Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 05:58 AM EDT

PDB ID	:	3TUZ
Title	:	Inward facing conformations of the MetNI methionine ABC transporter: CY5 SeMet soak crystal form
Authors	:	Johnson, E.; Nguyen, P.; Rees, D.C.
Deposited on	:	2011-09-19
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

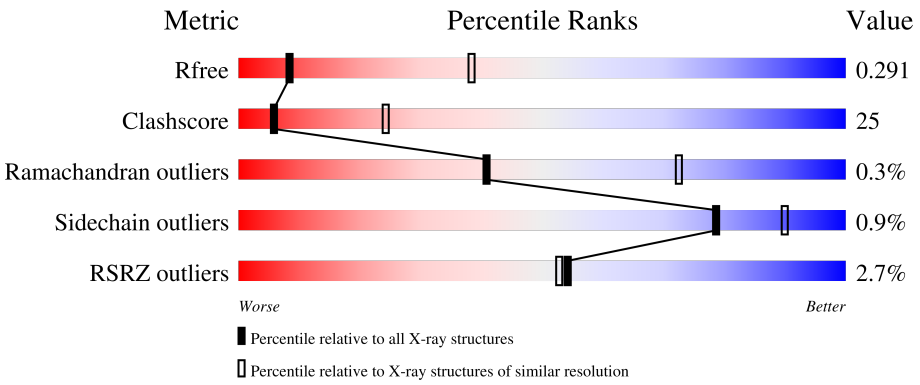
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	217	60% 38% •
1	B	217	% 55% 43% •
1	E	217	59% 40% •
1	F	217	2% 59% 40%
2	C	366	4% 62% 31% 6%

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Mol	Chain	Length	Quality of chain
2	D	366	5% 59% 34% 6%
2	G	366	2% 55% 37% 6%
2	H	366	4% 54% 38% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MSE	H	1000	-	-	X	-
4	ADP	C	2000	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17234 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 D-methionine transport system permease protein metI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1627	1079	266	272	10	0	0	0
1	B	216	1627	1079	266	272	10	0	0	0
1	E	215	1616	1073	262	271	10	0	0	0
1	F	216	1627	1079	266	272	10	0	0	0

- Molecule 2 is a protein called Methionine import ATP-binding protein MetN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	344	2661	1670	471	508	12	0	0	0
2	D	343	2651	1664	468	507	12	0	0	0
2	G	343	2651	1664	468	507	12	0	0	0
2	H	340	2630	1648	467	503	12	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	expression tag	UNP P30750
C	-21	GLY	-	expression tag	UNP P30750
C	-20	HIS	-	expression tag	UNP P30750
C	-19	HIS	-	expression tag	UNP P30750
C	-18	HIS	-	expression tag	UNP P30750
C	-17	HIS	-	expression tag	UNP P30750
C	-16	HIS	-	expression tag	UNP P30750
C	-15	HIS	-	expression tag	UNP P30750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP P30750
C	-13	HIS	-	expression tag	UNP P30750
C	-12	HIS	-	expression tag	UNP P30750
C	-11	HIS	-	expression tag	UNP P30750
C	-10	SER	-	expression tag	UNP P30750
C	-9	SER	-	expression tag	UNP P30750
C	-8	GLY	-	expression tag	UNP P30750
C	-7	HIS	-	expression tag	UNP P30750
C	-6	ILE	-	expression tag	UNP P30750
C	-5	ASP	-	expression tag	UNP P30750
C	-4	ASP	-	expression tag	UNP P30750
C	-3	ASP	-	expression tag	UNP P30750
C	-2	ASP	-	expression tag	UNP P30750
C	-1	LYS	-	expression tag	UNP P30750
C	0	HIS	-	expression tag	UNP P30750
C	166	GLN	GLU	engineered mutation	UNP P30750
D	-22	MET	-	expression tag	UNP P30750
D	-21	GLY	-	expression tag	UNP P30750
D	-20	HIS	-	expression tag	UNP P30750
D	-19	HIS	-	expression tag	UNP P30750
D	-18	HIS	-	expression tag	UNP P30750
D	-17	HIS	-	expression tag	UNP P30750
D	-16	HIS	-	expression tag	UNP P30750
D	-15	HIS	-	expression tag	UNP P30750
D	-14	HIS	-	expression tag	UNP P30750
D	-13	HIS	-	expression tag	UNP P30750
D	-12	HIS	-	expression tag	UNP P30750
D	-11	HIS	-	expression tag	UNP P30750
D	-10	SER	-	expression tag	UNP P30750
D	-9	SER	-	expression tag	UNP P30750
D	-8	GLY	-	expression tag	UNP P30750
D	-7	HIS	-	expression tag	UNP P30750
D	-6	ILE	-	expression tag	UNP P30750
D	-5	ASP	-	expression tag	UNP P30750
D	-4	ASP	-	expression tag	UNP P30750
D	-3	ASP	-	expression tag	UNP P30750
D	-2	ASP	-	expression tag	UNP P30750
D	-1	LYS	-	expression tag	UNP P30750
D	0	HIS	-	expression tag	UNP P30750
D	166	GLN	GLU	engineered mutation	UNP P30750
G	-22	MET	-	expression tag	UNP P30750
G	-21	GLY	-	expression tag	UNP P30750

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	HIS	-	expression tag	UNP P30750
G	-19	HIS	-	expression tag	UNP P30750
G	-18	HIS	-	expression tag	UNP P30750
G	-17	HIS	-	expression tag	UNP P30750
G	-16	HIS	-	expression tag	UNP P30750
G	-15	HIS	-	expression tag	UNP P30750
G	-14	HIS	-	expression tag	UNP P30750
G	-13	HIS	-	expression tag	UNP P30750
G	-12	HIS	-	expression tag	UNP P30750
G	-11	HIS	-	expression tag	UNP P30750
G	-10	SER	-	expression tag	UNP P30750
G	-9	SER	-	expression tag	UNP P30750
G	-8	GLY	-	expression tag	UNP P30750
G	-7	HIS	-	expression tag	UNP P30750
G	-6	ILE	-	expression tag	UNP P30750
G	-5	ASP	-	expression tag	UNP P30750
G	-4	ASP	-	expression tag	UNP P30750
G	-3	ASP	-	expression tag	UNP P30750
G	-2	ASP	-	expression tag	UNP P30750
G	-1	LYS	-	expression tag	UNP P30750
G	0	HIS	-	expression tag	UNP P30750
G	166	GLN	GLU	engineered mutation	UNP P30750
H	-22	MET	-	expression tag	UNP P30750
H	-21	GLY	-	expression tag	UNP P30750
H	-20	HIS	-	expression tag	UNP P30750
H	-19	HIS	-	expression tag	UNP P30750
H	-18	HIS	-	expression tag	UNP P30750
H	-17	HIS	-	expression tag	UNP P30750
H	-16	HIS	-	expression tag	UNP P30750
H	-15	HIS	-	expression tag	UNP P30750
H	-14	HIS	-	expression tag	UNP P30750
H	-13	HIS	-	expression tag	UNP P30750
H	-12	HIS	-	expression tag	UNP P30750
H	-11	HIS	-	expression tag	UNP P30750
H	-10	SER	-	expression tag	UNP P30750
H	-9	SER	-	expression tag	UNP P30750
H	-8	GLY	-	expression tag	UNP P30750
H	-7	HIS	-	expression tag	UNP P30750
H	-6	ILE	-	expression tag	UNP P30750
H	-5	ASP	-	expression tag	UNP P30750
H	-4	ASP	-	expression tag	UNP P30750
H	-3	ASP	-	expression tag	UNP P30750

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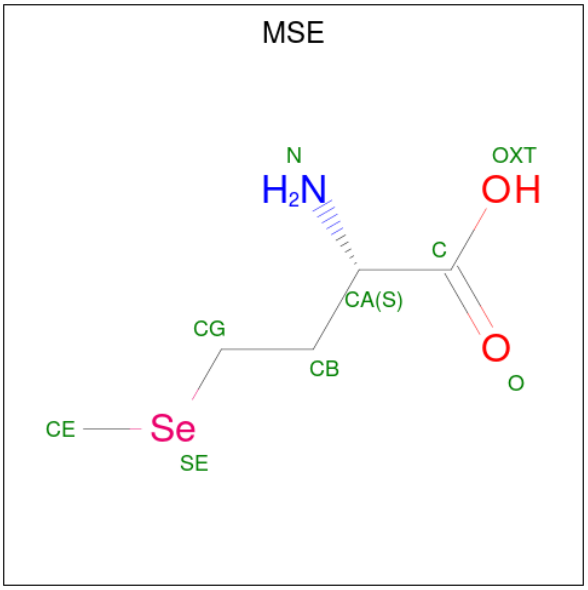
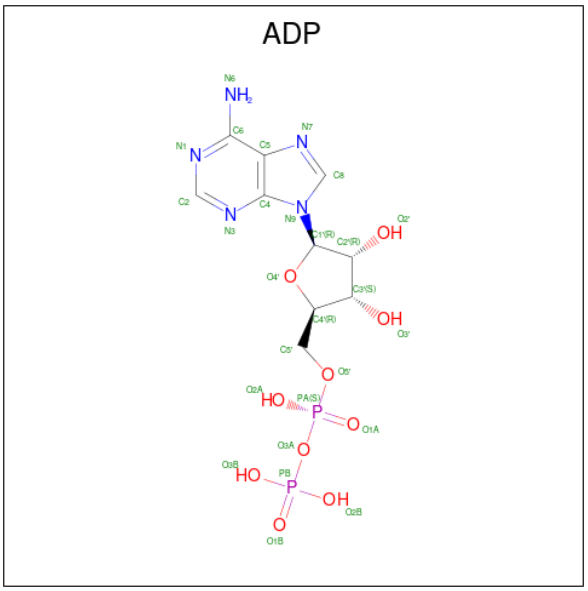
Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	ASP	-	expression tag	UNP P30750
H	-1	LYS	-	expression tag	UNP P30750
H	0	HIS	-	expression tag	UNP P30750
H	166	GLN	GLU	engineered mutation	UNP P30750

- Molecule 3 is SELENOMETHIONINE (three-letter code: MSE) (formula: $C_5H_{11}NO_2Se$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Se		
3	C	1	9	5	1	2	1	0	0
3	D	1	9	5	1	2	1	0	0
3	G	1	9	5	1	2	1	0	0
3	H	1	9	5	1	2	1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



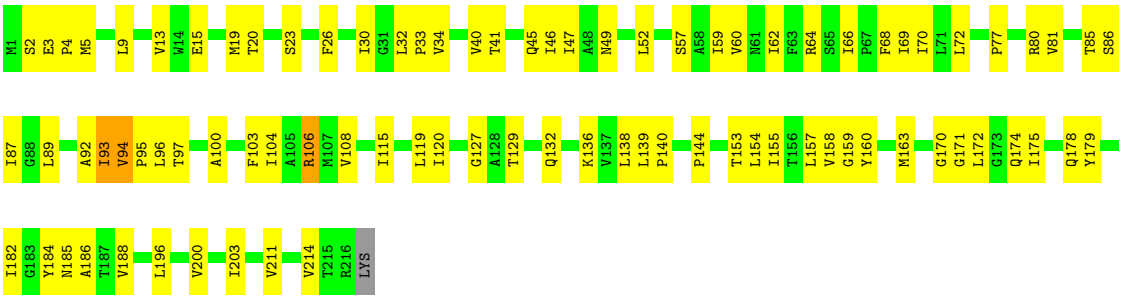
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

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

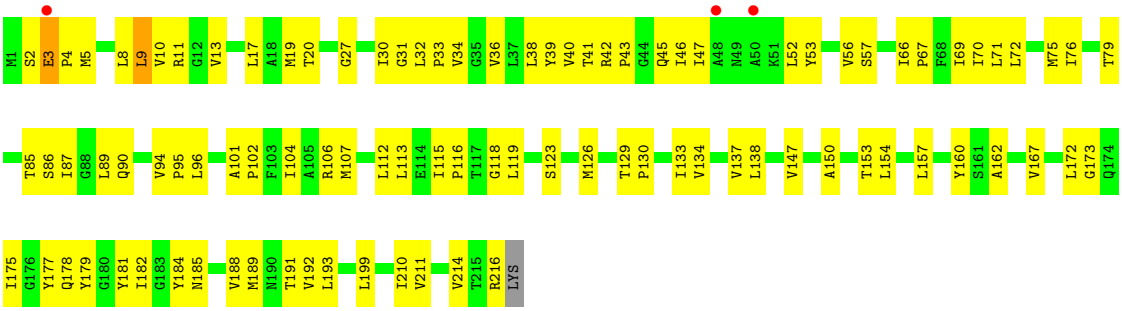
• Molecule 1: D-methionine transport system permease protein metI

Chain A: 60% 38%



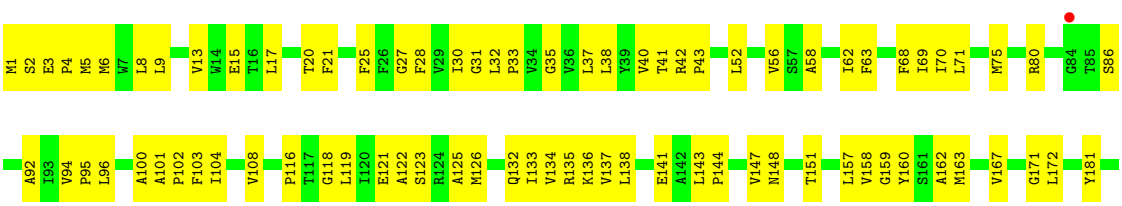
• Molecule 1: D-methionine transport system permease protein metI

Chain B: % 55% 43%



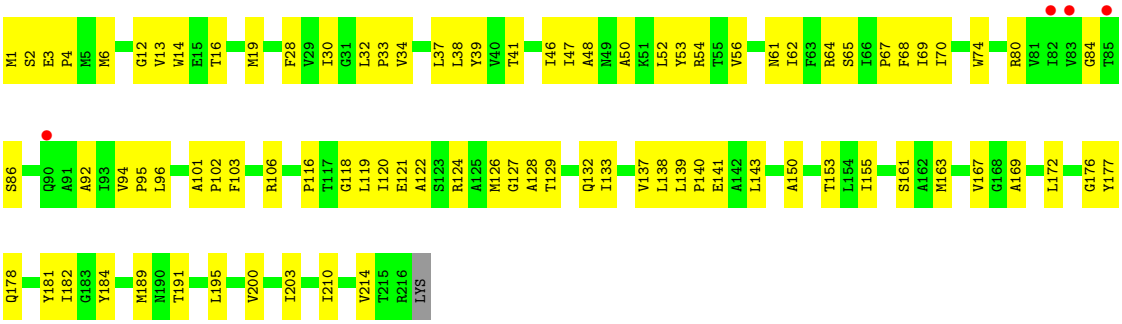
• Molecule 1: D-methionine transport system permease protein metI

Chain E: 59% 40%



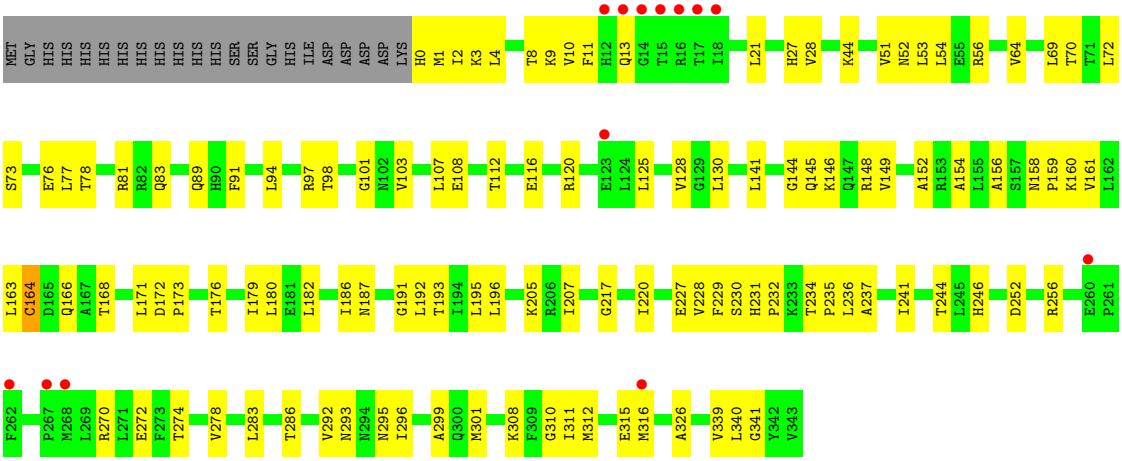
• Molecule 1: D-methionine transport system permease protein metI

