



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 05:00 PM BST

PDB ID : 4HNV
Title : Crystal structure of R54E mutant of *S. aureus* Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

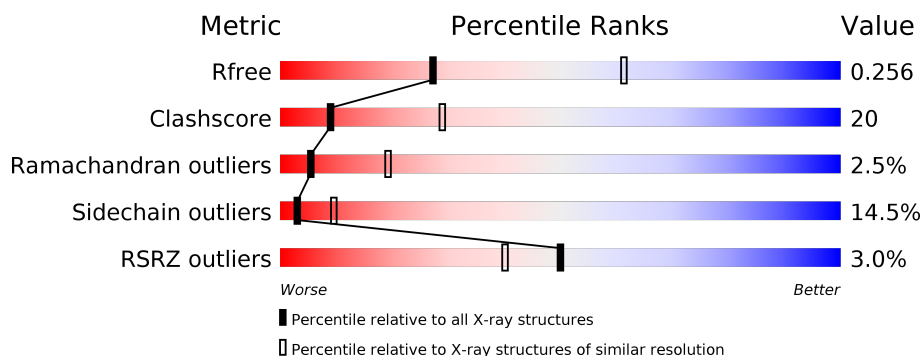
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1173	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>6%</div> <div>••</div> </div> </div>
1	B	1173	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>30%</div> <div>6%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	1173	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>28%</div> <div>7%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	1173	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>27%</div> <div>6%</div> <div>•</div> <div>9%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTI	B	1201	-	-	X	-
4	BTI	B	1202	-	-	X	-
6	CL	D	1201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34066 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1133	Total	C	N	O	S	0	0	0
			8938	5663	1502	1743	30			
1	B	1033	Total	C	N	O	S	0	0	0
			8155	5169	1375	1583	28			
1	C	1067	Total	C	N	O	S	0	0	0
			8439	5349	1418	1642	30			
1	D	1067	Total	C	N	O	S	0	0	0
			8411	5333	1413	1636	29			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q99UY8
A	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	13	SER	-	EXPRESSION TAG	UNP Q99UY8
A	14	SER	-	EXPRESSION TAG	UNP Q99UY8
A	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	21	SER	-	EXPRESSION TAG	UNP Q99UY8
A	22	SER	-	EXPRESSION TAG	UNP Q99UY8
A	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
A	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
A	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
A	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
A	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	29	SER	-	EXPRESSION TAG	UNP Q99UY8
A	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	31	MET	-	EXPRESSION TAG	UNP Q99UY8

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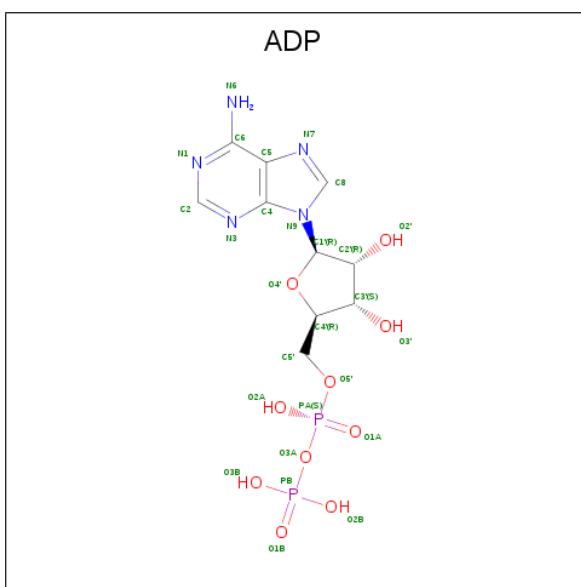
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
A	54	GLU	ARG	ENGINEERED MUTATION	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	21	SER	-	EXPRESSION TAG	UNP Q99UY8
B	22	SER	-	EXPRESSION TAG	UNP Q99UY8
B	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
B	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
B	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
B	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
B	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	29	SER	-	EXPRESSION TAG	UNP Q99UY8
B	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	31	MET	-	EXPRESSION TAG	UNP Q99UY8
B	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
B	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	54	GLU	ARG	ENGINEERED MUTATION	UNP Q99UY8
C	11	MET	-	EXPRESSION TAG	UNP Q99UY8
C	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	13	SER	-	EXPRESSION TAG	UNP Q99UY8
C	14	SER	-	EXPRESSION TAG	UNP Q99UY8
C	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	21	SER	-	EXPRESSION TAG	UNP Q99UY8
C	22	SER	-	EXPRESSION TAG	UNP Q99UY8
C	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
C	25	VAL	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
C	54	GLU	ARG	ENGINEERED MUTATION	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
D	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	13	SER	-	EXPRESSION TAG	UNP Q99UY8
D	14	SER	-	EXPRESSION TAG	UNP Q99UY8
D	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	21	SER	-	EXPRESSION TAG	UNP Q99UY8
D	22	SER	-	EXPRESSION TAG	UNP Q99UY8
D	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
D	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
D	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
D	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
D	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	29	SER	-	EXPRESSION TAG	UNP Q99UY8
D	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	31	MET	-	EXPRESSION TAG	UNP Q99UY8
D	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
D	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	54	GLU	ARG	ENGINEERED MUTATION	UNP Q99UY8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

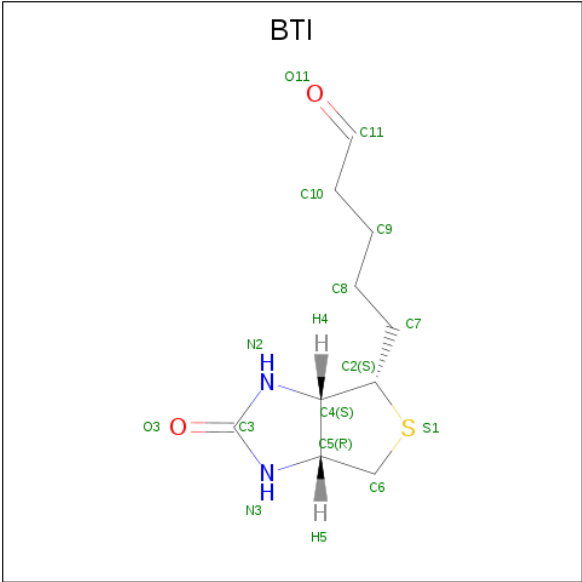


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

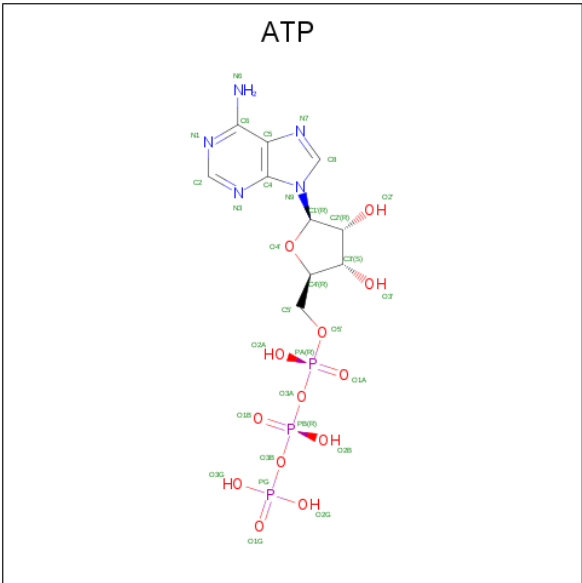
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

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



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

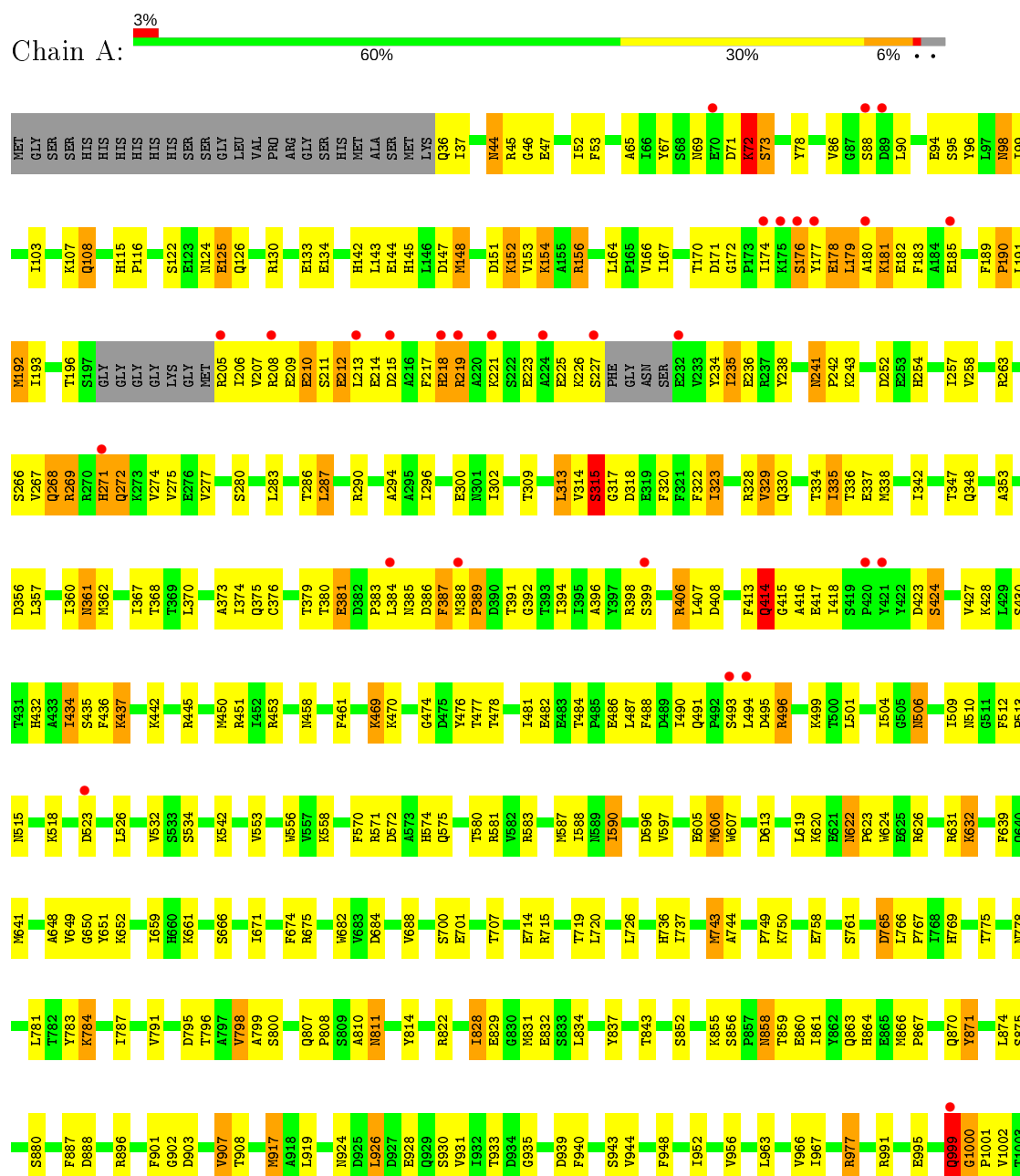
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

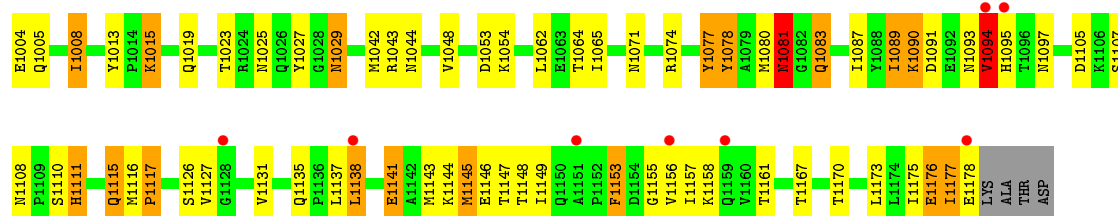
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

3 Residue-property plots [i](#)

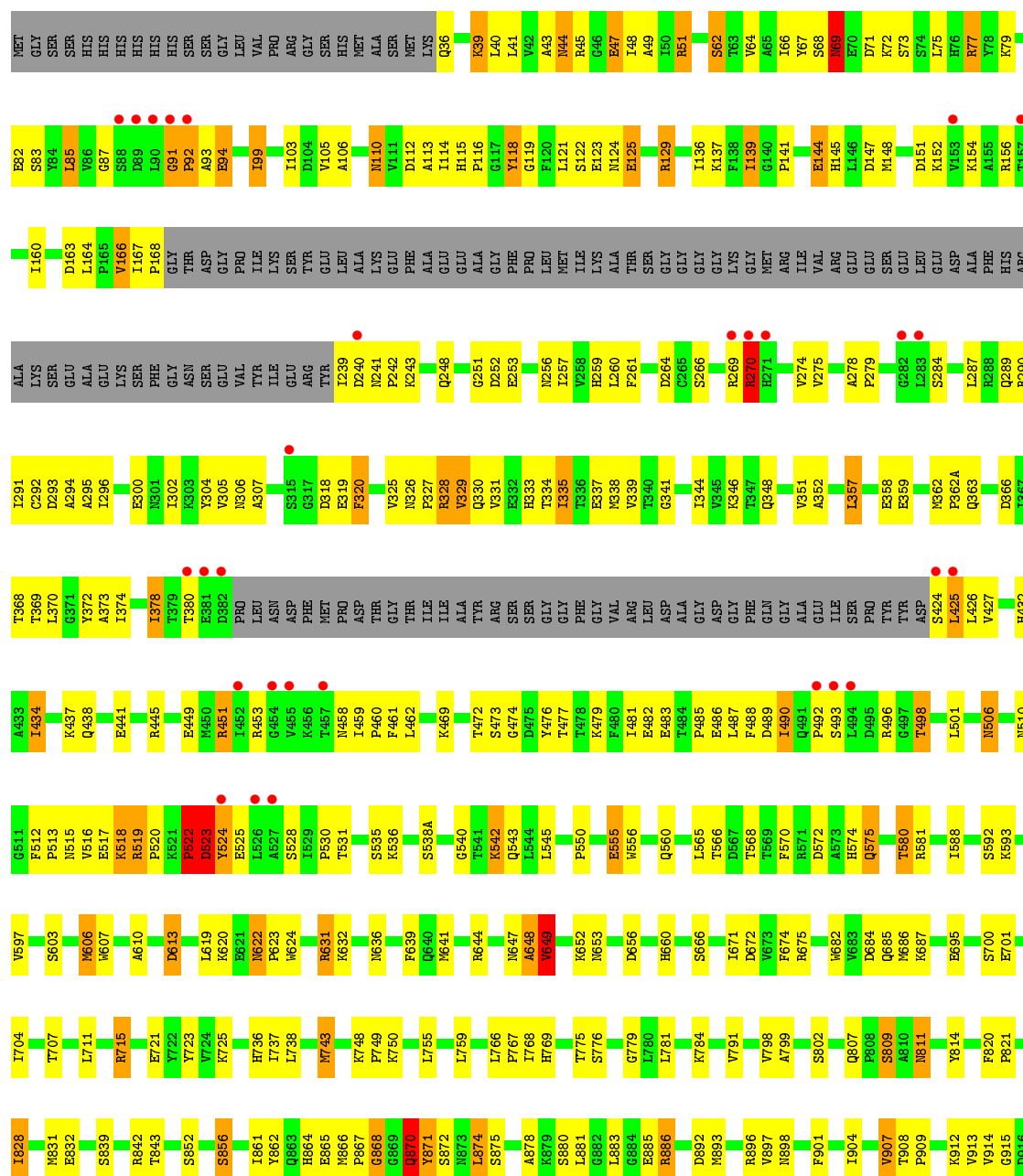
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

