Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:19 pm BST

PDB ID	:	3OPY
Title	:	Crystal structure of Pichia pastoris phosphofructokinase in the T-state
Authors	:	Strater, N.; Marek, S.; Kuettner, E.B.; Kloos, M.; Keim, A.; Bruser, A.; Kirchberger, J.; Schoneberg, T.
Deposited on	:	2010-09-02
Resolution	:	3.05 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:

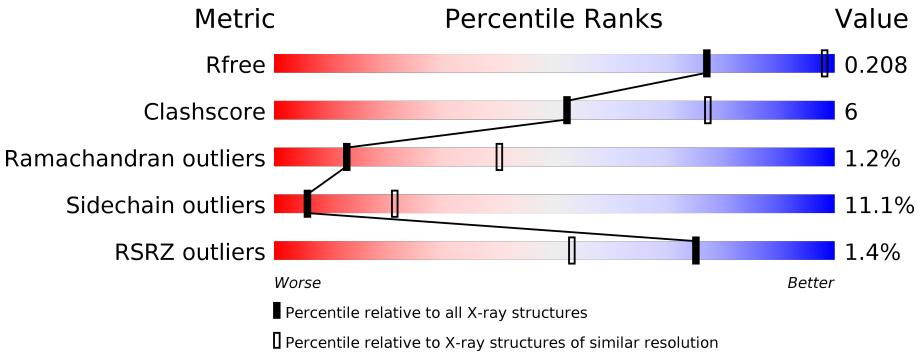
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 <=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	989	75% 18% • 5%
1	C	989	75% 17% • 5%
1	E	989	75% 17% • 5%
1	G	989	75% 17% • 5%
2	B	941	76% 16% • 6%
2	D	941	77% 16% • 6%

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Mol	Chain	Length	Quality of chain
2	F	941	3% 76% 16% 6%
2	H	941	2% 76% 16% 6%
3	I	351	65% 24% 8%
3	J	351	61% 28% 8%
3	K	351	% 67% 22% 8%
3	L	351	66% 23% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	991	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65025 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6-phosphofructo-1-kinase alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	C	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	E	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	G	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			

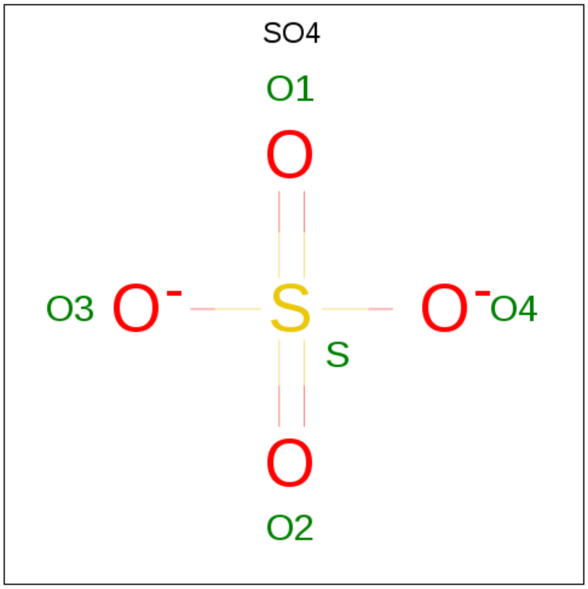
- Molecule 2 is a protein called 6-phosphofructo-1-kinase beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	D	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	F	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	H	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			

- Molecule 3 is a protein called 6-phosphofructo-1-kinase gamma-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	J	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	K	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	L	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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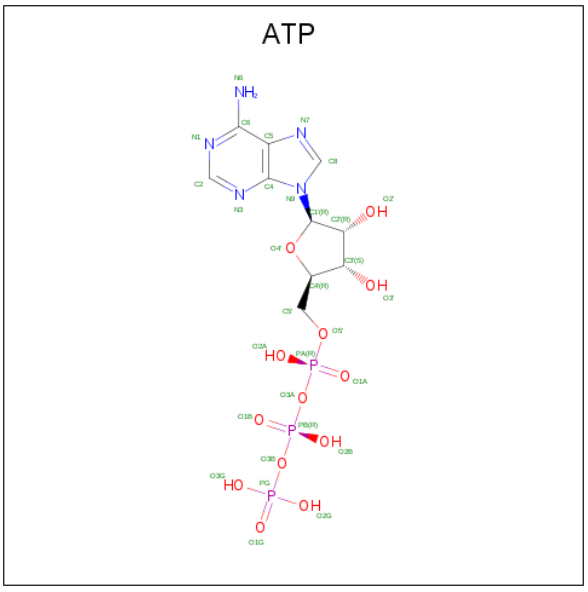
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O P 31 10 5 13 3	0	0

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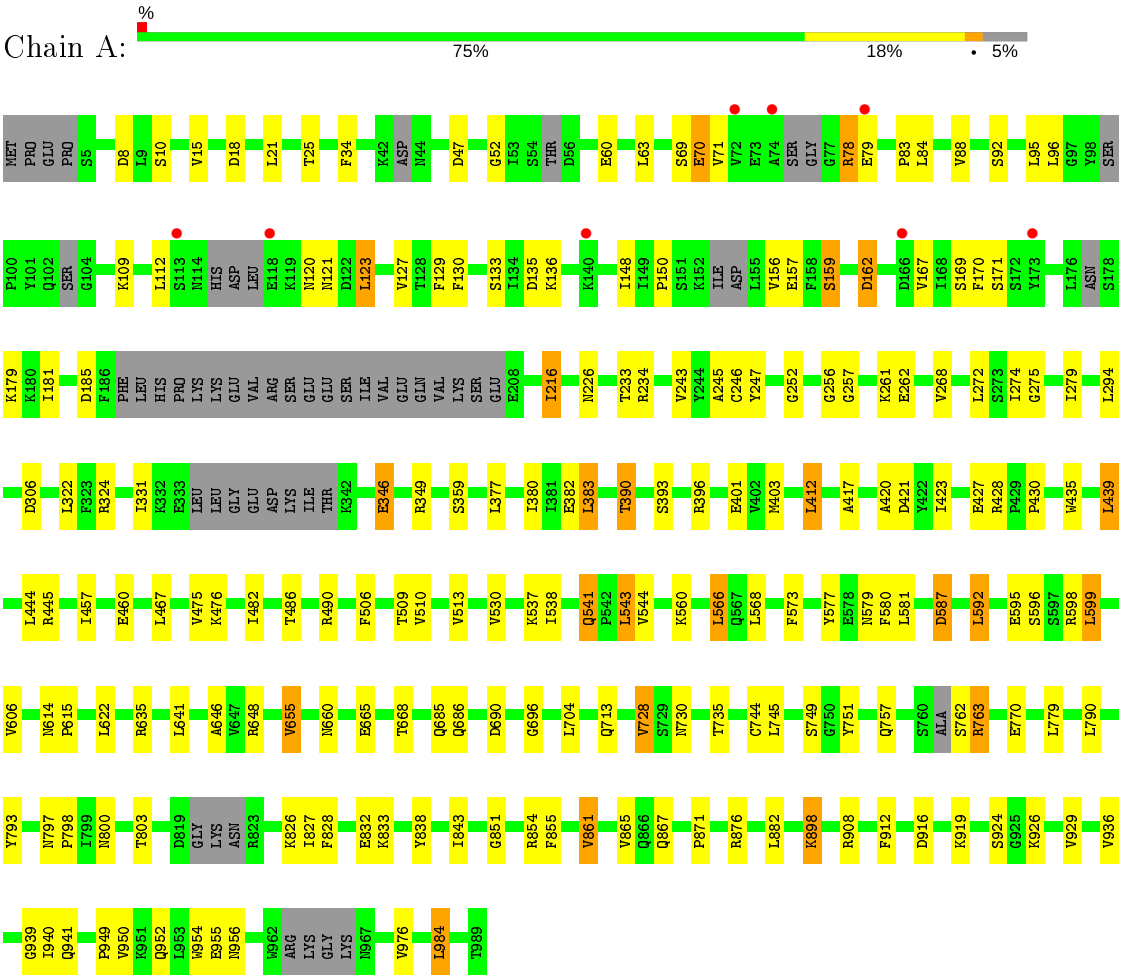
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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.

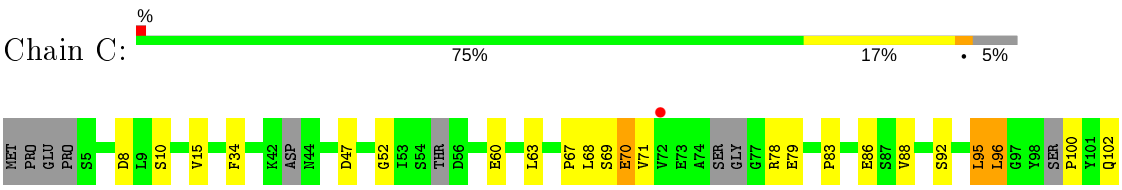
- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

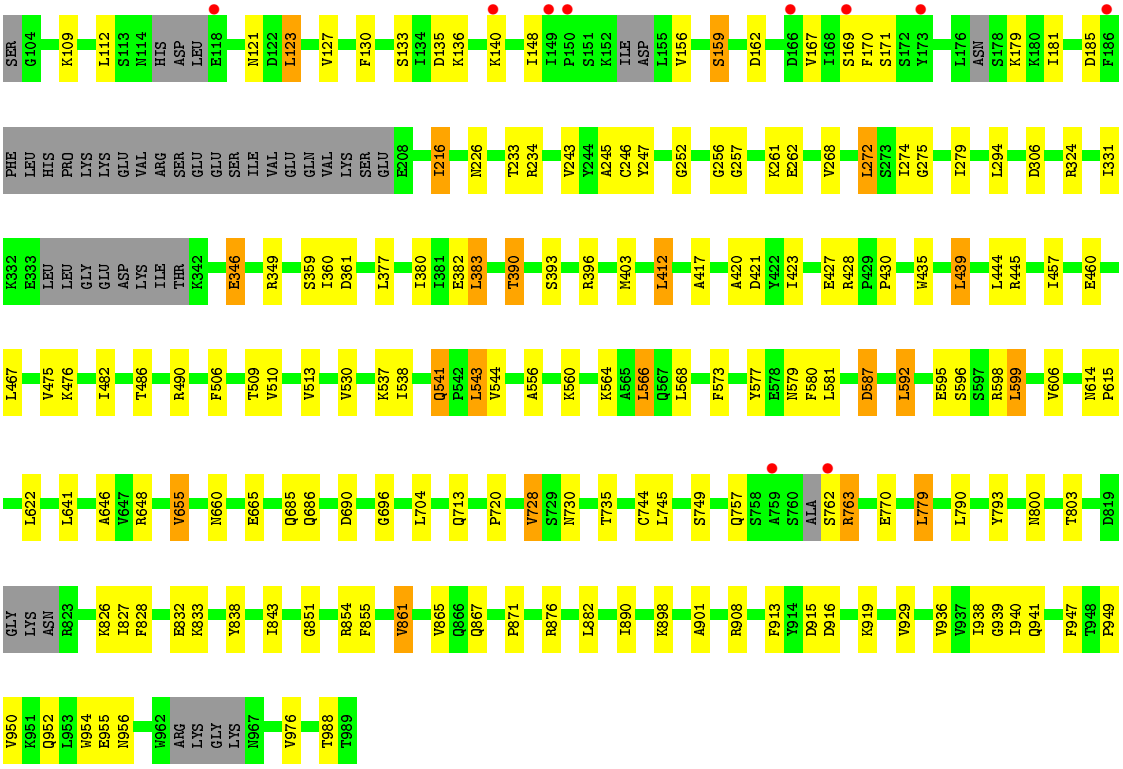
Chain A:



- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

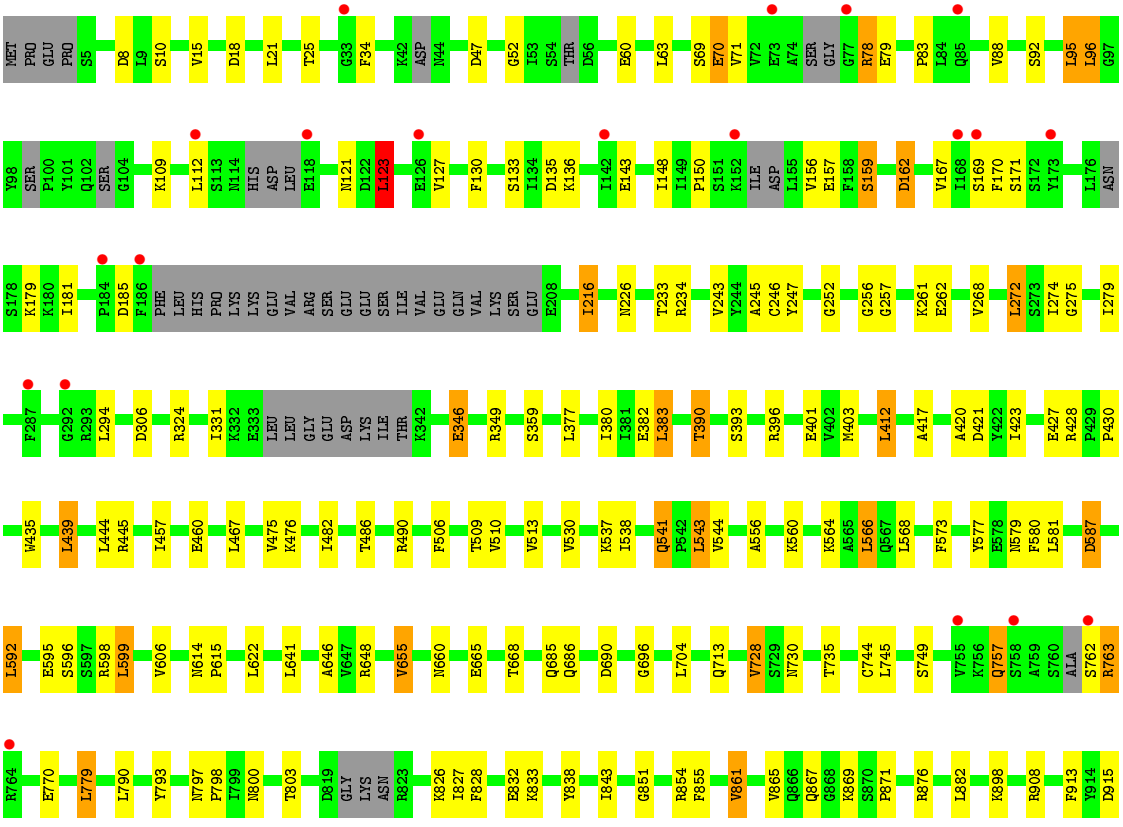
Chain C:

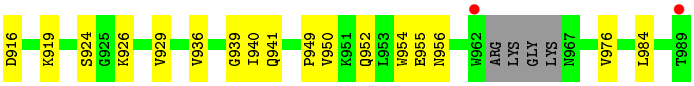




• Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

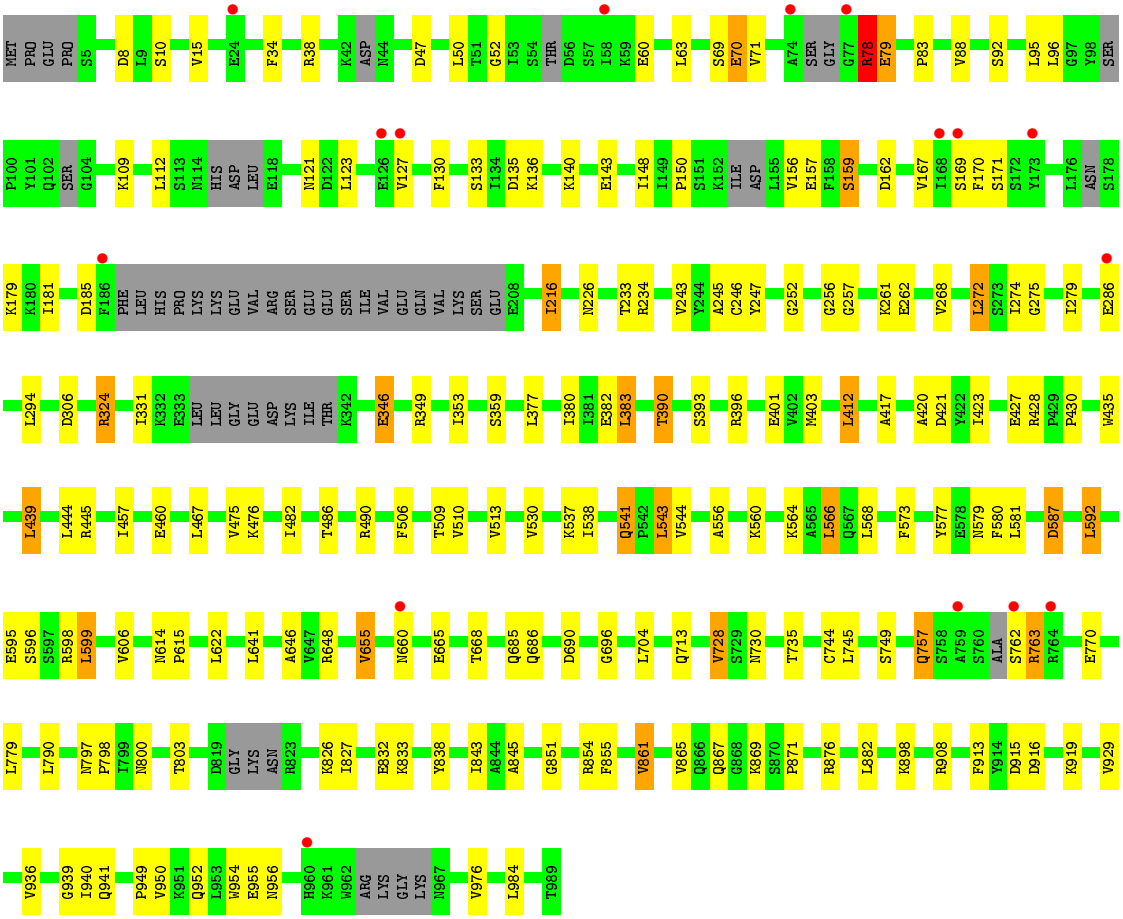
Chain E:





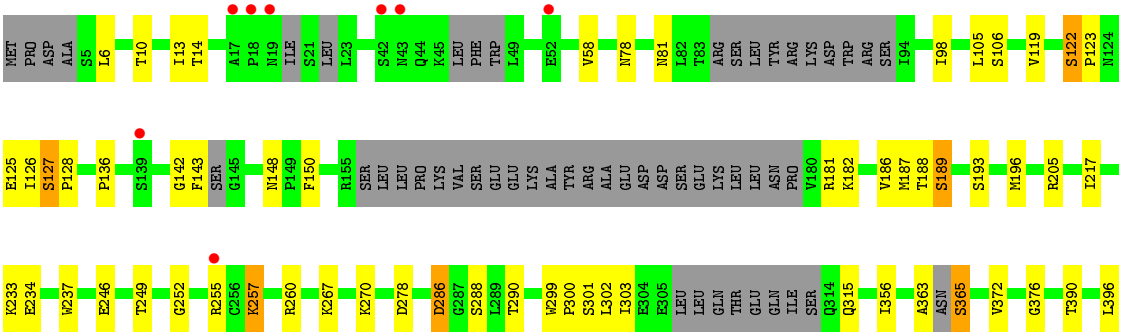
• Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

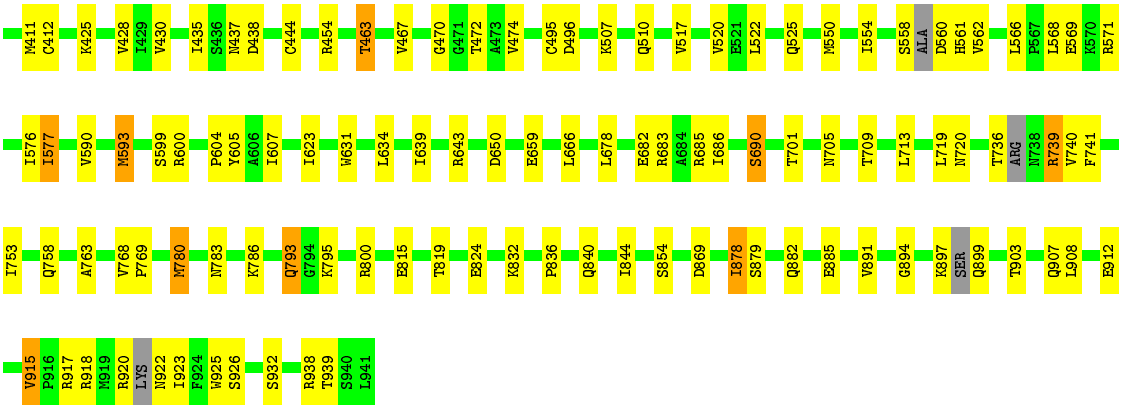
Chain G:



