLU:OE1	1:K:441:ARG:NH1	2.34	0.61
2:B:16:GLY:O	2:B:18:LYS:N	2.32	0.60
1:A:261:TYR:CE2	1:A:423:GLY:HA2	2.36	0.60
1:A:252:TYR:CG	1:A:253:PRO:HD2	2.36	0.60
1:C:566:LEU:HD21	1:C:611:ILE:HD11	1.82	0.60
1:E:401:GLU:O	1:E:402:GLU:HG2	2.01	0.60
1:E:223:LYS:HD2	1:E:498:PRO:HB2	1.84	0.60
1:E:403:ARG:HH11	1:K:571:TRP:HE1	1.50	0.60
1:K:275:GLU:HB3	1:K:610:HIS:HB3	1.82	0.60
2:D:148:ILE:H	2:D:148:ILE:HD13	1.65	0.60
1:G:23:HIS:CE1	1:G:220:HIS:HD2	2.17	0.60
1:C:59:VAL:HG12	1:C:188:ILE:HG23	1.83	0.59
1:K:85:ASN:HD22	1:K:85:ASN:H	1.48	0.59
1:G:359:LEU:HD11	1:G:400:PRO:HB2	1.84	0.59
1:I:74:LEU:HA	1:I:385:MET:HB3	1.85	0.59
2:D:65:ARG:NH2	2:D:65:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:TRP:CZ3	1:C:400:PRO:HG3	2.37	0.59
1:E:276:ASN:ND2	1:E:421:CYS:H	1.99	0.59
1:E:455:GLU:HG3	1:E:489:TRP:CH2	2.36	0.59
2:L:137:VAL:HG22	2:L:138:PRO:HD2	1.85	0.59
1:A:262:THR:HG21	1:A:602:TRP:HB3	1.85	0.59
1:E:275:GLU:HB3	1:E:610:HIS:HB3	1.84	0.59
1:E:102:ARG:NH1	1:E:426:ALA:O	2.36	0.58
1:I:137:LEU:HA	1:I:141:GLN:HE21	1.67	0.58
1:C:102:ARG:NH2	1:C:104:ASP:OD1	2.36	0.58
1:C:162:GLN:HE21	1:C:162:GLN:N	2.00	0.58
1:E:258:GLY:O	1:E:262:THR:HG22	2.03	0.58
1:A:262:THR:HG23	1:A:603:THR:OG1	2.03	0.58
1:G:182:LEU:O	1:G:186:ARG:HD3	2.03	0.58
1:K:459:THR:HG23	1:K:464:VAL:HG12	1.85	0.58
1:I:262:THR:HG22	1:I:602:TRP:HB3	1.85	0.58
1:C:296:LEU:HD22	1:C:374:LEU:HD12	1.84	0.58
1:C:20:ILE:HD11	1:C:508:LYS:HD2	1.86	0.58
1:C:464:VAL:HG22	1:C:470:LYS:HE3	1.85	0.58
1:C:460:CYS:HB3	1:C:482:VAL:HG21	1.84	0.58
1:C:70:VAL:HG13	1:C:74:LEU:HG	1.86	0.58
1:I:471:PHE:HB3	3:I:1000:FAD:O2	2.04	0.58
1:A:502:GLU:HG3	1:A:507:LEU:HD21	1.86	0.58
1:E:234:ALA:HB3	1:E:414:LEU:HB2	1.86	0.57
2:H:167:ARG:HD2	1:I:158:SER:HB3	1.85	0.57
1:E:228:VAL:HG13	1:E:482:VAL:HG11	1.86	0.57
1:C:262:THR:CG2	1:C:602:TRP:HB3	2.33	0.57
1:E:543:ARG:NH2	2:L:72:PRO:HB3	2.20	0.57
1:A:551:TYR:OH	1:G:284:LYS:HE2	2.03	0.57
1:A:471:PHE:HB3	3:A:1000:FAD:O2	2.05	0.57
1:C:23:HIS:CE1	1:C:220:HIS:HD2	2.22	0.57
1:C:210:VAL:CG1	1:C:221:ILE:HG13	2.34	0.56
1:A:262:THR:HG22	1:A:602:TRP:HB3	1.85	0.56
1:C:228:VAL:HG22	1:C:486:MET:SD	2.46	0.56
1:E:418:HIS:CD2	1:E:419:SER:H	2.22	0.56
1:I:111:ARG:NH1	2:J:135:LEU:HD13	2.20	0.56
1:K:279:VAL:HG13	1:K:622:PHE:CD1	2.40	0.56
1:C:551:TYR:OH	1:I:284:LYS:HE2	2.06	0.56
1:G:252:TYR:CG	1:G:253:PRO:HD2	2.40	0.56
1:A:381:ASP:O	1:A:385:MET:HB3	2.05	0.56
1:K:139:GLY:H	1:K:166:ASN:ND2	2.03	0.56
1:K:354:ASP:O	1:K:356:LYS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:135:HIS:O	1:K:136:ASN:HB2	2.04	0.56
1:K:158:SER:HB2	1:K:295:LEU:HD21	1.86	0.56
1:K:139:GLY:H	1:K:166:ASN:HD21	1.53	0.56
1:A:59:VAL:HG12	1:A:188:ILE:HG23	1.88	0.56
1:A:205:ARG:NH2	1:A:205:ARG:HG2	2.16	0.56
1:E:275:GLU:HB2	1:E:611:ILE:HG22	1.87	0.56
1:G:471:PHE:HB3	3:G:1000:FAD:O2	2.05	0.55
1:K:127:VAL:HG11	1:K:149:LEU:HD11	1.89	0.55
1:I:464:VAL:HG21	1:I:478:GLU:OE1	2.07	0.55
1:A:195:LYS:O	1:A:196:LEU:HB2	2.07	0.55
1:A:393:TRP:CZ3	1:A:400:PRO:HG3	2.42	0.55
1:G:393:TRP:CZ3	1:G:400:PRO:HG3	2.42	0.55
1:K:228:VAL:HG11	1:K:482:VAL:CG1	2.32	0.55
1:C:111:ARG:HB3	2:D:136:THR:HG22	1.89	0.55
1:E:162:GLN:H	1:E:162:GLN:HE21	1.53	0.55
1:K:410:THR:HG21	1:K:413:TYR:HE1	1.72	0.55
1:A:25:VAL:HG21	1:A:57:LEU:HB2	1.88	0.54
1:C:200:LYS:HB2	1:C:501:VAL:HG13	1.89	0.54
1:I:275:GLU:HB2	1:I:611:ILE:HG22	1.89	0.54
1:C:74:LEU:HA	1:C:385:MET:HB3	1.89	0.54
1:E:497:LYS:HG3	1:E:497:LYS:O	2.07	0.54
1:I:11:ARG:HG3	1:I:11:ARG:O	2.07	0.54
1:C:137:LEU:HA	1:C:141:GLN:HE21	1.73	0.54
1:A:460:CYS:HB2	1:A:478:GLU:HB3	1.90	0.54
1:G:340:MET:HE3	1:G:409:PRO:HD3	1.90	0.54
1:K:4:ILE:HD11	1:K:526:THR:HB	1.90	0.54
1:G:262:THR:CG2	1:G:602:TRP:HB3	2.38	0.53
1:C:70:VAL:HB	1:C:171:LYS:HB2	1.90	0.53
1:I:359:LEU:HD11	1:I:400:PRO:HB2	1.91	0.53
1:K:278:PHE:CE1	1:K:419:SER:HB2	2.43	0.53
1:E:182:LEU:HD22	1:E:186:ARG:HB2	1.90	0.53
1:G:69:ALA:HA	1:G:253:PRO:HG3	1.90	0.53
1:K:252:TYR:CG	1:K:253:PRO:HD2	2.43	0.53
1:K:461:ALA:O	1:K:462:ASP:HB3	2.08	0.53
1:C:130:LYS:HE3	2:F:166:ASN:HD22	1.73	0.53
1:I:634:SER:HB3	1:K:329:HIS:CG	2.44	0.53
1:C:23:HIS:HE1	1:C:220:HIS:HD2	1.55	0.53
1:C:560:ASN:HD21	1:C:626:ALA:HB2	1.74	0.53
1:C:275:GLU:HB2	1:C:611:ILE:HG22	1.91	0.53
1:G:262:THR:HG22	1:G:602:TRP:HB3	1.91	0.53
1:A:137:LEU:HA	1:A:141:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:518:TYR:HB2	1:I:584:ALA:HB1	1.91	0.52
1:I:275:GLU:OE2	1:I:640:VAL:HB	2.10	0.52
1:C:537:PRO:HG3	1:C:594:CYS:SG	2.50	0.52
1:E:340:MET:HG3	1:E:351:ILE:HD13	1.90	0.52
1:I:196:LEU:HB2	1:I:267:VAL:HG21	1.92	0.52
1:G:279:VAL:HG22	1:G:622:PHE:CD1	2.45	0.52
1:G:70:VAL:HG13	1:G:74:LEU:HG	1.92	0.52
1:I:496:PHE:CE1	1:I:498:PRO:HB3	2.44	0.52
1:K:455:GLU:HG3	1:K:489:TRP:HH2	1.74	0.52
1:G:23:HIS:HE1	1:G:220:HIS:CD2	2.21	0.52
1:K:70:VAL:HG13	1:K:74:LEU:HG	1.91	0.52
1:K:228:VAL:HG12	1:K:458:TRP:CB	2.40	0.52
1:C:557:THR:HG23	1:C:560:ASN:H	1.74	0.52
1:E:284:LYS:HG3	1:E:408:MET:HB2	1.91	0.52
2:F:65:ARG:NH2	2:F:65:ARG:HG2	2.11	0.52
1:K:111:ARG:HB3	2:L:136:THR:HG23	1.92	0.52
1:C:366:MET:HB2	1:C:371:GLN:OE1	2.10	0.52
1:I:326:ALA:O	1:I:327:LYS:HB3	2.09	0.52
1:K:154:LYS:HE2	1:K:155:PRO:HD2	1.91	0.52
1:E:235:VAL:HG21	1:E:254:VAL:HA	1.91	0.52
1:G:70:VAL:O	1:G:70:VAL:HG12	2.09	0.52
1:I:14:ALA:O	1:I:15:ILE:HG22	2.09	0.52
1:I:12:GLY:HA2	2:J:31:ILE:HD13	1.91	0.52
1:A:126:PRO:HB2	1:A:166:ASN:HB2	1.92	0.51
2:F:73:MET:O	2:F:93:ARG:HD2	2.10	0.51
1:G:139:GLY:H	1:G:166:ASN:HD21	1.56	0.51
1:I:197:LEU:HD11	1:I:210:VAL:HG22	1.91	0.51
2:H:152:GLU:HB2	1:I:300:LYS:NZ	2.25	0.51
1:E:353:MET:HG3	1:E:407:ILE:HD11	1.92	0.51
1:K:45:ARG:HG2	2:L:130:PHE:CD1	2.45	0.51
1:G:24:SER:HB3	5:G:665:HOH:O	2.10	0.51
2:B:33:ASP:OD1	1:G:4:ILE:HG22	2.11	0.51
1:C:638:CYS:HB2	1:C:656:LYS:O	2.10	0.51
1:C:639:PHE:HB2	1:C:656:LYS:HB3	1.91	0.51
1:G:157:ARG:HB3	2:L:166:ASN:ND2	2.25	0.51
1:K:126:PRO:HB2	1:K:166:ASN:HB2	1.93	0.51
1:A:226:ALA:HB2	1:A:489:TRP:CD1	2.46	0.51
1:I:577:GLU:HG3	1:I:605:ARG:NH2	2.24	0.51
1:E:25:VAL:O	1:E:224:ALA:HA	2.11	0.51
2:J:35:GLU:OE2	2:J:36:GLU:HG2	2.11	0.51
1:K:471:PHE:HB3	3:K:1000:FAD:O2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:SER:OG	1:E:476:HIS:HD2	1.93	0.51
1:G:408:MET:HG3	1:G:409:PRO:HD2	1.92	0.51
1:A:126:PRO:HB2	1:A:166:ASN:HD22	1.76	0.50
1:A:461:ALA:HB2	1:A:475:SER:HA	1.93	0.50
1:C:337:ASN:C	1:C:337:ASN:HD22	2.15	0.50
1:G:337:ASN:O	1:G:341:LEU:HB2	2.11	0.50
1:I:464:VAL:CG2	1:I:470:LYS:HE3	2.35	0.50
1:G:279:VAL:O	1:G:279:VAL:HG23	2.10	0.50
1:G:356:LYS:HD2	1:G:401:GLU:O	2.11	0.50
1:G:80:TYR:O	1:G:157:ARG:NH2	2.45	0.50
2:B:153:THR:HB	2:B:155:GLN:H	1.76	0.50
1:E:359:LEU:CD1	1:E:400:PRO:HB2	2.41	0.50
1:I:139:GLY:H	1:I:166:ASN:HD21	1.60	0.50
1:I:262:THR:HG23	1:I:603:THR:OG1	2.12	0.50
1:K:277:ARG:HD3	1:K:412:PRO:HB3	1.93	0.50
1:C:262:THR:HG22	1:C:602:TRP:HB3	1.93	0.50
1:G:195:LYS:O	1:G:196:LEU:HB2	2.12	0.50
1:A:249:ARG:HB2	2:B:67:TYR:CZ	2.47	0.50
1:E:162:GLN:N	1:E:162:GLN:HE21	2.09	0.50
1:K:51:ALA:HB2	1:K:491:LEU:HD21	1.94	0.50
1:K:450:ARG:NH1	1:K:478:GLU:OE1	2.46	0.49
1:C:514:PRO:HA	1:C:583:LEU:O	2.12	0.49
1:E:359:LEU:HD13	1:E:400:PRO:HB2	1.94	0.49
1:E:284:LYS:HE2	1:K:551:TYR:OH	2.13	0.49
1:K:85:ASN:ND2	1:K:85:ASN:H	2.10	0.49
1:C:138:ASP:HB2	1:C:166:ASN:HD21	1.77	0.49
1:A:196:LEU:HD11	1:A:229:VAL:HG21	1.95	0.49
1:E:65:GLU:HG3	1:E:172:VAL:HG23	1.95	0.49
1:G:321:GLU:HG2	1:G:326:ALA:HB3	1.94	0.49
1:A:234:ALA:HB3	1:A:414:LEU:HB2	1.95	0.49
2:F:13:CYS:HB2	2:F:19:THR:HG22	1.94	0.49
1:A:353:MET:HG3	1:A:407:ILE:HD11	1.95	0.49
1:C:399:ALA:HB3	1:C:402:GLU:HG2	1.95	0.49
1:G:464:VAL:HG21	1:G:478:GLU:OE1	2.13	0.49
1:C:577:GLU:HG3	1:C:605:ARG:NH2	2.27	0.49
2:L:160:LEU:O	2:L:162:CYS:N	2.46	0.49
1:E:514:PRO:HG2	1:E:591:LEU:HD12	1.94	0.49
2:H:7:PRO:O	2:H:38:LYS:HE3	2.13	0.49
1:K:197:LEU:HD11	1:K:210:VAL:HG22	1.95	0.49
1:K:208:GLY:HA3	1:K:222:PHE:O	2.12	0.48
1:C:111:ARG:HB3	2:D:136:THR:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:VAL:O	1:E:292:ALA:N	2.46	0.48
1:G:357:THR:HA	1:G:360:GLN:HG2	1.95	0.48
2:L:65:ARG:HG2	2:L:65:ARG:NH2	2.16	0.48
1:A:10:PRO:O	1:A:11:ARG:HG2	2.12	0.48
1:A:261:TYR:HE2	1:A:423:GLY:HA2	1.78	0.48
2:B:158:PHE:O	2:B:159:ASP:CB	2.61	0.48
1:C:562:SER:HB3	1:C:626:ALA:HB3	1.95	0.48
1:I:278:PHE:CE1	1:I:419:SER:HB2	2.48	0.48
1:I:267:VAL:HG12	1:I:454:VAL:HG21	1.95	0.48
1:K:226:ALA:HB2	1:K:489:TRP:CD1	2.48	0.48
1:I:228:VAL:HG22	1:I:486:MET:SD	2.54	0.48
1:I:276:ASN:ND2	1:I:421:CYS:H	2.11	0.48
2:B:2:PRO:HD3	2:B:67:TYR:CD2	2.48	0.48
1:G:190:ARG:NH2	2:H:25:CYS:O	2.46	0.48
1:K:235:VAL:HG11	1:K:252:TYR:HB3	1.96	0.48
1:C:130:LYS:HE3	2:F:166:ASN:HB3	1.95	0.48
1:G:78:ASN:HB2	1:G:471:PHE:CG	2.49	0.48
1:K:89:TYR:O	1:K:93:VAL:HG23	2.14	0.48
2:B:166:ASN:HB3	1:E:157:ARG:O	2.13	0.48
1:I:262:THR:HG21	1:I:599:HIS:O	2.13	0.48
1:C:238:TYR:CD1	1:C:412:PRO:HG2	2.47	0.48
1:E:235:VAL:HG11	1:E:252:TYR:HB3	1.96	0.48
1:E:430:ASP:HB2	1:E:447:VAL:HG22	1.96	0.48
1:I:69:ALA:HB1	3:I:1000:FAD:HM81	1.96	0.48
2:J:113:LYS:HE2	2:J:114:PRO:HD2	1.95	0.48
1:C:262:THR:HG21	1:C:599:HIS:O	2.13	0.47
2:H:20:ALA:HB1	2:H:56:ILE:HG12	1.95	0.47
2:H:65:ARG:HG2	2:H:65:ARG:NH2	2.12	0.47
1:I:537:PRO:HG3	1:I:594:CYS:SG	2.54	0.47
1:K:574:GLU:HA	1:K:577:GLU:HB2	1.96	0.47
2:B:65:ARG:NH2	2:B:65:ARG:HG2	2.23	0.47
1:C:262:THR:HG23	1:C:603:THR:OG1	2.15	0.47
1:G:196:LEU:HD11	1:G:229:VAL:HG21	1.97	0.47
1:I:70:VAL:HG13	1:I:74:LEU:HG	1.94	0.47
1:K:35:GLY:O	1:K:479:GLY:HA3	2.14	0.47
1:E:57:LEU:HD11	1:E:188:ILE:HG12	1.96	0.47
1:E:608:MET:HA	1:E:611:ILE:HG12	1.96	0.47
1:I:77:ILE:HG23	1:I:473:SER:OG	2.15	0.47
2:J:148:ILE:H	2:J:148:ILE:HD13	1.80	0.47
1:C:195:LYS:HB3	1:C:210:VAL:HG23	1.95	0.47
1:A:210:VAL:HG21	1:A:507:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:PRO:HB2	1:E:166:ASN:HB2	1.95	0.47
1:K:12:GLY:HA3	1:K:587:ASP:OD2	2.15	0.47
1:K:228:VAL:HG12	1:K:458:TRP:HB2	1.96	0.47
1:A:310:CYS:SG	2:D:155:GLN:HG2	2.54	0.47
1:K:279:VAL:HG22	1:K:279:VAL:O	2.14	0.47
1:G:519:GLU:HA	1:G:522:LYS:HD2	1.96	0.47
1:I:296:LEU:HD22	1:I:374:LEU:HD22	1.96	0.47
1:K:455:GLU:HG3	1:K:489:TRP:CH2	2.49	0.47
1:A:14:ALA:O	1:A:15:ILE:HG22	2.15	0.46
1:C:15:ILE:HA	1:C:217:ASN:ND2	2.21	0.46
1:C:23:HIS:CE1	1:C:220:HIS:CD2	2.95	0.46
1:E:471:PHE:HB3	3:E:1000:FAD:O2	2.14	0.46
1:K:102:ARG:NH2	1:K:105:LEU:HG	2.30	0.46
1:K:9:THR:O	1:K:11:ARG:N	2.48	0.46
1:A:450:ARG:NH1	1:A:478:GLU:OE1	2.49	0.46
2:B:160:LEU:O	2:B:162:CYS:N	2.48	0.46
1:C:33:GLY:HA3	3:C:1000:FAD:O5B	2.15	0.46
1:I:395:ALA:O	2:J:72:PRO:HG2	2.15	0.46
2:J:17:GLU:HG2	2:J:18:LYS:N	2.30	0.46
1:C:248:GLY:HA2	1:C:254:VAL:HG21	1.97	0.46
1:A:243:VAL:HG22	1:G:239:ARG:HH11	1.81	0.46
2:H:166:ASN:HD21	1:I:130:LYS:HG3	1.81	0.46
1:K:261:TYR:CE2	1:K:423:GLY:HA2	2.51	0.46
1:C:243:VAL:HG11	1:I:243:VAL:HG21	1.97	0.46
1:E:410:THR:OG1	1:E:411:GLU:N	2.48	0.46
1:I:367:SER:OG	1:I:370:GLN:HB2	2.16	0.46
1:A:593:ARG:NH1	1:A:596:GLU:OE2	2.49	0.46
1:C:277:ARG:HD3	1:C:412:PRO:HB3	1.97	0.46
1:C:62:ALA:O	1:C:189:GLU:HB2	2.15	0.46
1:E:80:TYR:O	1:E:157:ARG:NH2	2.47	0.46
1:A:548:THR:HA	1:A:608:MET:HE1	1.98	0.46
1:C:45:ARG:HE	2:D:120:GLU:HA	1.79	0.46
1:E:548:THR:HA	1:E:608:MET:HE1	1.98	0.46
2:H:152:GLU:HB2	1:I:300:LYS:HZ1	1.80	0.46
1:I:241:ARG:HE	1:I:408:MET:HG2	1.79	0.46
1:K:59:VAL:HG12	1:K:188:ILE:HB	1.98	0.46
1:K:70:VAL:O	1:K:70:VAL:HG12	2.16	0.46
1:K:471:PHE:HB3	3:K:1000:FAD:C2	2.45	0.46
