Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 10:26 AM JST

PDB ID	:	6LKN
Title	:	Crystal structure of ATP11C-CDC50A in PtdSer-bound E2P state
Authors	:	Abe, K.; Irie, K.; Nakanishi, H.; Hasegawa, K.
Deposited on	:	2019-12-19
Resolution	:	3.90 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:

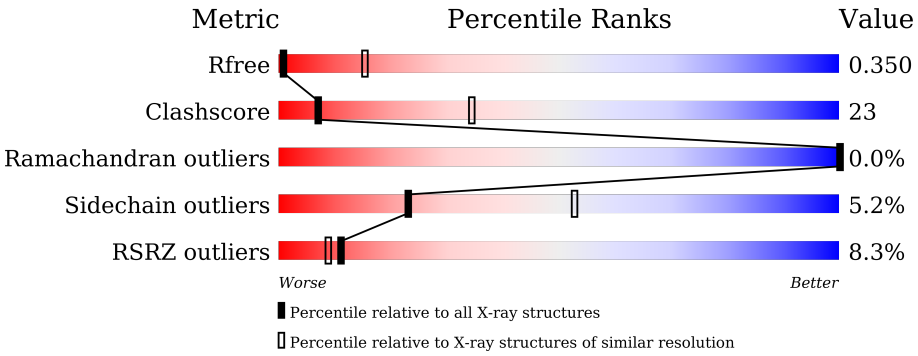
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	1129	4% 56% 35% · 6%
1	E	1129	8% 57% 34% · 6%
1	I	1129	9% 65% 27% · 6%
1	M	1129	11% 65% 27% · 6%
2	C	361	59% 29% · 10%
2	F	361	% 58% 29% · 10%

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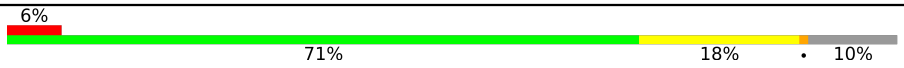
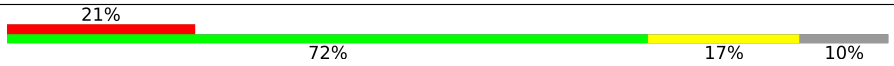
Mol	Chain	Length	Quality of chain
2	J	361	
2	N	361	

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
1	BFD	E	409	-	-	X	-
5	NAG	F	405	-	-	X	-
5	NAG	J	404	-	-	X	-
5	NAG	J	405	-	-	X	-
5	NAG	N	401	-	-	-	X
5	NAG	N	405	-	-	X	-
6	AH2	N	403	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 45252 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 Phospholipid-transporting ATPase IG.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			
1	E	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			
1	I	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			
1	M	1064	Total	Be	C	F	N	O	S	0	0	0
			8601	1	5556	3	1401	1594	46			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NB49
A	2	PHE	-	expression tag	UNP Q8NB49
A	3	ARG	-	expression tag	UNP Q8NB49
A	4	ARG	-	expression tag	UNP Q8NB49
A	5	SER	-	expression tag	UNP Q8NB49
A	6	LEU	-	expression tag	UNP Q8NB49
A	7	ASN	-	expression tag	UNP Q8NB49
A	8	ARG	-	expression tag	UNP Q8NB49
A	9	PHE	-	expression tag	UNP Q8NB49
A	111	TRP	CYS	engineered mutation	UNP Q8NB49
E	1	MET	-	initiating methionine	UNP Q8NB49
E	2	PHE	-	expression tag	UNP Q8NB49
E	3	ARG	-	expression tag	UNP Q8NB49
E	4	ARG	-	expression tag	UNP Q8NB49
E	5	SER	-	expression tag	UNP Q8NB49
E	6	LEU	-	expression tag	UNP Q8NB49
E	7	ASN	-	expression tag	UNP Q8NB49
E	8	ARG	-	expression tag	UNP Q8NB49
E	9	PHE	-	expression tag	UNP Q8NB49
E	111	TRP	CYS	engineered mutation	UNP Q8NB49
I	1	MET	-	initiating methionine	UNP Q8NB49

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Chain	Residue	Modelled	Actual	Comment	Reference
I	2	PHE	-	expression tag	UNP Q8NB49
I	3	ARG	-	expression tag	UNP Q8NB49
I	4	ARG	-	expression tag	UNP Q8NB49
I	5	SER	-	expression tag	UNP Q8NB49
I	6	LEU	-	expression tag	UNP Q8NB49
I	7	ASN	-	expression tag	UNP Q8NB49
I	8	ARG	-	expression tag	UNP Q8NB49
I	9	PHE	-	expression tag	UNP Q8NB49
I	111	TRP	CYS	engineered mutation	UNP Q8NB49
M	1	MET	-	initiating methionine	UNP Q8NB49
M	2	PHE	-	expression tag	UNP Q8NB49
M	3	ARG	-	expression tag	UNP Q8NB49
M	4	ARG	-	expression tag	UNP Q8NB49
M	5	SER	-	expression tag	UNP Q8NB49
M	6	LEU	-	expression tag	UNP Q8NB49
M	7	ASN	-	expression tag	UNP Q8NB49
M	8	ARG	-	expression tag	UNP Q8NB49
M	9	PHE	-	expression tag	UNP Q8NB49
M	111	TRP	CYS	engineered mutation	UNP Q8NB49

- Molecule 2 is a protein called Cell cycle control protein 50A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	F	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	J	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	N	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	190	GLN	ASN	engineered mutation	UNP Q9NV96
C	292	TRP	SER	engineered mutation	UNP Q9NV96
F	190	GLN	ASN	engineered mutation	UNP Q9NV96
F	292	TRP	SER	engineered mutation	UNP Q9NV96
J	190	GLN	ASN	engineered mutation	UNP Q9NV96
J	292	TRP	SER	engineered mutation	UNP Q9NV96
N	190	GLN	ASN	engineered mutation	UNP Q9NV96

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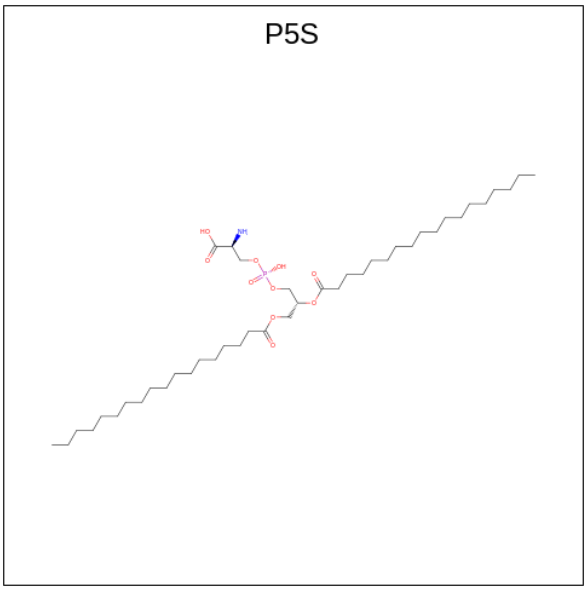
Chain	Residue	Modelled	Actual	Comment	Reference
N	292	TRP	SER	engineered mutation	UNP Q9NV96

- Molecule 3 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 11 3 1 6 1	0	0
3	C	1	Total C N O P 54 42 1 10 1	0	0
3	E	1	Total C N O P 11 3 1 6 1	0	0
3	E	1	Total C N O P 11 3 1 6 1	0	0
3	I	1	Total C N O P 11 3 1 6 1	0	0
3	I	1	Total C N O P 11 3 1 6 1	0	0
3	M	1	Total C N O P 11 3 1 6 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

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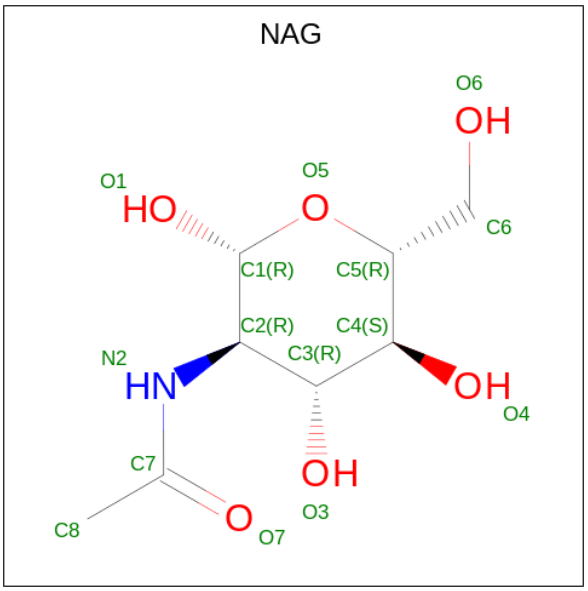
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 13 8 1 4	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 13 8 1 4	0	0

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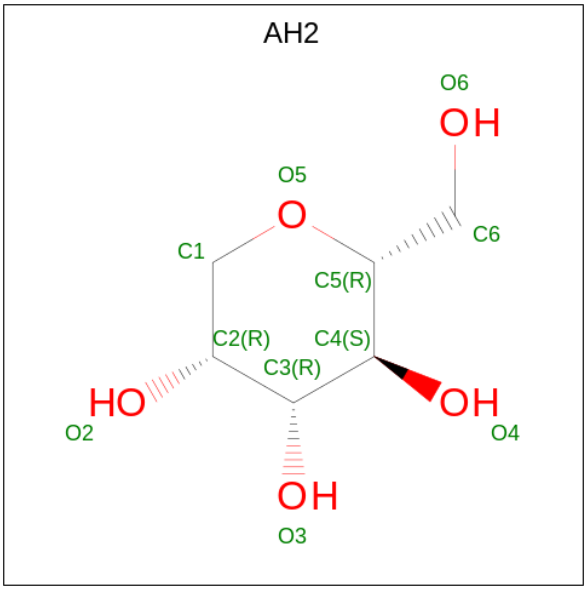
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total C N O 14 8 1 5	0	0
5	J	1	Total C N O 14 8 1 5	0	0
5	J	1	Total C N O 14 8 1 5	0	0
5	J	1	Total C N O 13 8 1 4	0	0
5	N	1	Total C N O 14 8 1 5	0	0
5	N	1	Total C N O 14 8 1 5	0	0
5	N	1	Total C N O 14 8 1 5	0	0
5	N	1	Total C N O 13 8 1 4	0	0

- Molecule 6 is 1-deoxy-alpha-D-mannopyranose (three-letter code: AH2) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 11 6 5	0	0
6	F	1	Total C O 11 6 5	0	0
6	J	1	Total C O 11 6 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total C O 11 6 5	0	0

- Molecule 7 is water.

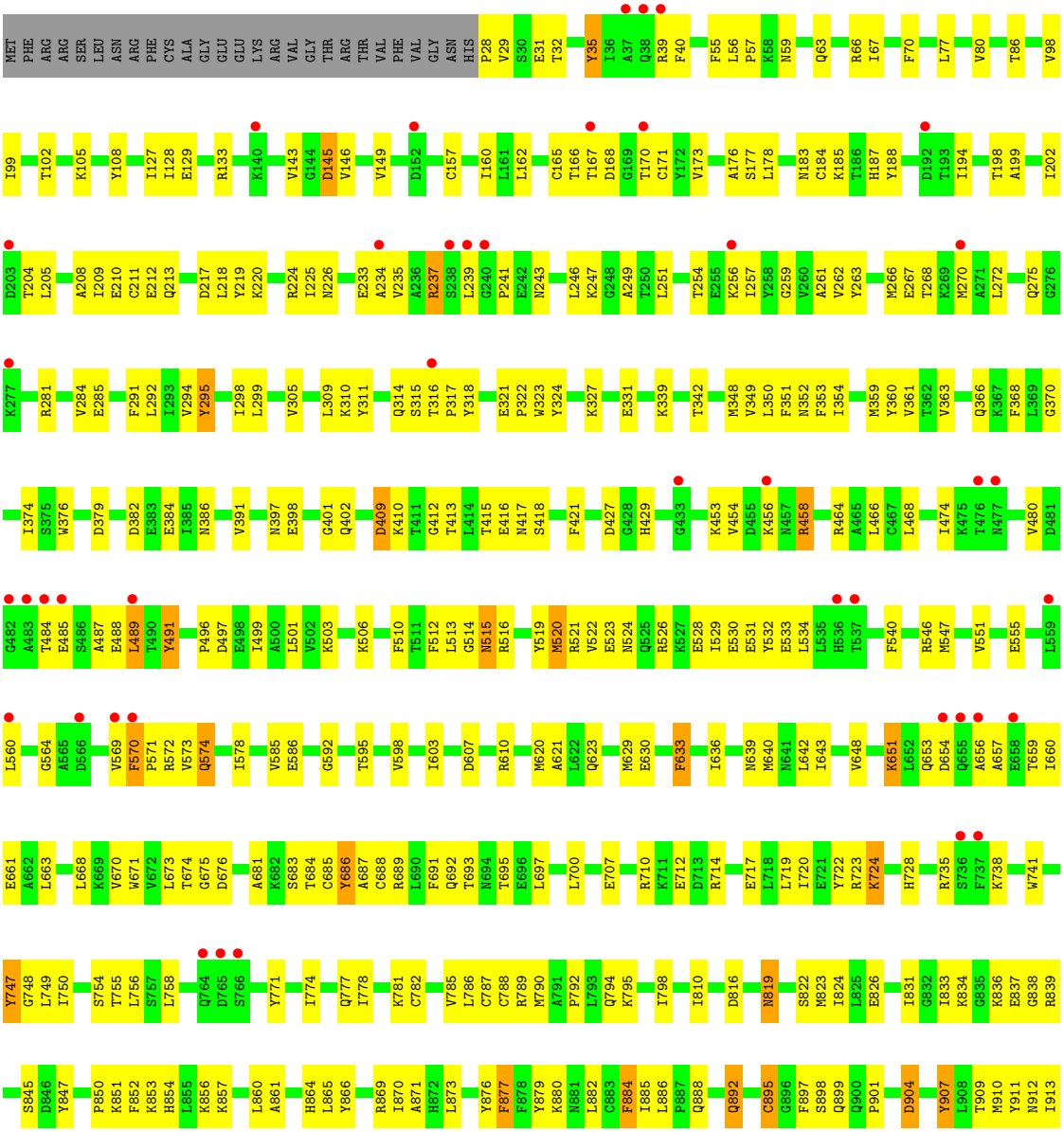
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	E	2	Total O 2 2	0	0
7	I	2	Total O 2 2	0	0
7	M	2	Total O 2 2	0	0

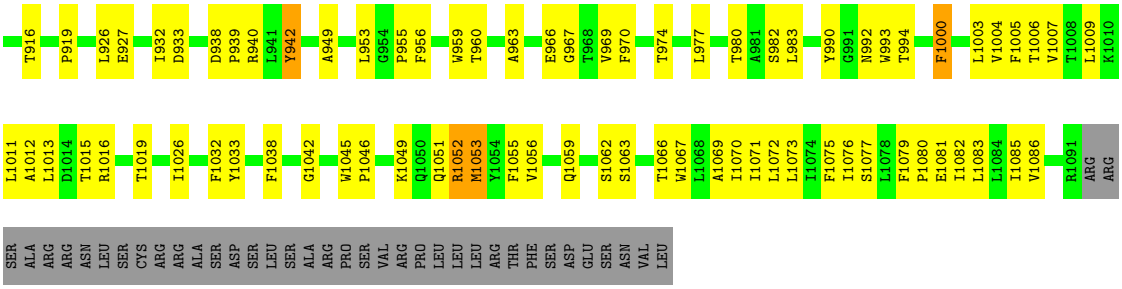
3 Residue-property plots (i)

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: Phospholipid-transporting ATPase IG

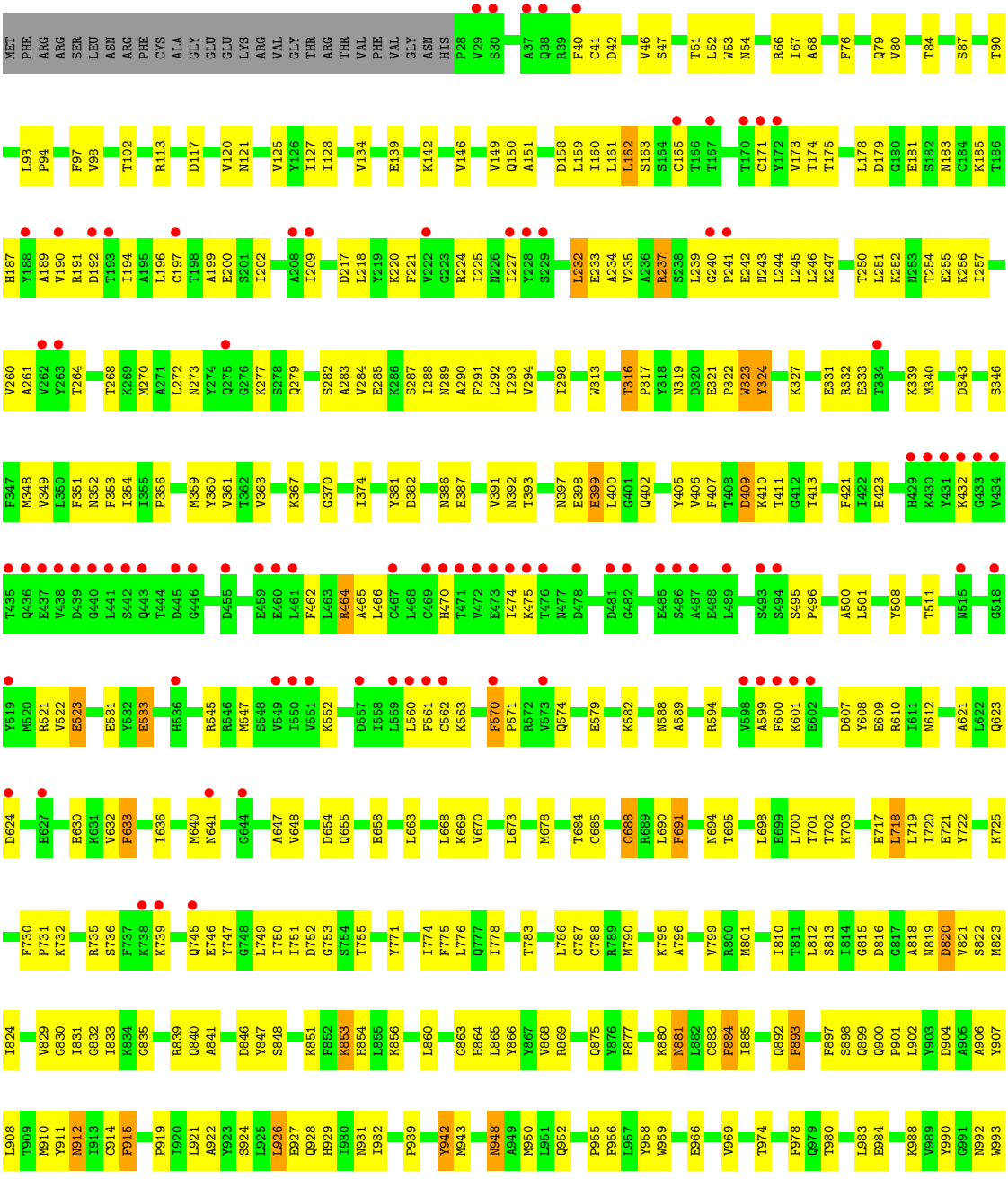
Chain A:

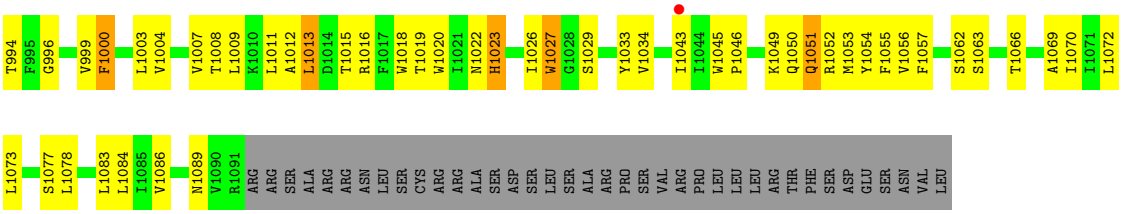


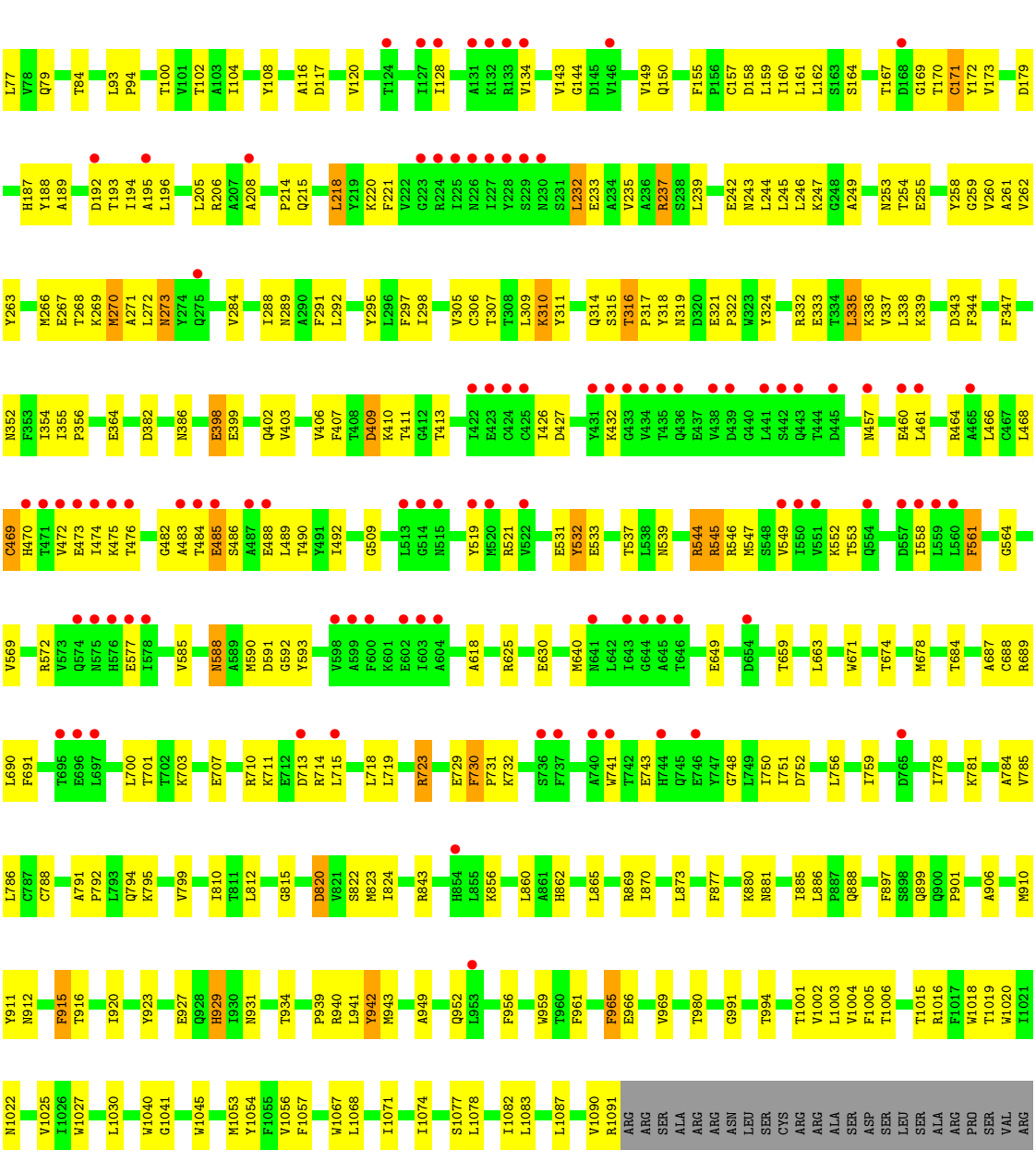


• Molecule 1: Phospholipid-transporting ATPase IG

Chain E:





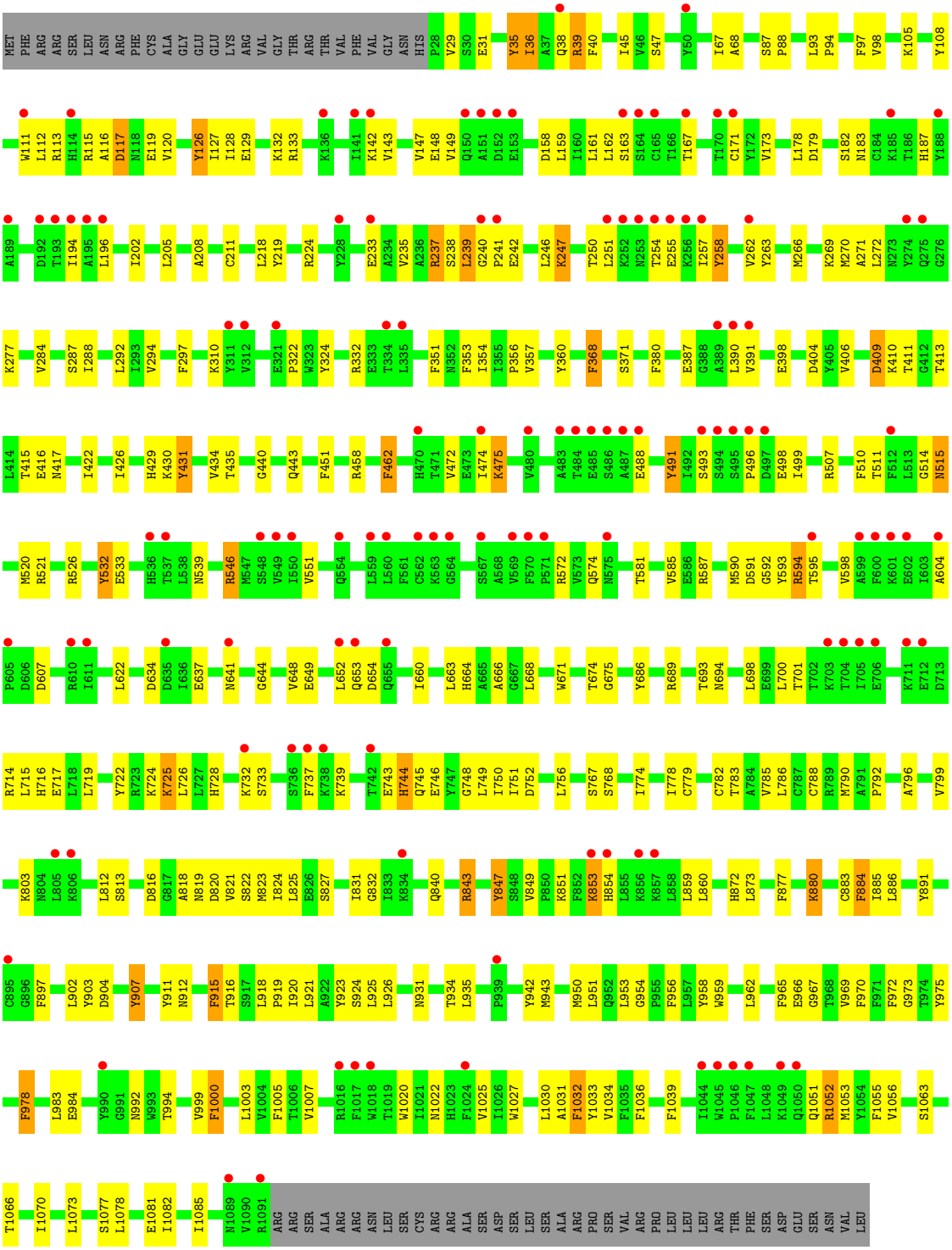


• Molecule 1: Phospholipid-transporting ATPase IG

Chain I:

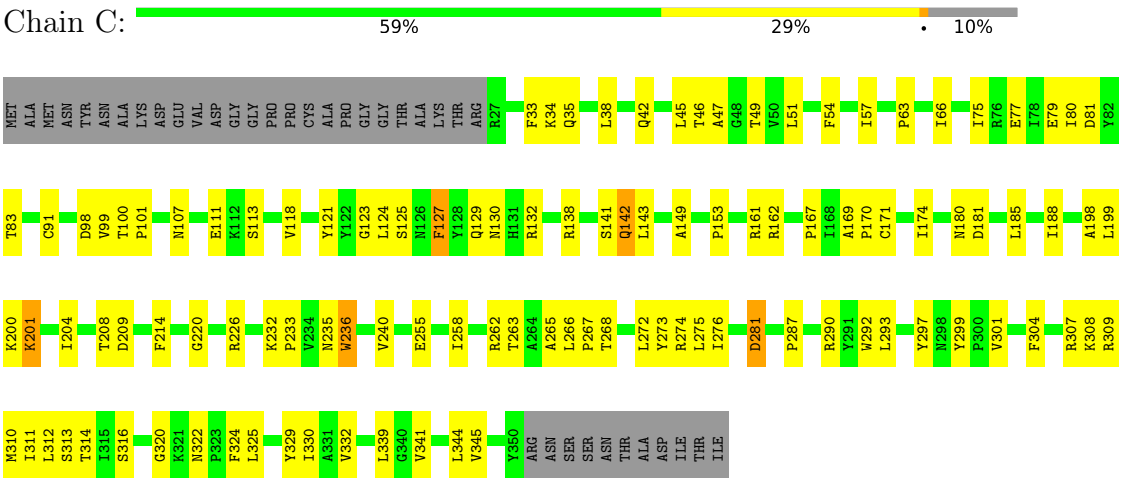
• Molecule 1: Phospholipid-transporting ATPase IG

Chain M:



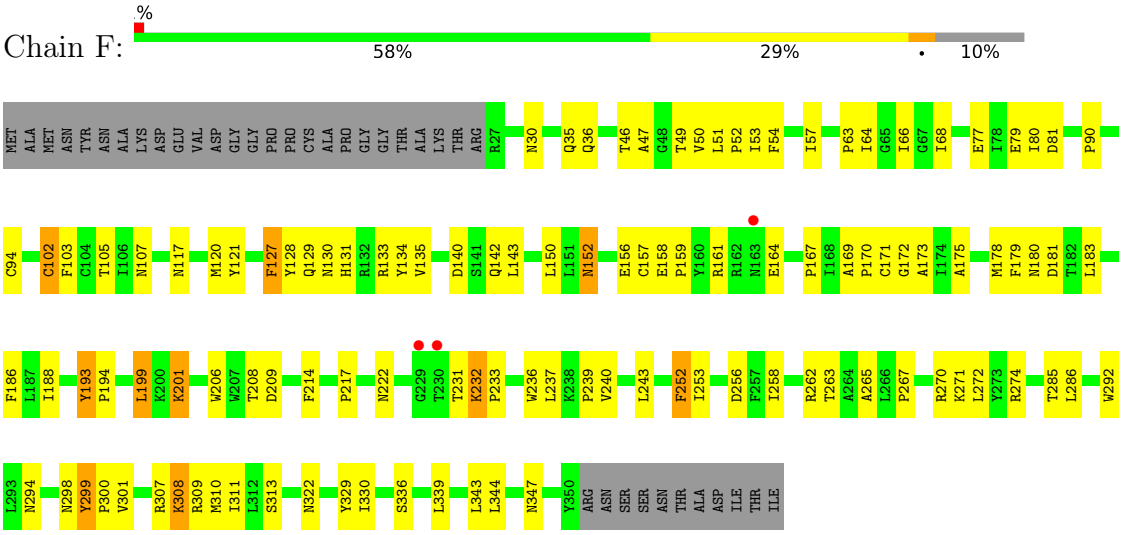
• Molecule 2: Cell cycle control protein 50A

Chain C:



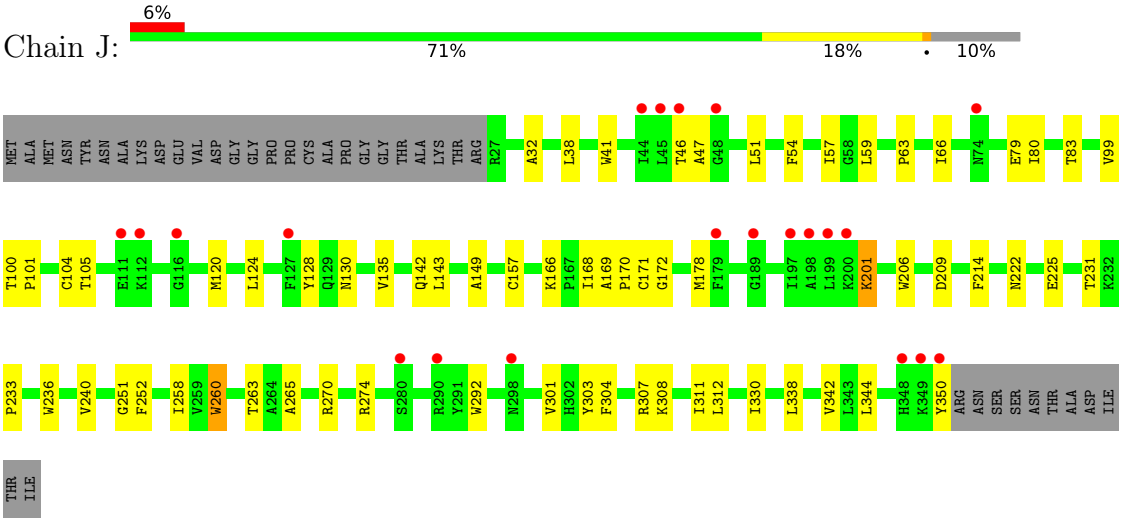
• Molecule 2: Cell cycle control protein 50A

Chain F:



• Molecule 2: Cell cycle control protein 50A

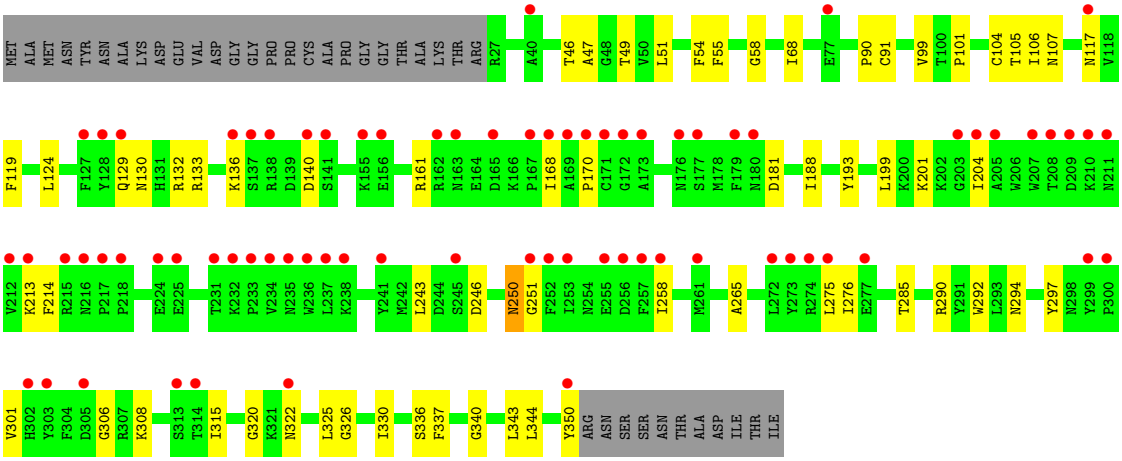
Chain J:



• Molecule 2: Cell cycle control protein 50A

Chain N:


21%
72%
17%
10%


MET ALA MET ASN TYR ASN ALA LYS ASP GLU VAL ASP GLY GLY PRO PRO CYS ALA PRO GLY GLY THR ALA LYS THR ARG R27 A40 T46 A47 G48 T49 V50 L51 F54 F55 G58 I68 E77 P90 C91 V99 T100 P101 C104 T105 I106 N107 N117 V118
F119 L124 F127 Y128 Q129 N130 H131 R132 R133 K136 S137 R138 D139 D140 S141 K155 E156 R161 R162 N163 E164 D165 K166 P167 I168 A169 P170 C171 G172 A173 N176 S177 M178 F179 N180 D181 I188 Y193 L199 K200 K201 K202 G203 I204 A205 W206 W207 T208 D209 K210 N211
V212 K213 F214 R215 N216 P217 P218 E224 E225 T231 K232 P233 V234 N235 W236 L237 K238 Y241 M242 L243 D244 S245 D246 N250 G251 F252 I253 N254 E255 D256 F257 I258 M261 A265 L272 Y273 R274 L275 I276 E277 T285 R290 Y291 W292 L293 N294 Y297 N298 Y299 P300
V301 H302 Y303 F304 D305 G306 R307 K308 S313 T314 I315 G320 K321 N322 L325 G326 I330 S336 F337 G340 L343 L344 Y350 ARG ASN SER SER ASN THR ALA ASP ILE THR ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.46Å 232.83Å 492.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.90 49.97 – 3.78	Depositor EDS
% Data completeness (in resolution range)	71.4 (49.97-3.90) 65.4 (49.97-3.78)	Depositor EDS
R_{merge}	1.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.281 , 0.350 0.281 , 0.350	Depositor DCC
R_{free} test set	3779 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 92.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	45252	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: MG, BFD, P5S, NAG, AH2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/8777	0.64	0/11883
1	E	0.34	0/8777	0.64	0/11883
1	I	0.29	0/8777	0.59	0/11883
1	M	0.29	0/8777	0.58	0/11883
2	C	0.33	0/2690	0.64	0/3659
2	F	0.33	0/2690	0.64	0/3659
2	J	0.27	0/2690	0.55	0/3659
2	N	0.28	0/2690	0.53	0/3659
All	All	0.31	0/45868	0.61	0/62168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8601	0	8587	591	0
1	E	8601	0	8588	436	0
1	I	8601	0	8587	461	0
1	M	8601	0	8588	267	0
2	C	2613	0	2592	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2613	0	2594	107	0
2	J	2613	0	2592	68	0
2	N	2613	0	2592	84	0
3	A	11	0	5	0	0
3	C	54	0	80	2	0
3	E	22	0	10	1	0
3	I	22	0	10	9	0
3	M	11	0	5	1	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
4	M	1	0	0	0	0
5	C	55	0	50	3	0
5	F	55	0	50	23	0
5	J	55	0	50	18	0
5	N	55	0	49	15	0
6	C	11	0	0	0	0
6	F	11	0	0	0	0
6	J	11	0	0	0	0
6	N	11	0	0	0	0
7	A	2	0	0	0	0
7	E	2	0	0	4	0
7	I	2	0	0	1	0
7	M	2	0	0	1	0
All	All	45252	0	45029	2057	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 23.