• Molecule 2: 6-phosphofructo-1-kinase beta-subunit

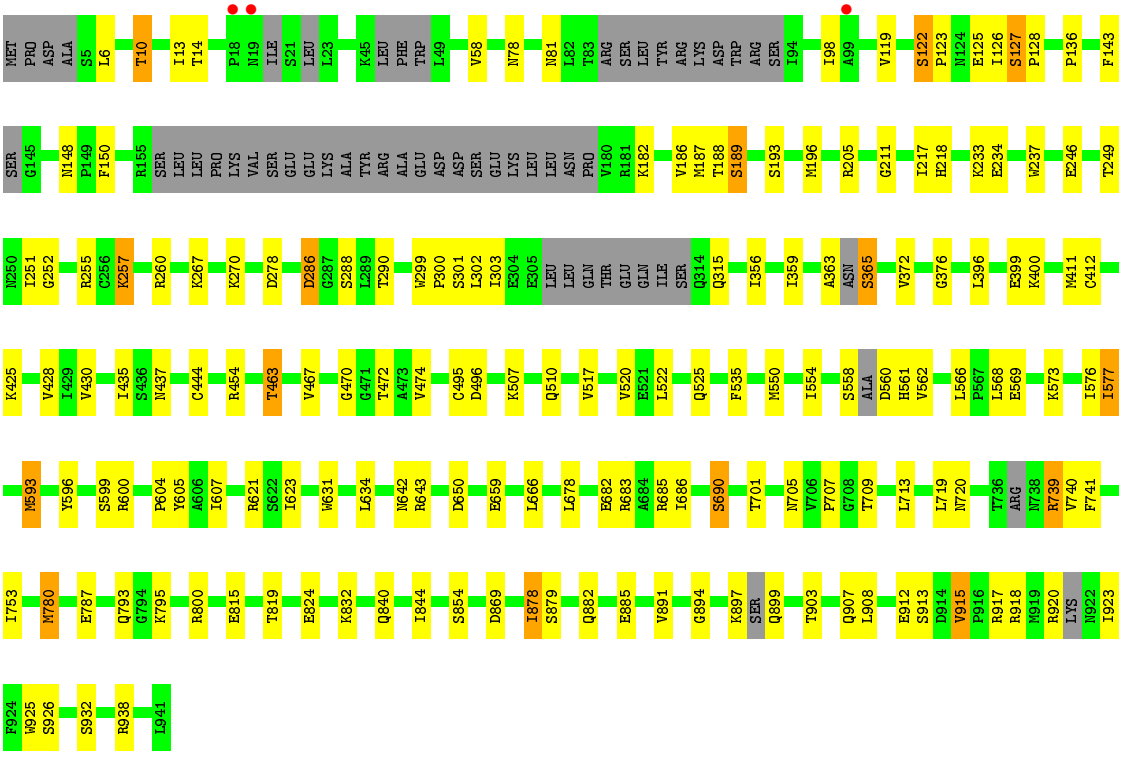
Chain B:





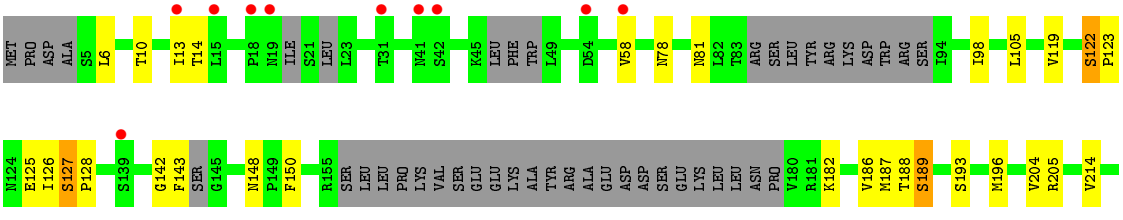
• Molecule 2: 6-phosphofructo-1-kinase beta-subunit

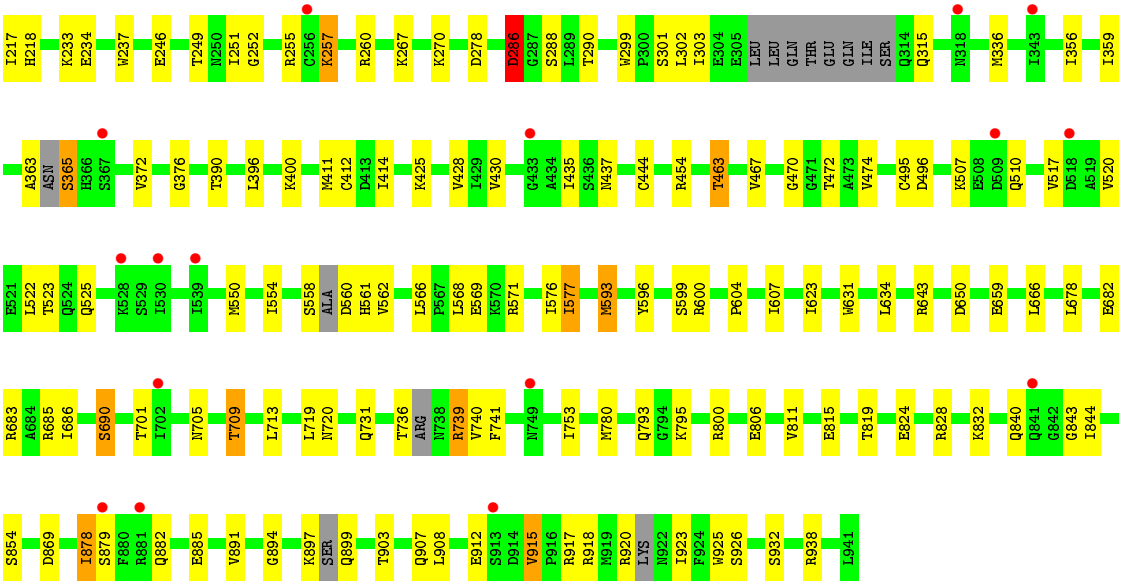
Chain D:



• Molecule 2: 6-phosphofructo-1-kinase beta-subunit

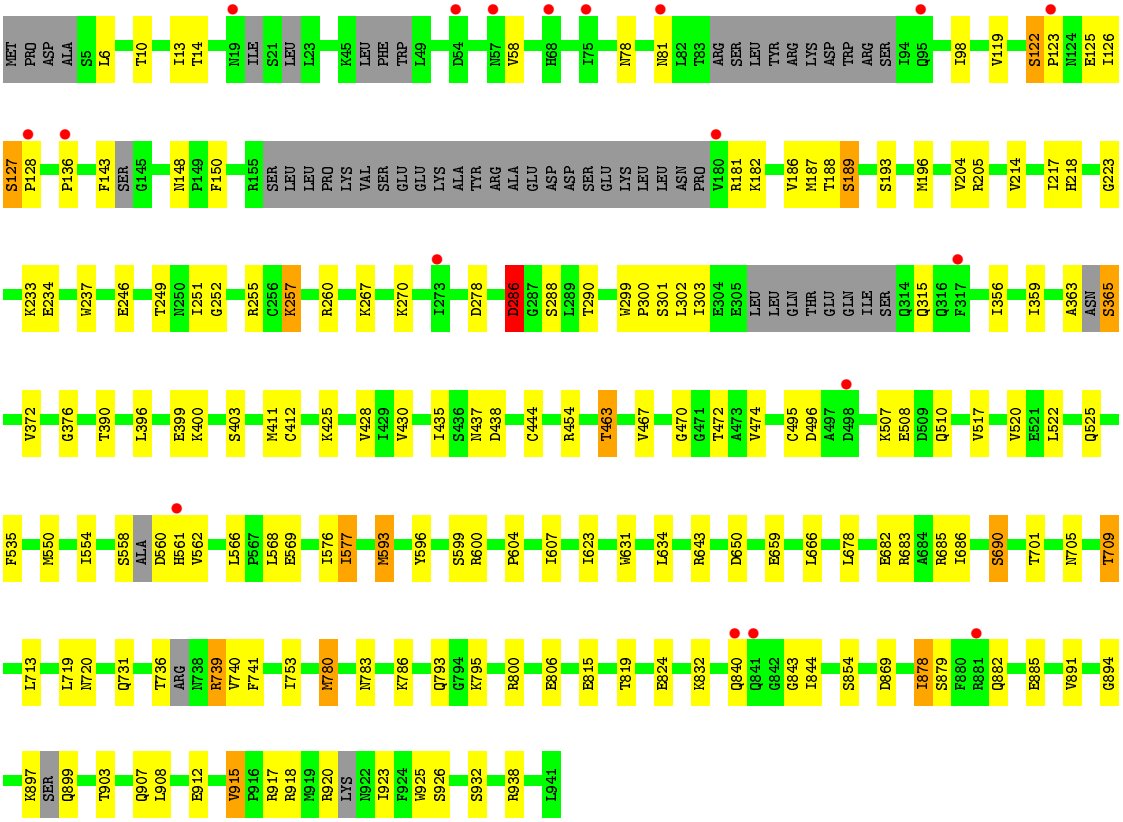
Chain F:





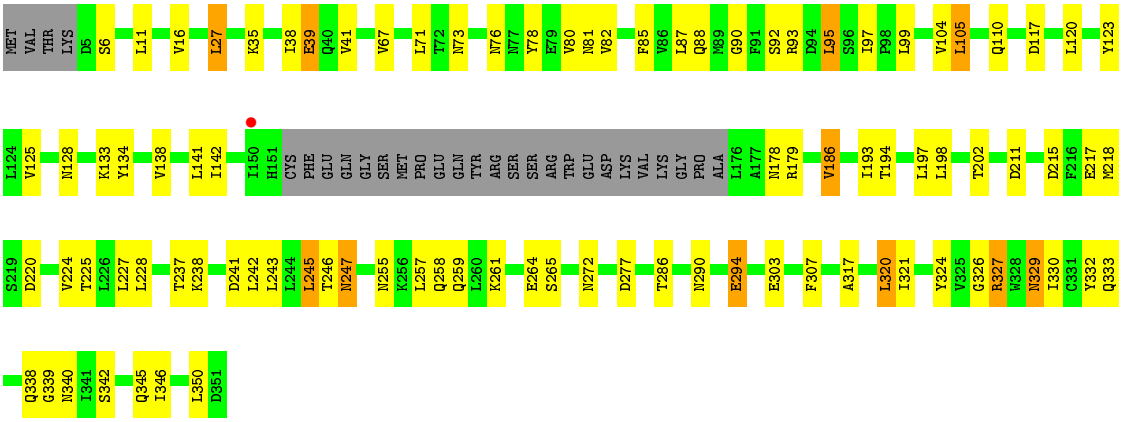
- Molecule 2: 6-phosphofructo-1-kinase beta-subunit

Chain H:



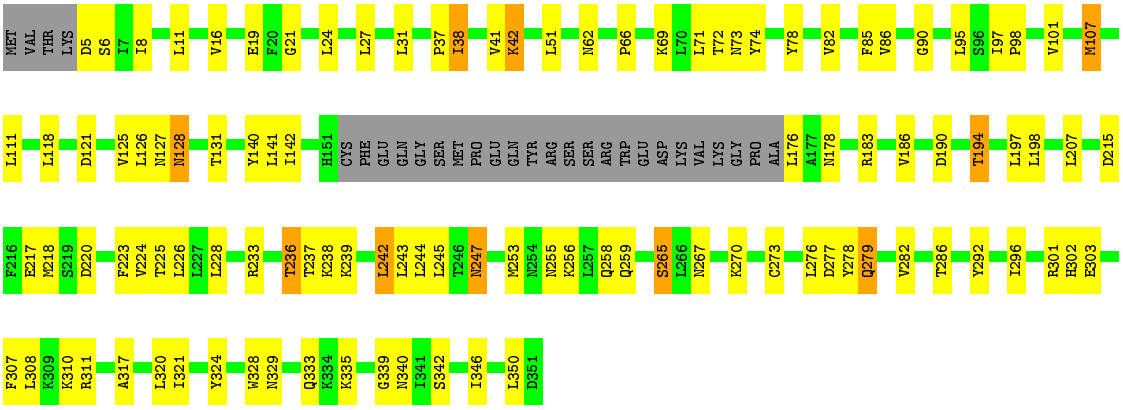
- Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain I:



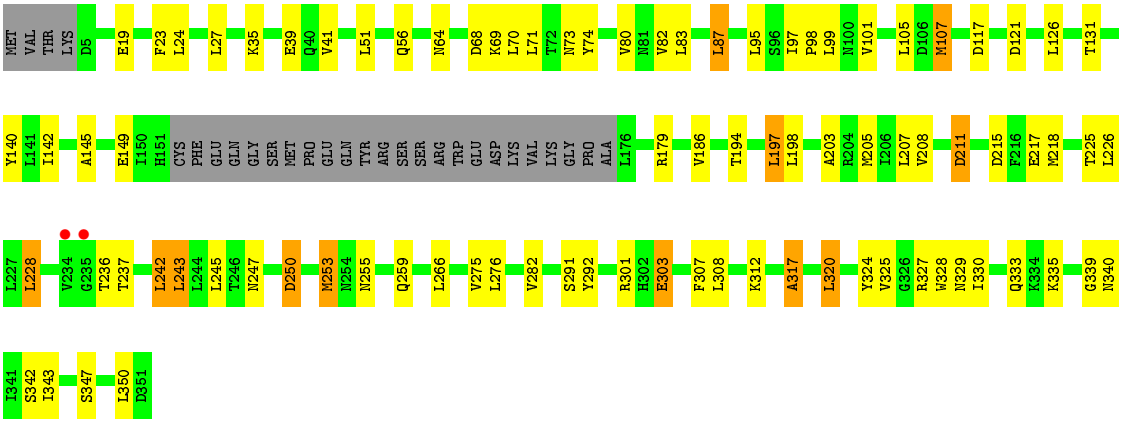
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain J:



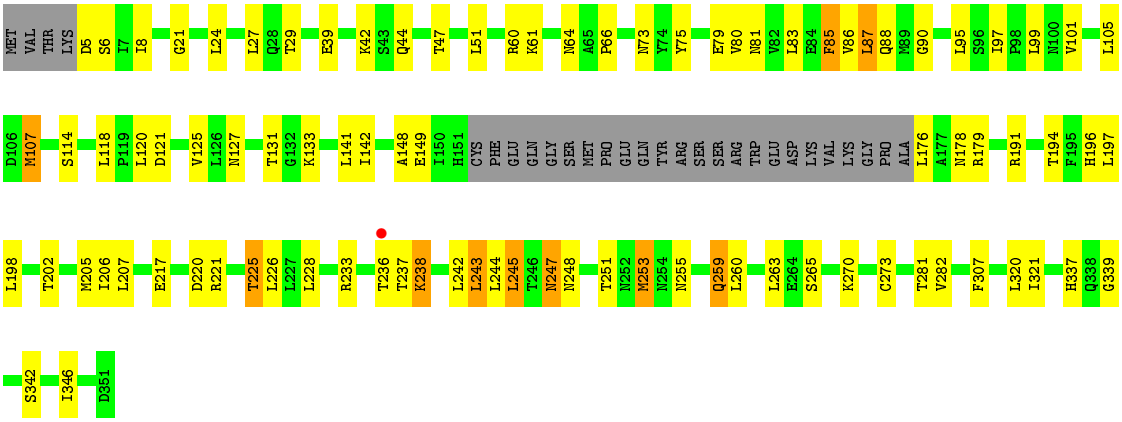
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain K:



• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain L:


MET VAL THR LYS D5 S6 I7 I8 G21 L24 L27 Q28 T29 E39 K42 S43 Q44 T47 L51 R60 K61 N64 A65 P66 N73 Y74 Y75 E79 V80 N81 V82 L83 E84 F85 V86 L87 Q88 M89 G90 L95 S96 I97 P98 L99 N100 V101 L105
D106 M107 S114 L118 P119 L120 D121 V125 L126 N127 T131 G132 K133 L141 I142 A148 E149 I150 H151 CYS PHE GLU GLN GLY SER MET PRO GLU GLN TYR ARG SER SER ARG TRP GLU ASP LYS VAL LYS GLY PRO ALA L176 A177 N178 R179 R191 T194 F195 H196 L197
L198 T202 M205 I206 L207 E217 D220 R221 T225 L226 L227 L228 R233 T236 T237 K238 L242 L243 L244 L245 T246 N247 N248 T251 N252 M253 N254 N255 Q259 L260 L263 E264 S265 K270 C273 T281 V282 F307 L320 I321 H337 Q338 G339
S342 I346 D351