1:A:179:LYS:O	1:A:183:GLY:N	2.41	0.46
1:C:434:VAL:HB	1:C:439:LYS:HE2	1.97	0.46
1:C:540:PHE:HZ	1:C:601:LEU:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:HG13	1:E:74:LEU:HG	1.97	0.46
2:F:4:TYR:OH	1:K:532:PRO:HG3	2.16	0.46
1:A:602:TRP:HZ3	1:A:606:LEU:HD22	1.81	0.46
1:C:450:ARG:HA	1:C:450:ARG:HD3	1.66	0.46
1:E:226:ALA:HB2	1:E:489:TRP:CD1	2.51	0.46
1:E:551:TYR:OH	1:K:284:LYS:HE2	2.16	0.46
1:I:459:THR:HG23	1:I:464:VAL:HG13	1.99	0.46
1:A:488:ARG:HD2	2:B:124:LEU:O	2.16	0.45
1:C:28:LEU:O	1:C:227:MET:HA	2.16	0.45
1:C:332:PRO:HG2	1:C:335:LEU:HD12	1.97	0.45
1:G:262:THR:HG21	1:G:599:HIS:O	2.16	0.45
1:A:102:ARG:NH1	1:A:426:ALA:O	2.50	0.45
1:A:130:LYS:HE3	2:D:166:ASN:OD1	2.15	0.45
1:K:461:ALA:O	1:K:462:ASP:CB	2.64	0.45
1:C:102:ARG:HH21	1:C:102:ARG:HB3	1.80	0.45
1:C:439:LYS:HB3	1:C:447:VAL:HG21	1.99	0.45
1:C:111:ARG:HG3	1:C:111:ARG:H	1.63	0.45
2:D:160:LEU:O	2:D:162:CYS:N	2.50	0.45
1:E:356:LYS:HD3	1:E:402:GLU:H	1.80	0.45
2:J:137:VAL:HG22	2:J:138:PRO:HD2	1.97	0.45
1:K:540:PHE:HZ	1:K:601:LEU:HD12	1.80	0.45
2:L:65:ARG:HH21	2:L:65:ARG:CG	2.19	0.45
1:C:151:ASN:HB3	1:C:153:ASP:OD2	2.17	0.45
1:C:318:LYS:HB3	1:C:319:PRO:HD3	1.97	0.45
1:C:276:ASN:ND2	1:C:421:CYS:H	2.14	0.45
2:D:65:ARG:CG	2:D:65:ARG:NH2	2.71	0.45
1:E:228:VAL:HG11	1:E:482:VAL:HG11	1.97	0.45
1:K:464:VAL:HG22	1:K:470:LYS:HE3	1.97	0.45
1:K:514:PRO:HG2	1:K:591:LEU:HD13	1.98	0.45
1:I:139:GLY:H	1:I:166:ASN:ND2	2.15	0.45
1:I:279:VAL:O	1:I:279:VAL:HG22	2.16	0.45
1:A:294:PHE:O	1:A:298:LYS:HA	2.17	0.45
1:C:228:VAL:HG13	1:C:482:VAL:HG11	1.99	0.45
1:C:430:ASP:HB2	1:C:447:VAL:HG22	1.97	0.45
2:F:65:ARG:HH21	2:F:65:ARG:CG	2.14	0.45
1:G:274:MET:HA	1:G:422:CYS:HB2	1.99	0.45
1:E:126:PRO:HB3	1:E:139:GLY:HA3	1.99	0.45
1:E:260:THR:HG21	1:E:463:GLY:HA2	1.99	0.45
1:G:484:LYS:NZ	2:H:126:ASN:OD1	2.49	0.45
1:A:262:THR:O	1:A:266:GLN:HB2	2.17	0.45
1:A:287:TYR:CE2	1:A:410:THR:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ASP:HB2	1:E:166:ASN:HD21	1.82	0.45
1:C:278:PHE:CZ	1:C:280:PRO:HB3	2.52	0.44
1:E:139:GLY:H	1:E:166:ASN:ND2	2.15	0.44
1:G:139:GLY:H	1:G:166:ASN:ND2	2.15	0.44
1:E:366:MET:HG3	1:E:370:GLN:HB2	1.99	0.44
1:C:239:ARG:HA	1:C:240:PRO:HD3	1.89	0.44
1:E:383:LEU:HG	2:F:88:TRP:CG	2.52	0.44
1:G:29:MET:HA	1:G:228:VAL:HG23	1.98	0.44
1:A:275:GLU:HB3	1:A:610:HIS:HB3	1.99	0.44
1:C:356:LYS:HD2	1:C:401:GLU:O	2.18	0.44
1:C:450:ARG:NH1	1:C:478:GLU:OE1	2.51	0.44
1:G:62:ALA:HA	1:G:190:ARG:NH1	2.32	0.44
1:G:455:GLU:HG3	1:G:489:TRP:HH2	1.83	0.44
2:D:87:MET:HG2	2:D:101:LYS:HD3	1.99	0.44
1:E:497:LYS:O	1:E:497:LYS:CG	2.66	0.44
1:A:51:ALA:HB2	1:A:491:LEU:HD21	2.00	0.44
1:A:541:MET:HG2	1:A:597:ASN:ND2	2.33	0.44
2:B:71:ALA:HA	2:B:72:PRO:HD2	1.90	0.44
1:G:337:ASN:HD22	1:G:337:ASN:C	2.20	0.44
1:I:279:VAL:HG13	1:I:622:PHE:CD1	2.53	0.44
1:K:137:LEU:HA	1:K:141:GLN:HE21	1.82	0.44
1:A:548:THR:HG22	1:A:608:MET:HE3	2.00	0.44
1:A:656:LYS:HA	1:A:657:PRO:HD3	1.89	0.44
1:C:14:ALA:O	1:C:15:ILE:HG22	2.18	0.44
1:C:359:LEU:O	1:C:363:PHE:HB2	2.18	0.44
1:C:532:PRO:HD3	2:J:4:TYR:CZ	2.53	0.44
2:H:158:PHE:O	2:H:159:ASP:HB2	2.18	0.43
1:I:261:TYR:CE2	1:I:423:GLY:HA2	2.52	0.43
1:K:176:GLU:CD	2:L:105:ARG:HH22	2.20	0.43
1:A:271:MET:HE1	1:A:424:ILE:HG12	1.99	0.43
1:E:9:THR:HA	1:E:10:PRO:HD3	1.89	0.43
1:K:328:GLY:O	1:K:330:VAL:N	2.51	0.43
1:K:262:THR:HG22	1:K:602:TRP:HB3	1.96	0.43
1:C:234:ALA:HB3	1:C:414:LEU:HB2	2.00	0.43
1:C:561:THR:HA	1:C:565:LEU:HD23	2.01	0.43
1:E:540:PHE:HZ	1:E:601:LEU:HD12	1.84	0.43
1:K:341:LEU:O	1:K:345:ARG:HG2	2.18	0.43
1:A:5:PRO:HB2	1:A:528:PRO:HD2	2.00	0.43
2:F:2:PRO:HD3	2:F:67:TYR:CD2	2.53	0.43
1:G:298:LYS:HE2	1:G:298:LYS:HA	2.01	0.43
1:C:78:ASN:HB2	1:C:471:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:PHE:O	2:F:159:ASP:HB2	2.19	0.43
2:H:29:LEU:HD22	2:H:43:GLU:HB3	2.01	0.43
1:I:223:LYS:HG2	1:I:500:PHE:CZ	2.53	0.43
1:A:295:LEU:HD21	2:D:167:ARG:HG3	1.99	0.43
1:K:293:TRP:CH2	1:K:400:PRO:HG2	2.54	0.43
1:C:130:LYS:HE2	1:C:156:VAL:HG22	2.00	0.43
1:C:6:SER:HA	1:C:528:PRO:HG3	2.00	0.43
1:C:45:ARG:HB2	2:D:115:PHE:CE2	2.53	0.43
1:G:235:VAL:CG1	1:G:256:ASN:HB2	2.49	0.43
1:K:262:THR:HG21	1:K:599:HIS:O	2.19	0.43
1:A:276:ASN:ND2	1:A:421:CYS:H	2.16	0.43
1:E:182:LEU:HD22	1:E:186:ARG:CB	2.47	0.43
1:E:632:ASP:HB3	1:E:636:TRP:HD1	1.84	0.43
1:I:340:MET:CG	1:I:351:ILE:HD13	2.49	0.43
1:K:274:MET:HB2	1:K:610:HIS:CD2	2.54	0.43
1:K:662:ILE:HA	1:K:663:PRO:HD3	1.90	0.43
1:C:238:TYR:CG	1:C:412:PRO:HG2	2.54	0.43
1:C:282:ARG:NH2	2:F:159:ASP:OD1	2.51	0.43
1:G:109:LEU:HB2	1:G:450:ARG:HH22	1.84	0.43
2:H:71:ALA:HA	2:H:72:PRO:HD3	1.90	0.43
1:K:424:ILE:HB	1:K:459:THR:HG21	2.00	0.43
1:G:128:TRP:HB3	1:G:156:VAL:CG2	2.49	0.43
1:G:617:SER:HB2	1:G:629:LEU:O	2.19	0.43
1:A:39:ALA:HA	1:A:479:GLY:O	2.18	0.42
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.90	0.42
1:C:196:LEU:HD11	1:C:229:VAL:HG21	2.01	0.42
1:G:279:VAL:HG12	1:G:412:PRO:HA	2.00	0.42
1:K:196:LEU:HD11	1:K:229:VAL:HG21	2.00	0.42
1:E:228:VAL:HG22	1:E:486:MET:SD	2.60	0.42
1:G:223:LYS:HB3	1:G:498:PRO:HG2	2.00	0.42
2:H:65:ARG:NH2	2:H:65:ARG:CG	2.81	0.42
1:K:233:GLY:O	1:K:256:ASN:HB3	2.19	0.42
1:A:471:PHE:HB3	3:A:1000:FAD:C2	2.48	0.42
1:C:182:LEU:O	1:C:186:ARG:HD3	2.19	0.42
1:C:380:GLU:O	1:C:384:ASP:HB2	2.20	0.42
1:E:51:ALA:HB2	1:E:491:LEU:HD21	2.01	0.42
1:K:125:LEU:HA	1:K:126:PRO:HD3	1.91	0.42
2:L:25:CYS:HA	2:L:26:PRO:HD3	1.88	0.42
2:L:78:ILE:HB	2:L:89:THR:HG23	2.02	0.42
1:C:300:LYS:NZ	2:F:153:THR:HG21	2.34	0.42
1:I:73:GLY:HA3	1:I:167:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:28:LEU:O	1:K:227:MET:HA	2.19	0.42
1:C:274:MET:HB2	1:C:610:HIS:CG	2.55	0.42
1:E:66:ARG:HG3	2:F:24:ILE:HD11	2.00	0.42
1:G:608:MET:O	1:G:611:ILE:HG22	2.20	0.42
1:C:30:VAL:HG13	1:C:193:ILE:HG13	2.01	0.42
1:I:278:PHE:CZ	1:I:280:PRO:HB3	2.55	0.42
1:A:82:GLY:O	1:A:83:ASP:CB	2.65	0.42
1:A:89:TYR:O	1:A:93:VAL:HG23	2.20	0.42
1:C:461:ALA:C	1:C:463:GLY:H	2.22	0.42
1:C:25:VAL:HG22	1:C:55:LYS:O	2.19	0.42
1:E:366:MET:HB2	1:E:369:ALA:HB3	2.00	0.42
1:E:403:ARG:HB2	1:E:403:ARG:HH21	1.85	0.42
1:E:502:GLU:HG3	1:E:507:LEU:HD21	2.00	0.42
1:G:132:GLU:CD	1:G:132:GLU:H	2.21	0.42
1:G:537:PRO:HG3	1:G:594:CYS:SG	2.59	0.42
1:I:217:ASN:ND2	1:I:512:TYR:OH	2.51	0.42
1:A:151:ASN:HB3	1:A:153:ASP:OD2	2.20	0.42
1:E:253:PRO:HA	2:F:48:TRP:CE2	2.55	0.42
1:E:42:GLU:O	1:E:46:TRP:HD1	2.02	0.42
1:K:235:VAL:CG2	1:K:254:VAL:HA	2.50	0.42
1:K:262:THR:HG23	1:K:603:THR:OG1	2.20	0.42
1:K:85:ASN:N	1:K:85:ASN:HD22	2.16	0.42
1:C:367:SER:HB2	1:C:368:PRO:HD2	2.02	0.42
1:G:74:LEU:HA	1:G:385:MET:HB3	2.02	0.42
1:I:109:LEU:HD11	1:I:474:GLY:HA3	2.02	0.42
1:I:80:TYR:O	1:I:157:ARG:NH2	2.53	0.42
1:C:575:MET:HE3	2:J:72:PRO:HG3	2.02	0.42
1:K:15:ILE:HA	1:K:217:ASN:ND2	2.33	0.42
1:C:129:ILE:HG21	1:C:147:LYS:HB3	2.02	0.41
1:G:337:ASN:HA	1:G:340:MET:HB3	2.01	0.41
1:I:459:THR:OG1	1:I:463:GLY:HA3	2.19	0.41
1:C:353:MET:CG	1:C:407:ILE:HD11	2.49	0.41
1:E:212:PHE:HZ	1:E:592:LEU:HA	1.86	0.41
1:G:418:HIS:CG	1:G:419:SER:H	2.38	0.41
1:I:45:ARG:NH1	2:J:115:PHE:HB3	2.36	0.41
1:A:274:MET:HA	1:A:422:CYS:HB2	2.02	0.41
1:E:157:ARG:HG2	1:E:162:GLN:O	2.20	0.41
1:E:25:VAL:HG23	1:E:55:LYS:HB3	2.01	0.41
1:K:393:TRP:CZ3	1:K:400:PRO:HG3	2.55	0.41
1:K:80:TYR:O	1:K:157:ARG:NH2	2.53	0.41
1:A:231:CYS:HB3	3:A:1000:FAD:C8A	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG13	1:A:622:PHE:CD1	2.56	0.41
1:E:208:GLY:HA3	1:E:222:PHE:O	2.20	0.41
1:E:69:ALA:HA	1:E:253:PRO:HG3	2.03	0.41
1:I:15:ILE:HA	1:I:217:ASN:ND2	2.29	0.41
1:I:77:ILE:HD12	1:I:165:ILE:HD13	2.02	0.41
1:C:126:PRO:HB3	1:C:139:GLY:HA3	2.02	0.41
1:C:538:LYS:HB2	1:C:538:LYS:HE3	1.85	0.41
1:E:279:VAL:HG13	1:E:622:PHE:CD1	2.55	0.41
1:A:192:PHE:HB2	1:A:214:LEU:HD11	2.02	0.41
1:A:380:GLU:O	1:A:384:ASP:HB2	2.21	0.41
1:E:264:CYS:O	1:E:267:VAL:HG12	2.20	0.41
1:E:267:VAL:HG13	1:E:454:VAL:HG21	2.03	0.41
1:G:102:ARG:NH2	1:G:104:ASP:OD2	2.54	0.41
1:G:45:ARG:HG2	2:H:130:PHE:CD1	2.56	0.41
2:H:2:PRO:N	2:H:49:GLU:OE1	2.53	0.41
1:A:608:MET:HA	1:A:611:ILE:HG12	2.03	0.41
1:A:662:ILE:HA	1:A:663:PRO:HD3	1.89	0.41
1:A:446:LYS:HE3	2:B:125:GLU:OE2	2.20	0.41
1:C:249:ARG:HB2	2:D:67:TYR:CZ	2.56	0.41
1:C:235:VAL:CG1	1:C:256:ASN:HB2	2.41	0.41
1:C:561:THR:HG21	1:C:611:ILE:HD12	2.03	0.41
2:J:158:PHE:C	2:J:160:LEU:H	2.24	0.41
1:C:261:TYR:CE2	1:C:423:GLY:HA2	2.55	0.41
1:C:461:ALA:HB1	1:C:475:SER:HB3	2.02	0.41
1:E:18:PRO:HA	1:E:217:ASN:HB3	2.02	0.41
1:E:418:HIS:C	1:E:420:GLY:H	2.24	0.41
1:E:112:HIS:CE1	2:F:129:LEU:HD13	2.56	0.41
1:G:14:ALA:O	1:G:15:ILE:HG22	2.21	0.41
1:G:276:ASN:ND2	1:G:421:CYS:H	2.19	0.41
1:I:45:ARG:HA	1:I:45:ARG:HD2	1.90	0.41
2:D:69:ASP:HA	1:I:543:ARG:HB2	2.03	0.41
1:A:15:ILE:HA	1:A:217:ASN:ND2	2.32	0.41
2:D:63:THR:HG22	2:D:64:ALA:N	2.36	0.41
1:G:279:VAL:CG2	1:G:279:VAL:O	2.68	0.41
2:H:166:ASN:HB3	1:I:156:VAL:O	2.21	0.41
1:I:205:ARG:NH2	1:I:205:ARG:CG	2.67	0.41
1:I:418:HIS:C	1:I:420:GLY:H	2.24	0.41
1:K:280:PRO:HB2	1:K:282:ARG:HE	1.85	0.41
1:K:639:PHE:HB2	1:K:656:LYS:HB3	2.03	0.41
1:I:235:VAL:CG1	1:I:256:ASN:HB2	2.44	0.41
2:J:25:CYS:HA	2:J:26:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:ARG:HG2	1:K:161:TRP:CE2	2.56	0.41
1:K:614:ARG:NH2	1:K:640:VAL:HG23	2.36	0.41
2:L:158:PHE:O	2:L:159:ASP:HB2	2.21	0.41
1:A:190:ARG:HG3	1:A:214:LEU:HB2	2.03	0.41
1:C:111:ARG:HD3	2:D:135:LEU:HD22	2.03	0.41
2:D:20:ALA:HB3	4:D:2000:SF4:S4	2.61	0.41
1:E:155:PRO:HG2	1:E:157:ARG:HG3	2.03	0.41
1:G:380:GLU:O	1:G:384:ASP:HB2	2.21	0.41
1:I:12:GLY:HA3	1:I:587:ASP:OD1	2.21	0.41
1:I:656:LYS:HA	1:I:657:PRO:HD2	1.85	0.41
1:K:182:LEU:O	1:K:186:ARG:HD3	2.21	0.41
1:A:154:LYS:HE2	1:A:155:PRO:HD2	2.03	0.40
1:C:139:GLY:H	1:C:166:ASN:HD21	1.68	0.40
1:C:607:HIS:O	1:C:611:ILE:HG23	2.22	0.40
1:E:125:LEU:HA	1:E:126:PRO:HD3	1.94	0.40
1:G:518:TYR:CE2	1:G:586:ARG:HG2	2.56	0.40
1:K:303:ASN:HB2	1:K:348:ARG:O	2.21	0.40
1:A:239:ARG:HA	1:A:240:PRO:HD3	1.84	0.40
1:E:178:ALA:O	1:E:182:LEU:HB2	2.21	0.40
1:E:544:LEU:O	1:E:548:THR:HG23	2.21	0.40
1:G:208:GLY:HA3	1:G:222:PHE:O	2.20	0.40
1:I:92:MET:HG2	1:I:161:TRP:NE1	2.36	0.40
1:A:271:MET:HG3	1:A:606:LEU:HD21	2.02	0.40
1:C:614:ARG:NH2	1:C:640:VAL:HG23	2.37	0.40
1:E:296:LEU:HD22	1:E:374:LEU:HD22	2.03	0.40
2:J:159:ASP:OD1	1:K:282:ARG:NH2	2.55	0.40
1:K:355:THR:OG1	1:K:404:GLY:HA2	2.22	0.40
1:K:548:THR:HG22	1:K:608:MET:HE1	2.02	0.40
2:B:25:CYS:HA	2:B:26:PRO:HD3	1.94	0.40
1:E:279:VAL:HG22	1:E:279:VAL:O	2.22	0.40
1:E:88:ASP:HA	1:E:91:ARG:HB2	2.03	0.40
1:G:274:MET:HB2	1:G:610:HIS:CG	2.56	0.40
1:K:321:GLU:HB3	1:K:326:ALA:HB3	2.03	0.40
1:A:274:MET:HB2	1:A:610:HIS:CG	2.57	0.40
1:C:139:GLY:H	1:C:166:ASN:ND2	2.19	0.40
1:G:239:ARG:HA	1:G:240:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	660/662 (100%)	600 (91%)	45 (7%)	15 (2%)	6	34
1	C	660/662 (100%)	612 (93%)	42 (6%)	6 (1%)	17	56
1	E	660/662 (100%)	604 (92%)	45 (7%)	11 (2%)	9	42
1	G	660/662 (100%)	618 (94%)	32 (5%)	10 (2%)	10	44
1	I	660/662 (100%)	610 (92%)	36 (6%)	14 (2%)	7	37
1	K	660/662 (100%)	612 (93%)	32 (5%)	16 (2%)	6	34
2	B	164/166 (99%)	147 (90%)	12 (7%)	5 (3%)	4	28
2	D	164/166 (99%)	145 (88%)	17 (10%)	2 (1%)	13	49
2	F	164/166 (99%)	145 (88%)	15 (9%)	4 (2%)	6	34
2	H	164/166 (99%)	142 (87%)	19 (12%)	3 (2%)	8	41
2	J	164/166 (99%)	154 (94%)	7 (4%)	3 (2%)	8	41
2	L	164/166 (99%)	147 (90%)	14 (8%)	3 (2%)	8	41
All	All	4944/4968 (100%)	4536 (92%)	316 (6%)	92 (2%)	8	39