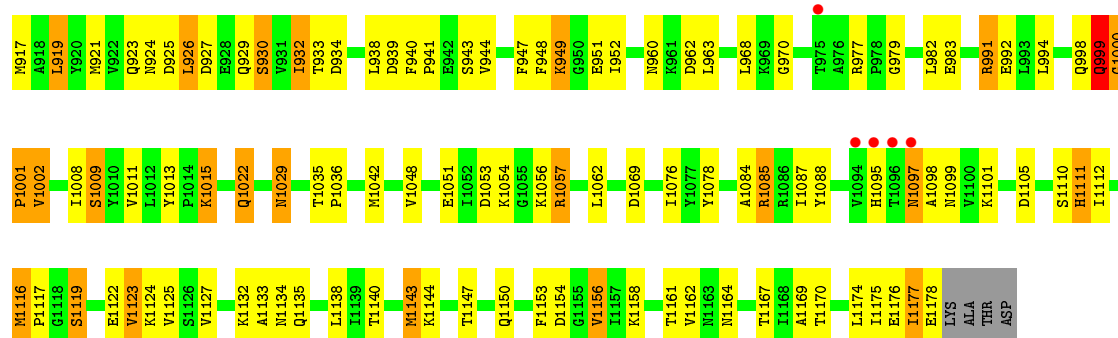
• Molecule 1: Pyruvate carboxylase



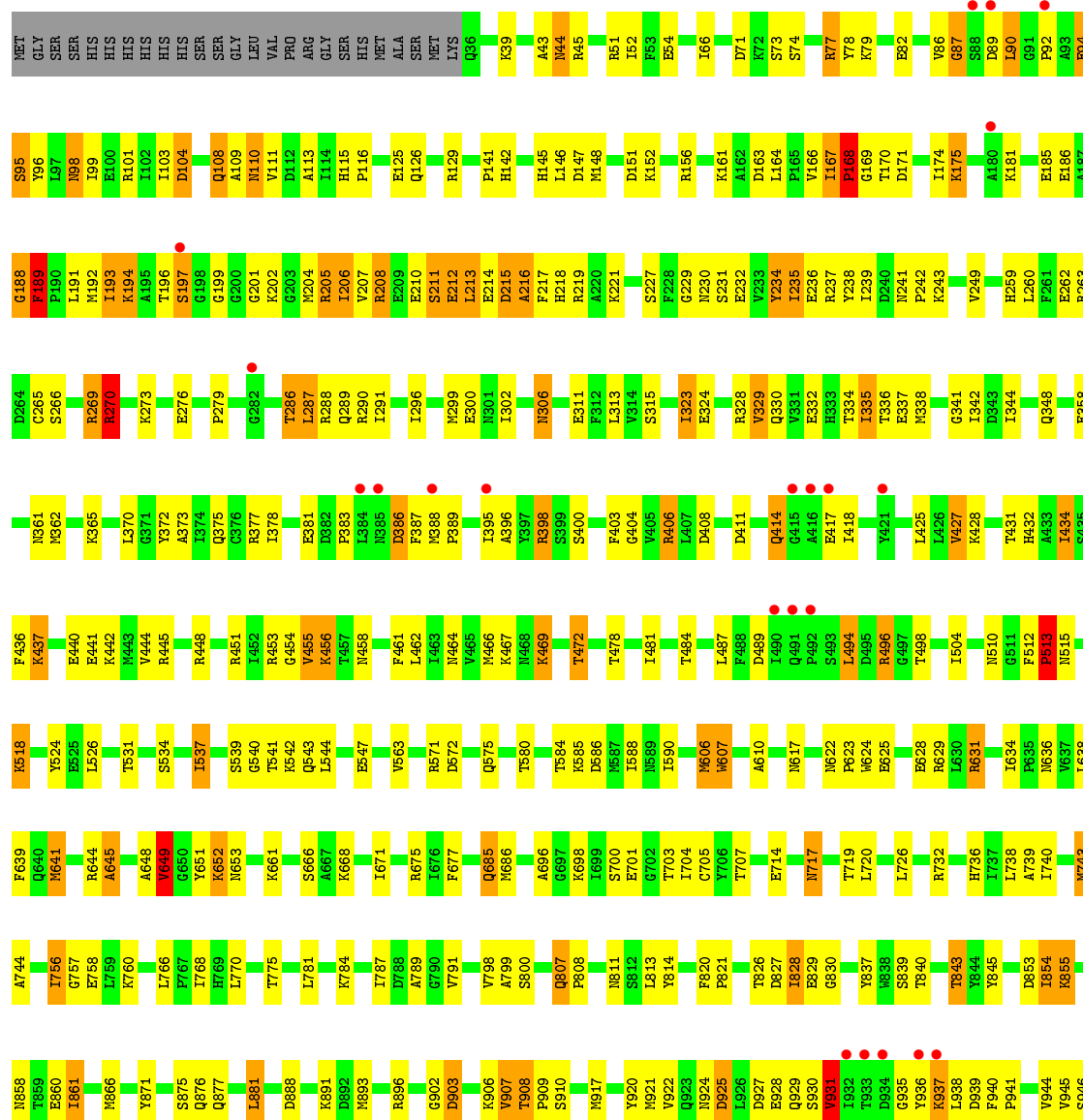


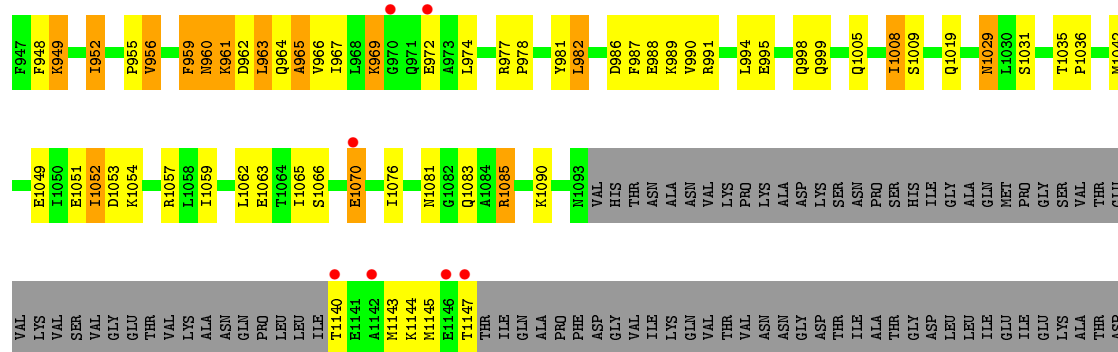
• Molecule 1: Pyruvate carboxylase



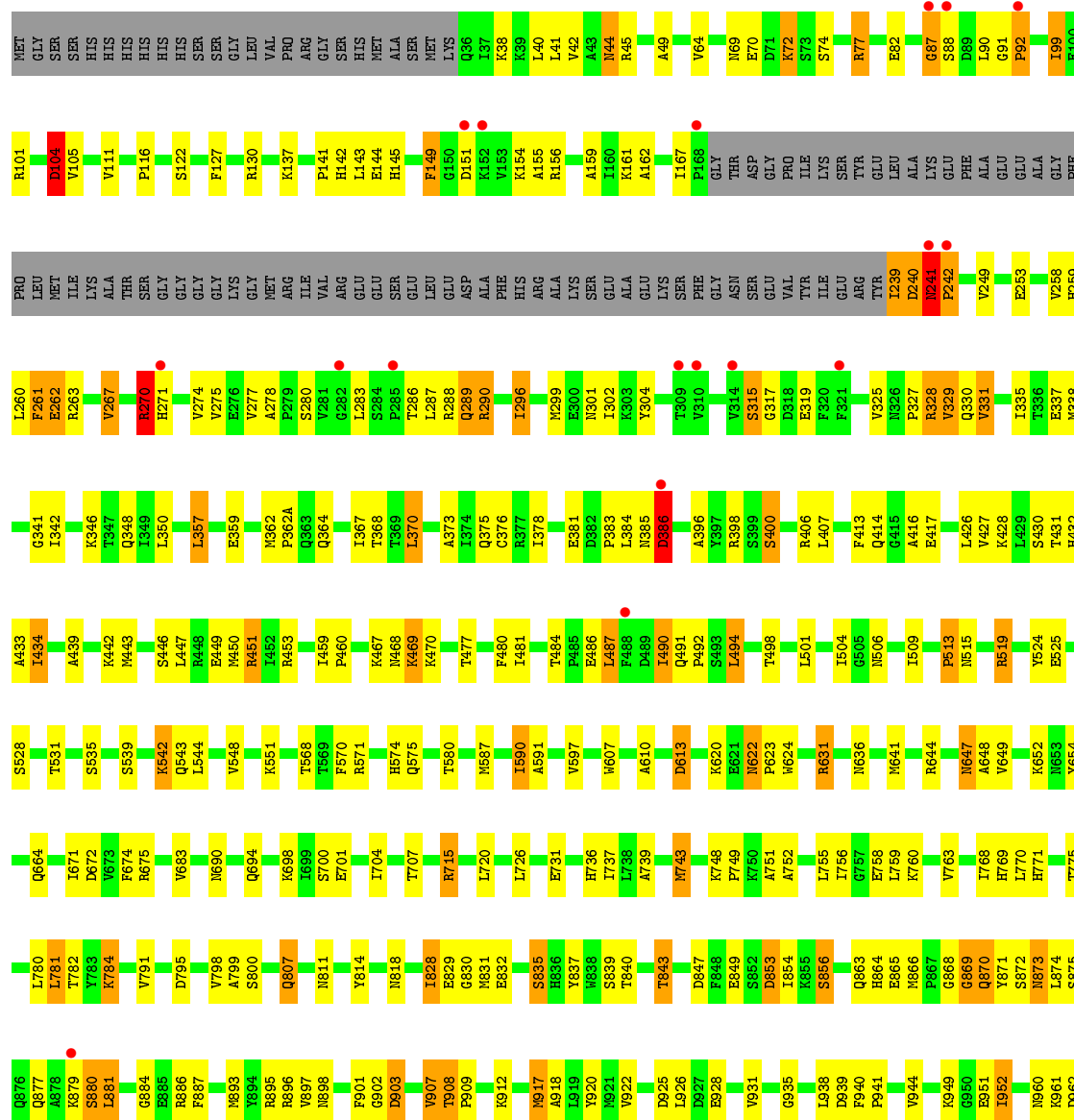


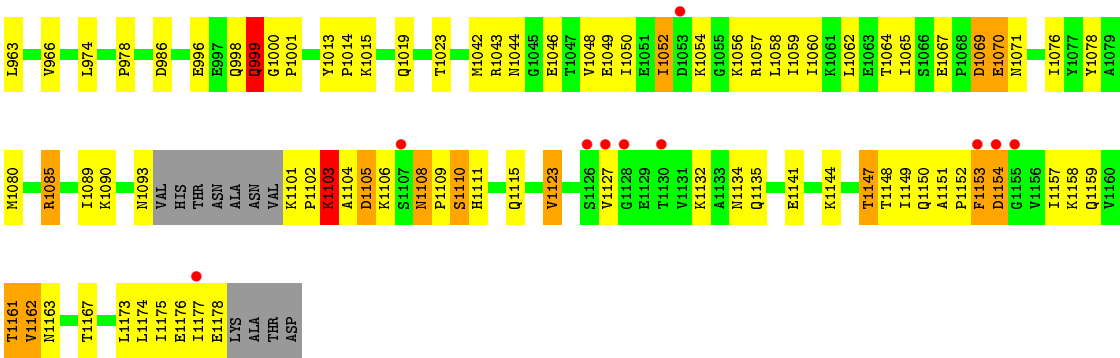
• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.43 Å 256.74 Å 127.05 Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.80) 93.1 (30.00-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.194 , 0.262 0.192 , 0.256	Depositor DCC
R_{free} test set	6647 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34066	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, BTI, ATP, ADP, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/9106	0.66	1/12319 (0.0%)
1	B	0.49	0/8305	0.60	0/11239
1	C	0.53	1/8601 (0.0%)	0.63	2/11625 (0.0%)
1	D	0.56	1/8569 (0.0%)	0.66	2/11596 (0.0%)
All	All	0.54	2/34581 (0.0%)	0.64	5/46779 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	D	0	2
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	8.04	1.69	1.52
1	D	513	PRO	CA-C	5.45	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	SER	CA-C-N	6.84	129.87	116.20
1	D	290	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	C	315	SER	CA-C-N	-6.03	104.15	116.20
1	C	315	SER	C-N-CA	5.30	133.44	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	849	GLU	CA-C-N	5.19	128.61	117.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	TYR	Peptide
1	A	1080	MET	Peptide
1	A	271	HIS	Peptide
1	A	494	LEU	Peptide
1	B	522	PRO	Peptide
1	B	92	PRO	Peptide
1	B	94	GLU	Peptide
1	D	1110	SER	Peptide
1	D	270	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8938	0	8865	364	0
1	B	8155	0	8127	343	0
1	C	8439	0	8345	376	0
1	D	8411	0	8357	324	0
2	A	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	30	0	32	17	0
4	C	15	0	16	1	0
4	D	15	0	16	5	0
5	C	31	0	12	6	0
6	D	1	0	0	3	0
All	All	34066	0	33782	1372	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 20.