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	161.66Å 188.30Å 231.56Å 90.00° 92.85° 90.00°	Depositor
Resolution (Å)	29.80 – 3.05 29.82 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.80-3.05) 84.0 (29.82-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.06Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.200 , 0.232 0.216 , 0.208	Depositor DCC
R_{free} test set	5145 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	65025	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.49	0/7125	0.73	0/9664
1	C	0.50	0/7125	0.73	0/9664
1	E	0.46	0/7125	0.72	0/9664
1	G	0.47	0/7125	0.72	0/9664
2	B	0.51	0/6651	0.74	1/9002 (0.0%)
2	D	0.51	0/6651	0.74	1/9002 (0.0%)
2	F	0.47	0/6651	0.72	1/9002 (0.0%)
2	H	0.48	0/6651	0.73	1/9002 (0.0%)
3	I	0.61	0/2640	0.85	1/3578 (0.0%)
3	J	0.57	0/2640	0.85	0/3578
3	K	0.53	0/2640	0.80	0/3578
3	L	0.54	0/2640	0.78	0/3578
All	All	0.50	0/65664	0.75	5/88976 (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	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	67	VAL	C-N-CA	5.33	135.04	121.70
2	F	125	GLU	C-N-CA	5.15	134.57	121.70
2	B	125	GLU	C-N-CA	5.12	134.49	121.70
2	H	125	GLU	C-N-CA	5.03	134.27	121.70
2	D	125	GLU	C-N-CA	5.02	134.26	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	915	VAL	Mainchain
2	D	915	VAL	Mainchain
1	E	123	LEU	Mainchain
2	F	915	VAL	Mainchain
2	H	915	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7008	0	6692	83	0
1	C	7008	0	6692	81	0
1	E	7008	0	6692	81	0
1	G	7008	0	6692	76	0
2	B	6546	0	6253	68	0
2	D	6546	0	6253	69	0
2	F	6546	0	6253	66	0
2	H	6546	0	6253	67	0
3	I	2590	0	2509	41	0
3	J	2590	0	2509	54	0
3	K	2590	0	2509	36	0
3	L	2590	0	2509	42	0
4	A	65	0	0	1	0
4	B	10	0	0	0	0
4	C	50	0	0	3	0
4	D	15	0	0	0	0
4	E	40	0	0	2	0
4	F	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	40	0	0	0	0
4	H	20	0	0	0	0
4	I	25	0	0	0	0
4	J	15	0	0	0	0
4	K	15	0	0	0	0
4	L	15	0	0	0	0
5	B	31	0	12	0	0
5	D	31	0	12	0	0
5	F	31	0	12	1	0
5	H	31	0	12	1	0
All	All	65025	0	61864	702	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (702) 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)
2:B:650:ASP:CB	2:D:148:ASN:HB2	2.01	0.90
2:F:148:ASN:HB2	2:H:650:ASP:CB	2.06	0.85
1:C:622:LEU:HD21	1:C:655:VAL:HG11	1.59	0.84
1:E:216:ILE:HG22	1:E:246:CYS:HB3	1.60	0.84
3:I:255:ASN:O	3:I:259:GLN:HG3	1.78	0.84
1:C:216:ILE:HG22	1:C:246:CYS:HB3	1.60	0.84
1:G:216:ILE:HG22	1:G:246:CYS:HB3	1.60	0.83
1:A:216:ILE:HG22	1:A:246:CYS:HB3	1.60	0.82
1:A:622:LEU:HD21	1:A:655:VAL:HG11	1.62	0.81
1:G:622:LEU:HD21	1:G:655:VAL:HG11	1.65	0.79
2:B:148:ASN:HB2	2:D:650:ASP:CB	2.13	0.79
1:E:622:LEU:HD21	1:E:655:VAL:HG11	1.65	0.78
2:D:780:MET:HE1	3:J:265:SER:HB3	1.66	0.78
3:K:225:THR:HG22	3:K:320:LEU:HD22	1.68	0.75
3:J:86:VAL:HG22	3:J:242:LEU:HB3	1.67	0.74
1:G:467:LEU:HD23	1:G:560:LYS:HG2	1.70	0.73
1:E:467:LEU:HD23	1:E:560:LYS:HG2	1.71	0.73
1:A:467:LEU:HD23	1:A:560:LYS:HG2	1.71	0.73
1:G:393:SER:HB2	1:G:396:ARG:HG3	1.70	0.73
1:A:393:SER:HB2	1:A:396:ARG:HG3	1.70	0.72
1:E:445:ARG:HE	1:E:587:ASP:HB2	1.55	0.72
2:H:122:SER:HB3	2:H:123:PRO:HD3	1.72	0.72
1:G:445:ARG:HE	1:G:587:ASP:HB2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:SER:HB2	1:E:396:ARG:HG3	1.70	0.71
2:B:122:SER:HB3	2:B:123:PRO:HD3	1.72	0.71
1:C:393:SER:HB2	1:C:396:ARG:HG3	1.73	0.71
2:D:780:MET:CE	3:J:265:SER:HB3	2.20	0.71
1:C:445:ARG:HE	1:C:587:ASP:HB2	1.56	0.70
2:F:650:ASP:CB	2:H:148:ASN:HB2	2.20	0.70
1:C:467:LEU:HD23	1:C:560:LYS:HG2	1.73	0.70
2:F:122:SER:HB3	2:F:123:PRO:HD3	1.72	0.70
1:A:445:ARG:HE	1:A:587:ASP:HB2	1.56	0.70
3:J:282:VAL:HG22	3:J:340:ASN:HD21	1.57	0.70
3:L:225:THR:HG22	3:L:320:LEU:HD22	1.74	0.69
3:J:282:VAL:HG22	3:J:340:ASN:ND2	2.07	0.69
2:D:122:SER:HB3	2:D:123:PRO:HD3	1.73	0.68
1:C:390:THR:HG23	2:D:470:GLY:HA2	1.74	0.68
2:H:189:SER:HB3	2:H:288:SER:HB3	1.75	0.68
2:F:189:SER:HB3	2:F:288:SER:HB3	1.74	0.68
3:L:75:TYR:HB3	3:L:79:GLU:HB2	1.74	0.68
1:A:294:LEU:HD11	1:A:331:ILE:HD12	1.75	0.66
3:K:228:LEU:HD22	3:K:320:LEU:HD21	1.77	0.66
3:I:264:GLU:HG2	3:I:330:ILE:HD12	1.78	0.66
3:J:307:PHE:HD2	3:J:308:LEU:HD12	1.59	0.66
2:B:189:SER:HB3	2:B:288:SER:HB3	1.77	0.66
3:I:329:ASN:H	3:I:329:ASN:HD22	1.42	0.65
1:A:390:THR:HG23	2:B:470:GLY:HA2	1.78	0.65
2:D:709:THR:CG2	2:D:894:GLY:HA2	2.27	0.65
1:G:728:VAL:HG22	1:G:744:CYS:HB2	1.78	0.64
3:I:123:TYR:HD1	3:I:198:LEU:HD11	1.62	0.64
2:H:709:THR:CG2	2:H:894:GLY:HA2	2.27	0.64
2:D:189:SER:HB3	2:D:288:SER:HB3	1.78	0.64
2:F:709:THR:CG2	2:F:894:GLY:HA2	2.28	0.64
3:I:290:ASN:O	3:I:294:GLU:HB2	1.96	0.64
1:C:728:VAL:HG22	1:C:744:CYS:HB2	1.78	0.63
1:G:390:THR:HG23	2:H:470:GLY:HA2	1.79	0.63
3:I:247:ASN:H	3:I:247:ASN:HD22	1.47	0.63
1:A:728:VAL:HG22	1:A:744:CYS:HB2	1.80	0.63
2:F:290:THR:HG22	2:F:520:VAL:HG13	1.81	0.63
2:B:412:CYS:SG	2:B:454:ARG:HD2	2.38	0.63
1:E:728:VAL:HG22	1:E:744:CYS:HB2	1.81	0.63
3:I:257:LEU:HG	3:I:261:LYS:HD2	1.81	0.63
2:B:709:THR:CG2	2:B:894:GLY:HA2	2.29	0.62
3:L:221:ARG:HG3	3:L:253:MET:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:LEU:HD11	1:E:331:ILE:HD12	1.82	0.62
1:G:294:LEU:HD11	1:G:331:ILE:HD12	1.79	0.62
3:J:125:VAL:HG22	3:J:198:LEU:HD12	1.82	0.62
2:H:412:CYS:SG	2:H:454:ARG:HD2	2.40	0.61
3:I:120:LEU:HD23	3:I:193:ILE:HD12	1.82	0.61
3:I:95:LEU:HB3	3:I:99:LEU:HD23	1.83	0.61
2:F:412:CYS:SG	2:F:454:ARG:HD2	2.42	0.60
2:B:577:ILE:HD11	2:B:666:LEU:HD21	1.83	0.60
1:G:412:LEU:HD21	1:G:577:TYR:HA	1.84	0.60
3:J:11:LEU:HD22	3:J:16:VAL:HG11	1.84	0.60
3:K:307:PHE:HD2	3:K:308:LEU:HD12	1.66	0.60
1:C:762:SER:HB3	2:D:643:ARG:HG3	1.84	0.60
2:F:577:ILE:HD11	2:F:666:LEU:HD21	1.84	0.60
2:D:188:THR:OG1	2:D:249:THR:HG21	2.02	0.59
1:C:294:LEU:HD11	1:C:331:ILE:HD12	1.83	0.59
2:F:188:THR:OG1	2:F:249:THR:HG21	2.02	0.59
3:K:228:LEU:HD21	3:K:266:LEU:HD11	1.83	0.59
2:B:290:THR:HG22	2:B:520:VAL:HG13	1.83	0.59
2:H:286:ASP:O	2:H:290:THR:HG23	2.03	0.59
2:F:286:ASP:O	2:F:290:THR:HG23	2.03	0.59
2:H:918:ARG:HD2	2:H:920:ARG:HH21	1.68	0.59
2:B:286:ASP:O	2:B:290:THR:HG23	2.03	0.59
3:I:90:GLY:HA2	3:I:125:VAL:O	2.02	0.59
2:B:188:THR:OG1	2:B:249:THR:HG21	2.02	0.58
2:H:577:ILE:HD11	2:H:666:LEU:HD21	1.84	0.58
2:D:577:ILE:HD11	2:D:666:LEU:HD21	1.84	0.58
1:C:412:LEU:HD21	1:C:577:TYR:HA	1.85	0.58
1:E:412:LEU:HD21	1:E:577:TYR:HA	1.84	0.58
3:L:179:ARG:HG3	3:L:202:THR:HG23	1.85	0.58
1:E:390:THR:HG23	2:F:470:GLY:HA2	1.85	0.58
2:B:918:ARG:HD2	2:B:920:ARG:HH21	1.67	0.57
2:D:286:ASP:O	2:D:290:THR:HG23	2.04	0.57
2:D:412:CYS:SG	2:D:454:ARG:HD2	2.45	0.57
3:I:320:LEU:HG	3:I:324:TYR:HD2	1.69	0.57
2:H:188:THR:OG1	2:H:249:THR:HG21	2.03	0.57
1:A:412:LEU:HD21	1:A:577:TYR:HA	1.85	0.57
1:C:686:GLN:HE21	1:G:685:GLN:HE21	1.51	0.57
3:J:247:ASN:HD22	3:J:247:ASN:H	1.53	0.57
2:D:918:ARG:HD2	2:D:920:ARG:HH21	1.68	0.57
1:A:129:PHE:HD1	2:D:10:THR:HG23	1.70	0.56
2:D:290:THR:HG22	2:D:520:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:709:THR:HG22	2:F:894:GLY:HA2	1.88	0.56
2:H:903:THR:HB	2:H:908:LEU:HD11	1.87	0.56
3:K:69:LYS:O	3:K:73:ASN:HB2	2.05	0.56
1:A:762:SER:HB3	2:B:643:ARG:HG3	1.87	0.56
3:J:69:LYS:O	3:J:73:ASN:ND2	2.39	0.56
2:F:918:ARG:HD2	2:F:920:ARG:HH21	1.68	0.56
3:J:307:PHE:HZ	3:J:321:ILE:HD12	1.70	0.56
3:K:312:LYS:HE3	3:K:317:ALA:HA	1.88	0.56
1:A:130:PHE:HD1	1:A:170:PHE:HA	1.70	0.56
1:G:247:TYR:HE2	1:G:261:LYS:HB2	1.71	0.56
1:G:668:THR:O	2:H:736:THR:HG22	2.06	0.56
2:D:211:GLY:HA3	3:J:296:ILE:HG21	1.88	0.56
3:L:247:ASN:H	3:L:247:ASN:HD22	1.53	0.55
1:E:130:PHE:HD1	1:E:170:PHE:HA	1.72	0.55
1:A:668:THR:O	2:B:736:THR:HG22	2.07	0.55
2:F:903:THR:HB	2:F:908:LEU:HD11	1.88	0.55
1:A:247:TYR:HE2	1:A:261:LYS:HB2	1.72	0.55
1:G:130:PHE:HD1	1:G:170:PHE:HA	1.70	0.55
2:H:709:THR:HG22	2:H:894:GLY:HA2	1.87	0.55
1:A:427:GLU:HG3	1:A:573:PHE:CZ	2.42	0.55
1:G:427:GLU:HG3	1:G:573:PHE:CZ	2.41	0.55
3:J:307:PHE:CD2	3:J:308:LEU:HD12	2.40	0.55
2:D:123:PRO:HD2	2:D:126:ILE:HA	1.89	0.55
1:E:427:GLU:HG3	1:E:573:PHE:CZ	2.41	0.55
3:K:51:LEU:HD11	3:K:98:PRO:HB2	1.87	0.55
2:B:709:THR:HG22	2:B:894:GLY:HA2	1.88	0.55
2:D:709:THR:HG22	2:D:894:GLY:HA2	1.88	0.55
1:A:686:GLN:HE21	1:E:685:GLN:HE21	1.55	0.54
1:C:427:GLU:HG3	1:C:573:PHE:CZ	2.42	0.54
2:H:290:THR:HG22	2:H:520:VAL:HG13	1.88	0.54
3:J:51:LEU:HD21	3:J:98:PRO:HB2	1.90	0.54
1:C:592:LEU:CD1	1:C:598:ARG:HH12	2.20	0.54
2:F:123:PRO:HD2	2:F:126:ILE:HA	1.89	0.54
2:D:903:THR:HB	2:D:908:LEU:HD11	1.89	0.54
1:E:592:LEU:CD1	1:E:598:ARG:HH12	2.20	0.54
2:F:182:LYS:HB2	2:F:278:ASP:HB2	1.89	0.54
2:F:267:LYS:HA	2:F:270:LYS:HD2	1.90	0.54
3:J:69:LYS:HB2	3:J:72:THR:HB	1.90	0.54
2:B:903:THR:HB	2:B:908:LEU:HD11	1.90	0.54
2:D:182:LYS:HB2	2:D:278:ASP:HB2	1.90	0.54
2:B:123:PRO:HD2	2:B:126:ILE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:592:LEU:CD1	1:G:598:ARG:HH12	2.20	0.54
3:J:310:LYS:HD3	3:J:311:ARG:HG3	1.89	0.54
2:D:709:THR:HG23	2:D:894:GLY:HA2	1.89	0.54
1:C:130:PHE:HD1	1:C:170:PHE:HA	1.72	0.53
1:E:226:ASN:HD22	1:E:275:GLY:H	1.56	0.53
1:E:383:LEU:HD13	2:F:467:VAL:HG21	1.89	0.53
2:H:123:PRO:HD2	2:H:126:ILE:HA	1.89	0.53
2:H:182:LYS:HB2	2:H:278:ASP:HB2	1.90	0.53
1:A:123:LEU:HD22	2:D:136:PRO:HD2	1.90	0.53
1:C:383:LEU:HD13	2:D:467:VAL:HG21	1.89	0.53
1:E:247:TYR:HE2	1:E:261:LYS:HB2	1.72	0.53
3:J:66:PRO:HG2	3:J:73:ASN:ND2	2.22	0.53
3:K:276:LEU:HG	3:K:343:ILE:HG12	1.90	0.53
1:C:247:TYR:HE2	1:C:261:LYS:HB2	1.72	0.53
1:G:882:LEU:HD11	1:G:940:ILE:HD11	1.90	0.53
2:B:363:ALA:O	2:B:365:SER:N	2.42	0.53
2:B:474:VAL:HG13	2:B:720:ASN:HD21	1.73	0.53
1:G:226:ASN:HD22	1:G:275:GLY:H	1.56	0.53
3:L:83:LEU:HD22	3:L:242:LEU:HB2	1.91	0.53
1:G:148:ILE:HB	1:G:159:SER:HB3	1.91	0.53
3:K:71:LEU:HD11	3:K:107:MET:HG3	1.90	0.53
3:K:97:ILE:O	3:K:101:VAL:HG23	2.09	0.53
2:F:709:THR:HG23	2:F:894:GLY:HA2	1.91	0.52
2:H:709:THR:HG23	2:H:894:GLY:HA2	1.90	0.52
3:I:92:SER:HB2	3:I:246:THR:OG1	2.10	0.52
3:J:292:TYR:HD1	3:J:303:GLU:HG2	1.74	0.52
1:A:148:ILE:HB	1:A:159:SER:HB3	1.92	0.52
1:A:420:ALA:HB2	1:A:457:ILE:HD12	1.91	0.52
2:D:193:SER:O	2:D:196:MET:HG3	2.10	0.52
1:C:770:GLU:HB3	1:C:861:VAL:HG13	1.92	0.52
1:A:592:LEU:CD1	1:A:598:ARG:HH12	2.23	0.52
1:C:530:VAL:HG23	1:C:543:LEU:HA	1.91	0.52
1:C:615:PRO:HG3	1:C:871:PRO:HG3	1.92	0.52
1:A:78:ARG:HE	2:B:571:ARG:HH12	1.58	0.52
2:D:267:LYS:HA	2:D:270:LYS:HD2	1.92	0.52
2:H:577:ILE:HG23	2:H:607:ILE:HB	1.90	0.52
2:B:193:SER:O	2:B:196:MET:HG3	2.09	0.52
1:C:882:LEU:HD11	1:C:940:ILE:HD11	1.92	0.52
1:C:439:LEU:HD11	1:C:475:VAL:HG13	1.92	0.52
1:E:78:ARG:HE	2:F:571:ARG:HH12	1.58	0.52
1:E:530:VAL:HG23	1:E:543:LEU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:307:PHE:HZ	3:I:321:ILE:HD12	1.74	0.52
2:B:267:LYS:HA	2:B:270:LYS:HD2	1.91	0.52
2:B:566:LEU:HD12	2:B:600:ARG:HB3	1.92	0.52
1:G:420:ALA:HB2	1:G:457:ILE:HD12	1.92	0.52
2:H:363:ALA:O	2:H:365:SER:N	2.43	0.52
2:B:182:LYS:HB2	2:B:278:ASP:HB2	1.92	0.51
1:E:148:ILE:HB	1:E:159:SER:HB3	1.90	0.51
2:H:631:TRP:HA	2:H:634:LEU:HD12	1.92	0.51
1:E:439:LEU:HD11	1:E:475:VAL:HG13	1.92	0.51
1:E:490:ARG:HB2	2:F:463:THR:HG23	1.92	0.51
4:E:991:SO4:O3	2:F:739:ARG:NH2	2.43	0.51
1:A:530:VAL:HG23	1:A:543:LEU:HA	1.91	0.51
1:E:444:LEU:HD11	1:E:482:ILE:HD12	1.92	0.51
2:F:363:ALA:O	2:F:365:SER:N	2.43	0.51
3:J:256:LYS:HZ2	3:J:277:ASP:HB2	1.74	0.51
1:A:226:ASN:HD22	1:A:275:GLY:H	1.57	0.51
3:L:66:PRO:HB2	3:L:73:ASN:HD21	1.76	0.51
2:D:363:ALA:O	2:D:365:SER:N	2.44	0.51
2:F:566:LEU:HD12	2:F:600:ARG:HB3	1.93	0.51
1:G:606:VAL:O	1:G:696:GLY:HA3	2.11	0.51
3:K:333:GLN:HB2	3:K:347:SER:HB3	1.92	0.51
1:A:606:VAL:O	1:A:696:GLY:HA3	2.11	0.51
1:E:420:ALA:HB2	1:E:457:ILE:HD12	1.93	0.51
1:G:599:LEU:HB3	1:G:690:ASP:HB2	1.93	0.51
2:H:193:SER:O	2:H:196:MET:HG3	2.11	0.51
2:H:566:LEU:HD12	2:H:600:ARG:HB3	1.92	0.51
3:I:320:LEU:HG	3:I:324:TYR:CD2	2.46	0.51
1:E:790:LEU:HG	1:E:826:LYS:HE3	1.93	0.51
1:G:444:LEU:HD11	1:G:482:ILE:HD12	1.92	0.51
3:L:95:LEU:HD22	3:L:99:LEU:HD23	1.93	0.51
2:B:577:ILE:HG23	2:B:607:ILE:HB	1.92	0.51
3:I:88:GLN:HE22	3:I:104:VAL:HG22	1.75	0.51
3:J:273:CYS:HB3	3:J:346:ILE:HD12	1.93	0.51
3:L:81:ASN:ND2	3:L:114:SER:H	2.08	0.51
1:C:599:LEU:HB3	1:C:690:ASP:HB2	1.93	0.51
1:E:615:PRO:HG3	1:E:871:PRO:HG3	1.92	0.51
2:F:193:SER:O	2:F:196:MET:HG3	2.11	0.51
2:F:631:TRP:HA	2:F:634:LEU:HD12	1.92	0.51
1:G:615:PRO:HG3	1:G:871:PRO:HG3	1.92	0.51
2:D:566:LEU:HD12	2:D:600:ARG:HB3	1.92	0.50
2:D:474:VAL:HG13	2:D:720:ASN:HD21	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:LYS:HA	2:H:270:LYS:HD2	1.93	0.50
3:I:11:LEU:HD22	3:I:16:VAL:HG11	1.93	0.50
2:B:709:THR:HG23	2:B:894:GLY:HA2	1.92	0.50
1:G:383:LEU:HD13	2:H:467:VAL:HG21	1.93	0.50
1:A:595:GLU:HG3	1:A:598:ARG:HH21	1.76	0.50
3:J:24:LEU:HD22	3:J:140:TYR:HD2	1.75	0.50
1:C:606:VAL:O	1:C:696:GLY:HA3	2.11	0.50
2:D:299:TRP:O	2:D:301:SER:N	2.44	0.50
1:G:530:VAL:HG23	1:G:543:LEU:HA	1.92	0.50
1:C:949:PRO:HB2	1:C:952:GLN:HE21	1.77	0.50
2:D:659:GLU:HB2	2:D:690:SER:HB3	1.93	0.50
3:I:38:ILE:HD11	3:I:105:LEU:O	2.11	0.50
3:I:245:LEU:O	3:I:277:ASP:HA	2.11	0.50
1:A:898:LYS:HG2	3:K:117:ASP:O	2.12	0.50
2:D:577:ILE:HG23	2:D:607:ILE:HB	1.92	0.50
2:F:577:ILE:HG23	2:F:607:ILE:HB	1.93	0.50
1:E:762:SER:HB3	2:F:643:ARG:HG3	1.94	0.50
1:E:668:THR:O	2:F:736:THR:HG22	2.12	0.50
2:H:659:GLU:HB2	2:H:690:SER:HB3	1.94	0.50
1:A:882:LEU:HD11	1:A:940:ILE:HD11	1.94	0.50
1:C:420:ALA:HB2	1:C:457:ILE:HD12	1.94	0.50
2:B:257:LYS:HA	2:B:260:ARG:HE	1.77	0.50
1:C:226:ASN:HD22	1:C:275:GLY:H	1.59	0.50
2:D:396:LEU:HD13	2:D:430:VAL:HG22	1.94	0.50
1:E:882:LEU:HD11	1:E:940:ILE:HD11	1.93	0.50
3:L:127:ASN:HD21	3:L:248:ASN:CG	2.15	0.50
1:G:541:GLN:HA	1:G:541:GLN:HE21	1.77	0.49
3:K:292:TYR:HD1	3:K:303:GLU:HG2	1.77	0.49
1:A:444:LEU:HD11	1:A:482:ILE:HD12	1.93	0.49
1:C:790:LEU:HG	1:C:826:LYS:HE3	1.94	0.49
2:F:356:ILE:HG12	2:F:372:VAL:HG21	1.94	0.49
2:F:659:GLU:HB2	2:F:690:SER:HB3	1.95	0.49
1:A:439:LEU:HD11	1:A:475:VAL:HG13	1.93	0.49
2:F:474:VAL:HG13	2:F:720:ASN:HD21	1.76	0.49
2:H:299:TRP:O	2:H:301:SER:N	2.45	0.49
3:I:78:TYR:CZ	3:I:82:VAL:HG21	2.47	0.49
3:K:41:VAL:HG11	3:K:145:ALA:HB2	1.93	0.49
1:A:599:LEU:HB3	1:A:690:ASP:HB2	1.95	0.49
1:A:513:VAL:HG21	1:A:976:VAL:HG13	1.95	0.49
2:D:356:ILE:HG12	2:D:372:VAL:HG21	1.94	0.49
1:G:790:LEU:HG	1:G:826:LYS:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:292:TYR:CD1	3:J:303:GLU:HG2	2.47	0.49
3:L:81:ASN:HD21	3:L:114:SER:H	1.60	0.49
2:H:474:VAL:HG13	2:H:720:ASN:HD21	1.77	0.49
1:A:615:PRO:HG3	1:A:871:PRO:HG3	1.94	0.49
2:B:631:TRP:HA	2:B:634:LEU:HD12	1.95	0.49
1:C:148:ILE:HB	1:C:159:SER:HB3	1.93	0.49
1:G:595:GLU:HG3	1:G:598:ARG:HH21	1.78	0.49
3:I:255:ASN:HB3	3:I:258:GLN:HB2	1.94	0.49
3:K:83:LEU:HD22	3:K:242:LEU:HB2	1.95	0.49
1:A:129:PHE:CD1	2:D:10:THR:HG23	2.48	0.49
1:A:383:LEU:HD13	2:B:467:VAL:HG21	1.95	0.49
1:G:439:LEU:HD11	1:G:475:VAL:HG13	1.94	0.49
1:C:444:LEU:HD11	1:C:482:ILE:HD12	1.94	0.49
1:E:599:LEU:HB3	1:E:690:ASP:HB2	1.94	0.49
2:H:205:ARG:HG2	2:H:237:TRP:CD2	2.48	0.49
3:L:107:MET:HG2	3:L:244:LEU:HD11	1.95	0.49
3:L:207:LEU:HD11	3:L:226:LEU:HD13	1.95	0.49
1:A:949:PRO:HB2	1:A:952:GLN:HE21	1.78	0.48
2:H:739:ARG:HD3	2:H:741:PHE:CE2	2.48	0.48
2:B:780:MET:O	3:I:327:ARG:NH2	2.45	0.48
2:F:257:LYS:HA	2:F:260:ARG:HE	1.78	0.48
2:F:396:LEU:HD13	2:F:430:VAL:HG22	1.94	0.48
1:G:762:SER:HB3	2:H:643:ARG:HG3	1.95	0.48
1:G:949:PRO:HB2	1:G:952:GLN:HE21	1.79	0.48
1:E:949:PRO:HB2	1:E:952:GLN:HE21	1.78	0.48
2:B:396:LEU:HD13	2:B:430:VAL:HG22	1.94	0.48
1:C:361:ASP:HB2	4:C:991:SO4:O3	2.13	0.48
1:G:919:LYS:HE2	1:G:929:VAL:HG21	1.95	0.48
3:I:71:LEU:HD12	3:I:110:GLN:HB2	1.95	0.48
1:A:490:ARG:HB2	2:B:463:THR:HG23	1.96	0.48
1:C:592:LEU:HD13	1:C:598:ARG:HH12	1.78	0.48
2:D:739:ARG:HD3	2:D:741:PHE:CE2	2.49	0.48
3:I:264:GLU:HG2	3:I:330:ILE:CD1	2.42	0.48
3:J:62:ASN:ND2	3:J:340:ASN:HB2	2.29	0.48
2:F:205:ARG:HG2	2:F:237:TRP:CD2	2.49	0.48
2:F:739:ARG:HD3	2:F:741:PHE:CE2	2.48	0.48
3:L:90:GLY:HA2	3:L:125:VAL:O	2.14	0.48
2:B:356:ILE:HG12	2:B:372:VAL:HG21	1.95	0.48
2:D:631:TRP:HA	2:D:634:LEU:HD12	1.94	0.48
2:F:299:TRP:O	2:F:301:SER:N	2.45	0.48
2:H:356:ILE:HG12	2:H:372:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:558:SER:O	2:F:560:ASP:N	2.47	0.48
1:E:513:VAL:HG21	1:E:976:VAL:HG13	1.96	0.48
1:E:95:LEU:HB3	1:E:96:LEU:H	1.61	0.48
1:G:490:ARG:HB2	2:H:463:THR:HG23	1.96	0.48
3:J:5:ASP:HA	3:J:8:ILE:HD12	1.96	0.48
2:B:659:GLU:HB2	2:B:690:SER:HB3	1.95	0.48
1:C:541:GLN:HE21	1:C:541:GLN:HA	1.79	0.48
1:C:901:ALA:HB2	3:L:118:LEU:HD13	1.96	0.48
2:D:257:LYS:HA	2:D:260:ARG:HE	1.78	0.48
1:G:60:GLU:HG2	1:G:109:LYS:HA	1.96	0.47
2:H:257:LYS:HA	2:H:260:ARG:HE	1.79	0.47
2:H:878:ILE:HG22	2:H:879:SER:H	1.79	0.47
3:I:81:ASN:ND2	3:I:117:ASP:OD2	2.47	0.47
3:J:78:TYR:CE2	3:J:82:VAL:HG21	2.49	0.47
3:L:255:ASN:O	3:L:259:GLN:HB2	2.14	0.47
1:A:592:LEU:HD13	1:A:598:ARG:HH12	1.79	0.47
1:A:635:ARG:NH2	4:A:993:SO4:O1	2.47	0.47
1:A:790:LEU:HG	1:A:826:LYS:HE3	1.95	0.47
1:E:869:LYS:HA	2:F:731:GLN:HE22	1.79	0.47
1:G:592:LEU:HD13	1:G:598:ARG:HH12	1.80	0.47
2:D:205:ARG:HG2	2:D:237:TRP:CD2	2.50	0.47
2:D:558:SER:O	2:D:560:ASP:N	2.47	0.47
3:J:126:LEU:HG	3:J:197:LEU:HD11	1.95	0.47