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLU
1	A	329	HIS
1	A	441	ARG
2	B	17	GLU
2	B	161	PRO
2	D	161	PRO
1	E	291	GLY
1	G	496	PHE
2	H	147	GLN
1	I	11	ARG
1	I	13	VAL
1	K	10	PRO

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Mol	Chain	Res	Type
1	K	327	LYS
1	K	329	HIS
1	K	355	THR
2	L	161	PRO
1	A	14	ALA
1	A	82	GLY
2	B	165	GLY
1	C	461	ALA
2	D	152	GLU
1	E	290	VAL
1	E	366	MET
1	E	402	GLU
1	E	441	ARG
2	F	162	CYS
1	I	157	ARG
1	I	328	GLY
1	I	329	HIS
1	I	441	ARG
1	K	13	VAL
1	K	461	ALA
2	L	164	GLY
1	A	15	ILE
1	A	154	LYS
1	A	327	LYS
1	A	430	ASP
1	A	461	ALA
2	B	147	GLN
2	B	159	ASP
1	E	11	ARG
2	F	67	TYR
2	F	161	PRO
1	G	15	ILE
1	G	136	ASN
1	G	441	ARG
2	H	164	GLY
1	I	14	ALA
2	J	147	GLN
1	K	11	ARG
1	K	14	ALA
1	K	136	ASN
1	K	154	LYS
1	K	160	ARG