Chain F:



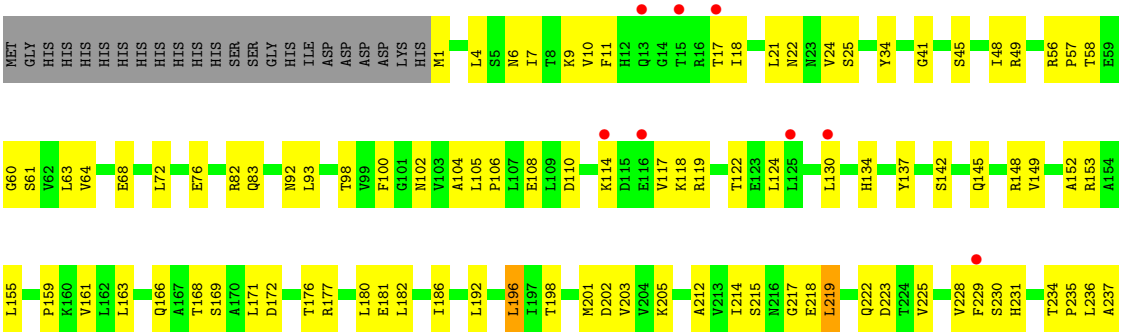
• Molecule 2: Methionine import ATP-binding protein MetN

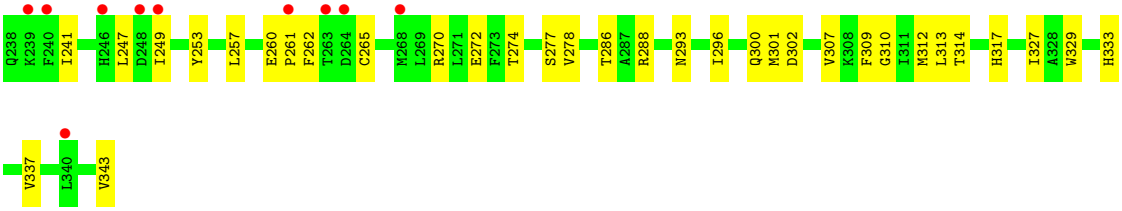
Chain C:



• Molecule 2: Methionine import ATP-binding protein MetN

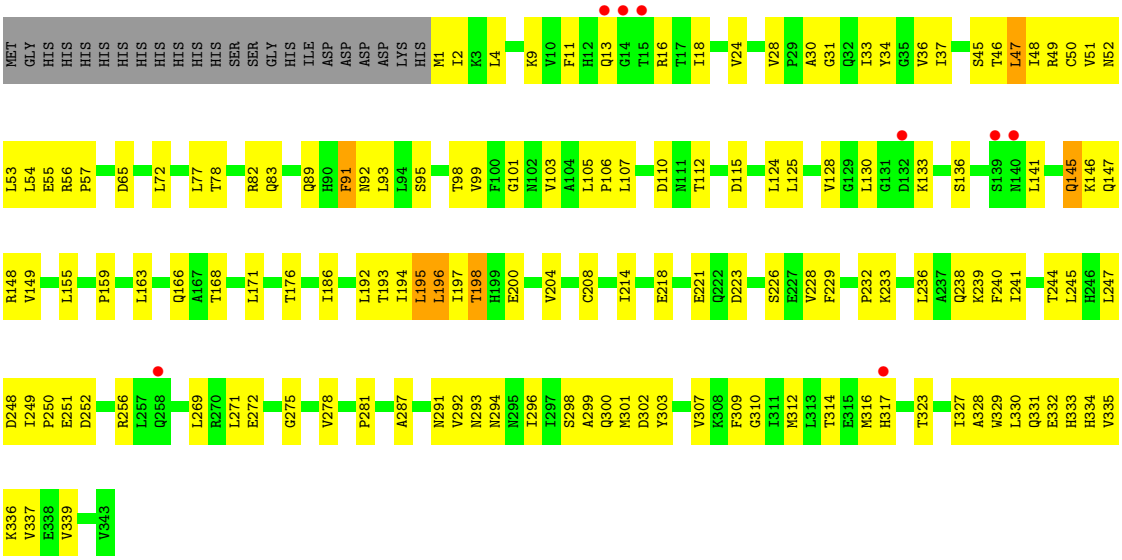
Chain D:





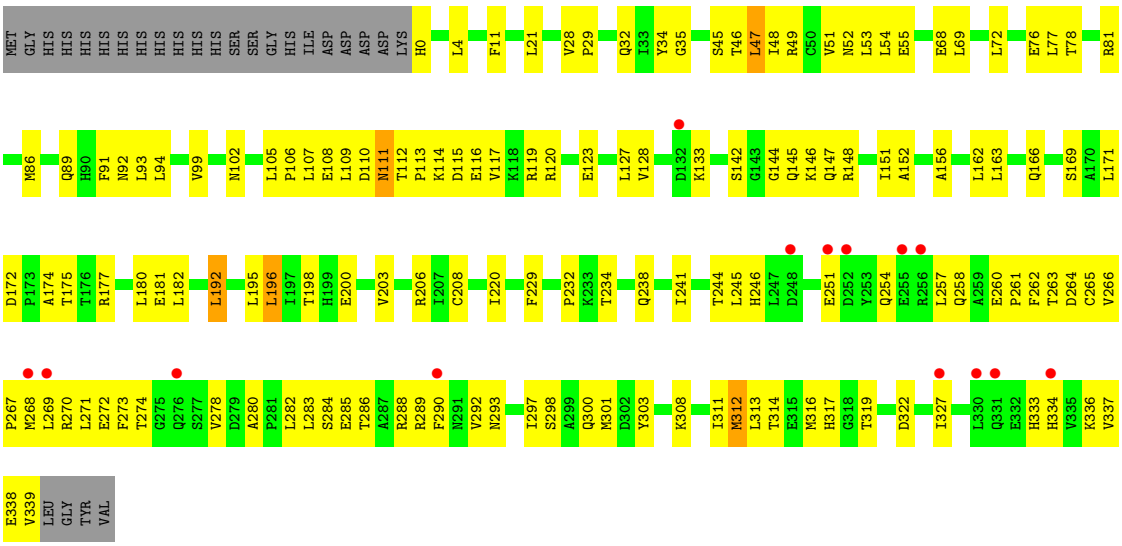
• Molecule 2: Methionine import ATP-binding protein MetN

Chain G:



• Molecule 2: Methionine import ATP-binding protein MetN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.31Å 138.89Å 147.51Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	38.80 – 3.40 39.46 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.4 (38.80-3.40) 84.1 (39.46-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.260 , 0.305 0.247 , 0.291	Depositor DCC
R_{free} test set	2337 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 23.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	17234	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.57	0/1660	0.67	0/2267
1	B	0.63	3/1660 (0.2%)	0.71	0/2267
1	E	0.55	1/1649 (0.1%)	0.69	1/2253 (0.0%)
1	F	0.54	0/1660	0.68	1/2267 (0.0%)
2	C	0.51	1/2701 (0.0%)	0.65	0/3662
2	D	0.51	0/2690	0.70	1/3647 (0.0%)
2	G	0.57	0/2690	0.75	3/3647 (0.1%)
2	H	0.55	0/2669	0.71	1/3618 (0.0%)
All	All	0.55	5/17379 (0.0%)	0.70	7/23628 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GLU	CD-OE1	-7.93	1.17	1.25
2	C	164	CYS	CB-SG	-5.60	1.72	1.81
1	B	3	GLU	CG-CD	-5.41	1.43	1.51
1	E	1	MET	CG-SD	-5.40	1.67	1.81
1	B	3	GLU	CD-OE2	-5.20	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	47	LEU	CA-CB-CG	7.78	133.20	115.30
2	G	196	LEU	CA-CB-CG	7.45	132.44	115.30
2	G	195	LEU	CA-CB-CG	5.63	128.25	115.30
2	D	196	LEU	CA-CB-CG	5.54	128.03	115.30
2	H	192	LEU	CA-CB-CG	5.49	127.92	115.30
1	F	1	MET	CG-SD-CE	5.46	108.93	100.20
1	E	1	MET	CG-SD-CE	5.18	108.48	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1627	0	1746	91	0
1	B	1627	0	1746	121	0
1	E	1616	0	1733	83	0
1	F	1627	0	1746	92	0
2	C	2661	0	2714	125	0
2	D	2651	0	2707	116	0
2	G	2651	0	2707	133	0
2	H	2630	0	2682	173	0
3	C	9	0	8	2	0
3	D	9	0	8	1	0
3	G	9	0	8	2	0
3	H	9	0	8	6	0
4	C	27	0	12	12	0
4	D	27	0	12	5	0
4	G	27	0	12	1	0
4	H	27	0	12	5	0
All	All	17234	0	17861	884	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 25.