2:F:815:GLU:O	2:F:819:THR:HG23	2.14	0.47
3:I:272:ASN:HB2	3:I:345:GLN:NE2	2.29	0.47
3:J:73:ASN:OD1	3:J:74:TYR:N	2.48	0.47
1:E:541:GLN:HE21	1:E:541:GLN:HA	1.79	0.47
2:F:576:ILE:HD13	2:F:593:MET:HG2	1.97	0.47
1:G:133:SER:HB3	1:G:136:LYS:HB2	1.94	0.47
3:L:97:ILE:HD11	3:L:131:THR:HG22	1.95	0.47
1:A:60:GLU:HG2	1:A:109:LYS:HA	1.97	0.47
1:A:15:VAL:HG22	1:A:109:LYS:HB2	1.97	0.47
1:C:95:LEU:HB3	1:C:96:LEU:H	1.61	0.47
1:E:133:SER:HB3	1:E:136:LYS:HB2	1.97	0.47
1:E:510:VAL:HG12	1:E:538:ILE:HG13	1.96	0.47
1:G:234:ARG:HD2	1:G:268:VAL:HG23	1.97	0.47
3:J:74:TYR:OH	3:J:335:LYS:HD3	2.14	0.47
1:E:606:VAL:O	1:E:696:GLY:HA3	2.15	0.47
1:G:150:PRO:HG3	1:G:157:GLU:O	2.15	0.47
2:H:396:LEU:HD13	2:H:430:VAL:HG22	1.95	0.47
3:K:80:VAL:HA	3:K:83:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:307:PHE:HZ	3:L:321:ILE:HD12	1.79	0.47
2:B:205:ARG:HG2	2:B:237:TRP:CD2	2.50	0.47
2:B:739:ARG:HD3	2:B:741:PHE:CE2	2.49	0.47
1:C:510:VAL:HG12	1:C:538:ILE:HG13	1.97	0.47
1:G:15:VAL:HG22	1:G:109:LYS:HB2	1.97	0.47
3:J:244:LEU:HD22	3:J:276:LEU:HD22	1.97	0.47
1:A:541:GLN:HA	1:A:541:GLN:HE21	1.80	0.47
1:A:851:GLY:HA3	1:A:854:ARG:HB2	1.97	0.47
1:A:770:GLU:HB3	1:A:861:VAL:HG13	1.96	0.47
1:C:513:VAL:HG21	1:C:976:VAL:HG13	1.97	0.47
2:D:211:GLY:HA3	3:J:296:ILE:CG2	2.45	0.47
1:A:133:SER:HB3	1:A:136:LYS:HB2	1.97	0.46
2:B:558:SER:O	2:B:560:ASP:N	2.48	0.46
1:E:770:GLU:HB3	1:E:861:VAL:HG13	1.97	0.46
2:F:257:LYS:HD3	2:F:257:LYS:H	1.81	0.46
2:H:908:LEU:HA	2:H:912:GLU:HB2	1.97	0.46
1:A:403:MET:HA	1:A:460:GLU:HB2	1.97	0.46
1:E:60:GLU:HG2	1:E:109:LYS:HA	1.97	0.46
2:B:908:LEU:HA	2:B:912:GLU:HB2	1.98	0.46
2:H:576:ILE:HD13	2:H:593:MET:HG2	1.96	0.46
3:J:244:LEU:HD23	3:J:276:LEU:HB3	1.96	0.46
1:G:757:GLN:OE1	2:H:843:GLY:HA2	2.15	0.46
3:L:21:GLY:HA2	3:L:24:LEU:HD12	1.97	0.46
1:C:133:SER:HB3	1:C:136:LYS:HB2	1.97	0.46
2:F:908:LEU:HA	2:F:912:GLU:HB2	1.98	0.46
1:G:513:VAL:HG21	1:G:976:VAL:HG13	1.97	0.46
1:G:838:TYR:HB3	1:G:843:ILE:HD11	1.98	0.46
2:H:558:SER:O	2:H:560:ASP:N	2.49	0.46
3:J:19:GLU:CD	3:J:19:GLU:H	2.18	0.46
3:L:179:ARG:HD2	3:L:206:ILE:HG13	1.98	0.46
2:D:576:ILE:HD13	2:D:593:MET:HG2	1.98	0.46
1:E:592:LEU:HD13	1:E:598:ARG:HH12	1.80	0.46
2:F:249:THR:HG22	2:F:252:GLY:H	1.81	0.46
1:G:510:VAL:HG12	1:G:538:ILE:HG13	1.96	0.46
1:G:851:GLY:HA3	1:G:854:ARG:HB2	1.98	0.46
1:G:770:GLU:HB3	1:G:861:VAL:HG13	1.96	0.46
3:I:134:TYR:O	3:I:138:VAL:HG23	2.16	0.46
3:L:86:VAL:HG23	3:L:120:LEU:HD11	1.97	0.46
1:A:233:THR:HA	1:A:243:VAL:HG21	1.98	0.46
3:J:183:ARG:HG2	3:J:194:THR:HB	1.97	0.46
3:K:255:ASN:O	3:K:259:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:THR:HA	1:G:243:VAL:HG21	1.98	0.46
1:A:798:PRO:HG2	3:J:233:ARG:HA	1.98	0.46
1:E:15:VAL:HG22	1:E:109:LYS:HB2	1.97	0.46
3:I:27:LEU:HD21	3:I:41:VAL:HG23	1.98	0.46
3:L:39:GLU:HA	3:L:42:LYS:HB2	1.97	0.46
1:C:60:GLU:HG2	1:C:109:LYS:HA	1.96	0.45
2:F:811:VAL:HG13	1:G:845:ALA:HB1	1.98	0.45
2:H:897:LYS:O	2:H:899:GLN:N	2.49	0.45
2:B:576:ILE:HD13	2:B:593:MET:HG2	1.98	0.45
3:J:37:PRO:O	3:J:41:VAL:HG12	2.15	0.45
2:H:127:SER:CB	2:H:128:PRO:HD3	2.47	0.45
2:H:815:GLU:O	2:H:819:THR:HG23	2.16	0.45
3:K:74:TYR:CE1	3:K:335:LYS:HB3	2.51	0.45
3:L:85:PHE:CD2	3:L:238:LYS:HB3	2.51	0.45
1:A:838:TYR:HB3	1:A:843:ILE:HD11	1.99	0.45
1:C:233:THR:HA	1:C:243:VAL:HG21	1.97	0.45
1:C:851:GLY:HA3	1:C:854:ARG:HB2	1.97	0.45
2:D:187:MET:HB3	2:D:217:ILE:HB	1.98	0.45
2:D:257:LYS:H	2:D:257:LYS:HD3	1.82	0.45
1:C:86:GLU:HG2	2:D:621:ARG:HH21	1.80	0.45
2:D:815:GLU:O	2:D:819:THR:HG23	2.17	0.45
1:A:685:GLN:HE21	1:E:686:GLN:HE21	1.64	0.45
3:L:243:LEU:HD22	3:L:245:LEU:HD13	1.98	0.45
1:E:423:ILE:HG22	1:E:457:ILE:HB	1.99	0.45
1:G:70:GLU:HB2	1:G:181:ILE:HA	1.99	0.45
3:J:218:MET:CE	3:J:226:LEU:HD12	2.47	0.45
2:B:249:THR:HG22	2:B:252:GLY:H	1.82	0.45
2:B:257:LYS:H	2:B:257:LYS:HD3	1.81	0.45
3:J:71:LEU:HD11	3:J:107:MET:HG3	1.99	0.45
2:B:299:TRP:O	2:B:301:SER:N	2.48	0.45
1:G:34:PHE:HB3	1:G:63:LEU:HB3	1.99	0.45
3:L:125:VAL:HG22	3:L:198:LEU:HD12	1.98	0.45
1:C:403:MET:HA	1:C:460:GLU:HB2	1.98	0.45
2:H:78:ASN:HA	2:H:81:ASN:HD22	1.82	0.45
3:L:220:ASP:HB2	3:L:253:MET:HG3	1.98	0.45
2:B:127:SER:CB	2:B:128:PRO:HD3	2.47	0.45
2:B:187:MET:HB3	2:B:217:ILE:HB	1.98	0.45
1:C:15:VAL:HG22	1:C:109:LYS:HB2	1.98	0.45
1:C:800:ASN:ND2	1:C:803:THR:HG23	2.31	0.45
3:I:81:ASN:HB3	3:I:117:ASP:OD1	2.17	0.45
3:K:87:LEU:HB3	3:K:243:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:VAL:HG12	1:A:538:ILE:HG13	1.98	0.45
2:B:136:PRO:HD2	1:C:123:LEU:HD22	1.99	0.45
2:B:918:ARG:HB3	2:B:920:ARG:HE	1.82	0.45
1:C:595:GLU:HG3	1:C:598:ARG:HH21	1.82	0.45
1:E:595:GLU:HG3	1:E:598:ARG:HH21	1.82	0.45
2:H:918:ARG:HB3	2:H:920:ARG:HE	1.82	0.45
1:C:838:TYR:HB3	1:C:843:ILE:HD11	1.99	0.44
2:F:187:MET:HB3	2:F:217:ILE:HB	1.99	0.44
1:C:234:ARG:HD2	1:C:268:VAL:HG23	1.98	0.44
1:E:233:THR:HA	1:E:243:VAL:HG21	1.99	0.44
1:E:272:LEU:H	1:E:272:LEU:HD23	1.82	0.44
1:E:403:MET:HA	1:E:460:GLU:HB2	1.98	0.44
1:G:403:MET:HA	1:G:460:GLU:HB2	1.98	0.44
3:L:5:ASP:HA	3:L:8:ILE:HD12	1.98	0.44
1:C:423:ILE:HG22	1:C:457:ILE:HB	1.99	0.44
3:K:308:LEU:HD21	3:K:325:VAL:HG11	1.99	0.44
3:K:327:ARG:HB2	3:K:330:ILE:CD1	2.48	0.44
3:L:120:LEU:HB2	3:L:191:ARG:CZ	2.47	0.44
2:B:143:PHE:CE1	2:B:148:ASN:O	2.71	0.44
1:C:417:ALA:O	1:C:876:ARG:HD3	2.17	0.44
1:E:851:GLY:HA3	1:E:854:ARG:HB2	1.98	0.44
2:F:414:ILE:HG12	5:F:942:ATP:H3'	1.99	0.44
1:C:685:GLN:HE21	1:G:686:GLN:HE21	1.64	0.44
2:H:249:THR:HG22	2:H:252:GLY:H	1.83	0.44
1:A:84:LEU:HD11	2:B:605:TYR:CE1	2.53	0.44
2:B:939:THR:HG21	3:I:326:GLY:O	2.18	0.44
1:C:919:LYS:HE2	1:C:929:VAL:HG21	2.00	0.44
2:H:604:PRO:HB2	2:H:623:ILE:HD12	2.00	0.44
3:I:76:ASN:O	3:I:80:VAL:HG12	2.18	0.44
3:K:320:LEU:HG	3:K:324:TYR:HD2	1.82	0.44
2:D:897:LYS:O	2:D:899:GLN:N	2.51	0.44
3:J:90:GLY:HA2	3:J:125:VAL:O	2.18	0.44
1:A:423:ILE:HG22	1:A:457:ILE:HB	2.00	0.44
2:B:815:GLU:O	2:B:819:THR:HG23	2.17	0.44
1:C:245:ALA:HB1	1:C:279:ILE:HG12	1.99	0.44
1:G:247:TYR:O	1:G:252:GLY:HA3	2.18	0.44
3:K:126:LEU:HD12	3:K:197:LEU:HD11	2.00	0.44
1:C:272:LEU:H	1:C:272:LEU:HD23	1.83	0.44
1:C:377:LEU:HA	1:C:380:ILE:HD12	1.99	0.44
2:D:878:ILE:HG22	2:D:879:SER:H	1.82	0.44
1:E:123:LEU:HD22	2:H:136:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:735:THR:HB	1:E:939:GLY:HA3	2.00	0.44
2:H:257:LYS:H	2:H:257:LYS:HD3	1.81	0.44
3:I:329:ASN:HB2	3:I:350:LEU:HB2	2.00	0.44
3:L:88:GLN:HA	3:L:244:LEU:HB2	1.99	0.44
1:C:396:ARG:NH1	4:C:996:SO4:O2	2.50	0.44
2:D:127:SER:CB	2:D:128:PRO:HD3	2.48	0.44
2:D:249:THR:HG22	2:D:252:GLY:H	1.83	0.44
2:F:918:ARG:HB3	2:F:920:ARG:HE	1.82	0.44
2:D:908:LEU:HA	2:D:912:GLU:HB2	2.00	0.43
1:E:377:LEU:HA	1:E:380:ILE:HD12	1.99	0.43
2:F:78:ASN:HA	2:F:81:ASN:HD22	1.82	0.43
2:F:878:ILE:HG22	2:F:879:SER:H	1.83	0.43
3:K:23:PHE:O	3:K:27:LEU:HB2	2.18	0.43
1:A:34:PHE:HB3	1:A:63:LEU:HB3	1.99	0.43
1:E:346:GLU:HG3	1:E:349:ARG:HH21	1.83	0.43
1:E:838:TYR:HB3	1:E:843:ILE:HD11	2.00	0.43
3:J:320:LEU:HG	3:J:324:TYR:HD2	1.82	0.43
1:A:417:ALA:O	1:A:876:ARG:HD3	2.18	0.43
2:D:78:ASN:HA	2:D:81:ASN:HD22	1.83	0.43
1:E:150:PRO:HG3	1:E:157:GLU:O	2.18	0.43
3:I:35:LYS:HE2	3:I:39:GLU:HB3	1.99	0.43
2:D:399:GLU:O	2:D:535:PHE:HB3	2.19	0.43
2:D:604:PRO:HB2	2:D:623:ILE:HD12	1.99	0.43
1:E:919:LYS:HE2	1:E:929:VAL:HG21	2.00	0.43
1:G:272:LEU:HD23	1:G:272:LEU:H	1.82	0.43
3:L:80:VAL:HA	3:L:83:LEU:HD12	1.99	0.43
1:A:763:ARG:HH11	1:A:763:ARG:HA	1.83	0.43
2:H:780:MET:HE1	3:L:265:SER:HB3	1.99	0.43
1:A:800:ASN:ND2	1:A:803:THR:HG23	2.33	0.43
1:G:140:LYS:HE3	1:G:140:LYS:HB2	1.83	0.43
2:H:411:MET:HE2	2:H:428:VAL:HG11	2.00	0.43
3:I:179:ARG:HG2	3:I:202:THR:HG23	2.01	0.43
3:I:332:TYR:CE1	3:I:346:ILE:HG12	2.53	0.43
2:D:741:PHE:HA	2:D:832:LYS:O	2.18	0.43
2:F:897:LYS:O	2:F:899:GLN:N	2.52	0.43
1:G:797:ASN:HA	1:G:798:PRO:HD3	1.91	0.43
2:H:187:MET:HB3	2:H:217:ILE:HB	2.00	0.43
3:J:255:ASN:HB3	3:J:258:GLN:HB2	2.00	0.43
3:K:126:LEU:HD22	3:K:131:THR:HB	2.01	0.43
3:K:208:VAL:HG23	3:K:211:ASP:H	1.84	0.43
1:C:140:LYS:HE3	1:C:140:LYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ALA:O	1:E:876:ARG:HD3	2.18	0.43
1:G:156:VAL:HA	1:G:169:SER:HB3	2.01	0.43
1:G:614:ASN:ND2	1:G:665:GLU:HG2	2.34	0.43
3:J:78:TYR:CZ	3:J:82:VAL:HG21	2.53	0.43
1:A:377:LEU:HA	1:A:380:ILE:HD12	2.01	0.43
1:A:614:ASN:ND2	1:A:665:GLU:HG2	2.33	0.43
1:C:70:GLU:HB2	1:C:181:ILE:HA	2.01	0.43
3:L:60:ARG:HH21	3:L:61:LYS:HE2	1.84	0.43
2:B:604:PRO:HB2	2:B:623:ILE:HD12	2.01	0.43
2:B:783:ASN:HA	2:B:786:LYS:HD3	2.01	0.43
2:D:682:GLU:HA	2:D:685:ARG:HD3	2.01	0.43
1:E:70:GLU:HB2	1:E:181:ILE:HA	2.01	0.43
1:G:423:ILE:HG22	1:G:457:ILE:HB	2.00	0.43
3:J:97:ILE:O	3:J:101:VAL:HG23	2.19	0.43
1:C:556:ALA:HB2	1:C:564:LYS:HD3	2.00	0.42
3:J:128:ASN:ND2	3:J:131:THR:H	2.17	0.42
3:K:179:ARG:HG3	3:K:205:MET:SD	2.58	0.42
1:E:779:LEU:HA	1:E:779:LEU:HD23	1.94	0.42
2:F:682:GLU:HA	2:F:685:ARG:HD3	2.01	0.42
1:G:800:ASN:ND2	1:G:803:THR:HG23	2.35	0.42
3:J:218:MET:HE2	3:J:223:PHE:HD1	1.84	0.42
3:K:218:MET:HE3	3:K:226:LEU:HD12	2.00	0.42
3:L:221:ARG:H	3:L:253:MET:HE3	1.83	0.42
1:A:346:GLU:HG3	1:A:349:ARG:HH21	1.83	0.42
2:B:78:ASN:HA	2:B:81:ASN:HD22	1.84	0.42
1:G:417:ALA:O	1:G:876:ARG:HD3	2.19	0.42
1:G:423:ILE:HG12	1:G:580:PHE:CE2	2.55	0.42
2:B:780:MET:HE1	3:I:265:SER:HB3	2.01	0.42
1:A:150:PRO:HG3	1:A:157:GLU:O	2.20	0.42
1:A:234:ARG:HD2	1:A:268:VAL:HG23	2.00	0.42
2:H:403:SER:HB3	5:H:942:ATP:O3G	2.19	0.42
3:K:292:TYR:CD1	3:K:303:GLU:HG2	2.54	0.42
3:L:273:CYS:HB3	3:L:346:ILE:HD12	2.00	0.42
1:A:156:VAL:HA	1:A:169:SER:HB3	2.01	0.42
1:A:272:LEU:H	1:A:272:LEU:HD23	1.84	0.42
1:A:430:PRO:HB2	1:A:435:TRP:HB3	2.02	0.42
1:A:476:LYS:HG2	1:A:486:THR:HB	2.01	0.42
1:C:346:GLU:HG3	1:C:349:ARG:HH21	1.84	0.42
1:C:34:PHE:HB3	1:C:63:LEU:HB3	2.00	0.42
1:C:614:ASN:ND2	1:C:665:GLU:HG2	2.34	0.42
2:D:411:MET:HE2	2:D:428:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:TYR:O	1:E:252:GLY:HA3	2.19	0.42
1:E:234:ARG:HD2	1:E:268:VAL:HG23	2.01	0.42
1:E:423:ILE:HG12	1:E:580:PHE:CE2	2.55	0.42
1:E:800:ASN:ND2	1:E:803:THR:HG23	2.34	0.42
2:F:127:SER:CB	2:F:128:PRO:HD3	2.49	0.42
3:J:8:ILE:HG12	3:J:21:GLY:HA2	2.02	0.42
2:B:356:ILE:HB	2:B:390:THR:HG21	2.02	0.42
2:B:758:GLN:HG3	2:B:763:ALA:HB3	2.00	0.42
1:E:428:ARG:HD3	1:E:566:LEU:HD13	2.02	0.42
2:H:127:SER:HB3	2:H:128:PRO:HD3	2.02	0.42
2:H:356:ILE:HB	2:H:390:THR:HG21	2.01	0.42
2:D:787:GLU:HG3	3:J:267:ASN:HB2	2.01	0.42
1:A:735:THR:HB	1:A:939:GLY:HA3	2.01	0.42
1:A:793:TYR:HE2	1:A:828:PHE:HD2	1.67	0.42
1:A:984:LEU:HD21	3:J:207:LEU:HB3	2.00	0.42
2:B:768:VAL:HA	2:B:769:PRO:HD3	1.96	0.42
1:E:614:ASN:ND2	1:E:665:GLU:HG2	2.35	0.42
2:F:741:PHE:HA	2:F:832:LYS:O	2.20	0.42
2:H:143:PHE:CE1	2:H:148:ASN:O	2.73	0.42
1:C:988:THR:O	3:I:218:MET:HA	2.19	0.42
3:K:250:ASP:OD1	3:K:253:MET:HG3	2.20	0.42
1:A:797:ASN:HA	1:A:798:PRO:HD3	1.92	0.42
2:B:741:PHE:HA	2:B:832:LYS:O	2.19	0.42
2:F:596:TYR:CZ	2:F:600:ARG:HD3	2.55	0.42
1:G:913:PHE:CE1	1:G:915:ASP:HB2	2.55	0.42
3:L:51:LEU:HD22	3:L:99:LEU:HB2	2.00	0.42
1:A:245:ALA:HB1	1:A:279:ILE:HG12	2.01	0.42
1:C:247:TYR:O	1:C:252:GLY:HA3	2.20	0.42
1:C:428:ARG:HD3	1:C:566:LEU:HD13	2.02	0.42
1:E:245:ALA:HB1	1:E:279:ILE:HG12	2.01	0.42
4:E:990:SO4:S	2:F:828:ARG:NH2	2.92	0.42
1:G:346:GLU:HG3	1:G:349:ARG:HH21	1.84	0.42
1:G:377:LEU:HA	1:G:380:ILE:HD12	2.02	0.42
3:J:247:ASN:H	3:J:247:ASN:ND2	2.16	0.42
1:A:762:SER:HB3	2:B:643:ARG:H	1.84	0.42
1:C:763:ARG:HH11	1:C:763:ARG:HA	1.84	0.42
2:D:218:HIS:HA	2:D:251:ILE:HG23	2.02	0.42
1:E:430:PRO:HB2	1:E:435:TRP:HB3	2.01	0.42
2:F:204:VAL:HA	2:F:214:VAL:HG11	2.01	0.42
2:F:411:MET:HE2	2:F:428:VAL:HG11	2.01	0.42
2:H:204:VAL:HA	2:H:214:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:682:GLU:HA	2:H:685:ARG:HD3	2.02	0.42
3:I:224:VAL:HA	3:I:227:LEU:HD12	2.01	0.42
3:K:218:MET:CE	3:K:226:LEU:HD12	2.50	0.42
3:L:243:LEU:HD11	3:L:263:LEU:HD12	2.01	0.42
1:A:70:GLU:HB2	1:A:181:ILE:HA	2.02	0.41
1:C:156:VAL:HA	1:C:169:SER:HB3	2.02	0.41
2:D:780:MET:HE1	3:J:265:SER:CB	2.44	0.41
2:F:143:PHE:CE1	2:F:148:ASN:O	2.72	0.41
2:F:356:ILE:HA	2:F:359:ILE:HD12	2.01	0.41
2:F:604:PRO:HB2	2:F:623:ILE:HD12	2.01	0.41
1:G:735:THR:HB	1:G:939:GLY:HA3	2.01	0.41
2:B:897:LYS:O	2:B:899:GLN:N	2.53	0.41
1:C:938:ILE:HG12	1:C:947:PHE:CD1	2.54	0.41
1:E:757:GLN:OE1	2:F:843:GLY:HA2	2.20	0.41
1:A:18:ASP:HB3	1:A:21:LEU:HB2	2.02	0.41
1:C:67:PRO:HB3	1:C:102:GLN:HA	2.01	0.41
1:E:34:PHE:HB3	1:E:63:LEU:HB3	2.01	0.41
1:E:913:PHE:CE1	1:E:915:ASP:HB2	2.55	0.41
1:G:430:PRO:HB2	1:G:435:TRP:HB3	2.03	0.41
3:K:95:LEU:HB3	3:K:99:LEU:HD23	2.02	0.41
1:C:735:THR:HB	1:C:939:GLY:HA3	2.02	0.41
2:D:143:PHE:CE1	2:D:148:ASN:O	2.72	0.41
2:D:918:ARG:HB3	2:D:920:ARG:HE	1.85	0.41
1:E:476:LYS:HG2	1:E:486:THR:HB	2.01	0.41
2:F:218:HIS:HA	2:F:251:ILE:HG23	2.03	0.41
1:G:78:ARG:HB3	1:G:79:GLU:H	1.77	0.41
1:C:793:TYR:HE2	1:C:828:PHE:HD2	1.68	0.41
1:G:401:GLU:HB3	1:G:490:ARG:HG2	2.03	0.41
2:H:218:HIS:HA	2:H:251:ILE:HG23	2.02	0.41
3:J:38:ILE:O	3:J:42:LYS:HB2	2.21	0.41
3:L:101:VAL:HG11	3:L:141:LEU:HD12	2.01	0.41
3:L:87:LEU:O	3:L:243:LEU:HD23	2.20	0.41
1:A:423:ILE:HG12	1:A:580:PHE:CE2	2.56	0.41
1:C:423:ILE:HG12	1:C:580:PHE:CE2	2.56	0.41
1:C:476:LYS:HG2	1:C:486:THR:HB	2.02	0.41
1:G:763:ARG:HA	1:G:763:ARG:HH11	1.85	0.41
3:I:329:ASN:ND2	3:I:329:ASN:H	2.14	0.41
3:J:278:TYR:O	3:J:279:GLN:HB3	2.20	0.41
1:A:401:GLU:HB3	1:A:490:ARG:HG2	2.03	0.41
1:A:751:TYR:OH	2:B:836:PRO:O	2.39	0.41
1:C:762:SER:N	2:D:642:ASN:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:797:ASN:HA	1:E:798:PRO:HD3	1.94	0.41
1:G:245:ALA:HB1	1:G:279:ILE:HG12	2.01	0.41
1:G:428:ARG:HD3	1:G:566:LEU:HD13	2.03	0.41
3:I:93:ARG:HG2	3:I:247:ASN:OD1	2.19	0.41
1:A:924:SER:HB2	1:A:926:LYS:HG3	2.03	0.41
2:B:780:MET:HE1	3:I:324:TYR:HA	2.02	0.41
1:E:156:VAL:HA	1:E:169:SER:HB3	2.02	0.41
1:E:18:ASP:HB3	1:E:21:LEU:HB2	2.03	0.41
2:F:336:MET:SD	2:F:523:THR:HG21	2.61	0.41
1:G:556:ALA:HB2	1:G:564:LYS:HD3	2.02	0.41
1:G:869:LYS:HA	2:H:731:GLN:HE22	1.86	0.41
2:H:741:PHE:HA	2:H:832:LYS:O	2.20	0.41
3:K:35:LYS:HE2	3:K:39:GLU:HB3	2.02	0.41
1:A:912:PHE:CD1	1:A:919:LYS:HE3	2.56	0.41
1:A:919:LYS:HE2	1:A:929:VAL:HG21	2.03	0.41
2:B:878:ILE:HG22	2:B:879:SER:H	1.85	0.41
1:C:430:PRO:HB2	1:C:435:TRP:HB3	2.01	0.41
1:C:490:ARG:HB2	2:D:463:THR:HG23	2.03	0.41
1:C:720:PRO:HB2	1:C:890:ILE:HA	2.03	0.41
1:C:360:ILE:N	4:C:991:SO4:O1	2.51	0.41
2:D:707:PRO:HG3	2:D:913:SER:HB3	2.02	0.41
1:G:324:ARG:HB3	1:G:353:ILE:HG21	2.02	0.41
2:H:596:TYR:CZ	2:H:600:ARG:HD3	2.56	0.41
2:D:780:MET:HE1	3:J:324:TYR:HA	2.02	0.41
3:J:66:PRO:HG2	3:J:73:ASN:HD21	1.86	0.41
1:A:428:ARG:HD3	1:A:566:LEU:HD13	2.02	0.41
2:B:590:VAL:HG21	2:B:639:ILE:HD12	2.03	0.41
2:D:356:ILE:HA	2:D:359:ILE:HD12	2.03	0.41
2:F:356:ILE:HB	2:F:390:THR:HG21	2.03	0.41
3:K:203:ALA:O	3:K:207:LEU:HG	2.21	0.41
3:L:179:ARG:HD3	3:L:205:MET:HB2	2.03	0.41
1:E:793:TYR:HE2	1:E:828:PHE:HD2	1.69	0.41
2:F:105:LEU:HD11	2:F:142:GLY:HA3	2.03	0.41
2:H:218:HIS:O	2:H:223:GLY:HA3	2.21	0.41
3:J:301:ARG:HD2	3:J:328:TRP:CE2	2.56	0.41
3:K:301:ARG:HD2	3:K:328:TRP:CE2	2.56	0.41
1:E:798:PRO:HG2	3:L:233:ARG:HA	2.03	0.41
1:A:247:TYR:O	1:A:252:GLY:HA3	2.21	0.40
1:E:482:ILE:HD13	1:E:482:ILE:HA	1.99	0.40
2:H:412:CYS:HG	2:H:454:ARG:HD2	1.86	0.40
3:L:179:ARG:CG	3:L:202:THR:HG23	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:573:LYS:HG2	2:D:605:TYR:HE2	1.86	0.40
1:E:556:ALA:HB2	1:E:564:LYS:HD3	2.02	0.40
2:H:356:ILE:HA	2:H:359:ILE:HD12	2.03	0.40
2:H:399:GLU:O	2:H:535:PHE:HB3	2.21	0.40
3:K:24:LEU:HD22	3:K:140:TYR:HD2	1.86	0.40
1:A:25:THR:HA	1:A:162:ASP:OD1	2.21	0.40
2:B:127:SER:HB3	2:B:128:PRO:HD3	2.03	0.40
2:B:411:MET:HE2	2:B:428:VAL:HG11	2.03	0.40
2:B:682:GLU:HA	2:B:685:ARG:HD3	2.03	0.40
2:D:596:TYR:CZ	2:D:600:ARG:HD3	2.56	0.40
1:E:401:GLU:HB3	1:E:490:ARG:HG2	2.03	0.40
1:E:763:ARG:HH11	1:E:763:ARG:HA	1.85	0.40
3:I:186:VAL:HB	3:I:193:ILE:HG21	2.03	0.40
3:L:337:HIS:HD2	3:L:342:SER:HB3	1.86	0.40
2:B:105:LEU:HD11	2:B:142:GLY:HA3	2.03	0.40
1:E:25:THR:HA	1:E:162:ASP:OD1	2.22	0.40
1:G:476:LYS:HG2	1:G:486:THR:HB	2.03	0.40
1:G:38:ARG:HH12	1:G:50:LEU:CB	2.34	0.40
1:C:68:LEU:O	1:C:100:PRO:HA	2.22	0.40
1:C:779:LEU:HA	1:C:779:LEU:HD23	1.93	0.40
1:C:913:PHE:CE1	1:C:915:ASP:HB2	2.56	0.40
1:E:924:SER:HB2	1:E:926:LYS:HG3	2.03	0.40
2:H:783:ASN:HA	2:H:786:LYS:HD3	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	908/989 (92%)	840 (92%)	58 (6%)	10 (1%)	14	42
1	C	908/989 (92%)	841 (93%)	57 (6%)	10 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	908/989 (92%)	841 (93%)	57 (6%)	10 (1%)	14	42
1	G	908/989 (92%)	843 (93%)	55 (6%)	10 (1%)	14	42
2	B	859/941 (91%)	800 (93%)	46 (5%)	13 (2%)	10	35
2	D	859/941 (91%)	803 (94%)	45 (5%)	11 (1%)	12	38
2	F	859/941 (91%)	803 (94%)	45 (5%)	11 (1%)	12	38
2	H	859/941 (91%)	800 (93%)	46 (5%)	13 (2%)	10	35
3	I	319/351 (91%)	296 (93%)	21 (7%)	2 (1%)	25	55
3	J	319/351 (91%)	285 (89%)	29 (9%)	5 (2%)	9	33
3	K	319/351 (91%)	286 (90%)	31 (10%)	2 (1%)	25	55
3	L	319/351 (91%)	283 (89%)	33 (10%)	3 (1%)	17	47
All	All	8344/9124 (92%)	7721 (92%)	523 (6%)	100 (1%)	13	40