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Mol	Chain	Res	Type
1	A	157	ARG
1	C	154	LYS
1	E	14	ALA
1	E	15	ILE
1	G	151	ASN
1	I	15	ILE
1	I	154	LYS
1	I	327	LYS
1	K	157	ARG
1	K	184	GLN
1	K	497	LYS
1	A	20	ILE
1	A	83	ASP
1	C	15	ILE
1	C	20	ILE
1	E	20	ILE
1	E	371	GLN
1	E	497	LYS
1	G	20	ILE
1	G	497	LYS
2	H	161	PRO
1	I	20	ILE
1	I	419	SER
1	I	496	PHE
2	J	162	CYS
1	K	15	ILE
1	K	20	ILE
2	L	147	GLN
1	A	328	GLY
1	G	14	ALA
2	J	161	PRO
1	C	10	PRO
1	G	328	GLY
1	G	663	PRO
1	A	497	LYS
2	F	164	GLY
1	C	13	VAL
1	I	663	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	540/540 (100%)	499 (92%)	41 (8%)	13	45
1	C	540/540 (100%)	494 (92%)	46 (8%)	10	38
1	E	540/540 (100%)	490 (91%)	50 (9%)	9	33
1	G	540/540 (100%)	494 (92%)	46 (8%)	10	38
1	I	540/540 (100%)	493 (91%)	47 (9%)	10	37
1	K	540/540 (100%)	499 (92%)	41 (8%)	13	45
2	B	139/139 (100%)	132 (95%)	7 (5%)	24	60
2	D	139/139 (100%)	130 (94%)	9 (6%)	17	51
2	F	139/139 (100%)	126 (91%)	13 (9%)	8	33
2	H	139/139 (100%)	133 (96%)	6 (4%)	29	64
2	J	139/139 (100%)	127 (91%)	12 (9%)	10	38
2	L	139/139 (100%)	121 (87%)	18 (13%)	4	19
All	All	4074/4074 (100%)	3738 (92%)	336 (8%)	11	41

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	25	VAL
1	A	57	LEU
1	A	92	MET
1	A	109	LEU
1	A	111	ARG
1	A	162	GLN
1	A	170	TYR
1	A	172	VAL
1	A	186	ARG
1	A	191	ILE
1	A	194	VAL
1	A	206	ILE
1	A	228	VAL

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Mol	Chain	Res	Type
1	A	249	ARG
1	A	267	VAL
1	A	279	VAL
1	A	295	LEU
1	A	331	ILE
1	A	337	ASN
1	A	341	LEU
1	A	342	ARG
1	A	343	GLU
1	A	381	ASP
1	A	383	LEU
1	A	408	MET
1	A	415	LEU
1	A	447	VAL
1	A	449	ASN
1	A	450	ARG
1	A	478	GLU
1	A	520	LYS
1	A	527	CYS
1	A	541	MET
1	A	560	ASN
1	A	565	LEU
1	A	601	LEU
1	A	602	TRP
1	A	629	LEU
1	A	631	LEU
1	A	651	THR
2	B	63	THR
2	B	80	LEU
2	B	85	ASP
2	B	91	LYS
2	B	129	LEU
2	B	136	THR
2	B	148	ILE
1	C	11	ARG
1	C	21	VAL
1	C	25	VAL
1	C	45	ARG
1	C	49	LYS
1	C	84	ASN
1	C	92	MET
1	C	109	LEU

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Mol	Chain	Res	Type
1	C	111	ARG
1	C	151	ASN
1	C	162	GLN
1	C	184	GLN
1	C	185	ASP
1	C	191	ILE
1	C	200	LYS
1	C	206	ILE
1	C	210	VAL
1	C	235	VAL
1	C	237	VAL
1	C	252	TYR
1	C	267	VAL
1	C	279	VAL
1	C	290	VAL
1	C	298	LYS
1	C	300	LYS
1	C	337	ASN
1	C	341	LEU
1	C	343	GLU
1	C	353	MET
1	C	371	GLN
1	C	381	ASP
1	C	408	MET
1	C	419	SER
1	C	446	LYS
1	C	447	VAL
1	C	450	ARG
1	C	455	GLU
1	C	501	VAL
1	C	538	LYS
1	C	560	ASN
1	C	565	LEU
1	C	575	MET
1	C	602	TRP
1	C	629	LEU
1	C	631	LEU
1	C	648	LYS
2	D	14	LYS
2	D	18	LYS
2	D	23	TYR
2	D	59	GLN

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Mol	Chain	Res	Type
2	D	65	ARG
2	D	101	LYS
2	D	148	ILE
2	D	152	GLU
2	D	163	GLU
1	E	15	ILE
1	E	19	ILE
1	E	21	VAL
1	E	61	LYS
1	E	64	LEU
1	E	92	MET
1	E	102	ARG
1	E	111	ARG
1	E	116	SER
1	E	150	ARG
1	E	162	GLN
1	E	170	TYR
1	E	182	LEU
1	E	184	GLN
1	E	185	ASP
1	E	191	ILE
1	E	210	VAL
1	E	228	VAL
1	E	249	ARG
1	E	267	VAL
1	E	273	MET
1	E	279	VAL
1	E	298	LYS
1	E	330	VAL
1	E	337	ASN
1	E	341	LEU
1	E	359	LEU
1	E	366	MET
1	E	383	LEU
1	E	401	GLU
1	E	403	ARG
1	E	408	MET
1	E	410	THR
1	E	415	LEU
1	E	447	VAL
1	E	449	ASN
1	E	450	ARG

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Mol	Chain	Res	Type
1	E	455	GLU
1	E	497	LYS
1	E	502	GLU
1	E	505	GLU
1	E	506	GLU
1	E	513	ARG
1	E	527	CYS
1	E	538	LYS
1	E	560	ASN
1	E	602	TRP
1	E	629	LEU
1	E	631	LEU
1	E	652	LYS
2	F	14	LYS
2	F	18	LYS
2	F	65	ARG
2	F	80	LEU
2	F	89	THR
2	F	91	LYS
2	F	99	ARG
2	F	104	ILE
2	F	125	GLU
2	F	131	THR
2	F	142	LEU
2	F	163	GLU
2	F	167	ARG
1	G	17	GLU
1	G	19	ILE
1	G	21	VAL
1	G	25	VAL
1	G	49	LYS
1	G	92	MET
1	G	95	THR
1	G	111	ARG
1	G	132	GLU
1	G	138	ASP
1	G	151	ASN
1	G	160	ARG
1	G	162	GLN
1	G	170	TYR
1	G	191	ILE
1	G	194	VAL

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Mol	Chain	Res	Type
1	G	200	LYS
1	G	201	ASN
1	G	228	VAL
1	G	235	VAL
1	G	249	ARG
1	G	252	TYR
1	G	254	VAL
1	G	300	LYS
1	G	312	THR
1	G	323	ARG
1	G	337	ASN
1	G	370	GLN
1	G	381	ASP
1	G	383	LEU
1	G	410	THR
1	G	437	ASP
1	G	447	VAL
1	G	449	ASN
1	G	505	GLU
1	G	506	GLU
1	G	509	THR
1	G	557	THR
1	G	568	THR
1	G	601	LEU
1	G	602	TRP
1	G	616	GLU
1	G	631	LEU
1	G	633	ASP
1	G	635	LYS
1	G	643	LYS
2	H	18	LYS
2	H	80	LEU
2	H	89	THR
2	H	129	LEU
2	H	136	THR
2	H	160	LEU
1	I	4	ILE
1	I	11	ARG
1	I	21	VAL
1	I	25	VAL
1	I	49	LYS
1	I	77	ILE

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Mol	Chain	Res	Type
1	I	92	MET
1	I	102	ARG
1	I	111	ARG
1	I	129	ILE
1	I	162	GLN
1	I	172	VAL
1	I	184	GLN
1	I	195	LYS
1	I	205	ARG
1	I	210	VAL
1	I	228	VAL
1	I	235	VAL
1	I	236	ASN
1	I	247	MET
1	I	249	ARG
1	I	252	TYR
1	I	276	ASN
1	I	279	VAL
1	I	282	ARG
1	I	295	LEU
1	I	322	GLU
1	I	337	ASN
1	I	353	MET
1	I	370	GLN
1	I	375	GLU
1	I	444	ASN
1	I	447	VAL
1	I	449	ASN
1	I	450	ARG
1	I	473	SER
1	I	505	GLU
1	I	506	GLU
1	I	508	LYS
1	I	527	CYS
1	I	541	MET
1	I	565	LEU
1	I	574	GLU
1	I	602	TRP
1	I	629	LEU
1	I	631	LEU
1	I	643	LYS
2	J	14	LYS