All (2057) 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:I:214:PRO:HB3	1:I:268:THR:CG2	1.23	1.60
1:I:678:MET:CE	1:I:700:LEU:HD13	1.27	1.60
1:A:28:PRO:CD	1:A:212:GLU:HA	1.15	1.58
1:A:519:TYR:HD2	1:A:532:TYR:CB	0.97	1.58
1:A:519:TYR:CE1	1:A:551:VAL:HG11	1.35	1.58
1:A:519:TYR:CD2	1:A:532:TYR:CB	1.80	1.58
1:I:159:LEU:HB2	1:I:262:VAL:CG2	1.30	1.56
1:I:314:GLN:HE22	3:I:1201:P5S:CB	1.13	1.56
1:A:790:MET:SD	1:A:794:GLN:HB3	1.46	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PRO:HD3	1:A:212:GLU:CA	1.33	1.55
1:I:159:LEU:CB	1:I:262:VAL:HG22	1.34	1.55
1:I:159:LEU:CD1	1:I:262:VAL:HG23	1.33	1.54
1:A:519:TYR:CE1	1:A:551:VAL:CG1	1.90	1.53
2:N:188:ILE:CD1	2:N:292:TRP:CD1	1.90	1.52
1:I:214:PRO:CB	1:I:268:THR:CG2	1.82	1.51
1:M:126:TYR:CE1	1:M:133:ARG:CD	1.95	1.49
2:N:188:ILE:HD12	2:N:292:TRP:CD1	0.99	1.48
1:I:143:VAL:HG13	1:I:263:TYR:CZ	1.47	1.48
1:M:126:TYR:CE1	1:M:133:ARG:HD3	1.46	1.46
1:A:654:ASP:OD2	1:A:853:LYS:CB	1.65	1.43
1:I:143:VAL:HG13	1:I:263:TYR:CE2	1.54	1.43
2:N:188:ILE:HD12	2:N:292:TRP:NE1	1.29	1.43
1:A:659:THR:HG21	1:A:852:PHE:CE2	1.55	1.40
1:I:314:GLN:NE2	3:I:1201:P5S:HBA	1.13	1.40
1:I:314:GLN:O	1:I:319:ASN:CB	1.70	1.40
1:A:519:TYR:CD2	1:A:532:TYR:HB3	1.43	1.36
1:A:833:ILE:HG12	1:A:836:LYS:CG	1.54	1.35
2:J:292:TRP:CZ3	5:J:405:NAG:O6	1.70	1.34
1:I:318:TYR:CZ	2:J:128:TYR:HE2	1.43	1.34
1:A:519:TYR:CZ	1:A:551:VAL:HG11	1.62	1.34
2:J:292:TRP:CD1	5:J:404:NAG:C6	2.11	1.33
1:I:214:PRO:CB	1:I:268:THR:HG22	1.49	1.32
1:A:792:PRO:O	1:A:823:MET:HE3	1.22	1.31
1:A:833:ILE:HD11	1:A:836:LYS:CD	1.61	1.31
1:I:678:MET:CE	1:I:700:LEU:CD1	2.10	1.30
1:A:28:PRO:CD	1:A:212:GLU:CA	1.90	1.30
1:E:717:GLU:OE1	1:E:774:ILE:HD12	1.29	1.28
1:A:519:TYR:CD2	1:A:532:TYR:HB2	1.52	1.28
1:I:318:TYR:O	1:I:322:PRO:CD	1.80	1.28
1:E:159:LEU:O	1:E:244:LEU:HD23	1.30	1.27
1:I:318:TYR:CE1	2:J:128:TYR:HE2	1.53	1.27
1:I:159:LEU:HD11	1:I:259:GLY:CA	1.65	1.26
1:A:176:ALA:HB3	1:A:837:GLU:OE2	1.36	1.25
1:A:28:PRO:N	1:A:212:GLU:HA	1.50	1.25
1:I:159:LEU:HD13	1:I:262:VAL:CG2	1.66	1.25
1:A:28:PRO:CA	1:A:211:CYS:O	1.85	1.25
1:I:158:ASP:O	1:I:262:VAL:HA	1.33	1.25
1:A:569:VAL:C	1:A:571:PRO:HD2	1.58	1.24
1:A:413:THR:O	1:A:653:GLN:NE2	1.70	1.24
1:I:143:VAL:CG1	1:I:263:TYR:CZ	2.20	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:LEU:CB	1:I:262:VAL:CG2	1.97	1.24
1:A:512:PHE:CZ	1:A:515:ASN:ND2	2.06	1.23
2:J:292:TRP:CD1	5:J:404:NAG:O6	1.91	1.23
2:N:107:ASN:ND2	5:N:405:NAG:H2	1.53	1.23
1:A:29:VAL:HG12	1:A:211:CYS:N	1.51	1.22
1:I:700:LEU:O	1:I:701:THR:CG2	1.86	1.22
1:I:310:LYS:HD2	1:I:311:TYR:N	1.53	1.21
1:A:519:TYR:OH	1:A:551:VAL:HG21	1.32	1.21
1:E:246:LEU:CD2	1:E:268:THR:HG21	1.69	1.21
1:I:472:VAL:O	1:I:475:LYS:NZ	1.73	1.21
1:A:489:LEU:HD11	1:A:503:LYS:NZ	1.55	1.20
1:E:717:GLU:CD	1:E:774:ILE:HD12	1.60	1.20
1:A:792:PRO:O	1:A:823:MET:CE	1.89	1.20
1:I:318:TYR:CZ	2:J:128:TYR:CE2	2.29	1.20
1:I:214:PRO:CB	1:I:268:THR:HG23	1.56	1.20
1:E:162:LEU:O	1:E:194:ILE:HG23	1.38	1.19
1:I:489:LEU:HD22	1:I:509:GLY:O	1.42	1.19
1:I:143:VAL:CG1	1:I:263:TYR:CE2	2.25	1.18
1:I:307:THR:O	1:I:310:LYS:HE3	1.37	1.18
1:A:654:ASP:OD2	1:A:853:LYS:HB2	1.01	1.18
1:I:678:MET:HE1	1:I:700:LEU:CD1	1.70	1.18
1:I:700:LEU:O	1:I:701:THR:HG22	1.01	1.18
1:E:717:GLU:CD	1:E:774:ILE:CD1	2.13	1.17
1:A:28:PRO:HA	1:A:211:CYS:O	1.39	1.16
1:E:1009:LEU:HD12	1:E:1078:LEU:HD22	1.26	1.16
2:J:292:TRP:NE1	5:J:404:NAG:H62	1.58	1.16
1:A:521:ARG:HD3	1:A:531:GLU:OE2	1.42	1.15
1:I:214:PRO:CA	1:I:268:THR:CG2	2.23	1.15
2:N:107:ASN:HD21	5:N:405:NAG:H2	0.99	1.15
1:I:159:LEU:CD1	1:I:259:GLY:HA3	1.74	1.15
2:J:292:TRP:CH2	5:J:405:NAG:O6	1.98	1.15
1:E:1009:LEU:HD12	1:E:1078:LEU:CD2	1.75	1.15
1:A:833:ILE:CG1	1:A:836:LYS:CG	2.23	1.14
1:E:185:LYS:HD3	1:E:245:LEU:HD11	1.30	1.14
1:I:700:LEU:HD23	1:I:751:ILE:C	1.67	1.14
1:I:700:LEU:HD22	1:I:788:CYS:HB3	1.15	1.14
1:I:482:GLY:HA3	1:I:490:THR:HG22	1.19	1.13
1:A:28:PRO:N	1:A:212:GLU:CA	2.04	1.13
1:A:519:TYR:HE1	1:A:551:VAL:CG1	1.39	1.13
1:A:311:TYR:O	1:A:315:SER:HB3	1.46	1.13
1:A:468:LEU:HD13	1:A:519:TYR:OH	1.46	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:ILE:HG12	1:I:261:ALA:HB3	1.24	1.13
1:M:715:LEU:O	1:M:719:LEU:HD13	1.43	1.13
1:I:318:TYR:CE1	2:J:128:TYR:CE2	2.37	1.12
1:I:700:LEU:HD23	1:I:752:ASP:N	1.63	1.13
1:I:678:MET:HE3	1:I:700:LEU:CD1	1.76	1.12
1:M:127:ILE:HD12	1:M:147:VAL:HG22	1.23	1.12
1:I:306:CYS:O	1:I:310:LYS:HG3	1.47	1.12
1:A:310:LYS:HE2	1:A:897:PHE:HB2	1.31	1.12
1:E:655:GLN:CG	1:E:658:GLU:HG2	1.78	1.12
1:M:126:TYR:HE1	1:M:133:ARG:CD	1.44	1.12
1:I:159:LEU:HD11	1:I:259:GLY:HA3	1.14	1.11
1:A:833:ILE:CD1	1:A:836:LYS:HD3	1.80	1.10
1:A:572:ARG:NE	1:A:639:ASN:HB2	1.66	1.10
1:E:47:SER:HB2	1:E:117:ASP:OD2	1.49	1.10
1:A:569:VAL:C	1:A:571:PRO:CD	2.20	1.10
1:I:482:GLY:CA	1:I:490:THR:HG22	1.80	1.10
1:A:512:PHE:CE1	1:A:515:ASN:ND2	2.20	1.10
1:A:524:ASN:HB2	1:A:530:GLU:OE1	1.51	1.09
2:F:292:TRP:HH2	5:F:405:NAG:C6	1.66	1.09
1:I:159:LEU:CD1	1:I:262:VAL:CG2	2.25	1.09
1:I:314:GLN:NE2	3:I:1201:P5S:CB	1.86	1.09
1:A:790:MET:SD	1:A:794:GLN:CB	2.39	1.09
1:I:318:TYR:O	1:I:322:PRO:HD3	1.39	1.09
1:A:833:ILE:CG1	1:A:836:LYS:HG2	1.81	1.09
1:I:489:LEU:CD2	1:I:509:GLY:O	2.00	1.09
1:M:113:ARG:O	1:M:117:ASP:OD1	1.71	1.09
1:A:792:PRO:HG3	1:A:819:ASN:O	1.52	1.09
2:F:143:LEU:HD22	2:F:252:PHE:CE2	1.86	1.09
1:I:690:LEU:HD12	1:I:691:PHE:N	1.68	1.09
1:A:28:PRO:N	1:A:211:CYS:O	1.84	1.08
1:M:47:SER:OG	1:M:843:ARG:CZ	1.99	1.08
1:I:690:LEU:HD11	1:I:691:PHE:CD2	1.87	1.08
1:A:519:TYR:CE2	1:A:532:TYR:HB3	1.86	1.08
1:I:678:MET:HE3	1:I:700:LEU:HD13	1.28	1.08
1:A:756:LEU:HD13	1:A:790:MET:HE1	1.34	1.08
1:A:833:ILE:CD1	1:A:836:LYS:CG	2.32	1.07
1:A:521:ARG:CD	1:A:531:GLU:OE2	2.02	1.07
1:I:310:LYS:HB2	1:I:897:PHE:HB2	1.33	1.07
1:I:160:ILE:CG1	1:I:261:ALA:HB3	1.84	1.07
1:A:570:PHE:N	1:A:571:PRO:CD	2.18	1.07
1:A:654:ASP:OD2	1:A:853:LYS:CA	2.03	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG21	1:A:31:GLU:OE2	1.54	1.06
1:A:28:PRO:CD	1:A:212:GLU:C	2.24	1.06
1:E:732:LYS:HG3	1:E:739:LYS:NZ	1.69	1.06
1:I:700:LEU:HD11	1:I:750:ILE:HG23	1.36	1.06
1:E:196:LEU:HD21	1:E:199:ALA:HB3	1.07	1.06
1:A:412:GLY:O	1:A:836:LYS:HB3	1.54	1.06
1:A:521:ARG:HB3	1:A:531:GLU:CD	1.74	1.06
1:A:176:ALA:CB	1:A:837:GLU:OE2	2.04	1.05
1:I:47:SER:OG	1:I:117:ASP:CG	1.93	1.05
1:A:654:ASP:CG	1:A:853:LYS:HB2	1.76	1.05
1:I:318:TYR:O	1:I:322:PRO:HD2	1.51	1.05
1:I:316:THR:HB	1:I:317:PRO:HD3	1.34	1.05
2:F:143:LEU:HD22	2:F:252:PHE:HE2	1.15	1.05
1:A:28:PRO:N	1:A:211:CYS:C	2.09	1.04
2:J:292:TRP:NE1	5:J:404:NAG:C6	2.16	1.04
1:A:519:TYR:CE1	1:A:551:VAL:HG12	1.90	1.04
1:E:163:SER:HB3	1:E:194:ILE:HG22	1.39	1.04
1:E:732:LYS:NZ	1:E:739:LYS:CE	2.20	1.03
1:I:158:ASP:O	1:I:262:VAL:CA	2.06	1.03
1:A:219:TYR:HA	1:A:235:VAL:CG1	1.86	1.03
1:I:700:LEU:CD2	1:I:751:ILE:C	2.27	1.03
1:A:570:PHE:N	1:A:571:PRO:HD3	1.72	1.03
1:A:219:TYR:CE2	1:A:235:VAL:O	2.11	1.03
1:A:316:THR:OG1	1:A:317:PRO:HD3	1.58	1.03
1:E:717:GLU:OE2	1:E:774:ILE:HD13	1.58	1.03
1:A:833:ILE:CD1	1:A:836:LYS:CD	2.33	1.03
1:E:159:LEU:HD11	1:E:261:ALA:H	1.22	1.03
1:E:191:ARG:N	1:E:194:ILE:HD12	1.73	1.03
1:I:159:LEU:CG	1:I:262:VAL:CG2	2.36	1.03
1:I:306:CYS:O	1:I:310:LYS:CG	2.07	1.03
1:A:519:TYR:OH	1:A:551:VAL:CG2	2.07	1.02
1:M:126:TYR:CE1	1:M:133:ARG:CG	2.41	1.02
1:A:31:GLU:HG3	1:A:209:ILE:HG23	1.39	1.02
1:E:732:LYS:HG3	1:E:739:LYS:HZ3	0.86	1.02
1:I:307:THR:C	1:I:310:LYS:HE3	1.80	1.02
1:E:185:LYS:CD	1:E:245:LEU:HD11	1.90	1.01
1:I:47:SER:OG	1:I:117:ASP:OD2	1.78	1.01
1:I:167:THR:HB	1:I:473:GLU:O	1.61	1.01
1:I:318:TYR:OH	2:J:128:TYR:CE2	2.12	1.01
1:E:640:MET:SD	1:E:641:ASN:O	2.18	1.01
1:I:678:MET:HE3	1:I:700:LEU:H	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:732:LYS:HZ2	1:E:739:LYS:HE2	1.23	1.01
1:A:519:TYR:HB2	1:A:533:GLU:CA	1.91	1.00
1:M:47:SER:OG	1:M:843:ARG:NH2	1.93	1.00
1:I:310:LYS:HB3	1:I:897:PHE:CG	1.95	1.00
1:I:678:MET:CE	1:I:700:LEU:H	1.75	1.00
1:A:833:ILE:CD1	1:A:836:LYS:HG3	1.89	0.99
2:N:117:ASN:ND2	2:N:119:PHE:CE2	2.29	0.99
1:E:196:LEU:CD2	1:E:199:ALA:HB3	1.92	0.99
1:E:246:LEU:HD22	1:E:268:THR:HG21	1.43	0.99
1:M:126:TYR:OH	1:M:133:ARG:HG3	1.60	0.99
1:A:31:GLU:O	1:A:208:ALA:HB1	1.62	0.99
1:A:519:TYR:CE2	1:A:532:TYR:CB	2.45	0.99
1:A:218:LEU:HB2	1:A:267:GLU:HG3	1.40	0.99
1:I:159:LEU:CA	1:I:262:VAL:HG22	1.91	0.99
1:A:311:TYR:O	1:A:315:SER:CB	2.11	0.98
1:E:732:LYS:NZ	1:E:739:LYS:HE3	1.77	0.98
1:M:126:TYR:CD1	1:M:133:ARG:HD3	1.98	0.98
1:I:690:LEU:CD1	1:I:691:PHE:CD2	2.46	0.98
1:I:700:LEU:CD2	1:I:788:CYS:HB3	1.91	0.98
1:I:159:LEU:HD11	1:I:259:GLY:C	1.81	0.98
1:A:219:TYR:HA	1:A:235:VAL:HG12	0.98	0.98
2:F:292:TRP:CH2	5:F:405:NAG:H61	1.98	0.98
1:I:214:PRO:HB2	1:I:268:THR:HG22	1.41	0.98
1:A:468:LEU:CD1	1:A:519:TYR:OH	2.10	0.98
1:I:307:THR:O	1:I:310:LYS:CE	2.11	0.98
1:A:468:LEU:HD13	1:A:519:TYR:CZ	1.99	0.97
1:E:717:GLU:OE2	1:E:774:ILE:CD1	2.10	0.97
1:A:219:TYR:CA	1:A:235:VAL:HG12	1.92	0.97
1:M:126:TYR:CE1	1:M:133:ARG:HD2	1.96	0.97
1:I:703:LYS:HE3	1:I:714:ARG:HD3	1.47	0.97
1:A:519:TYR:CZ	1:A:551:VAL:CG1	2.33	0.97
1:A:882:LEU:HD12	1:A:963:ALA:HB1	1.46	0.97
1:E:655:GLN:HG3	1:E:658:GLU:HG2	1.43	0.97
2:N:188:ILE:HD12	2:N:292:TRP:HD1	1.19	0.96
1:I:700:LEU:CD1	1:I:750:ILE:HG23	1.94	0.96
1:A:524:ASN:CB	1:A:530:GLU:OE1	2.12	0.96
1:I:143:VAL:HG13	1:I:263:TYR:CE1	2.00	0.96
1:M:126:TYR:HE1	1:M:133:ARG:CG	1.76	0.96
1:E:732:LYS:HZ2	1:E:739:LYS:CE	1.77	0.96
1:I:159:LEU:CG	1:I:259:GLY:HA3	1.94	0.96
1:I:474:ILE:C	1:I:475:LYS:HD2	1.86	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:PHE:CE2	1:A:515:ASN:ND2	2.34	0.96
2:J:292:TRP:HE1	5:J:404:NAG:H62	1.25	0.95
1:A:519:TYR:CZ	1:A:551:VAL:CB	2.49	0.95
1:I:307:THR:CA	1:I:310:LYS:HE3	1.96	0.95
1:E:1009:LEU:CD1	1:E:1078:LEU:HD22	1.97	0.95
1:I:314:GLN:C	1:I:319:ASN:HB2	1.86	0.95
1:I:310:LYS:NZ	1:I:343:ASP:OD2	1.99	0.95
2:N:188:ILE:CD1	2:N:292:TRP:NE1	2.08	0.94
1:M:434:VAL:HG23	1:M:440:GLY:O	1.65	0.94
1:A:28:PRO:N	1:A:212:GLU:N	2.15	0.94
1:E:125:VAL:HG13	1:E:127:ILE:HG22	1.50	0.94
1:E:698:LEU:HD11	1:E:719:LEU:HB3	1.50	0.94
1:I:159:LEU:CG	1:I:262:VAL:HG23	1.93	0.94
1:M:247:LYS:HE2	1:M:269:LYS:HA	1.50	0.94
1:M:126:TYR:CE1	1:M:133:ARG:HG3	2.03	0.94
1:A:519:TYR:OH	1:A:551:VAL:HG11	1.67	0.93
2:N:292:TRP:CZ3	5:N:405:NAG:O5	2.22	0.93
1:A:659:THR:HG21	1:A:852:PHE:HE2	1.29	0.93
1:A:659:THR:CG2	1:A:852:PHE:CE2	2.50	0.93
1:E:1003:LEU:O	1:E:1007:VAL:HG22	1.69	0.93
1:I:214:PRO:CA	1:I:268:THR:HG22	1.92	0.93
1:A:519:TYR:HD2	1:A:532:TYR:CA	1.81	0.93
1:I:159:LEU:HD21	1:I:259:GLY:HA3	1.50	0.93
2:F:292:TRP:HH2	5:F:405:NAG:H61	1.33	0.93
1:A:464:ARG:NH2	1:A:532:TYR:OH	2.01	0.92
1:E:165:CYS:HG	1:E:197:CYS:HG	0.96	0.92
1:E:233:GLU:OE1	1:E:243:ASN:N	2.02	0.92
1:I:485:GLU:HG3	1:I:488:GLU:CD	1.88	0.92
1:E:117:ASP:O	1:E:121:ASN:HB2	1.70	0.92
1:I:159:LEU:CD2	1:I:259:GLY:HA3	2.00	0.92
1:A:519:TYR:HB2	1:A:533:GLU:HA	1.47	0.91
1:A:29:VAL:H	1:A:211:CYS:H	1.18	0.91
1:A:489:LEU:HD11	1:A:503:LYS:HZ3	1.29	0.91
1:I:159:LEU:HB2	1:I:262:VAL:HG21	1.49	0.91
1:I:314:GLN:O	1:I:319:ASN:HB2	0.74	0.91
2:J:292:TRP:HZ3	5:J:405:NAG:O6	1.21	0.91
1:A:177:SER:HB3	1:A:837:GLU:HG3	1.53	0.91
1:A:833:ILE:HG12	1:A:836:LYS:HG2	0.93	0.91
1:I:700:LEU:HD22	1:I:788:CYS:CB	2.01	0.91
1:M:127:ILE:CD1	1:M:147:VAL:HG22	2.00	0.91
1:A:218:LEU:HB2	1:A:267:GLU:CG	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:PHE:CE1	1:A:520:MET:HG3	2.07	0.90
1:A:833:ILE:CG1	1:A:836:LYS:HG3	1.98	0.90
1:A:833:ILE:HD13	1:A:836:LYS:HG3	1.53	0.90
1:M:126:TYR:CZ	1:M:133:ARG:HG3	2.07	0.90
1:E:233:GLU:OE2	1:E:244:LEU:N	2.04	0.90
2:C:201:LYS:HD3	2:C:201:LYS:H	1.36	0.90
1:I:214:PRO:CA	1:I:268:THR:HG21	2.02	0.90
2:N:107:ASN:HB3	2:N:292:TRP:CE3	2.06	0.90
1:A:128:ILE:HD13	1:A:133:ARG:HA	1.53	0.90
1:A:792:PRO:CG	1:A:819:ASN:O	2.20	0.90
1:I:310:LYS:CB	1:I:897:PHE:HB2	2.02	0.89
1:E:185:LYS:HD3	1:E:245:LEU:CD1	2.03	0.89
2:N:130:ASN:HB3	2:N:265:ALA:HB1	1.53	0.89
2:F:301:VAL:HG21	2:F:308:LYS:HD3	1.51	0.89
1:I:157:CYS:HB2	1:I:262:VAL:CG1	2.01	0.89
2:N:290:ARG:HE	2:N:292:TRP:HE1	1.18	0.89
1:E:732:LYS:HZ3	1:E:739:LYS:HE3	1.31	0.89
2:N:290:ARG:CZ	2:N:292:TRP:HZ2	1.86	0.89
1:E:880:LYS:HG2	1:E:1007:VAL:HG11	1.55	0.88
1:E:163:SER:HB3	1:E:194:ILE:CG2	2.03	0.88
1:A:697:LEU:HA	1:A:747:TYR:HD2	1.38	0.88
1:E:233:GLU:CD	1:E:244:LEU:H	1.75	0.88
1:A:519:TYR:HD2	1:A:532:TYR:HB2	0.88	0.88
1:I:307:THR:HA	1:I:310:LYS:CE	2.04	0.88
2:J:292:TRP:CD1	5:J:404:NAG:H61	2.07	0.88
1:A:28:PRO:HD3	1:A:212:GLU:C	1.87	0.88
1:E:158:ASP:O	1:E:159:LEU:HD22	1.74	0.88
1:A:519:TYR:CB	1:A:533:GLU:CA	2.52	0.88
1:I:310:LYS:HB3	1:I:897:PHE:CD1	2.09	0.88
1:A:29:VAL:HG12	1:A:211:CYS:H	1.33	0.88
2:F:292:TRP:CE3	5:F:404:NAG:O6	2.26	0.88
1:E:915:PHE:HZ	1:E:1008:THR:CG2	1.87	0.87
2:J:292:TRP:HZ3	5:J:405:NAG:C6	1.87	0.87
1:E:1009:LEU:O	1:E:1009:LEU:HD13	1.74	0.87
1:A:521:ARG:CG	1:A:531:GLU:OE2	2.23	0.87
1:A:489:LEU:HD11	1:A:503:LYS:HZ2	1.39	0.86
1:A:572:ARG:HG2	1:A:640:MET:H	1.38	0.86
1:E:720:ILE:HD12	1:E:778:ILE:HG21	1.56	0.86
1:E:233:GLU:CD	1:E:244:LEU:N	2.28	0.86
2:F:292:TRP:CH2	5:F:405:NAG:C6	2.54	0.86
1:I:310:LYS:HD2	1:I:311:TYR:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:ASN:HA	1:M:499:ILE:HG13	1.57	0.86
2:N:290:ARG:CZ	2:N:292:TRP:CZ2	2.59	0.86
1:A:756:LEU:HD13	1:A:790:MET:CE	2.06	0.86
1:I:143:VAL:HG13	1:I:263:TYR:CD2	2.10	0.86
1:I:159:LEU:HD21	1:I:259:GLY:CA	2.05	0.86
2:N:117:ASN:HD21	2:N:119:PHE:HE2	1.24	0.86
1:A:219:TYR:CD2	1:A:235:VAL:O	2.29	0.85
1:A:512:PHE:HE1	1:A:520:MET:CG	1.89	0.85
1:I:473:GLU:HA	1:I:475:LYS:HZ3	1.41	0.85
1:A:520:MET:O	1:A:522:VAL:HG13	1.76	0.85
1:A:898:SER:O	2:C:132:ARG:NH2	2.08	0.85
1:E:127:ILE:HD11	1:E:146:VAL:HG23	1.58	0.85
1:M:115:ARG:O	1:M:119:GLU:HG3	1.76	0.85
1:I:678:MET:HE1	1:I:700:LEU:HD13	0.87	0.85
1:A:572:ARG:HD3	1:A:639:ASN:HA	1.58	0.85
1:E:162:LEU:O	1:E:194:ILE:CG2	2.24	0.85
1:E:196:LEU:HD21	1:E:199:ALA:CB	2.01	0.85
2:N:90:PRO:CG	5:N:405:NAG:H83	2.07	0.84
1:E:246:LEU:HD22	1:E:268:THR:CG2	2.06	0.84
1:A:31:GLU:HG3	1:A:209:ILE:CG2	2.06	0.84
1:A:519:TYR:CE1	1:A:551:VAL:CB	2.60	0.84
1:E:233:GLU:OE2	1:E:244:LEU:HB3	1.77	0.84
1:I:700:LEU:C	1:I:701:THR:HG22	1.97	0.84
1:A:833:ILE:HD11	1:A:836:LYS:HD3	0.88	0.84
1:E:246:LEU:HD21	1:E:268:THR:HG21	1.58	0.84
1:I:214:PRO:HA	1:I:268:THR:HG21	1.58	0.84
1:A:220:LYS:HB2	1:A:220:LYS:NZ	1.93	0.84
1:E:1009:LEU:HD13	1:E:1009:LEU:C	1.98	0.84
1:E:574:GLN:H	1:E:640:MET:HE3	1.43	0.84
1:I:473:GLU:HA	1:I:475:LYS:NZ	1.93	0.84
1:A:572:ARG:CZ	1:A:639:ASN:CB	2.55	0.83
1:A:468:LEU:HD13	1:A:519:TYR:HH	1.37	0.83
1:A:516:ARG:O	1:A:516:ARG:NE	2.12	0.83
1:A:569:VAL:O	1:A:571:PRO:HD2	1.76	0.83
1:I:159:LEU:HD12	1:I:160:ILE:H	1.43	0.83
1:I:700:LEU:HD11	1:I:750:ILE:CG2	2.09	0.83
1:I:678:MET:HE3	1:I:700:LEU:HD12	1.59	0.83
1:A:572:ARG:NE	1:A:639:ASN:CB	2.42	0.83
2:N:117:ASN:ND2	2:N:119:PHE:HE2	1.77	0.83
1:A:29:VAL:CG1	1:A:211:CYS:N	2.40	0.83
1:A:574:GLN:O	1:A:578:ILE:HG13	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:719:LEU:O	1:E:722:TYR:HB3	1.78	0.82
1:E:233:GLU:CG	1:E:244:LEU:HB3	2.09	0.82
1:A:519:TYR:CZ	1:A:551:VAL:HG21	2.14	0.82
1:I:307:THR:HA	1:I:310:LYS:HE3	1.58	0.82
1:A:521:ARG:HB3	1:A:531:GLU:OE2	1.79	0.82
2:F:292:TRP:CH2	5:F:405:NAG:O5	2.33	0.82
1:A:464:ARG:CZ	1:A:532:TYR:OH	2.26	0.82
1:E:339:LYS:NZ	1:E:343:ASP:CG	2.33	0.82
1:I:160:ILE:CG1	1:I:261:ALA:CB	2.58	0.82
1:M:354:ILE:HG13	1:M:885:ILE:HD13	1.62	0.81
1:M:1031:ALA:HA	1:M:1034:VAL:HG22	1.61	0.81
1:A:572:ARG:CZ	1:A:639:ASN:HB2	2.08	0.81
1:E:720:ILE:HG23	1:E:778:ILE:HB	1.60	0.81
1:E:1009:LEU:HD12	1:E:1078:LEU:HD21	1.62	0.81
1:E:127:ILE:HD12	1:E:128:ILE:H	1.45	0.81
1:E:640:MET:CE	1:E:641:ASN:O	2.29	0.81
1:I:468:LEU:O	1:I:468:LEU:HD13	1.81	0.81
1:A:31:GLU:CG	1:A:209:ILE:HG23	2.11	0.81
1:I:321:GLU:OE1	2:J:303:TYR:O	1.86	0.81
1:M:126:TYR:HE1	1:M:133:ARG:HD3	0.94	0.81
1:E:655:GLN:CD	1:E:658:GLU:HG2	2.02	0.81
1:M:127:ILE:HD12	1:M:147:VAL:CG2	2.10	0.80
1:E:717:GLU:CD	1:E:774:ILE:HD13	1.91	0.80
2:N:292:TRP:HH2	5:N:405:NAG:C4	1.91	0.80
1:E:185:LYS:CE	1:E:245:LEU:HD11	2.10	0.80
1:E:339:LYS:HZ3	1:E:343:ASP:CG	1.83	0.80
1:I:159:LEU:HD21	1:I:259:GLY:N	1.96	0.80
1:E:1009:LEU:CD1	1:E:1078:LEU:CD2	2.55	0.80
1:I:489:LEU:CD1	1:I:509:GLY:O	2.30	0.80
1:I:690:LEU:CD1	1:I:691:PHE:CG	2.64	0.80
1:I:700:LEU:CD2	1:I:750:ILE:HG12	2.12	0.80
1:I:310:LYS:CB	1:I:897:PHE:CB	2.60	0.79
1:E:191:ARG:HB2	1:E:194:ILE:CD1	2.13	0.79
1:E:190:VAL:C	1:E:194:ILE:HD12	2.01	0.79
1:I:143:VAL:HG22	1:I:263:TYR:CD2	2.17	0.79
1:I:703:LYS:HB3	1:I:711:LYS:HD2	1.64	0.79
1:E:158:ASP:OD2	1:E:268:THR:OG1	1.98	0.79
1:E:880:LYS:NZ	1:E:912:ASN:OD1	2.15	0.79
1:I:473:GLU:CA	1:I:475:LYS:NZ	2.45	0.79
1:E:640:MET:HE1	1:E:641:ASN:O	1.82	0.79
2:N:107:ASN:HB3	2:N:292:TRP:CZ3	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLN:NE2	1:A:826:GLU:H	1.81	0.79
1:E:233:GLU:HG2	1:E:244:LEU:CB	2.12	0.79
1:I:321:GLU:CD	2:J:303:TYR:O	2.21	0.78
1:A:519:TYR:HE1	1:A:551:VAL:HG12	1.29	0.78
1:E:339:LYS:NZ	1:E:343:ASP:OD2	2.17	0.78
1:A:756:LEU:CD1	1:A:790:MET:HE1	2.12	0.78
1:E:79:GLN:HB2	1:E:84:THR:HG21	1.65	0.78
1:E:655:GLN:OE1	1:E:658:GLU:HG2	1.83	0.78
2:N:107:ASN:ND2	2:N:292:TRP:CZ3	2.51	0.78
1:E:718:LEU:HD23	1:E:718:LEU:H	1.48	0.78
1:M:47:SER:CB	1:M:843:ARG:CZ	2.62	0.78
1:E:242:GLU:C	1:E:243:ASN:HD22	1.87	0.78
1:A:28:PRO:HD3	1:A:212:GLU:CB	2.13	0.78
1:A:697:LEU:HA	1:A:747:TYR:CD2	2.19	0.78
1:A:723:ARG:NH2	1:A:778:ILE:O	2.16	0.77
1:E:732:LYS:CG	1:E:739:LYS:HZ3	1.83	0.77
1:A:519:TYR:HH	1:A:551:VAL:HG11	1.45	0.77
1:I:880:LYS:HZ3	1:I:1003:LEU:HD21	1.50	0.77
1:M:237:ARG:NH1	1:M:409:BFD:F2	2.08	0.77
1:M:351:PHE:HA	1:M:885:ILE:HD11	1.65	0.77
1:A:176:ALA:HB3	1:A:837:GLU:CD	2.05	0.77
1:A:673:LEU:HD22	1:A:787:CYS:HB2	1.65	0.77
1:A:129:GLU:HB2	1:A:146:VAL:HG22	1.67	0.77
1:I:214:PRO:C	1:I:268:THR:HG22	2.05	0.77
1:I:700:LEU:HD21	1:I:750:ILE:HG12	1.67	0.77
1:A:176:ALA:C	1:A:837:GLU:OE2	2.23	0.76
1:A:176:ALA:CA	1:A:837:GLU:OE2	2.32	0.76
1:A:572:ARG:HD3	1:A:639:ASN:CB	2.14	0.76
1:A:177:SER:CB	1:A:837:GLU:HG3	2.15	0.76
2:F:308:LYS:N	2:F:308:LYS:HD2	2.00	0.76
1:I:489:LEU:HD13	1:I:509:GLY:O	1.84	0.76
1:I:700:LEU:HB3	1:I:752:ASP:HB3	1.68	0.76
2:N:290:ARG:NE	2:N:292:TRP:NE1	2.33	0.76
1:A:28:PRO:HD3	1:A:212:GLU:HA	0.82	0.76
1:A:219:TYR:O	1:A:234:ALA:HA	1.85	0.76
1:A:1045:TRP:HB3	1:A:1051:GLN:HE21	1.50	0.76
1:I:310:LYS:HZ1	1:I:343:ASP:CG	1.88	0.76
1:A:384:GLU:O	1:A:386:ASN:OD1	2.03	0.75
1:A:519:TYR:CD2	1:A:532:TYR:C	2.57	0.75
1:A:660:ILE:HD11	1:A:670:VAL:HG21	1.68	0.75
1:A:657:ALA:O	1:A:661:GLU:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:VAL:O	1:A:529:ILE:O	2.04	0.75
2:F:167:PRO:O	2:F:231:THR:OG1	2.04	0.75
1:I:159:LEU:HD13	1:I:262:VAL:HG23	0.77	0.75
1:I:311:TYR:CE1	1:I:339:LYS:HG2	2.21	0.75
1:I:307:THR:OG1	1:I:347:PHE:CD2	2.37	0.75
2:N:91:CYS:HA	2:N:104:CYS:HB2	1.68	0.75
2:N:290:ARG:NH2	2:N:292:TRP:CZ2	2.55	0.75
1:E:233:GLU:CD	1:E:244:LEU:HB3	2.07	0.75
1:A:673:LEU:HD13	1:A:798:ILE:HD12	1.69	0.74
2:C:75:ILE:HD11	2:C:316:SER:HB3	1.69	0.74
1:A:792:PRO:CB	1:A:819:ASN:O	2.36	0.74
1:I:143:VAL:HG11	1:I:263:TYR:CE2	2.22	0.74
1:I:157:CYS:HB2	1:I:262:VAL:HG12	1.69	0.74
1:I:700:LEU:CD1	1:I:750:ILE:HG12	2.17	0.74
2:C:170:PRO:HD2	2:C:233:PRO:HD3	1.69	0.74
1:E:655:GLN:HB3	1:E:853:LYS:HG3	1.70	0.74
1:A:657:ALA:O	1:A:661:GLU:CB	2.36	0.74
1:A:519:TYR:OH	1:A:551:VAL:CG1	2.31	0.74
1:I:314:GLN:NE2	3:I:1201:P5S:CA	2.51	0.74
2:N:107:ASN:HD22	2:N:292:TRP:HZ3	1.34	0.74
1:E:159:LEU:CD1	1:E:261:ALA:H	2.00	0.74
1:I:688:CYS:SG	1:I:690:LEU:HG	2.27	0.74
1:A:1056:VAL:HG22	2:C:262:ARG:HH22	1.52	0.73
1:A:1072:LEU:HD11	2:C:332:VAL:HG21	1.68	0.73
1:E:717:GLU:OE2	1:E:774:ILE:HG21	1.87	0.73
1:A:512:PHE:HE1	1:A:520:MET:HG3	1.46	0.73
1:A:516:ARG:HE	1:A:516:ARG:C	1.92	0.73
1:E:159:LEU:HD11	1:E:261:ALA:N	2.03	0.73
2:N:292:TRP:HZ3	5:N:405:NAG:O5	1.69	0.73
1:E:246:LEU:CD2	1:E:268:THR:CG2	2.57	0.73
2:J:143:LEU:HD11	2:J:214:PHE:HD1	1.54	0.73
1:A:654:ASP:OD2	1:A:853:LYS:HA	1.88	0.73
2:C:201:LYS:H	2:C:201:LYS:CD	2.01	0.73
2:N:107:ASN:ND2	5:N:405:NAG:C2	2.43	0.73
2:N:290:ARG:NE	2:N:292:TRP:HE1	1.86	0.73
5:F:405:NAG:C7	5:F:405:NAG:H5	2.19	0.72
1:A:28:PRO:HD2	1:A:212:GLU:C	2.07	0.72
1:A:519:TYR:HB2	1:A:533:GLU:C	2.08	0.72
1:I:160:ILE:HG13	1:I:261:ALA:CB	2.18	0.72
1:E:233:GLU:HG2	1:E:244:LEU:HB3	1.70	0.72
1:I:315:SER:HA	1:I:319:ASN:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:405:NAG:H5	5:F:405:NAG:O7	1.89	0.72
1:A:653:GLN:NE2	1:A:836:LYS:HE2	2.03	0.72
1:A:834:LYS:HE2	1:A:839:ARG:NE	2.05	0.72
1:E:233:GLU:OE2	1:E:244:LEU:CA	2.38	0.72
1:A:521:ARG:CB	1:A:531:GLU:OE2	2.38	0.72
1:A:911:TYR:OH	1:A:1004:VAL:HG21	1.90	0.72
1:I:700:LEU:HD21	1:I:751:ILE:N	2.05	0.72
1:I:475:LYS:HD2	1:I:475:LYS:N	2.03	0.71
1:M:179:ASP:O	1:M:237:ARG:NH2	2.23	0.71
1:I:315:SER:HA	1:I:319:ASN:HD22	1.54	0.71
1:M:47:SER:HB3	1:M:843:ARG:NE	2.05	0.71
1:A:574:GLN:HA	1:A:574:GLN:HE21	1.56	0.71
1:E:246:LEU:HD22	1:E:268:THR:CB	2.19	0.71
1:I:703:LYS:CE	1:I:714:ARG:HD3	2.19	0.71
1:A:519:TYR:CZ	1:A:551:VAL:HB	2.24	0.71
1:A:569:VAL:CA	1:A:571:PRO:HD2	2.20	0.71
1:A:790:MET:SD	1:A:794:GLN:C	2.69	0.71
1:E:351:PHE:HA	1:E:885:ILE:HD11	1.73	0.71
1:I:158:ASP:O	1:I:262:VAL:HG13	1.89	0.71
1:M:113:ARG:O	1:M:117:ASP:CG	2.29	0.71
1:A:512:PHE:CD1	1:A:515:ASN:ND2	2.59	0.71
1:A:572:ARG:CD	1:A:639:ASN:CB	2.69	0.71
1:E:732:LYS:HZ3	1:E:739:LYS:CE	1.95	0.71
1:E:992:ASN:HA	2:F:265:ALA:HB2	1.73	0.71
1:A:712:GLU:HG3	1:A:771:TYR:CZ	2.26	0.71
1:I:564:GLY:HA3	1:I:569:VAL:HG21	1.73	0.70
2:N:301:VAL:HG23	2:N:306:GLY:HA3	1.73	0.70
1:A:574:GLN:HG2	1:A:642:LEU:HB2	1.71	0.70
1:A:653:GLN:HE22	1:A:836:LYS:HE2	1.55	0.70
1:E:185:LYS:HE2	1:E:245:LEU:HD11	1.71	0.70
1:I:315:SER:HA	1:I:319:ASN:CB	2.20	0.70
1:A:856:LYS:O	1:A:860:LEU:HB2	1.92	0.70
1:A:572:ARG:HD3	1:A:639:ASN:CA	2.21	0.70
1:A:700:LEU:HD13	1:A:749:LEU:HD12	1.71	0.70
1:E:655:GLN:HG3	1:E:658:GLU:CG	2.19	0.70
1:A:792:PRO:HB3	1:A:819:ASN:O	1.92	0.70
1:E:915:PHE:CZ	1:E:1008:THR:CG2	2.74	0.70
1:I:411:THR:O	7:I:1301:HOH:O	2.10	0.70
1:M:47:SER:HB2	1:M:117:ASP:OD2	1.90	0.70
1:M:962:LEU:O	1:M:966:GLU:HG2	1.92	0.70
1:A:370:GLY:O	1:A:866:TYR:OH	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:ALA:HB2	2:C:325:LEU:HD21	1.73	0.70
1:E:179:ASP:O	1:E:237:ARG:NH2	2.25	0.70
1:E:640:MET:SD	1:E:641:ASN:N	2.65	0.70
1:M:498:GLU:N	1:M:498:GLU:OE1	2.23	0.70
1:A:28:PRO:CD	1:A:213:GLN:N	2.54	0.70
2:C:199:LEU:HD23	2:C:199:LEU:H	1.56	0.70
1:I:128:ILE:HD13	1:I:134:VAL:HG22	1.74	0.70
1:I:700:LEU:HD11	1:I:750:ILE:HG12	1.74	0.70
1:I:750:ILE:HD11	1:I:788:CYS:HB2	1.74	0.70
1:A:904:ASP:HB3	1:A:907:TYR:HB2	1.73	0.69
1:I:316:THR:HB	1:I:317:PRO:CD	2.17	0.69
1:A:833:ILE:HG12	1:A:836:LYS:HG3	1.58	0.69
1:E:185:LYS:HD2	1:E:241:PRO:HB2	1.75	0.69
1:I:310:LYS:HZ2	1:I:311:TYR:HB2	1.55	0.69
1:A:29:VAL:O	1:A:210:GLU:HA	1.93	0.69
1:A:29:VAL:CG2	1:A:31:GLU:OE2	2.36	0.69
1:E:655:GLN:CG	1:E:658:GLU:CG	2.65	0.69
1:I:482:GLY:HA3	1:I:490:THR:CG2	2.10	0.69
1:I:956:PHE:HA	1:I:959:TRP:CD1	2.27	0.69
1:I:167:THR:CB	1:I:473:GLU:O	2.39	0.69
1:I:218:LEU:HD12	1:I:235:VAL:HG13	1.74	0.69
2:J:292:TRP:NE1	5:J:404:NAG:O6	2.18	0.69
1:M:973:GLY:HA3	1:M:1073:LEU:HD21	1.75	0.69
1:A:311:TYR:HA	1:A:315:SER:HB2	1.74	0.69
1:A:657:ALA:O	1:A:661:GLU:CG	2.41	0.69
1:I:314:GLN:HE22	3:I:1201:P5S:HB	1.46	0.69
1:I:316:THR:CB	1:I:317:PRO:HD3	2.16	0.69
1:M:904:ASP:OD1	1:M:1052:ARG:NH1	2.26	0.69
2:N:99:VAL:HG12	2:N:101:PRO:HD2	1.73	0.69
1:A:28:PRO:HD3	1:A:213:GLN:N	2.08	0.69
1:A:792:PRO:O	1:A:823:MET:HE1	1.93	0.69
2:N:188:ILE:CG1	2:N:292:TRP:CD1	2.73	0.69
1:A:409:BFD:OD1	1:A:410:LYS:N	2.26	0.68
1:E:233:GLU:OE2	1:E:244:LEU:CB	2.41	0.68
1:A:519:TYR:CZ	1:A:551:VAL:CG2	2.72	0.68
1:A:884:PHE:HA	1:A:1003:LEU:HD11	1.75	0.68
1:A:410:LYS:HE2	1:A:681:ALA:HA	1.75	0.68
1:E:158:ASP:OD1	1:E:247:LYS:N	2.26	0.68
1:E:67:ILE:HG13	1:E:292:LEU:HD11	1.74	0.68
1:I:700:LEU:HD21	1:I:751:ILE:C	2.13	0.68
1:M:491:TYR:OH	1:M:514:GLY:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:VAL:HG13	1:A:643:ILE:HG13	1.74	0.68
2:C:153:PRO:HG2	2:C:161:ARG:HG2	1.75	0.68
1:I:700:LEU:HD23	1:I:752:ASP:CA	2.22	0.68
1:E:1049:LYS:O	1:E:1051:GLN:NE2	2.25	0.68
1:I:472:VAL:C	1:I:475:LYS:NZ	2.47	0.68
1:A:468:LEU:CD1	1:A:519:TYR:CZ	2.72	0.68
2:C:220:GLY:O	2:C:226:ARG:NH2	2.27	0.68
2:F:66:ILE:HB	2:F:330:ILE:HD11	1.76	0.68
1:M:31:GLU:HB3	1:M:208:ALA:HB1	1.75	0.68
1:M:604:ALA:HB3	1:M:607:ASP:HB2	1.76	0.68
1:M:126:TYR:CD1	1:M:133:ARG:CD	2.68	0.67
1:M:916:THR:O	1:M:920:ILE:HG12	1.93	0.67
1:A:513:LEU:O	1:A:515:ASN:OD1	2.11	0.67
2:F:292:TRP:CZ2	5:F:405:NAG:H61	2.29	0.67
1:I:310:LYS:CD	1:I:311:TYR:N	2.47	0.67
1:E:178:LEU:HD13	1:E:246:LEU:HB2	1.76	0.67
1:M:235:VAL:HG23	1:M:241:PRO:HD3	1.76	0.67
1:I:335:LEU:HD13	1:I:338:LEU:HB2	1.75	0.67
1:A:756:LEU:CD1	1:A:790:MET:CE	2.71	0.67
2:C:204:ILE:HG12	2:C:255:GLU:HB3	1.76	0.67
1:E:185:LYS:CD	1:E:245:LEU:CD1	2.67	0.67
1:I:311:TYR:HE1	1:I:339:LYS:HG2	1.59	0.67
1:M:911:TYR:O	1:M:915:PHE:HD1	1.77	0.67
1:E:113:ARG:NH1	1:E:392:ASN:O	2.28	0.67
1:E:240:GLY:N	1:E:241:PRO:HD3	2.10	0.67
1:A:521:ARG:CB	1:A:531:GLU:CD	2.59	0.67
1:A:572:ARG:CZ	1:A:639:ASN:HB3	2.24	0.67
1:A:31:GLU:O	1:A:208:ALA:CB	2.41	0.66
1:A:171:CYS:SG	1:A:257:ILE:HG12	2.35	0.66
1:A:656:ALA:HB1	1:A:688:CYS:SG	2.34	0.66
1:I:485:GLU:HG3	1:I:488:GLU:CG	2.25	0.66
1:A:211:CYS:HG	1:A:263:TYR:HH	1.41	0.66
1:A:572:ARG:CD	1:A:639:ASN:HB2	2.26	0.66
1:E:718:LEU:HD23	1:E:718:LEU:N	2.09	0.66
2:J:166:LYS:HD3	2:J:231:THR:HG22	1.77	0.66
1:E:127:ILE:HD11	1:E:146:VAL:CG2	2.26	0.66
1:I:307:THR:OG1	1:I:347:PHE:HD2	1.79	0.66
2:C:199:LEU:HD23	2:C:199:LEU:N	2.11	0.66
1:E:915:PHE:HZ	1:E:1008:THR:HG23	1.61	0.66
1:M:983:LEU:HD11	1:M:1066:THR:HG23	1.76	0.66
1:A:29:VAL:HG12	1:A:211:CYS:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:CYS:SG	1:A:254:THR:HG21	2.36	0.66
1:A:572:ARG:NH1	1:A:639:ASN:HB3	2.10	0.66
1:E:718:LEU:H	1:E:718:LEU:CD2	2.08	0.66
2:C:185:LEU:HD11	2:C:312:LEU:HD21	1.78	0.65
1:I:700:LEU:HD12	1:I:700:LEU:N	2.10	0.65
2:J:292:TRP:CG	5:J:404:NAG:O6	2.30	0.65
2:N:188:ILE:CG1	2:N:292:TRP:HD1	2.09	0.65
1:A:218:LEU:CB	1:A:267:GLU:HG3	2.20	0.65
1:A:275:GLN:NE2	1:A:822:SER:O	2.29	0.65
2:N:90:PRO:CG	5:N:405:NAG:C8	2.74	0.65
1:E:732:LYS:HB2	1:E:736:SER:HB3	1.76	0.65
1:I:310:LYS:CB	1:I:897:PHE:CG	2.74	0.65
1:I:678:MET:HE1	1:I:700:LEU:CG	2.27	0.65
1:M:663:LEU:HG	1:M:668:LEU:HD12	1.79	0.65
1:E:821:VAL:HB	1:E:841:ALA:HB1	1.79	0.65
1:E:47:SER:HB2	1:E:117:ASP:CG	2.17	0.65
1:E:159:LEU:O	1:E:244:LEU:CD2	2.25	0.65
1:E:161:LEU:HD13	1:E:257:ILE:HG23	1.79	0.65
1:E:409:BFD:F2	7:E:1302:HOH:O	2.03	0.65
2:F:201:LYS:HA	2:F:274:ARG:HD2	1.77	0.65
2:N:130:ASN:HB3	2:N:265:ALA:CB	2.25	0.65
2:N:188:ILE:CD1	2:N:292:TRP:HD1	1.81	0.65
2:N:290:ARG:NH2	2:N:292:TRP:HZ2	1.93	0.65
1:A:220:LYS:HB2	1:A:220:LYS:HZ2	1.61	0.65
1:E:125:VAL:CG1	1:E:127:ILE:HG22	2.25	0.65
1:E:254:THR:HG22	1:E:255:GLU:H	1.62	0.65
1:A:318:TYR:HA	1:A:321:GLU:HG2	1.79	0.64
2:N:292:TRP:CH2	5:N:405:NAG:O5	2.50	0.64
1:A:519:TYR:HB2	1:A:534:LEU:N	2.12	0.64
1:A:659:THR:HG21	1:A:852:PHE:CZ	2.28	0.64
2:F:170:PRO:HA	2:F:252:PHE:CZ	2.32	0.64
1:I:159:LEU:HB2	1:I:262:VAL:HG22	0.68	0.64
1:E:233:GLU:HG2	1:E:244:LEU:HB2	1.78	0.64
1:I:795:LYS:HB3	1:I:823:MET:HG3	1.79	0.64
1:A:572:ARG:NH2	1:A:639:ASN:HD22	1.95	0.64
1:I:31:GLU:HB3	1:I:208:ALA:HB1	1.79	0.64
1:M:953:LEU:HD12	1:M:954:GLY:H	1.63	0.64
2:N:90:PRO:HG2	5:N:405:NAG:H83	1.79	0.64
1:E:574:GLN:HB3	1:E:640:MET:CE	2.28	0.64
1:I:309:LEU:HD22	1:I:309:LEU:N	2.11	0.64
2:C:124:LEU:HD22	2:C:308:LYS:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:984:GLU:HG2	1:M:1063:SER:HB2	1.79	0.64
1:A:560:LEU:HB2	1:A:603:ILE:HD11	1.79	0.64
1:A:723:ARG:NH1	1:A:777:GLN:O	2.31	0.64
2:C:169:ALA:HB3	2:C:170:PRO:HD3	1.80	0.64
1:E:574:GLN:HB3	1:E:640:MET:HE1	1.80	0.64
2:J:338:LEU:O	2:J:342:VAL:HG23	1.97	0.64
1:I:482:GLY:N	1:I:490:THR:HG22	2.11	0.64
1:A:32:THR:HB	1:A:35:TYR:HD2	1.62	0.64
1:I:29:VAL:HB	1:I:263:TYR:OH	1.97	0.64
1:I:700:LEU:CD2	1:I:752:ASP:N	2.50	0.64
1:A:63:GLN:OE1	1:A:102:THR:OG1	2.17	0.63
2:C:142:GLN:NE2	2:C:171:CYS:SG	2.70	0.63
1:M:202:ILE:HG23	1:M:205:LEU:HD12	1.80	0.63
1:A:29:VAL:HG12	1:A:211:CYS:CA	2.27	0.63
2:C:200:LYS:O	2:C:275:LEU:HD23	1.99	0.63
1:I:171:CYS:SG	1:I:172:TYR:N	2.71	0.63
2:N:107:ASN:CB	2:N:292:TRP:CE3	2.81	0.63
1:A:992:ASN:HB2	2:C:265:ALA:HB2	1.80	0.63
2:C:201:LYS:HD3	2:C:201:LYS:N	2.09	0.63
1:I:306:CYS:O	1:I:310:LYS:HG2	1.97	0.63
1:A:295:TYR:HH	1:A:959:TRP:HH2	1.43	0.63
2:C:80:ILE:O	2:C:80:ILE:HD12	1.99	0.63
1:I:214:PRO:C	1:I:268:THR:CG2	2.66	0.63
1:M:239:LEU:HD21	1:M:496:PRO:HB3	1.79	0.63
1:A:31:GLU:HB3	1:A:209:ILE:H	1.62	0.63
1:A:869:ARG:NH1	1:A:927:GLU:O	2.31	0.63
2:C:174:ILE:H	2:C:174:ILE:HD12	1.64	0.63
1:E:47:SER:CB	1:E:117:ASP:OD2	2.38	0.63
1:I:707:GLU:HB2	1:I:710:ARG:HB2	1.80	0.63
1:I:307:THR:O	1:I:310:LYS:CD	2.46	0.63
1:M:831:ILE:HD11	1:M:849:VAL:HG22	1.81	0.63
1:A:202:ILE:HG23	1:A:205:LEU:HD12	1.81	0.63
1:A:663:LEU:HG	1:A:668:LEU:HD12	1.79	0.63
1:A:993:TRP:CZ3	1:A:1052:ARG:HB2	2.34	0.63
1:E:189:ALA:O	1:E:194:ILE:HG21	1.99	0.63
1:E:892:GLN:HE22	1:E:900:GLN:N	1.97	0.63
2:F:143:LEU:HD22	2:F:252:PHE:CZ	2.33	0.63
1:M:163:SER:HB3	1:M:257:ILE:HA	1.81	0.63
1:E:354:ILE:HG23	1:E:885:ILE:HG21	1.80	0.63
1:I:710:ARG:O	1:I:714:ARG:HB2	1.99	0.63
1:I:218:LEU:HD12	1:I:235:VAL:CG1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:723:ARG:H	1:I:723:ARG:HD2	1.64	0.62
1:M:746:GLU:O	1:M:783:THR:N	2.32	0.62
2:N:107:ASN:CB	2:N:292:TRP:CZ3	2.81	0.62
1:E:233:GLU:CG	1:E:244:LEU:CB	2.75	0.62
1:M:178:LEU:HA	1:M:818:ALA:HB3	1.81	0.62
1:M:992:ASN:CB	2:N:265:ALA:HB2	2.29	0.62
2:N:132:ARG:O	2:N:136:LYS:HB3	1.99	0.62
1:E:233:GLU:CD	1:E:244:LEU:CB	2.67	0.62
1:E:1009:LEU:CD1	1:E:1009:LEU:C	2.67	0.62
1:I:159:LEU:HD22	1:I:262:VAL:HG21	1.81	0.62
1:I:310:LYS:HD2	1:I:310:LYS:C	2.18	0.62
1:M:36:ILE:C	1:M:36:ILE:HD12	2.18	0.62
1:A:524:ASN:N	1:A:530:GLU:OE1	2.32	0.62
1:M:953:LEU:HD12	1:M:954:GLY:N	2.14	0.62
2:F:292:TRP:HH2	5:F:405:NAG:C5	2.11	0.62
1:I:214:PRO:HB3	1:I:268:THR:HG23	0.63	0.62
1:M:47:SER:HB2	1:M:117:ASP:CG	2.19	0.62
1:E:242:GLU:O	1:E:243:ASN:ND2	2.28	0.62
1:E:1051:GLN:HG2	2:F:140:ASP:OD2	2.00	0.62
1:I:158:ASP:O	1:I:262:VAL:CB	2.48	0.62
1:I:940:ARG:HG3	1:I:941:LEU:H	1.65	0.62
1:A:217:ASP:O	1:A:218:LEU:HB3	2.00	0.61
1:E:254:THR:HG22	1:E:255:GLU:N	2.16	0.61