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	646	ALA
2	B	127	SER
2	B	150	PHE
2	B	303	ILE
1	C	646	ALA
2	D	127	SER
2	D	150	PHE
2	D	303	ILE
1	E	646	ALA
2	F	127	SER
2	F	150	PHE
2	F	303	ILE
1	G	646	ALA
2	H	127	SER
2	H	150	PHE
2	H	303	ILE
3	J	339	GLY
3	K	317	ALA
1	A	162	ASP
1	A	179	LYS
1	C	162	ASP
1	C	179	LYS
1	E	162	ASP

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Mol	Chain	Res	Type
1	E	179	LYS
1	G	162	ASP
1	G	179	LYS
3	I	317	ALA
3	I	339	GLY
3	J	279	GLN
3	K	339	GLY
3	L	64	ASN
3	L	339	GLY
1	A	171	SER
1	A	256	GLY
2	B	315	GLN
2	D	315	GLN
2	D	917	ARG
1	E	171	SER
2	F	315	GLN
1	G	78	ARG
1	G	171	SER
2	H	315	GLN
2	H	917	ARG
3	J	31	LEU
3	J	317	ALA
2	B	122	SER
2	B	840	GLN
2	B	917	ARG
2	B	925	TRP
1	C	78	ARG
1	C	171	SER
1	C	256	GLY
2	D	122	SER
1	E	78	ARG
1	E	256	GLY
2	F	122	SER
2	F	840	GLN
2	F	917	ARG
1	G	256	GLY
2	H	122	SER
2	H	840	GLN
3	J	236	THR
1	A	52	GLY
1	A	78	ARG
2	B	793	GLN

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Mol	Chain	Res	Type
2	B	878	ILE
1	C	52	GLY
2	D	840	GLN
2	D	925	TRP
2	F	286	ASP
2	F	925	TRP
2	H	286	ASP
2	H	925	TRP
3	L	148	ALA
2	B	438	ASP
2	D	878	ILE
1	E	52	GLY
2	F	878	ILE
1	G	52	GLY
2	H	438	ASP
2	H	878	ILE
1	A	83	PRO
1	A	274	ILE
1	C	274	ILE
1	E	274	ILE
1	G	274	ILE
1	C	83	PRO
1	E	83	PRO
1	G	83	PRO
2	H	376	GLY
2	B	376	GLY
1	C	257	GLY
1	E	257	GLY
2	F	376	GLY
1	A	257	GLY
2	D	300	PRO
2	D	376	GLY
1	G	257	GLY
2	B	300	PRO
2	H	300	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	725/835 (87%)	648 (89%)	77 (11%)	6 23
1	C	725/835 (87%)	650 (90%)	75 (10%)	7 24
1	E	725/835 (87%)	648 (89%)	77 (11%)	6 23
1	G	725/835 (87%)	646 (89%)	79 (11%)	6 22
2	B	670/799 (84%)	600 (90%)	70 (10%)	7 24
2	D	670/799 (84%)	602 (90%)	68 (10%)	7 25
2	F	670/799 (84%)	600 (90%)	70 (10%)	7 24
2	H	670/799 (84%)	598 (89%)	72 (11%)	6 23
3	I	282/322 (88%)	242 (86%)	40 (14%)	3 13
3	J	282/322 (88%)	239 (85%)	43 (15%)	3 10
3	K	282/322 (88%)	245 (87%)	37 (13%)	4 15
3	L	282/322 (88%)	248 (88%)	34 (12%)	5 17
All	All	6708/7824 (86%)	5966 (89%)	742 (11%)	6 21

All (742) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	10	SER
1	A	47	ASP
1	A	69	SER
1	A	70	GLU
1	A	71	VAL
1	A	79	GLU
1	A	88	VAL
1	A	92	SER
1	A	95	LEU
1	A	96	LEU
1	A	112	LEU
1	A	120	ASN
1	A	121	ASN
1	A	123	LEU
1	A	127	VAL
1	A	135	ASP
1	A	159	SER
1	A	167	VAL
1	A	185	ASP

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Mol	Chain	Res	Type
1	A	216	ILE
1	A	262	GLU
1	A	306	ASP
1	A	322	LEU
1	A	324	ARG
1	A	346	GLU
1	A	359	SER
1	A	382	GLU
1	A	383	LEU
1	A	390	THR
1	A	412	LEU
1	A	421	ASP
1	A	439	LEU
1	A	506	PHE
1	A	509	THR
1	A	537	LYS
1	A	541	GLN
1	A	543	LEU
1	A	544	VAL
1	A	566	LEU
1	A	568	LEU
1	A	579	ASN
1	A	581	LEU
1	A	587	ASP
1	A	592	LEU
1	A	596	SER
1	A	599	LEU
1	A	641	LEU
1	A	648	ARG
1	A	655	VAL
1	A	660	ASN
1	A	704	LEU
1	A	713	GLN
1	A	728	VAL
1	A	730	ASN
1	A	745	LEU
1	A	749	SER
1	A	757	GLN
1	A	763	ARG
1	A	779	LEU
1	A	827	ILE
1	A	832	GLU

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Mol	Chain	Res	Type
1	A	833	LYS
1	A	855	PHE
1	A	861	VAL
1	A	865	VAL
1	A	867	GLN
1	A	898	LYS
1	A	908	ARG
1	A	916	ASP
1	A	936	VAL
1	A	941	GLN
1	A	950	VAL
1	A	954	TRP
1	A	955	GLU
1	A	956	ASN
1	A	984	LEU
2	B	6	LEU
2	B	10	THR
2	B	13	ILE
2	B	14	THR
2	B	58	VAL
2	B	98	ILE
2	B	106	SER
2	B	119	VAL
2	B	181	ARG
2	B	186	VAL
2	B	189	SER
2	B	233	LYS
2	B	234	GLU
2	B	246	GLU
2	B	255	ARG
2	B	257	LYS
2	B	286	ASP
2	B	302	LEU
2	B	365	SER
2	B	425	LYS
2	B	435	ILE
2	B	437	ASN
2	B	444	CYS
2	B	463	THR
2	B	472	THR
2	B	495	CYS
2	B	496	ASP