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Mol	Chain	Res	Type
2	J	18	LYS
2	J	35	GLU
2	J	65	ARG
2	J	76	THR
2	J	80	LEU
2	J	89	THR
2	J	113	LYS
2	J	129	LEU
2	J	136	THR
2	J	148	ILE
2	J	166	ASN
1	K	9	THR
1	K	19	ILE
1	K	25	VAL
1	K	85	ASN
1	K	92	MET
1	K	102	ARG
1	K	111	ARG
1	K	129	ILE
1	K	164	MET
1	K	170	TYR
1	K	172	VAL
1	K	191	ILE
1	K	205	ARG
1	K	206	ILE
1	K	210	VAL
1	K	235	VAL
1	K	267	VAL
1	K	279	VAL
1	K	295	LEU
1	K	300	LYS
1	K	312	THR
1	K	318	LYS
1	K	337	ASN
1	K	341	LEU
1	K	346	GLU
1	K	370	GLN
1	K	371	GLN
1	K	374	LEU
1	K	381	ASP
1	K	401	GLU
1	K	408	MET

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Mol	Chain	Res	Type
1	K	446	LYS
1	K	447	VAL
1	K	449	ASN
1	K	450	ARG
1	K	541	MET
1	K	565	LEU
1	K	574	GLU
1	K	602	TRP
1	K	629	LEU
1	K	648	LYS
2	L	14	LYS
2	L	18	LYS
2	L	35	GLU
2	L	77	CYS
2	L	89	THR
2	L	90	ILE
2	L	101	LYS
2	L	109	GLU
2	L	113	LYS
2	L	118	LYS
2	L	125	GLU
2	L	129	LEU
2	L	136	THR
2	L	137	VAL
2	L	139	GLN
2	L	150	ASP
2	L	152	GLU
2	L	163	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	141	GLN
1	A	162	GLN
1	A	166	ASN
1	A	217	ASN
1	A	220	HIS
1	A	236	ASN
1	A	256	ASN
1	A	266	GLN
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	370	GLN
1	A	371	GLN
1	A	418	HIS
1	A	449	ASN
1	A	476	HIS
1	A	560	ASN
1	A	597	ASN
2	B	166	ASN
1	C	23	HIS
1	C	84	ASN
1	C	141	GLN
1	C	162	GLN
1	C	217	ASN
1	C	220	HIS
1	C	236	ASN
1	C	256	ASN
1	C	266	GLN
1	C	276	ASN
1	C	337	ASN
1	C	418	HIS
1	C	560	ASN
1	C	597	ASN
1	E	141	GLN
1	E	162	GLN
1	E	166	ASN
1	E	217	ASN
1	E	236	ASN
1	E	256	ASN
1	E	276	ASN
1	E	337	ASN
1	E	418	HIS
1	E	449	ASN
1	E	476	HIS
1	E	597	ASN
2	F	144	GLN
2	F	166	ASN
1	G	23	HIS
1	G	135	HIS
1	G	141	GLN
1	G	162	GLN
1	G	166	ASN

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Mol	Chain	Res	Type
1	G	217	ASN
1	G	220	HIS
1	G	236	ASN
1	G	256	ASN
1	G	276	ASN
1	G	337	ASN
1	G	371	GLN
1	G	418	HIS
1	G	449	ASN
1	G	597	ASN
2	H	166	ASN
1	I	23	HIS
1	I	141	GLN
1	I	162	GLN
1	I	166	ASN
1	I	217	ASN
1	I	220	HIS
1	I	236	ASN
1	I	256	ASN
1	I	266	GLN
1	I	276	ASN
1	I	337	ASN
1	I	444	ASN
1	I	449	ASN
1	I	597	ASN
2	J	155	GLN
1	K	23	HIS
1	K	85	ASN
1	K	141	GLN
1	K	151	ASN
1	K	166	ASN
1	K	217	ASN
1	K	220	HIS
1	K	236	ASN
1	K	256	ASN
1	K	276	ASN
1	K	337	ASN
1	K	370	GLN
1	K	373	HIS
1	K	449	ASN
1	K	560	ASN
1	K	597	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SF4	D	2000	2	0,12,12	0.00	-	-		
4	SF4	H	2000	2	0,12,12	0.00	-	-		
4	SF4	B	2000	2	0,12,12	0.00	-	-		
4	SF4	D	1000	2	0,12,12	0.00	-	-		
4	SF4	F	1000	2	0,12,12	0.00	-	-		
4	SF4	F	2000	2	0,12,12	0.00	-	-		
4	SF4	B	1000	2	0,12,12	0.00	-	-		
4	SF4	L	1000	2	0,12,12	0.00	-	-		
4	SF4	L	2000	2	0,12,12	0.00	-	-		
4	SF4	H	1000	2	0,12,12	0.00	-	-		
3	FAD	A	1000	-	51,58,58	1.43	6 (11%)	60,89,89	1.59	8 (13%)
4	SF4	J	1000	2	0,12,12	0.00	-	-		
3	FAD	C	1000	-	51,58,58	1.40	6 (11%)	60,89,89	1.62	9 (15%)
3	FAD	E	1000	-	51,58,58	1.43	6 (11%)	60,89,89	1.64	10 (16%)
3	FAD	G	1000	-	51,58,58	1.44	6 (11%)	60,89,89	1.63	8 (13%)
3	FAD	I	1000	-	51,58,58	1.40	6 (11%)	60,89,89	1.59	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	K	1000	-	51,58,58	1.41	6 (11%)	60,89,89	1.59	8 (13%)
4	SF4	J	2000	2	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	D	2000	2	-	-	0/6/5/5
4	SF4	H	2000	2	-	-	0/6/5/5
4	SF4	B	2000	2	-	-	0/6/5/5
4	SF4	D	1000	2	-	-	0/6/5/5
4	SF4	F	1000	2	-	-	0/6/5/5
4	SF4	F	2000	2	-	-	0/6/5/5
4	SF4	B	1000	2	-	-	0/6/5/5
4	SF4	L	1000	2	-	-	0/6/5/5
4	SF4	L	2000	2	-	-	0/6/5/5
4	SF4	H	1000	2	-	-	0/6/5/5
3	FAD	A	1000	-	-	5/30/50/50	0/6/6/6
4	SF4	J	1000	2	-	-	0/6/5/5
3	FAD	C	1000	-	-	2/30/50/50	0/6/6/6
3	FAD	E	1000	-	-	5/30/50/50	0/6/6/6
3	FAD	G	1000	-	-	7/30/50/50	0/6/6/6
3	FAD	I	1000	-	-	10/30/50/50	0/6/6/6
3	FAD	K	1000	-	-	8/30/50/50	0/6/6/6
4	SF4	J	2000	2	-	-	0/6/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C10-N1	4.65	1.39	1.33
3	E	1000	FAD	C10-N1	4.60	1.39	1.33
3	K	1000	FAD	C10-N1	4.58	1.39	1.33
3	C	1000	FAD	C10-N1	4.53	1.39	1.33
3	G	1000	FAD	C10-N1	4.51	1.39	1.33
3	I	1000	FAD	C10-N1	4.48	1.39	1.33
3	E	1000	FAD	C2A-N3A	4.35	1.39	1.32
3	C	1000	FAD	C2A-N3A	4.07	1.38	1.32
3	G	1000	FAD	C2A-N3A	4.07	1.38	1.32
3	I	1000	FAD	C2A-N3A	4.05	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	FAD	C2A-N3A	4.04	1.38	1.32
3	K	1000	FAD	C2A-N3A	3.87	1.38	1.32
3	K	1000	FAD	C4X-N5	3.65	1.38	1.33
3	A	1000	FAD	C4X-N5	3.55	1.38	1.33
3	G	1000	FAD	C4X-N5	3.50	1.38	1.33
3	I	1000	FAD	C4X-N5	3.49	1.38	1.33
3	E	1000	FAD	C4X-N5	3.43	1.38	1.33
3	C	1000	FAD	C4X-N5	3.34	1.38	1.33
3	C	1000	FAD	C4-N3	3.22	1.38	1.33
3	I	1000	FAD	C4-N3	3.18	1.38	1.33
3	G	1000	FAD	C1'-N10	3.18	1.51	1.48
3	E	1000	FAD	C4-N3	3.16	1.38	1.33
3	A	1000	FAD	C4-N3	3.10	1.38	1.33
3	G	1000	FAD	C4-N3	3.07	1.38	1.33
3	A	1000	FAD	C1'-N10	3.07	1.51	1.48
3	E	1000	FAD	C1'-N10	2.90	1.51	1.48
3	K	1000	FAD	C4-N3	2.86	1.38	1.33
3	C	1000	FAD	C1'-N10	2.85	1.51	1.48
3	K	1000	FAD	C1'-N10	2.77	1.51	1.48
3	E	1000	FAD	C2A-N1A	2.74	1.39	1.33
3	G	1000	FAD	C2A-N1A	2.73	1.39	1.33
3	I	1000	FAD	C1'-N10	2.71	1.51	1.48
3	A	1000	FAD	C2A-N1A	2.62	1.38	1.33
3	I	1000	FAD	C2A-N1A	2.61	1.38	1.33
3	K	1000	FAD	C2A-N1A	2.58	1.38	1.33
3	C	1000	FAD	C2A-N1A	2.49	1.38	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1000	FAD	C4-N3-C2	6.13	120.32	115.14
3	G	1000	FAD	C4-N3-C2	6.04	120.24	115.14
3	A	1000	FAD	C4-N3-C2	5.92	120.14	115.14
3	I	1000	FAD	N3A-C2A-N1A	-5.91	119.44	128.68
3	C	1000	FAD	C4-N3-C2	5.88	120.11	115.14
3	K	1000	FAD	C4-N3-C2	5.82	120.06	115.14
3	I	1000	FAD	C4-N3-C2	5.78	120.02	115.14
3	A	1000	FAD	N3A-C2A-N1A	-5.75	119.70	128.68
3	G	1000	FAD	N3A-C2A-N1A	-5.71	119.76	128.68
3	K	1000	FAD	N3A-C2A-N1A	-5.65	119.84	128.68
3	C	1000	FAD	N3A-C2A-N1A	-5.64	119.87	128.68
3	E	1000	FAD	N3A-C2A-N1A	-5.53	120.04	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1000	FAD	C5X-C9A-N10	3.86	120.51	117.72
3	G	1000	FAD	C5X-C9A-N10	3.70	120.40	117.72
3	K	1000	FAD	C5X-C9A-N10	3.70	120.39	117.72
3	G	1000	FAD	P-O3P-PA	-3.61	120.45	132.83
3	K	1000	FAD	C4X-N5-C5X	3.49	120.26	116.77
3	A	1000	FAD	C5X-C9A-N10	3.46	120.23	117.72
3	I	1000	FAD	C4X-N5-C5X	3.45	120.22	116.77
3	C	1000	FAD	C5X-C9A-N10	3.38	120.17	117.72
3	A	1000	FAD	C4X-N5-C5X	3.35	120.12	116.77
3	C	1000	FAD	P-O3P-PA	-3.30	121.50	132.83
3	I	1000	FAD	C5X-C9A-N10	3.29	120.10	117.72
3	C	1000	FAD	C4X-N5-C5X	3.24	120.01	116.77
3	I	1000	FAD	P-O3P-PA	-3.20	121.85	132.83
3	E	1000	FAD	C4X-N5-C5X	3.19	119.95	116.77
3	E	1000	FAD	P-O3P-PA	-3.17	121.94	132.83
3	A	1000	FAD	P-O3P-PA	-3.14	122.06	132.83
3	G	1000	FAD	C4X-N5-C5X	3.10	119.87	116.77
3	G	1000	FAD	C4X-C4-N3	-2.90	119.47	123.43
3	K	1000	FAD	P-O3P-PA	-2.85	123.06	132.83
3	E	1000	FAD	C4X-C4-N3	-2.65	119.81	123.43
3	G	1000	FAD	C9A-N10-C10	-2.65	118.44	121.91
3	E	1000	FAD	C8M-C8-C9	-2.63	114.06	120.34
3	C	1000	FAD	C4X-C4-N3	-2.59	119.89	123.43
3	A	1000	FAD	C4X-C4-N3	-2.54	119.95	123.43
3	A	1000	FAD	C8M-C8-C9	-2.54	114.27	120.34
3	E	1000	FAD	C1'-N10-C10	-2.54	116.14	118.41
3	E	1000	FAD	C9A-N10-C10	-2.49	118.65	121.91
3	I	1000	FAD	C4X-C4-N3	-2.47	120.05	123.43
3	K	1000	FAD	C9A-N10-C10	-2.43	118.72	121.91
3	C	1000	FAD	C9A-N10-C10	-2.42	118.74	121.91
3	K	1000	FAD	C4X-C4-N3	-2.41	120.14	123.43
3	G	1000	FAD	C8M-C8-C9	-2.38	114.66	120.34
3	E	1000	FAD	C5A-C6A-N6A	-2.28	116.89	120.35
3	C	1000	FAD	C8M-C8-C9	-2.25	114.97	120.34
3	K	1000	FAD	C8M-C8-C9	-2.20	115.08	120.34
3	A	1000	FAD	C9A-N10-C10	-2.19	119.03	121.91
3	I	1000	FAD	C9A-N10-C10	-2.18	119.06	121.91
3	C	1000	FAD	C1'-N10-C10	-2.08	116.55	118.41