All (1372) 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:C:1144:LYS:NZ	4:D:1202:BTI:H11	1.21	1.52
1:B:1144:LYS:NZ	4:B:1202:BTI:C11	1.74	1.46
1:A:864:HIS:CD2	1:A:866:MET:HG3	1.66	1.29
1:C:1144:LYS:NZ	4:D:1202:BTI:C11	1.91	1.29
1:C:1144:LYS:HZ1	4:D:1202:BTI:C11	1.44	1.29
1:B:1144:LYS:NZ	4:B:1202:BTI:H11	1.40	1.25
1:A:1144:LYS:NZ	4:B:1201:BTI:C11	2.00	1.23
1:A:1144:LYS:NZ	4:B:1201:BTI:H11	1.57	1.16
1:C:260:LEU:HD21	1:C:362:MET:CE	1.79	1.13
1:A:156:ARG:HD2	1:A:166:VAL:HG11	1.32	1.12
1:B:1144:LYS:HZ3	4:B:1202:BTI:C11	1.39	1.11
1:B:434:ILE:HD12	1:B:434:ILE:H	1.06	1.11
1:A:1144:LYS:HZ3	4:B:1201:BTI:H11	0.94	1.11
1:A:176:SER:O	1:A:179:LEU:HD22	1.51	1.10
1:C:960:ASN:HB2	1:C:963:LEU:HD23	1.31	1.10
1:A:156:ARG:HH11	1:A:156:ARG:HB3	1.08	1.08
1:D:357:LEU:O	1:D:362:MET:HB2	1.55	1.07
1:D:999:GLN:HG2	1:D:1000:GLY:N	1.58	1.07
1:D:999:GLN:CG	1:D:1000:GLY:H	1.67	1.06
1:C:960:ASN:CB	1:C:963:LEU:HD23	1.86	1.05
1:B:1085:ARG:HH11	1:B:1085:ARG:HG2	0.93	1.05
1:C:498:THR:OG1	1:C:1085:ARG:NH2	1.89	1.03
1:A:192:MET:HE2	1:A:238:TYR:HD1	1.23	1.03
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.20	1.03
1:A:406:ARG:HH11	1:A:406:ARG:HG2	1.21	1.03
1:B:137:LYS:HE3	1:B:352:ALA:O	1.58	1.02
1:B:1144:LYS:HZ1	4:B:1202:BTI:C11	1.48	1.02
1:B:1085:ARG:HG2	1:B:1085:ARG:NH1	1.61	1.02
1:A:179:LEU:H	1:A:179:LEU:HD23	1.22	1.01
1:A:434:ILE:HD12	1:A:434:ILE:H	1.25	1.01
1:A:1144:LYS:HZ3	4:B:1201:BTI:C11	1.62	1.00
1:D:960:ASN:ND2	1:D:963:LEU:H	1.58	1.00
1:C:260:LEU:HD21	1:C:362:MET:HE1	1.42	1.00
1:C:44:ASN:HD22	1:C:45:ARG:H	1.07	1.00
1:D:490:ILE:O	1:D:492:PRO:HD3	1.59	1.00
4:C:1203:BTI:O11	1:D:1144:LYS:NZ	1.94	1.00
1:C:828:ILE:HD12	1:C:828:ILE:H	1.27	1.00
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:HH11	1:A:156:ARG:CB	1.75	0.98
1:C:653:ASN:HD21	1:C:685:GLN:HE22	1.10	0.98
1:A:384:LEU:HD11	1:A:490:ILE:HD11	1.00	0.98
1:D:77:ARG:HG3	1:D:77:ARG:HH11	1.26	0.98
1:D:44:ASN:HD22	1:D:45:ARG:H	0.98	0.97
1:C:700:SER:H	1:C:736:HIS:HD2	1.12	0.97
1:A:384:LEU:CD1	1:A:490:ILE:HD11	1.93	0.95
1:C:398:ARG:NE	1:C:1083:GLN:HG2	1.81	0.95
1:A:44:ASN:HD22	1:A:45:ARG:H	0.96	0.94
1:B:1085:ARG:HH11	1:B:1085:ARG:CG	1.80	0.94
1:B:44:ASN:HD22	1:B:45:ARG:H	0.98	0.93
1:D:338:MET:HE2	1:D:430:SER:HB3	1.52	0.92
1:A:469:LYS:HD2	1:A:469:LYS:N	1.85	0.92
1:D:287:LEU:HD11	1:D:317:GLY:O	1.68	0.91
1:D:700:SER:H	1:D:736:HIS:HD2	1.17	0.91
1:A:1144:LYS:HZ1	4:B:1201:BTI:C11	1.71	0.91
1:D:879:LYS:HG2	1:D:884:GLY:HA3	1.52	0.91
1:D:864:HIS:CD2	1:D:866:MET:HG3	2.06	0.91
1:C:398:ARG:HE	1:C:1083:GLN:HG2	1.32	0.90
1:D:644:ARG:HH21	1:D:908:THR:HB	1.36	0.90
1:C:454:GLY:O	1:C:455:VAL:HG13	1.70	0.90
1:B:44:ASN:HD22	1:B:45:ARG:N	1.70	0.89
1:B:274:VAL:HG12	1:B:275:VAL:HG23	1.54	0.89
1:C:1051:GLU:HG3	1:C:1057:ARG:NH2	1.88	0.89
1:D:259:HIS:H	1:D:364:GLN:HE22	1.21	0.89
1:B:378:ILE:HG13	1:B:427:VAL:HG23	1.54	0.89
1:A:700:SER:H	1:A:736:HIS:HD2	1.20	0.88
1:D:999:GLN:HE21	1:D:1001:PRO:HD2	1.38	0.88
1:D:960:ASN:HD22	1:D:963:LEU:H	1.20	0.88
1:A:254:HIS:HD2	1:A:356:ASP:OD2	1.57	0.88
1:A:156:ARG:HD2	1:A:166:VAL:CG1	2.03	0.88
1:C:960:ASN:HB2	1:C:963:LEU:CD2	2.03	0.88
1:B:575:GLN:HB2	1:B:580:THR:HG23	1.57	0.87
1:A:181:LYS:O	1:A:185:GLU:HG3	1.72	0.87
1:A:406:ARG:HH11	1:A:406:ARG:CG	1.85	0.87
1:B:897:VAL:CG1	1:B:914:VAL:HG13	2.04	0.87
1:B:864:HIS:HD2	1:B:866:MET:H	1.22	0.87
1:D:873:ASN:H	1:D:873:ASN:HD22	1.20	0.87
1:C:191:LEU:HB3	1:C:235:ILE:HD11	1.57	0.86
1:A:384:LEU:HD11	1:A:490:ILE:CD1	1.97	0.86
1:C:263:ARG:HH21	1:C:330:GLN:NE2	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1069:ASP:OD2	1:D:1071:ASN:N	2.08	0.86
1:B:329:VAL:HG13	1:B:348:GLN:NE2	1.90	0.86
1:C:840:THR:O	1:C:843:THR:HB	1.76	0.85
1:B:434:ILE:N	1:B:434:ILE:HD12	1.89	0.85
1:B:44:ASN:ND2	1:B:45:ARG:H	1.74	0.85
1:A:622:ASN:ND2	1:A:624:TRP:H	1.74	0.85
1:B:1144:LYS:HZ1	4:B:1202:BTI:H11	0.69	0.85
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.58	0.85
1:C:1049:GLU:HG2	1:C:1059:ILE:HD12	1.55	0.85
1:D:509:ILE:HD13	1:D:1089:ILE:HG21	1.59	0.85
1:A:174:ILE:HD12	1:A:179:LEU:HB2	1.57	0.85
1:A:219:ARG:O	1:A:223:GLU:HB2	1.77	0.84
1:A:1115:GLN:CD	1:A:1115:GLN:H	1.79	0.84
1:D:1108:ASN:HB3	1:D:1109:PRO:HD3	1.58	0.84
1:B:897:VAL:HG12	1:B:914:VAL:HG13	1.59	0.84
1:A:558:LYS:HE2	1:A:765:ASP:O	1.77	0.84
1:B:241:ASN:HD22	1:B:477:THR:HG21	1.43	0.83
1:A:641:MET:HE2	1:A:674:PHE:CE1	2.14	0.83
1:D:338:MET:CE	1:D:430:SER:HB3	2.09	0.83
1:C:504:ILE:HD13	1:C:1042:MET:CE	2.08	0.83
1:B:434:ILE:HG13	1:D:341:GLY:O	1.79	0.83
1:A:1145:MET:CE	1:A:1145:MET:HA	2.09	0.83
1:C:572:ASP:HB3	1:C:807:GLN:HE22	1.45	0.82
1:C:44:ASN:ND2	1:C:45:ARG:H	1.77	0.82
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.44	0.82
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.58	0.82
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.44	0.82
1:C:700:SER:H	1:C:736:HIS:CD2	1.98	0.82
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.62	0.82
1:A:641:MET:CE	1:A:674:PHE:CE1	2.62	0.81
1:B:434:ILE:CD1	1:B:434:ILE:H	1.85	0.81
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.14	0.81
1:A:192:MET:HE2	1:A:238:TYR:CD1	2.14	0.81
1:C:828:ILE:HD12	1:C:828:ILE:N	1.94	0.81
1:D:840:THR:O	1:D:843:THR:HB	1.78	0.81
1:C:217:PHE:O	1:C:221:LYS:HB2	1.81	0.81
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.27	0.81
1:A:223:GLU:HA	1:A:226:LYS:HB3	1.63	0.81
1:A:176:SER:O	1:A:179:LEU:CD2	2.29	0.80
5:C:1202:ATP:O1G	5:C:1202:ATP:O3A	1.98	0.80
1:A:379:THR:HG22	1:A:424:SER:O	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:GLN:HG2	1:D:1000:GLY:H	0.75	0.80
1:C:152:LYS:NZ	5:C:1202:ATP:O1A	2.14	0.80
1:A:156:ARG:NH1	1:A:156:ARG:HB3	1.93	0.80
1:A:864:HIS:CD2	1:A:866:MET:CG	2.59	0.80
1:D:504:ILE:HD13	1:D:1042:MET:HE3	1.61	0.80
1:D:864:HIS:HD2	1:D:866:MET:H	1.30	0.80
1:C:196:THR:O	1:C:196:THR:HG22	1.82	0.80
1:C:306:ASN:OD1	1:C:348:GLN:HG2	1.82	0.80
1:A:315:SER:O	1:A:317:GLY:C	2.20	0.80
1:D:44:ASN:HD22	1:D:45:ARG:N	1.80	0.80
1:D:263:ARG:HH21	1:D:330:GLN:NE2	1.80	0.79
1:C:1144:LYS:HZ3	4:D:1202:BTI:C11	1.74	0.79
1:B:811:ASN:H	1:B:811:ASN:HD22	1.30	0.79
1:B:570:PHE:O	1:B:574:HIS:HE1	1.66	0.79
1:B:506:ASN:ND2	1:B:510:ASN:HD22	1.81	0.78
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.66	0.78
1:A:362:MET:CE	1:A:367:ILE:HD11	2.12	0.78
1:B:1095:HIS:HB3	1:B:1098:ALA:HB3	1.66	0.78
1:C:221:LYS:NZ	1:C:231:SER:O	2.17	0.78
1:D:470:LYS:HA	1:D:470:LYS:HE2	1.66	0.78
1:B:1110:SER:HB2	1:B:1177:ILE:O	1.83	0.78
1:C:269:ARG:HG3	1:C:270:ARG:H	1.48	0.78
1:C:196:THR:O	1:C:197:SER:HB3	1.84	0.78
1:C:87:GLY:HA3	1:C:90:LEU:HD22	1.66	0.78
1:D:1111:HIS:HB3	1:D:1173:LEU:CD1	2.13	0.77
1:B:291:ILE:HG12	1:B:320:PHE:HD2	1.49	0.77
1:A:179:LEU:CD2	1:A:179:LEU:H	1.96	0.77
1:C:440:GLU:OE1	1:C:466:MET:HB3	1.82	0.77
1:A:44:ASN:HD22	1:A:45:ARG:N	1.79	0.76
1:A:858:ASN:ND2	1:A:860:GLU:H	1.82	0.76
1:B:47:GLU:CD	1:B:47:GLU:H	1.87	0.76
1:D:620:LYS:HE2	1:D:1023:THR:OG1	1.85	0.76
1:D:1108:ASN:HB3	1:D:1109:PRO:CD	2.16	0.76
1:D:647:ASN:C	1:D:647:ASN:HD22	1.88	0.76
1:A:800:SER:HA	1:D:856:SER:OG	1.86	0.76
1:C:606:MET:HE1	1:C:607:TRP:HB2	1.67	0.76
1:C:396:ALA:HB3	1:C:453:ARG:HH11	1.49	0.76
1:C:206:ILE:HD11	1:C:208:ARG:HE	1.51	0.75
1:D:504:ILE:HD13	1:D:1042:MET:CE	2.15	0.75
1:A:496:ARG:HH11	1:A:496:ARG:HB3	1.52	0.75
1:A:864:HIS:HD2	1:A:866:MET:H	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:LYS:HA	1:C:469:LYS:HE3	1.67	0.75
1:A:445:ARG:NH1	1:C:54:GLU:HG2	2.02	0.75
1:D:337:GLU:HG2	1:D:342:ILE:O	1.87	0.75
1:D:259:HIS:H	1:D:364:GLN:NE2	1.83	0.75
1:B:1122:GLU:HA	1:B:1164:ASN:OD1	1.85	0.74
1:C:269:ARG:HH11	1:C:269:ARG:HB2	1.51	0.74
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.00	0.74
1:C:1051:GLU:HG3	1:C:1057:ARG:HH22	1.53	0.74
1:D:622:ASN:ND2	1:D:624:TRP:H	1.85	0.74
1:B:913:VAL:HG11	1:B:947:PHE:HB2	1.68	0.74
1:A:1145:MET:HA	1:A:1145:MET:HE3	1.70	0.74
1:A:999:GLN:HG2	1:A:1000:GLY:H	1.52	0.73
1:B:68:SER:O	1:B:85:LEU:HD12	1.88	0.73
1:C:260:LEU:HD21	1:C:362:MET:HE3	1.68	0.73
1:C:677:PHE:HA	1:C:686:MET:CE	2.18	0.73
1:B:141:PRO:HB2	1:B:145:HIS:HB2	1.70	0.73
1:C:337:GLU:HG2	1:C:344:ILE:HD12	1.70	0.73
1:D:999:GLN:HE21	1:D:1001:PRO:CD	2.00	0.73
1:D:240:ASP:O	1:D:241:ASN:HB2	1.87	0.73
1:D:77:ARG:CG	1:D:77:ARG:HH11	1.97	0.73
1:C:504:ILE:HD13	1:C:1042:MET:HE3	1.69	0.73
1:C:44:ASN:HD22	1:C:45:ARG:N	1.85	0.73
1:D:398:ARG:HH21	1:D:451:ARG:HD2	1.54	0.73
1:D:335:ILE:HG12	1:D:373:ALA:HB3	1.71	0.73
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.70	0.73
1:C:677:PHE:HA	1:C:686:MET:HE3	1.70	0.73
1:A:142:HIS:H	1:A:145:HIS:HD2	1.37	0.72
1:B:445:ARG:O	1:B:449:GLU:HG3	1.89	0.72
1:A:107:LYS:HD2	1:A:134:GLU:OE1	1.88	0.72
1:B:1105:ASP:H	1:B:1111:HIS:HD2	1.36	0.72
1:D:941:PRO:O	1:D:944:VAL:HG12	1.88	0.72
1:A:606:MET:HE1	1:A:671:ILE:HD13	1.70	0.72
1:C:437:LYS:O	1:C:441:GLU:HG3	1.89	0.72
1:B:828:ILE:N	1:B:828:ILE:HD12	2.05	0.72
1:C:572:ASP:HB3	1:C:807:GLN:NE2	2.04	0.72
1:A:1081:ASN:HB3	1:C:78:TYR:CE2	2.25	0.72
1:B:253:GLU:HG3	1:B:305:VAL:HG11	1.70	0.72
1:D:44:ASN:ND2	1:D:45:ARG:H	1.82	0.72
1:A:235:ILE:HG13	1:A:236:GLU:H	1.55	0.71
1:C:937:LYS:HD3	1:D:1152:PRO:CB	2.21	0.71
1:C:175:LYS:H	1:C:175:LYS:HD2	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ARG:HD2	1:A:407:LEU:N	2.04	0.71
1:C:263:ARG:NH2	1:C:330:GLN:HE21	1.87	0.71
1:C:188:GLY:HA3	1:C:237:ARG:HH22	1.55	0.71
1:D:575:GLN:NE2	1:D:610:ALA:H	1.87	0.71
1:A:434:ILE:HD12	1:A:434:ILE:N	2.04	0.71
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.20	0.71
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.55	0.71
1:A:513:PRO:O	1:A:515:ASN:HB2	1.90	0.71
1:A:924:ASN:HB2	1:A:926:LEU:HD22	1.73	0.71
1:B:1105:ASP:H	1:B:1111:HIS:CD2	2.09	0.71
1:C:145:HIS:HE1	1:C:302:ILE:O	1.73	0.71
1:A:1093:ASN:O	1:A:1094:VAL:HB	1.90	0.70
1:A:156:ARG:CD	1:A:166:VAL:HG11	2.18	0.70
1:B:99:ILE:HD12	1:B:99:ILE:H	1.57	0.70
1:C:820:PHE:HB3	1:C:821:PRO:CD	2.21	0.70
1:C:1144:LYS:HZ3	4:D:1202:BTI:H11	0.83	0.70
1:D:362:MET:HE1	1:D:367:ILE:HD11	1.73	0.70
1:B:927:ASP:H	1:B:930:SER:HB2	1.56	0.70
1:B:934:ASP:O	1:B:938:LEU:HG	1.90	0.70
1:D:784:LYS:HE3	6:D:1201:CL:CL	2.28	0.70
1:B:568:THR:OG1	1:B:807:GLN:HG3	1.92	0.70
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.05	0.70
1:C:494:LEU:HD22	1:C:494:LEU:H	1.57	0.69
1:D:941:PRO:HD2	1:D:944:VAL:HG11	1.74	0.69
1:A:44:ASN:ND2	1:A:45:ARG:H	1.81	0.69
1:A:263:ARG:HH21	1:A:330:GLN:NE2	1.89	0.69
1:A:406:ARG:HH12	1:C:403:PHE:HB2	1.55	0.69
1:D:142:HIS:HB3	1:D:144:GLU:OE1	1.91	0.69
1:D:828:ILE:HD12	1:D:828:ILE:N	2.07	0.69
1:C:338:MET:CE	1:C:373:ALA:HB1	2.22	0.69
1:B:243:LYS:HE3	1:B:264:ASP:OD1	1.92	0.69
1:D:509:ILE:HD13	1:D:1089:ILE:CG2	2.21	0.69
1:D:87:GLY:HA3	1:D:90:LEU:HG	1.75	0.69
1:A:413:PHE:CE1	1:A:416:ALA:HB3	2.27	0.69
1:A:622:ASN:C	1:A:622:ASN:HD22	1.94	0.69
1:B:1101:LYS:HE2	1:B:1162:VAL:HG12	1.75	0.69
1:C:191:LEU:HB3	1:C:235:ILE:CD1	2.23	0.69
1:B:261:PHE:CE1	1:B:368:THR:HA	2.28	0.68
1:B:927:ASP:N	1:B:930:SER:HB2	2.08	0.68
1:B:141:PRO:HB2	1:B:145:HIS:CB	2.23	0.68
1:C:978:PRO:HA	1:C:981:TYR:CE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:GLN:HE22	1:B:610:ALA:H	1.41	0.68
1:C:269:ARG:HG3	1:C:270:ARG:N	2.07	0.68
1:A:396:ALA:HB3	1:A:453:ARG:HB2	1.76	0.68
1:B:291:ILE:CG1	1:B:320:PHE:HD2	2.07	0.68
1:C:991:ARG:O	1:C:995:GLU:HG3	1.93	0.68
1:A:1146:GLU:O	1:A:1147:THR:HG23	1.94	0.68
1:B:329:VAL:HG13	1:B:348:GLN:HE22	1.57	0.68
1:C:210:GLU:O	1:C:211:SER:CB	2.41	0.68
1:A:235:ILE:HG13	1:A:236:GLU:N	2.06	0.68
1:A:177:TYR:O	1:A:178:GLU:C	2.32	0.68
1:A:362:MET:HE1	1:A:367:ILE:HD11	1.75	0.68
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.76	0.67
1:A:700:SER:H	1:A:736:HIS:CD2	2.07	0.67
1:C:1035:THR:HB	1:C:1036:PRO:HD3	1.77	0.67
1:D:286:THR:O	1:D:290:ARG:HG3	1.94	0.67
1:A:622:ASN:HD22	1:A:624:TRP:H	1.42	0.67
1:B:506:ASN:HD22	1:B:510:ASN:HD22	1.42	0.67
1:B:555:GLU:OE1	1:B:555:GLU:HA	1.94	0.67
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.76	0.67
1:C:1029:ASN:ND2	1:C:1031:SER:H	1.92	0.67
1:C:167:ILE:HG23	1:C:239:ILE:HD11	1.76	0.67
1:D:1049:GLU:HG2	1:D:1059:ILE:HD13	1.75	0.67
1:A:1044:ASN:HA	1:A:1062:LEU:HD23	1.77	0.67
1:A:1115:GLN:H	1:A:1115:GLN:NE2	1.93	0.67
1:D:239:ILE:HB	1:D:242:PRO:HG3	1.76	0.67
1:A:811:ASN:H	1:A:811:ASN:HD22	1.40	0.67
1:B:556:TRP:O	1:B:560:GLN:HG2	1.94	0.67
1:B:700:SER:H	1:B:736:HIS:HD2	1.40	0.67
1:A:406:ARG:NH1	1:C:403:PHE:HB2	2.09	0.67
1:D:641:MET:CE	1:D:674:PHE:CE1	2.78	0.67
1:C:653:ASN:HD21	1:C:685:GLN:NE2	1.90	0.67
1:B:370:LEU:HD21	1:D:341:GLY:HA3	1.76	0.67
1:C:700:SER:N	1:C:736:HIS:HD2	1.91	0.67
1:C:1049:GLU:HG2	1:C:1059:ILE:CD1	2.24	0.67
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.75	0.66
1:C:89:ASP:HB3	1:C:101:ARG:HH12	1.60	0.66
1:A:651:TYR:CE1	1:A:652:LYS:HG3	2.30	0.66
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.31	0.66
1:D:1108:ASN:CB	1:D:1109:PRO:HD3	2.23	0.66
1:D:909:PRO:HG2	1:D:952:ILE:HG13	1.77	0.66
1:A:499:LYS:NZ	1:A:1025:ASN:O	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:O	1:A:179:LEU:N	2.28	0.66
1:B:927:ASP:HB3	1:B:929:GLN:H	1.60	0.66
1:B:940:PHE:HB3	1:B:944:VAL:HG11	1.77	0.66
1:C:398:ARG:HE	1:C:1083:GLN:CG	2.04	0.66
1:A:215:ASP:O	1:A:218:HIS:HB2	1.95	0.66
1:B:451:ARG:HG2	1:B:453:ARG:HH21	1.61	0.66
1:A:156:ARG:NH1	1:A:156:ARG:CB	2.56	0.66
1:A:242:PRO:O	1:A:477:THR:HB	1.96	0.66
1:B:251:GLY:HA2	1:B:256:ASN:O	1.95	0.65
1:B:828:ILE:H	1:B:828:ILE:HD12	1.59	0.65
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.26	0.65
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.10	0.65
1:D:1044:ASN:HD22	1:D:1062:LEU:HD23	1.61	0.65
1:B:291:ILE:HG12	1:B:320:PHE:CD2	2.29	0.65
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.79	0.65
1:B:125:GLU:CD	1:B:125:GLU:H	2.00	0.65
1:B:144:GLU:O	1:B:148:MET:HB2	1.96	0.65
1:C:960:ASN:HB3	1:C:963:LEU:HD23	1.79	0.65
1:D:644:ARG:NH2	1:D:908:THR:HB	2.09	0.65
1:B:1000:GLY:H	1:B:1001:PRO:HD2	1.60	0.65
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.78	0.65
1:C:396:ALA:CB	1:C:453:ARG:NH1	2.60	0.65
1:D:400:SER:O	1:D:407:LEU:HD11	1.96	0.64
1:A:866:MET:HE1	1:A:874:LEU:HD22	1.77	0.64
1:D:1062:LEU:HD12	1:D:1078:TYR:CE2	2.32	0.64
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.79	0.64
1:A:47:GLU:CD	1:A:428:LYS:HE2	2.17	0.64
1:B:909:PRO:O	1:B:913:VAL:HG23	1.96	0.64
1:C:732:ARG:HG3	1:C:732:ARG:HH11	1.62	0.64
1:B:570:PHE:O	1:B:574:HIS:CE1	2.50	0.64
1:B:701:GLU:HG2	1:B:737:ILE:HB	1.78	0.64
1:C:539:SER:HA	1:C:543:GLN:HG3	1.78	0.64
1:D:853:ASP:OD2	1:D:853:ASP:N	2.27	0.64
1:B:1156:VAL:HG23	1:B:1178:GLU:HB2	1.80	0.64
1:C:215:ASP:HB3	1:C:219:ARG:HG3	1.79	0.64
1:C:1029:ASN:HD22	1:C:1029:ASN:C	2.01	0.64
1:A:381:GLU:HG2	1:A:387:PHE:O	1.98	0.64
1:B:99:ILE:O	1:B:103:ILE:HD12	1.98	0.64
1:D:72:LYS:O	1:D:77:ARG:CD	2.46	0.64
1:A:142:HIS:H	1:A:145:HIS:CD2	2.15	0.64
1:A:176:SER:O	1:A:179:LEU:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:MET:CE	1:B:373:ALA:HB1	2.28	0.64
1:C:411:ASP:HB3	1:C:418:ILE:HG22	1.80	0.64
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.33	0.63
1:A:620:LYS:CG	1:A:1023:THR:HG21	2.28	0.63
1:D:72:LYS:O	1:D:77:ARG:NE	2.31	0.63
1:A:501:LEU:HD13	1:A:1078:TYR:CD1	2.33	0.63
1:A:338:MET:HE3	1:A:373:ALA:HB1	1.80	0.63
1:A:828:ILE:HD12	1:A:829:GLU:H	1.63	0.63
1:B:1174:LEU:C	1:B:1175:ILE:HG12	2.19	0.63
1:C:142:HIS:H	1:C:145:HIS:HD2	1.46	0.63
1:D:259:HIS:N	1:D:364:GLN:HE22	1.93	0.63
1:D:869:GLY:O	1:D:871:TYR:N	2.31	0.63
1:C:917:MET:O	1:C:921:MET:HG3	1.97	0.63
1:A:1131:VAL:HG12	1:A:1135:GLN:NE2	2.14	0.63
1:B:341:GLY:O	1:D:434:ILE:HG12	1.99	0.63