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Mol	Chain	Res	Type
2	B	507	LYS
2	B	510	GLN
2	B	517	VAL
2	B	522	LEU
2	B	525	GLN
2	B	550	MET
2	B	554	ILE
2	B	561	HIS
2	B	562	VAL
2	B	568	LEU
2	B	569	GLU
2	B	577	ILE
2	B	593	MET
2	B	599	SER
2	B	678	LEU
2	B	683	ARG
2	B	686	ILE
2	B	690	SER
2	B	701	THR
2	B	705	ASN
2	B	713	LEU
2	B	719	LEU
2	B	739	ARG
2	B	740	VAL
2	B	753	ILE
2	B	780	MET
2	B	793	GLN
2	B	795	LYS
2	B	800	ARG
2	B	824	GLU
2	B	844	ILE
2	B	854	SER
2	B	869	ASP
2	B	882	GLN
2	B	885	GLU
2	B	891	VAL
2	B	907	GLN
2	B	915	VAL
2	B	922	ASN
2	B	923	ILE
2	B	926	SER
2	B	932	SER

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Mol	Chain	Res	Type
2	B	938	ARG
1	C	8	ASP
1	C	10	SER
1	C	47	ASP
1	C	69	SER
1	C	70	GLU
1	C	71	VAL
1	C	79	GLU
1	C	88	VAL
1	C	92	SER
1	C	95	LEU
1	C	96	LEU
1	C	112	LEU
1	C	121	ASN
1	C	123	LEU
1	C	127	VAL
1	C	135	ASP
1	C	159	SER
1	C	167	VAL
1	C	185	ASP
1	C	216	ILE
1	C	262	GLU
1	C	272	LEU
1	C	306	ASP
1	C	324	ARG
1	C	346	GLU
1	C	359	SER
1	C	382	GLU
1	C	383	LEU
1	C	390	THR
1	C	412	LEU
1	C	421	ASP
1	C	439	LEU
1	C	506	PHE
1	C	509	THR
1	C	537	LYS
1	C	541	GLN
1	C	543	LEU
1	C	544	VAL
1	C	566	LEU
1	C	568	LEU
1	C	579	ASN

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Mol	Chain	Res	Type
1	C	581	LEU
1	C	587	ASP
1	C	592	LEU
1	C	596	SER
1	C	599	LEU
1	C	641	LEU
1	C	648	ARG
1	C	655	VAL
1	C	660	ASN
1	C	704	LEU
1	C	713	GLN
1	C	728	VAL
1	C	730	ASN
1	C	745	LEU
1	C	749	SER
1	C	757	GLN
1	C	763	ARG
1	C	779	LEU
1	C	827	ILE
1	C	832	GLU
1	C	833	LYS
1	C	855	PHE
1	C	861	VAL
1	C	865	VAL
1	C	867	GLN
1	C	898	LYS
1	C	908	ARG
1	C	916	ASP
1	C	936	VAL
1	C	941	GLN
1	C	950	VAL
1	C	954	TRP
1	C	955	GLU
1	C	956	ASN
2	D	6	LEU
2	D	10	THR
2	D	13	ILE
2	D	14	THR
2	D	58	VAL
2	D	98	ILE
2	D	119	VAL
2	D	186	VAL

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Mol	Chain	Res	Type
2	D	189	SER
2	D	233	LYS
2	D	234	GLU
2	D	246	GLU
2	D	255	ARG
2	D	257	LYS
2	D	286	ASP
2	D	302	LEU
2	D	365	SER
2	D	400	LYS
2	D	425	LYS
2	D	435	ILE
2	D	437	ASN
2	D	444	CYS
2	D	463	THR
2	D	472	THR
2	D	495	CYS
2	D	496	ASP
2	D	507	LYS
2	D	510	GLN
2	D	517	VAL
2	D	522	LEU
2	D	525	GLN
2	D	550	MET
2	D	554	ILE
2	D	561	HIS
2	D	562	VAL
2	D	568	LEU
2	D	569	GLU
2	D	577	ILE
2	D	593	MET
2	D	599	SER
2	D	678	LEU
2	D	683	ARG
2	D	686	ILE
2	D	690	SER
2	D	701	THR
2	D	705	ASN
2	D	713	LEU
2	D	719	LEU
2	D	739	ARG
2	D	740	VAL

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Mol	Chain	Res	Type
2	D	753	ILE
2	D	780	MET
2	D	793	GLN
2	D	795	LYS
2	D	800	ARG
2	D	824	GLU
2	D	844	ILE
2	D	854	SER
2	D	869	ASP
2	D	882	GLN
2	D	885	GLU
2	D	891	VAL
2	D	907	GLN
2	D	915	VAL
2	D	923	ILE
2	D	926	SER
2	D	932	SER
2	D	938	ARG
1	E	8	ASP
1	E	10	SER
1	E	47	ASP
1	E	69	SER
1	E	70	GLU
1	E	71	VAL
1	E	79	GLU
1	E	88	VAL
1	E	92	SER
1	E	95	LEU
1	E	96	LEU
1	E	112	LEU
1	E	121	ASN
1	E	123	LEU
1	E	127	VAL
1	E	135	ASP
1	E	143	GLU
1	E	159	SER
1	E	167	VAL
1	E	185	ASP
1	E	216	ILE
1	E	262	GLU
1	E	272	LEU
1	E	306	ASP

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Mol	Chain	Res	Type
1	E	324	ARG
1	E	346	GLU
1	E	359	SER
1	E	382	GLU
1	E	383	LEU
1	E	390	THR
1	E	412	LEU
1	E	421	ASP
1	E	439	LEU
1	E	506	PHE
1	E	509	THR
1	E	537	LYS
1	E	541	GLN
1	E	543	LEU
1	E	544	VAL
1	E	566	LEU
1	E	568	LEU
1	E	579	ASN
1	E	581	LEU
1	E	587	ASP
1	E	592	LEU
1	E	596	SER
1	E	599	LEU
1	E	641	LEU
1	E	648	ARG
1	E	655	VAL
1	E	660	ASN
1	E	704	LEU
1	E	713	GLN
1	E	728	VAL
1	E	730	ASN
1	E	745	LEU
1	E	749	SER
1	E	757	GLN
1	E	763	ARG
1	E	779	LEU
1	E	827	ILE
1	E	832	GLU
1	E	833	LYS
1	E	855	PHE
1	E	861	VAL
1	E	865	VAL

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Mol	Chain	Res	Type
1	E	867	GLN
1	E	898	LYS
1	E	908	ARG
1	E	916	ASP
1	E	936	VAL
1	E	941	GLN
1	E	950	VAL
1	E	954	TRP
1	E	955	GLU
1	E	956	ASN
1	E	984	LEU
2	F	6	LEU
2	F	10	THR
2	F	13	ILE
2	F	14	THR
2	F	58	VAL
2	F	98	ILE
2	F	119	VAL
2	F	186	VAL
2	F	189	SER
2	F	233	LYS
2	F	234	GLU
2	F	246	GLU
2	F	255	ARG
2	F	257	LYS
2	F	286	ASP
2	F	302	LEU
2	F	365	SER
2	F	400	LYS
2	F	425	LYS
2	F	435	ILE
2	F	437	ASN
2	F	444	CYS
2	F	463	THR
2	F	472	THR
2	F	495	CYS
2	F	496	ASP
2	F	507	LYS
2	F	510	GLN
2	F	517	VAL
2	F	522	LEU
2	F	525	GLN

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Mol	Chain	Res	Type
2	F	550	MET
2	F	554	ILE
2	F	561	HIS
2	F	562	VAL
2	F	568	LEU
2	F	569	GLU
2	F	577	ILE
2	F	593	MET
2	F	599	SER
2	F	678	LEU
2	F	683	ARG
2	F	686	ILE
2	F	690	SER
2	F	701	THR
2	F	705	ASN
2	F	709	THR
2	F	713	LEU
2	F	719	LEU
2	F	739	ARG
2	F	740	VAL
2	F	753	ILE
2	F	780	MET
2	F	793	GLN
2	F	795	LYS
2	F	800	ARG
2	F	806	GLU
2	F	824	GLU
2	F	844	ILE
2	F	854	SER
2	F	869	ASP
2	F	882	GLN
2	F	885	GLU
2	F	891	VAL
2	F	907	GLN
2	F	915	VAL
2	F	923	ILE
2	F	926	SER
2	F	932	SER
2	F	938	ARG
1	G	8	ASP
1	G	10	SER
1	G	47	ASP

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Mol	Chain	Res	Type
1	G	69	SER
1	G	70	GLU
1	G	71	VAL
1	G	78	ARG
1	G	79	GLU
1	G	88	VAL
1	G	92	SER
1	G	95	LEU
1	G	96	LEU
1	G	112	LEU
1	G	121	ASN
1	G	123	LEU
1	G	127	VAL
1	G	135	ASP
1	G	143	GLU
1	G	159	SER
1	G	167	VAL
1	G	185	ASP
1	G	216	ILE
1	G	262	GLU
1	G	272	LEU
1	G	286	GLU
1	G	306	ASP
1	G	324	ARG
1	G	346	GLU
1	G	359	SER
1	G	382	GLU
1	G	383	LEU
1	G	390	THR
1	G	412	LEU
1	G	421	ASP
1	G	439	LEU
1	G	506	PHE
1	G	509	THR
1	G	537	LYS
1	G	541	GLN
1	G	543	LEU
1	G	544	VAL
1	G	566	LEU
1	G	568	LEU
1	G	579	ASN
1	G	581	LEU

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Mol	Chain	Res	Type
1	G	587	ASP
1	G	592	LEU
1	G	596	SER
1	G	599	LEU
1	G	641	LEU
1	G	648	ARG
1	G	655	VAL
1	G	660	ASN
1	G	704	LEU
1	G	713	GLN
1	G	728	VAL
1	G	730	ASN
1	G	745	LEU
1	G	749	SER
1	G	757	GLN
1	G	763	ARG
1	G	779	LEU
1	G	827	ILE
1	G	832	GLU
1	G	833	LYS
1	G	855	PHE
1	G	861	VAL
1	G	865	VAL
1	G	867	GLN
1	G	898	LYS
1	G	908	ARG
1	G	916	ASP
1	G	936	VAL
1	G	941	GLN
1	G	950	VAL
1	G	954	TRP
1	G	955	GLU
1	G	956	ASN
1	G	984	LEU
2	H	6	LEU
2	H	10	THR
2	H	13	ILE
2	H	14	THR
2	H	58	VAL
2	H	98	ILE
2	H	119	VAL
2	H	181	ARG

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Mol	Chain	Res	Type
2	H	186	VAL
2	H	189	SER
2	H	233	LYS
2	H	234	GLU
2	H	246	GLU
2	H	255	ARG
2	H	257	LYS
2	H	286	ASP
2	H	302	LEU
2	H	365	SER
2	H	400	LYS
2	H	425	LYS
2	H	435	ILE
2	H	437	ASN
2	H	444	CYS
2	H	463	THR
2	H	472	THR
2	H	495	CYS
2	H	496	ASP
2	H	507	LYS
2	H	508	GLU
2	H	510	GLN
2	H	517	VAL
2	H	522	LEU
2	H	525	GLN
2	H	550	MET
2	H	554	ILE
2	H	561	HIS
2	H	562	VAL
2	H	568	LEU
2	H	569	GLU
2	H	577	ILE
2	H	593	MET
2	H	599	SER
2	H	678	LEU
2	H	683	ARG
2	H	686	ILE
2	H	690	SER
2	H	701	THR
2	H	705	ASN
2	H	709	THR
2	H	713	LEU

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Mol	Chain	Res	Type
2	H	719	LEU
2	H	739	ARG
2	H	740	VAL
2	H	753	ILE
2	H	780	MET
2	H	793	GLN
2	H	795	LYS
2	H	800	ARG
2	H	806	GLU
2	H	824	GLU
2	H	844	ILE
2	H	854	SER
2	H	869	ASP
2	H	882	GLN
2	H	885	GLU
2	H	891	VAL
2	H	907	GLN
2	H	915	VAL
2	H	923	ILE
2	H	926	SER
2	H	932	SER
2	H	938	ARG
3	I	6	SER
3	I	27	LEU
3	I	39	GLU
3	I	73	ASN
3	I	85	PHE
3	I	87	LEU
3	I	95	LEU
3	I	97	ILE
3	I	105	LEU
3	I	128	ASN
3	I	133	LYS
3	I	141	LEU
3	I	142	ILE
3	I	178	ASN
3	I	186	VAL
3	I	194	THR
3	I	197	LEU
3	I	211	ASP
3	I	215	ASP
3	I	217	GLU

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Mol	Chain	Res	Type
3	I	220	ASP
3	I	225	THR
3	I	228	LEU
3	I	237	THR
3	I	238	LYS
3	I	241	ASP
3	I	242	LEU
3	I	243	LEU
3	I	245	LEU
3	I	247	ASN
3	I	286	THR
3	I	294	GLU
3	I	303	GLU
3	I	320	LEU
3	I	327	ARG
3	I	329	ASN
3	I	333	GLN
3	I	338	GLN
3	I	340	ASN
3	I	342	SER
3	J	6	SER
3	J	27	LEU
3	J	38	ILE
3	J	42	LYS
3	J	85	PHE
3	J	95	LEU
3	J	107	MET
3	J	111	LEU
3	J	118	LEU
3	J	121	ASP
3	J	127	ASN
3	J	128	ASN
3	J	141	LEU
3	J	142	ILE
3	J	176	LEU
3	J	178	ASN
3	J	186	VAL
3	J	190	ASP
3	J	194	THR
3	J	215	ASP
3	J	217	GLU
3	J	220	ASP

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Mol	Chain	Res	Type
3	J	224	VAL
3	J	225	THR
3	J	228	LEU
3	J	236	THR
3	J	237	THR
3	J	238	LYS
3	J	239	LYS
3	J	242	LEU
3	J	243	LEU
3	J	245	LEU
3	J	247	ASN
3	J	253	MET
3	J	259	GLN
3	J	265	SER
3	J	270	LYS
3	J	286	THR
3	J	302	HIS
3	J	329	ASN
3	J	333	GLN
3	J	342	SER
3	J	350	LEU
3	K	19	GLU
3	K	56	GLN
3	K	64	ASN
3	K	68	ASP
3	K	70	LEU
3	K	82	VAL
3	K	87	LEU
3	K	105	LEU
3	K	107	MET
3	K	121	ASP
3	K	142	ILE
3	K	149	GLU
3	K	186	VAL
3	K	194	THR
3	K	197	LEU
3	K	198	LEU
3	K	211	ASP
3	K	215	ASP
3	K	217	GLU
3	K	228	LEU
3	K	236	THR

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Mol	Chain	Res	Type
3	K	237	THR
3	K	242	LEU
3	K	243	LEU
3	K	245	LEU
3	K	247	ASN
3	K	250	ASP
3	K	253	MET
3	K	275	VAL
3	K	282	VAL
3	K	291	SER
3	K	303	GLU
3	K	320	LEU
3	K	329	ASN
3	K	340	ASN
3	K	342	SER
3	K	350	LEU
3	L	6	SER
3	L	27	LEU
3	L	29	THR
3	L	44	GLN
3	L	47	THR
3	L	85	PHE
3	L	87	LEU
3	L	105	LEU
3	L	107	MET
3	L	121	ASP
3	L	133	LYS
3	L	142	ILE
3	L	149	GLU
3	L	176	LEU
3	L	178	ASN
3	L	194	THR
3	L	196	HIS
3	L	197	LEU
3	L	217	GLU
3	L	225	THR
3	L	228	LEU
3	L	236	THR
3	L	237	THR
3	L	238	LYS
3	L	243	LEU
3	L	245	LEU

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Mol	Chain	Res	Type
3	L	247	ASN
3	L	251	THR
3	L	253	MET
3	L	259	GLN
3	L	260	LEU
3	L	270	LYS
3	L	281	THR
3	L	282	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	85	GLN
1	A	350	ASN
1	A	541	GLN
1	A	686	GLN
1	A	802	GLN
1	A	805	GLN
1	A	831	ASN
1	A	867	GLN
1	A	952	GLN
2	B	81	ASN
2	B	121	GLN
2	B	148	ASN
2	B	250	ASN
2	B	320	HIS
2	B	453	ASN
2	B	490	ASN
2	B	534	ASN
2	B	557	ASN
2	B	561	HIS
2	B	705	ASN
2	B	720	ASN
2	B	731	GLN
2	B	758	GLN
2	B	777	GLN
2	B	922	ASN
1	C	44	ASN
1	C	85	GLN
1	C	541	GLN
1	C	686	GLN

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Mol	Chain	Res	Type
1	C	802	GLN
1	C	831	ASN
1	C	867	GLN
1	C	952	GLN
1	C	972	GLN
2	D	81	ASN
2	D	121	GLN
2	D	148	ASN
2	D	250	ASN
2	D	320	HIS
2	D	490	ASN
2	D	534	ASN
2	D	557	ASN
2	D	561	HIS
2	D	705	ASN
2	D	720	ASN
2	D	731	GLN
2	D	758	GLN
2	D	777	GLN
2	D	922	ASN
1	E	44	ASN
1	E	85	GLN
1	E	350	ASN
1	E	541	GLN
1	E	686	GLN
1	E	802	GLN
1	E	805	GLN
1	E	831	ASN
1	E	867	GLN
1	E	899	HIS
1	E	900	ASN
1	E	952	GLN
2	F	81	ASN
2	F	121	GLN
2	F	148	ASN
2	F	250	ASN
2	F	320	HIS
2	F	490	ASN
2	F	534	ASN
2	F	561	HIS
2	F	705	ASN
2	F	720	ASN

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Mol	Chain	Res	Type
2	F	731	GLN
2	F	758	GLN
2	F	777	GLN
2	F	922	ASN
1	G	44	ASN
1	G	85	GLN
1	G	350	ASN
1	G	541	GLN
1	G	686	GLN
1	G	802	GLN
1	G	831	ASN
1	G	867	GLN
1	G	900	ASN
1	G	952	GLN
1	G	972	GLN
2	H	81	ASN
2	H	121	GLN
2	H	148	ASN
2	H	250	ASN
2	H	320	HIS
2	H	490	ASN
2	H	534	ASN
2	H	557	ASN
2	H	561	HIS
2	H	705	ASN
2	H	720	ASN
2	H	731	GLN
2	H	758	GLN
2	H	777	GLN
2	H	922	ASN
3	I	62	ASN
3	I	81	ASN
3	I	128	ASN
3	I	247	ASN
3	I	288	ASN
3	I	329	ASN
3	I	338	GLN
3	J	25	ASN
3	J	77	ASN
3	J	81	ASN
3	J	128	ASN
3	J	247	ASN

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Mol	Chain	Res	Type
3	J	267	ASN
3	J	288	ASN
3	J	290	ASN
3	J	329	ASN
3	J	338	GLN
3	J	340	ASN
3	K	81	ASN
3	K	128	ASN
3	K	247	ASN
3	K	329	ASN
3	K	337	HIS
3	L	62	ASN
3	L	73	ASN
3	L	81	ASN
3	L	127	ASN
3	L	128	ASN
3	L	247	ASN
3	L	248	ASN
3	L	259	GLN
3	L	288	ASN
3	L	329	ASN
3	L	333	GLN
3	L	337	HIS
3	L	338	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