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	FAD	C5'-O5'-P-O1P
3	A	1000	FAD	C5'-O5'-P-O2P
3	E	1000	FAD	C3'-C4'-C5'-O5'
3	E	1000	FAD	O4'-C4'-C5'-O5'
3	G	1000	FAD	O4'-C4'-C5'-O5'
3	G	1000	FAD	C5'-O5'-P-O1P
3	I	1000	FAD	C5B-O5B-PA-O2A
3	I	1000	FAD	C5B-O5B-PA-O3P
3	I	1000	FAD	C2'-C1'-N10-C9A
3	I	1000	FAD	O4'-C4'-C5'-O5'
3	I	1000	FAD	C5'-O5'-P-O3P
3	K	1000	FAD	C3'-C4'-C5'-O5'
3	K	1000	FAD	O4'-C4'-C5'-O5'
3	K	1000	FAD	C5'-O5'-P-O1P
3	K	1000	FAD	C5'-O5'-P-O2P
3	C	1000	FAD	O4B-C4B-C5B-O5B
3	C	1000	FAD	C3B-C4B-C5B-O5B
3	G	1000	FAD	C3'-C4'-C5'-O5'
3	I	1000	FAD	C3'-C4'-C5'-O5'
3	I	1000	FAD	O4B-C4B-C5B-O5B
3	A	1000	FAD	PA-O3P-P-O5'
3	E	1000	FAD	PA-O3P-P-O5'
3	G	1000	FAD	PA-O3P-P-O5'
3	I	1000	FAD	PA-O3P-P-O5'
3	K	1000	FAD	PA-O3P-P-O5'
3	K	1000	FAD	C5'-O5'-P-O3P
3	G	1000	FAD	PA-O3P-P-O1P
3	I	1000	FAD	C5B-O5B-PA-O1A
3	I	1000	FAD	C5'-O5'-P-O1P
3	A	1000	FAD	O4B-C4B-C5B-O5B
3	G	1000	FAD	O4B-C4B-C5B-O5B
3	A	1000	FAD	C5'-O5'-P-O3P
3	G	1000	FAD	C5'-O5'-P-O3P
3	K	1000	FAD	O4B-C4B-C5B-O5B
3	E	1000	FAD	PA-O3P-P-O1P
3	K	1000	FAD	PA-O3P-P-O1P
3	E	1000	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

7 monomers are involved in 11 short contacts:

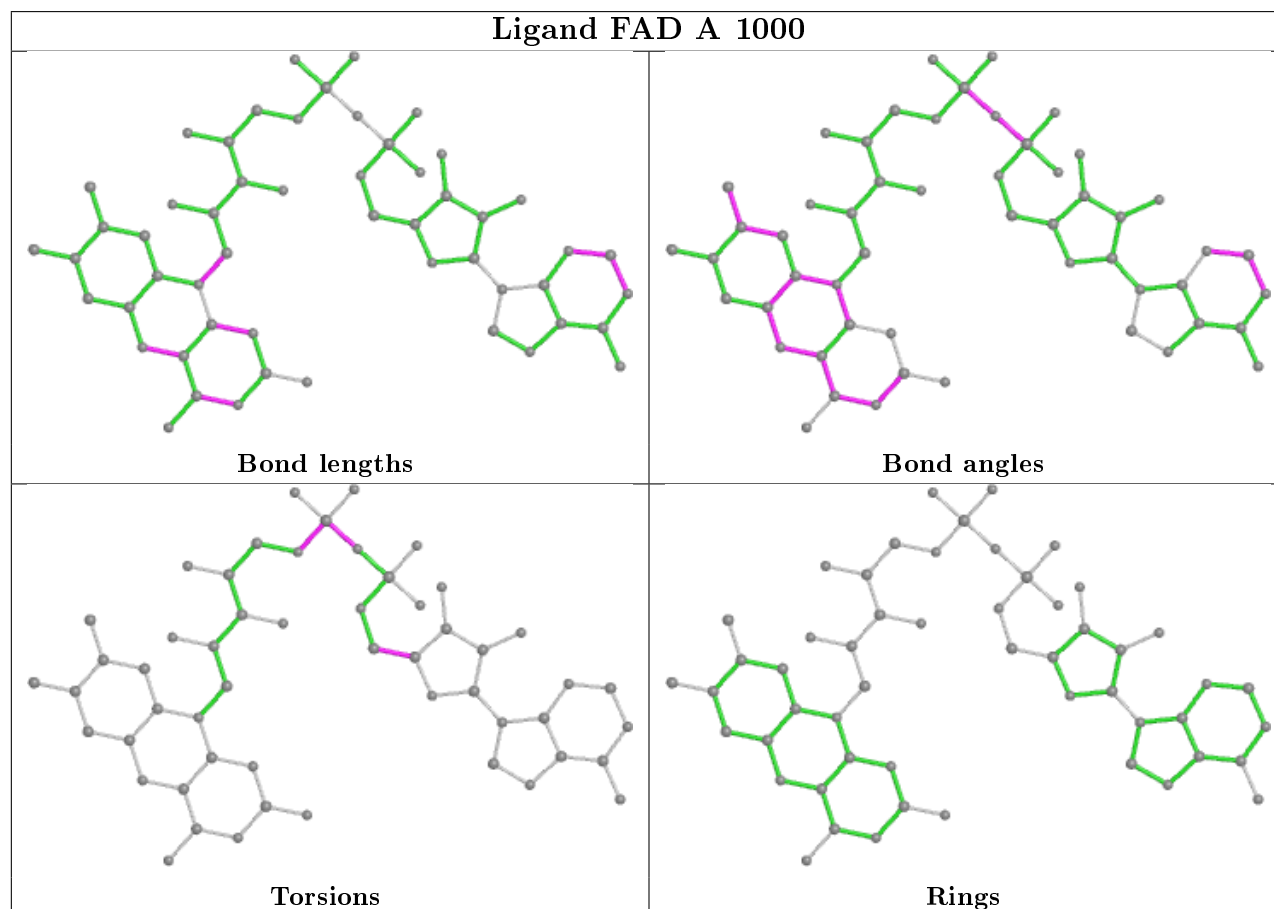
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2000	SF4	1	0

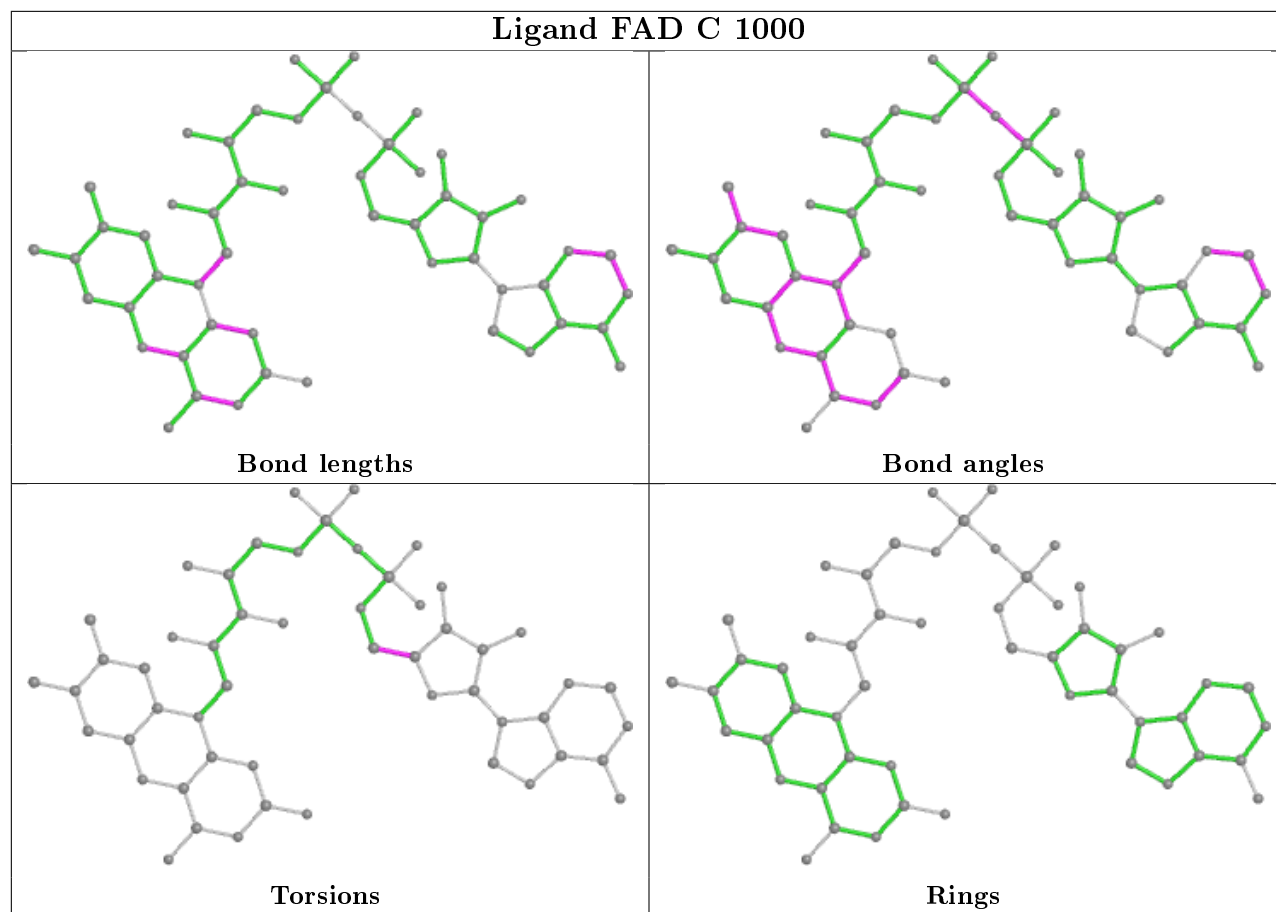
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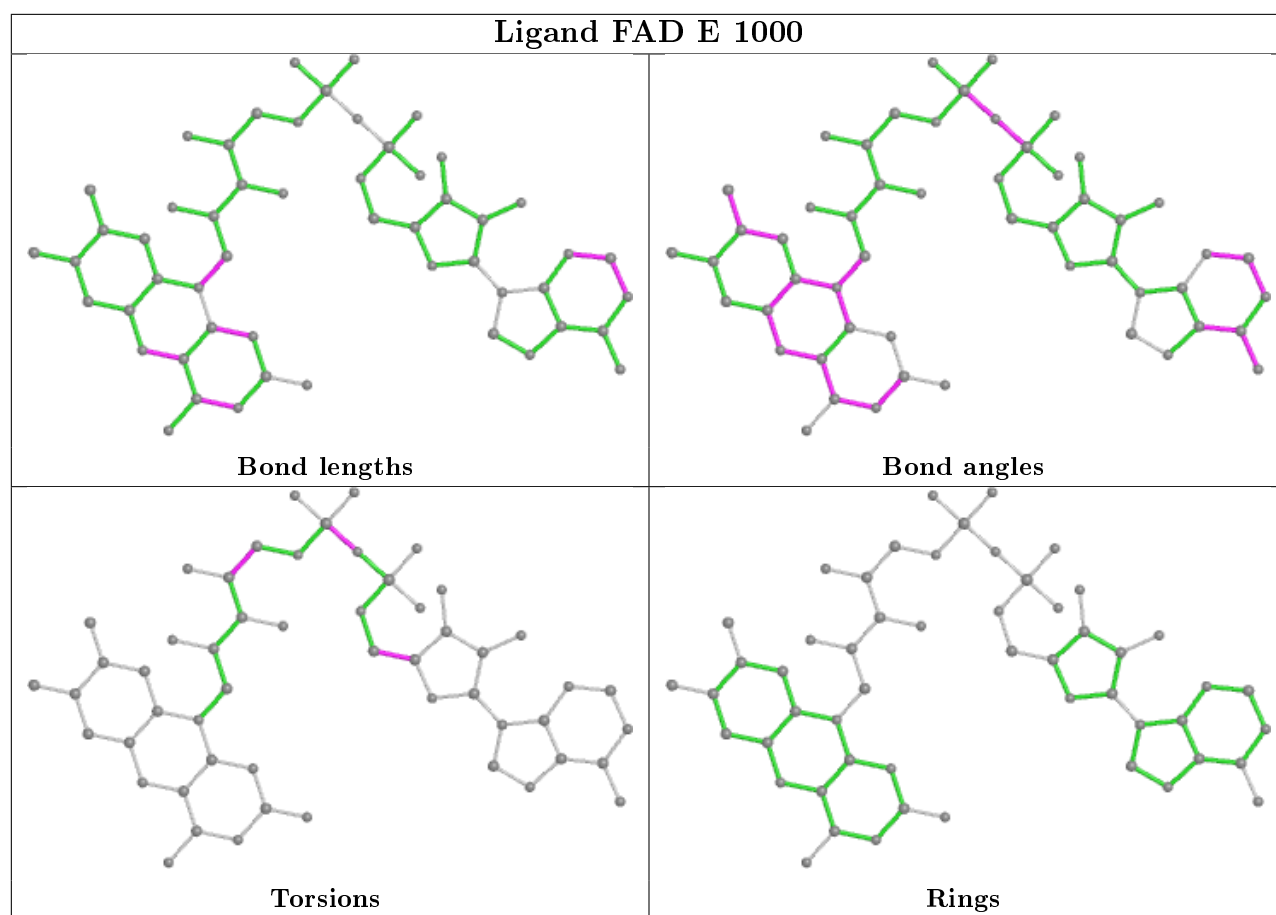
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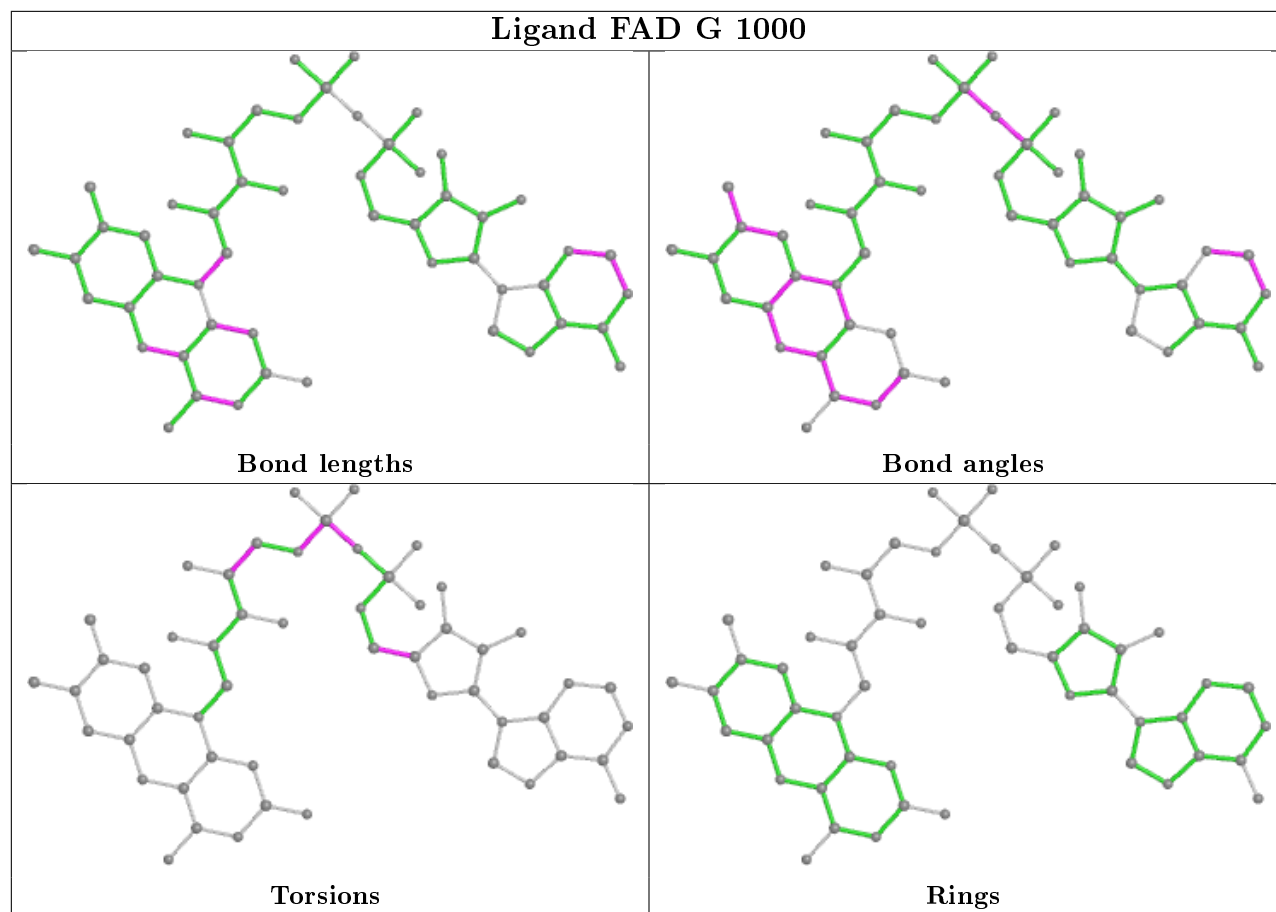
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	FAD	3	0
3	C	1000	FAD	1	0
3	E	1000	FAD	1	0
3	G	1000	FAD	1	0
3	I	1000	FAD	2	0
3	K	1000	FAD	2	0