1:A:208:ALA:O	1:A:225:ILE:HG13	2.01	0.61
1:I:170:THR:OG1	1:I:473:GLU:OE2	2.18	0.61
1:M:254:THR:HB	1:M:257:ILE:HD11	1.82	0.61
1:A:351:PHE:HA	1:A:885:ILE:HD11	1.81	0.61
1:A:750:ILE:HD12	1:A:786:LEU:HD13	1.81	0.61
1:E:159:LEU:HG	1:E:260:VAL:H	1.65	0.61
1:A:519:TYR:CE1	1:A:551:VAL:HB	2.35	0.61
1:A:816:ASP:OD2	1:A:837:GLU:CB	2.49	0.61
2:C:107:ASN:ND2	5:C:406:NAG:O5	2.33	0.61
2:J:292:TRP:HH2	5:J:405:NAG:O6	1.77	0.61
2:F:170:PRO:HA	2:F:252:PHE:HZ	1.66	0.61
1:E:409:BFD:HB3	1:E:815:GLY:HA2	1.81	0.61
1:A:28:PRO:HD2	1:A:213:GLN:N	2.15	0.61
2:C:75:ILE:HG23	2:C:314:THR:HG23	1.82	0.61
2:J:169:ALA:HB3	2:J:170:PRO:HD3	1.83	0.61
1:A:519:TYR:OH	1:A:551:VAL:CB	2.49	0.60
1:A:521:ARG:HB2	1:A:529:ILE:HD11	1.83	0.60
2:F:102:CYS:SG	2:F:103:PHE:N	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:ASP:HA	2:F:143:LEU:HG	1.83	0.60
2:J:292:TRP:HD1	5:J:404:NAG:H61	1.58	0.60
1:I:489:LEU:HD22	1:I:509:GLY:C	2.18	0.60
2:C:130:ASN:HB3	2:C:265:ALA:HA	1.84	0.60
1:E:655:GLN:HG3	1:E:655:GLN:O	2.01	0.60
1:E:906:ALA:O	1:E:910:MET:HB3	2.01	0.60
2:N:250:ASN:HD22	2:N:251:GLY:H	1.49	0.60
1:A:523:GLU:HA	1:A:528:GLU:O	2.01	0.60
1:I:310:LYS:NZ	1:I:311:TYR:HB2	2.16	0.60
1:I:473:GLU:C	1:I:475:LYS:NZ	2.55	0.60
1:M:47:SER:CB	1:M:843:ARG:NE	2.64	0.60
1:M:413:THR:N	1:M:816:ASP:OD2	2.33	0.60
1:M:435:THR:H	1:M:440:GLY:HA3	1.66	0.60
1:A:574:GLN:HE21	1:A:574:GLN:CA	2.14	0.60
1:E:904:ASP:OD1	1:E:1052:ARG:NH1	2.34	0.60
1:A:512:PHE:CD2	1:A:515:ASN:ND2	2.70	0.60
1:A:657:ALA:HB1	1:A:661:GLU:HG3	1.84	0.60
1:A:747:TYR:CG	1:A:748:GLY:N	2.69	0.60
1:A:1059:GLN:O	1:A:1062:SER:OG	2.19	0.60
1:E:952:GLN:O	1:E:956:PHE:HE2	1.85	0.60
1:I:466:LEU:HD23	1:I:470:HIS:ND1	2.17	0.60
1:A:879:TYR:HA	1:A:959:TRP:CZ3	2.36	0.60
1:I:473:GLU:C	1:I:475:LYS:HZ2	2.05	0.60
1:E:405:TYR:HE1	1:E:669:LYS:HB2	1.67	0.60
1:M:904:ASP:HB3	1:M:907:TYR:HB2	1.84	0.60
1:A:219:TYR:O	1:A:235:VAL:N	2.35	0.60
1:A:966:GLU:HB3	1:A:970:PHE:CZ	2.36	0.60
1:E:730:PHE:N	1:E:731:PRO:CD	2.64	0.60
1:I:690:LEU:HD12	1:I:690:LEU:C	2.22	0.60
1:M:970:PHE:CD2	1:M:1003:LEU:HD12	2.36	0.60
1:A:529:ILE:HG13	1:A:531:GLU:HG2	1.84	0.59
1:I:157:CYS:HB2	1:I:262:VAL:HG13	1.83	0.59
1:I:179:ASP:O	1:I:237:ARG:NH1	2.36	0.59
1:I:1083:LEU:O	1:I:1087:LEU:HD23	2.01	0.59
1:E:191:ARG:HB2	1:E:194:ILE:HD12	1.84	0.59
1:E:966:GLU:OE1	1:E:1077:SER:HB3	2.01	0.59
5:F:405:NAG:H83	5:F:405:NAG:C1	2.32	0.59
1:M:410:LYS:HD3	1:M:411:THR:HG23	1.84	0.59
1:M:426:ILE:HG22	1:M:430:LYS:HB2	1.83	0.59
1:E:720:ILE:CD1	1:E:778:ILE:HG21	2.32	0.59
1:A:516:ARG:HD3	1:E:202:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:922:ALA:HB1	1:E:1022:ASN:OD1	2.02	0.59
1:I:159:LEU:CD1	1:I:160:ILE:H	2.14	0.59
1:I:159:LEU:HD11	1:I:260:VAL:N	2.17	0.59
1:M:36:ILE:HG23	1:M:36:ILE:O	2.03	0.59
1:M:782:CYS:SG	1:M:783:THR:N	2.76	0.59
1:A:165:CYS:SG	1:A:166:THR:N	2.75	0.59
1:A:284:VAL:HG11	1:A:870:ILE:HD11	1.83	0.59
1:E:851:LYS:HD3	1:E:854:HIS:CG	2.37	0.59
1:I:307:THR:HA	1:I:310:LYS:HE2	1.84	0.59
1:A:1083:LEU:HD21	2:C:339:LEU:HD21	1.82	0.59
1:E:316:THR:HG23	1:E:317:PRO:HD3	1.85	0.59
1:I:310:LYS:HZ1	1:I:343:ASP:CB	2.14	0.59
1:I:700:LEU:CD2	1:I:751:ILE:CA	2.80	0.59
1:A:1053:MET:HB2	1:A:1056:VAL:HG21	1.84	0.59
1:I:235:VAL:HG13	1:I:235:VAL:O	2.02	0.59
2:J:168:ILE:HG22	2:J:170:PRO:HD2	1.85	0.59
1:M:886:LEU:HD23	1:M:967:GLY:HA3	1.83	0.59
1:A:956:PHE:HA	1:A:959:TRP:HD1	1.67	0.59
1:E:562:CYS:SG	1:E:563:LYS:N	2.74	0.59
1:E:655:GLN:OE1	1:E:658:GLU:CG	2.49	0.59
1:I:266:MET:HA	1:I:269:LYS:HZ3	1.68	0.59
1:I:678:MET:HE3	1:I:700:LEU:N	2.08	0.59
1:E:332:ARG:O	1:E:333:GLU:HG2	2.03	0.59
1:I:158:ASP:O	1:I:262:VAL:CG1	2.50	0.59
1:I:1068:LEU:HD13	1:I:1071:ILE:HD11	1.84	0.59
2:C:124:LEU:HD22	2:C:308:LYS:CD	2.33	0.58
1:E:654:ASP:O	1:E:853:LYS:HB2	2.03	0.58
1:E:68:ALA:HB2	1:E:292:LEU:HD22	1.84	0.58
1:E:980:THR:OG1	2:F:322:ASN:HB2	2.03	0.58
1:M:698:LEU:HD12	1:M:715:LEU:HD11	1.85	0.58
1:M:972:PHE:HA	1:M:975:TYR:CE1	2.39	0.58
2:N:107:ASN:HD21	5:N:405:NAG:C2	1.93	0.58
1:A:519:TYR:CD2	1:A:532:TYR:CA	2.66	0.58
1:A:992:ASN:CB	2:C:265:ALA:HB2	2.32	0.58
2:F:253:ILE:O	2:F:253:ILE:HG12	2.04	0.58
1:I:700:LEU:HD11	1:I:750:ILE:C	2.24	0.58
1:A:178:LEU:HD22	1:A:246:LEU:HD22	1.85	0.58
1:A:519:TYR:CG	1:A:533:GLU:C	2.77	0.58
1:A:980:THR:OG1	2:C:322:ASN:HB2	2.03	0.58
1:E:994:THR:HG22	1:E:1056:VAL:HG13	1.86	0.58
1:I:266:MET:HA	1:I:269:LYS:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:ARG:HB3	1:M:39:ARG:HH11	1.69	0.58
1:A:413:THR:C	1:A:653:GLN:NE2	2.54	0.58
1:E:339:LYS:NZ	1:E:343:ASP:CB	2.67	0.58
1:I:310:LYS:HB3	1:I:897:PHE:CB	2.31	0.58
1:I:585:VAL:HA	1:I:588:ASN:OD1	2.04	0.58
2:J:143:LEU:CD1	2:J:214:PHE:HD1	2.15	0.58
1:E:282:SER:HB2	1:E:399:GLU:OE1	2.04	0.58
1:I:160:ILE:HG13	1:I:261:ALA:HB2	1.84	0.58
2:J:292:TRP:CD1	5:J:404:NAG:H62	2.06	0.58
1:A:220:LYS:NZ	1:A:220:LYS:CB	2.66	0.58
1:A:895:CYS:O	1:A:897:PHE:N	2.35	0.58
1:E:574:GLN:CB	1:E:640:MET:HE1	2.33	0.58
2:N:188:ILE:CD1	2:N:292:TRP:HE1	2.12	0.58
1:E:98:VAL:HG22	1:E:361:VAL:HG13	1.85	0.58
2:J:178:MET:HG2	2:J:260:TRP:CD1	2.38	0.58
1:M:235:VAL:HG21	1:M:246:LEU:HD21	1.86	0.58
1:A:29:VAL:HG13	1:A:31:GLU:HG2	1.85	0.58
1:E:171:CYS:HG	1:E:187:HIS:CE1	2.19	0.58
1:E:409:BFD:F3	7:E:1301:HOH:O	2.06	0.58
1:I:160:ILE:HG12	1:I:261:ALA:CB	2.14	0.58
1:I:354:ILE:HG21	1:I:885:ILE:HG21	1.85	0.58
2:N:124:LEU:HD22	2:N:308:LYS:HE3	1.86	0.58
1:A:220:LYS:HB2	1:A:220:LYS:HZ3	1.69	0.57
1:A:994:THR:HG22	1:A:1056:VAL:HG13	1.85	0.57
1:I:295:TYR:HA	1:I:298:ILE:HD12	1.86	0.57
1:I:315:SER:HA	1:I:319:ASN:ND2	2.18	0.57
1:M:935:LEU:HD11	1:M:942:TYR:HB3	1.86	0.57
1:E:630:GLU:HA	1:E:633:PHE:HB3	1.85	0.57
1:I:700:LEU:HD21	1:I:751:ILE:CA	2.34	0.57
1:M:820:ASP:O	1:M:824:ILE:HG12	2.04	0.57
1:A:218:LEU:HD22	1:A:267:GLU:OE1	2.03	0.57
1:A:1081:GLU:O	1:A:1085:ILE:HG12	2.04	0.57
1:E:466:LEU:O	1:E:470:HIS:HB2	2.04	0.57
1:I:690:LEU:HD12	1:I:691:PHE:CB	2.34	0.57
1:A:489:LEU:HG	1:A:489:LEU:O	2.03	0.57
1:E:185:LYS:HE2	1:E:245:LEU:HD21	1.87	0.57
1:E:720:ILE:HD12	1:E:778:ILE:CG2	2.30	0.57
2:F:80:ILE:HD12	2:F:80:ILE:O	2.04	0.57
1:I:403:VAL:HA	1:I:810:ILE:HB	1.85	0.57
1:A:512:PHE:CZ	1:A:520:MET:HG3	2.39	0.57
2:C:99:VAL:HG12	2:C:101:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:309:LEU:HD22	1:I:309:LEU:H	1.68	0.57
1:I:544:ARG:HD2	1:I:546:ARG:NH1	2.20	0.57
1:I:678:MET:HE2	1:I:700:LEU:H	1.65	0.57
2:J:206:TRP:HB3	2:J:209:ASP:OD1	2.04	0.57
1:I:307:THR:HG23	1:I:310:LYS:CE	2.34	0.57
1:I:588:ASN:HD22	1:I:593:TYR:HB2	1.69	0.57
1:M:585:VAL:HG22	1:M:595:THR:HG21	1.86	0.57
1:E:983:LEU:HD21	1:E:990:TYR:CD1	2.39	0.57
2:F:307:ARG:C	2:F:308:LYS:HD2	2.24	0.57
1:I:403:VAL:HG21	1:I:812:LEU:HB2	1.85	0.57
1:I:472:VAL:O	1:I:472:VAL:HG13	2.04	0.57
1:I:690:LEU:HD11	1:I:691:PHE:HD2	1.60	0.57
1:A:519:TYR:HD1	1:A:534:LEU:CA	2.18	0.57
1:E:185:LYS:HE2	1:E:245:LEU:CD1	2.34	0.57
1:E:400:LEU:HB2	1:E:863:GLY:HA2	1.86	0.57
1:M:972:PHE:HA	1:M:975:TYR:CD1	2.39	0.57
1:A:598:VAL:HG22	1:A:643:ILE:HD11	1.86	0.57
2:C:132:ARG:NH1	3:C:401:P5S:O15	2.38	0.57
2:C:235:ASN:HD22	5:C:402:NAG:H61	1.69	0.57
1:M:35:TYR:CD2	1:M:35:TYR:N	2.73	0.57
1:A:171:CYS:HB2	1:A:187:HIS:CE1	2.39	0.57
1:A:421:PHE:HB2	1:A:648:VAL:HG12	1.87	0.57
1:E:574:GLN:CB	1:E:640:MET:CE	2.83	0.57
1:E:974:THR:HG21	1:E:999:VAL:HG12	1.87	0.57
2:F:47:ALA:HB2	2:F:347:ASN:HD22	1.70	0.57
1:I:468:LEU:HD13	1:I:468:LEU:C	2.24	0.57
1:M:380:PHE:HB3	1:M:854:HIS:CG	2.40	0.57
1:A:311:TYR:O	1:A:315:SER:HB2	2.00	0.56
1:M:912:ASN:HA	1:M:915:PHE:CE1	2.40	0.56
1:E:76:PHE:O	1:E:80:VAL:HG13	2.04	0.56
2:J:143:LEU:HD11	2:J:214:PHE:CD1	2.38	0.56
1:M:726:LEU:HD23	1:M:743:GLU:HG2	1.85	0.56
1:A:994:THR:HG22	1:A:1056:VAL:CG1	2.35	0.56
1:M:732:LYS:HD3	1:M:733:SER:H	1.70	0.56
1:A:32:THR:OG1	1:A:35:TYR:HB2	2.06	0.56
1:A:833:ILE:HG13	1:A:850:PRO:HA	1.87	0.56
1:A:870:ILE:HA	1:A:873:LEU:HB3	1.88	0.56
1:E:919:PRO:HB3	1:E:1026:ILE:HG12	1.87	0.56
1:I:489:LEU:CG	1:I:509:GLY:O	2.54	0.56
1:I:750:ILE:HD12	1:I:786:LEU:HD13	1.86	0.56
1:E:992:ASN:OD1	2:F:263:THR:OG1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:147:VAL:HG12	1:M:148:GLU:N	2.20	0.56
1:E:339:LYS:NZ	1:E:343:ASP:HB2	2.21	0.56
1:I:47:SER:OG	1:I:117:ASP:OD1	2.23	0.56
1:I:170:THR:HG21	1:I:473:GLU:HG3	1.87	0.56
1:I:314:GLN:HE22	3:I:1201:P5S:HBA	0.40	0.56
1:I:690:LEU:HD12	1:I:691:PHE:CA	2.35	0.56
1:A:31:GLU:CB	1:A:209:ILE:H	2.18	0.56
1:A:322:PRO:HB3	1:A:324:TYR:CE1	2.40	0.56
1:A:512:PHE:CE1	1:A:520:MET:CG	2.73	0.56
1:I:588:ASN:HA	1:I:591:ASP:HB2	1.87	0.56
1:M:126:TYR:CZ	1:M:133:ARG:CG	2.76	0.56
1:M:266:MET:O	1:M:270:MET:HG2	2.05	0.56
1:M:353:PHE:HA	1:M:356:PRO:HB3	1.88	0.56
1:A:519:TYR:CD1	1:A:533:GLU:C	2.78	0.56
1:I:116:ALA:O	1:I:120:VAL:HG12	2.06	0.56
1:I:915:PHE:CE2	1:I:1004:VAL:HG23	2.41	0.56
1:A:692:GLN:HB3	1:A:695:THR:HG23	1.87	0.55
1:E:353:PHE:HB3	1:E:881:ASN:OD1	2.06	0.55
1:I:966:GLU:HG2	1:I:1077:SER:HB3	1.87	0.55
1:A:524:ASN:H	1:A:530:GLU:CD	2.09	0.55
1:I:700:LEU:HD11	1:I:750:ILE:O	2.06	0.55
1:M:98:VAL:HG21	1:M:357:VAL:HB	1.88	0.55
1:M:724:LYS:HA	1:M:728:HIS:HB2	1.87	0.55
1:A:29:VAL:HG13	1:A:210:GLU:HA	1.87	0.55
1:A:171:CYS:HB2	1:A:187:HIS:HE1	1.71	0.55
1:A:218:LEU:HD22	1:A:267:GLU:CD	2.26	0.55
1:E:942:TYR:CG	1:E:943:MET:N	2.74	0.55
1:E:1072:LEU:HD22	2:F:329:TYR:CD1	2.42	0.55
1:I:592:GLY:HA3	1:I:687:ALA:HB2	1.88	0.55
1:I:700:LEU:HD11	1:I:750:ILE:CB	2.37	0.55
1:E:392:ASN:HB2	1:E:846:ASP:HA	1.87	0.55
2:F:142:GLN:NE2	2:F:169:ALA:O	2.40	0.55
1:A:719:LEU:CD1	1:A:720:ILE:HD12	2.36	0.55
1:M:272:LEU:HG	1:M:792:PRO:HB3	1.88	0.55
1:A:217:ASP:OD1	1:A:218:LEU:N	2.39	0.55
2:F:181:ASP:HB3	2:F:298:ASN:H	1.71	0.55
1:I:309:LEU:H	1:I:309:LEU:CD2	2.19	0.55
1:I:923:TYR:HA	1:I:927:GLU:HB2	1.88	0.55
1:M:1078:LEU:HB3	1:M:1082:ILE:HD13	1.88	0.55
1:A:167:THR:CG2	1:E:196:LEU:HD13	2.37	0.55
1:A:464:ARG:NE	1:A:532:TYR:OH	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ARG:HA	1:A:564:GLY:HA2	1.88	0.55
1:A:959:TRP:CZ3	1:A:963:ALA:HB2	2.42	0.55
1:E:127:ILE:CD1	1:E:146:VAL:HG23	2.34	0.55
1:E:522:VAL:O	1:E:523:GLU:HG3	2.07	0.55
1:I:539:ASN:HD22	1:I:547:MET:HB2	1.72	0.55
1:A:723:ARG:NH1	1:A:778:ILE:HA	2.22	0.55
2:C:181:ASP:N	2:C:181:ASP:OD1	2.40	0.55
1:E:409:BFD:F3	7:E:1302:HOH:O	2.08	0.55
1:E:983:LEU:H	1:E:983:LEU:HD23	1.72	0.55
1:I:33:GLU:HB2	1:I:205:LEU:HA	1.89	0.55
1:I:473:GLU:CA	1:I:475:LYS:HZ3	2.11	0.55
1:M:126:TYR:OH	1:M:133:ARG:CG	2.44	0.55
5:F:405:NAG:C7	5:F:405:NAG:C5	2.85	0.55
1:M:272:LEU:HD22	1:M:822:SER:H	1.72	0.55
2:F:292:TRP:CZ3	5:F:405:NAG:O5	2.60	0.54
1:A:834:LYS:HE3	1:A:839:ARG:NH2	2.23	0.54
1:E:695:THR:O	1:E:695:THR:HG23	2.07	0.54
1:I:150:GLN:HA	1:I:255:GLU:O	2.06	0.54
1:M:594:ARG:O	1:M:648:VAL:HG22	2.08	0.54
1:E:159:LEU:H	1:E:244:LEU:CD2	2.20	0.54
1:E:816:ASP:OD1	7:E:1301:HOH:O	2.18	0.54
2:F:240:VAL:O	2:F:243:LEU:HD22	2.08	0.54
1:I:678:MET:CE	1:I:700:LEU:N	2.59	0.54
1:M:883:CYS:O	1:M:1003:LEU:HD11	2.07	0.54
2:N:290:ARG:NE	2:N:292:TRP:CE2	2.75	0.54
2:C:125:SER:HA	2:C:268:THR:HG22	1.90	0.54
1:M:162:LEU:O	1:M:194:ILE:HG13	2.08	0.54
1:A:515:ASN:OD1	1:A:515:ASN:N	2.39	0.54
1:E:860:LEU:HD11	1:E:939:PRO:HB3	1.89	0.54
1:I:407:PHE:CE2	1:I:799:VAL:HG22	2.42	0.54
1:A:1055:PHE:CB	2:C:208:THR:HG21	2.37	0.54
2:C:83:THR:HG21	2:C:307:ARG:HD2	1.89	0.54
1:A:176:ALA:O	1:A:837:GLU:HG2	2.07	0.54
1:A:522:VAL:O	1:A:530:GLU:HB2	2.08	0.54
1:I:318:TYR:OH	2:J:128:TYR:CZ	2.27	0.54
1:M:149:VAL:HB	1:M:258:TYR:HE2	1.73	0.54
1:A:29:VAL:HG22	1:A:31:GLU:HG2	1.88	0.54
1:A:225:ILE:O	1:A:225:ILE:HG12	2.06	0.54
1:E:813:SER:OG	1:E:824:ILE:HA	2.08	0.54
1:E:983:LEU:HD12	1:E:1066:THR:HG23	1.89	0.54
1:I:337:VAL:HG23	1:I:338:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:90:PRO:CD	5:N:405:NAG:H83	2.36	0.54
2:N:107:ASN:ND2	2:N:292:TRP:CH2	2.74	0.54
1:A:67:ILE:HB	1:A:292:LEU:HD23	1.89	0.54
1:A:653:GLN:NE2	1:A:836:LYS:CE	2.71	0.54
1:E:162:LEU:C	1:E:194:ILE:HG23	2.23	0.54
1:I:161:LEU:HD11	1:I:187:HIS:CD2	2.43	0.54
1:I:474:ILE:N	1:I:475:LYS:HZ2	2.05	0.54
2:J:301:VAL:HG11	2:J:308:LYS:HE2	1.90	0.54
1:A:40:PHE:HB3	1:A:143:VAL:HG21	1.90	0.54
1:A:831:ILE:HD13	1:A:847:TYR:HB2	1.89	0.54
1:I:311:TYR:CE2	1:I:336:LYS:HG3	2.43	0.54
1:M:716:HIS:HA	1:M:719:LEU:HD22	1.89	0.54
1:A:29:VAL:N	1:A:211:CYS:H	1.97	0.53
1:A:218:LEU:HD21	1:A:246:LEU:HD23	1.90	0.53
1:E:367:LYS:O	1:E:397:ASN:ND2	2.41	0.53
1:E:926:LEU:HD11	1:E:1019:THR:HG21	1.90	0.53
1:E:1012:ALA:O	1:E:1015:THR:HG22	2.08	0.53
1:E:1045:TRP:HB2	1:E:1046:PRO:HD3	1.89	0.53
2:J:142:GLN:HA	2:J:149:ALA:HB1	1.89	0.53
1:M:714:ARG:O	1:M:717:GLU:HG3	2.08	0.53
1:A:519:TYR:CD1	1:A:534:LEU:CA	2.91	0.53
1:E:294:VAL:O	1:E:298:ILE:HG12	2.09	0.53
1:E:353:PHE:HB2	1:E:885:ILE:HD12	1.90	0.53
1:E:907:TYR:HH	1:E:1033:TYR:HE1	1.56	0.53
1:E:254:THR:HG21	1:E:257:ILE:CD1	2.38	0.53
1:E:869:ARG:HD3	1:E:924:SER:O	2.09	0.53
2:J:222:ASN:HD21	2:J:225:GLU:HB3	1.73	0.53
1:M:422:ILE:O	1:M:507:ARG:NH1	2.41	0.53
1:M:796:ALA:HB2	1:M:823:MET:SD	2.48	0.53
2:N:204:ILE:HG23	2:N:275:LEU:HD22	1.89	0.53
2:C:46:THR:H	2:C:49:THR:HG22	1.73	0.53
1:E:192:ASP:N	1:E:192:ASP:OD1	2.40	0.53
1:E:233:GLU:OE1	1:E:244:LEU:N	2.40	0.53
1:E:673:LEU:HD12	1:E:795:LYS:HE2	1.88	0.53
1:E:915:PHE:HD1	1:E:1029:SER:HB3	1.72	0.53
2:F:128:TYR:CE1	2:F:267:PRO:HB3	2.44	0.53
1:I:873:LEU:HD13	1:I:920:ILE:HG21	1.90	0.53
1:E:354:ILE:O	1:E:356:PRO:HD3	2.09	0.53
2:F:81:ASP:HA	2:F:309:ARG:HB3	1.91	0.53
1:I:144:GLY:N	1:I:263:TYR:CE1	2.76	0.53
1:I:856:LYS:O	1:I:860:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ILE:HA	1:A:777:GLN:HB2	1.90	0.53
1:E:864:HIS:CG	1:E:942:TYR:CE1	2.96	0.53
2:J:124:LEU:HD22	2:J:308:LYS:HE3	1.91	0.53
1:M:725:LYS:HE2	1:M:732:LYS:HG2	1.90	0.53
2:N:290:ARG:HH21	2:N:292:TRP:HE1	1.56	0.53
1:A:410:LYS:CE	1:A:681:ALA:HA	2.37	0.53
1:A:573:VAL:O	1:A:578:ILE:HD11	2.09	0.53
1:E:173:VAL:HG23	1:E:250:THR:O	2.09	0.53
1:E:244:LEU:HD13	1:E:244:LEU:C	2.28	0.53
1:E:752:ASP:OD1	1:E:755:THR:OG1	2.19	0.53
1:E:992:ASN:N	2:F:263:THR:O	2.42	0.53
2:F:285:THR:HG22	2:F:286:LEU:HD12	1.90	0.53
1:M:147:VAL:HG12	1:M:148:GLU:H	1.74	0.53
1:A:177:SER:HA	1:A:837:GLU:HG2	1.89	0.53
1:A:723:ARG:NH1	1:A:781:LYS:HB3	2.23	0.53
1:I:314:GLN:CD	3:I:1201:P5S:CB	2.71	0.53
1:I:544:ARG:NH2	1:I:569:VAL:HG13	2.24	0.53
1:M:472:VAL:HG21	1:M:491:TYR:CE1	2.43	0.53
2:N:168:ILE:HG22	2:N:170:PRO:HD2	1.90	0.53
1:A:374:ILE:HD11	1:A:391:VAL:HG23	1.91	0.53
1:A:514:GLY:C	1:A:515:ASN:OD1	2.47	0.53
1:A:569:VAL:CA	1:A:571:PRO:CD	2.85	0.53
1:A:938:ASP:OD1	1:A:940:ARG:HG3	2.09	0.53
2:F:51:LEU:HD21	2:F:344:LEU:HD12	1.91	0.53
1:M:117:ASP:OD1	1:M:117:ASP:N	2.41	0.53
1:M:147:VAL:HB	1:M:258:TYR:CD1	2.43	0.53
1:A:237:ARG:NE	1:A:789:ARG:HA	2.24	0.53
1:E:128:ILE:HD12	1:E:134:VAL:HG22	1.90	0.53
1:E:242:GLU:C	1:E:243:ASN:ND2	2.60	0.53
1:E:893:PHE:HA	1:E:897:PHE:HE1	1.74	0.53
1:E:939:PRO:O	1:E:943:MET:N	2.39	0.53
1:E:1073:LEU:O	1:E:1077:SER:OG	2.22	0.53
2:F:121:TYR:HD1	2:F:272:LEU:HA	1.73	0.53
1:I:292:LEU:HD11	1:I:355:ILE:HG23	1.90	0.53
1:I:911:TYR:CG	1:I:912:ASN:N	2.77	0.53
1:M:218:LEU:HD22	1:M:271:ALA:HB1	1.90	0.53
1:E:668:LEU:HD23	1:E:668:LEU:H	1.74	0.52
1:I:102:THR:HG22	1:I:364:GLU:HG3	1.90	0.52
1:I:703:LYS:HB3	1:I:711:LYS:CD	2.37	0.52
2:J:292:TRP:CH2	5:J:405:NAG:HO6	1.66	0.52
1:A:218:LEU:HG	1:A:218:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:PHE:HA	2:C:38:LEU:HD11	1.90	0.52
1:A:310:LYS:CE	1:A:897:PHE:HB2	2.21	0.52
1:A:966:GLU:HG2	1:A:1006:THR:HG21	1.90	0.52
1:E:393:THR:OG1	1:E:846:ASP:HB3	2.09	0.52
1:I:410:LYS:HD3	1:I:411:THR:HG23	1.92	0.52
1:I:700:LEU:CD1	1:I:750:ILE:CG2	2.76	0.52
1:M:539:ASN:ND2	1:M:546:ARG:O	2.43	0.52
1:A:295:TYR:OH	1:A:959:TRP:HH2	1.92	0.52
1:A:1051:GLN:OE1	1:A:1051:GLN:N	2.42	0.52
2:F:117:ASN:OD1	2:F:117:ASN:N	2.43	0.52
2:F:292:TRP:CE3	5:F:404:NAG:C6	2.92	0.52
1:I:75:ILE:HG12	1:I:352:ASN:HD21	1.74	0.52
1:I:743:GLU:OE2	1:I:781:LYS:NZ	2.42	0.52
2:N:90:PRO:HG2	5:N:405:NAG:C8	2.38	0.52
1:A:519:TYR:CB	1:A:533:GLU:C	2.75	0.52
1:A:29:VAL:CG1	1:A:211:CYS:H	2.12	0.52
1:A:512:PHE:HE1	1:A:520:MET:CB	2.22	0.52
1:A:574:GLN:CA	1:A:574:GLN:NE2	2.73	0.52
1:E:196:LEU:HD11	1:E:199:ALA:CB	2.39	0.52
1:I:35:TYR:HD1	1:I:38:GLN:HE22	1.57	0.52
1:M:39:ARG:CB	1:M:39:ARG:NH1	2.73	0.52
1:M:287:SER:HB2	1:M:951:LEU:HD13	1.91	0.52
2:N:68:ILE:HD12	2:N:325:LEU:HG	1.92	0.52
1:A:723:ARG:CZ	1:A:778:ILE:HA	2.40	0.52
1:A:884:PHE:HA	1:A:1003:LEU:CD1	2.40	0.52
1:A:888:GLN:O	1:A:892:GLN:NE2	2.42	0.52
1:E:736:SER:CB	1:E:739:LYS:HZ1	2.20	0.52
2:F:150:LEU:HD22	2:F:217:PRO:HG2	1.92	0.52
2:F:179:PHE:HA	2:F:299:TYR:CE2	2.45	0.52
1:I:354:ILE:O	1:I:356:PRO:HD3	2.10	0.52
1:A:209:ILE:HD12	1:A:224:ARG:O	2.10	0.52
1:A:592:GLY:HA3	1:A:687:ALA:HB2	1.91	0.52
1:E:382:ASP:OD2	1:E:386:ASN:ND2	2.42	0.52
1:I:164:SER:HB2	1:I:169:GLY:HA2	1.92	0.52
1:I:678:MET:SD	1:I:750:ILE:HD13	2.50	0.52
1:I:700:LEU:HD11	1:I:750:ILE:CG1	2.38	0.52
2:J:143:LEU:HD22	2:J:252:PHE:CD2	2.45	0.52
1:A:105:LYS:HE3	1:A:368:PHE:CG	2.45	0.52
1:A:510:PHE:HA	1:A:523:GLU:O	2.10	0.52
1:E:720:ILE:CG2	1:E:778:ILE:HB	2.38	0.52
1:I:485:GLU:CD	1:I:488:GLU:OE2	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:722:TYR:HA	1:M:725:LYS:HZ3	1.73	0.52
2:N:188:ILE:HD13	2:N:292:TRP:NE1	2.18	0.52
1:A:919:PRO:HB3	1:A:1026:ILE:HG12	1.91	0.52
1:E:277:LYS:HE3	1:E:279:GLN:HB2	1.91	0.52
2:F:64:ILE:O	2:F:68:ILE:HG12	2.10	0.52
1:I:270:MET:O	1:I:273:ASN:ND2	2.43	0.52
1:M:884:PHE:HA	1:M:1003:LEU:HD21	1.92	0.52
1:A:266:MET:O	1:A:270:MET:HG2	2.09	0.51
1:A:327:LYS:HG2	1:A:331:GLU:HA	1.91	0.51
1:A:512:PHE:HA	1:A:522:VAL:HG12	1.92	0.51
1:E:835:GLY:H	1:E:839:ARG:HD2	1.75	0.51
1:E:915:PHE:CD1	1:E:1029:SER:HB3	2.45	0.51
1:I:690:LEU:HD13	1:I:691:PHE:CD2	2.44	0.51
1:I:715:LEU:O	1:I:719:LEU:HB2	2.11	0.51
2:J:51:LEU:HD21	2:J:344:LEU:HD12	1.91	0.51
1:A:324:TYR:HE2	2:C:127:PHE:CZ	2.27	0.51
1:A:816:ASP:OD2	1:A:837:GLU:HB2	2.10	0.51
1:E:185:LYS:HG3	1:E:241:PRO:HD2	1.92	0.51
1:E:796:ALA:HB2	1:E:823:MET:HE3	1.91	0.51
2:F:159:PRO:HG2	2:F:173:ALA:HB2	1.92	0.51
1:I:284:VAL:O	1:I:288:ILE:HG13	2.10	0.51
1:I:310:LYS:HE2	1:I:347:PHE:HE2	1.75	0.51
1:A:860:LEU:HD21	1:A:939:PRO:HB3	1.92	0.51
1:E:158:ASP:CG	1:E:246:LEU:HA	2.31	0.51
1:E:688:CYS:SG	1:E:690:LEU:HD23	2.50	0.51
1:E:820:ASP:O	1:E:824:ILE:HG12	2.10	0.51
1:I:214:PRO:HA	1:I:268:THR:CG2	2.16	0.51
1:I:690:LEU:HD12	1:I:691:PHE:CG	2.46	0.51
1:I:700:LEU:CD1	1:I:700:LEU:N	2.73	0.51
2:N:250:ASN:HD22	2:N:251:GLY:N	2.08	0.51
1:A:177:SER:N	1:A:837:GLU:OE2	2.43	0.51
2:C:162:ARG:HG2	2:C:167:PRO:HA	1.93	0.51
1:E:533:GLU:HG3	1:E:552:LYS:HG2	1.91	0.51
1:E:932:ILE:HD11	2:F:36:GLN:HG2	1.93	0.51
1:I:100:THR:O	1:I:104:ILE:N	2.43	0.51
1:I:382:ASP:OD2	1:I:386:ASN:ND2	2.44	0.51
1:I:1041:GLY:HA2	1:I:1054:TYR:HB3	1.92	0.51
1:E:570:PHE:HB3	1:E:571:PRO:HD3	1.92	0.51
1:E:812:LEU:HA	1:E:829:VAL:HG12	1.91	0.51
1:E:179:ASP:N	1:E:179:ASP:OD1	2.41	0.51
2:F:179:PHE:HA	2:F:299:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:ARG:HB3	1:M:39:ARG:NH1	2.25	0.51
1:M:45:ILE:HD12	1:M:843:ARG:HH12	1.75	0.51
1:A:837:GLU:OE1	1:A:837:GLU:HA	2.10	0.51
1:A:880:LYS:NZ	1:A:912:ASN:OD1	2.41	0.51
2:C:301:VAL:HG12	2:C:304:PHE:CZ	2.45	0.51
1:E:159:LEU:HD12	1:E:260:VAL:HB	1.93	0.51
1:E:225:ILE:HG23	1:E:227:ILE:HG12	1.92	0.51
1:E:324:TYR:CE1	2:F:127:PHE:CZ	2.99	0.51
1:E:678:MET:N	1:E:788:CYS:SG	2.84	0.51
1:E:812:LEU:HG	1:E:829:VAL:HG11	1.92	0.51
2:F:199:LEU:HB2	2:F:274:ARG:HG2	1.91	0.51
1:A:354:ILE:HG12	1:A:885:ILE:HG21	1.93	0.51
1:A:657:ALA:HA	1:A:661:GLU:HG2	1.92	0.51
1:A:876:TYR:CE2	1:A:1011:LEU:HB2	2.46	0.51
1:E:875:GLN:HG3	1:E:955:PRO:HG3	1.91	0.51
1:E:1045:TRP:CE3	1:E:1051:GLN:HA	2.46	0.51
1:I:221:PHE:O	1:I:232:LEU:HA	2.10	0.51
1:I:310:LYS:HD2	1:I:311:TYR:CA	2.38	0.51
1:I:700:LEU:CD1	1:I:700:LEU:H	2.24	0.51
1:I:856:LYS:O	1:I:860:LEU:CB	2.58	0.51
1:M:472:VAL:HG21	1:M:491:TYR:CD1	2.46	0.51
1:E:191:ARG:HB2	1:E:194:ILE:HD11	1.92	0.51
2:F:233:PRO:HG2	2:F:236:TRP:CD1	2.45	0.51
1:I:473:GLU:CA	1:I:475:LYS:HZ2	2.22	0.51
1:A:412:GLY:HA3	1:A:816:ASP:CG	2.31	0.51
1:A:700:LEU:O	1:A:755:THR:OG1	2.27	0.51
1:E:601:LYS:HB2	1:E:641:ASN:HA	1.92	0.51
1:E:993:TRP:CZ3	1:E:1052:ARG:HB3	2.46	0.51
1:I:485:GLU:HG3	1:I:488:GLU:OE2	2.10	0.51
1:M:574:GLN:NE2	1:M:641:ASN:O	2.41	0.51
1:M:749:LEU:H	1:M:749:LEU:HD23	1.75	0.51
1:M:992:ASN:HB2	2:N:265:ALA:HB2	1.92	0.51
1:A:453:LYS:HG3	1:A:454:VAL:N	2.26	0.50
1:A:519:TYR:CD1	1:A:534:LEU:N	2.79	0.50
1:E:175:THR:O	1:E:175:THR:OG1	2.29	0.50
1:M:725:LYS:HE2	1:M:732:LYS:CG	2.41	0.50
1:M:958:TYR:O	1:M:962:LEU:HB2	2.11	0.50
1:M:1032:PHE:O	1:M:1036:PHE:HB3	2.10	0.50
1:A:316:THR:HG1	1:A:317:PRO:HD3	1.74	0.50
1:A:496:PRO:HA	1:A:499:ILE:HB	1.93	0.50
1:E:730:PHE:N	1:E:731:PRO:HD3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:746:GLU:HB3	1:E:783:THR:HG1	1.76	0.50
1:E:1055:PHE:CD2	2:F:208:THR:HG21	2.46	0.50
2:F:292:TRP:HH2	5:F:405:NAG:O6	1.93	0.50
1:I:671:TRP:CG	1:I:785:VAL:HG22	2.45	0.50
1:A:886:LEU:HD23	1:A:967:GLY:HA3	1.93	0.50
2:C:77:GLU:HB2	2:C:313:SER:HB3	1.93	0.50
1:I:318:TYR:CE1	2:J:128:TYR:CD2	2.98	0.50
1:I:880:LYS:HE3	1:I:911:TYR:HE2	1.76	0.50
2:J:79:GLU:HB3	2:J:311:ILE:HG23	1.93	0.50
1:A:66:ARG:HD3	1:A:360:TYR:CZ	2.46	0.50
1:A:834:LYS:HB2	1:A:839:ARG:HG3	1.93	0.50
1:E:51:THR:HG23	1:E:53:TRP:H	1.76	0.50
1:E:178:LEU:HD13	1:E:246:LEU:CB	2.42	0.50
1:E:413:THR:HG22	1:E:833:ILE:HG21	1.93	0.50
1:E:579:GLU:HA	1:E:582:LYS:HE3	1.93	0.50
1:I:464:ARG:HD3	1:I:561:PHE:HB2	1.94	0.50
1:I:678:MET:CE	1:I:700:LEU:HB2	2.41	0.50
1:M:237:ARG:NH1	1:M:409:BFD:F3	2.30	0.50
2:N:90:PRO:HG3	5:N:405:NAG:C8	2.41	0.50
1:A:412:GLY:O	1:A:836:LYS:CB	2.44	0.50
1:A:489:LEU:CD1	1:A:503:LYS:HZ3	2.13	0.50
2:C:233:PRO:HG2	2:C:236:TRP:HB2	1.94	0.50
1:E:983:LEU:HD21	1:E:990:TYR:CG	2.45	0.50
2:F:30:ASN:OD1	2:F:35:GLN:HG3	2.12	0.50
2:F:292:TRP:CD2	5:F:404:NAG:O6	2.59	0.50
1:M:824:ILE:O	1:M:827:SER:OG	2.24	0.50
1:A:484:THR:CG2	1:A:487:ALA:O	2.59	0.50
1:A:519:TYR:HD1	1:A:534:LEU:HB2	1.75	0.50
1:A:904:ASP:OD2	1:A:1052:ARG:HD2	2.12	0.50
2:C:185:LEU:CD1	2:C:312:LEU:HD21	2.41	0.50
1:I:869:ARG:NH1	1:I:927:GLU:O	2.45	0.50
1:E:406:VAL:HG13	1:E:670:VAL:HA	1.93	0.50
1:E:1054:TYR:HE2	2:F:208:THR:HB	1.76	0.50
2:F:53:ILE:O	2:F:57:ILE:HG12	2.12	0.50
2:F:292:TRP:CH2	5:F:405:NAG:C5	2.93	0.50
1:I:143:VAL:CG2	1:I:263:TYR:CD2	2.93	0.50
1:I:247:LYS:HD3	1:I:269:LYS:HE3	1.94	0.50
1:I:546:ARG:HD2	1:I:630:GLU:HB2	1.94	0.50
1:I:700:LEU:H	1:I:700:LEU:HD12	1.77	0.50
1:M:47:SER:HB3	1:M:843:ARG:CD	2.41	0.50
2:N:58:GLY:HA3	2:N:337:PHE:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:ILE:O	1:A:1086:VAL:HG23	2.11	0.50
1:E:158:ASP:HB2	1:E:264:THR:O	2.11	0.50
1:I:700:LEU:HD21	1:I:750:ILE:CG1	2.39	0.50
1:M:1022:ASN:HA	1:M:1025:VAL:HG22	1.92	0.50
1:A:305:VAL:O	1:A:309:LEU:HB2	2.12	0.50
1:A:398:GLU:HA	1:A:866:TYR:HB3	1.93	0.50
1:A:480:VAL:HG23	1:I:486:SER:HB3	1.93	0.50
1:E:171:CYS:HB2	1:E:254:THR:OG1	2.11	0.50
1:E:685:CYS:HB3	1:E:691:PHE:HD2	1.76	0.50
2:F:232:LYS:HB3	2:F:239:PRO:HG3	1.94	0.50
1:I:42:ASP:OD1	1:I:43:ASN:N	2.45	0.50
1:I:730:PHE:O	1:I:732:LYS:N	2.45	0.50
1:M:105:LYS:HG3	1:M:368:PHE:CE2	2.47	0.50
1:A:299:LEU:HD21	1:A:348:MET:HG2	1.92	0.49
1:A:397:ASN:ND2	1:A:847:TYR:OH	2.44	0.49
1:A:790:MET:HE3	1:A:798:ILE:HD11	1.93	0.49
1:A:904:ASP:HB3	1:A:907:TYR:CB	2.41	0.49
3:C:401:P5S:H42A	3:C:401:P5S:C17	2.42	0.49
1:E:159:LEU:N	1:E:244:LEU:CD2	2.75	0.49
1:E:609:GLU:O	1:E:612:ASN:ND2	2.42	0.49
1:E:1015:THR:HG23	1:E:1016:ARG:N	2.27	0.49
2:F:131:HIS:CD2	2:F:133:ARG:HG2	2.46	0.49
2:F:222:ASN:OD1	2:F:222:ASN:N	2.45	0.49
1:I:354:ILE:HA	1:I:881:ASN:HB3	1.93	0.49
1:M:182:SER:HA	1:M:417:ASN:HD21	1.76	0.49
1:M:843:ARG:HD2	1:M:843:ARG:C	2.33	0.49
1:M:966:GLU:OE1	1:M:1077:SER:OG	2.25	0.49
2:N:188:ILE:HD11	2:N:292:TRP:CD1	2.26	0.49
1:A:149:VAL:HG22	1:A:251:LEU:HD22	1.94	0.49
1:A:348:MET:O	1:A:352:ASN:N	2.44	0.49
1:A:724:LYS:H	1:A:724:LYS:HD2	1.78	0.49
1:I:162:LEU:C	1:I:194:ILE:HG23	2.33	0.49
1:M:127:ILE:HB	1:M:147:VAL:HG13	1.94	0.49
1:M:1052:ARG:H	1:M:1052:ARG:HE	1.58	0.49
1:A:480:VAL:HG23	1:I:486:SER:CA	2.43	0.49
1:A:851:LYS:HG3	1:A:854:HIS:HB2	1.94	0.49
1:A:856:LYS:O	1:A:860:LEU:CB	2.60	0.49
1:E:285:GLU:O	1:E:288:ILE:HG22	2.12	0.49
1:E:339:LYS:HZ1	1:E:343:ASP:HB2	1.77	0.49
1:I:723:ARG:HH21	1:I:778:ILE:CD1	2.24	0.49
1:M:38:GLN:HG3	1:M:142:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:994:THR:HG22	1:M:1056:VAL:HG22	1.95	0.49
1:A:574:GLN:HG2	1:A:642:LEU:CB	2.42	0.49
1:A:880:LYS:HD3	1:A:1007:VAL:HG11	1.93	0.49
1:E:51:THR:HG22	1:E:54:ASN:OD1	2.13	0.49
1:E:139:GLU:OE1	1:E:139:GLU:N	2.45	0.49
1:E:865:LEU:O	1:E:869:ARG:HG3	2.12	0.49
1:E:1023:HIS:O	1:E:1027:TRP:HB2	2.12	0.49
2:F:135:VAL:HG22	2:F:263:THR:HG21	1.94	0.49
1:I:171:CYS:HB2	1:I:254:THR:HG21	1.94	0.49
1:I:309:LEU:N	1:I:309:LEU:CD2	2.75	0.49
1:I:703:LYS:HE3	1:I:714:ARG:CD	2.32	0.49
1:I:723:ARG:HH21	1:I:778:ILE:HD13	1.77	0.49
1:I:1022:ASN:HA	1:I:1025:VAL:HG22	1.95	0.49
1:M:872:HIS:HB3	1:M:923:TYR:OH	2.12	0.49
1:A:237:ARG:NH1	1:A:789:ARG:H	2.09	0.49
1:A:484:THR:HG21	1:A:487:ALA:O	2.11	0.49
1:A:911:TYR:OH	1:A:1033:TYR:HB2	2.12	0.49
1:I:678:MET:CE	1:I:700:LEU:CB	2.90	0.49
1:M:859:LEU:C	1:M:859:LEU:HD12	2.33	0.49
1:A:291:PHE:CZ	1:A:956:PHE:HD2	2.30	0.49
1:A:353:PHE:HB2	1:A:885:ILE:HD12	1.94	0.49
1:A:519:TYR:HH	1:A:551:VAL:CG1	2.16	0.49
1:E:402:GLN:O	1:E:810:ILE:HD13	2.13	0.49
1:I:117:ASP:O	1:I:120:VAL:CG1	2.61	0.49
1:I:314:GLN:NE2	3:I:1201:P5S:HB	2.08	0.49
1:A:555:GLU:OE1	1:A:555:GLU:N	2.46	0.49
1:A:1079:PHE:CZ	2:C:339:LEU:HD22	2.47	0.49
2:C:266:LEU:HD22	2:C:267:PRO:HD2	1.95	0.49
1:E:948:ASN:O	1:E:950:MET:HG3	2.12	0.49
1:A:31:GLU:CD	1:A:209:ILE:HG23	2.32	0.49
1:A:480:VAL:HG23	1:I:486:SER:HA	1.95	0.49
1:A:489:LEU:HD12	1:A:491:TYR:OH	2.13	0.49
1:A:519:TYR:CD1	1:A:534:LEU:HA	2.47	0.49
1:A:572:ARG:HD3	1:A:639:ASN:HB3	1.94	0.49
1:A:912:ASN:O	1:A:916:THR:OG1	2.24	0.49
1:E:387:GLU:OE1	1:E:839:ARG:NH2	2.38	0.49
2:F:170:PRO:HD2	2:F:233:PRO:HG3	1.95	0.49
1:I:117:ASP:O	1:I:120:VAL:HG13	2.12	0.49
1:I:310:LYS:O	1:I:314:GLN:HB2	2.12	0.49
1:I:475:LYS:N	1:I:475:LYS:CD	2.73	0.49
1:I:1019:THR:HG23	1:I:1022:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:294:VAL:HG21	1:M:959:TRP:HH2	1.78	0.49
1:E:360:TYR:HA	1:E:363:VAL:HG12	1.94	0.49
1:E:868:VAL:HG11	1:E:929:HIS:CD2	2.48	0.49
1:E:911:TYR:HE2	1:E:1004:VAL:HG21	1.76	0.49
2:F:231:THR:OG1	2:F:232:LYS:N	2.45	0.49
2:F:339:LEU:O	2:F:343:LEU:HB2	2.13	0.49
1:I:159:LEU:O	1:I:245:LEU:N	2.22	0.49
1:I:406:VAL:HG23	1:I:812:LEU:HD22	1.94	0.49
1:I:649:GLU:N	1:I:649:GLU:OE1	2.46	0.49
1:M:415:THR:HA	1:M:653:GLN:HB2	1.94	0.49
1:M:430:LYS:O	1:M:430:LYS:HD3	2.13	0.49
1:M:719:LEU:HD23	1:M:778:ILE:HG12	1.93	0.49
1:M:992:ASN:HB3	2:N:265:ALA:HB2	1.93	0.49
1:I:307:THR:CA	1:I:310:LYS:CE	2.71	0.49
1:I:942:TYR:CG	1:I:943:MET:N	2.80	0.49
2:J:292:TRP:HZ3	5:J:405:NAG:HO6	0.50	0.49
1:M:671:TRP:CD2	1:M:785:VAL:HG22	2.48	0.49
2:N:290:ARG:NH2	2:N:292:TRP:HE1	2.11	0.49
1:A:63:GLN:OE1	1:A:99:ILE:HA	2.13	0.48
1:A:220:LYS:CB	1:A:220:LYS:HZ3	2.26	0.48
1:A:956:PHE:HA	1:A:959:TRP:CD1	2.47	0.48
1:E:465:ALA:HA	1:E:501:LEU:HD12	1.95	0.48
1:M:277:LYS:HB2	1:M:825:LEU:HB3	1.95	0.48
1:A:225:ILE:O	1:A:225:ILE:HG23	2.13	0.48
1:A:795:LYS:HD3	1:A:823:MET:HG3	1.95	0.48
1:A:824:ILE:HG12	1:A:845:SER:HA	1.95	0.48
1:A:834:LYS:HE2	1:A:839:ARG:HE	1.76	0.48
1:A:456:LYS:HD2	1:A:456:LYS:O	2.13	0.48
1:A:520:MET:N	1:A:520:MET:SD	2.86	0.48
2:C:273:TYR:O	2:C:274:ARG:HD3	2.13	0.48
1:E:594:ARG:HB2	1:E:648:VAL:CG2	2.44	0.48
1:I:233:GLU:HG2	1:I:244:LEU:H	1.78	0.48
1:A:314:GLN:HB3	1:A:318:TYR:HB2	1.94	0.48
1:A:630:GLU:HA	1:A:633:PHE:CE1	2.49	0.48
2:C:121:TYR:HE1	2:C:272:LEU:HD12	1.78	0.48
2:C:199:LEU:N	2:C:199:LEU:CD2	2.75	0.48
1:E:256:LYS:O	1:E:257:ILE:HD12	2.13	0.48
2:F:270:ARG:HD3	2:F:311:ILE:HD12	1.95	0.48
1:I:159:LEU:CA	1:I:262:VAL:CG2	2.70	0.48
1:A:384:GLU:C	1:A:386:ASN:OD1	2.52	0.48
1:A:574:GLN:O	1:A:578:ILE:CG1	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:MET:O	1:A:633:PHE:HD1	1.97	0.48
1:E:127:ILE:HD12	1:E:128:ILE:N	2.21	0.48
1:E:632:VAL:O	1:E:636:ILE:HG23	2.14	0.48
1:E:695:THR:OG1	1:E:747:TYR:CD2	2.66	0.48
2:F:180:ASN:HD21	2:F:298:ASN:HB3	1.77	0.48
1:I:46:VAL:HG21	1:I:270:MET:CE	2.42	0.48
1:M:956:PHE:HA	1:M:959:TRP:NE1	2.29	0.48
2:N:290:ARG:NH2	2:N:292:TRP:CE2	2.81	0.48
1:A:167:THR:HG23	1:E:196:LEU:HD13	1.96	0.48
2:C:81:ASP:OD2	2:C:83:THR:HG22	2.13	0.48
2:C:113:SER:HB2	2:C:287:PRO:HA	1.96	0.48
2:C:121:TYR:HD1	2:C:272:LEU:HA	1.79	0.48
2:C:123:GLY:O	2:C:124:LEU:HD23	2.13	0.48
1:E:465:ALA:HB1	1:E:501:LEU:HB3	1.96	0.48
2:F:206:TRP:CD1	2:F:208:THR:HG23	2.48	0.48
1:M:737:PHE:CE1	1:M:739:LYS:HB2	2.48	0.48
1:A:31:GLU:CG	1:A:209:ILE:CG2	2.82	0.48
1:A:402:GLN:O	1:A:810:ILE:HD13	2.13	0.48
1:A:1066:THR:O	1:A:1070:ILE:HG23	2.13	0.48
1:E:812:LEU:HD12	1:E:829:VAL:HG21	1.95	0.48
1:E:926:LEU:CD1	1:E:1019:THR:HG21	2.44	0.48
2:F:237:LEU:HB2	5:F:401:NAG:H82	1.95	0.48
2:J:201:LYS:HA	2:J:274:ARG:HD2	1.95	0.48
1:M:912:ASN:HA	1:M:915:PHE:HE1	1.76	0.48
2:C:180:ASN:HD21	5:C:402:NAG:C1	2.26	0.48
1:E:865:LEU:HD11	1:E:928:GLN:HB3	1.96	0.48
1:I:143:VAL:HG13	1:I:263:TYR:CD1	2.45	0.48
1:M:108:TYR:O	1:M:112:LEU:HD13	2.14	0.48
1:A:384:GLU:HB2	1:A:386:ASN:CG	2.33	0.48
1:A:401:GLY:HA3	1:A:864:HIS:N	2.28	0.48
1:I:162:LEU:HD21	1:I:260:VAL:HG23	1.96	0.48
1:I:700:LEU:HG	1:I:751:ILE:HA	1.95	0.48
1:I:718:LEU:HG	1:I:719:LEU:HD22	1.96	0.48
2:N:290:ARG:NH2	2:N:292:TRP:NE1	2.62	0.48
1:A:160:ILE:HG12	1:A:261:ALA:HB3	1.96	0.48
1:A:176:ALA:CB	1:A:837:GLU:CD	2.73	0.48
1:A:790:MET:SD	1:A:794:GLN:O	2.72	0.48
2:C:129:GLN:HG2	2:C:263:THR:HA	1.96	0.48
1:E:254:THR:HG21	1:E:257:ILE:HD11	1.96	0.48
1:E:321:GLU:N	1:E:322:PRO:HD2	2.29	0.48
1:E:840:GLN:OE1	1:E:840:GLN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1011:LEU:HD12	1:E:1011:LEU:O	2.14	0.48
1:E:1043:ILE:O	1:E:1046:PRO:HD2	2.14	0.48
1:I:305:VAL:O	1:I:309:LEU:HD23	2.13	0.48
1:I:310:LYS:CB	1:I:897:PHE:CD1	2.91	0.48
1:M:310:LYS:HD3	1:M:897:PHE:HB2	1.96	0.48
1:A:157:CYS:SG	1:A:262:VAL:HG13	2.54	0.47
1:A:834:LYS:CE	1:A:839:ARG:CZ	2.92	0.47
1:A:876:TYR:HE2	1:A:1011:LEU:HB2	1.78	0.47
1:A:1055:PHE:HB2	2:C:208:THR:HG21	1.96	0.47
1:E:290:ALA:O	1:E:293:ILE:HB	2.15	0.47
1:E:900:GLN:NE2	1:E:901:PRO:O	2.47	0.47
1:E:966:GLU:O	1:E:969:VAL:HG12	2.14	0.47
2:F:157:CYS:SG	2:F:171:CYS:HB2	2.54	0.47
1:I:187:HIS:HB3	1:I:242:GLU:O	2.14	0.47
1:M:284:VAL:HB	1:M:398:GLU:HG3	1.96	0.47