69 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	SO4	I	354	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	G	995	-	4,4,4	0.14	0	6,6,6	0.27	0
4	SO4	E	995	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	H	945	-	4,4,4	0.28	0	6,6,6	0.37	0
4	SO4	C	994	-	4,4,4	0.41	0	6,6,6	0.28	0
4	SO4	A	1001	-	4,4,4	0.52	0	6,6,6	0.23	0
4	SO4	D	944	-	4,4,4	0.28	0	6,6,6	0.41	0
4	SO4	C	997	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	E	990	-	4,4,4	0.26	0	6,6,6	0.11	0
4	SO4	C	993	-	4,4,4	0.15	0	6,6,6	0.48	0
4	SO4	A	1000	-	4,4,4	0.25	0	6,6,6	0.23	0
4	SO4	I	355	-	4,4,4	0.31	0	6,6,6	0.16	0
4	SO4	F	945	-	4,4,4	0.21	0	6,6,6	0.23	0
4	SO4	I	356	-	4,4,4	0.25	0	6,6,6	0.15	0
4	SO4	J	352	-	4,4,4	0.24	0	6,6,6	0.24	0
4	SO4	A	991	-	4,4,4	0.95	0	6,6,6	0.26	0
4	SO4	E	994	-	4,4,4	0.32	0	6,6,6	0.13	0
4	SO4	I	353	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	G	994	-	4,4,4	0.31	0	6,6,6	0.24	0
4	SO4	F	943	-	4,4,4	0.39	0	6,6,6	0.31	0
4	SO4	H	944	-	4,4,4	0.19	0	6,6,6	0.34	0
4	SO4	B	943	-	4,4,4	0.55	0	6,6,6	0.28	0
4	SO4	L	353	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	L	354	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	E	992	-	4,4,4	0.25	0	6,6,6	0.25	0
4	SO4	E	996	-	4,4,4	0.16	0	6,6,6	0.15	0
5	ATP	F	942	-	26,33,33	1.47	3 (11%)	31,52,52	1.26	2 (6%)
4	SO4	K	352	-	4,4,4	0.27	0	6,6,6	0.35	0
4	SO4	E	991	-	4,4,4	0.76	0	6,6,6	0.24	0
4	SO4	L	352	-	4,4,4	0.08	0	6,6,6	0.10	0
5	ATP	B	942	-	26,33,33	1.42	5 (19%)	31,52,52	1.31	4 (12%)
4	SO4	G	992	-	4,4,4	0.48	0	6,6,6	0.13	0
4	SO4	A	990	-	4,4,4	0.63	0	6,6,6	0.30	0
5	ATP	D	942	-	26,33,33	1.48	6 (23%)	31,52,52	1.52	7 (22%)
4	SO4	H	946	-	4,4,4	0.22	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	999	-	4,4,4	0.74	0	6,6,6	0.20	0
4	SO4	C	991	-	4,4,4	0.60	0	6,6,6	0.23	0
4	SO4	A	997	-	4,4,4	0.24	0	6,6,6	0.24	0
4	SO4	C	990	-	4,4,4	0.81	0	6,6,6	0.38	0
4	SO4	D	943	-	4,4,4	0.87	0	6,6,6	0.39	0
4	SO4	E	997	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	G	996	-	4,4,4	0.19	0	6,6,6	0.10	0
4	SO4	A	994	-	4,4,4	0.21	0	6,6,6	0.38	0
4	SO4	A	996	-	4,4,4	0.48	0	6,6,6	0.30	0
4	SO4	I	352	-	4,4,4	0.58	0	6,6,6	0.50	0
4	SO4	H	943	-	4,4,4	0.18	0	6,6,6	0.33	0
4	SO4	A	992	-	4,4,4	0.29	0	6,6,6	0.19	0
4	SO4	G	991	-	4,4,4	0.44	0	6,6,6	0.50	0
4	SO4	E	993	-	4,4,4	0.21	0	6,6,6	0.40	0
4	SO4	A	995	-	4,4,4	0.52	0	6,6,6	0.23	0
4	SO4	J	354	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	D	945	-	4,4,4	0.19	0	6,6,6	0.40	0
4	SO4	C	996	-	4,4,4	0.55	0	6,6,6	0.46	0
4	SO4	J	353	-	4,4,4	0.29	0	6,6,6	0.20	0
5	ATP	H	942	-	26,33,33	1.42	3 (11%)	31,52,52	1.42	6 (19%)
4	SO4	G	990	-	4,4,4	0.43	0	6,6,6	0.39	0
4	SO4	C	999	-	4,4,4	0.21	0	6,6,6	0.07	0
4	SO4	K	354	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	A	998	-	4,4,4	0.62	0	6,6,6	0.35	0
4	SO4	G	993	-	4,4,4	0.29	0	6,6,6	0.31	0
4	SO4	F	944	-	4,4,4	0.38	0	6,6,6	0.24	0
4	SO4	A	993	-	4,4,4	0.22	0	6,6,6	0.21	0
4	SO4	B	944	-	4,4,4	0.53	0	6,6,6	0.56	0
4	SO4	G	997	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	C	998	-	4,4,4	0.20	0	6,6,6	0.20	0
4	SO4	C	992	-	4,4,4	1.18	0	6,6,6	0.24	0
4	SO4	K	353	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	C	995	-	4,4,4	0.30	0	6,6,6	0.18	0
4	SO4	A	1002	-	4,4,4	0.24	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	H	942	-	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	942	-	-	1/18/38/38	0/3/3/3
5	ATP	D	942	-	-	1/18/38/38	0/3/3/3
5	ATP	F	942	-	-	4/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	942	ATP	O4'-C1'	4.38	1.47	1.41
5	D	942	ATP	O2'-C2'	4.24	1.53	1.43
5	F	942	ATP	C2-N3	3.33	1.37	1.32
5	H	942	ATP	C4-N3	3.31	1.40	1.35
5	F	942	ATP	C2-N1	2.82	1.39	1.33
5	B	942	ATP	C2'-C1'	2.74	1.57	1.53
5	H	942	ATP	C2-N1	2.73	1.39	1.33
5	D	942	ATP	C2-N3	2.73	1.36	1.32
5	H	942	ATP	C2-N3	2.68	1.36	1.32
5	B	942	ATP	C2-N3	2.60	1.36	1.32
5	D	942	ATP	C4-N3	2.56	1.39	1.35
5	D	942	ATP	O4'-C1'	2.46	1.44	1.41
5	D	942	ATP	PA-O1A	2.32	1.59	1.50
5	B	942	ATP	O2'-C2'	2.20	1.48	1.43
5	B	942	ATP	O4'-C4'	-2.14	1.40	1.45
5	D	942	ATP	C2-N1	2.08	1.37	1.33
5	B	942	ATP	C4-N3	2.03	1.38	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	942	ATP	O2G-PG-O3B	3.71	117.06	104.64
5	B	942	ATP	O2'-C2'-C1'	3.42	123.48	110.85
5	D	942	ATP	PA-O3A-PB	-3.34	121.37	132.83
5	H	942	ATP	C5-C6-N6	3.31	125.38	120.35
5	H	942	ATP	O2G-PG-O3B	3.14	115.18	104.64
5	D	942	ATP	C3'-C2'-C1'	-2.87	96.66	100.98
5	B	942	ATP	N3-C2-N1	-2.81	124.28	128.68
5	D	942	ATP	C5-C6-N6	2.76	124.54	120.35
5	D	942	ATP	N3-C2-N1	-2.41	124.91	128.68
5	F	942	ATP	C4-C5-N7	2.27	111.77	109.40
5	H	942	ATP	O3'-C3'-C4'	2.19	117.37	111.05
5	H	942	ATP	C3'-C2'-C1'	2.15	104.22	100.98
5	D	942	ATP	PB-O3B-PG	2.15	140.20	132.83
5	D	942	ATP	C1'-N9-C4	-2.15	122.86	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	942	ATP	O4'-C1'-C2'	-2.13	103.81	106.93
5	D	942	ATP	O5'-C5'-C4'	-2.11	101.73	108.99
5	H	942	ATP	PB-O3B-PG	2.11	140.06	132.83
5	B	942	ATP	C5-C6-N6	2.07	123.49	120.35
5	B	942	ATP	O3'-C3'-C4'	2.01	116.87	111.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	942	ATP	PB-O3A-PA-O5'
5	H	942	ATP	PB-O3A-PA-O5'
5	F	942	ATP	C5'-O5'-PA-O1A
5	F	942	ATP	O4'-C4'-C5'-O5'
5	D	942	ATP	PG-O3B-PB-O2B
5	F	942	ATP	C3'-C4'-C5'-O5'
5	B	942	ATP	C5'-O5'-PA-O1A

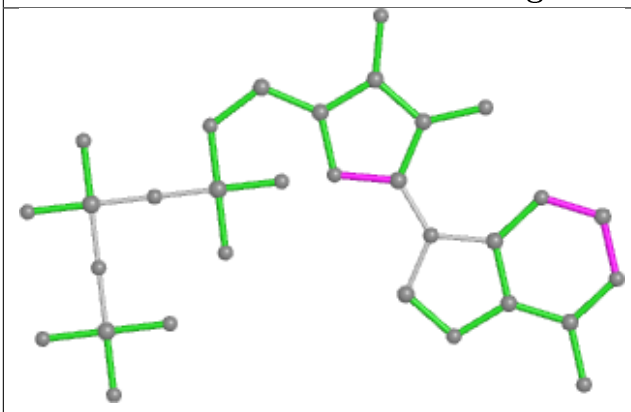
There are no ring outliers.

7 monomers are involved in 8 short contacts:

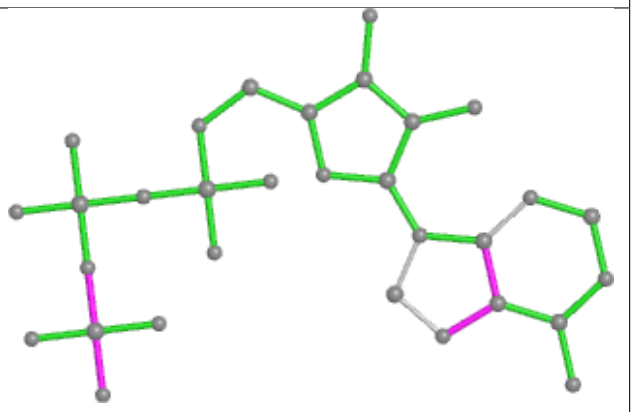
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	990	SO4	1	0
5	F	942	ATP	1	0
4	E	991	SO4	1	0
4	C	991	SO4	2	0
4	C	996	SO4	1	0
5	H	942	ATP	1	0
4	A	993	SO4	1	0

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 then 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.