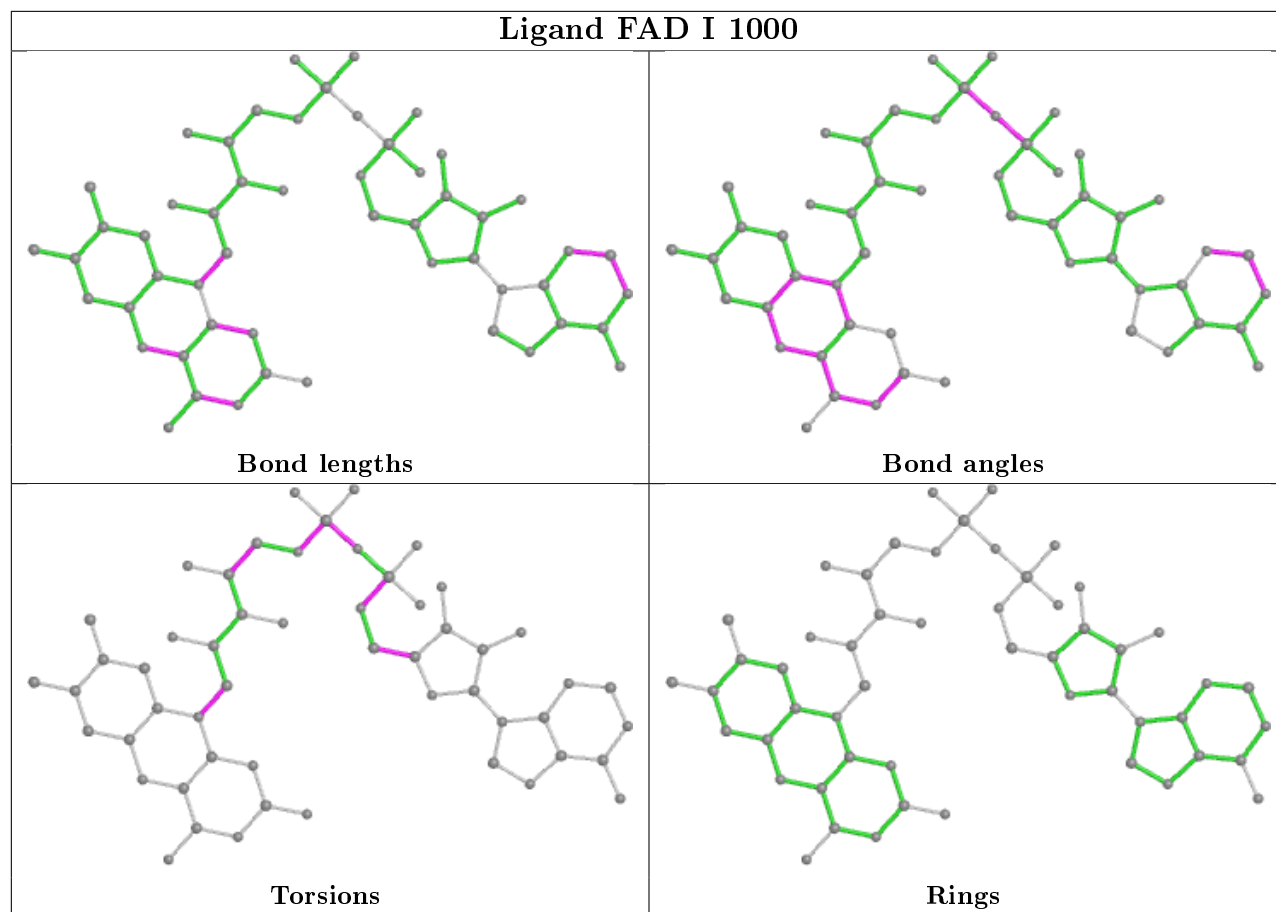
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

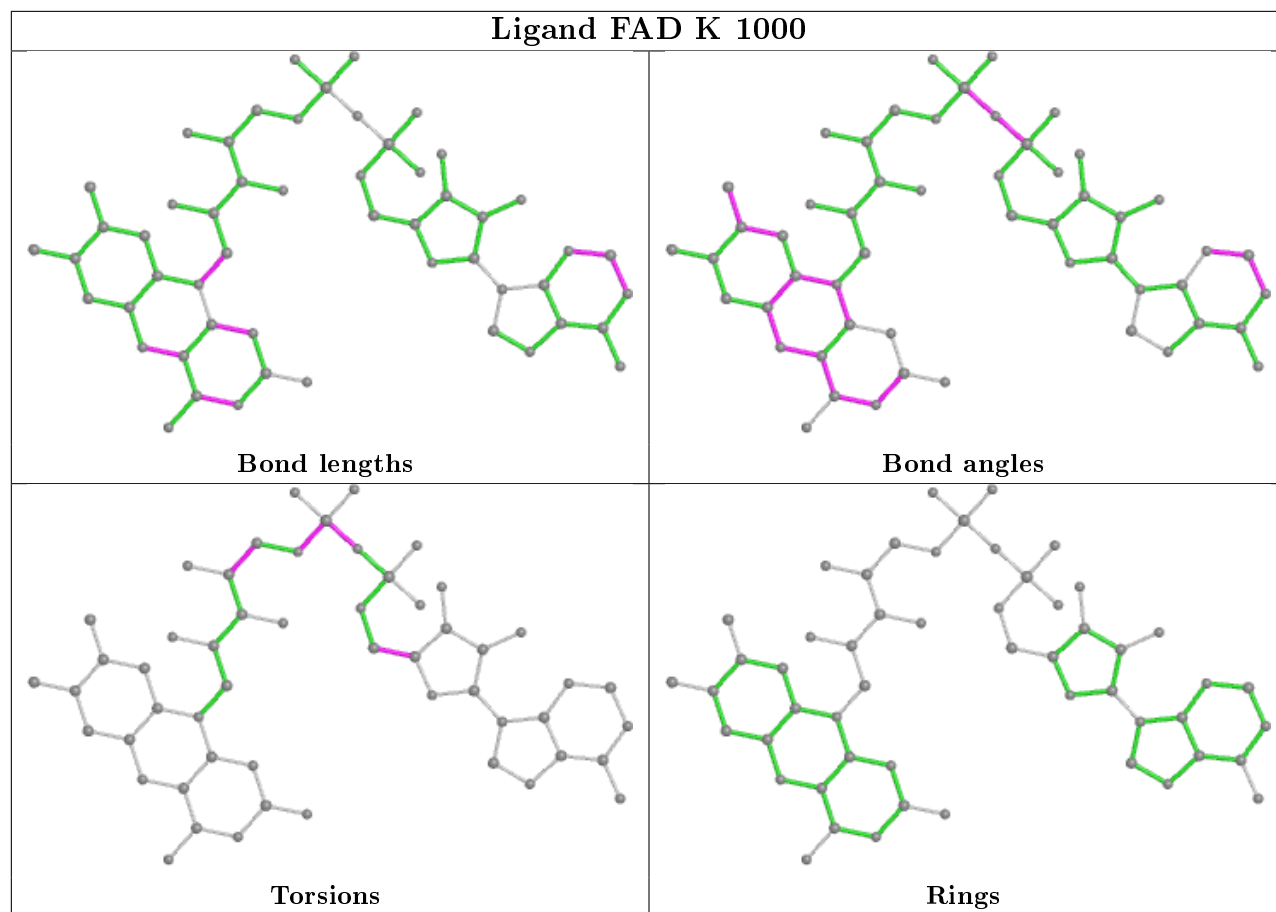












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	662/662 (100%)	-0.47	1 (0%) 95 94	32, 40, 56, 69	8 (1%)
1	C	662/662 (100%)	-0.49	2 (0%) 94 92	32, 41, 60, 73	8 (1%)
1	E	662/662 (100%)	-0.35	4 (0%) 89 83	34, 52, 69, 76	8 (1%)
1	G	662/662 (100%)	-0.45	1 (0%) 95 94	34, 44, 56, 63	8 (1%)
1	I	662/662 (100%)	-0.45	8 (1%) 79 67	28, 40, 59, 76	8 (1%)
1	K	662/662 (100%)	-0.46	3 (0%) 91 86	32, 41, 57, 66	9 (1%)
2	B	166/166 (100%)	-0.25	5 (3%) 50 34	34, 46, 73, 76	1 (0%)
2	D	166/166 (100%)	-0.27	2 (1%) 79 67	31, 43, 66, 72	1 (0%)
2	F	166/166 (100%)	-0.01	6 (3%) 42 27	43, 59, 69, 71	1 (0%)
2	H	166/166 (100%)	-0.12	8 (4%) 30 18	33, 44, 72, 78	1 (0%)
2	J	166/166 (100%)	-0.24	3 (1%) 68 55	34, 46, 59, 65	1 (0%)
2	L	166/166 (100%)	-0.20	3 (1%) 68 55	40, 50, 66, 73	1 (0%)
All	All	4968/4968 (100%)	-0.39	46 (0%) 84 75	28, 43, 64, 78	55 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	263	MET	5.3
1	C	263	MET	5.2
1	A	263	MET	4.8
2	B	17	GLU	4.2
2	B	152	GLU	3.6
1	I	329	HIS	3.5
1	K	263	MET	3.5
1	E	263	MET	3.4
2	H	15	GLY	3.4
2	D	150	ASP	3.3
1	G	263	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	133	HIS	3.1
2	L	151	ALA	3.0
1	I	364	ALA	2.9
2	J	150	ASP	2.9
2	F	17	GLU	2.9
1	C	329	HIS	2.7
2	H	17	GLU	2.6
2	H	150	ASP	2.6
2	H	152	GLU	2.6
2	B	150	ASP	2.5
1	E	328	GLY	2.5
2	J	15	GLY	2.5
2	H	144	GLN	2.5
1	K	327	LYS	2.4
2	F	153	THR	2.4
2	B	15	GLY	2.4
1	I	132	GLU	2.3
2	J	17	GLU	2.3
2	F	150	ASP	2.3
2	H	14	LYS	2.3
1	I	385	MET	2.2
2	B	16	GLY	2.2
1	I	135	HIS	2.2
1	E	146	GLY	2.2
2	D	15	GLY	2.2
1	E	133	HIS	2.1
2	H	147	GLN	2.1
1	I	365	THR	2.1
1	K	385	MET	2.1
2	F	15	GLY	2.1
2	L	150	ASP	2.1
2	F	123	ASP	2.1
2	H	83	SER	2.0
2	L	17	GLU	2.0
2	F	18	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