All (884) 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:F:13:VAL:HA	1:F:172:LEU:HD11	1.16	1.16
2:G:293:ASN:OD1	2:H:284:SER:HB2	1.48	1.13
2:G:31:GLY:H	2:G:193:THR:HG22	1.03	1.06
1:B:115:ILE:HD11	1:B:138:LEU:HD23	1.38	1.05
1:B:8:LEU:O	1:B:11:ARG:N	1.91	1.04
2:H:91:PHE:CD2	2:H:146:LYS:HG3	1.93	1.04
1:A:185:ASN:HB3	1:A:188:VAL:CG1	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:312:MET:HB3	3:H:1000:MSE:CE	1.91	1.01
1:A:185:ASN:HB3	1:A:188:VAL:HG12	1.46	0.97
2:D:307:VAL:HG13	2:D:309:PHE:HE1	1.27	0.97
1:A:2:SER:OG	1:A:5:MET:HB2	1.66	0.96
1:A:23:SER:HA	1:A:97:THR:HG22	1.44	0.95
2:C:241:ILE:O	2:C:244:THR:HG22	1.68	0.94
2:D:9:LYS:HA	2:D:58:THR:HG22	1.47	0.94
2:G:49:ARG:HB2	2:G:54:LEU:HB2	1.48	0.93
2:G:31:GLY:N	2:G:193:THR:HG22	1.83	0.93
2:D:182:LEU:HD11	2:D:186:ILE:HD11	1.50	0.92
1:A:170:GLY:HA2	1:A:174:GLN:HE21	1.33	0.92
2:D:307:VAL:HG13	2:D:309:PHE:CE1	2.03	0.92
1:F:13:VAL:CA	1:F:172:LEU:HD11	2.00	0.91
2:H:266:VAL:HG13	2:H:316:MET:O	1.69	0.91
1:E:41:THR:HG21	1:E:52:LEU:HD11	1.49	0.90
1:F:155:ILE:HB	1:F:203:ILE:HD11	1.55	0.88
1:B:2:SER:C	1:B:4:PRO:HD2	1.94	0.87
2:C:11:PHE:HE2	4:C:2000:ADP:C4	1.93	0.87
1:E:147:VAL:HG23	1:E:211:VAL:HG22	1.57	0.87
2:H:128:VAL:HG11	2:H:152:ALA:HB2	1.54	0.87
2:H:260:GLU:OE1	2:H:261:PRO:HD2	1.75	0.86
2:H:48:ILE:HD12	2:H:195:LEU:HD12	1.58	0.86
1:B:42:ARG:HH11	1:B:113:LEU:HD11	1.39	0.85
2:D:182:LEU:CD1	2:D:186:ILE:HD11	2.07	0.84
1:F:129:THR:H	1:F:132:GLN:HE21	1.26	0.84
1:A:5:MET:CE	1:A:188:VAL:HG23	2.09	0.83
2:H:114:LYS:HG2	2:H:115:ASP:H	1.42	0.82
2:C:11:PHE:HE2	4:C:2000:ADP:C5	1.97	0.82
2:C:2:ILE:HD11	2:C:28:VAL:HG23	1.62	0.82
1:E:118:GLY:O	2:G:92:ASN:ND2	2.11	0.82
1:B:20:THR:HG22	1:B:154:LEU:HD12	1.62	0.82
2:H:110:ASP:O	2:H:111:ASN:HB2	1.78	0.82
1:B:72:LEU:HD21	1:B:167:VAL:HG11	1.62	0.82
1:E:28:PHE:HA	1:E:104:ILE:HD12	1.62	0.82
2:D:72:LEU:HD12	2:D:76:GLU:HB3	1.63	0.81
1:E:143:LEU:HD23	1:E:214:VAL:HG21	1.62	0.81
1:E:172:LEU:HD11	1:E:195:LEU:HD22	1.61	0.81
1:B:179:TYR:HD1	1:B:188:VAL:HG21	1.46	0.81
1:F:80:ARG:HB2	1:F:86:SER:HB3	1.64	0.80
2:G:248:ASP:HB3	2:H:300:GLN:HE22	1.45	0.80
1:A:185:ASN:HB3	1:A:188:VAL:HG11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD13	1:B:70:ILE:HG13	1.63	0.80
2:C:2:ILE:HG22	2:C:64:VAL:HG13	1.63	0.80
1:A:13:VAL:HG22	1:A:172:LEU:HD11	1.64	0.80
2:G:9:LYS:HE2	2:G:56:ARG:O	1.82	0.79
2:H:312:MET:HB3	3:H:1000:MSE:HE2	1.64	0.79
2:C:11:PHE:CE2	4:C:2000:ADP:C4	2.70	0.79
1:E:118:GLY:C	2:G:92:ASN:ND2	2.35	0.79
1:E:134:VAL:HG12	1:E:138:LEU:HD12	1.65	0.79
1:F:92:ALA:HB2	1:F:169:ALA:HB1	1.65	0.79
2:G:329:TRP:CE2	2:G:333:HIS:NE2	2.51	0.79
2:D:98:THR:HG22	2:D:137:TYR:CE2	2.18	0.79
2:G:310:GLY:HA3	3:G:1000:MSE:CE	2.13	0.78
2:C:246:HIS:O	2:D:300:GLN:NE2	2.16	0.78
2:D:72:LEU:CD1	2:D:76:GLU:HB3	2.14	0.77
1:E:20:THR:HG21	1:E:158:VAL:HG22	1.66	0.77
2:H:11:PHE:HB3	4:H:2000:ADP:C2	2.18	0.77
1:B:211:VAL:HA	1:B:214:VAL:HG12	1.65	0.77
2:C:0:HIS:HA	2:C:27:HIS:NE2	2.00	0.76
2:D:182:LEU:HD13	2:D:182:LEU:C	2.06	0.76
1:E:42:ARG:HB3	1:E:43:PRO:HD2	1.65	0.76
1:E:133:ILE:O	1:E:137:VAL:HG22	1.85	0.76
2:H:114:LYS:HG2	2:H:115:ASP:N	2.01	0.76
1:A:185:ASN:CB	1:A:188:VAL:HG12	2.15	0.76
2:D:296:ILE:HG23	2:D:312:MET:CE	2.16	0.76
2:D:100:PHE:HD2	2:D:134:HIS:CE1	2.04	0.75
2:G:300:GLN:HE21	2:H:246:HIS:CD2	2.03	0.75
2:H:45:SER:OG	4:H:2000:ADP:O1B	2.02	0.75
2:C:2:ILE:HD11	2:C:28:VAL:CG2	2.16	0.75
1:E:32:LEU:HB3	1:E:33:PRO:HD3	1.69	0.75
2:G:99:VAL:HG11	2:G:141:LEU:HD11	1.68	0.75
2:H:174:ALA:HA	2:H:177:ARG:HH11	1.51	0.75
1:A:2:SER:OG	1:A:5:MET:CB	2.35	0.75
1:B:42:ARG:NH1	1:B:113:LEU:HD11	2.01	0.75
2:H:91:PHE:HD2	2:H:146:LYS:HG3	1.52	0.75
2:H:220:ILE:HG22	2:H:234:THR:HG21	1.67	0.75
2:D:296:ILE:HA	2:D:314:THR:HG22	1.67	0.74
2:G:300:GLN:HE21	2:H:246:HIS:HD2	1.35	0.74
2:H:91:PHE:CE2	2:H:146:LYS:HG3	2.22	0.74
1:E:13:VAL:HG22	1:E:195:LEU:HD21	1.68	0.74
2:G:1:MET:HB2	2:G:65:ASP:H	1.53	0.74
1:E:123:SER:HA	1:E:126:MET:HE3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:13:GLN:HB2	2:G:16:ARG:HB3	1.68	0.74
1:F:41:THR:HA	1:F:48:ALA:HA	1.70	0.74
1:F:137:VAL:O	1:F:141:GLU:HB2	1.87	0.74
2:G:99:VAL:CG1	2:G:141:LEU:HD11	2.18	0.73
2:H:48:ILE:CD1	2:H:195:LEU:HD12	2.18	0.73
2:D:6:ASN:H	2:D:25:SER:HB3	1.53	0.73
2:G:223:ASP:HB3	2:G:228:VAL:HG23	1.71	0.73
2:C:220:ILE:HD12	2:C:234:THR:HG21	1.70	0.73
1:F:118:GLY:C	2:H:92:ASN:ND2	2.42	0.73
1:F:46:ILE:HG22	1:F:124:ARG:HD3	1.69	0.73
1:F:143:LEU:HD23	1:F:214:VAL:HG21	1.70	0.73
2:D:4:LEU:HB3	2:D:7:ILE:HD12	1.68	0.72
1:E:172:LEU:CD1	1:E:195:LEU:HD22	2.19	0.72
1:B:178:GLN:OE1	1:B:182:ILE:HD12	1.89	0.72
1:B:72:LEU:CD2	1:B:167:VAL:HG11	2.18	0.72
2:D:182:LEU:HD13	2:D:182:LEU:O	1.90	0.72
1:B:188:VAL:HA	1:B:191:THR:HG22	1.72	0.72
1:A:5:MET:HE2	1:A:188:VAL:HG23	1.71	0.72
1:F:118:GLY:CA	2:H:92:ASN:HD21	2.02	0.72
1:B:32:LEU:HB3	1:B:33:PRO:HD3	1.72	0.71
2:D:307:VAL:CG1	2:D:309:PHE:HE1	2.02	0.71
2:D:230:SER:HG	2:D:231:HIS:CE1	2.08	0.71
2:D:142:SER:HB2	2:D:145:GLN:HG3	1.71	0.71
2:H:319:THR:HG23	2:H:322:ASP:HB2	1.73	0.71
2:C:1:MET:HE1	2:C:160:LYS:HB3	1.73	0.71
1:E:20:THR:HG21	1:E:158:VAL:CG2	2.21	0.71
2:C:98:THR:HG23	2:C:101:GLY:H	1.56	0.70
1:B:85:THR:HG22	1:B:87:ILE:H	1.56	0.70
2:G:45:SER:HA	2:G:48:ILE:HG22	1.73	0.70
2:H:53:LEU:HD12	2:H:69:LEU:HB3	1.72	0.70
1:A:2:SER:HG	1:A:5:MET:HB2	1.55	0.70
2:D:124:LEU:HD21	2:D:155:LEU:HB2	1.74	0.70
2:C:283:LEU:HD11	2:C:312:MET:SD	2.32	0.70
1:A:68:PHE:HZ	1:A:96:LEU:HD12	1.56	0.69
1:B:40:VAL:HG12	1:B:47:ILE:HD12	1.73	0.69
1:F:210:ILE:O	1:F:214:VAL:HG12	1.91	0.69
2:G:248:ASP:HB3	2:H:300:GLN:NE2	2.06	0.69
1:E:118:GLY:C	2:G:92:ASN:HD21	1.96	0.69
2:G:9:LYS:HE3	2:G:55:GLU:HG3	1.74	0.69
1:A:5:MET:HE1	1:A:188:VAL:HG23	1.75	0.69
2:D:168:THR:HA	2:D:171:LEU:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:LEU:HD11	2:D:203:VAL:HG12	1.75	0.69
1:B:177:TYR:O	1:B:181:TYR:HB3	1.92	0.69
2:G:91:PHE:O	2:G:92:ASN:HB2	1.92	0.69
2:H:35:GLY:HA2	2:H:196:LEU:HD13	1.74	0.69
1:A:154:LEU:HB3	1:A:203:ILE:HD11	1.74	0.68
1:A:200:VAL:O	1:A:203:ILE:HG22	1.91	0.68
2:H:269:LEU:HD12	2:H:337:VAL:HG13	1.75	0.68
1:F:3:GLU:N	1:F:4:PRO:HD2	2.08	0.68
2:C:310:GLY:HA3	3:C:1000:MSE:HE1	1.75	0.68
1:B:72:LEU:HD21	1:B:167:VAL:CG1	2.23	0.68
2:C:310:GLY:HA3	3:C:1000:MSE:CE	2.22	0.68
2:D:124:LEU:CD2	2:D:155:LEU:HB2	2.23	0.68
1:B:41:THR:HG22	1:B:41:THR:O	1.94	0.68
2:H:266:VAL:CG1	2:H:316:MET:O	2.40	0.68
1:B:211:VAL:HA	1:B:214:VAL:CG1	2.22	0.68
2:D:230:SER:HB3	2:D:309:PHE:CE2	2.29	0.68
1:B:41:THR:HG22	1:B:53:TYR:HB2	1.76	0.67
2:D:48:ILE:HD11	2:D:163:LEU:HB3	1.76	0.67
2:H:99:VAL:HG21	2:H:133:LYS:O	1.94	0.67
1:A:64:ARG:NH1	1:A:103:PHE:CD1	2.62	0.67
2:D:237:ALA:O	2:D:241:ILE:HG12	1.94	0.67
1:E:162:ALA:O	1:F:69:ILE:HD11	1.95	0.67
2:H:196:LEU:HD11	2:H:208:CYS:SG	2.34	0.67
2:H:107:LEU:HD11	2:H:156:ALA:O	1.93	0.67
1:B:118:GLY:O	2:D:92:ASN:ND2	2.27	0.67
2:G:125:LEU:O	2:G:130:LEU:N	2.22	0.67
2:H:112:THR:HG22	2:H:117:VAL:HG23	1.77	0.67
1:B:216:ARG:N	1:B:216:ARG:HD2	2.09	0.67
2:C:144:GLY:O	2:C:148:ARG:HG3	1.95	0.67
2:C:283:LEU:O	2:C:286:THR:HG22	1.95	0.67
1:E:80:ARG:HH12	1:F:184:TYR:HE2	1.41	0.67
2:C:274:THR:O	2:C:278:VAL:HG23	1.95	0.66
2:G:46:THR:OG1	4:G:2000:ADP:O1A	2.11	0.66
1:E:172:LEU:HD11	1:E:195:LEU:CD2	2.25	0.66
2:D:215:SER:CB	2:D:236:LEU:HD11	2.26	0.66
2:H:91:PHE:CE1	2:H:147:GLN:NE2	2.62	0.66
2:H:292:VAL:HG21	2:H:316:MET:HE2	1.77	0.66
2:H:303:TYR:OH	2:H:308:LYS:HD2	1.96	0.66
2:C:187:ASN:ND2	2:C:192:LEU:O	2.27	0.66
2:D:105:LEU:N	2:D:106:PRO:HD2	2.11	0.66
1:B:2:SER:CB	1:B:4:PRO:HD2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:GLY:O	1:E:104:ILE:HD11	1.96	0.66
2:G:329:TRP:CZ2	2:G:333:HIS:NE2	2.64	0.66
2:H:290:PHE:HB3	2:H:322:ASP:HB3	1.78	0.65
2:H:172:ASP:HB2	2:H:175:THR:OG1	1.96	0.65
2:G:45:SER:O	2:G:49:ARG:HG2	1.97	0.65
1:F:16:THR:HB	1:F:172:LEU:HD13	1.78	0.65
2:H:260:GLU:CD	2:H:261:PRO:HD2	2.16	0.65
2:C:301:MET:SD	2:C:308:LYS:HE2	2.37	0.65
2:D:182:LEU:CD1	2:D:186:ILE:CD1	2.74	0.65
1:B:172:LEU:CD2	1:B:192:VAL:HG13	2.27	0.65
1:F:16:THR:HB	1:F:172:LEU:CD1	2.27	0.65
2:G:46:THR:O	2:G:50:CYS:HB2	1.97	0.65
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.77	0.65
2:C:130:LEU:HD11	2:C:148:ARG:HB2	1.77	0.65
2:C:130:LEU:HD13	2:C:149:VAL:HG22	1.79	0.65
1:E:167:VAL:HG12	1:E:167:VAL:O	1.97	0.65
2:H:327:ILE:HG23	2:H:337:VAL:HG21	1.79	0.65
1:B:3:GLU:N	1:B:4:PRO:CD	2.60	0.64
2:C:1:MET:CE	2:C:160:LYS:HB3	2.27	0.64
2:C:231:HIS:N	2:C:232:PRO:HD3	2.13	0.64
2:G:328:ALA:O	2:G:332:GLU:HG3	1.96	0.64
1:A:23:SER:HA	1:A:97:THR:CG2	2.23	0.64
2:C:13:GLN:NE2	4:C:2000:ADP:C2	2.65	0.64
1:F:118:GLY:HA3	2:H:92:ASN:HD21	1.62	0.64
1:A:3:GLU:N	1:A:4:PRO:HD2	2.13	0.64
1:B:179:TYR:CD1	1:B:188:VAL:HG21	2.30	0.64
1:E:3:GLU:N	1:E:4:PRO:HD2	2.12	0.64
2:G:91:PHE:HD1	2:G:147:GLN:HE21	1.46	0.64
2:H:142:SER:N	2:H:145:GLN:OE1	2.28	0.64
1:F:38:LEU:HD21	1:F:106:ARG:NH1	2.13	0.64
1:B:185:ASN:HB3	1:B:188:VAL:HG22	1.80	0.63
1:B:119:LEU:O	1:B:123:SER:HB2	1.97	0.63
2:H:272:GLU:HB2	2:H:336:LYS:HB3	1.80	0.63
2:C:168:THR:HG22	2:C:171:LEU:HD12	1.80	0.63
1:F:129:THR:H	1:F:132:GLN:NE2	1.94	0.63
2:H:286:THR:HG22	2:H:292:VAL:CG2	2.28	0.63
1:F:46:ILE:HG13	1:F:46:ILE:O	1.98	0.63
1:A:103:PHE:HE2	1:A:160:TYR:HH	1.44	0.63
1:A:127:GLY:O	2:C:78:THR:HG23	1.99	0.63
2:C:2:ILE:HG13	2:C:28:VAL:HB	1.81	0.63
2:D:45:SER:HB3	4:D:2000:ADP:PA	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:VAL:HG22	1:E:195:LEU:CD2	2.28	0.63
2:D:145:GLN:O	2:D:149:VAL:HG23	1.99	0.62
1:E:71:LEU:O	1:E:75:MET:HG2	1.99	0.62
2:H:91:PHE:CD1	2:H:147:GLN:NE2	2.67	0.62
2:H:280:ALA:O	3:H:1000:MSE:N	2.32	0.62
1:A:26:PHE:O	1:A:30:ILE:HG22	1.99	0.62
1:B:3:GLU:N	1:B:4:PRO:HD2	2.14	0.62
2:D:41:GLY:HA2	4:D:2000:ADP:H3'	1.79	0.62
2:G:249:ILE:HG13	2:G:249:ILE:O	1.99	0.62
2:D:45:SER:O	2:D:49:ARG:HG2	1.98	0.62
2:G:198:THR:HB	2:G:200:GLU:H	1.65	0.62
2:C:53:LEU:CD1	2:C:69:LEU:HB3	2.29	0.62
1:F:47:ILE:HG12	1:F:47:ILE:O	1.98	0.62
1:B:40:VAL:HG12	1:B:47:ILE:CD1	2.30	0.62
2:D:166:GLN:HB3	2:D:169:SER:HB2	1.81	0.62
2:D:214:ILE:HA	2:D:219:LEU:HA	1.82	0.62
2:H:257:LEU:HG	2:H:258:GLN:O	2.00	0.62
1:A:93:ILE:HG22	1:A:93:ILE:O	1.99	0.62
1:B:45:GLN:HG3	1:B:46:ILE:H	1.64	0.62
1:B:36:VAL:HG12	1:B:112:LEU:HD11	1.81	0.61
1:F:167:VAL:HG12	1:F:167:VAL:O	2.00	0.61
2:H:220:ILE:CG2	2:H:234:THR:HG21	2.29	0.61
2:C:0:HIS:CA	2:C:27:HIS:NE2	2.64	0.61
1:F:176:GLY:O	1:F:189:MET:HE3	2.00	0.61
2:D:230:SER:HB3	2:D:309:PHE:CZ	2.35	0.61
2:D:307:VAL:CG1	2:D:309:PHE:CE1	2.81	0.61
2:D:106:PRO:HG3	2:D:153:ARG:HG3	1.81	0.61
2:C:94:LEU:HD12	2:C:97:ARG:HD3	1.82	0.61
1:E:27:GLY:C	1:E:104:ILE:HD11	2.20	0.61
1:B:42:ARG:HG3	1:B:43:PRO:HD2	1.82	0.61
2:C:0:HIS:N	2:C:27:HIS:NE2	2.48	0.61
2:H:262:PHE:CE1	2:H:265:CYS:HB2	2.35	0.61
2:H:91:PHE:HZ	2:H:171:LEU:HD21	1.65	0.61
2:G:293:ASN:O	2:G:317:HIS:HB2	2.01	0.60
1:F:139:LEU:HB2	1:F:140:PRO:HD3	1.82	0.60
1:F:64:ARG:HD2	1:F:103:PHE:HA	1.83	0.60
2:H:105:LEU:HB3	2:H:106:PRO:HD3	1.83	0.60
1:A:155:ILE:CG1	1:A:203:ILE:CG2	2.79	0.60
1:B:45:GLN:HG3	1:B:46:ILE:N	2.17	0.59
2:C:272:GLU:HG2	2:C:311:ILE:HG12	1.84	0.59
1:A:32:LEU:HB3	1:A:33:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:CG	1:B:43:PRO:HD2	2.32	0.59
2:C:13:GLN:NE2	4:C:2000:ADP:H2	2.00	0.59
2:H:300:GLN:HE21	2:H:301:MET:H	1.50	0.59
1:B:167:VAL:HG22	1:B:167:VAL:O	2.02	0.59
2:H:269:LEU:HD13	2:H:338:GLU:O	2.02	0.59
2:C:164:CYS:HB2	2:C:196:LEU:CD1	2.32	0.59
2:D:21:LEU:HA	2:D:217:GLY:HA2	1.83	0.59
2:D:118:LYS:O	2:D:122:THR:HG23	2.02	0.59
2:D:177:ARG:O	2:D:181:GLU:HB2	2.01	0.59
2:G:248:ASP:O	2:G:249:ILE:HG22	2.03	0.59
1:E:159:GLY:HA2	1:F:67:PRO:HB3	1.84	0.59
2:C:168:THR:HB	2:C:176:THR:HG22	1.85	0.59
2:H:112:THR:HB	2:H:117:VAL:CG2	2.33	0.59
1:B:115:ILE:HG13	1:B:115:ILE:O	2.02	0.59
2:H:274:THR:HG23	2:H:334:HIS:HD2	1.67	0.59
2:G:310:GLY:HA3	3:G:1000:MSE:HE1	1.84	0.58
2:D:260:GLU:HB2	2:D:261:PRO:HD2	1.84	0.58
1:A:30:ILE:O	1:A:34:VAL:HG23	2.03	0.58
1:F:118:GLY:C	2:H:92:ASN:HD22	2.07	0.58
2:G:293:ASN:OD1	2:H:284:SER:CB	2.40	0.58
1:F:118:GLY:CA	2:H:92:ASN:ND2	2.66	0.58
2:D:215:SER:HB2	2:D:236:LEU:HD11	1.84	0.58
2:G:98:THR:HG23	2:G:101:GLY:H	1.68	0.58
2:C:72:LEU:HD23	2:C:77:LEU:HD12	1.85	0.58
2:C:141:LEU:HB3	2:C:145:GLN:HB2	1.86	0.58
2:D:329:TRP:O	2:D:333:HIS:HD2	1.87	0.58
1:B:2:SER:HB2	1:B:5:MET:HB2	1.86	0.58
2:C:107:LEU:HB3	2:C:112:THR:HG21	1.86	0.58
2:G:2:ILE:HG12	2:G:2:ILE:O	2.04	0.58
1:E:17:LEU:HD21	1:E:199:LEU:HD22	1.85	0.57
2:H:45:SER:N	4:H:2000:ADP:O1B	2.37	0.57
2:G:2:ILE:HG23	2:G:28:VAL:HB	1.84	0.57
2:G:91:PHE:HD1	2:G:147:GLN:NE2	2.02	0.57
1:E:122:ALA:O	1:E:126:MET:HE3	2.04	0.57
1:A:155:ILE:HG12	1:A:203:ILE:CG2	2.34	0.57
2:G:294:ASN:HB3	2:G:316:MET:HA	1.87	0.57
2:G:327:ILE:O	2:G:331:GLN:HG3	2.05	0.57
2:H:268:MET:HE2	2:H:313:LEU:HD13	1.86	0.57
1:B:172:LEU:HD23	1:B:192:VAL:HG13	1.86	0.57
2:C:220:ILE:CD1	2:C:236:LEU:HD23	2.35	0.57
2:H:271:LEU:HD11	2:H:283:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:287:ALA:O	2:G:291:ASN:HA	2.05	0.57
1:A:20:THR:HG22	1:A:157:LEU:O	2.05	0.57
2:G:333:HIS:O	2:G:335:VAL:N	2.38	0.57
2:H:89:GLN:NE2	2:H:169:SER:HB3	2.19	0.57
1:A:23:SER:CA	1:A:97:THR:HG22	2.27	0.56
1:A:157:LEU:HA	1:A:160:TYR:HB2	1.87	0.56
2:G:323:THR:O	2:G:327:ILE:HD12	2.05	0.56
1:A:155:ILE:CG1	1:A:203:ILE:HG23	2.36	0.56
2:H:266:VAL:HG13	2:H:267:PRO:HD2	1.88	0.56
2:D:215:SER:OG	2:D:236:LEU:HD11	2.06	0.56
1:B:179:TYR:N	1:B:179:TYR:HD2	2.04	0.56
2:D:198:THR:HG21	2:D:203:VAL:CG2	2.36	0.56
1:E:31:GLY:HA3	1:E:104:ILE:HG13	1.86	0.56
2:G:51:VAL:HB	2:G:163:LEU:HD21	1.87	0.56
2:C:241:ILE:O	2:C:244:THR:CG2	2.50	0.56
1:B:179:TYR:N	1:B:179:TYR:CD2	2.73	0.56
1:F:16:THR:HA	1:F:19:MET:HE2	1.87	0.56
1:A:57:SER:OG	1:A:106:ARG:NH2	2.34	0.56
2:C:91:PHE:CD2	2:C:91:PHE:N	2.74	0.56
1:E:214:VAL:O	1:E:214:VAL:HG13	2.04	0.55
2:H:286:THR:HG22	2:H:292:VAL:HG21	1.86	0.55
2:H:319:THR:CG2	2:H:322:ASP:HB2	2.36	0.55
2:C:103:VAL:HG21	2:C:125:LEU:HD11	1.88	0.55
2:H:312:MET:HE2	2:H:314:THR:HB	1.87	0.55
2:D:274:THR:O	2:D:277:SER:HB2	2.07	0.55
2:G:232:PRO:HG2	2:G:238:GLN:HG2	1.87	0.55
2:D:223:ASP:HB3	2:D:228:VAL:HG23	1.89	0.55
2:G:28:VAL:HG22	2:G:34:TYR:CD2	2.41	0.55
1:A:144:PRO:HB3	1:A:214:VAL:HG21	1.88	0.55
1:F:128:ALA:HA	2:H:109:LEU:HD21	1.88	0.55
2:G:245:LEU:HD21	2:G:309:PHE:CZ	2.41	0.55
2:G:241:ILE:O	2:G:244:THR:HG22	2.05	0.55
2:H:47:LEU:C	2:H:47:LEU:HD12	2.26	0.55
2:C:182:LEU:CD1	2:C:186:ILE:HD11	2.37	0.55
1:E:125:ALA:HB1	2:G:52:ASN:HD21	1.72	0.55
1:A:196:LEU:CD1	1:B:70:ILE:HG13	2.33	0.55
2:H:112:THR:CG2	2:H:117:VAL:HG23	2.36	0.55
1:B:2:SER:HB3	1:B:4:PRO:HD2	1.89	0.55
2:C:141:LEU:HB2	2:C:146:LYS:HG3	1.88	0.55
2:D:172:ASP:O	2:D:176:THR:N	2.39	0.55
2:D:182:LEU:CD1	2:D:182:LEU:C	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:268:MET:CE	2:H:313:LEU:HD13	2.36	0.55
1:B:8:LEU:O	1:B:9:LEU:C	2.44	0.54
2:H:303:TYR:CE1	2:H:308:LYS:HB2	2.42	0.54
2:G:99:VAL:HG13	2:G:136:SER:O	2.07	0.54
2:H:4:LEU:HD21	2:H:51:VAL:HG22	1.90	0.54
1:F:92:ALA:CB	1:F:169:ALA:HB1	2.36	0.54
2:G:146:LYS:O	2:G:149:VAL:HG12	2.06	0.54
2:H:91:PHE:HE1	2:H:147:GLN:HE21	1.55	0.54
1:A:136:LYS:NZ	2:C:108:GLU:OE1	2.41	0.54
2:C:283:LEU:CD1	2:C:312:MET:SD	2.95	0.54
2:D:296:ILE:HG23	2:D:312:MET:HE1	1.88	0.54
2:G:247:LEU:HD22	2:G:298:SER:HB3	1.89	0.54
2:C:299:ALA:CB	2:C:312:MET:HG2	2.38	0.54
1:F:32:LEU:HB3	1:F:33:PRO:HD3	1.88	0.54
2:H:336:LYS:HE2	2:H:338:GLU:OE2	2.07	0.54
1:B:133:ILE:O	1:B:137:VAL:HG13	2.07	0.54
2:D:205:LYS:HG2	2:D:229:PHE:CZ	2.43	0.54
2:D:105:LEU:HD23	2:D:105:LEU:O	2.07	0.54
1:F:41:THR:OG1	1:F:53:TYR:HB2	2.08	0.54
2:C:1:MET:CE	2:C:161:VAL:HG23	2.38	0.54
2:G:110:ASP:O	2:G:112:THR:HG23	2.08	0.54
2:H:270:ARG:HH21	2:H:311:ILE:HD11	1.72	0.54
1:A:93:ILE:O	1:A:93:ILE:CG2	2.56	0.53
1:A:100:ALA:O	1:A:104:ILE:HG12	2.07	0.53
2:D:270:ARG:HH22	2:D:272:GLU:CD	2.12	0.53
1:B:150:ALA:O	1:B:154:LEU:HD23	2.09	0.53
2:G:272:GLU:HB2	2:G:336:LYS:HB3	1.91	0.53
1:F:191:THR:O	1:F:195:LEU:HB2	2.09	0.53
1:F:101:ALA:HB3	1:F:102:PRO:HD3	1.91	0.53
2:G:31:GLY:H	2:G:193:THR:CG2	1.97	0.53
2:H:47:LEU:HD12	2:H:47:LEU:O	2.08	0.53
2:D:286:THR:HG22	2:D:329:TRP:CE3	2.44	0.53
2:G:103:VAL:HG21	2:G:125:LEU:HD11	1.91	0.53
1:A:120:ILE:HD12	1:A:138:LEU:HD11	1.91	0.53
1:B:40:VAL:HA	1:B:45:GLN:HG2	1.90	0.53
2:G:252:ASP:O	2:G:256:ARG:HG2	2.08	0.53
1:A:40:VAL:HA	1:A:45:GLN:HG2	1.90	0.53
1:B:20:THR:CG2	1:B:154:LEU:HD12	2.38	0.53
1:B:185:ASN:HB3	1:B:188:VAL:CG2	2.40	0.52
2:C:11:PHE:CE2	4:C:2000:ADP:C5	2.89	0.52
2:H:312:MET:HB3	3:H:1000:MSE:HE3	1.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:316:MET:CE	2:C:326:ALA:HB3	2.40	0.52
1:E:13:VAL:HG21	1:E:195:LEU:HD11	1.92	0.52
1:E:20:THR:HG1	1:E:21:PHE:HD2	1.57	0.52
1:A:120:ILE:CD1	1:A:138:LEU:HD11	2.38	0.52
1:E:123:SER:HA	1:E:126:MET:CE	2.38	0.52
2:G:72:LEU:HD23	2:G:77:LEU:HD23	1.90	0.52
2:H:28:VAL:HG22	2:H:34:TYR:CD2	2.45	0.52
2:H:333:HIS:O	2:H:334:HIS:CG	2.62	0.52
1:F:13:VAL:HA	1:F:172:LEU:CD1	2.11	0.52
2:G:226:SER:HB2	2:G:307:VAL:CG1	2.40	0.52
2:C:103:VAL:HG21	2:C:125:LEU:CD1	2.40	0.52
2:G:245:LEU:HD11	2:G:302:ASP:HB2	1.92	0.52
2:H:112:THR:HB	2:H:117:VAL:HG22	1.92	0.52
1:F:119:LEU:HD23	2:H:94:LEU:HD23	1.92	0.52
1:B:177:TYR:CE2	1:B:181:TYR:CD2	2.98	0.52
2:H:263:THR:O	2:H:264:ASP:HB3	2.09	0.52
1:A:159:GLY:HA2	1:B:67:PRO:HB3	1.92	0.51
1:B:30:ILE:O	1:B:34:VAL:HG23	2.10	0.51
1:B:32:LEU:CB	1:B:33:PRO:HD3	2.36	0.51
2:C:182:LEU:HD13	2:C:186:ILE:CD1	2.40	0.51
2:D:262:PHE:O	2:D:265:CYS:HB3	2.10	0.51
2:G:271:LEU:HD23	2:G:337:VAL:HG13	1.90	0.51
2:C:182:LEU:HD11	2:C:186:ILE:HD11	1.92	0.51
2:G:107:LEU:O	2:G:110:ASP:O	2.27	0.51
2:G:124:LEU:O	2:G:128:VAL:HG22	2.10	0.51
2:G:287:ALA:O	2:H:288:ARG:NH1	2.43	0.51
2:H:162:LEU:HB2	2:H:192:LEU:HD11	1.91	0.51
2:H:198:THR:OG1	2:H:203:VAL:HG11	2.10	0.51
2:C:9:LYS:HD3	2:C:56:ARG:O	2.10	0.51
2:C:128:VAL:HB	2:C:148:ARG:HB3	1.93	0.51
2:D:11:PHE:CE2	4:D:2000:ADP:C4	2.98	0.51
2:D:34:TYR:OH	2:D:212:ALA:HB2	2.10	0.51
2:D:100:PHE:HD2	2:D:134:HIS:HE1	1.58	0.51
2:D:296:ILE:HG23	2:D:312:MET:HE3	1.91	0.51
2:C:53:LEU:HD12	2:C:69:LEU:HB3	1.91	0.51
2:C:234:THR:HG22	2:C:237:ALA:H	1.75	0.51
2:H:116:GLU:HA	2:H:119:ARG:NH1	2.25	0.51
2:D:249:ILE:HG12	2:D:313:LEU:HD11	1.92	0.51
1:E:104:ILE:O	1:E:108:VAL:HG23	2.11	0.51
2:C:220:ILE:HD11	2:C:236:LEU:HD23	1.92	0.51
2:C:299:ALA:HB1	2:C:312:MET:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:TYR:OH	2:D:222:GLN:HG3	2.10	0.51
2:D:293:ASN:HB2	2:D:317:HIS:HB2	1.92	0.51
1:E:52:LEU:O	1:E:56:VAL:N	2.37	0.51
2:G:49:ARG:HG3	2:G:55:GLU:HB2	1.92	0.51
2:G:302:ASP:OD1	2:G:303:TYR:N	2.41	0.51
1:B:172:LEU:HD21	1:B:192:VAL:HG13	1.92	0.51
2:C:52:ASN:HB3	2:C:54:LEU:HD12	1.93	0.51
1:E:143:LEU:HD23	1:E:214:VAL:CG2	2.38	0.51
1:F:30:ILE:O	1:F:34:VAL:HG23	2.11	0.51
1:F:37:LEU:HD11	1:F:52:LEU:HD21	1.92	0.51
1:A:94:VAL:H	1:A:95:PRO:HD2	1.76	0.51
2:C:234:THR:HG23	2:C:235:PRO:HD2	1.92	0.51
1:E:189:MET:HB3	1:F:74:TRP:HD1	1.76	0.51
1:B:177:TYR:CE2	1:B:181:TYR:HD2	2.29	0.51
1:E:96:LEU:CD2	1:E:160:TYR:HB3	2.40	0.51
2:G:93:LEU:HD11	2:G:149:VAL:CG1	2.41	0.51
2:H:91:PHE:CD2	2:H:146:LYS:CG	2.82	0.51
2:H:91:PHE:HD2	2:H:146:LYS:CG	2.21	0.51
2:H:283:LEU:HD11	2:H:312:MET:SD	2.50	0.51
1:B:104:ILE:HD11	1:B:153:THR:HG21	1.93	0.50
2:G:91:PHE:CD2	2:G:91:PHE:N	2.60	0.50
2:G:24:VAL:HG11	2:G:47:LEU:HD23	1.93	0.50
1:A:179:TYR:HB3	1:A:188:VAL:HG11	1.92	0.50
2:D:182:LEU:HD13	2:D:186:ILE:CD1	2.40	0.50
1:B:57:SER:OG	1:B:106:ARG:NH2	2.33	0.50
2:G:1:MET:CB	2:G:65:ASP:H	2.23	0.50
2:C:44:LYS:HE2	4:C:2000:ADP:O3B	2.11	0.50
2:C:52:ASN:HB3	2:C:54:LEU:CD1	2.41	0.50
2:D:83:GLN:O	2:D:159:PRO:HB2	2.11	0.50