1:D:895:ARG:O	1:D:898:ASN:HB3	1.99	0.63
1:C:458:ASN:ND2	1:C:462:LEU:HD11	2.14	0.63
1:B:864:HIS:CD2	1:B:866:MET:H	2.11	0.62
1:B:921:MET:HG2	1:B:926:LEU:CB	2.29	0.62
1:B:960:ASN:HB3	1:B:963:LEU:HB3	1.80	0.62
1:C:606:MET:CE	1:C:607:TRP:HB2	2.28	0.62
1:D:141:PRO:HG3	1:D:304:TYR:OH	1.99	0.62
1:B:912:LYS:NZ	1:B:943:SER:HB3	2.14	0.62
1:C:496:ARG:HD3	1:C:496:ARG:H	1.64	0.62
1:B:39:LYS:HD2	1:B:110:ASN:O	1.99	0.62
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.30	0.62
1:A:243:LYS:NZ	1:A:474:GLY:O	2.32	0.62
1:D:866:MET:CE	1:D:871:TYR:HA	2.29	0.62
1:A:496:ARG:NH1	1:A:496:ARG:HB3	2.14	0.62
1:A:606:MET:CE	1:A:639:PHE:HB3	2.29	0.62
1:B:40:LEU:C	1:B:40:LEU:HD23	2.19	0.62
1:B:861:ILE:HG13	1:B:862:TYR:N	2.14	0.62
1:A:1158:LYS:HB3	1:A:1176:GLU:HB3	1.81	0.62
1:C:649:VAL:HG13	1:C:649:VAL:O	2.00	0.62
1:D:91:GLY:O	1:D:92:PRO:O	2.18	0.62
1:C:189:PHE:O	1:C:189:PHE:HD2	1.82	0.62
1:A:124:ASN:OD1	1:A:126:GLN:HB2	2.00	0.62
1:A:361:ASN:HB3	1:C:434:ILE:HD13	1.82	0.62
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.52	0.62
1:C:396:ALA:CB	1:C:453:ARG:HH11	2.13	0.62
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD12	1:A:353:ALA:HB2	1.81	0.61
1:A:53:PHE:CZ	1:A:65:ALA:HB2	2.35	0.61
1:A:864:HIS:NE2	1:A:866:MET:HG3	2.14	0.61
1:B:927:ASP:CB	1:B:930:SER:H	2.12	0.61
1:D:570:PHE:O	1:D:574:HIS:HE1	1.82	0.61
1:D:743:MET:HG3	1:D:907:VAL:CG1	2.30	0.61
1:B:339:VAL:O	1:B:369:THR:HA	2.00	0.61
1:C:738:LEU:HD23	1:C:768:ILE:HG12	1.81	0.61
1:A:225:GLU:HA	1:A:225:GLU:OE2	2.01	0.61
1:D:260:LEU:O	1:D:261:PHE:HB2	2.01	0.61
1:A:1110:SER:O	1:A:1177:ILE:HD12	2.00	0.61
1:A:1144:LYS:CE	4:B:1201:BTI:H11	2.30	0.61
1:B:490:ILE:O	1:B:492:PRO:HD3	2.01	0.61
1:A:241:ASN:HD22	1:A:477:THR:HG21	1.64	0.60
1:A:434:ILE:CD1	1:A:434:ILE:H	2.00	0.60
1:D:960:ASN:HD22	1:D:963:LEU:N	1.97	0.60
1:B:1144:LYS:CE	4:B:1202:BTI:C11	2.74	0.60
1:D:864:HIS:HD2	1:D:866:MET:HG3	1.66	0.60
1:A:902:GLY:O	1:A:903:ASP:HB3	2.01	0.60
1:A:98:ASN:C	1:A:98:ASN:HD22	2.04	0.60
1:C:448:ARG:HH22	1:C:467:LYS:NZ	1.99	0.60
1:A:661:LYS:NZ	1:A:1004:GLU:OE2	2.28	0.60
1:D:1067:GLU:HA	1:D:1067:GLU:OE1	2.02	0.60
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.82	0.60
1:C:436:PHE:HE2	1:C:472:THR:HA	1.66	0.60
1:C:86:VAL:HG12	1:C:86:VAL:O	2.00	0.60
1:C:931:VAL:HA	1:C:935:GLY:H	1.67	0.60
1:D:375:GLN:HG2	1:D:376:CYS:N	2.16	0.60
1:B:112:ASP:C	1:B:136:ILE:HG23	2.21	0.60
1:B:927:ASP:HB2	1:B:930:SER:HB2	1.82	0.60
1:C:411:ASP:HB3	1:C:418:ILE:CG2	2.32	0.60
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.83	0.60
1:A:1081:ASN:HB2	1:C:78:TYR:CG	2.36	0.60
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.05	0.60
1:D:880:SER:O	1:D:881:LEU:HD23	2.02	0.60
1:A:180:ALA:O	1:A:183:PHE:N	2.27	0.60
1:D:1111:HIS:HB3	1:D:1173:LEU:HD13	1.84	0.60
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.84	0.60
1:B:555:GLU:OE1	1:B:555:GLU:CA	2.49	0.60
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.83	0.60
1:C:624:TRP:O	1:C:628:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:ILE:H	1:C:828:ILE:CD1	1.96	0.60
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.53	0.59
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.32	0.59
1:D:587:MET:O	1:D:590:ILE:HD12	2.02	0.59
1:A:1105:ASP:H	1:A:1111:HIS:HD2	1.50	0.59
1:A:156:ARG:CD	1:A:166:VAL:CG1	2.76	0.59
1:B:593:LYS:O	1:B:597:VAL:HG23	2.02	0.59
1:C:893:MET:HG3	1:C:922:VAL:HG23	1.84	0.59
1:D:641:MET:HE2	1:D:674:PHE:CE1	2.37	0.59
1:C:205:ARG:HB2	1:C:205:ARG:HH11	1.67	0.59
1:D:999:GLN:NE2	1:D:1001:PRO:HD2	2.14	0.59
1:D:1109:PRO:HG2	1:D:1111:HIS:CE1	2.38	0.59
1:D:315:SER:O	1:D:319:GLU:HB3	2.03	0.59
1:A:1145:MET:HA	1:A:1145:MET:HE2	1.83	0.59
1:B:519:ARG:HB2	1:B:520:PRO:HD3	1.84	0.59
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.85	0.59
1:C:396:ALA:HB1	1:C:453:ARG:NH1	2.18	0.59
1:A:1015:LYS:HE2	1:A:1019:GLN:NE2	2.17	0.59
1:A:214:GLU:HB3	1:A:215:ASP:OD1	2.03	0.59
1:B:622:ASN:ND2	1:B:624:TRP:H	2.01	0.59
1:C:937:LYS:HD3	1:D:1152:PRO:HB3	1.84	0.58
1:D:874:LEU:O	1:D:887:PHE:HE1	1.85	0.58
1:A:277:VAL:HG11	1:A:436:PHE:CE1	2.38	0.58
1:A:948:PHE:CD1	1:A:967:ILE:HD12	2.38	0.58
1:C:213:LEU:HD12	1:C:213:LEU:O	2.03	0.58
1:C:276:GLU:O	1:C:335:ILE:HD11	2.03	0.58
1:D:575:GLN:HE22	1:D:610:ALA:H	1.50	0.58
1:A:144:GLU:O	1:A:148:MET:HB3	2.04	0.58
1:A:210:GLU:O	1:A:212:GLU:N	2.37	0.58
1:B:114:ILE:O	1:B:139:ILE:HG13	2.04	0.58
1:D:877:GLN:O	1:D:881:LEU:HG	2.03	0.58
1:A:641:MET:CE	1:A:674:PHE:HE1	2.17	0.58
1:B:1042:MET:CE	1:B:1062:LEU:HB2	2.33	0.58
1:C:323:ILE:HG22	1:C:324:GLU:N	2.18	0.58
1:B:99:ILE:H	1:B:99:ILE:CD1	2.12	0.58
1:D:1161:THR:O	1:D:1162:VAL:HG13	2.04	0.58
1:D:263:ARG:HH21	1:D:330:GLN:HE21	1.49	0.58
1:D:40:LEU:CD2	1:D:42:VAL:HG23	2.34	0.58
1:D:544:LEU:O	1:D:548:VAL:HG22	2.04	0.58
1:D:896:ARG:HD2	1:D:928:GLU:OE2	2.03	0.58
1:C:378:ILE:N	1:C:378:ILE:HD13	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:GLN:HE22	1:A:1149:ILE:HD11	1.69	0.58
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.69	0.58
1:A:622:ASN:ND2	1:A:624:TRP:N	2.49	0.57
1:B:167:ILE:HG23	1:B:168:PRO:HD2	1.86	0.57
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.85	0.57
1:D:870:GLN:O	1:D:871:TYR:C	2.42	0.57
1:A:328:ARG:HD2	1:A:329:VAL:O	2.04	0.57
1:A:254:HIS:CD2	1:A:356:ASP:OD2	2.49	0.57
1:B:1116:MET:CB	1:B:1117:PRO:HD2	2.33	0.57
1:D:378:ILE:HG13	1:D:450:MET:CE	2.34	0.57
1:C:740:ILE:HB	1:C:770:LEU:HD12	1.87	0.57
1:A:179:LEU:HD11	1:A:217:PHE:CZ	2.38	0.57
1:A:362:MET:HE1	1:A:367:ILE:CD1	2.34	0.57
1:D:700:SER:H	1:D:736:HIS:CD2	2.09	0.57
1:C:196:THR:O	1:C:197:SER:CB	2.52	0.57
1:D:828:ILE:O	1:D:832:GLU:HG2	2.05	0.57
1:A:631:ARG:O	1:A:631:ARG:HD3	2.04	0.57
1:B:451:ARG:HG2	1:B:453:ARG:NH2	2.19	0.57
1:A:177:TYR:C	1:A:179:LEU:N	2.58	0.57
1:B:253:GLU:HG3	1:B:305:VAL:CG1	2.35	0.57
1:B:41:LEU:HD22	1:B:114:ILE:HG12	1.85	0.57
1:D:142:HIS:H	1:D:145:HIS:HD2	1.51	0.57
1:D:690:ASN:O	1:D:694:GLN:HG2	2.05	0.57
1:A:1064:THR:HG22	1:A:1065:ILE:N	2.19	0.57
1:A:116:PRO:HB2	1:A:122:SER:HA	1.86	0.57
1:B:543:GLN:H	1:B:543:GLN:NE2	2.03	0.57
1:C:1029:ASN:C	1:C:1029:ASN:ND2	2.57	0.57
1:C:675:ARG:HA	1:C:701:GLU:HB3	1.86	0.57
1:D:960:ASN:ND2	1:D:963:LEU:N	2.42	0.57
1:A:52:ILE:HD13	1:A:115:HIS:CG	2.40	0.57
1:B:325:VAL:O	1:B:327:PRO:HD3	2.05	0.57
1:D:873:ASN:H	1:D:873:ASN:ND2	1.94	0.57
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.40	0.56
1:C:732:ARG:NH1	1:C:732:ARG:HG3	2.20	0.56
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.69	0.56
1:A:210:GLU:C	1:A:212:GLU:H	2.08	0.56
1:D:1127:VAL:O	1:D:1157:ILE:O	2.23	0.56
1:B:334:THR:HA	1:B:337:GLU:OE2	2.05	0.56
1:B:513:PRO:O	1:B:515:ASN:HB2	2.05	0.56
1:B:738:LEU:HD23	1:B:768:ILE:HG13	1.87	0.56
1:B:921:MET:HG2	1:B:926:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:TYR:HE1	1:C:891:LYS:HD3	1.70	0.56
1:B:370:LEU:O	1:B:432:HIS:HE1	1.89	0.56
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.87	0.56
1:A:1081:ASN:CB	1:C:78:TYR:CD2	2.88	0.56
1:A:386:ASP:O	1:A:387:PHE:HB2	2.04	0.56
1:A:67:TYR:O	1:A:86:VAL:HG23	2.05	0.56
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.56
1:D:1015:LYS:O	1:D:1019:GLN:HG3	2.06	0.56
1:D:149:PHE:HA	1:D:155:ALA:HB2	1.88	0.56
1:D:799:ALA:H	1:D:811:ASN:ND2	2.04	0.56
1:A:1110:SER:HB3	1:A:1176:GLU:HG2	1.87	0.56
1:A:512:PHE:CD2	1:A:513:PRO:HD2	2.41	0.56
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.88	0.56
1:B:1053:ASP:HB3	1:B:1056:LYS:HG2	1.86	0.56
1:B:1116:MET:HB3	1:B:1117:PRO:HD2	1.87	0.56
1:C:286:THR:O	1:C:290:ARG:HG3	2.06	0.56
1:C:937:LYS:HD3	1:D:1152:PRO:HB2	1.88	0.56
1:D:381:GLU:O	1:D:383:PRO:HD3	2.06	0.56
1:A:406:ARG:C	1:A:406:ARG:HD2	2.24	0.56
1:C:191:LEU:CB	1:C:235:ILE:HD11	2.32	0.56
1:C:652:LYS:HA	1:C:952:ILE:CD1	2.35	0.56
1:A:275:VAL:HG22	1:A:376:CYS:HB3	1.87	0.56
1:A:90:LEU:CD1	1:A:98:ASN:HB2	2.36	0.56
1:B:501:LEU:HB3	1:B:1078:TYR:CE1	2.41	0.56
1:C:1008:ILE:HD12	1:C:1009:SER:H	1.71	0.56
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.87	0.56
1:A:866:MET:CE	1:A:870:GLN:HG2	2.36	0.56
1:C:311:GLU:OE2	5:C:1202:ATP:O1G	2.24	0.56
1:B:40:LEU:HA	1:B:113:ALA:O	2.07	0.55
1:C:238:TYR:CE1	5:C:1202:ATP:C2	2.94	0.55
1:D:468:ASN:OD1	1:D:469:LYS:N	2.40	0.55
1:C:404:GLY:HA3	1:C:442:LYS:HE2	1.88	0.55
1:B:287:LEU:O	1:B:287:LEU:HD22	2.06	0.55
1:B:424:SER:O	1:B:425:LEU:C	2.44	0.55
1:B:445:ARG:NH1	1:B:449:GLU:OE1	2.39	0.55
1:C:927:ASP:OD1	1:C:929:GLN:HG2	2.05	0.55
1:D:641:MET:HE3	1:D:674:PHE:CE1	2.40	0.55
1:A:606:MET:HE1	1:A:639:PHE:HB3	1.86	0.55
1:D:1069:ASP:C	1:D:1069:ASP:OD2	2.45	0.55
1:D:1111:HIS:HB3	1:D:1173:LEU:HD11	1.87	0.55
1:D:864:HIS:CD2	1:D:866:MET:H	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:920:TYR:OH	1:D:938:LEU:O	2.25	0.55
1:A:622:ASN:HD21	1:A:624:TRP:HB2	1.71	0.55
1:B:519:ARG:HB2	1:B:520:PRO:CD	2.37	0.55
1:C:206:ILE:HG13	1:C:206:ILE:O	2.05	0.55
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.71	0.55
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.40	0.55
1:B:923:GLN:HG3	1:B:923:GLN:O	2.06	0.55
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.42	0.55
1:C:358:GLU:HA	1:C:358:GLU:OE1	2.05	0.55
1:C:456:LYS:N	1:C:456:LYS:HD3	2.22	0.55
1:A:313:LEU:HD22	1:A:323:ILE:HG13	1.88	0.55
1:B:67:TYR:CD1	1:B:77:ARG:HG3	2.42	0.55
1:A:180:ALA:O	1:A:181:LYS:C	2.44	0.55
1:A:896:ARG:HD2	1:A:928:GLU:OE2	2.06	0.55
1:B:252:ASP:OD1	1:B:357:LEU:N	2.40	0.55
1:B:641:MET:HE2	1:B:671:ILE:HG21	1.89	0.55
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.72	0.55
1:D:524:TYR:CD2	1:D:843:THR:CG2	2.90	0.55
1:A:296:ILE:O	1:A:300:GLU:HB2	2.07	0.55
1:A:864:HIS:CD2	1:A:866:MET:H	2.19	0.55
1:A:935:GLY:HA3	1:A:966:VAL:CG1	2.36	0.55
1:D:647:ASN:C	1:D:647:ASN:ND2	2.59	0.55
1:D:335:ILE:HD11	1:D:373:ALA:O	2.07	0.54
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.40	0.54
1:B:438:GLN:HA	1:B:441:GLU:HG2	1.89	0.54
1:D:1135:GLN:O	1:D:1150:GLN:HA	2.08	0.54
1:A:1137:LEU:O	1:A:1138:LEU:HB2	2.07	0.54
1:D:384:LEU:HD21	1:D:490:ILE:HG23	1.89	0.54
1:D:814:TYR:CZ	1:D:828:ILE:HG13	2.43	0.54
1:B:1144:LYS:NZ	4:B:1202:BTI:O11	2.29	0.54
1:A:1145:MET:HG3	1:B:515:ASN:OD1	2.07	0.54
1:C:1005:GLN:O	1:C:1008:ILE:HD12	2.07	0.54
1:C:170:THR:HG21	1:C:174:ILE:HD11	1.90	0.54
1:A:268:GLN:HB3	1:A:272:GLN:O	2.08	0.54
1:C:238:TYR:CD1	5:C:1202:ATP:C2	2.96	0.54
1:C:960:ASN:O	1:C:961:LYS:C	2.45	0.54
1:D:1123:VAL:HG12	1:D:1163:ASN:O	2.07	0.54
1:C:930:SER:O	1:C:931:VAL:HG23	2.06	0.54
1:D:385:ASN:O	1:D:386:ASP:HB2	2.08	0.54
1:A:1015:LYS:HE2	1:A:1019:GLN:HE22	1.73	0.54
1:A:1029:ASN:HD22	1:A:1029:ASN:C	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:MET:HE2	1:A:674:PHE:CD1	2.42	0.54
1:B:1053:ASP:HB3	1:B:1056:LYS:CG	2.38	0.54
1:A:515:ASN:HA	1:B:1143:MET:HG3	1.88	0.54
1:C:504:ILE:HG21	1:C:1042:MET:HE2	1.89	0.54
1:D:811:ASN:H	1:D:811:ASN:HD22	1.55	0.54
1:A:207:VAL:HG12	1:A:209:GLU:H	1.73	0.54
1:B:814:TYR:CZ	1:B:828:ILE:HG13	2.43	0.54
1:B:434:ILE:CG1	1:D:341:GLY:O	2.53	0.54
1:C:174:ILE:HG22	1:C:217:PHE:HE1	1.73	0.54
1:C:330:GLN:HB3	1:C:332:GLU:OE2	2.08	0.54
1:D:622:ASN:HD22	1:D:623:PRO:N	2.06	0.54
1:A:179:LEU:HD21	1:A:217:PHE:CE2	2.43	0.54
1:A:413:PHE:HE1	1:A:416:ALA:HB3	1.73	0.53
1:B:1132:LYS:HA	1:B:1154:ASP:OD1	2.09	0.53
1:D:1105:ASP:HB3	1:D:1109:PRO:HD2	1.90	0.53
1:B:606:MET:HE1	1:B:671:ILE:HD13	1.89	0.53
1:B:932:ILE:HG13	1:B:933:THR:N	2.23	0.53
1:A:1081:ASN:HB3	1:C:78:TYR:CD2	2.43	0.53
1:D:743:MET:CG	1:D:907:VAL:HG13	2.37	0.53
1:A:178:GLU:HG3	1:A:181:LYS:HB2	1.91	0.53
1:C:370:LEU:O	1:C:432:HIS:HE1	1.91	0.53
1:C:696:ALA:O	1:C:698:LYS:HG2	2.09	0.53
1:C:949:LYS:HE3	1:C:974:LEU:HG	1.90	0.53
1:A:504:ILE:HG21	1:A:1042:MET:HE2	1.90	0.53
1:A:309:THR:HG21	1:A:330:GLN:HE22	1.73	0.53
1:C:98:ASN:HD22	1:C:98:ASN:C	2.12	0.53
1:D:704:ILE:HG12	1:D:726:LEU:HD23	1.89	0.53
1:D:77:ARG:NH1	1:D:77:ARG:HG3	2.08	0.53
1:B:335:ILE:HD11	1:B:374:ILE:CA	2.39	0.53
1:B:545:LEU:HD11	1:B:550:PRO:HD3	1.90	0.53
1:A:335:ILE:HD11	1:A:375:GLN:N	2.23	0.53
1:B:641:MET:CE	1:B:674:PHE:CE1	2.92	0.53
1:B:695:GLU:O	1:B:695:GLU:HG2	2.07	0.53
1:C:169:GLY:CA	1:C:236:GLU:HA	2.39	0.53
1:C:265:CYS:HB3	1:C:273:LYS:HD3	1.89	0.53
1:D:151:ASP:HB3	1:D:154:LYS:HG3	1.90	0.53
1:B:1053:ASP:HB3	1:B:1056:LYS:CD	2.38	0.53
1:B:472:THR:O	1:B:474:GLY:N	2.41	0.53
1:B:641:MET:HE1	1:B:666:SER:HB3	1.91	0.53
1:C:111:VAL:HG12	1:C:113:ALA:H	1.74	0.53
1:C:234:TYR:HD2	1:C:234:TYR:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG11	1:A:436:PHE:HE1	1.73	0.53
1:A:1081:ASN:HB2	1:C:78:TYR:CD2	2.44	0.53
1:A:179:LEU:O	1:A:182:GLU:HG2	2.09	0.53
1:B:337:GLU:HG2	1:B:344:ILE:HD12	1.91	0.53
1:B:871:TYR:CD1	1:B:871:TYR:O	2.62	0.53
1:C:826:THR:OG1	1:C:827:ASP:N	2.40	0.53
1:A:337:GLU:HB3	1:A:342:ILE:O	2.09	0.52
1:C:398:ARG:NH1	1:C:451:ARG:NH1	2.57	0.52
1:A:1117:PRO:HD3	1:A:1170:THR:OG1	2.09	0.52
1:C:811:ASN:H	1:C:811:ASN:HD22	1.55	0.52
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.23	0.52
1:D:647:ASN:HB2	1:D:654:TYR:CE1	2.44	0.52
1:A:45:ARG:HH11	1:A:45:ARG:HG3	1.74	0.52
1:A:458:ASN:O	1:A:461:PHE:HB3	2.09	0.52
1:B:335:ILE:HG12	1:B:373:ALA:CB	2.40	0.52
1:B:572:ASP:HB3	1:B:807:GLN:HE21	1.73	0.52
1:C:323:ILE:HG22	1:C:324:GLU:H	1.73	0.52
1:A:263:ARG:HH21	1:A:330:GLN:HE22	1.57	0.52
1:C:188:GLY:HA3	1:C:237:ARG:NH2	2.23	0.52
1:D:400:SER:HB3	1:D:449:GLU:CD	2.29	0.52
1:B:575:GLN:NE2	1:B:610:ALA:H	2.06	0.52
1:B:927:ASP:HB2	1:B:930:SER:H	1.73	0.52
1:C:337:GLU:CG	1:C:344:ILE:HD12	2.39	0.52
1:C:644:ARG:CZ	1:C:908:THR:HG21	2.38	0.52
1:C:756:ILE:HG22	1:C:789:ALA:HB1	1.90	0.52
1:D:509:ILE:CD1	1:D:1089:ILE:HG21	2.34	0.52
1:D:1159:GLN:NE2	1:D:1176:GLU:OE1	2.30	0.52
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.43	0.52
1:A:414:GLN:CA	1:A:414:GLN:HE21	2.22	0.52
1:B:921:MET:HG2	1:B:926:LEU:HB2	1.90	0.52
1:C:296:ILE:O	1:C:300:GLU:HB2	2.09	0.52
1:D:749:PRO:HG3	1:D:781:LEU:HB3	1.91	0.52
1:D:952:ILE:O	1:D:952:ILE:CG2	2.58	0.52
1:B:137:LYS:CE	1:B:352:ALA:O	2.47	0.52
1:B:506:ASN:ND2	1:B:510:ASN:ND2	2.56	0.52
1:B:871:TYR:HD1	1:B:871:TYR:O	1.93	0.52
1:C:174:ILE:HG22	1:C:217:PHE:CE1	2.44	0.52
1:C:652:LYS:HA	1:C:952:ILE:HD11	1.91	0.52
1:D:263:ARG:NH2	1:D:330:GLN:HE21	2.08	0.52
1:A:991:ARG:O	1:A:995:GLU:HG3	2.10	0.52
1:B:1097:ASN:HD22	1:B:1097:ASN:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:O	1:B:148:MET:N	2.41	0.52
1:C:896:ARG:HB3	1:C:928:GLU:OE2	2.10	0.52
1:A:571:ARG:HH11	1:A:575:GLN:NE2	2.07	0.52
1:B:1087:ILE:HG22	1:B:1088:TYR:N	2.24	0.52
1:B:363:GLN:HB2	1:B:366:ASP:OD2	2.10	0.52
1:C:571:ARG:HH11	1:C:575:GLN:HE22	1.58	0.52
1:C:649:VAL:CG1	1:C:649:VAL:O	2.58	0.52
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.41	0.52
1:B:145:HIS:HE1	1:B:302:ILE:O	1.93	0.52
1:B:358:GLU:OE2	1:B:358:GLU:HA	2.10	0.52
1:B:820:PHE:HB3	1:B:821:PRO:HD2	1.91	0.52
1:C:964:GLN:O	1:C:965:ALA:C	2.48	0.52
1:D:866:MET:HE2	1:D:871:TYR:HA	1.91	0.52
1:A:125:GLU:CD	1:A:125:GLU:H	2.14	0.51
1:A:580:THR:HG22	1:A:580:THR:O	2.10	0.51
1:C:893:MET:HE1	1:C:921:MET:SD	2.50	0.51
1:D:1069:ASP:OD2	1:D:1070:GLU:N	2.43	0.51
1:B:1177:ILE:HD13	1:B:1177:ILE:N	2.25	0.51
1:B:641:MET:HE2	1:B:674:PHE:CE1	2.45	0.51
1:C:206:ILE:HD11	1:C:208:ARG:NE	2.24	0.51
1:C:940:PHE:HB3	1:C:944:VAL:HG11	1.92	0.51
1:D:370:LEU:O	1:D:432:HIS:HE1	1.92	0.51
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.57	0.51
1:A:688:VAL:HG21	1:A:977:ARG:NH2	2.26	0.51
1:A:513:PRO:O	1:A:515:ASN:CB	2.50	0.51
1:A:622:ASN:HD22	1:A:623:PRO:N	2.08	0.51
1:A:796:THR:HB	1:A:810:ALA:HB2	1.91	0.51
1:B:893:MET:CE	1:B:896:ARG:HH21	2.24	0.51