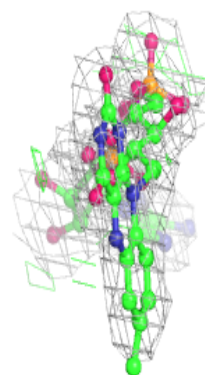
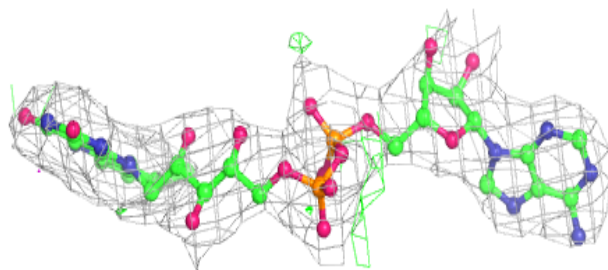
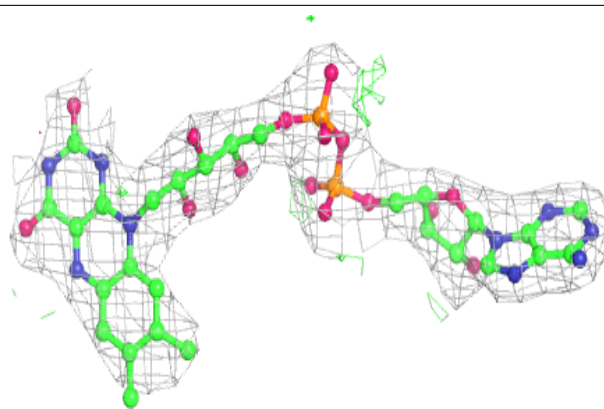
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	A	1000	53/53	0.96	0.14	31,33,38,38	0
3	FAD	I	1000	53/53	0.96	0.15	26,31,37,37	0
3	FAD	K	1000	53/53	0.96	0.15	33,35,38,38	0
3	FAD	G	1000	53/53	0.97	0.14	34,36,38,38	0
3	FAD	C	1000	53/53	0.97	0.15	32,34,41,42	0
3	FAD	E	1000	53/53	0.97	0.14	38,39,44,44	0
4	SF4	F	2000	8/8	0.98	0.06	57,59,60,60	0
4	SF4	J	2000	8/8	0.98	0.07	44,45,46,47	0
4	SF4	L	2000	8/8	0.99	0.08	52,53,54,55	0
4	SF4	H	1000	8/8	0.99	0.14	30,31,32,32	0
4	SF4	H	2000	8/8	0.99	0.07	42,44,44,45	0
4	SF4	J	1000	8/8	0.99	0.12	34,35,35,35	0
4	SF4	B	2000	8/8	0.99	0.09	49,50,50,52	0
4	SF4	D	1000	8/8	0.99	0.14	30,31,31,32	0
4	SF4	F	1000	8/8	0.99	0.13	43,44,45,45	0
4	SF4	D	2000	8/8	0.99	0.07	39,41,42,42	0
4	SF4	B	1000	8/8	0.99	0.12	33,34,34,35	0
4	SF4	L	1000	8/8	0.99	0.13	41,41,42,42	0

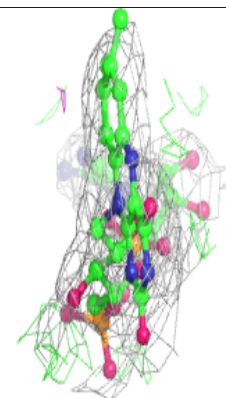
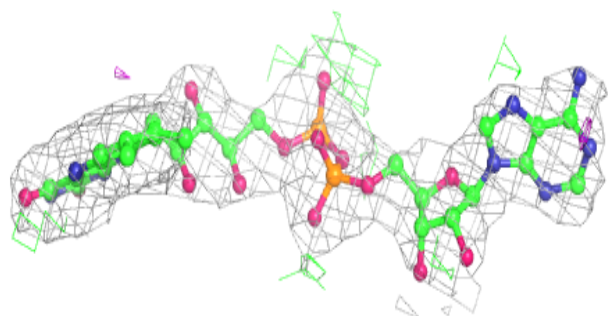
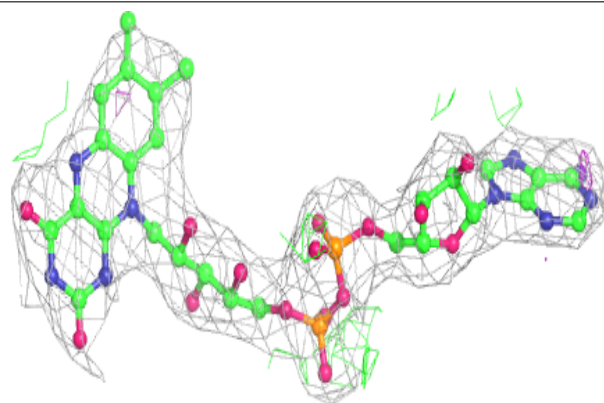
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1000:

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

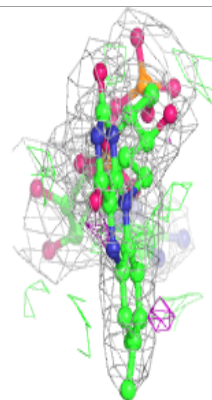
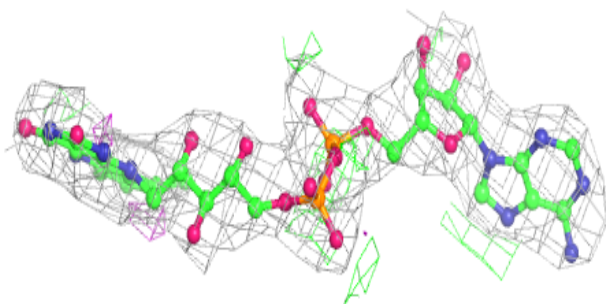
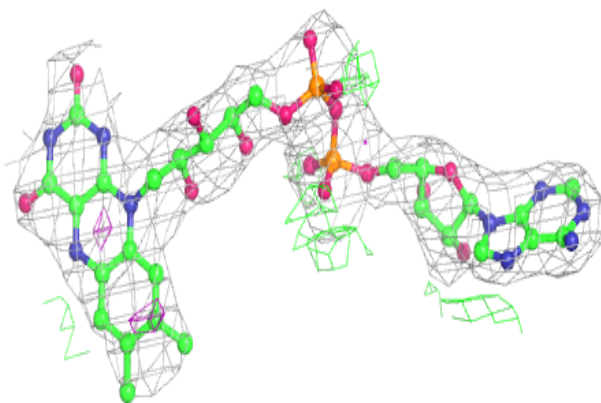
**Electron density around FAD I 1000:**

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

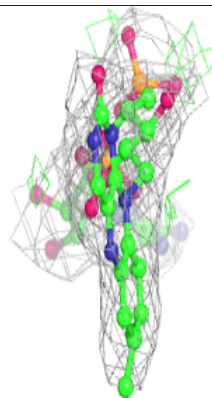
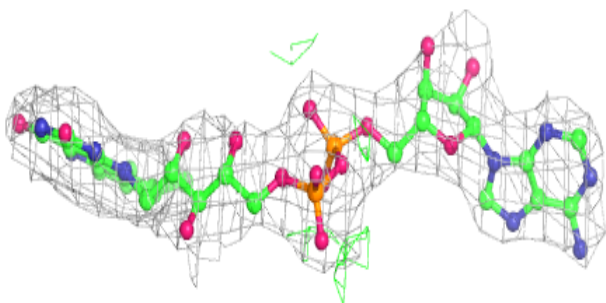
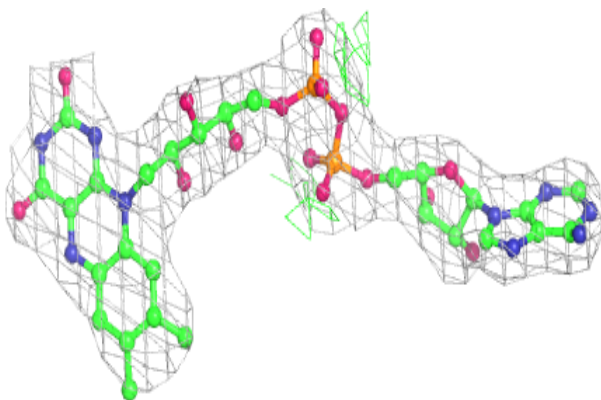


Electron density around FAD K 1000:

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

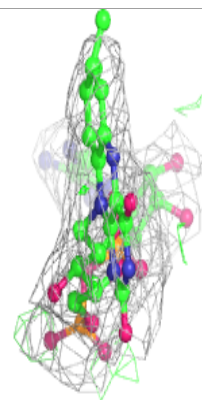
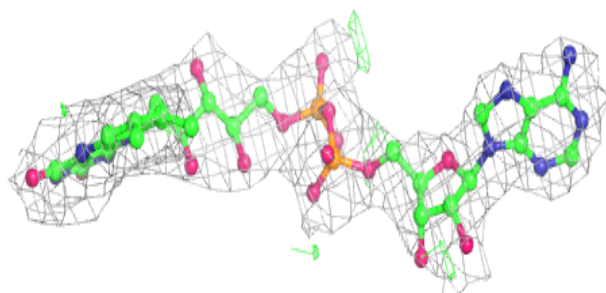
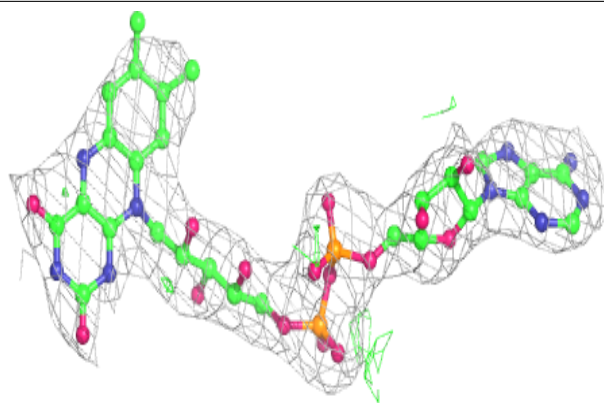
**Electron density around FAD G 1000:**

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

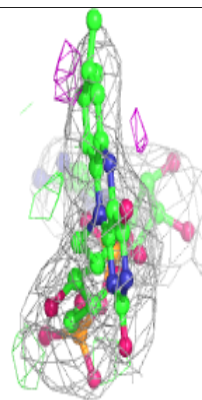
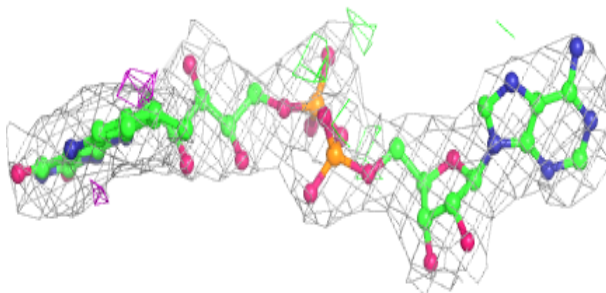
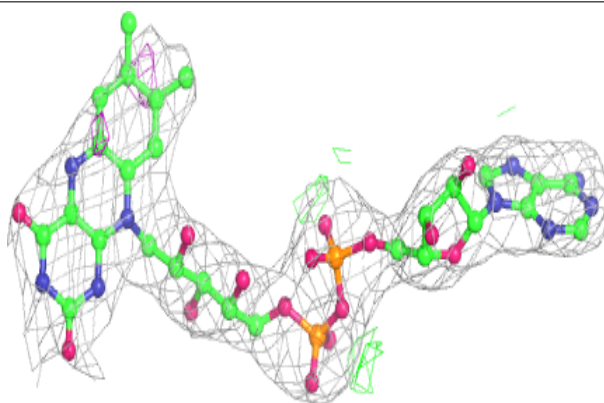


Electron density around FAD C 1000:

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

**Electron density around FAD E 1000:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.