1:E:134:VAL:HA	1:E:138:LEU:HB2	1.93	0.50
1:F:28:PHE:HZ	1:F:150:ALA:HA	1.77	0.50
1:A:139:LEU:HB2	1:A:140:PRO:HD3	1.94	0.50
2:G:204:VAL:HA	2:G:208:CYS:SG	2.52	0.50
2:H:49:ARG:HB2	2:H:54:LEU:HB2	1.94	0.50
2:H:110:ASP:O	2:H:111:ASN:CB	2.56	0.50
2:D:296:ILE:HG12	2:D:312:MET:HE1	1.93	0.50
2:G:105:LEU:N	2:G:106:PRO:HD2	2.26	0.50
2:G:296:ILE:HG13	2:G:296:ILE:O	2.12	0.50
1:A:127:GLY:HA2	2:C:81:ARG:HD3	1.93	0.50
2:C:234:THR:HG22	2:C:236:LEU:N	2.27	0.50
1:F:200:VAL:O	1:F:203:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:THR:HG21	2:H:203:VAL:HG13	1.94	0.49
2:H:303:TYR:CZ	2:H:308:LYS:HD2	2.46	0.49
1:A:2:SER:HB2	1:A:4:PRO:HD2	1.94	0.49
1:B:101:ALA:HB3	1:B:102:PRO:HD3	1.94	0.49
2:C:164:CYS:HB2	2:C:196:LEU:HD13	1.94	0.49
2:D:278:VAL:HG12	2:D:301:MET:HE2	1.92	0.49
1:E:58:ALA:O	1:E:62:ILE:HG12	2.13	0.49
2:G:30:ALA:HA	2:G:193:THR:CG2	2.42	0.49
2:H:273:PHE:HE1	2:H:282:LEU:HD12	1.76	0.49
2:H:319:THR:HG23	2:H:322:ASP:H	1.77	0.49
2:H:333:HIS:O	2:H:334:HIS:ND1	2.45	0.49
2:G:50:CYS:SG	2:G:57:PRO:HG3	2.52	0.49
2:H:120:ARG:NH2	2:H:156:ALA:O	2.45	0.49
1:B:8:LEU:O	1:B:11:ARG:HB3	2.12	0.49
1:B:17:LEU:HD21	1:B:199:LEU:HD11	1.94	0.49
2:C:73:SER:OG	2:C:76:GLU:HB2	2.12	0.49
2:C:286:THR:O	2:C:292:VAL:HG22	2.13	0.49
2:D:100:PHE:CD2	2:D:134:HIS:CE1	2.94	0.49
1:E:118:GLY:HA2	1:E:121:GLU:HB2	1.93	0.49
1:F:30:ILE:HD11	1:F:101:ALA:HB2	1.93	0.49
2:G:155:LEU:HD11	2:G:186:ILE:HD13	1.93	0.49
2:G:236:LEU:O	2:G:239:LYS:HB2	2.12	0.49
2:H:273:PHE:CE1	2:H:282:LEU:HD12	2.47	0.49
2:C:128:VAL:HG11	2:C:152:ALA:HB2	1.95	0.49
2:D:225:VAL:HG13	2:D:229:PHE:CE2	2.47	0.49
2:D:327:ILE:HG23	2:D:337:VAL:HG11	1.94	0.49
1:E:207:GLY:O	1:E:211:VAL:HG23	2.13	0.49
2:G:301:MET:HG3	2:H:297:ILE:HG23	1.95	0.49
2:C:205:LYS:HB3	2:C:229:PHE:CZ	2.48	0.49
1:F:133:ILE:HG22	1:F:138:LEU:HG	1.94	0.49
2:G:36:VAL:HB	2:G:197:ILE:HG22	1.94	0.49
1:A:41:THR:HG21	1:A:52:LEU:HD12	1.95	0.48
1:B:211:VAL:CA	1:B:214:VAL:HG12	2.39	0.48
1:F:19:MET:CE	1:F:161:SER:OG	2.61	0.48
2:G:226:SER:HB2	2:G:307:VAL:HG11	1.95	0.48
2:H:29:PRO:HG2	2:H:32:GLN:OE1	2.13	0.48
2:H:89:GLN:HE21	2:H:169:SER:HB3	1.77	0.48
2:C:1:MET:HE3	2:C:161:VAL:HG23	1.95	0.48
2:G:105:LEU:O	2:G:105:LEU:HD23	2.13	0.48
1:B:45:GLN:CG	1:B:46:ILE:H	2.26	0.48
2:D:262:PHE:HZ	2:D:343:VAL:C	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:PHE:HB3	1:E:102:PRO:HG2	1.94	0.48
2:G:299:ALA:HB2	2:G:312:MET:HG3	1.95	0.48
2:H:105:LEU:O	2:H:108:GLU:HB2	2.13	0.48
2:H:114:LYS:CG	2:H:115:ASP:N	2.70	0.48
1:A:45:GLN:HG3	1:A:46:ILE:H	1.78	0.48
2:C:8:THR:HG23	2:C:21:LEU:O	2.13	0.48
2:C:145:GLN:O	2:C:149:VAL:HG23	2.13	0.48
1:B:42:ARG:HE	1:B:113:LEU:HD21	1.77	0.48
1:B:66:ILE:HG22	1:B:71:LEU:HB2	1.96	0.48
1:F:68:PHE:CZ	1:F:96:LEU:HD23	2.48	0.48
2:G:93:LEU:HD11	2:G:149:VAL:HG13	1.94	0.48
1:A:211:VAL:O	1:A:214:VAL:HG22	2.14	0.48
2:C:252:ASP:O	2:C:256:ARG:HG3	2.14	0.48
2:D:93:LEU:HB3	2:D:102:ASN:HD21	1.77	0.48
2:D:234:THR:HG23	2:D:235:PRO:HD2	1.94	0.48
2:G:93:LEU:CD1	2:G:149:VAL:CG1	2.92	0.48
1:A:115:ILE:HG23	1:A:119:LEU:HD12	1.96	0.48
1:B:89:LEU:HD12	1:B:90:GLN:N	2.29	0.48
1:E:69:ILE:HG23	1:E:70:ILE:HD12	1.96	0.48
1:F:46:ILE:O	1:F:47:ILE:HG22	2.13	0.48
2:G:83:GLN:HA	2:G:159:PRO:HA	1.96	0.48
1:B:189:MET:HE2	1:B:189:MET:HA	1.94	0.48
2:D:329:TRP:O	2:D:333:HIS:CD2	2.66	0.48
1:E:100:ALA:O	1:E:103:PHE:HB2	2.13	0.48
2:G:316:MET:HE3	2:G:323:THR:HA	1.95	0.48
2:D:130:LEU:HD11	2:D:148:ARG:HB2	1.96	0.47
2:G:89:GLN:HB2	2:G:166:GLN:HB2	1.96	0.47
2:H:0:HIS:CB	2:H:29:PRO:HA	2.44	0.47
2:H:333:HIS:C	2:H:334:HIS:ND1	2.67	0.47
2:C:53:LEU:HD11	2:C:69:LEU:HB3	1.96	0.47
2:D:225:VAL:O	2:D:229:PHE:HD2	1.97	0.47
1:E:30:ILE:HD11	1:E:101:ALA:HB2	1.95	0.47
1:E:35:GLY:HA2	1:E:38:LEU:HD12	1.96	0.47
1:F:2:SER:C	1:F:4:PRO:HD2	2.34	0.47
2:G:278:VAL:HG12	2:G:301:MET:SD	2.54	0.47
1:A:30:ILE:O	1:A:33:PRO:HD2	2.14	0.47
1:A:103:PHE:HE2	1:A:160:TYR:OH	1.95	0.47
1:B:2:SER:CA	1:B:4:PRO:HD2	2.44	0.47
2:G:301:MET:O	2:G:302:ASP:HB2	2.15	0.47
2:H:72:LEU:HG	2:H:76:GLU:HB2	1.95	0.47
2:C:163:LEU:HD23	2:C:195:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ILE:HG13	1:E:163:MET:HE2	1.97	0.47
2:H:89:GLN:HB2	2:H:166:GLN:HB2	1.97	0.47
1:E:3:GLU:N	1:E:4:PRO:CD	2.78	0.47
2:G:30:ALA:HA	2:G:193:THR:HG21	1.96	0.47
2:G:168:THR:HB	2:G:176:THR:HG23	1.97	0.47
2:G:248:ASP:O	2:G:249:ILE:CG2	2.62	0.47
1:A:19:MET:HG3	1:A:89:LEU:HD22	1.97	0.47
1:A:155:ILE:HG12	1:A:203:ILE:HG21	1.96	0.47
1:E:148:ASN:O	1:E:151:THR:HB	2.14	0.47
1:F:118:GLY:HA3	2:H:92:ASN:ND2	2.25	0.47
2:G:11:PHE:HB2	2:G:18:ILE:HG22	1.95	0.47
1:B:172:LEU:HD23	1:B:172:LEU:O	2.14	0.47
2:C:172:ASP:O	2:C:176:THR:HG23	2.14	0.47
1:B:179:TYR:O	1:B:184:TYR:HA	2.15	0.47
2:C:4:LEU:HD11	2:C:51:VAL:HG22	1.96	0.47
2:C:164:CYS:HB2	2:C:196:LEU:HD12	1.96	0.47
2:D:63:LEU:O	2:D:63:LEU:HD12	2.15	0.47
1:F:12:GLY:O	1:F:172:LEU:HD12	2.15	0.47
2:H:105:LEU:HD23	2:H:105:LEU:C	2.35	0.47
1:B:32:LEU:HD12	1:B:32:LEU:HA	1.68	0.47
2:D:124:LEU:HD22	2:D:152:ALA:O	2.15	0.47
1:E:27:GLY:C	1:E:104:ILE:CD1	2.83	0.47
1:F:176:GLY:HA2	1:F:189:MET:CE	2.45	0.47
2:G:37:ILE:HG12	2:G:240:PHE:CE1	2.50	0.47
1:A:3:GLU:N	1:A:4:PRO:CD	2.78	0.46
1:A:129:THR:OG1	1:A:132:GLN:HG3	2.15	0.46
2:C:3:LYS:HG2	2:C:27:HIS:CD2	2.50	0.46
2:C:171:LEU:HD13	2:C:179:ILE:HG13	1.97	0.46
1:F:129:THR:N	1:F:132:GLN:HE21	2.04	0.46
2:H:45:SER:HB2	4:H:2000:ADP:PA	2.55	0.46
1:E:92:ALA:O	1:E:95:PRO:HD2	2.16	0.46
1:A:155:ILE:HD11	1:A:203:ILE:HG23	1.97	0.46
1:B:41:THR:O	1:B:41:THR:CG2	2.62	0.46
1:E:141:GLU:OE2	2:G:95:SER:HB2	2.15	0.46
2:H:313:LEU:HD23	2:H:313:LEU:HA	1.76	0.46
1:B:8:LEU:O	1:B:11:ARG:CA	2.63	0.46
1:B:38:LEU:HD21	1:B:56:VAL:HG12	1.97	0.46
2:C:130:LEU:CD1	2:C:148:ARG:HB2	2.44	0.46
2:D:11:PHE:CZ	4:D:2000:ADP:C5	3.03	0.46
2:D:105:LEU:HD23	2:D:105:LEU:C	2.36	0.46
2:G:296:ILE:HG22	2:G:314:THR:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:273:PHE:CZ	3:H:1000:MSE:HG3	2.51	0.46
2:D:119:ARG:O	2:D:122:THR:OG1	2.33	0.46
2:D:176:THR:HG22	2:D:180:LEU:CD1	2.46	0.46
1:E:68:PHE:CZ	1:E:96:LEU:HD23	2.51	0.46
1:F:50:ALA:O	1:F:54:ARG:HB2	2.14	0.46
1:F:189:MET:CE	1:F:189:MET:HA	2.45	0.46
1:B:66:ILE:CG2	1:B:71:LEU:HB2	2.46	0.46
2:C:293:ASN:OD1	2:D:288:ARG:NH1	2.44	0.46
2:G:331:GLN:HA	2:G:335:VAL:O	2.15	0.46
1:B:27:GLY:O	1:B:31:GLY:N	2.48	0.46
2:C:154:ALA:O	2:C:159:PRO:HG3	2.16	0.46
2:G:221:GLU:CD	2:G:233:LYS:H	2.18	0.46
1:E:5:MET:O	1:E:8:LEU:HB3	2.14	0.46
1:E:42:ARG:HB3	1:E:43:PRO:CD	2.38	0.46
2:D:230:SER:HB3	2:D:309:PHE:HE2	1.77	0.46
2:D:329:TRP:CE2	2:D:333:HIS:NE2	2.84	0.46
1:E:37:LEU:HA	1:E:40:VAL:HG22	1.97	0.46
1:F:119:LEU:HD23	2:H:94:LEU:CD2	2.46	0.46
2:H:286:THR:O	2:H:292:VAL:HG22	2.16	0.46
2:C:3:LYS:CG	2:C:27:HIS:HD2	2.29	0.46
2:C:182:LEU:HD13	2:C:182:LEU:C	2.36	0.46
2:D:198:THR:HG21	2:D:203:VAL:HG23	1.96	0.46
1:F:16:THR:CB	1:F:172:LEU:HD13	2.44	0.46
2:H:45:SER:HB2	4:H:2000:ADP:O2A	2.15	0.46
2:H:270:ARG:HA	2:H:313:LEU:HD23	1.98	0.46
1:A:60:VAL:O	1:A:64:ARG:HB3	2.15	0.45
1:A:72:LEU:C	1:A:72:LEU:HD23	2.37	0.45
1:A:154:LEU:HB3	1:A:203:ILE:CD1	2.42	0.45
2:C:2:ILE:CG2	2:C:64:VAL:HG13	2.42	0.45
2:C:11:PHE:CD2	4:C:2000:ADP:N3	2.84	0.45
1:F:3:GLU:N	1:F:4:PRO:CD	2.79	0.45
2:C:160:LYS:O	2:C:192:LEU:HD12	2.16	0.45
1:F:178:GLN:O	1:F:182:ILE:HG13	2.16	0.45
2:H:268:MET:O	2:H:339:VAL:HA	2.16	0.45
2:D:234:THR:HG22	2:D:236:LEU:H	1.81	0.45
1:E:6:MET:C	1:E:8:LEU:H	2.18	0.45
2:G:47:LEU:O	2:G:50:CYS:HB3	2.17	0.45
1:A:155:ILE:CG1	1:A:203:ILE:HG21	2.47	0.45
1:B:123:SER:HA	1:B:126:MET:HE2	1.98	0.45
2:C:316:MET:HE1	2:C:326:ALA:HB3	1.98	0.45
2:D:9:LYS:HA	2:D:58:THR:CG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:TYR:CD1	1:F:167:VAL:HG13	2.52	0.45
1:F:41:THR:HG21	1:F:52:LEU:HD23	1.98	0.45
2:H:273:PHE:HB3	2:H:278:VAL:HG22	1.98	0.45
2:H:312:MET:CE	2:H:314:THR:HB	2.46	0.45
1:A:62:ILE:O	1:A:66:ILE:HG13	2.17	0.45
1:F:101:ALA:N	1:F:102:PRO:CD	2.79	0.45
2:H:52:ASN:OD1	2:H:54:LEU:HG	2.17	0.45
1:B:76:ILE:HD12	1:B:86:SER:OG	2.17	0.45
1:F:128:ALA:HA	2:H:109:LEU:CD2	2.46	0.45
1:A:77:PRO:O	1:A:81:VAL:HG23	2.17	0.45
1:A:175:ILE:O	1:A:175:ILE:HG22	2.17	0.45
1:B:9:LEU:HA	1:B:175:ILE:HD13	1.98	0.45
2:C:172:ASP:HB2	2:C:173:PRO:HD2	1.98	0.45
1:E:13:VAL:CG2	1:E:195:LEU:HD21	2.43	0.45
1:E:80:ARG:HD3	1:E:86:SER:HB2	1.98	0.45
2:H:180:LEU:CD1	2:H:203:VAL:HG23	2.46	0.45
2:D:201:MET:HE2	2:D:229:PHE:CZ	2.52	0.45
1:E:100:ALA:HB2	1:E:157:LEU:HD21	1.98	0.45
1:F:28:PHE:CZ	1:F:150:ALA:HA	2.52	0.45
2:G:293:ASN:HD21	2:H:285:GLU:N	2.14	0.45
1:A:139:LEU:N	1:A:140:PRO:CD	2.80	0.45
2:C:270:ARG:HB3	2:C:340:LEU:HD11	1.99	0.45
2:H:4:LEU:HD13	2:H:47:LEU:HD11	1.99	0.45
2:H:271:LEU:CD1	2:H:283:LEU:HD21	2.46	0.45
1:B:41:THR:CG2	1:B:53:TYR:HB2	2.47	0.45
2:D:10:VAL:HG11	2:D:17:THR:HG23	1.99	0.45
1:E:2:SER:HB2	1:E:4:PRO:HD2	1.99	0.45
1:E:144:PRO:O	1:E:148:ASN:HB2	2.17	0.45
1:F:19:MET:HE3	1:F:161:SER:OG	2.17	0.45
1:F:62:ILE:O	1:F:65:SER:HB3	2.17	0.45
1:B:19:MET:HE2	1:B:96:LEU:HD11	1.98	0.44
2:C:13:GLN:CD	4:C:2000:ADP:H2	2.20	0.44
2:D:11:PHE:CE2	4:D:2000:ADP:C5	3.04	0.44
2:G:292:VAL:O	2:G:292:VAL:HG13	2.17	0.44
2:H:68:GLU:O	2:H:72:LEU:HD13	2.18	0.44
1:F:127:GLY:O	2:H:78:THR:HG23	2.16	0.44
1:E:25:PHE:CD2	1:E:25:PHE:C	2.90	0.44
2:H:232:PRO:HB2	2:H:238:GLN:HG3	1.98	0.44
2:H:300:GLN:NE2	2:H:300:GLN:HA	2.32	0.44
2:H:314:THR:HG23	2:H:314:THR:O	2.17	0.44
1:B:13:VAL:HG22	1:B:172:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:ASN:HD22	2:C:54:LEU:HD11	1.83	0.44
2:H:0:HIS:HB3	2:H:29:PRO:HA	1.99	0.44
1:B:4:PRO:HG2	1:B:5:MET:H	1.83	0.44
2:D:82:ARG:HH21	2:D:110:ASP:HB2	1.82	0.44
1:F:13:VAL:N	1:F:172:LEU:HD11	2.32	0.44
1:B:147:VAL:HG11	1:B:210:ILE:HG23	2.00	0.44
2:D:10:VAL:HG13	2:D:18:ILE:O	2.18	0.44
2:D:93:LEU:HD22	2:D:102:ASN:HD21	1.82	0.44
2:D:114:LYS:HA	2:D:117:VAL:HG22	1.99	0.44
2:D:310:GLY:HA3	3:D:1000:MSE:HE2	1.98	0.44
2:H:72:LEU:HG	2:H:76:GLU:CB	2.48	0.44
2:C:220:ILE:HD13	2:C:236:LEU:HD23	1.99	0.44
2:C:231:HIS:N	2:C:232:PRO:CD	2.79	0.44
2:D:234:THR:CG2	2:D:235:PRO:HD2	2.47	0.44
2:D:105:LEU:N	2:D:106:PRO:CD	2.80	0.44
2:D:249:ILE:HG12	2:D:313:LEU:CD1	2.47	0.44
1:F:106:ARG:HA	1:F:106:ARG:HD3	1.65	0.44
1:B:4:PRO:CD	1:B:5:MET:H	2.31	0.44
1:F:121:GLU:OE1	2:H:49:ARG:NH2	2.51	0.44
2:G:78:THR:O	2:G:82:ARG:HG3	2.17	0.44
2:H:260:GLU:O	2:H:262:PHE:HD2	2.01	0.44
1:B:134:VAL:HA	1:B:138:LEU:HB2	1.98	0.43
2:D:230:SER:OG	2:D:231:HIS:ND1	2.21	0.43
2:D:253:TYR:O	2:D:257:LEU:N	2.51	0.43
2:G:251:GLU:OE2	2:H:206:ARG:NH2	2.48	0.43
2:H:112:THR:CB	2:H:117:VAL:HG23	2.48	0.43
1:B:4:PRO:HG2	1:B:5:MET:N	2.33	0.43
1:B:129:THR:O	1:B:133:ILE:N	2.44	0.43
1:B:154:LEU:HD13	1:B:154:LEU:HA	1.87	0.43
2:C:56:ARG:NH1	2:C:70:THR:O	2.50	0.43
1:E:137:VAL:HG23	1:E:138:LEU:N	2.33	0.43
2:G:275:GLY:O	2:G:278:VAL:HG23	2.18	0.43
1:A:19:MET:HG3	1:A:89:LEU:CD2	2.48	0.43
1:B:72:LEU:CG	1:B:167:VAL:HG11	2.48	0.43
2:C:83:GLN:HA	2:C:159:PRO:HA	2.00	0.43
2:C:116:GLU:O	2:C:120:ARG:HG2	2.18	0.43
1:E:69:ILE:HD12	1:F:163:MET:HA	2.01	0.43
1:F:94:VAL:HB	1:F:95:PRO:HD3	2.01	0.43
2:H:303:TYR:CZ	2:H:308:LYS:HB2	2.51	0.43
1:B:134:VAL:HA	1:B:138:LEU:HD12	1.99	0.43
1:B:167:VAL:O	1:B:167:VAL:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:CA	1:B:191:THR:HG22	2.46	0.43
2:G:269:LEU:HD23	2:G:339:VAL:HG13	2.01	0.43
1:A:85:THR:HG22	1:A:87:ILE:H	1.84	0.43
1:B:2:SER:HB3	1:B:4:PRO:CD	2.47	0.43
2:G:281:PRO:CB	2:H:293:ASN:HB3	2.48	0.43
2:G:334:HIS:N	2:G:334:HIS:CD2	2.84	0.43
1:A:59:ILE:HG13	1:A:60:VAL:N	2.33	0.43
1:A:178:GLN:HA	1:A:182:ILE:HD12	2.01	0.43
1:B:42:ARG:HG2	1:B:43:PRO:N	2.34	0.43
1:B:52:LEU:O	1:B:56:VAL:HG23	2.18	0.43
2:G:145:GLN:HA	2:G:148:ARG:HB2	2.00	0.43
2:G:251:GLU:HG2	2:H:177:ARG:HH21	1.83	0.43
2:H:288:ARG:HG3	2:H:289:ARG:N	2.34	0.43
2:C:1:MET:HG2	2:C:193:THR:HG21	2.00	0.43
1:F:47:ILE:O	1:F:47:ILE:CG1	2.63	0.43
2:G:91:PHE:O	2:G:92:ASN:CB	2.62	0.43
1:B:8:LEU:O	1:B:10:VAL:N	2.52	0.43
1:B:66:ILE:HA	1:B:67:PRO:HD3	1.86	0.43
2:D:247:LEU:O	2:D:247:LEU:HG	2.19	0.43
1:E:162:ALA:HB1	1:F:70:ILE:HD13	2.01	0.43
1:F:13:VAL:HG12	1:F:172:LEU:HD21	2.00	0.43
1:A:69:ILE:HD12	1:A:163:MET:HE1	2.01	0.43
1:B:41:THR:HA	1:B:47:ILE:HB	2.01	0.43
2:C:21:LEU:HD23	2:C:217:GLY:HA2	2.00	0.43
2:H:48:ILE:HD11	2:H:163:LEU:HB3	2.00	0.43
2:D:56:ARG:HG3	2:D:57:PRO:HD2	2.00	0.43
1:E:134:VAL:HG23	1:E:135:ARG:N	2.34	0.43
1:F:61:ASN:OD1	1:F:106:ARG:NH2	2.45	0.43
1:F:176:GLY:HA2	1:F:189:MET:HE1	2.01	0.43
2:G:168:THR:HA	2:G:171:LEU:HD12	2.00	0.43
2:H:292:VAL:HG21	2:H:316:MET:CE	2.46	0.43
2:C:53:LEU:HD11	2:C:69:LEU:CB	2.48	0.42
2:D:61:SER:HB2	2:D:68:GLU:OE2	2.19	0.42
1:E:162:ALA:C	1:F:69:ILE:HD11	2.39	0.42
1:F:177:TYR:O	1:F:181:TYR:HB3	2.19	0.42
2:G:24:VAL:HG11	2:G:47:LEU:CD2	2.49	0.42
2:G:124:LEU:HD12	2:G:124:LEU:N	2.34	0.42
2:H:21:LEU:HD11	2:H:47:LEU:HA	2.01	0.42
2:H:91:PHE:CZ	2:H:171:LEU:HD21	2.51	0.42
1:B:4:PRO:CG	1:B:5:MET:N	2.81	0.42
2:C:182:LEU:CD1	2:C:186:ILE:CD1	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:ASN:HB3	2:G:54:LEU:HG	2.00	0.42
1:A:80:ARG:CG	1:A:86:SER:HB2	2.49	0.42
1:B:133:ILE:O	1:B:137:VAL:CG1	2.66	0.42
1:B:188:VAL:HA	1:B:191:THR:CG2	2.46	0.42
2:C:11:PHE:HD2	4:C:2000:ADP:N3	2.17	0.42
2:C:339:VAL:HG12	2:C:341:GLY:H	1.83	0.42
1:E:17:LEU:HD21	1:E:199:LEU:CD2	2.49	0.42
1:E:162:ALA:HB1	1:F:70:ILE:CD1	2.49	0.42
1:F:38:LEU:HD13	1:F:56:VAL:HG12	2.01	0.42
2:G:98:THR:HG23	2:G:101:GLY:N	2.34	0.42
1:B:4:PRO:CG	1:B:5:MET:H	2.32	0.42
1:B:45:GLN:CG	1:B:46:ILE:N	2.82	0.42
2:C:10:VAL:O	2:C:11:PHE:HD1	2.02	0.42
1:F:80:ARG:CB	1:F:86:SER:HB3	2.43	0.42
2:G:330:LEU:O	2:G:335:VAL:HB	2.19	0.42
2:H:86:MET:HG3	2:H:163:LEU:HB2	2.00	0.42
1:A:69:ILE:HD12	1:A:163:MET:CE	2.50	0.42
2:D:302:ASP:O	2:D:309:PHE:HB2	2.19	0.42
1:E:132:GLN:O	1:E:136:LYS:HB2	2.20	0.42
1:E:143:LEU:HA	1:E:143:LEU:HD12	1.79	0.42
2:G:9:LYS:CE	2:G:56:ARG:O	2.59	0.42
2:G:236:LEU:HA	2:G:239:LYS:HD2	2.00	0.42
1:A:178:GLN:HB2	1:A:179:TYR:CD1	2.54	0.42
1:B:40:VAL:CG1	1:B:47:ILE:HD12	2.47	0.42
1:B:75:MET:O	1:B:79:THR:N	2.40	0.42
1:B:157:LEU:HA	1:B:160:TYR:HB2	2.01	0.42
2:C:3:LYS:CG	2:C:27:HIS:CD2	3.02	0.42
2:C:227:GLU:O	2:C:230:SER:O	2.38	0.42
2:D:7:ILE:HA	2:D:60:GLY:HA3	2.01	0.42
2:G:229:PHE:HA	2:G:241:ILE:CD1	2.49	0.42
1:A:26:PHE:HB2	1:A:97:THR:HG21	2.02	0.42
1:A:155:ILE:HG13	1:A:203:ILE:CG2	2.49	0.42
2:H:123:GLU:O	2:H:127:LEU:HG	2.20	0.42
1:A:20:THR:HG21	1:A:158:VAL:HA	2.01	0.42
2:D:1:MET:HE2	2:D:161:VAL:HG23	2.01	0.42
2:H:251:GLU:HA	2:H:254:GLN:HB3	2.01	0.42
1:A:104:ILE:O	1:A:108:VAL:HG23	2.20	0.42
1:B:20:THR:HG22	1:B:154:LEU:CD1	2.42	0.42
2:C:72:LEU:HG	2:C:76:GLU:HB3	2.02	0.42
2:D:1:MET:O	2:D:64:VAL:HA	2.19	0.42
1:E:116:PRO:O	1:E:119:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:LEU:HD12	2:H:146:LYS:HB2	2.01	0.42
2:H:114:LYS:CG	2:H:115:ASP:H	2.12	0.42
2:H:144:GLY:O	2:H:148:ARG:HG3	2.20	0.42
1:B:115:ILE:HA	1:B:116:PRO:HD3	1.86	0.42
1:B:130:PRO:O	1:B:134:VAL:HG23	2.20	0.42
2:C:1:MET:HE2	2:C:161:VAL:HG23	2.01	0.42
1:B:42:ARG:CG	1:B:43:PRO:CD	2.97	0.41
2:C:89:GLN:HB2	2:C:166:GLN:HB2	2.02	0.41
2:C:283:LEU:HA	2:C:286:THR:HG22	2.02	0.41
1:F:2:SER:O	1:F:6:MET:HG2	2.20	0.41
1:F:13:VAL:HG23	1:F:14:TRP:N	2.35	0.41
2:G:103:VAL:O	2:G:106:PRO:HD2	2.20	0.41
2:H:319:THR:HG23	2:H:322:ASP:CB	2.44	0.41
2:G:33:ILE:HG12	2:G:194:ILE:HB	2.01	0.41
2:G:214:ILE:HA	2:G:218:GLU:O	2.20	0.41
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.81	0.41
1:B:147:VAL:HB	1:B:211:VAL:HG22	2.00	0.41
1:B:210:ILE:O	1:B:214:VAL:HG12	2.21	0.41
2:C:44:LYS:CE	4:C:2000:ADP:O3B	2.67	0.41
2:D:24:VAL:HG13	2:D:219:LEU:HD12	2.01	0.41
1:E:195:LEU:HD23	1:E:195:LEU:O	2.21	0.41
1:F:150:ALA:O	1:F:153:THR:HB	2.21	0.41
2:H:107:LEU:HA	2:H:110:ASP:OD1	2.20	0.41
2:H:241:ILE:O	2:H:244:THR:HG22	2.20	0.41
1:A:68:PHE:CZ	1:A:96:LEU:HD12	2.46	0.41
2:C:11:PHE:CD2	4:C:2000:ADP:C4	3.08	0.41
2:C:182:LEU:HD13	2:C:182:LEU:O	2.20	0.41
1:F:116:PRO:C	1:F:118:GLY:N	2.74	0.41
2:G:99:VAL:HG12	2:G:141:LEU:HD11	1.96	0.41
2:H:28:VAL:HA	2:H:29:PRO:HD2	1.92	0.41
2:H:298:SER:O	2:H:312:MET:HB2	2.21	0.41
2:D:201:MET:CE	2:D:229:PHE:CZ	3.04	0.41
2:G:99:VAL:HG21	2:G:133:LYS:O	2.21	0.41
2:H:257:LEU:HD12	2:H:258:GLN:H	1.84	0.41
1:A:104:ILE:HD11	1:A:153:THR:CG2	2.51	0.41
1:F:54:ARG:HD2	1:F:54:ARG:HA	1.85	0.41
2:G:53:LEU:HD23	2:G:53:LEU:HA	1.84	0.41
2:H:300:GLN:HE21	2:H:300:GLN:HA	1.86	0.41
1:A:184:TYR:OH	1:A:186:ALA:HA	2.21	0.41
2:D:104:ALA:O	2:D:108:GLU:HG3	2.20	0.41
2:D:312:MET:HE2	2:D:314:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4:LEU:O	2:G:4:LEU:HD12	2.20	0.41
2:H:180:LEU:HD11	2:H:203:VAL:HG23	2.02	0.41
2:H:200:GLU:O	2:H:203:VAL:HG12	2.21	0.41
1:A:70:ILE:HG22	1:B:193:LEU:HD12	2.03	0.41
1:E:125:ALA:CB	2:G:52:ASN:HD21	2.32	0.41
1:F:30:ILE:CD1	1:F:101:ALA:HB2	2.50	0.41
1:F:80:ARG:O	1:F:84:GLY:HA2	2.20	0.41
1:F:122:ALA:O	1:F:126:MET:HG3	2.21	0.41
2:G:241:ILE:HA	2:G:244:THR:HG22	2.03	0.41
2:H:77:LEU:HD21	2:H:81:ARG:NH1	2.35	0.41
1:A:13:VAL:CG2	1:A:172:LEU:HD11	2.45	0.41
1:A:15:GLU:HB2	1:A:171:GLY:HA2	2.03	0.41
1:A:41:THR:HA	1:A:47:ILE:O	2.21	0.41
1:B:13:VAL:HG22	1:B:172:LEU:HD12	2.03	0.41
1:B:39:TYR:HE1	1:B:113:LEU:HA	1.85	0.41
1:B:42:ARG:HG2	1:B:43:PRO:HD2	2.03	0.41
1:B:104:ILE:O	1:B:107:MET:N	2.54	0.41
2:C:180:LEU:O	2:C:207:ILE:HG21	2.20	0.41
2:C:295:ASN:HB3	2:C:315:GLU:HG3	2.02	0.41
2:C:296:ILE:HD11	2:D:312:MET:SD	2.61	0.41
2:D:230:SER:CB	2:D:309:PHE:HE2	2.34	0.41
1:E:9:LEU:O	1:E:13:VAL:HG23	2.21	0.41
1:E:15:GLU:OE2	1:E:171:GLY:N	2.54	0.41
1:E:94:VAL:HB	1:E:95:PRO:HD3	2.02	0.41
2:G:56:ARG:HA	2:G:57:PRO:HD3	1.87	0.41
2:G:296:ILE:HG12	3:H:1000:MSE:OXT	2.20	0.41
2:H:93:LEU:HA	2:H:93:LEU:HD23	1.89	0.41
2:H:266:VAL:HG21	2:H:317:HIS:HA	2.03	0.41
1:A:49:ASN:HB2	1:A:52:LEU:HB3	2.03	0.41
1:B:162:ALA:HA	1:B:173:GLY:HA3	2.03	0.41
2:C:156:ALA:C	2:C:158:ASN:H	2.23	0.41
2:H:49:ARG:HG3	2:H:55:GLU:HB2	2.03	0.41
2:H:244:THR:HG23	2:H:245:LEU:HD13	2.03	0.41
1:A:92:ALA:C	1:A:94:VAL:H	2.24	0.40
2:C:4:LEU:HD21	2:C:51:VAL:HG22	2.02	0.40
2:C:130:LEU:CD1	2:C:149:VAL:HG22	2.49	0.40
2:G:48:ILE:HD12	2:G:195:LEU:HD12	2.03	0.40
2:G:245:LEU:HD21	2:G:309:PHE:CE2	2.56	0.40
2:H:46:THR:HG23	2:H:55:GLU:HG2	2.03	0.40
2:H:148:ARG:HA	2:H:151:ILE:HD12	2.02	0.40
2:C:231:HIS:NE2	2:C:274:THR:HG21	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:280:ALA:O	2:H:282:LEU:N	2.50	0.40
2:H:288:ARG:O	2:H:289:ARG:C	2.60	0.40
1:A:60:VAL:O	1:A:64:ARG:CB	2.70	0.40
1:A:64:ARG:HG3	1:A:64:ARG:HH11	1.85	0.40
1:B:69:ILE:HD12	1:B:69:ILE:HA	1.93	0.40
1:E:104:ILE:HD13	1:E:104:ILE:HG21	1.80	0.40
2:H:35:GLY:CA	2:H:196:LEU:HD13	2.47	0.40
2:H:93:LEU:HD22	2:H:102:ASN:CG	2.42	0.40
2:D:22:ASN:ND2	2:D:218:GLU:OE1	2.55	0.40
2:H:257:LEU:HG	2:H:258:GLN:N	2.36	0.40
2:H:283:LEU:CD1	2:H:312:MET:SD	3.09	0.40
1:A:5:MET:HE3	1:A:9:LEU:HG	2.03	0.40
2:C:187:ASN:O	2:C:191:GLY:N	2.48	0.40
2:C:228:VAL:O	2:C:232:PRO:HG3	2.21	0.40
1:F:39:TYR:OH	1:F:120:ILE:HD11	2.22	0.40
2:H:270:ARG:HE	2:H:311:ILE:HD11	1.87	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	214/217 (99%)	208 (97%)	4 (2%)	2 (1%)	17 49
1	B	214/217 (99%)	206 (96%)	7 (3%)	1 (0%)	29 61
1	E	213/217 (98%)	202 (95%)	11 (5%)	0	100 100
1	F	214/217 (99%)	206 (96%)	8 (4%)	0	100 100
2	C	342/366 (93%)	333 (97%)	9 (3%)	0	100 100
2	D	341/366 (93%)	322 (94%)	19 (6%)	0	100 100
2	G	341/366 (93%)	320 (94%)	20 (6%)	1 (0%)	41 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	338/366 (92%)	321 (95%)	15 (4%)	2 (1%)	25	57
All	All	2217/2332 (95%)	2118 (96%)	93 (4%)	6 (0%)	41	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	111	ASN
2	H	113	PRO
1	B	9	LEU
2	G	250	PRO
1	A	93	ILE
1	A	94	VAL