1:M:1030:LEU:O	1:M:1034:VAL:HG13	2.14	0.47
1:A:497:ASP:N	1:A:497:ASP:OD1	2.47	0.47
1:A:966:GLU:CG	1:A:1077:SER:HB3	2.44	0.47
2:C:169:ALA:HB3	2:C:232:LYS:HZ2	1.78	0.47
1:E:753:GLY:N	1:E:788:CYS:O	2.47	0.47
2:F:292:TRP:HH2	5:F:405:NAG:O5	1.85	0.47
1:M:622:LEU:O	1:M:622:LEU:HD23	2.15	0.47
1:M:749:LEU:HD12	1:M:751:ILE:HD11	1.96	0.47
1:A:382:ASP:HB3	1:A:386:ASN:ND2	2.30	0.47
1:A:572:ARG:HG2	1:A:640:MET:N	2.19	0.47
1:A:621:ALA:HB1	1:A:623:GLN:HE22	1.79	0.47
1:A:880:LYS:HZ3	1:A:1003:LEU:HD21	1.80	0.47
1:I:66:ARG:HA	1:I:289:ASN:HD21	1.79	0.47
1:I:426:ILE:HG12	1:I:427:ASP:H	1.79	0.47
1:M:598:VAL:HG22	1:M:644:GLY:O	2.14	0.47
1:M:660:ILE:HG23	1:M:664:HIS:CE1	2.50	0.47
2:C:142:GLN:OE1	2:C:149:ALA:O	2.32	0.47
1:E:240:GLY:H	1:E:241:PRO:HD3	1.79	0.47
1:E:284:VAL:O	1:E:287:SER:OG	2.23	0.47
1:E:464:ARG:HG2	1:E:547:MET:SD	2.55	0.47
1:E:908:LEU:O	1:E:912:ASN:HB2	2.14	0.47
1:I:961:PHE:O	1:I:965:PHE:HB2	2.14	0.47
1:M:593:TYR:CD1	1:M:649:GLU:HG2	2.50	0.47
1:M:880:LYS:HZ2	1:M:1007:VAL:HG11	1.78	0.47
1:A:480:VAL:CG2	1:I:486:SER:HA	2.45	0.47
1:A:671:TRP:CD2	1:A:785:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ILE:HA	1:A:786:LEU:O	2.14	0.47
2:C:232:LYS:HB3	2:C:233:PRO:HD2	1.95	0.47
1:I:314:GLN:NE2	3:I:1201:P5S:N	2.62	0.47
1:M:233:GLU:HG2	1:M:242:GLU:H	1.80	0.47
1:M:475:LYS:H	1:M:475:LYS:HD3	1.79	0.47
1:M:873:LEU:HD13	1:M:924:SER:HB3	1.97	0.47
1:A:184:CYS:SG	1:A:185:LYS:N	2.87	0.47
1:A:1053:MET:HB2	1:A:1056:VAL:CG2	2.44	0.47
1:E:40:PHE:CZ	1:E:142:LYS:HA	2.50	0.47
1:E:323:TRP:HH2	2:F:300:PRO:O	1.96	0.47
1:I:71:TYR:O	1:I:74:ILE:HG22	2.13	0.47
1:I:483:ALA:O	1:I:484:THR:C	2.51	0.47
2:J:292:TRP:CE2	5:J:404:NAG:O6	2.67	0.47
1:M:31:GLU:OE2	1:M:224:ARG:NH2	2.47	0.47
1:M:674:THR:O	1:M:788:CYS:HA	2.14	0.47
1:A:211:CYS:SG	1:A:212:GLU:N	2.87	0.47
1:A:899:GLN:HG2	2:C:132:ARG:NH2	2.29	0.47
1:A:966:GLU:HG2	1:A:1077:SER:HB3	1.96	0.47
2:C:301:VAL:HG12	2:C:304:PHE:HZ	1.80	0.47
1:E:339:LYS:C	1:E:339:LYS:HD3	2.35	0.47
1:E:410:LYS:HG3	1:E:684:THR:HG21	1.96	0.47
1:E:717:GLU:OE2	1:E:774:ILE:CG2	2.58	0.47
1:I:307:THR:CG2	1:I:310:LYS:HE3	2.45	0.47
1:I:410:LYS:HE2	1:I:684:THR:HG21	1.97	0.47
2:J:301:VAL:HG21	2:J:308:LYS:HD3	1.96	0.47
1:M:532:TYR:CE1	1:M:551:VAL:HG22	2.50	0.47
1:M:634:ASP:HA	1:M:637:GLU:HG2	1.96	0.47
2:C:322:ASN:OD1	2:C:324:PHE:HB3	2.15	0.47
1:E:397:ASN:HB3	1:E:866:TYR:CD2	2.49	0.47
1:E:750:ILE:HD12	1:E:786:LEU:HD13	1.97	0.47
1:E:915:PHE:CZ	1:E:1008:THR:HG21	2.48	0.47
2:F:63:PRO:HA	2:F:66:ILE:HG22	1.95	0.47
1:M:891:TYR:CD1	1:M:902:LEU:HD23	2.50	0.47
2:N:54:PHE:CD1	2:N:336:SER:HB2	2.49	0.47
1:E:98:VAL:O	1:E:102:THR:OG1	2.23	0.47
1:I:730:PHE:N	1:I:731:PRO:HD2	2.29	0.47
1:M:744:HIS:O	1:M:745:GLN:HG2	2.15	0.47
1:M:918:LEU:HB2	1:M:919:PRO:HD3	1.96	0.47
1:A:354:ILE:CG1	1:A:885:ILE:HG21	2.45	0.47
1:A:382:ASP:OD1	1:A:851:LYS:HE2	2.15	0.47
2:C:232:LYS:HE3	2:C:233:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:LEU:HD13	1:E:264:THR:OG1	2.15	0.47
1:I:284:VAL:HG11	1:I:870:ILE:HD13	1.96	0.47
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.84	0.46
1:A:519:TYR:CE2	1:A:532:TYR:HB2	2.26	0.46
1:A:519:TYR:CG	1:A:533:GLU:N	2.75	0.46
1:A:574:GLN:NE2	1:A:574:GLN:N	2.63	0.46
1:E:339:LYS:HD3	1:E:340:MET:N	2.30	0.46
1:I:949:ALA:HA	1:I:952:GLN:HG2	1.97	0.46
1:M:387:GLU:N	1:M:387:GLU:OE1	2.48	0.46
1:A:386:ASN:OD1	1:A:386:ASN:N	2.47	0.46
1:A:953:LEU:HD23	1:A:953:LEU:H	1.80	0.46
1:E:898:SER:HG	2:F:131:HIS:CD2	2.29	0.46
5:F:405:NAG:C1	5:F:405:NAG:C8	2.93	0.46
1:M:241:PRO:HG3	1:M:246:LEU:HD13	1.96	0.46
2:N:290:ARG:CZ	2:N:292:TRP:CE2	2.97	0.46
1:A:570:PHE:H	1:A:571:PRO:HD3	1.69	0.46
1:E:196:LEU:HD11	1:E:199:ALA:HB2	1.97	0.46
1:E:234:ALA:O	1:E:241:PRO:HA	2.15	0.46
1:E:407:PHE:HB3	1:E:673:LEU:HD12	1.96	0.46
1:E:776:LEU:HD11	1:E:801:MET:SD	2.56	0.46
1:I:270:MET:SD	1:I:270:MET:C	2.94	0.46
1:M:435:THR:N	1:M:440:GLY:HA3	2.29	0.46
1:M:668:LEU:HD21	1:M:943:MET:HG2	1.98	0.46
2:N:326:GLY:O	2:N:330:ILE:HG12	2.15	0.46
1:A:671:TRP:CG	1:A:785:VAL:HG22	2.51	0.46
1:I:46:VAL:HG21	1:I:270:MET:HE2	1.97	0.46
1:E:200:GLU:HG3	1:E:200:GLU:O	2.14	0.46
1:E:405:TYR:CE1	1:E:669:LYS:HB2	2.49	0.46
1:E:893:PHE:HA	1:E:897:PHE:CE1	2.50	0.46
1:I:266:MET:SD	1:I:266:MET:C	2.94	0.46
2:N:129:GLN:HB3	2:N:265:ALA:HA	1.97	0.46
1:A:177:SER:CA	1:A:837:GLU:CG	2.93	0.46
1:A:275:GLN:HE21	1:A:826:GLU:HB2	1.81	0.46
1:A:294:VAL:O	1:A:298:ILE:HG12	2.16	0.46
1:A:692:GLN:HG3	1:A:693:THR:H	1.80	0.46
1:A:888:GLN:HE21	1:A:901:PRO:HA	1.80	0.46
1:A:1070:ILE:HG13	1:A:1071:ILE:N	2.29	0.46
1:E:270:MET:O	1:E:273:ASN:HB2	2.16	0.46
1:I:188:TYR:CG	1:I:189:ALA:N	2.84	0.46
2:J:240:VAL:HG22	2:J:251:GLY:HA2	1.98	0.46
1:M:700:LEU:HD13	1:M:751:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:46:THR:H	2:N:49:THR:HG22	1.81	0.46
1:A:247:LYS:HG2	1:A:268:THR:HG21	1.97	0.46
1:A:519:TYR:O	1:A:532:TYR:HB2	2.15	0.46
1:E:406:VAL:HG23	1:E:812:LEU:HD23	1.96	0.46
1:E:588:ASN:OD1	1:E:589:ALA:N	2.48	0.46
1:I:158:ASP:HA	1:I:246:LEU:HA	1.96	0.46
1:I:159:LEU:CD2	1:I:262:VAL:HG21	2.46	0.46
1:I:956:PHE:HA	1:I:959:TRP:NE1	2.31	0.46
2:J:104:CYS:SG	2:J:105:THR:N	2.89	0.46
2:J:130:ASN:HB3	2:J:265:ALA:HA	1.97	0.46
1:M:966:GLU:HA	1:M:969:VAL:HG12	1.98	0.46
1:A:1069:ALA:O	1:A:1073:LEU:HD23	2.15	0.46
1:E:751:ILE:O	1:E:787:CYS:HA	2.15	0.46
2:F:107:ASN:OD1	5:F:405:NAG:C1	2.64	0.46
1:I:315:SER:CA	1:I:319:ASN:HB3	2.44	0.46
1:I:723:ARG:H	1:I:723:ARG:CD	2.26	0.46
1:I:906:ALA:O	1:I:910:MET:CB	2.64	0.46
1:M:163:SER:HA	1:M:194:ILE:HG21	1.97	0.46
1:M:238:SER:O	1:M:240:GLY:N	2.46	0.46
1:M:272:LEU:N	1:M:272:LEU:HD12	2.31	0.46
1:M:750:ILE:HB	1:M:786:LEU:HD13	1.97	0.46
1:A:382:ASP:OD1	1:A:851:LYS:CE	2.64	0.46
1:A:521:ARG:HB2	1:A:529:ILE:CD1	2.44	0.46
1:A:939:PRO:HA	1:A:942:TYR:HB3	1.97	0.46
2:F:294:ASN:ND2	5:F:404:NAG:H2	2.30	0.46
1:M:68:ALA:HB3	1:M:360:TYR:CE2	2.51	0.46
1:M:767:SER:OG	1:M:768:SER:N	2.49	0.46
1:E:185:LYS:HE2	1:E:245:LEU:CD2	2.46	0.46
1:E:191:ARG:H	1:E:194:ILE:HB	1.81	0.46
1:E:832:GLY:O	1:E:848:SER:HA	2.16	0.46
2:F:77:GLU:HB3	2:F:313:SER:HB2	1.96	0.46
1:I:307:THR:HG23	1:I:310:LYS:NZ	2.30	0.46
1:I:310:LYS:NZ	1:I:343:ASP:CG	2.58	0.46
1:I:537:THR:HA	1:I:549:VAL:HG11	1.98	0.46
1:M:415:THR:OG1	1:M:416:GLU:N	2.49	0.46
2:N:290:ARG:CZ	2:N:292:TRP:HE1	2.28	0.46
2:C:54:PHE:CE2	2:C:339:LEU:HD23	2.51	0.45
2:F:170:PRO:HB2	2:F:175:ALA:CB	2.46	0.45
1:I:820:ASP:N	1:I:820:ASP:OD1	2.49	0.45
1:I:1015:THR:HG21	1:I:1018:TRP:CE2	2.52	0.45
2:N:292:TRP:CH2	5:N:405:NAG:C4	2.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:340:GLY:HA2	2:N:343:LEU:HD12	1.98	0.45
1:A:198:THR:HG22	1:A:204:THR:OG1	2.16	0.45
1:A:376:TRP:HB2	2:C:34:LYS:HE2	1.99	0.45
1:A:1045:TRP:HB2	1:A:1046:PRO:HD3	1.98	0.45
2:C:46:THR:OG1	2:C:47:ALA:N	2.49	0.45
1:E:40:PHE:CE2	1:E:42:ASP:HA	2.51	0.45
1:E:240:GLY:N	1:E:241:PRO:CD	2.79	0.45
1:E:398:GLU:O	1:E:399:GLU:HB2	2.16	0.45
1:I:457:ASN:HA	1:I:460:GLU:HB3	1.99	0.45
1:I:940:ARG:HG3	1:I:941:LEU:N	2.29	0.45
1:M:873:LEU:HD22	1:M:924:SER:HB2	1.99	0.45
1:A:366:GLN:HG2	1:A:870:ILE:HG22	1.97	0.45
1:A:861:ALA:O	1:A:865:LEU:HG	2.17	0.45
2:C:66:ILE:HB	2:C:330:ILE:HD11	1.98	0.45
1:E:1015:THR:HG21	1:E:1018:TRP:CZ2	2.52	0.45
1:I:723:ARG:HD2	1:I:723:ARG:N	2.30	0.45
1:I:886:LEU:HD12	1:I:886:LEU:HA	1.74	0.45
1:M:47:SER:HB3	1:M:843:ARG:CZ	2.36	0.45
1:A:520:MET:O	1:A:521:ARG:C	2.52	0.45
1:E:246:LEU:HD22	1:E:268:THR:HB	1.98	0.45
1:E:640:MET:CG	1:E:641:ASN:H	2.30	0.45
1:E:907:TYR:OH	1:E:1033:TYR:HE1	1.99	0.45
2:F:181:ASP:OD1	2:F:181:ASP:N	2.49	0.45
1:I:159:LEU:HG	1:I:160:ILE:N	2.32	0.45
1:I:271:ALA:O	1:I:272:LEU:C	2.54	0.45
2:J:46:THR:OG1	2:J:47:ALA:N	2.49	0.45
1:M:751:ILE:HG22	1:M:752:ASP:H	1.80	0.45
1:A:173:VAL:CG1	1:A:249:ALA:HB1	2.47	0.45
1:A:384:GLU:HB2	1:A:386:ASN:ND2	2.32	0.45
1:A:412:GLY:O	1:A:836:LYS:HE3	2.16	0.45
1:A:724:LYS:HD2	1:A:724:LYS:N	2.31	0.45
2:C:79:GLU:HB3	2:C:311:ILE:HG23	1.97	0.45
1:E:174:THR:OG1	1:E:181:GLU:O	2.34	0.45
2:F:152:ASN:O	2:F:152:ASN:ND2	2.49	0.45
1:I:179:ASP:OD1	1:I:179:ASP:N	2.50	0.45
1:M:732:LYS:HD3	1:M:733:SER:N	2.31	0.45
1:A:524:ASN:CA	1:A:530:GLU:OE1	2.65	0.45
1:A:574:GLN:CG	1:A:642:LEU:HB2	2.42	0.45
1:A:719:LEU:HD11	1:A:720:ILE:HD12	1.98	0.45
1:A:1012:ALA:O	1:A:1015:THR:HG22	2.16	0.45
1:I:544:ARG:NH1	1:I:545:ARG:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:671:TRP:CH2	1:M:779:CYS:HB3	2.51	0.45
2:N:214:PHE:CD2	2:N:258:ILE:HD12	2.52	0.45
1:A:29:VAL:CG1	1:A:211:CYS:CB	2.95	0.45
1:A:529:ILE:CG1	1:A:531:GLU:HG2	2.45	0.45
2:C:188:ILE:HD11	2:C:292:TRP:CD1	2.52	0.45
1:I:159:LEU:CG	1:I:160:ILE:N	2.80	0.45
1:M:701:THR:HG21	1:M:752:ASP:HB3	1.97	0.45
1:A:427:ASP:HB3	1:A:429:HIS:ND1	2.32	0.45
1:E:220:LYS:HA	1:E:234:ALA:HA	1.99	0.45
1:E:245:LEU:HD22	1:E:245:LEU:N	2.31	0.45
1:E:702:THR:HG23	1:E:703:LYS:HG2	1.99	0.45
1:I:457:ASN:HB2	1:I:461:LEU:HG	1.99	0.45
1:M:426:ILE:H	1:M:430:LYS:HB3	1.82	0.45
1:M:832:GLY:N	1:M:847:TYR:O	2.50	0.45
1:A:235:VAL:HA	1:A:241:PRO:HD3	1.99	0.45
1:A:512:PHE:CE1	1:A:520:MET:HB3	2.52	0.45
1:A:707:GLU:HB2	1:A:710:ARG:HB2	1.99	0.45
1:A:926:LEU:HD13	1:A:1019:THR:HG21	1.98	0.45
1:A:1072:LEU:HB2	2:C:329:TYR:HE1	1.81	0.45
1:E:812:LEU:HA	1:E:829:VAL:CG1	2.46	0.45
1:I:931:ASN:HB2	1:I:934:THR:HG22	1.99	0.45
2:J:83:THR:HG21	2:J:307:ARG:HD2	1.98	0.45
1:A:218:LEU:HD13	1:A:267:GLU:HG3	1.99	0.45
1:A:415:THR:OG1	1:A:416:GLU:N	2.50	0.45
1:A:512:PHE:HE1	1:A:520:MET:HB3	1.82	0.45
1:A:521:ARG:CB	1:A:529:ILE:HD11	2.47	0.45
1:A:683:SER:OG	1:A:684:THR:N	2.50	0.45
2:C:63:PRO:HA	2:C:66:ILE:HG22	1.99	0.45
2:C:118:VAL:CG2	2:C:276:ILE:HB	2.47	0.45
1:E:717:GLU:OE1	1:E:717:GLU:HA	2.16	0.45
1:E:1000:PHE:O	1:E:1003:LEU:HG	2.17	0.45
1:M:903:TYR:CD1	1:M:1000:PHE:CE2	3.05	0.45
1:A:464:ARG:HH21	1:A:532:TYR:HH	1.64	0.44
1:A:574:GLN:NE2	1:A:574:GLN:H	2.13	0.44
1:A:982:SER:OG	2:C:320:GLY:N	2.44	0.44
1:E:407:PHE:CE2	1:E:799:VAL:HG22	2.52	0.44
1:E:787:CYS:HB3	1:E:790:MET:HE3	2.00	0.44
2:F:188:ILE:HG13	2:F:292:TRP:HD1	0.98	0.44
2:F:214:PHE:CD2	2:F:258:ILE:HD12	2.52	0.44
1:I:214:PRO:HG2	1:I:267:GLU:HB2	1.99	0.44
1:I:690:LEU:CD1	1:I:690:LEU:C	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:LEU:O	2:J:63:PRO:HG3	2.17	0.44
1:M:171:CYS:HB2	1:M:251:LEU:HD21	2.00	0.44
1:M:911:TYR:O	1:M:915:PHE:CD1	2.66	0.44
1:A:29:VAL:CG1	1:A:31:GLU:HG2	2.47	0.44
1:A:788:CYS:SG	1:A:789:ARG:N	2.90	0.44
1:A:1072:LEU:CD1	2:C:332:VAL:HG21	2.44	0.44
1:E:370:GLY:O	1:E:866:TYR:OH	2.27	0.44
1:I:40:PHE:HB3	1:I:143:VAL:HG21	1.99	0.44
1:I:552:LYS:HB3	1:I:558:ILE:HG23	1.98	0.44
1:I:700:LEU:CD1	1:I:750:ILE:O	2.66	0.44
1:M:254:THR:HG22	1:M:255:GLU:H	1.81	0.44
1:M:590:MET:HB3	1:M:693:THR:HA	2.00	0.44
2:N:290:ARG:NE	2:N:292:TRP:CZ2	2.84	0.44
1:A:524:ASN:N	1:A:530:GLU:CD	2.69	0.44
1:A:685:CYS:HB3	1:A:691:PHE:CE1	2.52	0.44
1:A:697:LEU:HD22	1:A:747:TYR:CD2	2.53	0.44
1:A:714:ARG:O	1:A:717:GLU:HG2	2.17	0.44
1:A:949:ALA:O	1:A:955:PRO:HG3	2.18	0.44
1:E:40:PHE:O	1:E:41:CYS:HB3	2.17	0.44
2:F:156:GLU:C	2:F:158:GLU:H	2.20	0.44
1:I:50:TYR:HD1	1:I:58:LYS:HD3	1.83	0.44
1:I:159:LEU:CD2	1:I:262:VAL:CG2	2.92	0.44
1:I:468:LEU:C	1:I:468:LEU:CD1	2.86	0.44
1:A:410:LYS:HZ3	1:A:674:THR:HG21	1.83	0.44
1:A:516:ARG:HE	1:A:516:ARG:CA	2.29	0.44
1:E:120:VAL:HG12	1:E:120:VAL:O	2.16	0.44
1:E:183:ASN:ND2	1:E:183:ASN:H	2.15	0.44
1:E:209:ILE:HD12	1:E:224:ARG:O	2.17	0.44
1:E:856:LYS:O	1:E:860:LEU:HB2	2.18	0.44
2:F:140:ASP:OD1	2:F:140:ASP:N	2.41	0.44
1:A:756:LEU:CD1	1:A:790:MET:HE3	2.48	0.44
1:E:217:ASP:O	1:E:218:LEU:HG	2.17	0.44
1:E:409:BFD:F3	1:E:411:THR:OG1	2.25	0.44
2:F:50:VAL:O	2:F:53:ILE:HB	2.17	0.44
1:I:321:GLU:CG	2:J:304:PHE:HB3	2.39	0.44
1:M:510:PHE:O	1:M:511:THR:HG23	2.18	0.44
1:A:959:TRP:HZ3	1:A:963:ALA:HB2	1.79	0.44
1:A:1076:ILE:HD13	2:C:332:VAL:HG22	1.99	0.44
2:C:111:GLU:OE1	2:C:111:GLU:N	2.38	0.44
1:E:218:LEU:HD12	1:E:235:VAL:O	2.18	0.44
1:E:283:ALA:HB3	1:E:399:GLU:CG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:521:ARG:HD2	1:E:531:GLU:N	2.32	0.44
1:E:732:LYS:NZ	1:E:739:LYS:HE2	1.98	0.44
1:E:942:TYR:CD1	1:E:942:TYR:C	2.88	0.44
1:E:988:LYS:HE3	2:F:206:TRP:HE3	1.83	0.44
1:E:1069:ALA:O	1:E:1073:LEU:HD23	2.18	0.44
2:F:130:ASN:HB3	2:F:265:ALA:HA	1.99	0.44
1:I:162:LEU:HB2	1:I:258:TYR:C	2.38	0.44
1:I:398:GLU:H	1:I:398:GLU:CD	2.20	0.44
1:I:1071:ILE:HA	1:I:1074:ILE:HG12	1.99	0.44
1:M:434:VAL:HG23	1:M:440:GLY:C	2.34	0.44
1:M:716:HIS:NE2	1:M:774:ILE:O	2.51	0.44
2:N:91:CYS:HB2	2:N:106:ILE:HD11	1.99	0.44
1:A:657:ALA:O	1:A:661:GLU:HG2	2.18	0.44
1:A:686:TYR:HA	1:A:691:PHE:HB2	1.99	0.44
1:E:323:TRP:CH2	2:F:300:PRO:O	2.71	0.44
1:E:462:PHE:HE2	1:E:511:THR:HA	1.82	0.44
2:F:79:GLU:HB2	2:F:311:ILE:HG12	1.99	0.44
1:I:489:LEU:HD21	1:I:509:GLY:O	2.10	0.44
1:M:67:ILE:HG13	1:M:292:LEU:HD23	2.00	0.44
1:M:128:ILE:HG21	1:M:132:LYS:HB2	1.99	0.44
1:M:161:LEU:HA	1:M:161:LEU:HD23	1.76	0.44
1:M:821:VAL:HG13	1:M:822:SER:H	1.83	0.44
1:A:127:ILE:HD11	1:A:145:ASP:HB3	1.99	0.44
1:A:217:ASP:O	1:A:218:LEU:CB	2.66	0.44
1:A:522:VAL:O	1:A:529:ILE:C	2.55	0.44
2:C:143:LEU:HB3	2:C:214:PHE:CD1	2.53	0.44
1:E:46:VAL:O	1:E:117:ASP:OD2	2.36	0.44
2:F:63:PRO:O	2:F:66:ILE:HG22	2.18	0.44
1:I:143:VAL:HG13	1:I:263:TYR:CG	2.52	0.44
1:I:413:THR:HG21	1:I:815:GLY:HA2	2.00	0.44
2:J:99:VAL:HG12	2:J:101:PRO:HD2	1.99	0.44
1:A:316:THR:OG1	1:A:317:PRO:CD	2.48	0.44
1:A:321:GLU:N	1:A:322:PRO:CD	2.80	0.44
1:A:379:ASP:OD2	2:C:35:GLN:NE2	2.50	0.44
1:A:754:SER:O	1:A:758:LEU:HD13	2.18	0.44
1:E:884:PHE:HZ	1:E:908:LEU:HD21	1.82	0.44
1:I:162:LEU:HB2	1:I:258:TYR:O	2.18	0.44
1:I:315:SER:O	1:I:315:SER:OG	2.28	0.44
1:I:700:LEU:CD2	1:I:751:ILE:O	2.65	0.44
1:M:171:CYS:O	1:M:187:HIS:NE2	2.51	0.44
1:A:489:LEU:HD12	1:A:491:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:CYS:HB3	2:F:172:GLY:HA2	1.99	0.43
2:F:186:PHE:HB3	2:F:194:PRO:HB2	1.99	0.43
1:I:1027:TRP:CE3	1:I:1030:LEU:HD21	2.53	0.43
1:M:475:LYS:H	1:M:475:LYS:CD	2.31	0.43
1:A:480:VAL:HG23	1:I:486:SER:CB	2.49	0.43
1:A:816:ASP:O	1:A:838:GLY:O	2.35	0.43
1:A:909:THR:O	1:A:913:ILE:HG23	2.18	0.43
1:E:346:SER:O	1:E:349:VAL:HG12	2.18	0.43
1:E:599:ALA:HB3	1:E:641:ASN:CB	2.48	0.43
1:I:192:ASP:OD1	1:I:193:THR:N	2.51	0.43
1:I:994:THR:HG22	1:I:1056:VAL:HG22	1.99	0.43
1:M:654:ASP:HB3	1:M:853:LYS:HB2	2.00	0.43
1:M:1052:ARG:HE	1:M:1052:ARG:N	2.16	0.43
1:A:354:ILE:HG13	1:A:885:ILE:HD13	2.01	0.43
1:A:519:TYR:HD1	1:A:534:LEU:CB	2.31	0.43
1:A:910:MET:SD	1:A:911:TYR:N	2.91	0.43
2:C:51:LEU:HD11	2:C:344:LEU:HD12	1.99	0.43
1:E:348:MET:O	1:E:352:ASN:N	2.51	0.43
1:E:717:GLU:OE2	1:E:774:ILE:CB	2.67	0.43
1:I:73:LEU:O	1:I:77:LEU:HD13	2.18	0.43
1:I:260:VAL:HG12	1:I:260:VAL:O	2.18	0.43
1:I:335:LEU:CD1	1:I:338:LEU:HB2	2.44	0.43
1:I:474:ILE:O	1:I:475:LYS:HD2	2.15	0.43
1:I:1002:VAL:O	1:I:1006:THR:OG1	2.20	0.43
2:J:100:THR:HB	2:J:101:PRO:HD3	2.00	0.43
1:M:147:VAL:HB	1:M:258:TYR:CG	2.54	0.43
1:M:211:CYS:HG	1:M:263:TYR:HH	1.61	0.43
1:M:272:LEU:HD12	1:M:272:LEU:H	1.83	0.43
1:M:526:ARG:NE	1:M:526:ARG:HA	2.33	0.43
1:A:173:VAL:HG22	1:A:251:LEU:HD12	2.01	0.43
1:A:673:LEU:HD12	1:A:795:LYS:HG3	1.99	0.43
1:A:816:ASP:OD2	1:A:837:GLU:HB3	2.16	0.43
2:C:143:LEU:HB3	2:C:214:PHE:CE1	2.53	0.43
2:C:258:ILE:HD13	2:C:258:ILE:HA	1.84	0.43
1:E:113:ARG:HD3	1:E:392:ASN:HB3	2.00	0.43
1:E:423:GLU:HB3	1:E:647:ALA:HB3	2.00	0.43
2:F:128:TYR:CD1	2:F:267:PRO:HB3	2.53	0.43
1:I:929:HIS:HB2	1:I:1016:ARG:HE	1.84	0.43
1:M:322:PRO:HB2	1:M:324:TYR:CE2	2.53	0.43
1:M:371:SER:HB2	1:M:391:VAL:HG22	1.99	0.43
1:M:999:VAL:O	1:M:1003:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE2	1:A:243:ASN:N	2.51	0.43
1:A:311:TYR:CA	1:A:315:SER:HB2	2.45	0.43
1:A:353:PHE:CZ	1:A:909:THR:HG22	2.54	0.43
1:A:932:ILE:HD12	1:A:933:ASP:N	2.33	0.43
2:C:281:ASP:N	2:C:281:ASP:OD1	2.51	0.43
1:E:984:GLU:OE2	1:E:1062:SER:OG	2.36	0.43
1:I:233:GLU:HB2	1:I:243:ASN:HB3	1.99	0.43
1:M:493:SER:HB3	1:M:498:GLU:OE2	2.19	0.43
1:M:581:THR:O	1:M:585:VAL:HG23	2.18	0.43
1:A:218:LEU:HD22	1:A:267:GLU:CG	2.47	0.43
1:A:384:GLU:C	1:A:386:ASN:N	2.71	0.43
1:A:468:LEU:CD2	1:A:520:MET:HB2	2.48	0.43
1:A:572:ARG:HG3	1:A:574:GLN:HE22	1.83	0.43
1:A:1009:LEU:O	1:A:1013:LEU:HG	2.18	0.43
2:C:141:SER:HB2	2:C:149:ALA:HB2	2.00	0.43
1:E:233:GLU:OE1	1:E:243:ASN:CA	2.66	0.43
1:E:421:PHE:HB3	1:E:648:VAL:HA	2.01	0.43
1:E:695:THR:HG1	1:E:747:TYR:HD2	1.61	0.43
1:E:880:LYS:C	1:E:880:LYS:HD3	2.38	0.43
1:I:173:VAL:HG21	1:I:249:ALA:HB1	2.00	0.43
1:I:311:TYR:CD1	1:I:339:LYS:HG2	2.53	0.43
1:I:791:ALA:HB3	1:I:794:GLN:HE22	1.83	0.43
1:I:865:LEU:HD22	1:I:869:ARG:HH12	1.82	0.43
1:M:284:VAL:HG21	1:M:398:GLU:HB2	2.01	0.43
1:M:462:PHE:HZ	1:M:521:ARG:HE	1.65	0.43
1:A:56:LEU:HB2	1:A:57:PRO:HD3	2.01	0.43
1:A:359:MET:HA	1:A:877:PHE:CE2	2.54	0.43
1:A:719:LEU:HD22	1:A:778:ILE:HB	2.01	0.43
1:E:94:PRO:HB3	3:E:1202:P5S:HB	2.00	0.43
1:E:560:LEU:HG	1:E:561:PHE:N	2.34	0.43
2:F:54:PHE:HB3	2:F:336:SER:O	2.18	0.43
2:F:129:GLN:HG3	2:F:134:TYR:CE1	2.54	0.43
1:I:748:GLY:HA2	1:I:784:ALA:O	2.18	0.43
2:J:66:ILE:HB	2:J:330:ILE:HD11	2.01	0.43
1:M:750:ILE:HA	1:M:786:LEU:O	2.19	0.43
1:A:384:GLU:C	1:A:386:ASN:H	2.20	0.43
1:A:1072:LEU:HB2	2:C:329:TYR:CE1	2.53	0.43
2:C:341:VAL:O	2:C:345:VAL:HG23	2.19	0.43
1:E:474:ILE:HG12	1:E:475:LYS:H	1.84	0.43
1:E:500:ALA:HB2	1:E:594:ARG:NH2	2.34	0.43
1:E:721:GLU:O	1:E:725:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:SER:OG	1:M:843:ARG:NH1	2.47	0.43
1:M:158:ASP:O	1:M:159:LEU:HD13	2.18	0.43
1:M:272:LEU:HD11	1:M:818:ALA:O	2.19	0.43
1:A:528:GLU:HA	1:A:528:GLU:OE2	2.19	0.43
1:A:1042:GLY:HA2	1:A:1045:TRP:CZ2	2.54	0.43
1:E:356:PRO:O	1:E:359:MET:HG2	2.19	0.43
1:E:694:ASN:HB2	1:E:745:GLN:CB	2.49	0.43
1:E:831:ILE:HD13	1:E:847:TYR:HB2	2.00	0.43
1:I:888:GLN:HE22	1:I:901:PRO:CB	2.31	0.43
2:J:80:ILE:HD12	2:J:80:ILE:O	2.19	0.43
2:J:135:VAL:HG22	2:J:263:THR:HG21	2.01	0.43
1:M:143:VAL:HA	1:M:262:VAL:HB	2.01	0.43
1:M:750:ILE:HD12	1:M:786:LEU:HD22	2.01	0.43
2:N:290:ARG:CZ	2:N:292:TRP:NE1	2.82	0.43
1:A:218:LEU:CD2	1:A:246:LEU:HD23	2.49	0.43
1:A:723:ARG:NH2	1:A:781:LYS:O	2.52	0.43
2:C:121:TYR:CE1	2:C:272:LEU:HD12	2.54	0.43
1:E:127:ILE:HG12	1:E:146:VAL:O	2.19	0.43
1:I:93:LEU:HB3	1:I:94:PRO:HD3	2.01	0.43
1:I:590:MET:O	1:I:689:ARG:NH2	2.52	0.43
1:I:756:LEU:O	1:I:759:ILE:HG22	2.19	0.43
1:M:237:ARG:HD2	1:M:675:GLY:O	2.18	0.43
1:A:77:LEU:O	1:A:80:VAL:HG22	2.18	0.42
1:A:128:ILE:HG12	1:A:199:ALA:HB2	2.00	0.42
1:A:146:VAL:HA	1:A:259:GLY:O	2.18	0.42
1:A:360:TYR:O	1:A:363:VAL:HG12	2.19	0.42
1:A:519:TYR:CD2	1:A:519:TYR:O	2.72	0.42
1:A:633:PHE:HA	1:A:636:ILE:HD12	2.00	0.42
1:A:656:ALA:CB	1:A:688:CYS:SG	3.07	0.42
1:E:464:ARG:C	1:E:464:ARG:HD3	2.39	0.42
1:E:735:ARG:HG3	1:E:735:ARG:O	2.19	0.42
1:E:1009:LEU:HD13	1:E:1013:LEU:HD23	2.01	0.42
2:F:262:ARG:O	2:F:271:LYS:NZ	2.51	0.42
2:J:157:CYS:HB3	2:J:172:GLY:HA2	2.00	0.42
1:M:167:THR:HG21	1:M:474:ILE:HD13	2.01	0.42
1:M:1081:GLU:O	1:M:1085:ILE:HG12	2.19	0.42
1:A:98:VAL:HG22	1:A:361:VAL:HG13	2.01	0.42
1:E:829:VAL:HG13	1:E:830:GLY:N	2.34	0.42
1:I:195:ALA:O	1:I:196:LEU:HB2	2.19	0.42
2:J:258:ILE:HD13	2:J:258:ILE:HA	1.91	0.42
1:M:149:VAL:HB	1:M:258:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:CA	1:A:837:GLU:HG2	2.48	0.42
1:A:474:ILE:HG22	1:A:491:TYR:HB3	2.00	0.42
1:A:792:PRO:HG3	1:A:819:ASN:C	2.33	0.42
2:C:301:VAL:HG21	2:C:308:LYS:HD3	2.01	0.42
1:M:205:LEU:HD23	1:M:205:LEU:HA	1.87	0.42
1:M:284:VAL:O	1:M:288:ILE:HG12	2.19	0.42
1:M:860:LEU:HD11	1:M:942:TYR:CE2	2.54	0.42
1:E:958:TYR:OH	1:E:1084:LEU:HD22	2.18	0.42
1:I:273:ASN:HA	1:I:822:SER:CB	2.50	0.42
1:I:492:ILE:O	1:I:492:ILE:HG13	2.19	0.42
1:I:572:ARG:HG2	1:I:640:MET:HG3	2.01	0.42
1:M:700:LEU:HD22	1:M:751:ILE:HG12	2.02	0.42
1:A:29:VAL:CG2	1:A:31:GLU:HG2	2.49	0.42
1:A:321:GLU:HG2	1:A:322:PRO:HD3	2.01	0.42
1:E:374:ILE:HD11	1:E:391:VAL:CG1	2.49	0.42
1:E:574:GLN:CB	1:E:640:MET:HE3	2.49	0.42
1:E:621:ALA:HB3	1:E:623:GLN:HE21	1.85	0.42
1:E:921:LEU:HD23	1:E:921:LEU:HA	1.94	0.42
1:M:921:LEU:HD22	1:M:925:LEU:HD11	2.01	0.42
2:N:46:THR:OG1	2:N:47:ALA:N	2.52	0.42
2:C:232:LYS:HZ3	2:C:240:VAL:HG12	1.85	0.42
2:C:293:LEU:HD11	2:C:310:MET:HE1	2.02	0.42
1:E:159:LEU:HD21	1:E:261:ALA:O	2.20	0.42
1:E:1015:THR:HG21	1:E:1018:TRP:CE2	2.54	0.42
2:F:310:MET:HG2	2:F:311:ILE:N	2.34	0.42
1:M:592:GLY:CA	1:M:686:TYR:HB2	2.50	0.42
1:A:194:ILE:O	1:A:198:THR:HG23	2.19	0.42
1:A:512:PHE:CE1	1:A:520:MET:CB	3.02	0.42
1:E:127:ILE:CD1	1:E:128:ILE:H	2.24	0.42
1:E:291:PHE:CE2	1:E:959:TRP:HZ3	2.38	0.42
1:E:574:GLN:HB3	1:E:640:MET:HE3	2.02	0.42
1:E:988:LYS:HE3	2:F:206:TRP:CE3	2.55	0.42
1:I:399:GLU:HG2	1:I:399:GLU:O	2.19	0.42
1:I:659:THR:O	1:I:663:LEU:HD13	2.20	0.42
1:I:843:ARG:H	1:I:843:ARG:HG3	1.68	0.42
1:M:812:LEU:HD23	1:M:813:SER:N	2.34	0.42
1:M:907:TYR:O	1:M:911:TYR:HB3	2.19	0.42
1:A:790:MET:SD	1:A:794:GLN:CA	3.07	0.42
2:C:81:ASP:HA	2:C:309:ARG:HB3	2.02	0.42
1:I:273:ASN:HA	1:I:822:SER:HB3	2.02	0.42
1:I:880:LYS:HE3	1:I:911:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1005:PHE:HE1	1:I:1030:LEU:HD13	1.84	0.42
1:M:194:ILE:O	1:M:196:LEU:N	2.51	0.42
1:M:818:ALA:HB2	1:M:840:GLN:HE21	1.84	0.42
1:A:514:GLY:O	1:A:515:ASN:CB	2.68	0.42
1:E:663:LEU:HD11	1:E:668:LEU:HD11	2.02	0.42
1:E:1063:SER:O	1:E:1066:THR:OG1	2.32	0.42
1:I:485:GLU:CG	1:I:488:GLU:HB2	2.49	0.42
1:I:703:LYS:CD	1:I:714:ARG:HD3	2.50	0.42
1:M:406:VAL:HG23	1:M:812:LEU:HD22	2.02	0.42
1:M:992:ASN:HB2	2:N:265:ALA:CB	2.49	0.42
1:A:66:ARG:NE	1:A:285:GLU:OE1	2.39	0.42
1:A:237:ARG:NH1	1:A:676:ASP:O	2.53	0.42
1:A:350:LEU:HD11	1:A:888:GLN:HE22	1.84	0.42
1:A:485:GLU:OE1	1:A:485:GLU:N	2.53	0.42
2:C:100:THR:HB	2:C:101:PRO:HD3	2.01	0.42
1:E:272:LEU:HA	1:E:822:SER:HB3	2.02	0.42
1:E:1050:GLN:CD	1:E:1052:ARG:HD3	2.40	0.42
1:I:321:GLU:HG2	2:J:304:PHE:HB3	2.02	0.42
1:I:588:ASN:HB2	1:I:593:TYR:CD1	2.55	0.42
1:M:310:LYS:HE2	3:M:1201:P5S:HN	1.85	0.42
1:M:748:GLY:CA	1:M:782:CYS:HB2	2.50	0.42
1:A:29:VAL:H	1:A:211:CYS:N	2.00	0.41
1:A:585:VAL:HG13	1:A:595:THR:HG21	2.02	0.41
2:C:185:LEU:HD11	2:C:312:LEU:CD2	2.49	0.41
1:E:66:ARG:NH2	1:E:285:GLU:OE1	2.51	0.41
1:E:87:SER:HB3	1:E:90:THR:HB	2.02	0.41
1:E:149:VAL:HG22	1:E:251:LEU:HD13	2.02	0.41
1:E:160:ILE:HD13	1:E:160:ILE:HA	1.97	0.41
1:E:187:HIS:HA	1:E:242:GLU:O	2.20	0.41
1:E:339:LYS:HZ1	1:E:343:ASP:CB	2.31	0.41
1:E:1019:THR:HG23	1:E:1022:ASN:H	1.84	0.41
1:I:295:TYR:O	1:I:298:ILE:HB	2.19	0.41
1:M:178:LEU:HD22	1:M:246:LEU:HD23	2.02	0.41
1:M:515:ASN:C	1:M:515:ASN:HD22	2.24	0.41
1:A:168:ASP:HB2	1:A:170:THR:HG22	2.02	0.41
1:A:724:LYS:O	1:A:728:HIS:ND1	2.53	0.41
1:A:974:THR:O	1:A:977:LEU:HG	2.20	0.41
1:E:413:THR:CG2	1:E:833:ILE:HG21	2.49	0.41
1:E:856:LYS:O	1:E:860:LEU:CB	2.68	0.41
1:E:902:LEU:O	1:E:996:GLY:HA3	2.21	0.41
2:F:299:TYR:O	2:F:301:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:468:LEU:HD12	1:I:469:CYS:SG	2.60	0.41
2:J:120:MET:HB2	2:J:312:LEU:HD12	2.02	0.41
2:J:233:PRO:HB2	2:J:236:TRP:HB2	2.02	0.41
1:M:29:VAL:HB	1:M:40:PHE:HZ	1.85	0.41
1:M:966:GLU:HB3	1:M:970:PHE:CE2	2.56	0.41
1:A:673:LEU:CD2	1:A:787:CYS:HB2	2.43	0.41
1:A:960:THR:O	1:A:963:ALA:N	2.53	0.41
1:E:771:TYR:HA	1:E:774:ILE:HD11	2.02	0.41
1:E:883:CYS:SG	1:E:966:GLU:HB2	2.60	0.41
2:F:209:ASP:O	2:F:214:PHE:HD2	2.03	0.41
1:I:149:VAL:HG11	1:I:155:PHE:CZ	2.55	0.41
1:I:159:LEU:HA	1:I:262:VAL:HG22	1.95	0.41
1:I:873:LEU:CD1	1:I:920:ILE:HG21	2.50	0.41
1:A:516:ARG:NE	1:A:516:ARG:CA	2.83	0.41
1:E:346:SER:HB3	1:E:899:GLN:HG2	2.01	0.41
1:E:1086:VAL:HG21	2:F:50:VAL:HG21	2.01	0.41
2:F:46:THR:OG1	2:F:47:ALA:N	2.54	0.41
1:I:820:ASP:O	1:I:824:ILE:HG12	2.20	0.41
1:I:939:PRO:HA	1:I:942:TYR:CD1	2.55	0.41
1:M:147:VAL:HG12	1:M:258:TYR:CE2	2.55	0.41
1:M:147:VAL:CG1	1:M:258:TYR:CE2	3.03	0.41
1:M:821:VAL:HG13	1:M:822:SER:N	2.36	0.41
1:M:950:MET:HG3	1:M:950:MET:O	2.21	0.41
2:N:51:LEU:HD13	2:N:344:LEU:HB2	2.02	0.41
1:A:466:LEU:HD21	1:A:501:LEU:HB3	2.01	0.41
2:C:273:TYR:CD2	2:C:274:ARG:HG2	2.55	0.41
1:E:185:LYS:HD2	1:E:241:PRO:CB	2.44	0.41
2:F:193:TYR:HD1	2:F:194:PRO:HD2	1.86	0.41
1:I:253:ASN:O	1:I:474:ILE:HD11	2.21	0.41
1:I:310:LYS:CD	1:I:310:LYS:C	2.86	0.41
1:M:294:VAL:HG21	1:M:959:TRP:CH2	2.55	0.41
1:M:593:TYR:CE1	1:M:649:GLU:HG2	2.56	0.41
1:M:975:TYR:HA	1:M:978:PHE:HB2	2.03	0.41
1:A:176:ALA:C	1:A:837:GLU:HG2	2.41	0.41
1:A:339:LYS:O	1:A:342:THR:HG22	2.19	0.41
1:A:458:ARG:NH1	1:A:458:ARG:HB3	2.36	0.41
1:A:1071:ILE:HG13	1:A:1072:LEU:N	2.36	0.41
2:C:63:PRO:O	2:C:66:ILE:HG22	2.20	0.41
2:C:107:ASN:HD22	2:C:290:ARG:HH21	1.68	0.41
2:C:198:ALA:O	2:C:276:ILE:HG23	2.20	0.41
1:E:865:LEU:HD12	1:E:869:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:678:MET:HE2	1:I:700:LEU:HB2	2.03	0.41
1:I:862:HIS:HA	1:I:865:LEU:HD12	2.02	0.41
1:M:116:ALA:O	1:M:120:VAL:HG23	2.21	0.41
1:M:173:VAL:HG23	1:M:250:THR:C	2.41	0.41
1:M:819:ASN:HB3	7:M:1302:HOH:O	2.20	0.41
1:M:880:LYS:HZ3	1:M:1007:VAL:HG21	1.85	0.41
1:M:1055:PHE:CE1	2:N:213:LYS:HE2	2.55	0.41
1:A:237:ARG:HH11	1:A:675:GLY:HA2	1.85	0.41
1:A:488:GLU:OE1	1:A:488:GLU:HA	2.21	0.41
1:A:983:LEU:HB2	1:A:990:TYR:HE2	1.85	0.41
1:E:327:LYS:CG	1:E:331:GLU:H	2.34	0.41
1:E:673:LEU:CD1	1:E:795:LYS:HE2	2.51	0.41
1:E:700:LEU:O	1:E:701:THR:HG22	2.20	0.41
1:I:332:ARG:O	1:I:335:LEU:HG	2.21	0.41
1:I:521:ARG:HD2	1:I:531:GLU:HG3	2.02	0.41
2:J:32:ALA:HB1	2:J:38:LEU:HA	2.03	0.41
2:J:79:GLU:HB3	2:J:311:ILE:HG12	2.03	0.41
1:A:173:VAL:HG11	1:A:249:ALA:HB1	2.03	0.41
2:C:45:LEU:HA	2:C:49:THR:HG21	2.02	0.41
1:E:818:ALA:O	1:E:821:VAL:HG12	2.21	0.41
2:F:90:PRO:HG2	2:F:105:THR:O	2.20	0.41
2:F:120:MET:SD	2:F:183:LEU:HD13	2.61	0.41
1:I:314:GLN:C	1:I:319:ASN:CB	2.66	0.41
1:I:321:GLU:N	1:I:322:PRO:HD2	2.35	0.41
1:I:409:BFD:F1	1:I:674:THR:OG1	2.20	0.41
1:M:183:ASN:OD1	1:M:239:LEU:HB3	2.20	0.41
1:A:29:VAL:HG13	1:A:209:ILE:O	2.21	0.41
1:A:219:TYR:O	1:A:234:ALA:CA	2.64	0.41
1:A:409:BFD:OD2	1:A:409:BFD:F3	2.29	0.41
1:A:909:THR:OG1	1:A:910:MET:N	2.53	0.41
1:A:1000:PHE:O	1:A:1003:LEU:HB3	2.21	0.41
1:A:1004:VAL:HG13	1:A:1005:PHE:HD1	1.86	0.41
1:A:1067:TRP:O	1:A:1071:ILE:HG23	2.20	0.41
1:A:1075:PHE:CZ	2:C:57:ILE:HD12	2.56	0.41
2:C:233:PRO:HG2	2:C:236:TRP:CB	2.51	0.41
2:C:339:LEU:HD12	2:C:339:LEU:HA	1.97	0.41
1:E:67:ILE:CD1	1:E:293:ILE:HG12	2.51	0.41
1:E:67:ILE:HD11	1:E:289:ASN:O	2.20	0.41
1:E:151:ALA:HB2	1:E:255:GLU:HA	2.03	0.41
1:E:178:LEU:O	1:E:819:ASN:HB2	2.21	0.41
1:E:254:THR:CG2	1:E:255:GLU:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:THR:CG2	1:E:255:GLU:N	2.84	0.41
1:E:381:TYR:H	1:E:851:LYS:HZ2	1.68	0.41
1:E:495:SER:HB2	1:E:496:PRO:HD2	2.03	0.41
1:E:775:PHE:O	1:E:778:ILE:HG22	2.20	0.41
1:E:952:GLN:O	1:E:956:PHE:CE2	2.69	0.41
2:F:51:LEU:N	2:F:52:PRO:HD2	2.36	0.41
1:I:159:LEU:HD21	1:I:258:TYR:C	2.40	0.41
1:I:173:VAL:CG2	1:I:249:ALA:HB1	2.50	0.41
1:I:618:ALA:HB3	1:I:625:ARG:HH11	1.86	0.41
1:I:822:SER:HB2	1:I:823:MET:HE3	2.03	0.41
1:I:915:PHE:CG	1:I:916:THR:N	2.88	0.41
1:M:93:LEU:HB3	1:M:94:PRO:HD3	2.02	0.41
1:M:143:VAL:HG13	1:M:263:TYR:H	1.86	0.41
1:M:666:ALA:HB1	1:M:943:MET:CB	2.51	0.41
1:M:799:VAL:O	1:M:803:LYS:HG3	2.20	0.41
1:M:992:ASN:CB	2:N:265:ALA:CB	2.97	0.41
1:A:59:ASN:O	1:A:63:GLN:HB2	2.21	0.41
1:A:458:ARG:HB3	1:A:458:ARG:HH11	1.85	0.41
1:E:150:GLN:HE21	1:E:150:GLN:HB3	1.68	0.41
1:E:218:LEU:O	1:E:235:VAL:HG13	2.21	0.41
1:E:232:LEU:HD12	1:E:242:GLU:OE1	2.21	0.41
1:E:397:ASN:HA	1:E:847:TYR:OH	2.21	0.41
1:E:1066:THR:O	1:E:1070:ILE:HG12	2.21	0.41
1:I:402:GLN:O	1:I:810:ILE:HD13	2.21	0.41
1:M:587:ARG:O	1:M:591:ASP:HB2	2.21	0.41
1:M:1070:ILE:HA	1:M:1073:LEU:HB2	2.03	0.41
2:N:315:ILE:HG22	2:N:320:GLY:HA2	2.03	0.41
1:A:712:GLU:HG3	1:A:771:TYR:CE2	2.56	0.40
1:E:93:LEU:N	1:E:94:PRO:HD2	2.36	0.40
1:E:1045:TRP:CZ2	1:E:1053:MET:O	2.74	0.40
2:F:46:THR:H	2:F:49:THR:CG2	2.33	0.40
2:F:292:TRP:HH2	5:F:405:NAG:HO6	1.58	0.40
1:I:79:GLN:HB2	1:I:84:THR:HG21	2.04	0.40
2:J:54:PHE:HA	2:J:57:ILE:HG12	2.04	0.40
2:J:178:MET:HG2	2:J:260:TRP:NE1	2.36	0.40
1:M:756:LEU:HD13	1:M:790:MET:HE1	2.03	0.40
1:M:931:ASN:HB3	1:M:934:THR:HG22	2.03	0.40
2:N:105:THR:HG22	2:N:294:ASN:HB3	2.02	0.40
1:A:268:THR:O	1:A:272:LEU:HG	2.21	0.40
1:A:966:GLU:HA	1:A:969:VAL:HG12	2.02	0.40
1:E:860:LEU:CD1	1:E:939:PRO:HB3	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1034:VAL:HG12	1:E:1057:PHE:CZ	2.57	0.40
1:I:489:LEU:HD22	1:I:509:GLY:CA	2.50	0.40
1:I:966:GLU:O	1:I:969:VAL:HG12	2.20	0.40
1:I:991:GLY:O	1:I:994:THR:OG1	2.39	0.40
1:M:287:SER:HB2	1:M:951:LEU:HD22	2.03	0.40
1:A:379:ASP:OD2	1:A:857:LYS:NZ	2.54	0.40
1:A:870:ILE:HG13	1:A:871:ALA:N	2.37	0.40
1:A:1079:PHE:N	1:A:1080:PRO:HD2	2.35	0.40
2:C:113:SER:CB	2:C:287:PRO:HA	2.51	0.40
1:E:52:LEU:HD22	1:E:52:LEU:H	1.86	0.40
1:E:914:CYS:SG	1:E:915:PHE:N	2.94	0.40
1:I:272:LEU:HD11	1:I:792:PRO:CG	2.52	0.40
1:I:476:THR:CG2	1:I:492:ILE:HD11	2.52	0.40
1:I:485:GLU:CG	1:I:488:GLU:OE2	2.69	0.40
1:I:980:THR:O	2:J:270:ARG:NH1	2.55	0.40
1:I:1005:PHE:CE1	1:I:1030:LEU:HB2	2.56	0.40
1:M:429:HIS:HB3	1:M:431:TYR:CE2	2.56	0.40
1:M:953:LEU:HA	1:M:956:PHE:HB3	2.03	0.40
1:A:86:THR:HG21	1:A:349:VAL:HG21	2.02	0.40
1:A:689:ARG:HA	1:A:689:ARG:HE	1.86	0.40
1:A:697:LEU:HD22	1:A:747:TYR:CE2	2.57	0.40
1:E:599:ALA:CB	1:E:641:ASN:HB3	2.51	0.40
1:I:319:ASN:C	1:I:322:PRO:HD2	2.41	0.40
1:I:1001:THR:HA	1:I:1004:VAL:HG12	2.03	0.40
1:M:873:LEU:HD11	1:M:920:ILE:HD12	2.04	0.40
2:N:276:ILE:HG21	2:N:285:THR:HG21	2.04	0.40
1:A:321:GLU:HG3	1:A:322:PRO:N	2.37	0.40
1:A:418:SER:HB2	1:A:651:LYS:HZ1	1.87	0.40
1:A:572:ARG:HD2	1:A:573:VAL:H	1.87	0.40
1:E:183:ASN:OD1	1:E:239:LEU:HD21	2.21	0.40
1:I:64:PHE:CE1	1:I:73:LEU:HD22	2.56	0.40
1:I:532:TYR:HD1	1:I:553:THR:HG21	1.85	0.40
1:I:906:ALA:O	1:I:910:MET:HB2	2.22	0.40
1:I:1078:LEU:HB3	1:I:1082:ILE:HD13	2.04	0.40
1:I:1090:VAL:O	1:I:1091:ARG:HB2	2.21	0.40
2:J:222:ASN:HD21	2:J:225:GLU:CB	2.32	0.40
1:M:87:SER:HA	1:M:88:PRO:HD3	1.93	0.40
1:M:451:PHE:HB3	1:M:526:ARG:NH2	2.37	0.40
1:M:1051:GLN:OE1	2:N:140:ASP:N	2.53	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	1061/1129 (94%)	917 (86%)	143 (14%)	1 (0%)	51 84
1	E	1061/1129 (94%)	875 (82%)	186 (18%)	0	100 100
1	I	1061/1129 (94%)	878 (83%)	182 (17%)	1 (0%)	51 84
1	M	1061/1129 (94%)	885 (83%)	176 (17%)	0	100 100
2	C	322/361 (89%)	266 (83%)	56 (17%)	0	100 100
2	F	322/361 (89%)	275 (85%)	47 (15%)	0	100 100
2	J	322/361 (89%)	281 (87%)	41 (13%)	0	100 100
2	N	322/361 (89%)	297 (92%)	25 (8%)	0	100 100
All	All	5532/5960 (93%)	4674 (84%)	856 (16%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	316	THR
1	A	570	PHE