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.45	0.51
1:C:814:TYR:CZ	1:C:828:ILE:HG13	2.45	0.51
1:C:590:ILE:CG1	1:C:837:TYR:CE2	2.94	0.51
1:C:775:THR:CG2	1:C:861:ILE:HG13	2.41	0.51
1:A:641:MET:CE	1:A:674:PHE:CD1	2.93	0.51
1:B:620:LYS:HG2	4:B:1201:BTI:H63	1.93	0.51
1:B:701:GLU:OE2	1:B:769:HIS:ND1	2.44	0.51
1:B:991:ARG:HG3	1:B:992:GLU:N	2.24	0.51
1:C:215:ASP:O	1:C:216:ALA:C	2.49	0.51
1:D:671:ILE:O	1:D:698:LYS:HE3	2.11	0.51
1:D:641:MET:HE3	1:D:674:PHE:HE1	1.74	0.51
1:A:167:ILE:HD12	1:A:323:ILE:HD11	1.92	0.51
1:A:451:ARG:NH1	1:A:495:ASP:OD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:MET:HG3	1:C:206:ILE:HG22	1.92	0.51
1:C:644:ARG:O	1:C:645:ALA:C	2.49	0.51
1:C:893:MET:HG3	1:C:922:VAL:CG2	2.40	0.51
1:D:263:ARG:HG2	1:D:278:ALA:HB2	1.91	0.51
1:A:650:GLY:HA2	1:A:1013:TYR:CE1	2.46	0.51
1:B:1133:ALA:O	1:B:1134:ASN:HB2	2.10	0.51
1:B:897:VAL:HG11	1:B:914:VAL:HG13	1.86	0.51
1:C:938:LEU:HA	1:D:1115:GLN:HE22	1.76	0.51
1:D:597:VAL:HG22	1:D:830:GLY:HA3	1.93	0.51
1:A:896:ARG:NH1	1:A:928:GLU:OE1	2.44	0.51
1:B:1000:GLY:N	1:B:1001:PRO:HD2	2.26	0.51
1:B:802:SER:OG	1:B:809:SER:HB2	2.11	0.51
1:C:194:LYS:HD2	1:C:234:TYR:CZ	2.46	0.51
1:C:43:ALA:HA	1:C:66:ILE:HD11	1.92	0.51
1:C:959:PHE:N	1:C:959:PHE:CD1	2.78	0.51
1:D:74:SER:O	1:D:77:ARG:HB3	2.11	0.51
1:D:784:LYS:CE	6:D:1201:CL:CL	2.96	0.51
1:B:144:GLU:O	1:B:148:MET:CB	2.58	0.51
1:B:71:ASP:C	1:B:73:SER:H	2.14	0.51
1:C:115:HIS:ND1	1:C:116:PRO:HD2	2.26	0.51
1:C:210:GLU:O	1:C:211:SER:HB3	2.11	0.51
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.41	0.51
1:D:542:LYS:HE3	1:D:672:ASP:OD1	2.10	0.51
1:A:572:ASP:HB3	1:A:807:GLN:NE2	2.25	0.51
1:C:90:LEU:HB3	1:C:95:SER:HB2	1.93	0.51
1:D:470:LYS:HB2	1:D:480:PHE:HE1	1.76	0.51
1:D:960:ASN:HD22	1:D:963:LEU:CB	2.23	0.51
1:A:166:VAL:CG1	1:A:167:ILE:N	2.74	0.50
1:A:257:ILE:HG22	1:A:296:ILE:CD1	2.41	0.50
1:A:553:VAL:O	1:A:556:TRP:HB3	2.11	0.50
1:B:40:LEU:HD23	1:B:41:LEU:N	2.27	0.50
1:B:711:LEU:HD11	1:B:750:LYS:HB3	1.93	0.50
1:C:703:THR:HG22	1:C:704:ILE:N	2.26	0.50
1:D:143:LEU:H	1:D:143:LEU:HD12	1.77	0.50
1:D:524:TYR:HD2	1:D:843:THR:CG2	2.24	0.50
1:D:641:MET:HE2	1:D:671:ILE:HG21	1.93	0.50
1:B:748:LYS:HB3	1:B:749:PRO:HD2	1.93	0.50
1:B:828:ILE:H	1:B:828:ILE:CD1	2.14	0.50
1:B:870:GLN:C	1:B:872:SER:H	2.15	0.50
1:C:496:ARG:CD	1:C:496:ARG:N	2.75	0.50
1:B:370:LEU:HD21	1:D:341:GLY:CA	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:PHE:CZ	1:D:416:ALA:HB2	2.46	0.50
1:A:179:LEU:N	1:A:179:LEU:HD23	2.07	0.50
1:B:121:LEU:O	1:B:124:ASN:HB3	2.10	0.50
1:B:530:PRO:HB2	1:B:593:LYS:HD3	1.94	0.50
1:B:71:ASP:C	1:B:73:SER:N	2.64	0.50
1:C:77:ARG:HD3	1:C:78:TYR:CD2	2.47	0.50
1:B:856:SER:OG	1:C:800:SER:HA	2.12	0.50
1:A:828:ILE:O	1:A:832:GLU:HG2	2.11	0.50
1:C:677:PHE:CA	1:C:686:MET:HE3	2.41	0.50
1:C:820:PHE:HB3	1:C:821:PRO:HD3	1.91	0.50
1:D:917:MET:HA	1:D:917:MET:CE	2.41	0.50
1:A:622:ASN:ND2	1:A:624:TRP:HB2	2.27	0.50
1:B:811:ASN:ND2	1:B:811:ASN:H	2.04	0.50
1:C:181:LYS:O	1:C:185:GLU:HG2	2.11	0.50
1:C:338:MET:HE1	1:C:373:ALA:HB1	1.91	0.50
1:B:335:ILE:HG12	1:B:373:ALA:HB1	1.93	0.50
1:D:328:ARG:HD3	1:D:329:VAL:O	2.11	0.50
1:A:504:ILE:HG21	1:A:1042:MET:HE3	1.93	0.50
1:A:606:MET:HE2	1:A:639:PHE:HB3	1.93	0.50
1:A:622:ASN:C	1:A:622:ASN:ND2	2.64	0.50
1:B:118:TYR:CE2	1:B:331:VAL:HA	2.46	0.50
1:C:99:ILE:O	1:C:103:ILE:HD12	2.12	0.50
1:C:1143:MET:O	1:C:1144:LYS:HB2	2.11	0.50
1:C:51:ARG:HD3	1:C:406:ARG:HH12	1.77	0.50
1:C:448:ARG:HH22	1:C:467:LYS:HZ1	1.58	0.50
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.93	0.50
1:B:1095:HIS:CB	1:B:1098:ALA:HB3	2.40	0.50
1:C:425:LEU:C	1:C:425:LEU:HD23	2.32	0.50
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.09	0.50
1:B:498:THR:HG23	1:B:1085:ARG:HH22	1.77	0.50
1:B:682:TRP:CE3	1:B:685:GLN:HG2	2.47	0.50
1:C:1065:ILE:HG12	1:C:1076:ILE:HG12	1.94	0.50
1:C:717:ASN:C	1:C:717:ASN:HD22	2.14	0.50
1:D:770:LEU:HD12	1:D:771:HIS:H	1.76	0.50
1:D:871:TYR:CE1	1:D:887:PHE:HE2	2.29	0.50
1:B:568:THR:OG1	1:B:807:GLN:CG	2.58	0.49
1:A:902:GLY:O	1:A:903:ASP:CB	2.61	0.49
1:C:563:VAL:HG21	1:C:787:ILE:HG12	1.93	0.49
1:C:641:MET:HB3	1:C:671:ILE:HD12	1.95	0.49
1:A:871:TYR:O	1:A:871:TYR:CD1	2.65	0.49
1:B:755:LEU:O	1:B:759:LEU:HG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:GLN:HA	1:C:1008:ILE:HD11	1.94	0.49
1:A:269:ARG:HD3	1:A:272:GLN:OE1	2.12	0.49
1:A:335:ILE:HD11	1:A:374:ILE:C	2.33	0.49
1:C:461:PHE:CE1	1:C:487:LEU:HB3	2.48	0.49
1:D:141:PRO:HB2	1:D:145:HIS:HB2	1.94	0.49
1:D:490:ILE:O	1:D:492:PRO:CD	2.48	0.49
1:A:811:ASN:N	1:A:811:ASN:HD22	2.09	0.49
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.47	0.49
1:B:307:ALA:HB3	1:B:348:GLN:HE21	1.78	0.49
1:B:40:LEU:C	1:B:40:LEU:CD2	2.81	0.49
1:B:542:LYS:HE2	1:B:631:ARG:NH2	2.26	0.49
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.95	0.49
1:C:90:LEU:HD11	1:C:98:ASN:OD1	2.13	0.49
1:C:939:ASP:O	1:D:1147:THR:CG2	2.60	0.49
1:D:1153:PHE:O	1:D:1154:ASP:HB2	2.13	0.49
1:A:192:MET:CE	1:A:238:TYR:HD1	2.10	0.49
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.27	0.49
1:B:115:HIS:NE2	1:B:348:GLN:OE1	2.45	0.49
1:B:715:ARG:O	1:B:715:ARG:HD2	2.13	0.49
1:B:927:ASP:HB2	1:B:930:SER:CB	2.42	0.49
1:C:71:ASP:O	1:C:73:SER:N	2.46	0.49
1:D:1105:ASP:HB3	1:D:1109:PRO:CD	2.42	0.49
1:D:918:ALA:O	1:D:922:VAL:HG23	2.12	0.49
1:D:998:GLN:O	1:D:999:GLN:O	2.31	0.49
1:A:509:ILE:HD12	1:A:1089:ILE:HG21	1.94	0.49
1:B:43:ALA:HB3	1:B:116:PRO:HA	1.95	0.49
1:B:912:LYS:HZ2	1:B:943:SER:HB3	1.77	0.49
1:C:166:VAL:HG12	1:C:167:ILE:N	2.28	0.49
1:A:90:LEU:HD11	1:A:98:ASN:HB2	1.94	0.49
1:B:842:ARG:CZ	1:C:855:LYS:HE2	2.43	0.49
1:B:949:LYS:HG2	1:B:968:LEU:HD21	1.95	0.49
1:C:991:ARG:HG3	1:C:995:GLU:HG3	1.95	0.49
1:D:262:GLU:OE2	1:D:288:ARG:HG3	2.13	0.49
1:A:174:ILE:HG13	1:A:174:ILE:O	2.13	0.49
1:A:783:TYR:O	1:A:787:ILE:HG13	2.12	0.49
1:B:1112:ILE:CD1	1:B:1177:ILE:HD11	2.43	0.49
1:B:606:MET:CE	1:B:639:PHE:HB3	2.43	0.49
1:C:152:LYS:HG3	1:C:197:SER:HA	1.94	0.49
1:C:544:LEU:O	1:C:547:GLU:HB2	2.13	0.49
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.48	0.49
1:D:241:ASN:HD22	1:D:477:THR:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ASN:C	1:D:622:ASN:HD22	2.16	0.49
1:D:622:ASN:C	1:D:622:ASN:ND2	2.66	0.49
1:B:156:ARG:NH2	1:B:167:ILE:HG13	2.28	0.48
1:B:472:THR:C	1:B:474:GLY:N	2.65	0.48
1:C:235:ILE:HG13	1:C:236:GLU:N	2.27	0.48
1:C:931:VAL:HA	1:C:935:GLY:N	2.28	0.48
1:C:969:LYS:HA	1:C:969:LYS:HE2	1.94	0.48
1:A:632:LYS:HE2	1:A:632:LYS:HB3	1.57	0.48
1:B:1022:GLN:NE2	1:B:1022:GLN:HA	2.28	0.48
1:B:1101:LYS:HD2	1:B:1161:THR:HG22	1.95	0.48
1:D:748:LYS:O	1:D:751:ALA:HB3	2.13	0.48
1:A:1071:ASN:O	1:A:1090:LYS:HE2	2.13	0.48
1:A:394:ILE:HD11	1:A:418:ILE:HD11	1.95	0.48
1:B:485:PRO:HD2	1:B:486:GLU:OE1	2.14	0.48
1:B:811:ASN:N	1:B:811:ASN:HD22	2.03	0.48
1:C:193:ILE:HD13	1:C:193:ILE:C	2.33	0.48
1:C:381:GLU:O	1:C:383:PRO:HD3	2.13	0.48
1:C:924:ASN:O	1:C:925:ASP:C	2.52	0.48
1:D:622:ASN:ND2	1:D:623:PRO:HD2	2.22	0.48
1:C:259:HIS:HB3	1:C:296:ILE:HD11	1.95	0.48
1:D:239:ILE:O	1:D:242:PRO:HD3	2.14	0.48
1:A:1064:THR:CG2	1:A:1065:ILE:N	2.76	0.48
1:A:1077:TYR:N	1:A:1077:TYR:CD1	2.81	0.48
1:C:866:MET:HE2	1:C:891:LYS:HG2	1.95	0.48
1:B:656:ASP:OD1	1:B:977:ARG:NH2	2.47	0.48
1:B:915:GLY:O	1:B:919:LEU:HD22	2.14	0.48
1:C:269:ARG:NH1	1:C:269:ARG:HB2	2.26	0.48
1:C:677:PHE:HA	1:C:686:MET:HE1	1.93	0.48
1:A:784:LYS:HE3	6:D:1201:CL:CL	2.50	0.48
1:A:380:THR:N	1:A:424:SER:OG	2.38	0.48
1:C:167:ILE:HD12	1:C:167:ILE:H	1.77	0.48
1:C:572:ASP:CB	1:C:807:GLN:HE22	2.22	0.48
1:A:778:ASN:ND2	1:D:780:LEU:HD13	2.29	0.48
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.49	0.48
1:C:496:ARG:HD3	1:C:496:ARG:N	2.28	0.48
1:C:703:THR:CG2	1:C:704:ILE:N	2.77	0.48
1:D:104:ASP:O	1:D:105:VAL:C	2.52	0.48
1:D:156:ARG:O	1:D:159:ALA:HB3	2.13	0.48
1:D:683:VAL:HG23	1:D:726:LEU:HD11	1.94	0.48
1:A:991:ARG:HG3	1:A:995:GLU:HG3	1.95	0.48
1:B:129:ARG:HH11	1:B:129:ARG:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:ASP:OD1	1:C:988:GLU:HB2	2.14	0.48
1:D:40:LEU:HD21	1:D:42:VAL:HG23	1.95	0.48
1:A:130:ARG:NH1	1:A:133:GLU:OE1	2.43	0.48
1:A:210:GLU:C	1:A:212:GLU:N	2.66	0.48
1:B:338:MET:HE2	1:B:373:ALA:HB1	1.95	0.48
1:D:385:ASN:O	1:D:386:ASP:CB	2.60	0.48
1:D:77:ARG:CG	1:D:77:ARG:NH1	2.68	0.48
1:A:192:MET:HE3	2:A:1201:ADP:C6	2.48	0.47
1:C:775:THR:HG21	1:C:861:ILE:HG13	1.96	0.47
1:D:286:THR:HG22	1:D:290:ARG:HD3	1.96	0.47
1:C:1144:LYS:HE2	1:D:513:PRO:HD3	1.95	0.47
1:B:870:GLN:NE2	1:B:874:LEU:HD13	2.28	0.47
1:C:328:ARG:HG3	1:C:329:VAL:O	2.14	0.47
1:D:287:LEU:CD1	1:D:317:GLY:O	2.54	0.47
1:D:484:THR:HB	1:D:487:LEU:HD22	1.96	0.47
1:A:176:SER:O	1:A:179:LEU:CB	2.62	0.47
1:C:87:GLY:HA3	1:C:90:LEU:CD2	2.40	0.47
1:C:955:PRO:O	1:C:956:VAL:C	2.52	0.47
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.80	0.47
1:D:262:GLU:OE2	1:D:288:ARG:NH1	2.46	0.47
1:D:362:MET:HE3	1:D:362(A):PRO:O	2.14	0.47
1:A:744:ALA:HB2	1:A:867:PRO:HA	1.96	0.47
1:B:105:VAL:O	1:B:106:ALA:C	2.52	0.47
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.11	0.47
1:A:99:ILE:O	1:A:103:ILE:HG12	2.13	0.47
1:B:1176:GLU:C	1:B:1177:ILE:HD13	2.35	0.47
1:D:396:ALA:HB3	1:D:453:ARG:HB2	1.97	0.47
1:A:856:SER:OG	1:D:800:SER:HA	2.14	0.47
1:A:512:PHE:CG	1:A:513:PRO:HD2	2.49	0.47
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.47
1:B:1161:THR:O	1:B:1161:THR:HG22	2.15	0.47
1:C:71:ASP:OD2	1:C:96:TYR:OH	2.17	0.47
1:C:743:MET:CG	1:C:907:VAL:HG13	2.45	0.47
1:C:798:VAL:O	1:C:799:ALA:C	2.53	0.47
1:D:1158:LYS:HB2	1:D:1176:GLU:HG3	1.96	0.47
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.47	0.47
1:D:902:GLY:O	1:D:903:ASP:HB3	2.14	0.47
1:A:1144:LYS:O	1:A:1145:MET:HE3	2.15	0.47
1:D:470:LYS:CA	1:D:470:LYS:HE2	2.42	0.47
1:A:370:LEU:O	1:A:432:HIS:HE1	1.97	0.47
1:B:1001:PRO:HB2	1:B:1002:VAL:H	1.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:PRO:HB2	1:C:145:HIS:HB2	1.96	0.47
1:C:189:PHE:O	1:C:189:PHE:CD2	2.66	0.47
1:C:342:ILE:HG12	1:C:362:MET:HE3	1.97	0.47
1:A:156:ARG:NH2	1:A:170:THR:O	2.48	0.47
1:A:258:VAL:HG21	1:A:362:MET:HE2	1.96	0.47
1:A:252:ASP:HB3	1:A:357:LEU:HG	1.97	0.47
1:B:878:ALA:HB1	1:B:883:LEU:HB2	1.97	0.47
1:B:913:VAL:HG13	1:B:943:SER:HB2	1.97	0.47
1:B:91:GLY:O	1:B:93:ALA:N	2.47	0.47
1:C:194:LYS:HD2	1:C:234:TYR:OH	2.15	0.47
1:C:586:ASP:OD1	1:C:845:TYR:OH	2.25	0.47
1:C:720:LEU:HD21	1:C:758:GLU:HG3	1.96	0.47
1:D:446:SER:O	1:D:450:MET:HG2	2.15	0.47
1:B:1053:ASP:CG	1:B:1054:LYS:H	2.19	0.47
1:A:263:ARG:NH2	1:A:330:GLN:NE2	2.58	0.47
1:A:413:PHE:CZ	1:A:416:ALA:HB3	2.49	0.47
1:A:45:ARG:HD2	1:A:96:TYR:CE1	2.50	0.47
1:A:71:ASP:O	1:A:73:SER:N	2.47	0.47
1:C:414:GLN:O	1:C:414:GLN:HG3	2.15	0.47
1:D:1050:ILE:HB	1:D:1058:LEU:HB3	1.97	0.47
1:D:116:PRO:HB2	1:D:122:SER:HA	1.96	0.47
1:D:755:LEU:O	1:D:759:LEU:HG	2.14	0.47
1:B:129:ARG:HH11	1:B:129:ARG:HB2	1.80	0.46
1:B:644:ARG:HD2	1:B:647:ASN:OD1	2.15	0.46
1:C:373:ALA:HA	1:C:431:THR:O	2.15	0.46
1:C:77:ARG:HD3	1:C:78:TYR:CE2	2.50	0.46
1:C:768:ILE:HG22	1:C:791:VAL:HG23	1.96	0.46
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.50	0.46
1:A:999:GLN:CG	1:A:1000:GLY:H	2.21	0.46
1:A:461:PHE:HE1	1:A:488:PHE:CE2	2.33	0.46
1:A:571:ARG:HH21	1:A:605:GLU:CD	2.18	0.46
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.80	0.46
1:C:210:GLU:O	1:C:211:SER:HB2	2.14	0.46
1:D:41:LEU:HB2	1:D:111:VAL:HG21	1.97	0.46
1:D:338:MET:HE1	1:D:430:SER:HB3	1.93	0.46
1:C:287:LEU:HD22	1:C:291:ILE:HD11	1.98	0.46
1:C:936:TYR:HE2	1:C:966:VAL:CG1	2.29	0.46
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.06	0.46
1:D:431:THR:HG21	1:D:443:MET:HA	1.98	0.46
1:A:1127:VAL:HG13	1:A:1158:LYS:O	2.14	0.46
1:B:269:ARG:O	1:B:270:ARG:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:ASN:ND2	1:B:811:ASN:N	2.63	0.46
1:C:39:LYS:NZ	1:C:109:ALA:O	2.45	0.46
1:D:325:VAL:HG12	1:D:327:PRO:HD3	1.97	0.46
1:C:540:GLY:HA3	1:C:636:ASN:O	2.15	0.46
1:C:705:CYS:HB3	1:C:743:MET:SD	2.55	0.46
1:D:1103:LYS:HB2	1:D:1104:ALA:H	1.61	0.46
1:D:866:MET:CE	1:D:870:GLN:HB3	2.46	0.46
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.43	0.46
1:C:196:THR:O	1:C:196:THR:CG2	2.53	0.46
1:C:249:VAL:HG21	1:C:299:MET:HG3	1.98	0.46
1:D:799:ALA:HB3	1:D:835:SER:OG	2.16	0.46
1:A:152:LYS:HB3	1:A:234:TYR:CE2	2.51	0.46
1:A:570:PHE:O	1:A:574:HIS:HE1	1.99	0.46
1:A:597:VAL:HG21	1:A:834:LEU:HG	1.96	0.46
1:B:41:LEU:CD2	1:B:114:ILE:HG12	2.46	0.46
1:B:248:GLN:HB3	1:B:260:LEU:HB2	1.98	0.46
1:B:909:PRO:HG2	1:B:952:ILE:HG12	1.97	0.46
1:C:269:ARG:CG	1:C:270:ARG:H	2.24	0.46
1:C:148:MET:SD	1:C:302:ILE:HG21	2.55	0.46
1:D:620:LYS:HE2	1:D:1023:THR:HG1	1.79	0.46
1:A:130:ARG:HD2	1:A:133:GLU:OE1	2.15	0.46
1:A:166:VAL:HG12	1:A:167:ILE:N	2.30	0.46
1:B:828:ILE:O	1:B:832:GLU:HG2	2.15	0.46
1:C:52:ILE:HD13	1:C:115:HIS:CG	2.50	0.46
1:C:986:ASP:O	1:C:990:VAL:HG23	2.15	0.46
1:D:1101:LYS:O	1:D:1102:PRO:C	2.54	0.46
1:A:1141:GLU:HA	1:A:1145:MET:O	2.16	0.46
1:A:180:ALA:O	1:A:182:GLU:N	2.49	0.46
1:A:164:LEU:HD13	1:A:294:ALA:HB1	1.97	0.46
1:A:71:ASP:O	1:A:72:LYS:C	2.54	0.46
1:B:1116:MET:CB	1:B:1117:PRO:CD	2.93	0.46
1:B:479:LYS:O	1:B:483:GLU:HG2	2.16	0.46
1:B:512:PHE:HB3	1:B:516:VAL:HB	1.97	0.46
1:B:927:ASP:HB3	1:B:930:SER:H	1.80	0.46
1:C:141:PRO:HG2	1:C:146:LEU:HD11	1.97	0.46
1:A:47:GLU:OE2	1:A:428:LYS:HE2	2.16	0.46
1:A:558:LYS:CE	1:A:765:ASP:O	2.57	0.46
1:A:796:THR:CB	1:A:810:ALA:HB2	2.46	0.46
1:A:858:ASN:HD21	1:A:860:GLU:H	1.60	0.46
1:B:426:LEU:O	1:B:427:VAL:HG13	2.17	0.46
1:C:241:ASN:N	1:C:242:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:VAL:CG2	1:D:348:GLN:HE22	2.10	0.46
1:C:403:PHE:O	1:C:442:LYS:HE3	2.15	0.45
1:C:677:PHE:HB3	1:C:703:THR:HB	1.97	0.45
1:D:501:LEU:HB3	1:D:1078:TYR:CE1	2.52	0.45
1:D:378:ILE:HG23	1:D:459:ILE:HG13	1.97	0.45
1:A:414:GLN:HA	1:A:414:GLN:HE21	1.81	0.45
1:B:1062:LEU:HD11	1:B:1076:ILE:HG23	1.98	0.45
1:C:175:LYS:H	1:C:175:LYS:CD	2.27	0.45
1:C:854:ILE:H	1:C:854:ILE:HG13	1.60	0.45
1:D:396:ALA:HB3	1:D:453:ARG:CG	2.46	0.45
1:B:1135:GLN:O	1:B:1150:GLN:HA	2.17	0.45
1:B:252:ASP:HA	1:B:351:VAL:HG13	1.98	0.45
1:B:326:ASN:ND2	1:B:330:GLN:NE2	2.65	0.45
1:B:653:ASN:ND2	1:B:951:GLU:O	2.41	0.45
1:D:872:SER:O	1:D:875:SER:HB2	2.16	0.45
1:D:875:SER:OG	1:D:887:PHE:CZ	2.65	0.45
1:B:1008:ILE:HD12	1:B:1009:SER:N	2.31	0.45
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.82	0.45
1:B:994:LEU:O	1:B:998:GLN:HG3	2.15	0.45
1:C:631:ARG:HD3	1:C:631:ARG:C	2.35	0.45
1:A:1161:THR:OG1	1:A:1173:LEU:O	2.33	0.45
1:A:720:LEU:HD21	1:A:758:GLU:HG3	1.98	0.45
1:B:924:ASN:O	1:B:925:ASP:HB2	2.16	0.45
1:C:260:LEU:CD2	1:C:362:MET:CE	2.73	0.45
1:C:813:LEU:O	1:C:814:TYR:C	2.53	0.45
1:C:939:ASP:O	1:D:1147:THR:HG21	2.17	0.45
1:B:1123:VAL:HA	1:B:1138:LEU:HD12	1.98	0.45
1:B:522:PRO:C	1:B:524:TYR:N	2.69	0.45
1:B:979:GLY:HA2	1:B:982:LEU:HD12	1.98	0.45
1:C:948:PHE:CD2	1:C:964:GLN:HB2	2.52	0.45
1:A:778:ASN:HD22	1:D:780:LEU:HD13	1.81	0.45
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.48	0.45
1:B:252:ASP:OD1	1:B:357:LEU:HB2	2.16	0.45
1:B:64:VAL:HG22	1:B:82:GLU:HB2	1.98	0.45
1:C:398:ARG:HH21	1:C:1083:GLN:HB3	1.80	0.45
1:C:820:PHE:HB3	1:C:821:PRO:HD2	1.98	0.45
1:C:524:TYR:CD2	1:C:843:THR:CG2	3.00	0.45
1:D:259:HIS:HD2	1:D:261:PHE:H	1.65	0.45
1:D:350:LEU:HD22	1:D:359:GLU:HB3	1.99	0.45
1:D:752:ALA:HB2	1:D:782:THR:HG23	1.97	0.45
1:A:190:PRO:O	1:A:191:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG12	1:A:274:VAL:HB	1.99	0.45
1:A:322:PHE:O	1:A:323:ILE:HD13	2.17	0.45
1:A:277:VAL:CG1	1:A:436:PHE:HE1	2.29	0.45
1:B:867:PRO:O	1:B:868:GLY:C	2.54	0.45
1:C:625:GLU:O	1:C:629:ARG:HG3	2.17	0.45