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	171/172 (99%)	170 (99%)	1 (1%)	86	94
1	B	171/172 (99%)	171 (100%)	0	100	100
1	E	170/172 (99%)	170 (100%)	0	100	100
1	F	171/172 (99%)	171 (100%)	0	100	100
2	C	299/319 (94%)	299 (100%)	0	100	100
2	D	298/319 (93%)	294 (99%)	4 (1%)	69	84
2	G	298/319 (93%)	292 (98%)	6 (2%)	55	77
2	H	296/319 (93%)	290 (98%)	6 (2%)	55	77
All	All	1874/1964 (95%)	1857 (99%)	17 (1%)	78	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ARG
2	D	192	LEU

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Mol	Chain	Res	Type
2	D	196	LEU
2	D	202	ASP
2	D	219	LEU
2	G	91	PHE
2	G	115	ASP
2	G	145	GLN
2	G	192	LEU
2	G	196	LEU
2	G	198	THR
2	H	47	LEU
2	H	181	GLU
2	H	182	LEU
2	H	196	LEU
2	H	229	PHE
2	H	312	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	178	GLN
2	C	13	GLN
2	D	102	ASN
1	F	132	GLN
2	G	52	ASN
2	G	92	ASN
2	G	145	GLN
2	G	147	GLN
2	G	276	GLN
2	G	334	HIS
2	H	89	GLN
2	H	92	ASN
2	H	246	HIS
2	H	294	ASN
2	H	300	GLN
2	H	320	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	ADP	D	2000	-	24,29,29	1.06	2 (8%)	29,45,45	1.36	3 (10%)
4	ADP	C	2000	-	24,29,29	1.16	4 (16%)	29,45,45	1.45	5 (17%)
3	MSE	G	1000	-	5,8,8	1.03	1 (20%)	5,9,9	2.22	2 (40%)
3	MSE	H	1000	-	5,8,8	1.15	1 (20%)	5,9,9	1.87	2 (40%)
3	MSE	D	1000	-	5,8,8	0.91	0	5,9,9	1.81	2 (40%)
3	MSE	C	1000	-	5,8,8	1.11	1 (20%)	5,9,9	1.85	2 (40%)
4	ADP	G	2000	-	24,29,29	1.19	3 (12%)	29,45,45	1.42	4 (13%)
4	ADP	H	2000	-	24,29,29	1.26	3 (12%)	29,45,45	1.51	3 (10%)