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	946/1004 (94%)	890 (94%)	56 (6%)	19 49
1	E	946/1004 (94%)	895 (95%)	51 (5%)	22 52
1	I	946/1004 (94%)	897 (95%)	49 (5%)	23 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	946/1004 (94%)	888 (94%)	58 (6%)	18 48
2	C	288/316 (91%)	276 (96%)	12 (4%)	30 57
2	F	288/316 (91%)	273 (95%)	15 (5%)	23 53
2	J	288/316 (91%)	283 (98%)	5 (2%)	60 78
2	N	288/316 (91%)	275 (96%)	13 (4%)	27 56
All	All	4936/5280 (94%)	4677 (95%)	259 (5%)	23 53

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	A	39	ARG
1	A	55	PHE
1	A	70	PHE
1	A	108	TYR
1	A	145	ASP
1	A	183	ASN
1	A	188	TYR
1	A	226	ASN
1	A	237	ARG
1	A	239	LEU
1	A	256	LYS
1	A	281	ARG
1	A	295	TYR
1	A	323	TRP
1	A	417	ASN
1	A	458	ARG
1	A	489	LEU
1	A	491	TYR
1	A	506	LYS
1	A	515	ASN
1	A	520	MET
1	A	526	ARG
1	A	540	PHE
1	A	547	MET
1	A	574	GLN
1	A	586	GLU
1	A	607	ASP
1	A	610	ARG
1	A	620	MET