1:D:145:HIS:HE1	1:D:302:ILE:O	2.00	0.45
1:D:494:LEU:HD23	1:D:494:LEU:N	2.31	0.45
1:D:613:ASP:HB2	1:D:1013:TYR:CZ	2.52	0.45
1:D:814:TYR:CE2	1:D:828:ILE:HG13	2.52	0.45
1:A:108:GLN:HG2	1:A:108:GLN:O	2.17	0.45
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.81	0.45
1:B:999:GLN:HG2	1:B:1001:PRO:HD2	1.99	0.45
1:C:386:ASP:O	1:C:387:PHE:HB2	2.17	0.45
1:D:1060:ILE:HG12	1:D:1080:MET:HG3	1.98	0.45
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.98	0.45
1:D:99:ILE:HG23	1:D:127:PHE:CD1	2.51	0.45
2:A:1201:ADP:O1A	2:A:1201:ADP:O1B	2.35	0.44
1:A:219:ARG:O	1:A:223:GLU:CB	2.59	0.44
1:B:472:THR:C	1:B:474:GLY:H	2.20	0.44
1:C:907:VAL:O	1:C:910:SER:N	2.50	0.44
1:C:661:LYS:HD2	1:C:987:PHE:CZ	2.52	0.44
1:D:484:THR:HG22	1:D:486:GLU:HG2	1.98	0.44
1:A:1156:VAL:HG22	1:A:1178:GLU:HB2	1.97	0.44
1:B:425:LEU:HD23	1:B:425:LEU:C	2.37	0.44
1:C:323:ILE:HA	1:C:323:ILE:HD13	1.58	0.44
1:C:739:ALA:C	1:C:740:ILE:HD13	2.37	0.44
1:C:828:ILE:O	1:C:829:GLU:C	2.54	0.44
1:B:118:TYR:O	1:B:118:TYR:HD1	2.01	0.44
1:B:68:SER:OG	1:B:69:ASN:N	2.49	0.44
1:C:170:THR:HG22	1:C:171:ASP:N	2.32	0.44
1:D:1042:MET:HB3	1:D:1046:GLU:OE2	2.17	0.44
1:D:267:VAL:HG12	1:D:481:ILE:HD11	1.98	0.44
1:D:270:ARG:HB3	1:D:271:HIS:H	1.65	0.44
1:A:650:GLY:HA2	1:A:1013:TYR:CZ	2.52	0.44
1:A:581:ARG:HD3	1:A:581:ARG:HA	1.62	0.44
1:B:768:ILE:HG22	1:B:791:VAL:HG23	2.00	0.44
1:D:952:ILE:HA	1:D:952:ILE:HD12	1.74	0.44
1:A:268:GLN:HA	1:A:274:VAL:HG23	2.00	0.44
1:A:98:ASN:C	1:A:98:ASN:ND2	2.70	0.44
1:B:1127:VAL:HG13	1:B:1158:LYS:O	2.18	0.44
1:B:294:ALA:O	1:B:295:ALA:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:ILE:N	1:B:828:ILE:CD1	2.70	0.44
1:B:927:ASP:HB3	1:B:929:GLN:N	2.31	0.44
1:C:211:SER:C	1:C:213:LEU:N	2.71	0.44
1:C:404:GLY:O	1:C:431:THR:HA	2.17	0.44
1:C:756:ILE:HG22	1:C:757:GLY:N	2.33	0.44
1:D:433:ALA:H	1:D:439:ALA:HB2	1.82	0.44
1:D:494:LEU:H	1:D:494:LEU:HD23	1.83	0.44
1:D:64:VAL:HG22	1:D:82:GLU:HB2	1.99	0.44
1:D:866:MET:HE1	1:D:871:TYR:HA	1.97	0.44
1:A:858:ASN:HD22	1:A:858:ASN:C	2.20	0.44
1:B:333:HIS:O	1:B:334:THR:C	2.55	0.44
1:B:540:GLY:H	1:B:543:GLN:NE2	2.15	0.44
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.53	0.44
1:C:986:ASP:CG	1:C:989:LYS:HG3	2.38	0.44
1:D:1044:ASN:HA	1:D:1062:LEU:HD23	1.99	0.44
1:D:433:ALA:HB2	1:D:442:LYS:NZ	2.32	0.44
1:D:731:GLU:OE2	1:D:763:VAL:HG12	2.18	0.44
1:A:435:SER:OG	1:A:437:LYS:HG2	2.17	0.44
1:B:1087:ILE:CG2	1:B:1088:TYR:N	2.81	0.44
1:B:1169:ALA:O	1:B:1170:THR:C	2.54	0.44
1:B:239:ILE:O	1:B:239:ILE:HG22	2.17	0.44
1:B:368:THR:OG1	1:B:369:THR:N	2.50	0.44
1:C:169:GLY:HA3	1:C:236:GLU:HB3	2.00	0.44
1:D:304:TYR:OH	1:D:327:PRO:HA	2.18	0.44
1:D:760:LYS:HG2	1:D:768:ILE:HD12	2.00	0.44
1:A:170:THR:HB	1:A:172:GLY:O	2.18	0.44
1:A:952:ILE:O	1:A:952:ILE:HG22	2.18	0.44
1:B:647:ASN:O	1:B:648:ALA:HB3	2.18	0.44
1:B:798:VAL:O	1:B:799:ALA:C	2.54	0.44
1:D:378:ILE:HG23	1:D:459:ILE:CG1	2.47	0.44
1:D:675:ARG:HH22	1:D:795:ASP:CG	2.21	0.44
1:A:347:THR:HG23	1:A:360:ILE:HG12	2.00	0.44
1:A:392:GLY:O	1:A:418:ILE:N	2.50	0.44
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.82	0.44
1:B:944:VAL:O	1:B:948:PHE:HD1	2.01	0.44
1:C:541:THR:OG1	1:C:638:LEU:HG	2.18	0.44
1:C:964:GLN:O	1:C:967:ILE:N	2.34	0.44
1:D:130:ARG:HA	1:D:130:ARG:HD2	1.82	0.44
1:D:568:THR:OG1	1:D:807:GLN:HG3	2.17	0.44
1:D:941:PRO:HD2	1:D:944:VAL:CG1	2.47	0.44
1:A:381:GLU:O	1:A:383:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:H	1:A:384:LEU:HD12	1.82	0.43
1:B:519:ARG:CB	1:B:520:PRO:CD	2.96	0.43
1:B:606:MET:HE1	1:B:639:PHE:HB3	1.98	0.43
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.66	0.43
1:C:71:ASP:O	1:C:74:SER:N	2.37	0.43
1:D:951:GLU:O	1:D:952:ILE:HD13	2.17	0.43
1:A:1087:ILE:HG22	1:A:1089:ILE:HD12	2.00	0.43
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.04	0.43
1:A:506:ASN:ND2	1:A:510:ASN:HD22	2.16	0.43
1:C:756:ILE:HG22	1:C:789:ALA:CB	2.48	0.43
1:D:999:GLN:CG	1:D:1000:GLY:N	2.42	0.43
1:A:1077:TYR:N	1:A:1077:TYR:HD1	2.16	0.43
1:A:532:VAL:HG21	1:A:596:ASP:HB2	2.00	0.43
1:B:647:ASN:O	1:B:649:VAL:N	2.46	0.43
1:B:66:ILE:O	1:B:66:ILE:HG13	2.18	0.43
1:C:323:ILE:CG2	1:C:324:GLU:N	2.81	0.43
1:C:456:LYS:H	1:C:456:LYS:HD3	1.83	0.43
1:C:462:LEU:O	1:C:466:MET:HG2	2.18	0.43
1:C:606:MET:HE1	1:C:671:ILE:HD11	2.00	0.43
1:C:941:PRO:O	1:C:945:VAL:HG13	2.18	0.43
1:C:941:PRO:O	1:C:944:VAL:HG12	2.19	0.43
1:C:981:TYR:CE1	1:C:982:LEU:HD23	2.53	0.43
1:A:1111:HIS:ND1	1:A:1176:GLU:HG3	2.33	0.43
1:A:144:GLU:CD	1:A:144:GLU:H	2.22	0.43
1:B:898:ASN:ND2	1:B:904:ILE:H	2.16	0.43
1:D:142:HIS:O	1:D:143:LEU:C	2.55	0.43
1:D:40:LEU:HD21	1:D:42:VAL:CG2	2.48	0.43
1:B:1053:ASP:CG	1:B:1054:LYS:N	2.72	0.43
1:C:201:GLY:HA2	1:C:204:MET:HE3	2.01	0.43
1:C:378:ILE:HG12	1:C:427:VAL:HG23	2.00	0.43
1:C:931:VAL:CA	1:C:935:GLY:H	2.29	0.43
1:D:470:LYS:HB2	1:D:480:PHE:CE1	2.53	0.43
1:A:1153:PHE:HE1	1:A:1177:ILE:HB	1.83	0.43
1:A:266:SER:O	1:A:478:THR:HA	2.18	0.43
1:A:571:ARG:NH2	1:A:605:GLU:OE2	2.46	0.43
1:B:536:LYS:HE3	1:B:536:LYS:HB3	1.81	0.43
1:B:613:ASP:HB2	1:B:1013:TYR:CZ	2.52	0.43
1:B:799:ALA:H	1:B:811:ASN:ND2	2.15	0.43
1:C:188:GLY:CA	1:C:237:ARG:HH22	2.29	0.43
1:C:940:PHE:HB3	1:C:944:VAL:HG13	2.00	0.43
1:D:818:ASN:HD22	1:D:818:ASN:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:SER:HA	1:D:856:SER:HG	1.79	0.43
1:C:994:LEU:O	1:C:998:GLN:HB2	2.19	0.43
1:A:509:ILE:HD12	1:A:1089:ILE:CG2	2.49	0.43
1:A:1108:ASN:C	1:A:1108:ASN:OD1	2.56	0.43
1:B:1051:GLU:OE1	1:B:1057:ARG:CZ	2.66	0.43
1:C:104:ASP:O	1:C:108:GLN:OE1	2.35	0.43
1:C:641:MET:CE	1:C:666:SER:HB3	2.48	0.43
1:C:651:TYR:O	1:C:952:ILE:HD11	2.19	0.43
1:C:977:ARG:HA	1:C:978:PRO:HD3	1.83	0.43
1:D:1132:LYS:O	1:D:1151:ALA:CB	2.66	0.43
1:A:620:LYS:HG3	1:A:1023:THR:HG21	2.01	0.43
1:C:141:PRO:HG2	1:C:146:LEU:CD1	2.49	0.43
1:D:590:ILE:O	1:D:591:ALA:C	2.58	0.43
1:A:571:ARG:HH11	1:A:575:GLN:HE22	1.65	0.43
1:A:798:VAL:O	1:A:799:ALA:C	2.57	0.43
1:B:51:ARG:CG	1:B:51:ARG:HH11	2.31	0.43
1:B:51:ARG:CG	1:B:51:ARG:NH1	2.81	0.43
1:C:287:LEU:HD22	1:C:291:ILE:CD1	2.48	0.43
1:C:375:GLN:HE22	1:C:428:LYS:HD3	1.81	0.43
1:C:584:THR:O	1:C:585:LYS:C	2.56	0.43
1:C:877:GLN:O	1:C:881:LEU:HD12	2.18	0.43
1:D:1132:LYS:O	1:D:1151:ALA:HB3	2.19	0.43
1:D:513:PRO:O	1:D:515:ASN:HB2	2.19	0.43
1:D:866:MET:HE3	1:D:870:GLN:HB3	2.01	0.43
1:D:869:GLY:O	1:D:870:GLN:C	2.57	0.43
1:A:1008:ILE:N	1:A:1008:ILE:HD12	2.34	0.42
1:B:335:ILE:HD11	1:B:374:ILE:HA	2.00	0.42
1:B:261:PHE:HE1	1:B:368:THR:HA	1.82	0.42
1:B:738:LEU:HD21	1:B:759:LEU:HD13	2.01	0.42
1:B:99:ILE:HD12	1:B:99:ILE:N	2.30	0.42
1:C:234:TYR:N	1:C:234:TYR:CD2	2.87	0.42
1:C:814:TYR:CE2	1:C:828:ILE:CG1	3.02	0.42
1:D:739:ALA:HA	1:D:769:HIS:O	2.19	0.42
1:A:90:LEU:HD13	1:A:94:GLU:HG3	2.00	0.42
1:B:892:ASP:O	1:B:896:ARG:HG3	2.20	0.42
1:C:624:TRP:HB3	1:C:1005:GLN:NE2	2.34	0.42
1:C:215:ASP:O	1:C:218:HIS:N	2.48	0.42
1:C:512:PHE:CG	1:C:513:PRO:HD2	2.54	0.42
1:D:1159:GLN:CG	1:D:1176:GLU:HG2	2.50	0.42
1:D:1159:GLN:HG3	1:D:1176:GLU:HG2	2.00	0.42
1:A:930:SER:HA	1:A:933:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:HA	1:B:62:SER:O	2.20	0.42
1:B:886:ARG:HG3	1:B:886:ARG:H	1.59	0.42
1:C:744:ALA:O	1:C:861:ILE:HD12	2.20	0.42
1:C:920:TYR:OH	1:C:938:LEU:HB3	2.20	0.42
1:D:142:HIS:CB	1:D:144:GLU:OE1	2.63	0.42
1:A:241:ASN:N	1:A:242:PRO:HD3	2.35	0.42
1:A:470:LYS:NZ	1:A:484:THR:HG23	2.35	0.42
1:A:682:TRP:CZ3	1:A:977:ARG:HB2	2.54	0.42
1:B:1015:LYS:HD3	1:B:1015:LYS:HA	1.78	0.42
1:B:622:ASN:HD22	1:B:623:PRO:CD	2.31	0.42
1:A:1064:THR:OG1	1:C:1066:SER:HB3	2.19	0.42
1:C:641:MET:HE3	1:C:666:SER:HB3	2.00	0.42
1:D:167:ILE:HG13	1:D:167:ILE:H	1.68	0.42
1:D:241:ASN:H	1:D:242:PRO:HD3	1.84	0.42
1:D:375:GLN:CG	1:D:376:CYS:N	2.82	0.42
1:D:459:ILE:HB	1:D:460:PRO:HD3	2.02	0.42
1:A:338:MET:CE	1:A:430:SER:HB3	2.49	0.42
1:B:1144:LYS:CE	4:B:1202:BTI:O11	2.67	0.42
1:C:167:ILE:HA	1:C:168:PRO:HD2	1.92	0.42
1:C:266:SER:O	1:C:478:THR:HA	2.19	0.42
1:C:936:TYR:HA	1:C:936:TYR:HD2	1.72	0.42
1:C:964:GLN:O	1:C:966:VAL:N	2.53	0.42
1:A:179:LEU:O	1:A:182:GLU:CG	2.68	0.42
1:B:125:GLU:CD	1:B:125:GLU:N	2.70	0.42
1:B:522:PRO:HB2	1:B:523:ASP:H	1.76	0.42
1:C:828:ILE:C	1:C:830:GLY:N	2.70	0.42
1:C:948:PHE:CD1	1:C:967:ILE:HD12	2.55	0.42
1:D:770:LEU:HD12	1:D:771:HIS:N	2.35	0.42
1:A:287:LEU:HD21	1:A:318:ASP:O	2.19	0.42
1:A:583:ARG:HG2	1:A:619:LEU:HD22	2.00	0.42
1:B:1095:HIS:CG	1:B:1098:ALA:HB3	2.55	0.42
1:B:296:ILE:O	1:B:300:GLU:HB2	2.19	0.42
1:B:48:ILE:HG23	1:B:49:ALA:N	2.35	0.42
1:B:878:ALA:O	1:B:883:LEU:N	2.40	0.42
1:C:335:ILE:CG2	1:C:336:THR:N	2.83	0.42
1:D:908:THR:HA	1:D:909:PRO:HA	1.66	0.42
1:A:381:GLU:HG2	1:A:387:PHE:HB3	2.00	0.42
1:A:379:THR:N	1:A:458:ASN:OD1	2.42	0.42
1:B:1144:LYS:HZ3	4:B:1202:BTI:C10	2.22	0.42
1:B:897:VAL:HG22	1:B:921:MET:HE1	2.02	0.42
1:C:335:ILE:HG22	1:C:336:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:MET:HE3	1:C:373:ALA:CB	2.49	0.42
1:D:1085:ARG:CG	1:D:1085:ARG:HH11	2.33	0.42
1:B:588:ILE:HA	1:B:588:ILE:HD13	1.81	0.42
1:B:927:ASP:H	1:B:930:SER:CB	2.30	0.42
1:C:631:ARG:NH1	1:C:634:ILE:O	2.53	0.42
1:C:39:LYS:NZ	1:C:82:GLU:OE2	2.49	0.42
1:C:590:ILE:HG12	1:C:837:TYR:CD2	2.55	0.42
1:A:1138:LEU:HD22	1:A:1175:ILE:HD11	2.01	0.42
1:A:791:VAL:O	1:A:822:ARG:NH2	2.38	0.42
1:A:866:MET:HE2	1:A:870:GLN:HG2	2.02	0.42
1:C:1008:ILE:HD12	1:C:1009:SER:N	2.34	0.42
1:C:45:ARG:NH1	1:C:71:ASP:OD1	2.53	0.42
1:D:1134:ASN:N	1:D:1151:ALA:HB3	2.34	0.42
1:D:289:GLN:HA	1:D:289:GLN:HE21	1.85	0.42
1:D:798:VAL:O	1:D:799:ALA:C	2.57	0.42
1:D:811:ASN:H	1:D:811:ASN:ND2	2.17	0.42
1:A:481:ILE:O	1:A:482:GLU:C	2.57	0.41
1:A:940:PHE:CD1	1:A:967:ILE:HA	2.55	0.41
1:B:362:MET:HA	1:B:362(A):PRO:HD3	1.87	0.41
1:C:199:GLY:HA2	5:C:1202:ATP:O1B	2.20	0.41
1:C:909:PRO:HG2	1:C:952:ILE:HG13	2.02	0.41
1:D:42:VAL:HG11	1:D:49:ALA:HA	2.02	0.41
1:A:145:HIS:HE1	1:A:302:ILE:O	2.02	0.41
1:A:334:THR:O	1:A:338:MET:HG3	2.20	0.41
1:A:78:TYR:CE2	1:C:1081:ASN:HA	2.54	0.41
1:B:1000:GLY:N	1:B:1001:PRO:CD	2.75	0.41
1:B:1069:ASP:O	1:B:1099:ASN:HB3	2.20	0.41
1:B:983:GLU:HA	1:B:983:GLU:OE1	2.19	0.41
1:C:164:LEU:O	1:C:166:VAL:HG23	2.20	0.41
1:C:167:ILE:CD1	1:C:167:ILE:H	2.30	0.41
1:C:311:GLU:O	1:C:323:ILE:HB	2.20	0.41
1:C:939:ASP:OD1	1:D:1149:ILE:HG12	2.19	0.41
1:D:342:ILE:N	1:D:342:ILE:HD12	2.35	0.41
1:A:486:GLU:C	1:A:488:PHE:H	2.24	0.41
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.35	0.41
1:B:241:ASN:N	1:B:242:PRO:CD	2.83	0.41
1:B:715:ARG:HH12	1:B:865:GLU:CD	2.23	0.41
1:C:358:GLU:CA	1:C:358:GLU:OE1	2.68	0.41
1:C:902:GLY:O	1:C:903:ASP:HB3	2.20	0.41
1:B:290:ARG:HB3	1:B:320:PHE:HE2	1.86	0.41
1:B:737:ILE:HG23	1:B:767:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1029:ASN:HD22	1:C:1031:SER:H	1.68	0.41
1:C:215:ASP:HB3	1:C:219:ARG:CG	2.50	0.41
1:C:540:GLY:H	1:C:543:GLN:HG2	1.85	0.41
1:D:1108:ASN:CB	1:D:1109:PRO:CD	2.89	0.41
1:D:828:ILE:HD12	1:D:829:GLU:H	1.86	0.41
1:D:998:GLN:O	1:D:999:GLN:C	2.58	0.41
1:A:1064:THR:OG1	1:C:1066:SER:CB	2.69	0.41
1:A:286:THR:O	1:A:290:ARG:HG3	2.21	0.41
1:B:620:LYS:CG	4:B:1201:BTI:H63	2.50	0.41
1:B:438:GLN:HG2	1:D:346:LYS:NZ	2.36	0.41
1:B:512:PHE:CD2	1:B:513:PRO:HD2	2.55	0.41
1:B:572:ASP:HB3	1:B:807:GLN:NE2	2.36	0.41
1:C:652:LYS:HD3	1:C:653:ASN:O	2.20	0.41
1:B:305:VAL:O	1:B:306:ASN:HB2	2.20	0.41
1:C:858:ASN:OD1	1:C:860:GLU:HB2	2.21	0.41
1:D:378:ILE:O	1:D:426:LEU:HB2	2.21	0.41
1:D:69:ASN:O	1:D:72:LYS:HB2	2.21	0.41
1:D:701:GLU:HG2	1:D:737:ILE:HB	2.02	0.41
1:D:893:MET:O	1:D:897:VAL:HG23	2.21	0.41
1:D:986:ASP:OD2	1:D:986:ASP:C	2.57	0.41
1:A:153:VAL:O	1:A:154:LYS:C	2.59	0.41
1:A:272:GLN:HB2	1:A:272:GLN:HE21	1.62	0.41
1:A:263:ARG:NH1	1:A:336:THR:OG1	2.46	0.41
1:A:46:GLY:O	1:A:47:GLU:C	2.59	0.41
1:A:631:ARG:HD3	1:A:631:ARG:C	2.34	0.41
1:B:462:LEU:HD23	1:B:462:LEU:HA	1.82	0.41
1:B:79:LYS:HD3	1:B:79:LYS:HA	1.84	0.41
1:C:1052:ILE:O	1:C:1053:ASP:HB2	2.21	0.41
1:A:434:ILE:HG13	1:C:341:GLY:O	2.21	0.41
1:A:597:VAL:HG11	1:A:831:MET:HG2	2.03	0.41
1:B:1035:THR:HB	1:B:1036:PRO:HD3	2.01	0.41
1:B:479:LYS:HB3	1:B:483:GLU:OE2	2.20	0.41
1:B:581:ARG:O	1:B:619:LEU:HD21	2.20	0.41
1:C:212:GLU:H	1:C:212:GLU:HG3	1.49	0.41
1:C:534:SER:O	1:C:537:ILE:HB	2.21	0.41
1:C:90:LEU:CB	1:C:95:SER:HB2	2.51	0.41
1:D:259:HIS:HB3	1:D:296:ILE:HD13	2.03	0.41
1:A:641:MET:HE1	1:A:666:SER:HB3	2.02	0.41
1:A:858:ASN:HD22	1:A:859:THR:N	2.19	0.41
1:A:948:PHE:CD1	1:A:967:ILE:CD1	3.04	0.41
1:A:948:PHE:CZ	1:A:963:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASP:C	1:B:242:PRO:HD3	2.42	0.41
1:B:328:ARG:HD2	1:B:329:VAL:O	2.21	0.41
1:B:498:THR:HG23	1:B:1085:ARG:NH2	2.36	0.41
1:B:908:THR:HA	1:B:909:PRO:HA	1.67	0.41
1:C:995:GLU:O	1:C:999:GLN:HA	2.21	0.41
1:D:941:PRO:O	1:D:944:VAL:CG1	2.64	0.41
1:A:1143:MET:O	1:B:513:PRO:HA	2.21	0.41
1:A:268:GLN:O	1:A:481:ILE:HD12	2.21	0.41
1:B:151:ASP:HB3	1:B:154:LYS:H	1.86	0.41
1:B:304:TYR:OH	1:B:327:PRO:HA	2.20	0.41
1:B:459:ILE:N	1:B:460:PRO:HD2	2.36	0.41
1:C:622:ASN:ND2	1:C:623:PRO:HD2	2.25	0.41
1:C:807:GLN:CB	1:C:808:PRO:CD	2.98	0.41
1:D:917:MET:HE1	1:D:940:PHE:HD2	1.86	0.41
1:D:999:GLN:HE21	1:D:1001:PRO:N	2.18	0.41
1:A:1155:GLY:HA3	1:A:1177:ILE:HG22	2.01	0.41
1:B:1124:LYS:C	1:B:1125:VAL:HG13	2.42	0.41
1:C:437:LYS:CD	1:C:437:LYS:H	2.33	0.41
1:D:1151:ALA:HA	1:D:1152:PRO:HD2	1.90	0.41
1:D:1153:PHE:HB3	1:D:1154:ASP:H	1.47	0.41
1:D:277:VAL:HA	1:D:335:ILE:HD11	2.03	0.41
1:D:447:LEU:O	1:D:450:MET:HB2	2.20	0.41
1:D:715:ARG:HH12	1:D:865:GLU:CD	2.22	0.41
1:D:864:HIS:CD2	1:D:866:MET:CG	2.93	0.41
1:A:206:ILE:HD12	1:A:206:ILE:H	1.86	0.40
1:A:314:VAL:HG22	1:A:320:PHE:HB3	2.03	0.40
1:A:499:LYS:HB3	1:A:1027:TYR:HA	2.03	0.40
1:A:875:SER:HA	1:A:887:PHE:CE1	2.56	0.40
1:B:278:ALA:CB	1:B:335:ILE:HG23	2.51	0.40
1:B:335:ILE:HA	1:B:338:MET:HE2	2.03	0.40
1:B:279:PRO:HD2	1:B:372:TYR:CD2	2.56	0.40
1:A:313:LEU:HD22	1:A:323:ILE:CG1	2.51	0.40
1:A:587:MET:SD	1:A:626:ARG:HD3	2.60	0.40
1:A:783:TYR:CE1	1:A:808:PRO:HG2	2.57	0.40
1:B:1119:SER:O	1:B:1140:THR:HA	2.21	0.40
1:B:545:LEU:CD1	1:B:550:PRO:HD3	2.51	0.40
1:C:375:GLN:CD	1:C:428:LYS:HD3	2.41	0.40
1:C:575:GLN:NE2	1:C:610:ALA:H	2.18	0.40
1:C:641:MET:HE2	1:C:671:ILE:HG13	2.02	0.40
1:C:952:ILE:HD12	1:C:952:ILE:HA	1.76	0.40
1:D:41:LEU:HD23	1:D:42:VAL:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:GLN:HB3	1:A:1083:GLN:HE21	1.65	0.40
1:A:388:MET:HA	1:A:389:PRO:HD3	1.91	0.40
1:A:743:MET:CG	1:A:907:VAL:HG13	2.46	0.40
1:A:999:GLN:HG2	1:A:1000:GLY:N	2.27	0.40
1:B:259:HIS:O	1:B:260:LEU:HD23	2.20	0.40
1:B:458:ASN:O	1:B:461:PHE:HB3	2.21	0.40
1:C:71:ASP:C	1:C:73:SER:H	2.25	0.40
1:D:396:ALA:HB3	1:D:453:ARG:HG3	2.03	0.40
1:A:399:SER:HB2	1:A:407:LEU:HD13	2.02	0.40
1:B:566:THR:HG23	1:B:603:SER:OG	2.22	0.40
1:C:338:MET:HE3	1:C:338:MET:HB2	1.81	0.40
1:C:606:MET:HE2	1:C:639:PHE:HB3	2.02	0.40
1:D:938:LEU:HD23	1:D:938:LEU:HA	1.74	0.40
1:D:974:LEU:HD13	1:D:978:PRO:HA	2.03	0.40
1:A:1053:ASP:O	1:A:1054:LYS:C	2.60	0.40
1:A:659:ILE:H	1:A:659:ILE:HG12	1.74	0.40
1:B:119:GLY:N	1:B:122:SER:OG	2.54	0.40
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.57	0.40
1:B:715:ARG:HD2	1:B:715:ARG:C	2.40	0.40
1:C:814:TYR:CZ	1:C:828:ILE:CG1	3.05	0.40
1:C:866:MET:CE	1:C:891:LYS:HG2	2.50	0.40
1:D:1065:ILE:HG12	1:D:1076:ILE:HG12	2.03	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	1127/1173 (96%)	1022 (91%)	81 (7%)	24 (2%)	7	23
1	B	1027/1173 (88%)	906 (88%)	92 (9%)	29 (3%)	5	17
1	C	1063/1173 (91%)	926 (87%)	105 (10%)	32 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1061/1173 (90%)	947 (89%)	90 (8%)	24 (2%)	6	21
All	All	4278/4692 (91%)	3801 (89%)	368 (9%)	109 (2%)	5	19