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	ADP	D	2000	-	-	3/12/32/32	0/3/3/3
4	ADP	C	2000	-	-	8/12/32/32	0/3/3/3
3	MSE	G	1000	-	-	0/7/8/8	-
3	MSE	H	1000	-	-	5/7/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MSE	D	1000	-	-	3/7/8/8	-
3	MSE	C	1000	-	-	2/7/8/8	-
4	ADP	G	2000	-	-	1/12/32/32	0/3/3/3
4	ADP	H	2000	-	-	1/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2000	ADP	C5-C4	3.22	1.49	1.40
4	G	2000	ADP	C5-C4	3.15	1.49	1.40
4	C	2000	ADP	C5-C4	3.08	1.49	1.40
4	H	2000	ADP	C2-N3	2.87	1.36	1.32
4	D	2000	ADP	C5-C4	2.70	1.48	1.40
4	G	2000	ADP	O4'-C1'	2.42	1.44	1.41
3	H	1000	MSE	OXT-C	-2.39	1.22	1.30
3	C	1000	MSE	OXT-C	-2.37	1.22	1.30
4	G	2000	ADP	C2-N3	2.31	1.35	1.32
4	D	2000	ADP	O4'-C1'	2.25	1.44	1.41
3	G	1000	MSE	OXT-C	-2.22	1.23	1.30
4	H	2000	ADP	C6-C5	2.22	1.51	1.43
4	C	2000	ADP	C2-N3	2.22	1.35	1.32
4	C	2000	ADP	C6-C5	2.12	1.51	1.43
4	C	2000	ADP	O4'-C1'	2.12	1.44	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2000	ADP	C4-C5-N7	-4.16	105.06	109.40
4	H	2000	ADP	C4-C5-N7	-3.73	105.51	109.40
3	G	1000	MSE	OXT-C-O	-3.68	115.73	124.09
4	D	2000	ADP	N3-C2-N1	-3.53	123.16	128.68
4	H	2000	ADP	N3-C2-N1	-3.29	123.54	128.68
3	D	1000	MSE	OXT-C-O	-3.14	116.97	124.09
3	C	1000	MSE	OXT-C-O	-3.12	117.00	124.09
3	G	1000	MSE	OXT-C-CA	3.06	123.82	113.38
4	G	2000	ADP	C3'-C2'-C1'	3.04	105.55	100.98
4	G	2000	ADP	C4-C5-N7	-2.95	106.32	109.40
4	C	2000	ADP	PA-O3A-PB	-2.95	122.71	132.83
4	H	2000	ADP	C3'-C2'-C1'	2.94	105.40	100.98
4	G	2000	ADP	N3-C2-N1	-2.88	124.17	128.68
3	H	1000	MSE	OXT-C-O	-2.85	117.61	124.09
3	H	1000	MSE	OXT-C-CA	2.83	123.01	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2000	ADP	C4-C5-N7	-2.69	106.59	109.40
4	G	2000	ADP	PA-O3A-PB	-2.68	123.63	132.83
3	C	1000	MSE	OXT-C-CA	2.68	122.51	113.38
3	D	1000	MSE	OXT-C-CA	2.53	121.99	113.38
4	C	2000	ADP	C3'-C2'-C1'	2.28	104.41	100.98
4	D	2000	ADP	C2-N1-C6	2.24	122.59	118.75
4	C	2000	ADP	N3-C2-N1	-2.16	125.30	128.68
4	C	2000	ADP	C5-C6-N6	2.09	123.53	120.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1000	MSE	O-C-CA-N
3	H	1000	MSE	N-CA-CB-CG
4	C	2000	ADP	PA-O3A-PB-O2B
4	C	2000	ADP	C5'-O5'-PA-O1A
4	C	2000	ADP	C5'-O5'-PA-O2A
4	C	2000	ADP	O4'-C4'-C5'-O5'
4	D	2000	ADP	O4'-C4'-C5'-O5'
3	H	1000	MSE	OXT-C-CA-N
3	C	1000	MSE	OXT-C-CA-N
4	C	2000	ADP	C3'-C4'-C5'-O5'
4	D	2000	ADP	PB-O3A-PA-O1A
3	D	1000	MSE	CA-CB-CG-SE
3	C	1000	MSE	O-C-CA-N
3	H	1000	MSE	C-CA-CB-CG
3	D	1000	MSE	O-C-CA-CB
3	D	1000	MSE	OXT-C-CA-CB
4	D	2000	ADP	PB-O3A-PA-O2A
4	C	2000	ADP	PA-O3A-PB-O3B
4	C	2000	ADP	C5'-O5'-PA-O3A
4	H	2000	ADP	PB-O3A-PA-O1A
3	H	1000	MSE	OXT-C-CA-CB
4	G	2000	ADP	C5'-O5'-PA-O1A
4	C	2000	ADP	PA-O3A-PB-O1B