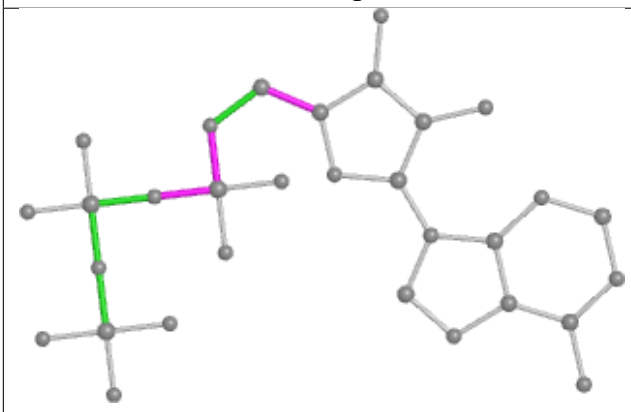
Ligand ATP F 942



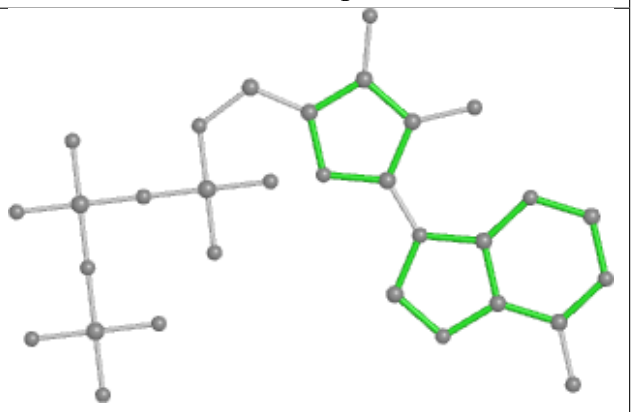
Bond lengths



Bond angles

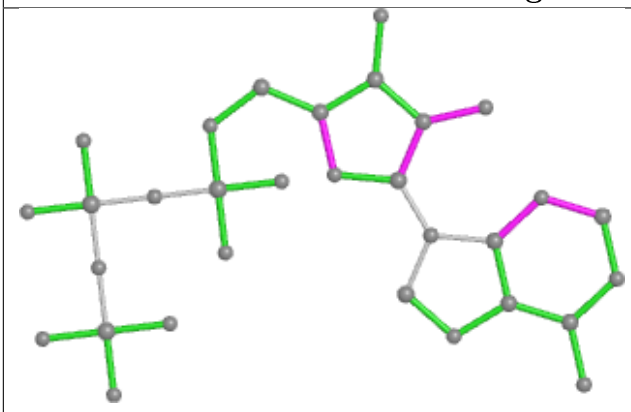


Torsions

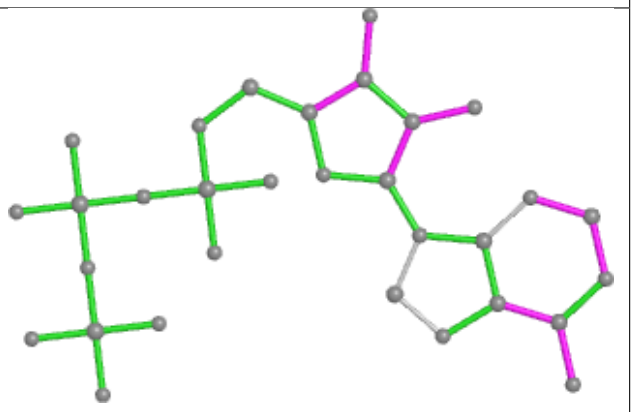


Rings

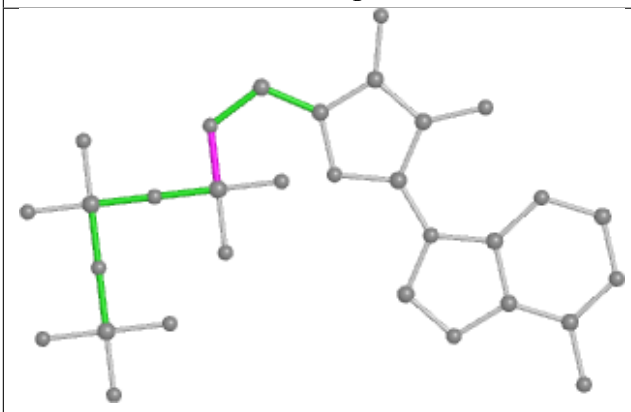
Ligand ATP B 942



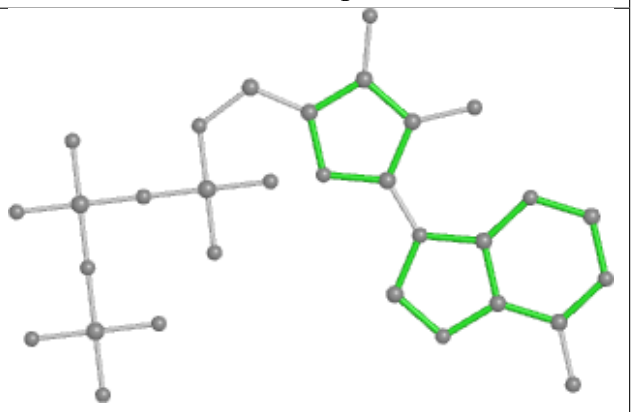
Bond lengths



Bond angles

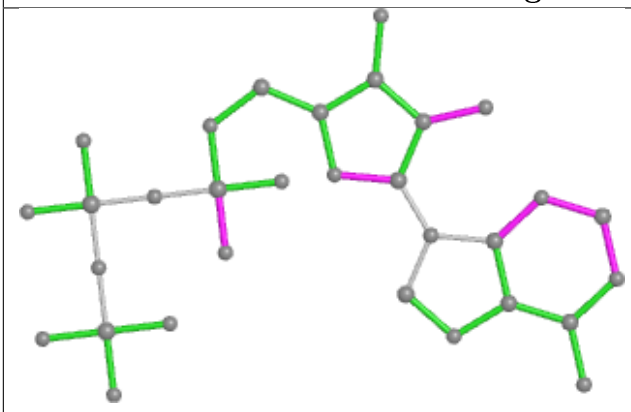


Torsions

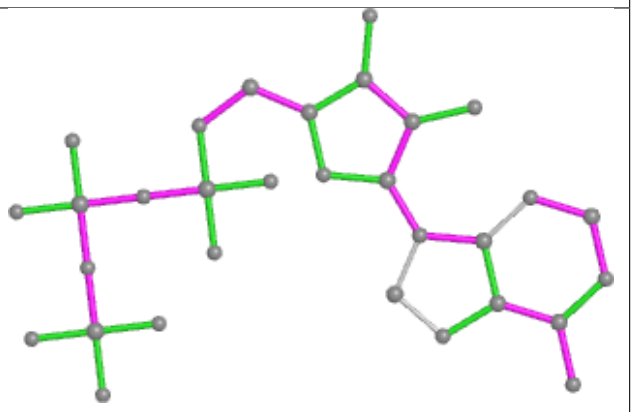


Rings

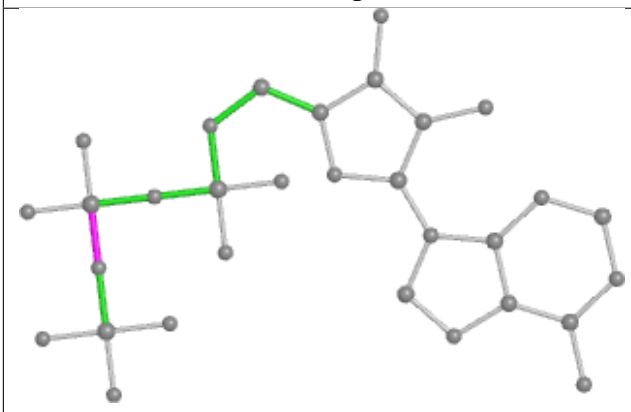
Ligand ATP D 942



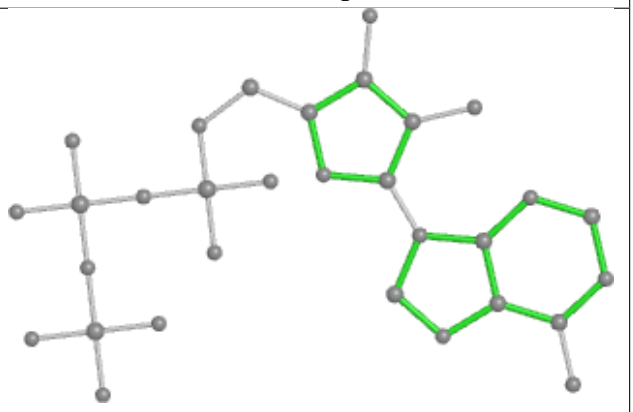
Bond lengths



Bond angles

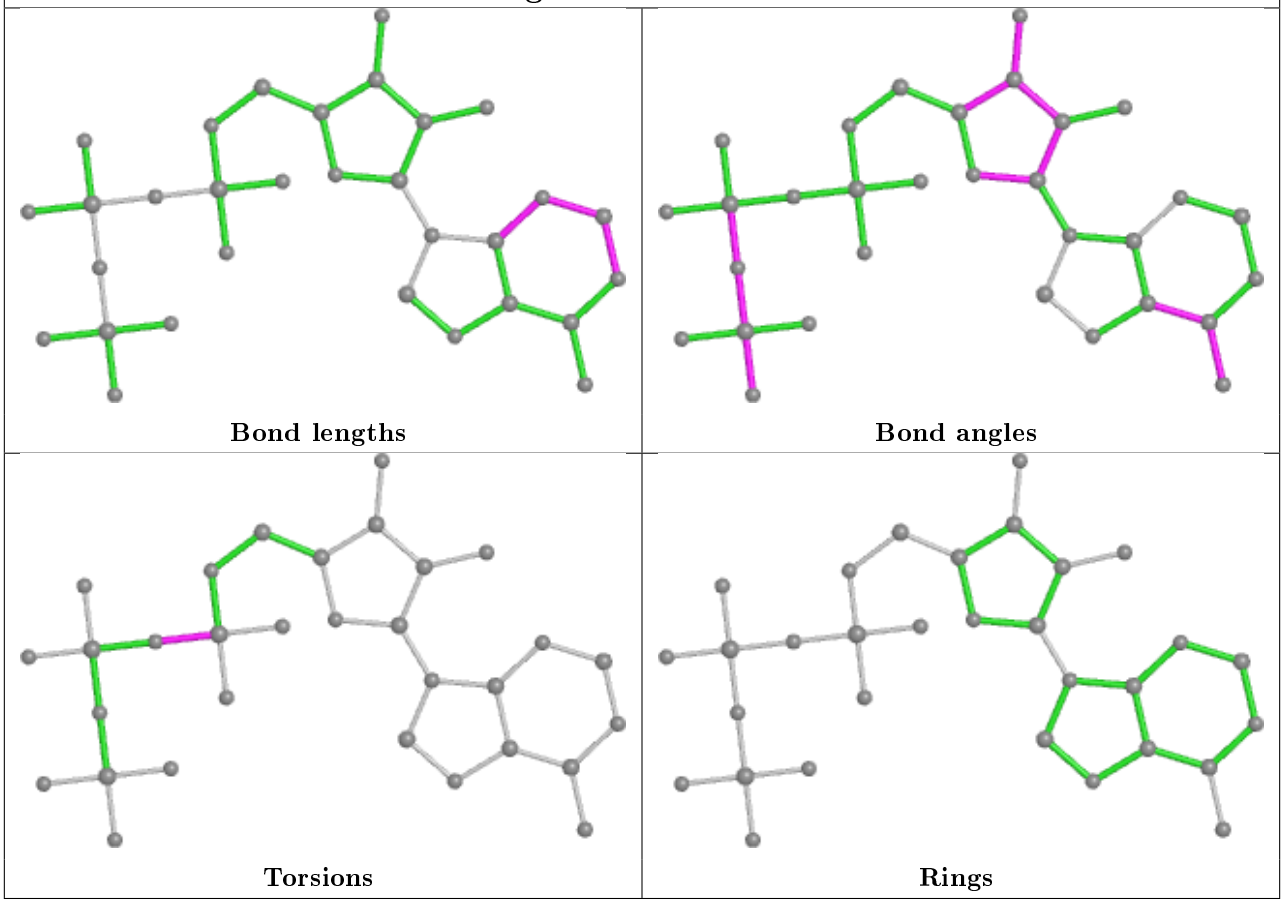


Torsions



Rings

Ligand ATP H 942



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, 95^{th} 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	936/989 (94%)	-0.10	8 (0%) 84 66	19, 52, 102, 146	0
1	C	936/989 (94%)	-0.07	11 (1%) 79 58	21, 53, 107, 163	0
1	E	936/989 (94%)	0.13	22 (2%) 59 34	31, 75, 120, 163	0
1	G	936/989 (94%)	0.06	16 (1%) 70 46	31, 70, 114, 160	0
2	B	884/941 (93%)	-0.09	8 (0%) 84 66	20, 52, 109, 163	0
2	D	884/941 (93%)	-0.08	3 (0%) 94 85	20, 51, 113, 186	0
2	F	884/941 (93%)	0.19	26 (2%) 51 26	43, 83, 126, 191	0
2	H	884/941 (93%)	0.11	18 (2%) 65 41	38, 72, 133, 184	0
3	I	323/351 (92%)	-0.30	1 (0%) 94 85	22, 47, 84, 106	0
3	J	323/351 (92%)	-0.31	0 100 100	17, 47, 84, 113	0
3	K	323/351 (92%)	-0.17	2 (0%) 89 76	38, 66, 96, 121	0
3	L	323/351 (92%)	-0.07	1 (0%) 94 85	47, 72, 104, 125	0
All	All	8572/9124 (93%)	-0.02	116 (1%) 75 53	17, 64, 116, 191	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	173	TYR	7.5
1	E	77	GLY	7.1
1	C	173	TYR	6.6
1	E	989	THR	6.3
1	E	764	ARG	5.8
2	H	54	ASP	5.7
1	A	173	TYR	5.6
1	G	762	SER	5.3
2	D	19	ASN	5.2
1	G	764	ARG	5.1
1	G	74	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	759	ALA	4.2
1	E	152	LYS	4.2
2	F	41	ASN	4.1
1	G	759	ALA	4.0
1	E	173	TYR	3.9
1	E	762	SER	3.9
2	B	43	ASN	3.9
1	E	118	GLU	3.8
1	A	166	ASP	3.8
2	H	95	GLN	3.8
2	F	256	CYS	3.7
1	E	112	LEU	3.7
2	F	31	THR	3.7
2	F	530	ILE	3.6
1	C	762	SER	3.6
1	C	150	PRO	3.5
1	C	186	PHE	3.5
1	E	186	PHE	3.5
1	E	168	ILE	3.4
1	E	962	TRP	3.4
2	F	58	VAL	3.3
1	G	286	GLU	3.3
2	H	561	HIS	3.3
1	E	169	SER	3.2
3	L	236	THR	3.2
2	H	136	PRO	3.2
2	F	881	ARG	3.2
2	B	19	ASN	3.2
1	E	287	PHE	3.0
1	E	33	GLY	2.9
2	F	879	SER	2.9
2	H	19	ASN	2.8
2	F	19	ASN	2.8
2	F	54	ASP	2.8
1	A	72	VAL	2.8
2	H	317	PHE	2.8
2	H	498	ASP	2.8
1	G	24	GLU	2.8
2	F	318	ASN	2.8
2	H	840	GLN	2.8
1	E	126	GLU	2.8
1	A	74	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	18	PRO	2.7
2	H	57	ASN	2.7
1	C	169	SER	2.7
2	B	17	ALA	2.6
1	G	77	GLY	2.6
2	H	881	ARG	2.6
1	A	118	GLU	2.6
2	F	509	ASP	2.6
2	H	128	PRO	2.6
2	F	343	ILE	2.6
2	F	367	SER	2.6
2	B	52	GLU	2.5
1	A	113	SER	2.5
1	C	166	ASP	2.5
1	E	758	SER	2.5
2	F	18	PRO	2.5
1	G	169	SER	2.5
2	F	433	GLY	2.5
2	D	18	PRO	2.5
2	H	68	HIS	2.4
1	G	660	ASN	2.4
2	D	99	ALA	2.4
2	F	528	LYS	2.4
1	E	85	GLN	2.4
2	F	139	SER	2.4
2	H	180	VAL	2.4
1	C	140	LYS	2.4
3	I	150	ILE	2.4
2	F	539	ILE	2.4
3	K	234	VAL	2.3
1	G	168	ILE	2.3
2	F	42	SER	2.3
1	E	292	GLY	2.3
2	B	255	ARG	2.3
1	G	127	VAL	2.3
2	B	139	SER	2.3
1	G	126	GLU	2.2
2	H	123	PRO	2.2
2	F	13	ILE	2.2
1	G	186	PHE	2.2
1	G	960	HIS	2.2
2	F	702	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	749	ASN	2.2
3	K	235	GLY	2.2
2	B	42	SER	2.1
1	C	118	GLU	2.1
1	E	73	GLU	2.1
2	H	273	ILE	2.1
2	H	75	ILE	2.1
2	F	913	SER	2.1
1	C	149	ILE	2.1
2	F	841	GLN	2.1
2	F	518	ASP	2.1
1	E	184	PRO	2.1
1	C	72	VAL	2.1
2	H	841	GLN	2.1
2	H	81	ASN	2.1
1	A	140	LYS	2.1
1	A	79	GLU	2.1
1	G	58	ILE	2.0
2	F	15	LEU	2.0
1	E	142	ILE	2.0
1	E	755	VAL	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, 95^{th} 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
4	SO4	I	354	5/5	0.76	0.28	160,164,165,166	0
4	SO4	C	999	5/5	0.76	0.25	147,152,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	998	5/5	0.80	0.18	119,123,124,125	0
4	SO4	J	354	5/5	0.83	0.16	140,144,145,145	0
4	SO4	L	354	5/5	0.84	0.21	129,133,134,135	0
4	SO4	L	352	5/5	0.85	0.15	122,127,128,128	0
4	SO4	I	355	5/5	0.85	0.24	131,135,136,137	0
4	SO4	I	356	5/5	0.85	0.17	125,129,130,130	0
4	SO4	G	997	5/5	0.85	0.17	135,139,139,140	0
4	SO4	K	354	5/5	0.85	0.16	136,141,141,142	0
4	SO4	E	996	5/5	0.86	0.18	123,127,128,129	0
4	SO4	L	353	5/5	0.88	0.21	165,169,170,170	0
4	SO4	A	995	5/5	0.88	0.16	116,120,121,122	0
4	SO4	A	1000	5/5	0.88	0.13	105,109,110,110	0
4	SO4	C	997	5/5	0.89	0.18	113,117,118,118	0
4	SO4	E	990	5/5	0.89	0.21	110,114,115,115	0
4	SO4	F	945	5/5	0.89	0.17	113,118,118,119	0
4	SO4	A	1002	5/5	0.89	0.16	131,136,136,137	0
4	SO4	H	946	5/5	0.90	0.18	116,120,121,121	0
4	SO4	A	998	5/5	0.90	0.22	84,87,89,90	0
4	SO4	E	997	5/5	0.90	0.21	124,128,129,129	0
4	SO4	E	994	5/5	0.90	0.17	118,122,123,124	0
4	SO4	J	352	5/5	0.90	0.19	104,108,109,109	0
4	SO4	K	352	5/5	0.91	0.18	88,92,93,94	0
5	ATP	H	942	31/31	0.92	0.17	69,70,102,104	0
4	SO4	A	1001	5/5	0.92	0.15	90,94,95,96	0
4	SO4	G	996	5/5	0.92	0.11	133,137,138,139	0
4	SO4	G	993	5/5	0.93	0.17	97,101,102,103	0
4	SO4	D	944	5/5	0.94	0.14	79,83,83,85	0
4	SO4	H	944	5/5	0.94	0.16	94,99,99,100	0
4	SO4	A	997	5/5	0.95	0.17	102,106,107,108	0
4	SO4	K	353	5/5	0.95	0.17	95,100,100,100	0
5	ATP	F	942	31/31	0.95	0.17	83,87,104,105	0
4	SO4	E	995	5/5	0.96	0.14	95,99,100,100	0
4	SO4	I	353	5/5	0.96	0.22	91,95,97,97	0
4	SO4	E	992	5/5	0.96	0.16	94,99,100,100	0
4	SO4	J	353	5/5	0.96	0.17	83,87,88,88	0
4	SO4	C	992	5/5	0.96	0.17	61,65,65,66	0
4	SO4	I	352	5/5	0.96	0.19	66,69,71,71	0
4	SO4	E	991	5/5	0.96	0.15	66,70,72,72	0
4	SO4	G	995	5/5	0.97	0.16	96,101,101,102	0
4	SO4	G	994	5/5	0.97	0.17	86,89,92,92	0
4	SO4	A	992	5/5	0.97	0.15	76,80,80,82	0
5	ATP	D	942	31/31	0.97	0.16	38,42,53,56	0

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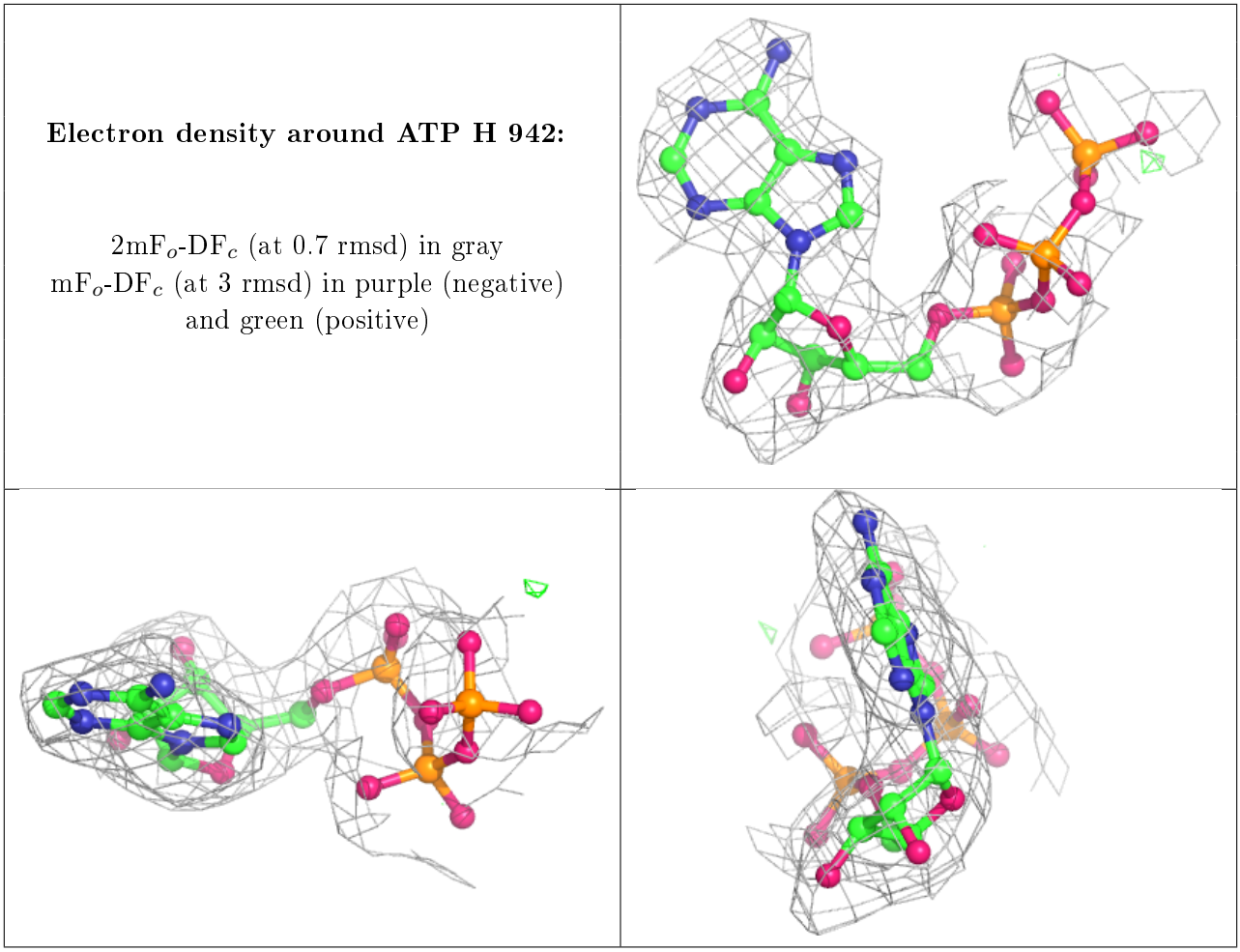
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	E	993	5/5	0.97	0.16	93,97,99,99	0
4	SO4	C	994	5/5	0.97	0.17	87,91,92,92	0
4	SO4	A	994	5/5	0.97	0.19	61,65,66,68	0
4	SO4	C	995	5/5	0.97	0.17	85,89,90,90	0
4	SO4	G	990	5/5	0.97	0.20	63,66,69,70	0
5	ATP	B	942	31/31	0.98	0.18	34,36,55,57	0
4	SO4	G	992	5/5	0.98	0.15	79,83,84,85	0
4	SO4	A	990	5/5	0.98	0.14	70,74,75,76	0
4	SO4	F	944	5/5	0.98	0.18	79,84,84,85	0
4	SO4	A	996	5/5	0.98	0.19	45,48,50,53	0
4	SO4	H	943	5/5	0.98	0.20	69,73,74,75	0
4	SO4	A	993	5/5	0.98	0.14	82,87,88,88	0
4	SO4	F	943	5/5	0.98	0.18	68,73,74,74	0
4	SO4	G	991	5/5	0.98	0.18	55,58,60,61	0
4	SO4	A	991	5/5	0.98	0.15	57,61,62,64	0
4	SO4	C	990	5/5	0.98	0.19	43,45,48,50	0
4	SO4	C	996	5/5	0.98	0.21	46,49,51,53	0
4	SO4	C	993	5/5	0.98	0.17	57,60,61,64	0
4	SO4	B	944	5/5	0.99	0.21	36,40,41,42	0
4	SO4	C	991	5/5	0.99	0.17	58,61,63,65	0
4	SO4	B	943	5/5	0.99	0.21	45,49,50,50	0
4	SO4	D	945	5/5	0.99	0.19	49,53,55,55	0
4	SO4	H	945	5/5	0.99	0.17	59,64,65,66	0
4	SO4	D	943	5/5	0.99	0.22	33,36,38,40	0
4	SO4	A	999	5/5	0.99	0.19	46,50,51,52	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.

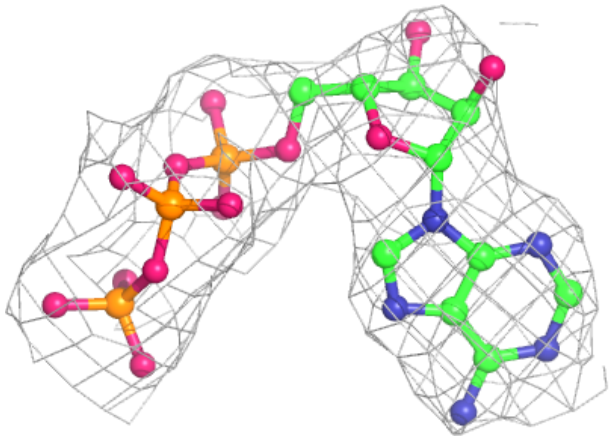
Electron density around ATP H 942:

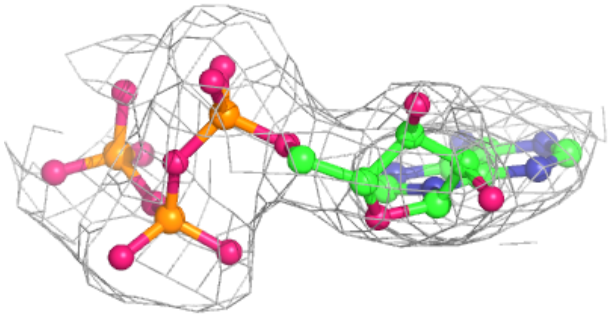
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

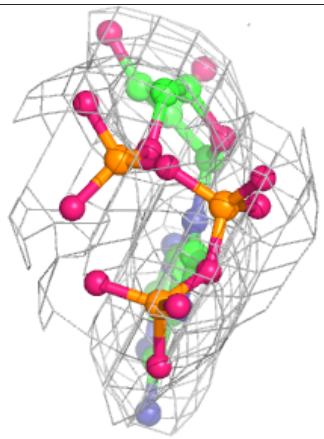


Electron density around ATP F 942:

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

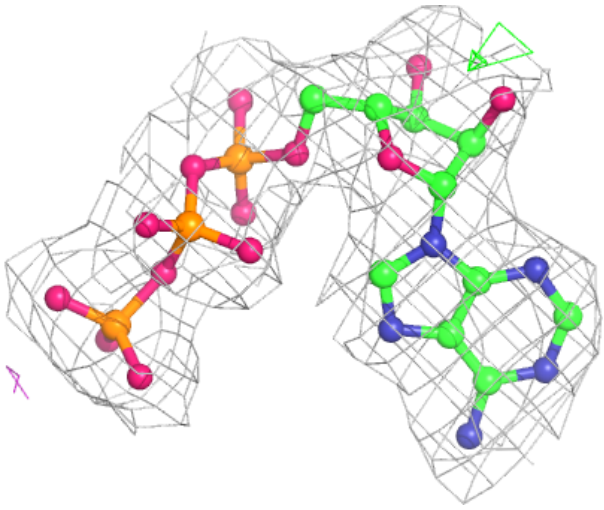


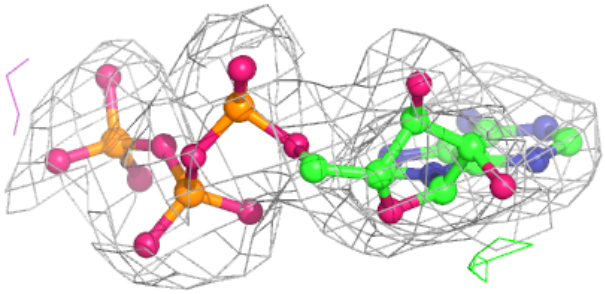


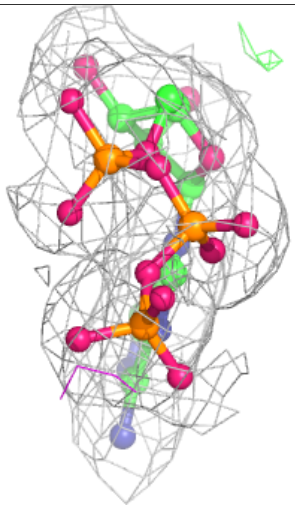


Electron density around ATP D 942:

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

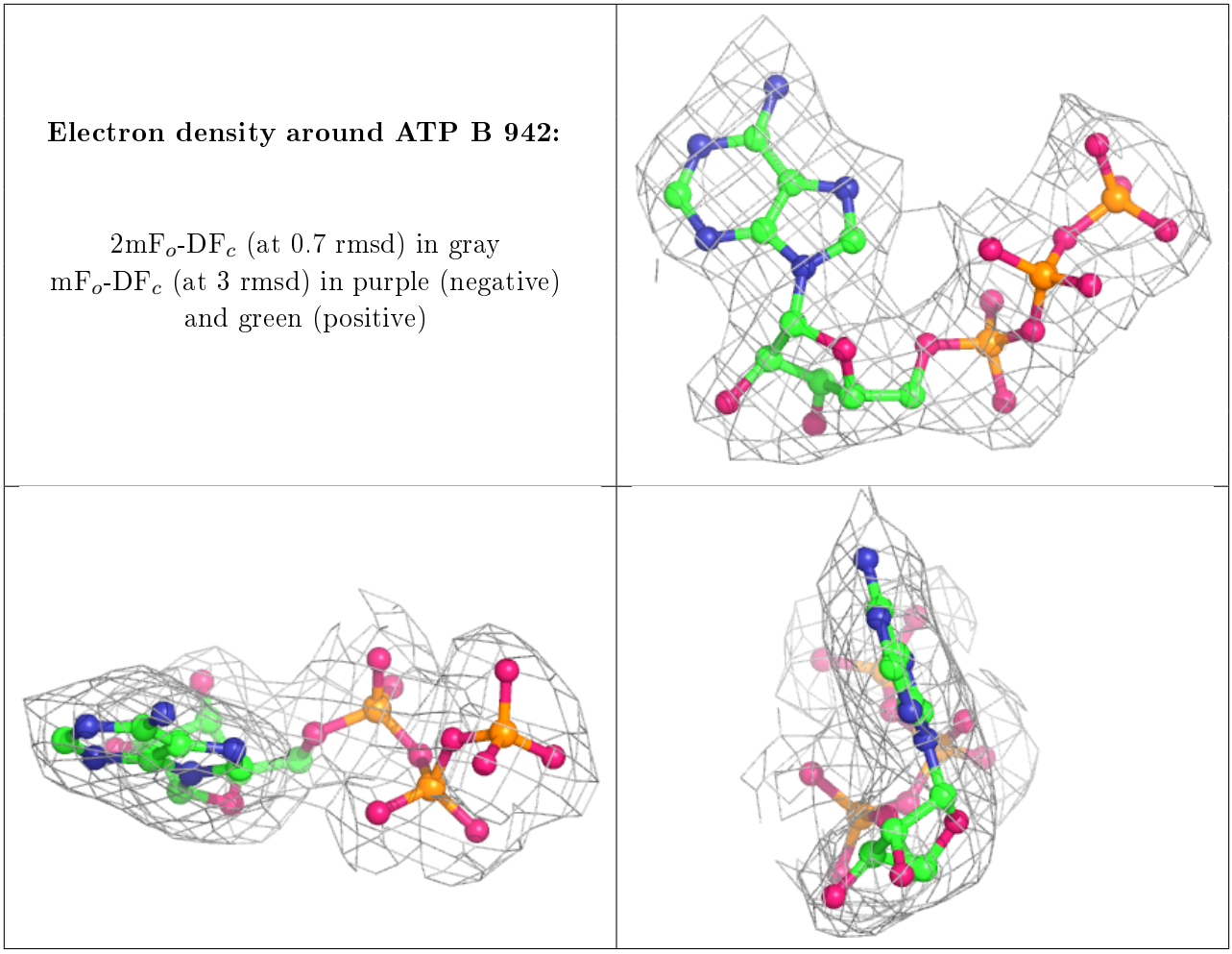






Electron density around ATP B 942:

$2mF_o$-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.