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	181	LYS
1	A	211	SER
1	A	956	VAL
1	A	1094	VAL
1	A	1095	HIS
1	A	1138	LEU
1	B	270	ARG
1	B	868	GLY
1	B	870	GLN
1	B	1001	PRO
1	C	92	PRO
1	C	168	PRO
1	C	211	SER
1	C	270	ARG
1	C	518	LYS
1	C	937	LYS
1	C	956	VAL
1	D	92	PRO
1	D	241	ASN
1	D	870	GLN
1	D	880	SER
1	D	999	GLN
1	D	1103	LYS
1	D	1108	ASN
1	D	1154	ASP
1	A	72	LYS
1	A	385	ASN
1	A	387	PHE
1	A	389	PRO
1	A	414	GLN
1	A	648	ALA
1	A	1081	ASN
1	B	87	GLY
1	B	91	GLY
1	B	163	ASP

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Mol	Chain	Res	Type
1	B	166	VAL
1	B	425	LEU
1	B	522	PRO
1	B	649	VAL
1	B	779	GLY
1	B	871	TYR
1	B	999	GLN
1	B	1002	VAL
1	C	87	GLY
1	C	188	GLY
1	C	197	SER
1	C	216	ALA
1	C	306	ASN
1	C	455	VAL
1	C	903	ASP
1	C	931	VAL
1	C	965	ALA
1	D	87	GLY
1	D	261	PHE
1	D	868	GLY
1	D	1052	ILE
1	D	1106	LYS
1	A	999	GLN
1	A	1001	PRO
1	A	1117	PRO
1	B	328	ARG
1	B	518	LYS
1	B	939	ASP
1	B	941	PRO
1	B	1000	GLY
1	C	189	PHE
1	C	645	ALA
1	C	648	ALA
1	C	1070	GLU
1	A	210	GLU
1	A	424	SER
1	B	69	ASN
1	B	72	LYS
1	B	473	SER
1	B	523	ASP
1	C	125	GLU
1	C	215	ASP