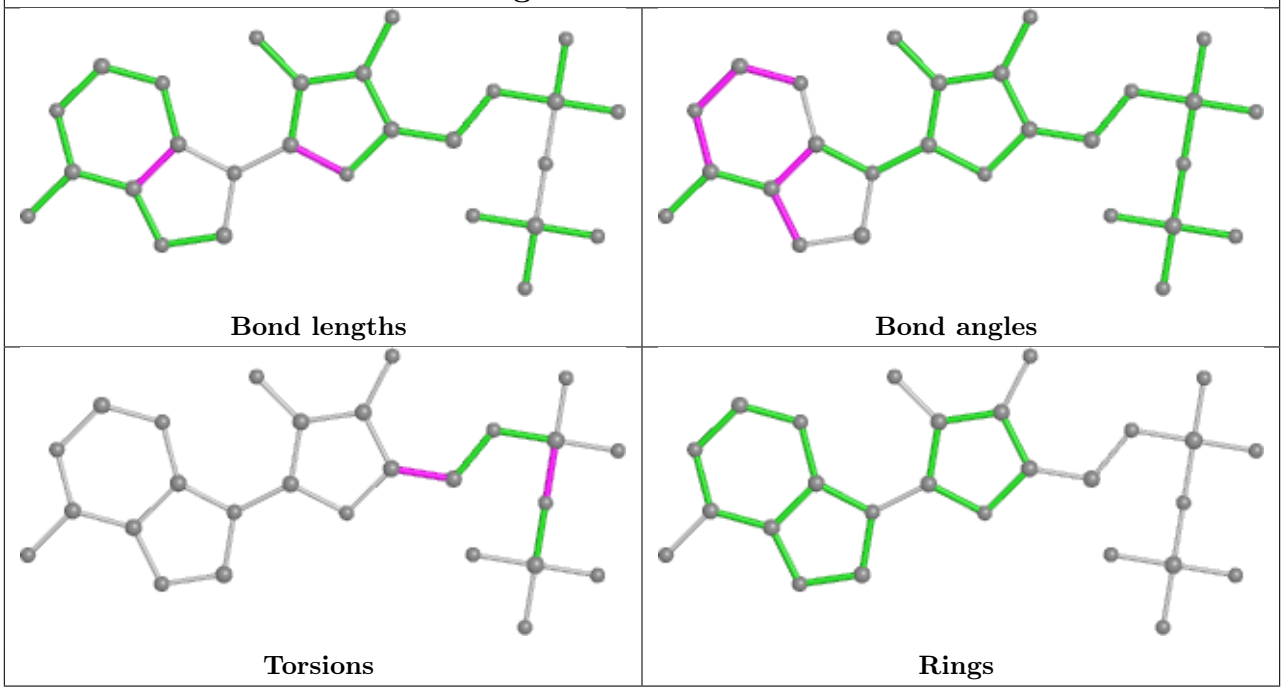
There are no ring outliers.

8 monomers are involved in 34 short contacts:

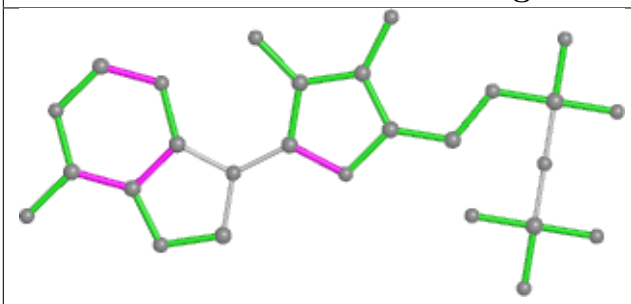
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2000	ADP	5	0
4	C	2000	ADP	12	0
3	G	1000	MSE	2	0
3	H	1000	MSE	6	0
3	D	1000	MSE	1	0
3	C	1000	MSE	2	0
4	G	2000	ADP	1	0
4	H	2000	ADP	5	0

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.