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Mol	Chain	Res	Type
1	A	633	PHE
1	A	651	LYS
1	A	686	TYR
1	A	722	TYR
1	A	724	LYS
1	A	735	ARG
1	A	738	LYS
1	A	741	TRP
1	A	747	TYR
1	A	782	CYS
1	A	819	ASN
1	A	877	PHE
1	A	884	PHE
1	A	892	GLN
1	A	895	CYS
1	A	904	ASP
1	A	907	TYR
1	A	942	TYR
1	A	1000	PHE
1	A	1016	ARG
1	A	1032	PHE
1	A	1038	PHE
1	A	1049	LYS
1	A	1052	ARG
1	A	1053	MET
1	A	1063	SER
2	C	42	GLN
2	C	91	CYS
2	C	98	ASP
2	C	127	PHE
2	C	138	ARG
2	C	142	GLN
2	C	201	LYS
2	C	209	ASP
2	C	236	TRP
2	C	281	ASP
2	C	297	TYR
2	C	299	TYR
1	E	97	PHE
1	E	162	LEU
1	E	221	PHE
1	E	232	LEU

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Mol	Chain	Res	Type
1	E	237	ARG
1	E	252	LYS
1	E	313	TRP
1	E	316	THR
1	E	319	ASN
1	E	323	TRP
1	E	324	TYR
1	E	399	GLU
1	E	432	LYS
1	E	464	ARG
1	E	508	TYR
1	E	523	GLU
1	E	533	GLU
1	E	545	ARG
1	E	570	PHE
1	E	600	PHE
1	E	607	ASP
1	E	608	TYR
1	E	610	ARG
1	E	624	ASP
1	E	633	PHE
1	E	688	CYS
1	E	691	PHE
1	E	718	LEU
1	E	749	LEU
1	E	820	ASP
1	E	853	LYS
1	E	877	PHE
1	E	881	ASN
1	E	884	PHE
1	E	893	PHE
1	E	912	ASN
1	E	915	PHE
1	E	926	LEU
1	E	927	GLU
1	E	931	ASN
1	E	942	TYR
1	E	948	ASN
1	E	978	PHE
1	E	1000	PHE
1	E	1013	LEU
1	E	1020	TRP

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Mol	Chain	Res	Type
1	E	1023	HIS
1	E	1027	TRP
1	E	1051	GLN
1	E	1083	LEU
1	E	1089	ASN
2	F	94	CYS
2	F	102	CYS
2	F	127	PHE
2	F	152	ASN
2	F	161	ARG
2	F	164	GLU
2	F	178	MET
2	F	193	TYR
2	F	199	LEU
2	F	201	LYS
2	F	232	LYS
2	F	252	PHE
2	F	256	ASP
2	F	299	TYR
2	F	308	LYS
1	I	50	TYR
1	I	108	TYR
1	I	171	CYS
1	I	206	ARG
1	I	215	GLN
1	I	218	LEU
1	I	220	LYS
1	I	232	LEU
1	I	237	ARG
1	I	239	LEU
1	I	270	MET
1	I	273	ASN
1	I	291	PHE
1	I	297	PHE
1	I	310	LYS
1	I	324	TYR
1	I	333	GLU
1	I	335	LEU
1	I	344	PHE
1	I	398	GLU
1	I	432	LYS
1	I	469	CYS

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Mol	Chain	Res	Type
1	I	485	GLU
1	I	519	TYR
1	I	532	TYR
1	I	533	GLU
1	I	544	ARG
1	I	545	ARG
1	I	561	PHE
1	I	577	GLU
1	I	588	ASN
1	I	713	ASP
1	I	723	ARG
1	I	729	GLU
1	I	730	PHE
1	I	741	TRP
1	I	820	ASP
1	I	877	PHE
1	I	899	GLN
1	I	915	PHE
1	I	929	HIS
1	I	942	TYR
1	I	965	PHE
1	I	1020	TRP
1	I	1040	TRP
1	I	1045	TRP
1	I	1053	MET
1	I	1057	PHE
1	I	1067	TRP
2	J	41	TRP
2	J	171	CYS
2	J	201	LYS
2	J	260	TRP
2	J	350	TYR
1	M	35	TYR
1	M	36	ILE
1	M	39	ARG
1	M	97	PHE
1	M	111	TRP
1	M	117	ASP
1	M	126	TYR
1	M	129	GLU
1	M	219	TYR
1	M	237	ARG

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Mol	Chain	Res	Type
1	M	239	LEU
1	M	247	LYS
1	M	258	TYR
1	M	297	PHE
1	M	332	ARG
1	M	368	PHE
1	M	390	LEU
1	M	404	ASP
1	M	431	TYR
1	M	443	GLN
1	M	458	ARG
1	M	462	PHE
1	M	475	LYS
1	M	488	GLU
1	M	491	TYR
1	M	515	ASN
1	M	520	MET
1	M	532	TYR
1	M	533	GLU
1	M	546	ARG
1	M	572	ARG
1	M	594	ARG
1	M	652	LEU
1	M	689	ARG
1	M	694	ASN
1	M	725	LYS
1	M	744	HIS
1	M	843	ARG
1	M	847	TYR
1	M	851	LYS
1	M	853	LYS
1	M	877	PHE
1	M	880	LYS
1	M	884	PHE
1	M	907	TYR
1	M	915	PHE
1	M	926	LEU
1	M	965	PHE
1	M	978	PHE
1	M	1000	PHE
1	M	1005	PHE
1	M	1020	TRP

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Mol	Chain	Res	Type
1	M	1027	TRP
1	M	1032	PHE
1	M	1033	TYR
1	M	1039	PHE
1	M	1052	ARG
1	M	1053	MET
2	N	55	PHE
2	N	133	ARG
2	N	161	ARG
2	N	181	ASP
2	N	193	TYR
2	N	199	LEU
2	N	201	LYS
2	N	243	LEU
2	N	246	ASP
2	N	250	ASN
2	N	297	TYR
2	N	322	ASN
2	N	350	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	275	GLN
1	A	397	ASN
1	A	574	GLN
1	A	655	GLN
2	C	142	GLN
1	E	243	ASN
1	E	329	GLN
1	E	623	GLN
1	E	892	GLN
2	F	92	ASN
2	F	142	GLN
1	I	38	GLN
1	I	273	ASN
1	I	314	GLN
1	I	881	ASN
1	M	402	GLN
1	M	694	ASN
1	M	840	GLN

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Mol	Chain	Res	Type
2	N	107	ASN
2	N	117	ASN
2	N	142	GLN
2	N	250	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	BFD	A	409	1,4	8,11,12	5.58	3 (37%)	3,15,17	1.72	1 (33%)
1	BFD	I	409	1	8,11,12	5.60	3 (37%)	3,15,17	2.12	1 (33%)
1	BFD	E	409	1	8,11,12	5.57	3 (37%)	3,15,17	1.14	0
1	BFD	M	409	1	8,11,12	5.62	3 (37%)	3,15,17	1.77	1 (33%)

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
1	BFD	A	409	1,4	-	2/5/11/13	-
1	BFD	I	409	1	-	2/5/11/13	-
1	BFD	E	409	1	-	4/5/11/13	-
1	BFD	M	409	1	-	4/5/11/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	409	BFD	F3-BE	9.39	1.77	1.54
1	I	409	BFD	F3-BE	9.38	1.77	1.54
1	A	409	BFD	F3-BE	9.33	1.76	1.54
1	E	409	BFD	F3-BE	9.32	1.76	1.54
1	M	409	BFD	F2-BE	9.01	1.76	1.54
1	M	409	BFD	F1-BE	8.93	1.75	1.54
1	E	409	BFD	F2-BE	8.93	1.75	1.54
1	I	409	BFD	F2-BE	8.93	1.75	1.54
1	I	409	BFD	F1-BE	8.91	1.75	1.54
1	A	409	BFD	F2-BE	8.89	1.75	1.54
1	A	409	BFD	F1-BE	8.88	1.75	1.54
1	E	409	BFD	F1-BE	8.87	1.75	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	409	BFD	CA-CB-CG	-3.26	106.02	112.86
1	M	409	BFD	CA-CB-CG	-2.65	107.30	112.86
1	A	409	BFD	OD2-CG-CB	-2.62	118.94	124.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	409	BFD	N-CA-CB-CG
1	I	409	BFD	C-CA-CB-CG
1	M	409	BFD	C-CA-CB-CG
1	M	409	BFD	N-CA-CB-CG
1	A	409	BFD	CA-CB-CG-OD2
1	A	409	BFD	CA-CB-CG-OD1
1	E	409	BFD	C-CA-CB-CG
1	E	409	BFD	N-CA-CB-CG
1	E	409	BFD	CA-CB-CG-OD2
1	M	409	BFD	CA-CB-CG-OD2
1	E	409	BFD	CA-CB-CG-OD1
1	M	409	BFD	CA-CB-CG-OD1

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	409	BFD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	409	BFD	1	0
1	E	409	BFD	5	0
1	M	409	BFD	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	F	401	-	14,14,15	1.12	1 (7%)	17,19,21	1.00	2 (11%)
5	NAG	C	405	-	14,14,15	0.63	1 (7%)	17,19,21	0.82	1 (5%)
5	NAG	C	402	-	14,14,15	1.24	1 (7%)	17,19,21	0.63	0
6	AH2	F	403	-	11,11,11	0.99	0	15,15,15	1.14	1 (6%)
6	AH2	N	403	-	11,11,11	0.81	0	15,15,15	1.39	3 (20%)
5	NAG	J	402	-	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	F	402	-	14,14,15	0.51	0	17,19,21	0.45	0
5	NAG	J	401	-	14,14,15	0.18	0	17,19,21	0.49	0
5	NAG	F	405	-	13,13,15	0.34	0	14,17,21	0.59	0
5	NAG	N	405	-	13,13,15	0.35	0	14,17,21	0.53	0
5	NAG	N	404	-	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
3	P5S	I	1202	-	9,10,53	0.92	0	12,14,60	1.12	0
5	NAG	J	405	-	13,13,15	0.56	0	14,17,21	0.71	0
6	AH2	C	404	-	11,11,11	0.72	0	15,15,15	1.16	1 (6%)
5	NAG	C	403	-	14,14,15	0.56	0	17,19,21	0.97	2 (11%)
5	NAG	J	404	-	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
5	NAG	N	401	-	14,14,15	0.40	0	17,19,21	0.38	0
3	P5S	A	1201	-	9,10,53	0.93	0	12,14,60	1.18	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	P5S	E	1202	-	9,10,53	0.92	0	12,14,60	1.35	2 (16%)
5	NAG	C	406	-	13,13,15	0.49	0	14,17,21	0.52	0
3	P5S	E	1201	-	9,10,53	0.92	0	12,14,60	1.09	1 (8%)
3	P5S	I	1201	-	9,10,53	0.91	0	12,14,60	1.44	3 (25%)
3	P5S	C	401	-	52,53,53	0.98	2 (3%)	56,60,60	1.09	2 (3%)
6	AH2	J	403	-	11,11,11	0.83	0	15,15,15	1.28	1 (6%)
5	NAG	F	404	-	14,14,15	0.25	0	17,19,21	0.61	1 (5%)
5	NAG	N	402	-	14,14,15	0.22	0	17,19,21	0.42	0
3	P5S	M	1201	-	9,10,53	0.91	0	12,14,60	1.28	3 (25%)

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	NAG	F	401	-	-	4/6/23/26	0/1/1/1
5	NAG	C	405	-	-	1/6/23/26	0/1/1/1
5	NAG	C	402	-	-	4/6/23/26	0/1/1/1
6	AH2	F	403	-	-	1/2/19/19	0/1/1/1
6	AH2	N	403	-	-	1/2/19/19	1/1/1/1
5	NAG	J	402	-	-	1/6/23/26	0/1/1/1
5	NAG	F	402	-	-	1/6/23/26	0/1/1/1
5	NAG	J	401	-	-	3/6/23/26	0/1/1/1
5	NAG	F	405	-	-	3/6/19/26	1/1/1/1
5	NAG	N	405	-	-	1/6/19/26	0/1/1/1
5	NAG	N	404	-	-	2/6/23/26	0/1/1/1
3	P5S	I	1202	-	-	2/10/10/59	-
5	NAG	J	405	-	-	3/6/19/26	1/1/1/1
6	AH2	C	404	-	-	1/2/19/19	1/1/1/1
5	NAG	C	403	-	-	2/6/23/26	0/1/1/1
5	NAG	J	404	-	-	2/6/23/26	0/1/1/1
5	NAG	N	401	-	-	2/6/23/26	0/1/1/1
3	P5S	A	1201	-	-	3/10/10/59	-
3	P5S	E	1202	-	-	3/10/10/59	-
5	NAG	C	406	-	-	2/6/19/26	0/1/1/1
3	P5S	E	1201	-	-	9/10/10/59	-
3	P5S	I	1201	-	-	5/10/10/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P5S	C	401	-	-	19/59/59/59	-
6	AH2	J	403	-	-	2/2/19/19	1/1/1/1
5	NAG	F	404	-	-	1/6/23/26	0/1/1/1
5	NAG	N	402	-	-	0/6/23/26	0/1/1/1
3	P5S	M	1201	-	-	4/10/10/59	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	P5S	O37-C38	4.53	1.47	1.34
3	C	401	P5S	O19-C17	4.43	1.46	1.33
5	C	402	NAG	O5-C1	-4.43	1.36	1.43
5	F	401	NAG	O5-C1	-3.72	1.37	1.43
5	C	405	NAG	O5-C1	2.07	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	P5S	O37-C38-C39	4.42	121.02	111.50
6	J	403	AH2	C1-O5-C5	3.87	117.44	112.19
6	N	403	AH2	C1-O5-C5	3.75	117.27	112.19
6	C	404	AH2	C1-O5-C5	3.38	116.78	112.19
3	I	1201	P5S	OG-CB-CA	3.25	110.89	108.06
5	C	405	NAG	C1-O5-C5	3.10	116.39	112.19
3	C	401	P5S	O19-C17-C20	2.79	120.66	111.91
6	F	403	AH2	C1-O5-C5	2.70	115.85	112.19
5	J	404	NAG	C1-O5-C5	2.67	115.81	112.19
5	C	403	NAG	C1-O5-C5	2.65	115.78	112.19
3	E	1202	P5S	OG-CB-CA	2.59	110.31	108.06
3	M	1201	P5S	OG-CB-CA	2.53	110.26	108.06
3	A	1201	P5S	OXT-C-O	-2.47	118.48	124.09
5	C	403	NAG	C3-C4-C5	2.37	114.46	110.24
5	N	404	NAG	C1-O5-C5	2.31	115.32	112.19
5	F	401	NAG	C1-O5-C5	-2.30	109.07	112.19
6	N	403	AH2	O5-C1-C2	2.24	114.24	110.77
6	N	403	AH2	O2-C2-C3	-2.23	105.67	110.14
3	E	1202	P5S	OXT-C-O	-2.22	119.05	124.09
3	I	1201	P5S	OXT-C-O	-2.16	119.19	124.09
5	F	401	NAG	C2-N2-C7	2.15	125.96	122.90
5	F	404	NAG	C1-O5-C5	2.11	115.05	112.19
3	M	1201	P5S	OXT-C-CA	2.09	120.51	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1201	P5S	OXT-C-O	-2.09	119.35	124.09
3	I	1201	P5S	OXT-C-CA	2.04	120.34	113.38
3	E	1201	P5S	OXT-C-O	-2.02	119.51	124.09

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	P5S	C-CA-CB-OG
3	A	1201	P5S	N-CA-CB-OG
3	C	401	P5S	O-C-CA-N
3	C	401	P5S	N-CA-CB-OG
3	C	401	P5S	C39-C38-O37-C2
3	E	1201	P5S	O-C-CA-N
3	E	1201	P5S	O-C-CA-CB
3	E	1201	P5S	OXT-C-CA-CB
3	E	1201	P5S	C-CA-CB-OG
3	E	1201	P5S	N-CA-CB-OG
3	E	1201	P5S	CB-OG-P12-O13
3	E	1202	P5S	C-CA-CB-OG
3	E	1202	P5S	N-CA-CB-OG
3	I	1201	P5S	C-CA-CB-OG
3	I	1201	P5S	N-CA-CB-OG
3	I	1201	P5S	CB-OG-P12-O13
5	C	406	NAG	C4-C5-C6-O6
5	C	406	NAG	O5-C5-C6-O6
5	F	405	NAG	C1-C2-N2-C7
5	F	405	NAG	C8-C7-N2-C2
5	F	405	NAG	O7-C7-N2-C2
5	J	405	NAG	O5-C5-C6-O6
3	C	401	P5S	O47-C38-O37-C2
5	F	401	NAG	O5-C5-C6-O6
5	C	403	NAG	O5-C5-C6-O6
3	M	1201	P5S	OXT-C-CA-N
5	C	402	NAG	O5-C5-C6-O6
6	J	403	AH2	O5-C5-C6-O6
5	J	404	NAG	O5-C5-C6-O6
5	F	401	NAG	C4-C5-C6-O6
5	C	403	NAG	C4-C5-C6-O6
3	E	1201	P5S	OXT-C-CA-N
5	C	402	NAG	C8-C7-N2-C2
5	C	402	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	F	401	NAG	C8-C7-N2-C2
5	F	401	NAG	O7-C7-N2-C2
5	J	401	NAG	C8-C7-N2-C2
5	J	401	NAG	O7-C7-N2-C2
5	N	401	NAG	C8-C7-N2-C2
5	N	401	NAG	O7-C7-N2-C2
5	C	402	NAG	C4-C5-C6-O6
5	N	405	NAG	C1-C2-N2-C7
5	N	404	NAG	O5-C5-C6-O6
6	J	403	AH2	C4-C5-C6-O6
3	C	401	P5S	C20-C21-C22-C23
3	C	401	P5S	OXT-C-CA-N
5	C	405	NAG	O5-C5-C6-O6
6	N	403	AH2	O5-C5-C6-O6
5	J	404	NAG	C4-C5-C6-O6
3	C	401	P5S	C25-C26-C27-C28
3	C	401	P5S	C-CA-CB-OG
6	C	404	AH2	O5-C5-C6-O6
6	F	403	AH2	O5-C5-C6-O6
5	J	402	NAG	O5-C5-C6-O6
3	C	401	P5S	C45-C46-C48-C49
5	J	401	NAG	O5-C5-C6-O6
3	C	401	P5S	O19-C1-C2-C3
3	M	1201	P5S	O-C-CA-N
3	C	401	P5S	C22-C23-C24-C25
3	I	1201	P5S	CB-OG-P12-O16
3	I	1201	P5S	CA-CB-OG-P12
3	C	401	P5S	C20-C17-O19-C1
3	C	401	P5S	O18-C17-O19-C1
3	C	401	P5S	O19-C1-C2-O37
3	C	401	P5S	C39-C40-C41-C42
3	C	401	P5S	CB-OG-P12-O16
3	C	401	P5S	C3-O16-P12-OG
3	I	1202	P5S	O-C-CA-CB
3	M	1201	P5S	O-C-CA-CB
3	M	1201	P5S	OXT-C-CA-CB
5	N	404	NAG	C4-C5-C6-O6
5	F	404	NAG	C1-C2-N2-C7
3	C	401	P5S	C44-C45-C46-C48
3	E	1201	P5S	CB-OG-P12-O16
3	E	1202	P5S	CB-OG-P12-O15
3	C	401	P5S	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
3	A	1201	P5S	CA-CB-OG-P12
3	E	1201	P5S	CA-CB-OG-P12
3	I	1202	P5S	OXT-C-CA-CB
5	F	402	NAG	C3-C2-N2-C7
5	J	405	NAG	C3-C2-N2-C7
5	J	405	NAG	C4-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	405	NAG	C1-C2-C3-C4-C5-O5
6	N	403	AH2	C1-C2-C3-C4-C5-O5
6	J	403	AH2	C1-C2-C3-C4-C5-O5
6	C	404	AH2	C1-C2-C3-C4-C5-O5
5	J	405	NAG	C1-C2-C3-C4-C5-O5

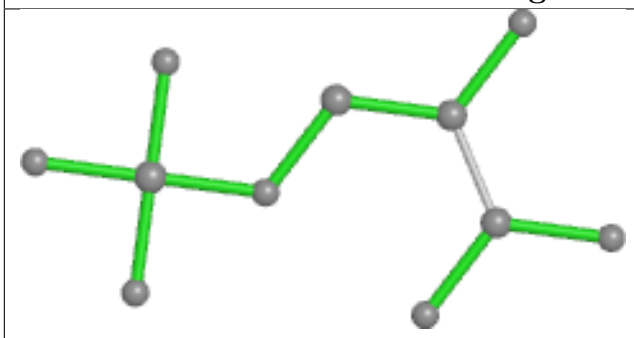
12 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	401	NAG	1	0
5	C	402	NAG	2	0
5	F	405	NAG	18	0
5	N	405	NAG	15	0
5	J	405	NAG	7	0
5	J	404	NAG	11	0
3	E	1202	P5S	1	0
5	C	406	NAG	1	0
3	I	1201	P5S	9	0
3	C	401	P5S	2	0
5	F	404	NAG	4	0
3	M	1201	P5S	1	0

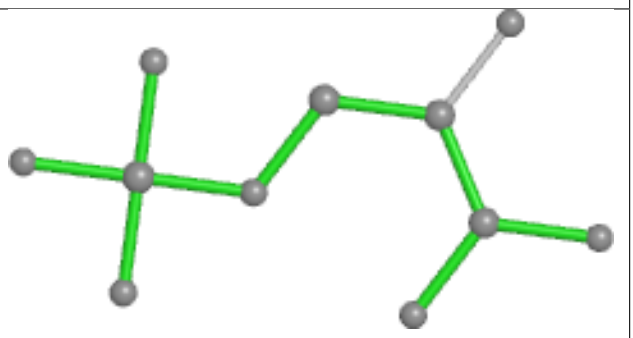
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

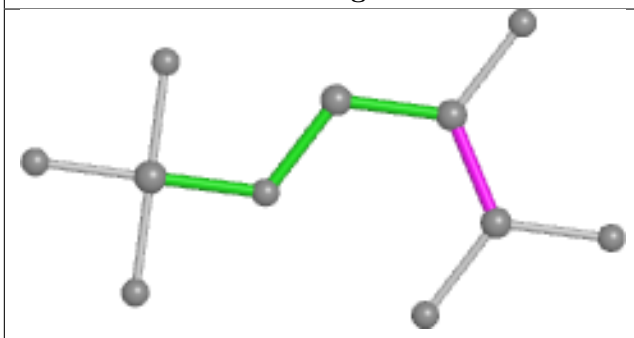
Ligand P5S I 1202



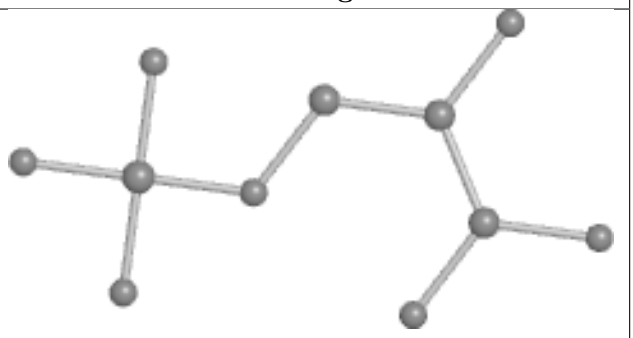
Bond lengths



Bond angles

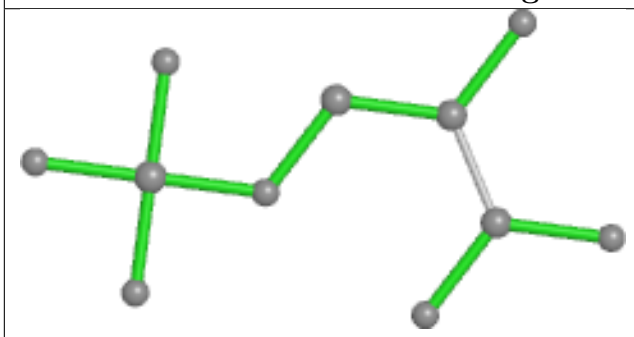


Torsions

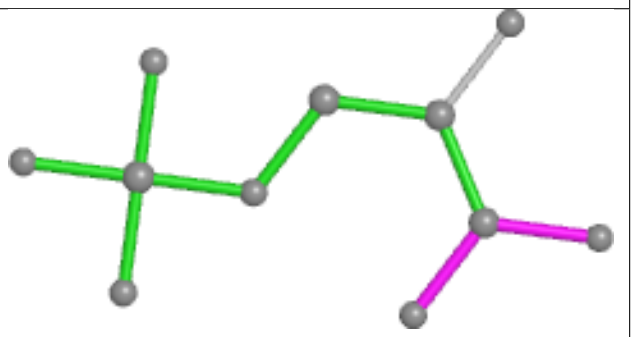


Rings

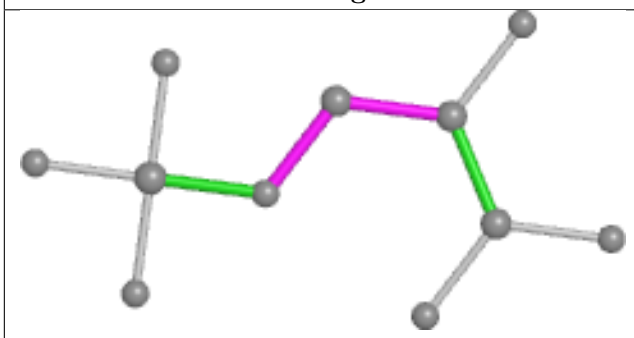
Ligand P5S A 1201



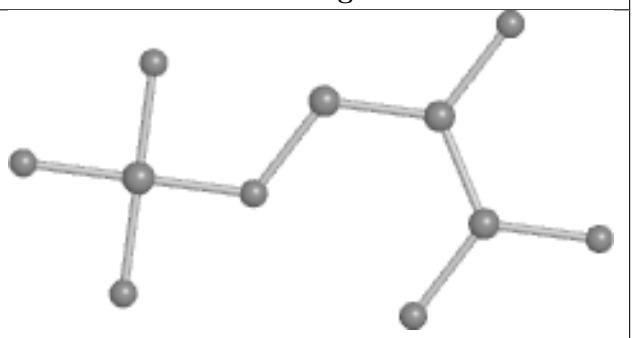
Bond lengths



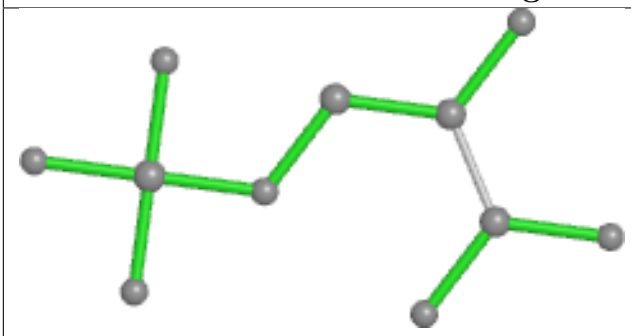
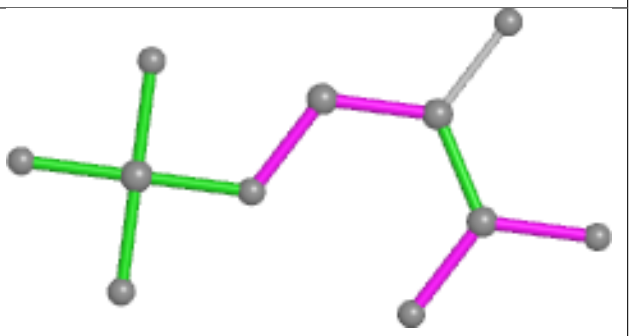
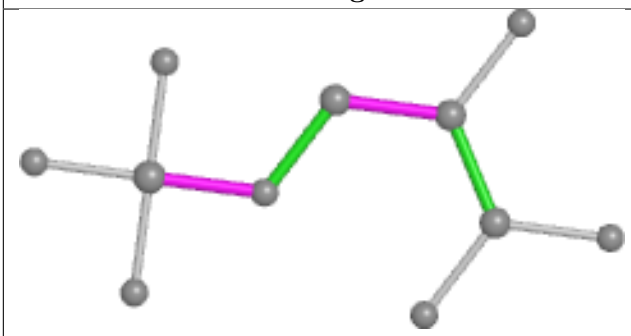
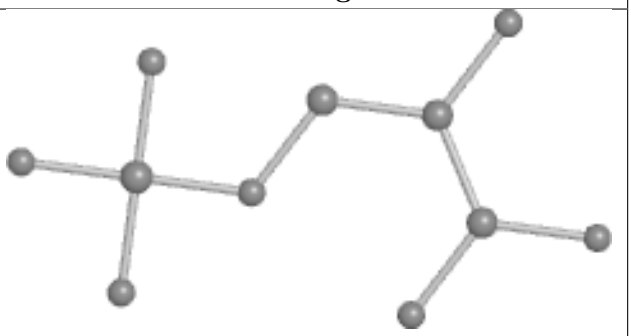
Bond angles

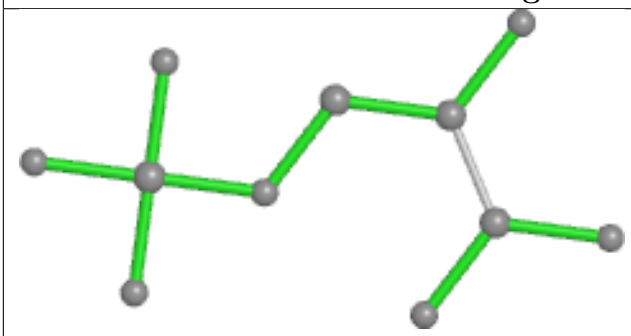
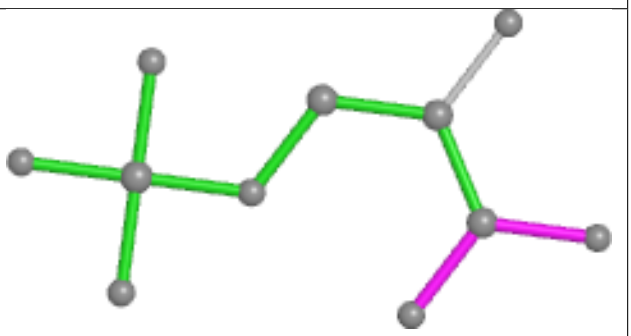
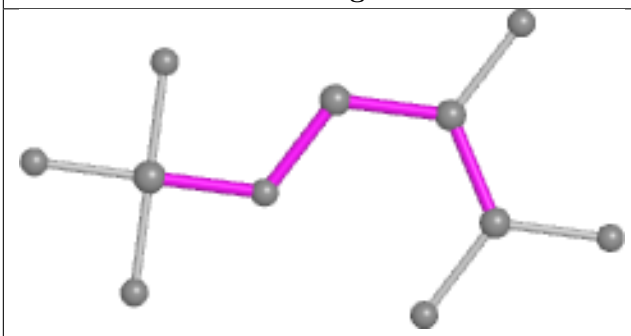
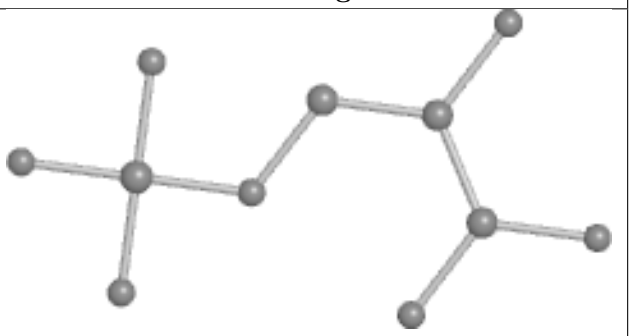


Torsions

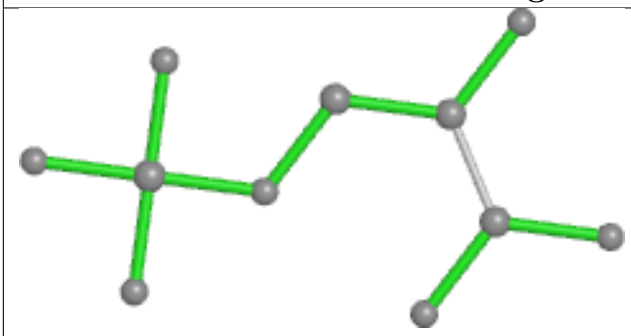


Rings

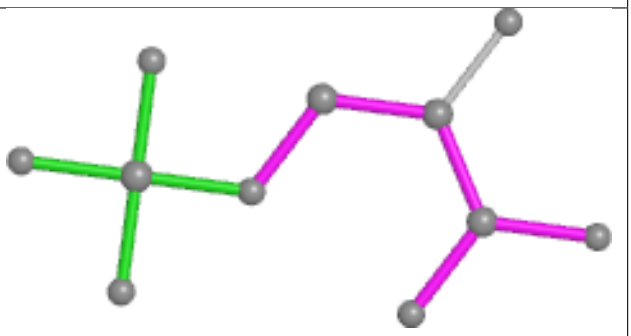
Ligand P5S E 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand P5S E 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

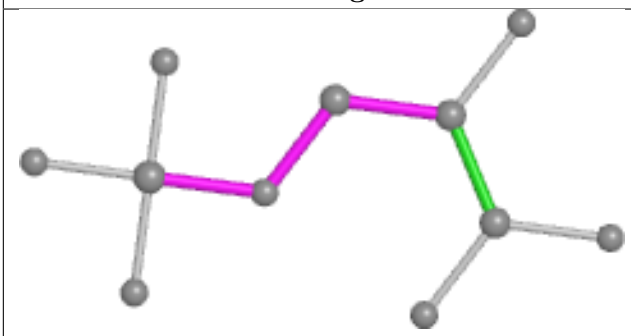
Ligand P5S I 1201



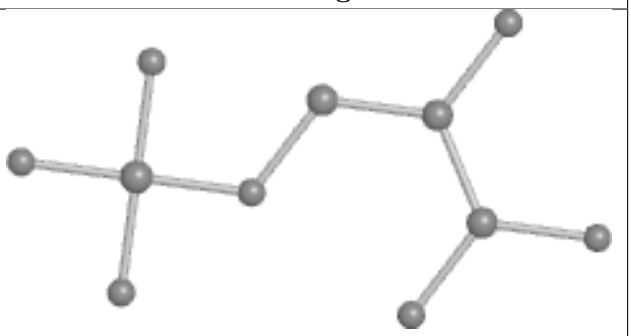
Bond lengths



Bond angles

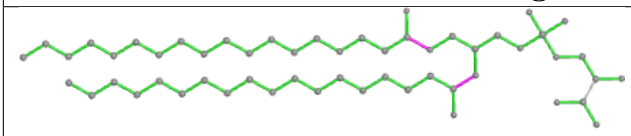


Torsions

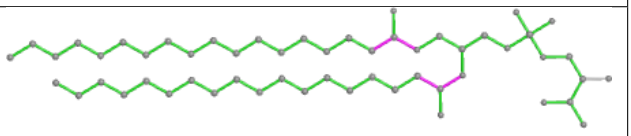


Rings

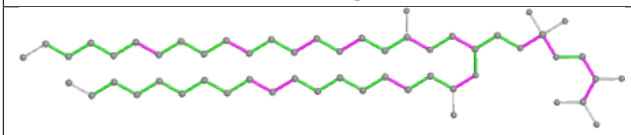
Ligand P5S C 401



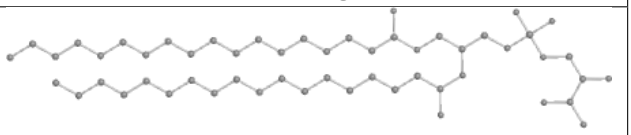
Bond lengths



Bond angles

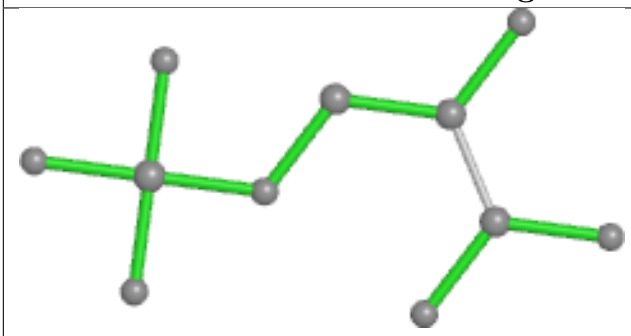


Torsions

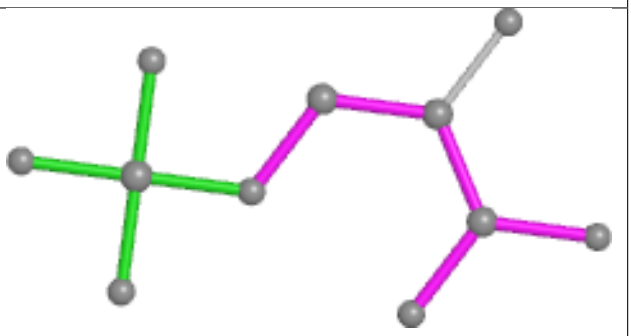


Rings

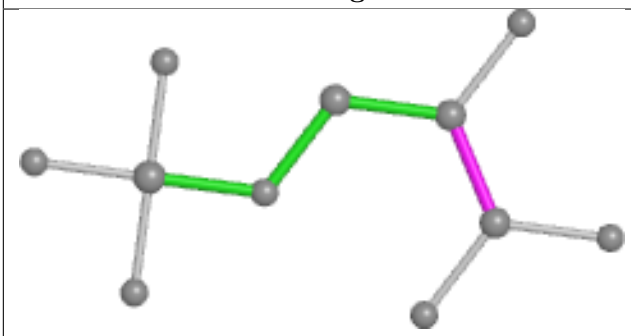
Ligand P5S M 1201



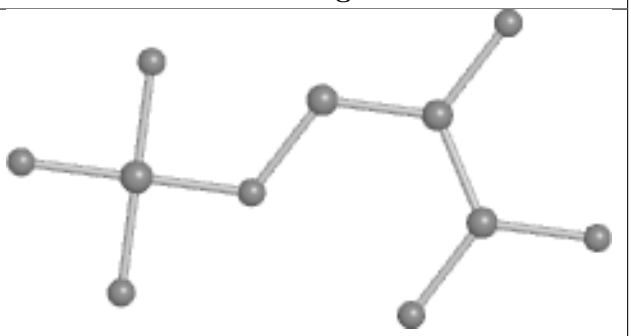
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1063/1129 (94%)	-0.16	42 (3%) 38 30	24, 120, 194, 235	0
1	E	1063/1129 (94%)	0.05	93 (8%) 10 8	31, 115, 211, 246	0
1	I	1063/1129 (94%)	0.18	101 (9%) 8 6	96, 173, 226, 261	0
1	M	1063/1129 (94%)	0.33	125 (11%) 4 4	124, 214, 315, 367	0
2	C	324/361 (89%)	-0.60	0 100 100	21, 79, 153, 183	0
2	F	324/361 (89%)	-0.58	3 (0%) 84 77	25, 71, 136, 166	0
2	J	324/361 (89%)	-0.05	21 (6%) 18 13	118, 189, 255, 281	0
2	N	324/361 (89%)	0.86	75 (23%) 0 0	204, 340, 392, 416	0
All	All	5548/5960 (93%)	0.05	460 (8%) 11 9	21, 164, 320, 416	0