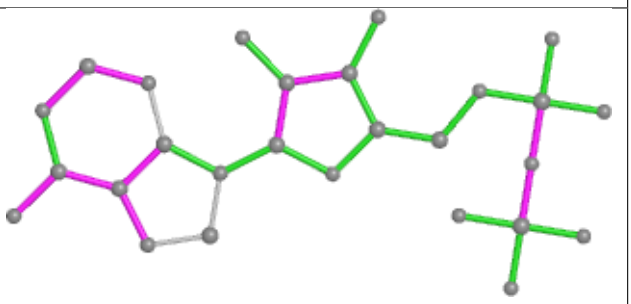
Ligand ADP D 2000



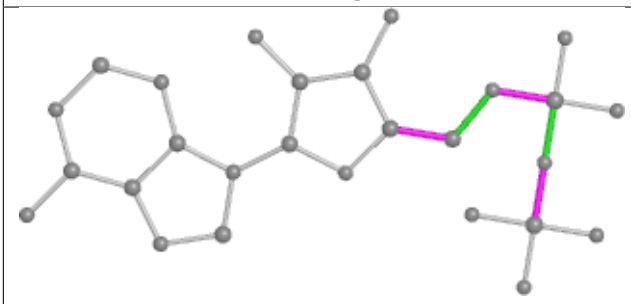
Ligand ADP C 2000



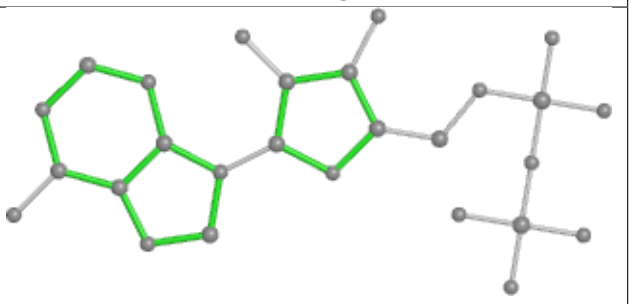
Bond lengths



Bond angles

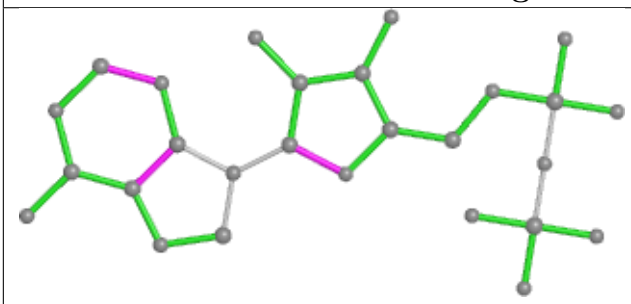


Torsions

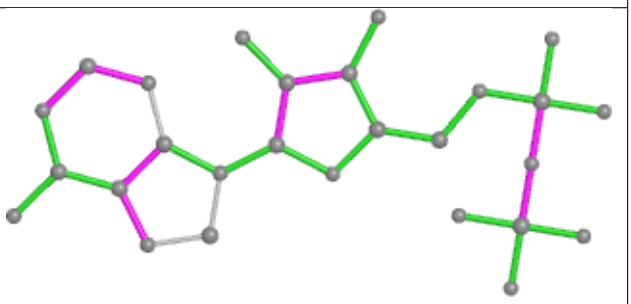


Rings

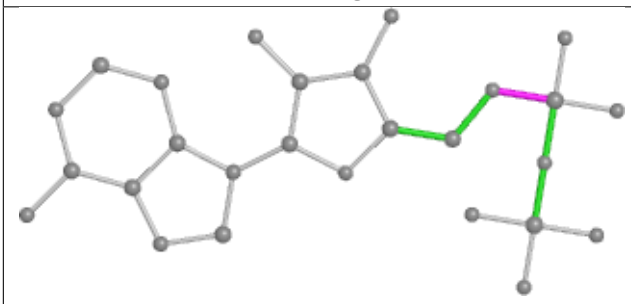
Ligand ADP G 2000



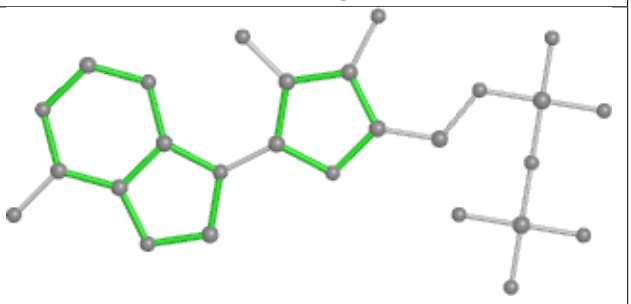
Bond lengths



Bond angles

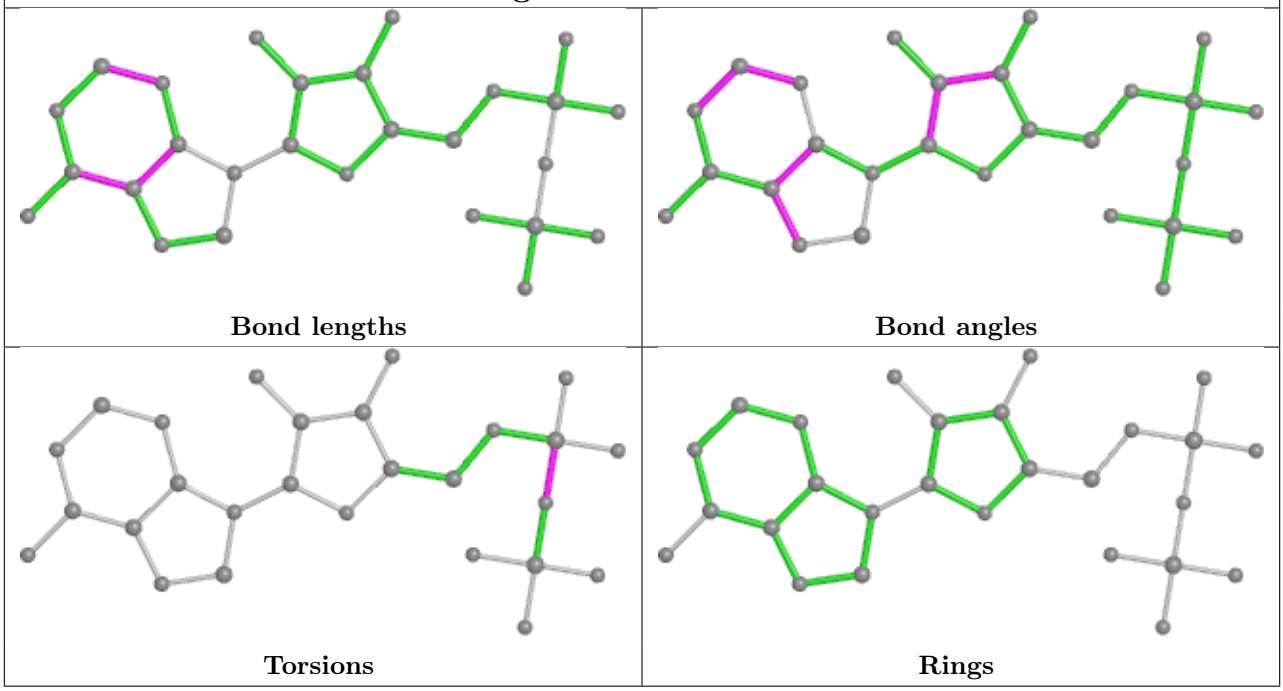


Torsions



Rings

Ligand ADP H 2000



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	216/217 (99%)	-0.12	0	100	100	43, 67, 100, 113	0
1	B	216/217 (99%)	-0.06	3 (1%)	75	74	48, 70, 109, 150	0
1	E	215/217 (99%)	-0.14	1 (0%)	91	90	48, 72, 98, 119	0
1	F	216/217 (99%)	-0.09	4 (1%)	66	65	51, 68, 104, 148	0
2	C	344/366 (93%)	0.09	13 (3%)	40	39	38, 73, 122, 146	0
2	D	343/366 (93%)	0.22	18 (5%)	27	27	48, 89, 150, 198	0
2	G	343/366 (93%)	-0.06	8 (2%)	60	59	41, 69, 112, 143	0
2	H	340/366 (92%)	0.19	14 (4%)	37	36	39, 83, 152, 168	0
All	All	2233/2332 (95%)	0.03	61 (2%)	54	53	38, 74, 130, 198	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	248	ASP	5.8
2	C	13	GLN	5.5
2	D	17	THR	4.2
2	C	18	ILE	4.1
2	H	255	GLU	4.0
1	F	90	GLN	3.9
2	D	239	LYS	3.7
2	C	15	THR	3.6
2	D	246	HIS	3.6
2	H	334	HIS	3.6
2	H	290	PHE	3.5
2	D	264	ASP	3.5
1	F	83	VAL	3.4
2	H	256	ARG	3.3
2	D	116	GLU	3.2
2	G	15	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	331	GLN	3.2
2	H	269	LEU	3.2
2	H	327	ILE	3.1
2	D	340	LEU	3.1
2	H	252	ASP	3.1
2	C	17	THR	3.1
2	H	268	MET	3.0
2	G	132	ASP	3.0
2	D	13	GLN	3.0
2	C	123	GLU	3.0
2	C	12	HIS	2.9
2	D	114	LYS	2.9
1	F	85	THR	2.7
2	C	267	PRO	2.7
2	G	258	GLN	2.7
2	G	13	GLN	2.6
2	D	130	LEU	2.6
2	H	276	GLN	2.6
2	D	240	PHE	2.5
2	D	249	ILE	2.5
2	H	132	ASP	2.4
1	B	50	ALA	2.4
2	G	139	SER	2.4
2	C	260	GLU	2.4
1	B	48	ALA	2.3
2	C	16	ARG	2.3
2	H	251	GLU	2.3
2	D	125	LEU	2.3
2	D	263	THR	2.3
1	B	3	GLU	2.2
2	G	14	GLY	2.2
2	D	15	THR	2.2
2	G	140	ASN	2.2
2	C	262	PHE	2.1
2	H	330	LEU	2.1
1	E	84	GLY	2.1
2	D	268	MET	2.1
2	G	317	HIS	2.1
1	F	82	ILE	2.1
2	C	316	MET	2.1
2	H	248	ASP	2.1
2	C	14	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	268	MET	2.1
2	D	261	PRO	2.1
2	D	229	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

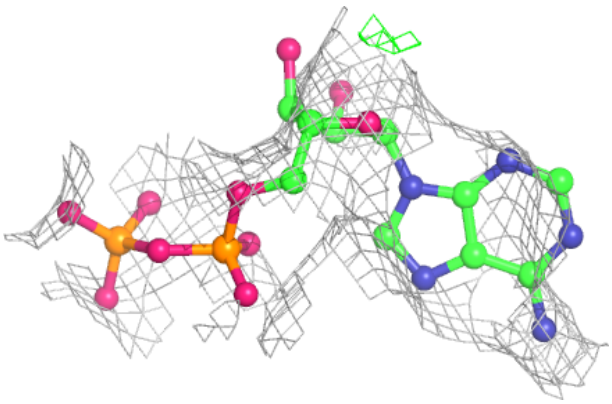
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

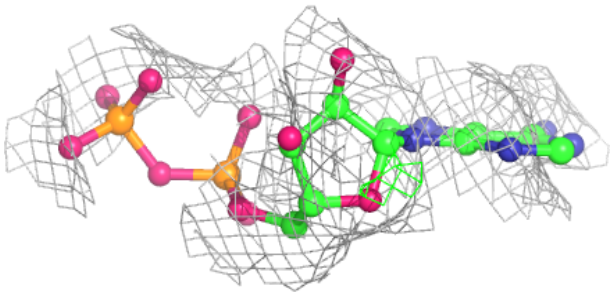
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ADP	D	2000	27/27	0.82	0.21	103,152,169,172	0
4	ADP	C	2000	27/27	0.84	0.22	82,118,144,149	0
4	ADP	G	2000	27/27	0.89	0.21	84,124,142,145	0
3	MSE	H	1000	9/9	0.90	0.19	89,98,115,130	0
4	ADP	H	2000	27/27	0.92	0.17	69,84,91,94	0
3	MSE	D	1000	9/9	0.95	0.19	73,75,78,123	0
3	MSE	G	1000	9/9	0.96	0.22	61,71,77,106	0
3	MSE	C	1000	9/9	0.97	0.21	77,84,87,113	0

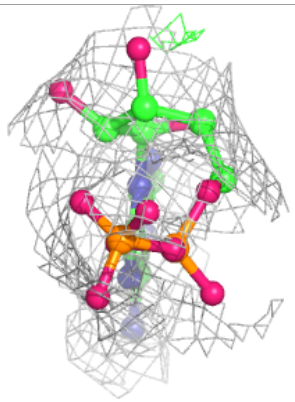
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 2000:

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

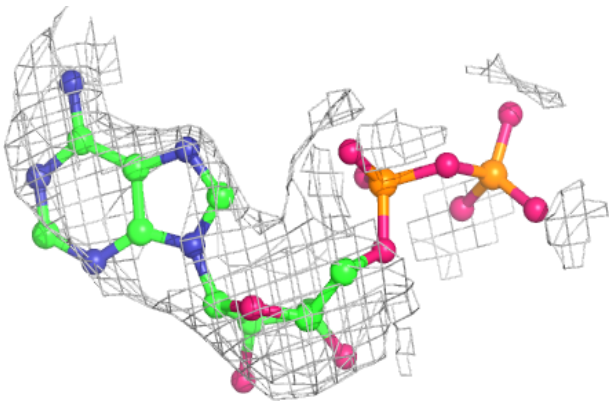


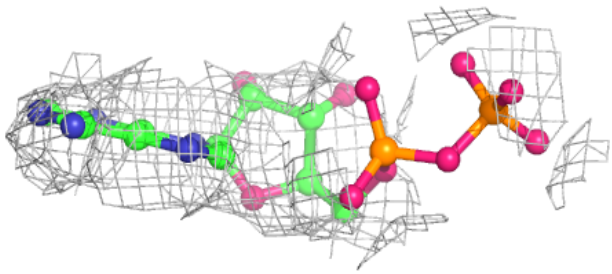


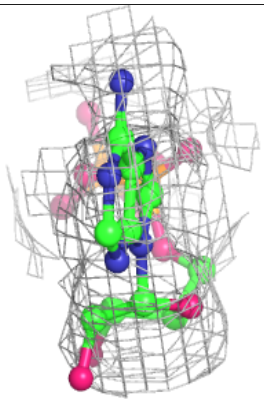


Electron density around ADP C 2000:

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

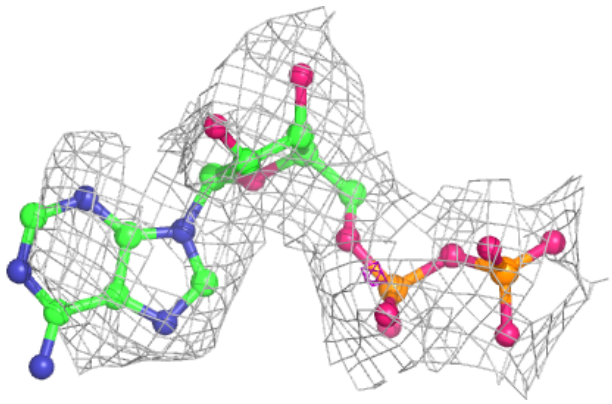


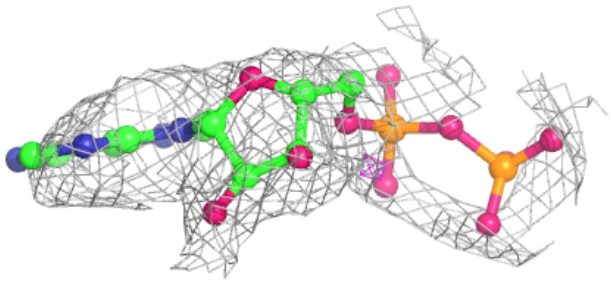


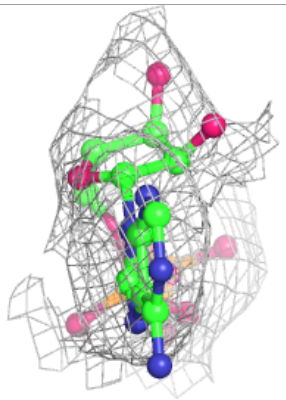


Electron density around ADP G 2000:

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

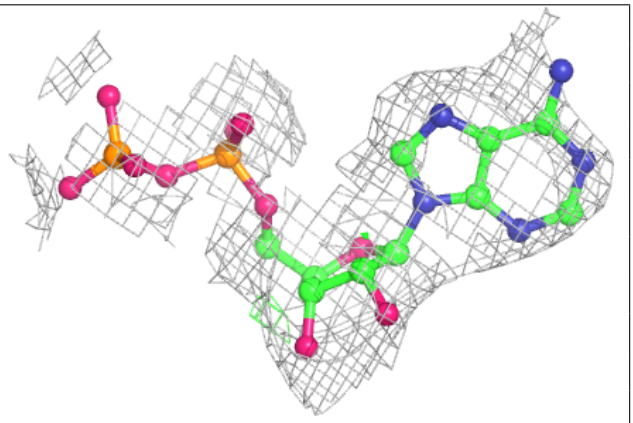


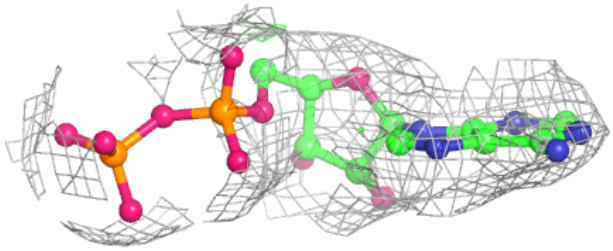


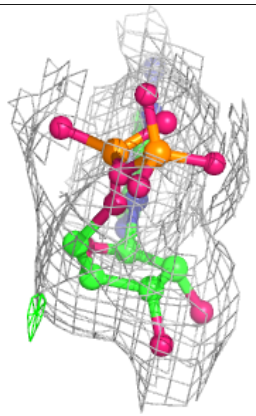


Electron density around ADP H 2000:

$2mF_o$-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.