All (460) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	172	GLY	13.3
1	E	37	ALA	10.7
2	N	176	ASN	10.2
1	E	431	TYR	9.9
1	E	432	LYS	9.1
1	E	193	THR	8.6
1	M	241	PRO	8.6
1	I	744	HIS	8.4
1	M	1089	ASN	8.4
2	N	233	PRO	8.4
2	N	273	TYR	8.3
1	I	432	LYS	8.1
1	E	599	ALA	8.1
1	M	240	GLY	8.0
1	A	37	ALA	8.0
1	I	435	THR	8.0

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Mol	Chain	Res	Type	RSRZ
1	I	134	VAL	7.8
1	E	560	LEU	7.7
1	M	549	VAL	7.6
1	M	704	THR	7.5
1	M	1046	PRO	7.5
1	I	577	GLU	7.3
1	E	561	PHE	7.3
1	E	438	VAL	7.0
1	M	602	GLU	7.0
1	I	559	LEU	6.8
1	E	550	ILE	6.7
1	E	439	ASP	6.6
1	I	599	ALA	6.6
1	E	433	GLY	6.5
1	A	38	GLN	6.4
1	E	600	PHE	6.4
2	N	204	ILE	6.3
1	I	696	GLU	6.3
1	I	740	ALA	6.2
1	M	484	THR	6.1
1	E	485	GLU	6.0
1	E	559	LEU	6.0
2	N	215	ARG	5.9
2	N	167	PRO	5.9
2	N	137	SER	5.9
1	E	549	VAL	5.9
2	N	217	PRO	5.9
1	I	576	HIS	5.9
2	N	170	PRO	5.9
1	I	515	ASN	5.8
1	M	854	HIS	5.7
1	E	38	GLN	5.7
1	I	226	ASN	5.7
1	E	551	VAL	5.6
1	I	433	GLY	5.6
1	M	152	ASP	5.5
1	E	434	VAL	5.4
1	M	251	LEU	5.4
2	N	234	VAL	5.4
1	M	497	ASP	5.4
1	E	229	SER	5.4
1	A	240	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	M	853	LYS	5.3
1	I	227	ILE	5.3
1	E	602	GLU	5.3
1	M	1047	PHE	5.3
2	N	258	ILE	5.2
1	I	741	TRP	5.2
1	I	434	VAL	5.1
2	N	299	TYR	5.0
1	M	570	PHE	5.0
1	E	435	THR	4.9
1	I	423	GLU	4.9
1	M	194	ILE	4.9
1	I	695	THR	4.9
1	I	128	ILE	4.9
2	N	136	LYS	4.9
1	A	192	ASP	4.9
2	N	177	SER	4.8
1	M	189	ALA	4.8
1	E	460	GLU	4.8
1	I	442	SER	4.8
2	N	216	ASN	4.7
1	A	484	THR	4.7
1	I	474	ILE	4.7
1	I	557	ASP	4.7
2	N	171	CYS	4.7
1	I	737	PHE	4.7
2	N	211	ASN	4.6
1	M	1044	ILE	4.6
1	M	188	TYR	4.5
1	E	471	THR	4.5
2	N	129	GLN	4.5
1	E	240	GLY	4.5
1	I	575	ASN	4.5
1	M	1045	TRP	4.5
1	E	192	ASP	4.5
1	I	436	GLN	4.5
1	I	522	VAL	4.4
1	M	153	GLU	4.4
1	I	229	SER	4.4
1	I	223	GLY	4.4
1	A	736	SER	4.4
1	E	459	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
2	N	257	PHE	4.3
1	M	641	ASN	4.3
1	I	513	LEU	4.3
2	N	252	PHE	4.3
1	I	514	GLY	4.3
1	M	737	PHE	4.3
1	I	424	CYS	4.3
1	I	560	LEU	4.3
1	M	705	ILE	4.3
1	M	493	SER	4.3
1	E	437	GLU	4.3
1	I	228	TYR	4.3
1	I	603	ILE	4.2
1	A	483	ALA	4.2
1	A	140	LYS	4.2
1	I	550	ILE	4.2
1	E	641	ASN	4.2
1	A	203	ASP	4.2
2	N	180	ASN	4.2
1	I	644	GLY	4.1
1	I	484	THR	4.1
1	I	471	THR	4.1
1	M	165	CYS	4.1
1	E	738	LYS	4.1
1	A	234	ALA	4.1
1	I	602	GLU	4.0
2	N	168	ILE	4.0
1	A	559	LEU	4.0
2	J	199	LEU	4.0
1	M	334	THR	4.0
2	N	163	ASN	4.0
2	J	197	ILE	4.0
2	N	210	LYS	4.0
2	J	127	PHE	4.0
1	E	1043	ILE	3.9
1	I	195	ALA	3.9
2	N	212	VAL	3.9
2	N	179	PHE	3.9
2	N	237	LEU	3.9
2	N	208	THR	3.9
2	J	348	HIS	3.9
1	E	562	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	746	GLU	3.9
1	M	554	GLN	3.9
2	N	300	PRO	3.8
1	E	30	SER	3.8
2	N	162	ARG	3.8
1	E	519	TYR	3.8
1	I	470	HIS	3.8
2	N	322	ASN	3.8
1	M	600	PHE	3.8
1	A	654	ASP	3.8
1	E	624	ASP	3.8
1	M	255	GLU	3.8
1	I	192	ASP	3.7
1	E	472	VAL	3.7
1	E	470	HIS	3.7
1	I	422	ILE	3.7
1	M	474	ILE	3.7
2	N	350	TYR	3.7
1	M	550	ILE	3.7
1	E	493	SER	3.6
1	M	567	SER	3.6
2	J	198	ALA	3.6
1	M	496	PRO	3.6
2	N	213	LYS	3.6
1	E	627	GLU	3.6
1	I	558	ILE	3.6
1	I	488	GLU	3.6
1	M	575	ASN	3.6
1	M	257	ILE	3.5
1	E	478	ASP	3.5
1	E	227	ILE	3.5
2	N	155	LYS	3.5
1	I	275	GLN	3.5
1	M	610	ARG	3.5
1	I	438	VAL	3.5
1	M	569	VAL	3.5
1	I	600	PHE	3.5
1	A	658	GLU	3.5
1	A	655	GLN	3.5
1	M	1091	ARG	3.4
1	E	481	ASP	3.4
1	M	706	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	133	ARG	3.4
1	E	557	ASP	3.4
1	M	390	LEU	3.4
1	M	256	LYS	3.4
1	M	167	THR	3.4
2	N	205	ALA	3.4
1	M	321	GLU	3.4
1	E	573	VAL	3.4
1	M	563	LYS	3.4
2	N	225	GLU	3.4
2	N	218	PRO	3.4
1	M	233	GLU	3.4
1	I	551	VAL	3.4
1	I	208	ALA	3.4
1	I	443	GLN	3.4
1	M	193	THR	3.4
1	M	595	THR	3.3
1	M	274	TYR	3.3
1	M	335	LEU	3.3
2	N	274	ARG	3.3
1	M	136	LYS	3.3
2	N	140	ASP	3.3
1	A	270	MET	3.3
1	M	311	TYR	3.2
2	N	261	MET	3.2
2	J	280	SER	3.2
1	A	476	THR	3.2
2	F	229	GLY	3.2
2	N	314	THR	3.2
1	M	653	GLN	3.2
1	A	489	LEU	3.2
1	I	230	ASN	3.2
1	I	472	VAL	3.2
1	E	334	THR	3.2
1	M	601	LYS	3.2
2	N	275	LEU	3.1
1	E	228	TYR	3.1
2	N	138	ARG	3.1
1	M	170	THR	3.1
1	I	225	ILE	3.1
2	J	189	GLY	3.1
1	E	262	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	40	PHE	3.1
1	I	441	LEU	3.1
1	M	536	HIS	3.1
1	A	485	GLU	3.1
2	J	298	ASN	3.1
2	N	169	ALA	3.1
1	I	519	TYR	3.0
1	M	635	ASP	3.0
1	E	473	GLU	3.0
1	M	252	LYS	3.0
1	E	429	HIS	3.0
1	M	192	ASP	3.0
1	E	442	SER	3.0
1	M	275	GLN	3.0
1	I	641	ASN	3.0
1	M	253	ASN	3.0
2	N	156	GLU	2.9
2	N	236	TRP	2.9
1	E	171	CYS	2.9
1	M	195	ALA	2.9
1	E	570	PHE	2.9
2	N	256	ASP	2.9
1	I	697	LEU	2.9
1	M	495	SER	2.9
1	I	476	THR	2.9
1	A	764	GLN	2.9
1	A	765	ASP	2.9
1	M	391	VAL	2.9
1	E	170	THR	2.9
1	E	536	HIS	2.9
2	N	203	GLY	2.9
2	N	277	GLU	2.9
1	A	277	LYS	2.9
1	M	389	ALA	2.9
1	M	895	CYS	2.9
1	M	164	SER	2.9
1	M	470	HIS	2.9
1	I	425	CYS	2.9
1	M	1018	TRP	2.9
1	E	482	GLY	2.8
1	M	736	SER	2.8
1	M	857	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	736	SER	2.8
1	E	188	TYR	2.8
1	I	520	MET	2.8
1	E	436	GLN	2.8
1	I	461	LEU	2.8
1	M	856	LYS	2.8
1	M	742	THR	2.8
2	J	46	THR	2.8
1	I	431	TYR	2.8
1	M	559	LEU	2.8
2	J	44	ILE	2.8
1	I	604	ALA	2.8
1	I	475	LYS	2.8
1	E	209	ILE	2.8
1	I	124	THR	2.8
1	E	167	THR	2.8
1	I	549	VAL	2.8
1	M	611	ILE	2.8
2	N	253	ILE	2.8
1	A	482	GLY	2.8
1	A	737	PHE	2.8
1	I	485	GLU	2.8
1	M	494	SER	2.7
1	I	473	GLU	2.7
1	M	939	PRO	2.7
2	J	200	LYS	2.7
2	N	117	ASN	2.7
1	M	114	HIS	2.7
1	I	460	GLU	2.7
1	M	483	ALA	2.7
1	A	477	ASN	2.7
1	E	515	ASN	2.7
2	N	231	THR	2.7
1	M	228	TYR	2.7
1	M	1049	LYS	2.7
1	M	488	GLU	2.6
2	N	77	GLU	2.6
1	E	165	CYS	2.6
1	M	151	ALA	2.6
1	M	548	SER	2.6
2	N	209	ASP	2.6
2	J	350	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	745	GLN	2.6
1	M	486	SER	2.6
1	I	487	ALA	2.6
1	M	312	VAL	2.6
1	I	574	GLN	2.6
2	N	141	SER	2.6
1	E	487	ALA	2.6
1	E	486	SER	2.6
2	N	313	SER	2.6
1	E	461	LEU	2.6
1	A	656	ALA	2.6
1	I	483	ALA	2.6
1	E	489	LEU	2.6
1	M	652	LEU	2.6
1	M	537	THR	2.6
2	N	165	ASP	2.6
1	M	738	LYS	2.6
1	E	222	VAL	2.6
1	I	168	ASP	2.5
1	I	598	VAL	2.5
1	M	150	GLN	2.5
1	E	430	LYS	2.5
1	E	494	SER	2.5
1	E	190	VAL	2.5
1	I	646	THR	2.5
2	J	111	GLU	2.5
1	A	536	HIS	2.5
1	E	440	GLY	2.5
1	M	487	ALA	2.5
2	J	116	GLY	2.5
1	M	485	GLU	2.5
2	N	127	PHE	2.5
1	I	578	ILE	2.5
1	M	254	THR	2.5
1	M	512	PHE	2.5
1	M	564	GLY	2.5
1	E	445	ASP	2.5
2	N	173	ALA	2.5
1	A	167	THR	2.5
1	E	474	ILE	2.5
1	M	834	LYS	2.5
2	N	245	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	456	LYS	2.5
1	I	645	ALA	2.5
2	N	235	ASN	2.4
2	N	40	ALA	2.4
1	E	467	CYS	2.4
1	I	643	ILE	2.4
2	N	255	GLU	2.4
1	M	599	ALA	2.4
1	M	703	LYS	2.4
2	N	224	GLU	2.4
1	E	518	GLY	2.4
1	I	131	ALA	2.4
1	I	465	ALA	2.4
1	I	127	ILE	2.4
1	I	654	ASP	2.4
1	M	38	GLN	2.4
1	M	50	TYR	2.4
1	M	655	GLN	2.4
1	M	806	LYS	2.4
1	I	457	ASN	2.4
1	E	475	LYS	2.4
1	M	262	VAL	2.3
1	M	1016	ARG	2.3
1	E	739	LYS	2.3
1	M	171	CYS	2.3
2	N	251	GLY	2.3
1	E	476	THR	2.3
1	I	765	ASP	2.3
1	M	1024	PHE	2.3
2	F	230	THR	2.3
2	N	128	TYR	2.3
1	A	766	SER	2.3
1	M	111	TRP	2.3
1	M	142	LYS	2.3
1	E	263	TYR	2.3
1	M	805	LEU	2.3
2	J	290	ARG	2.3
1	M	732	LYS	2.3
1	M	141	ILE	2.3
1	M	196	LEU	2.3
1	E	172	TYR	2.3
1	E	241	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	303	TYR	2.3
1	I	146	VAL	2.3
1	E	197	CYS	2.3
1	A	433	GLY	2.3
1	I	224	ARG	2.3
1	A	569	VAL	2.2
2	J	179	PHE	2.2
2	N	302	HIS	2.2
1	M	605	PRO	2.2
1	E	275	GLN	2.2
1	M	1017	PHE	2.2
1	A	170	THR	2.2
1	M	185	LYS	2.2
2	J	74	ASN	2.2
1	E	29	VAL	2.2
1	A	256	LYS	2.2
1	I	132	LYS	2.2
2	F	163	ASN	2.2
1	E	455	ASP	2.2
1	I	439	ASP	2.2
2	N	272	LEU	2.2
1	E	644	GLY	2.2
2	J	48	GLY	2.2
1	I	554	GLN	2.2
1	M	163	SER	2.2
1	E	598	VAL	2.2
2	N	207	TRP	2.2
1	A	537	THR	2.2
1	I	713	ASP	2.2
1	E	443	GLN	2.2
1	M	711	LYS	2.2
1	A	152	ASP	2.1
1	A	570	PHE	2.1
2	N	305	ASP	2.1
1	A	316	THR	2.1
1	A	239	LEU	2.1
1	M	604	ALA	2.1
1	E	469	CYS	2.1
1	A	238	SER	2.1
1	M	571	PRO	2.1
1	I	445	ASP	2.1
2	J	112	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	39	ARG	2.1
1	A	39	ARG	2.1
1	A	566	ASP	2.1
1	A	560	LEU	2.1
1	M	990	TYR	2.1
1	M	1050	GLN	2.1
1	M	560	LEU	2.1
1	I	953	LEU	2.1
1	E	208	ALA	2.1
2	N	232	LYS	2.1
2	N	238	LYS	2.1
1	I	31	GLU	2.0
1	I	715	LEU	2.0
1	M	562	CYS	2.0
2	J	45	LEU	2.0
2	J	349	LYS	2.0
1	E	601	LYS	2.0
1	E	446	GLY	2.0
2	N	241	TYR	2.0
1	I	38	GLN	2.0
1	M	480	VAL	2.0
1	M	712	GLU	2.0
1	E	441	LEU	2.0
1	I	854	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	BFD	M	409	12/13	0.81	0.32	184,209,238,250	0
1	BFD	I	409	12/13	0.87	0.29	148,153,162,162	0
1	BFD	A	409	12/13	0.95	0.27	70,84,106,109	0
1	BFD	E	409	12/13	0.95	0.23	59,78,88,89	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

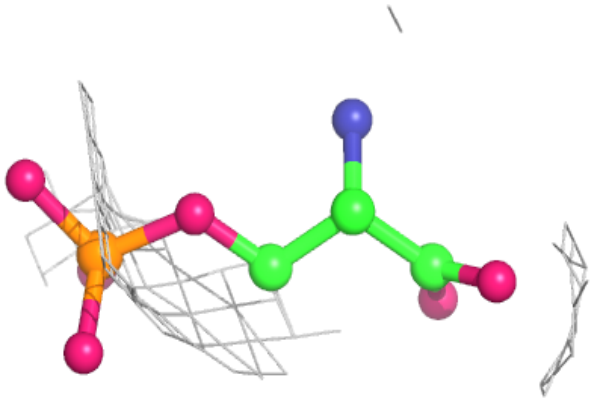
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

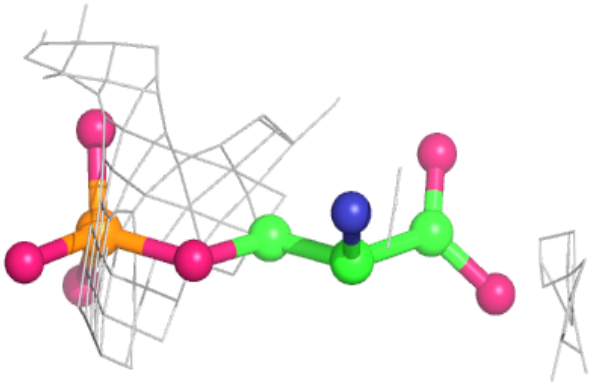
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	AH2	N	403	11/11	-0.02	0.90	347,350,356,359	0
5	NAG	N	404	14/15	0.55	0.25	398,409,413,415	0
3	P5S	M	1201	11/54	0.60	0.21	293,299,310,312	0
5	NAG	J	405	13/15	0.63	0.21	255,269,274,276	0
5	NAG	N	401	14/15	0.68	0.47	335,342,344,344	0
6	AH2	F	403	11/11	0.71	0.24	143,165,168,170	0
6	AH2	J	403	11/11	0.78	0.22	155,161,168,172	0
5	NAG	J	404	14/15	0.78	0.20	238,242,246,249	0
6	AH2	C	404	11/11	0.79	0.27	117,126,144,145	0
3	P5S	I	1201	11/54	0.80	0.26	220,231,238,239	0
5	NAG	J	401	14/15	0.80	0.22	145,176,183,185	0
3	P5S	I	1202	11/54	0.81	0.34	151,162,189,189	0
5	NAG	F	405	13/15	0.83	0.20	125,133,149,153	0
3	P5S	E	1202	11/54	0.85	0.25	78,97,159,160	0
3	P5S	C	401	54/54	0.86	0.33	92,120,135,141	0
5	NAG	N	402	14/15	0.87	0.53	309,312,317,319	0
5	NAG	N	405	13/15	0.87	0.16	356,362,366,367	0
3	P5S	A	1201	11/54	0.90	0.37	107,117,167,172	0
4	MG	I	1203	1/1	0.90	0.27	139,139,139,139	0
5	NAG	C	406	13/15	0.90	0.19	70,93,122,127	0
5	NAG	F	404	14/15	0.90	0.23	61,100,139,145	0
5	NAG	C	405	14/15	0.92	0.19	99,111,127,137	0
5	NAG	F	402	14/15	0.93	0.16	45,82,110,113	0
5	NAG	J	402	14/15	0.93	0.13	156,172,186,190	0
5	NAG	F	401	14/15	0.94	0.18	66,80,102,109	0
5	NAG	C	402	14/15	0.95	0.18	41,71,97,98	0
5	NAG	C	403	14/15	0.95	0.16	75,107,121,124	0
4	MG	M	1202	1/1	0.97	0.40	185,185,185,185	0
4	MG	E	1203	1/1	0.97	0.33	91,91,91,91	0
3	P5S	E	1201	11/54	0.97	0.18	70,85,102,110	0
4	MG	A	1202	1/1	0.99	0.28	172,172,172,172	0

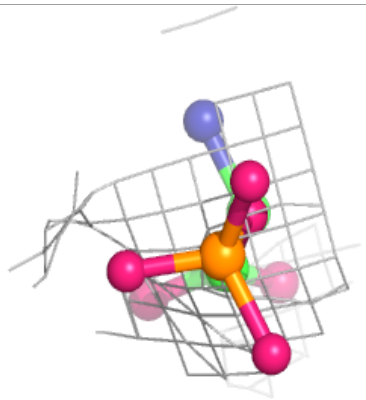
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P5S M 1201:

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

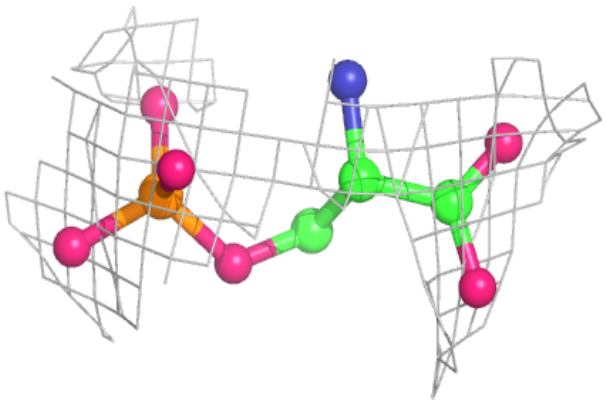


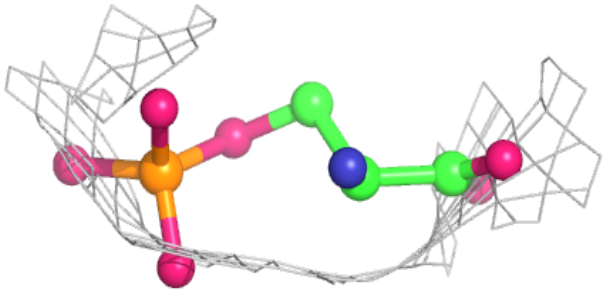


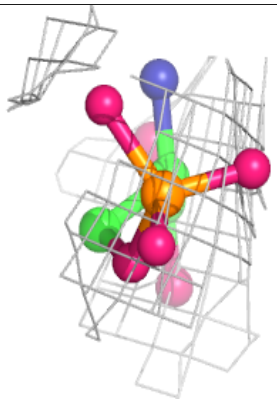


Electron density around P5S I 1201:

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

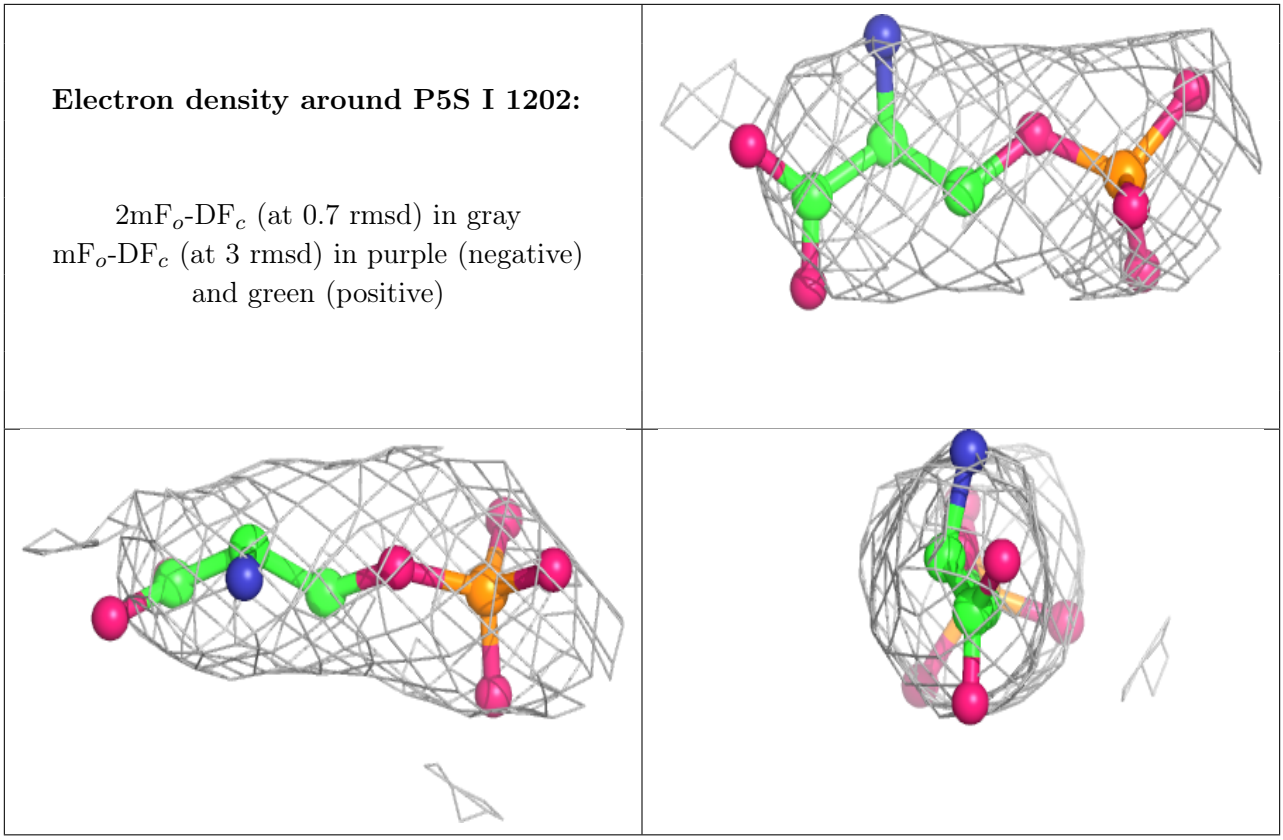






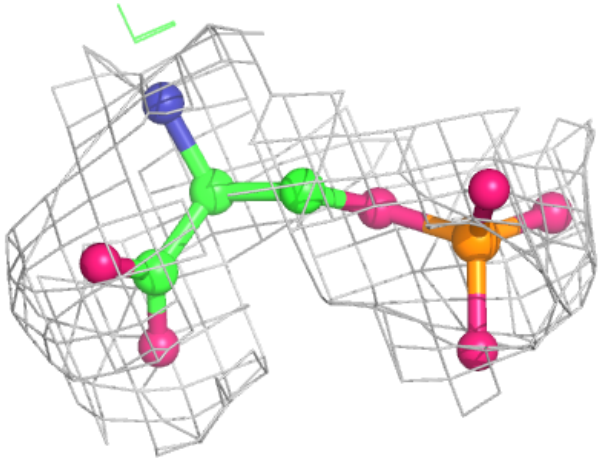
Electron density around P5S I 1202:

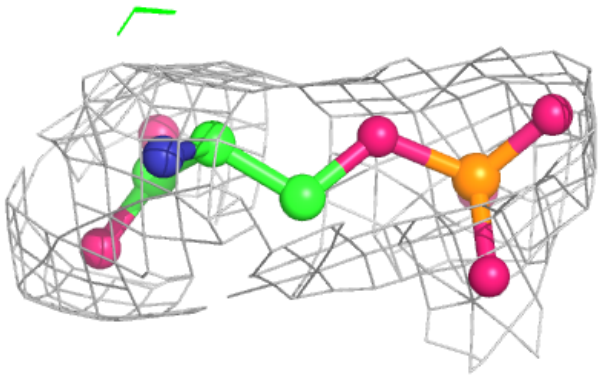
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

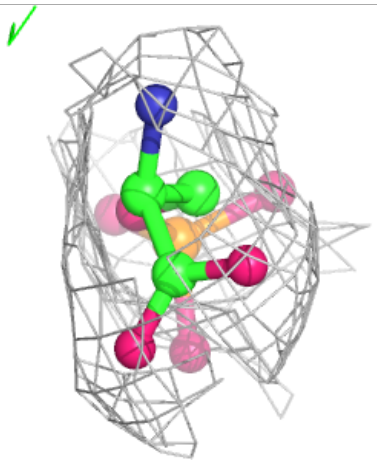


Electron density around P5S E 1202:

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

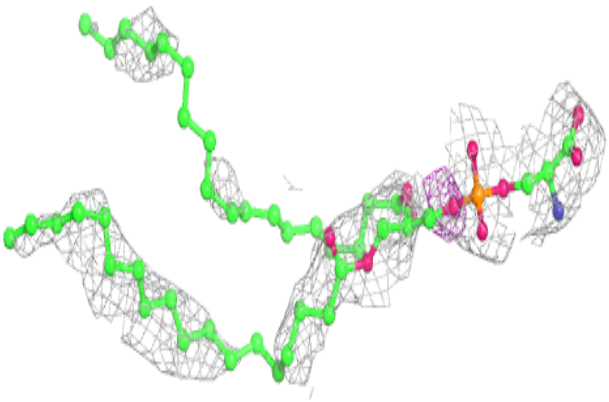


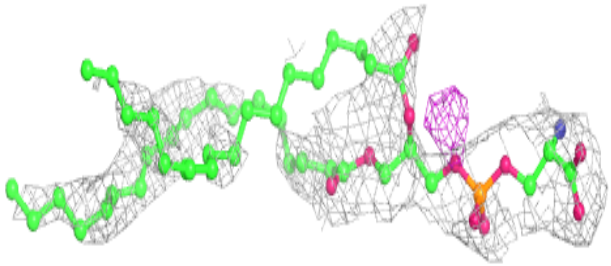




Electron density around P5S C 401:

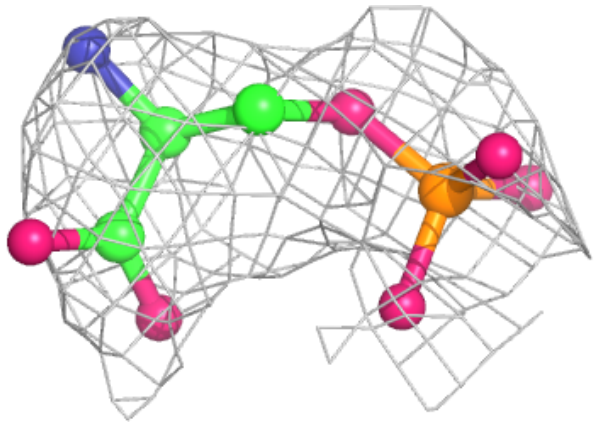
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

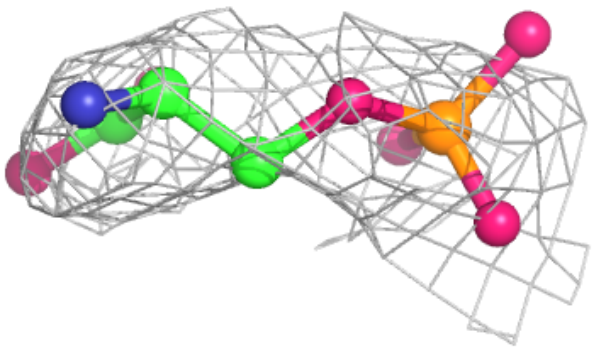


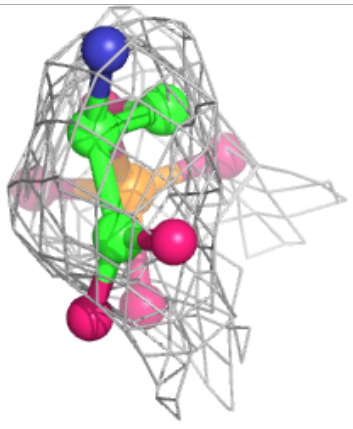


Electron density around P5S A 1201:

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

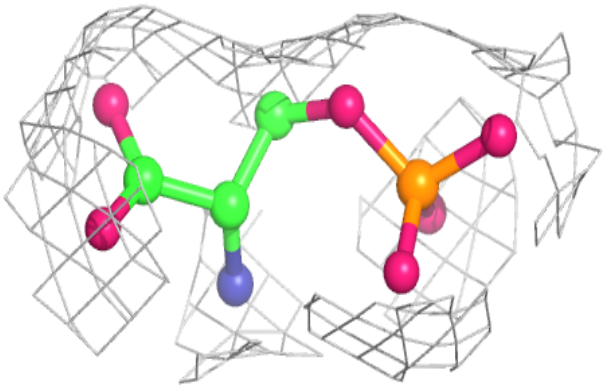


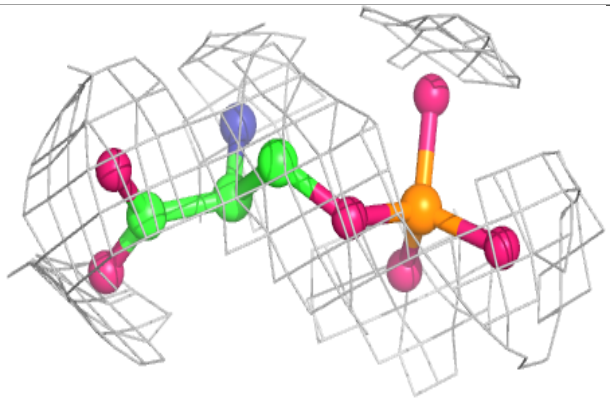


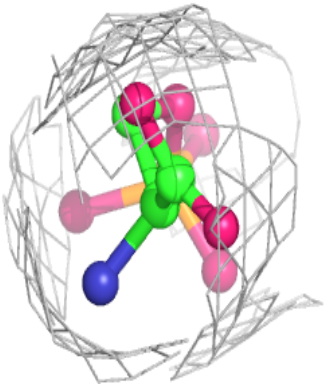


Electron density around P5S E 1201:

$2mF_o$-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.