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Mol	Chain	Res	Type
1	C	229	GLY
1	C	925	ASP
1	D	386	ASP
1	D	648	ALA
1	D	869	GLY
1	A	190	PRO
1	A	221	LYS
1	A	476	TYR
1	B	519	ARG
1	B	648	ALA
1	C	94	GLU
1	C	214	GLU
1	C	961	LYS
1	D	104	ASP
1	D	491	GLN
1	D	854	ILE
1	D	903	ASP
1	D	939	ASP
1	A	415	GLY
1	B	1084	ALA
1	C	110	ASN
1	C	186	GLU
1	D	242	PRO
1	B	92	PRO
1	D	1014	PRO
1	B	970	GLY
1	D	331	VAL
1	A	1000	GLY
1	C	513	PRO
1	C	389	PRO
1	C	649	VAL

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	977/1006 (97%)	837 (86%)	140 (14%)	3 10
1	B	897/1006 (89%)	763 (85%)	134 (15%)	3 9
1	C	917/1006 (91%)	775 (84%)	142 (16%)	2 8
1	D	922/1006 (92%)	798 (87%)	124 (13%)	4 12
All	All	3713/4024 (92%)	3173 (86%)	540 (14%)	3 9

All (540) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	44	ASN
1	A	69	ASN
1	A	72	LYS
1	A	73	SER
1	A	88	SER
1	A	95	SER
1	A	98	ASN
1	A	108	GLN
1	A	125	GLU
1	A	143	LEU
1	A	147	ASP
1	A	148	MET
1	A	152	LYS
1	A	154	LYS
1	A	156	ARG
1	A	171	ASP
1	A	176	SER
1	A	179	LEU
1	A	189	PHE
1	A	192	MET
1	A	193	ILE
1	A	196	THR
1	A	205	ARG
1	A	208	ARG
1	A	212	GLU
1	A	213	LEU
1	A	218	HIS
1	A	219	ARG
1	A	227	SER

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Mol	Chain	Res	Type
1	A	235	ILE
1	A	241	ASN
1	A	268	GLN
1	A	269	ARG
1	A	271	HIS
1	A	272	GLN
1	A	280	SER
1	A	283	LEU
1	A	287	LEU
1	A	313	LEU
1	A	315	SER
1	A	323	ILE
1	A	329	VAL
1	A	335	ILE
1	A	361	ASN
1	A	368	THR
1	A	381	GLU
1	A	391	THR
1	A	398	ARG
1	A	406	ARG
1	A	408	ASP
1	A	414	GLN
1	A	417	GLU
1	A	423	ASP
1	A	427	VAL
1	A	434	ILE
1	A	437	LYS
1	A	442	LYS
1	A	450	MET
1	A	469	LYS
1	A	487	LEU
1	A	491	GLN
1	A	493	SER
1	A	496	ARG
1	A	506	ASN
1	A	518	LYS
1	A	523	ASP
1	A	526	LEU
1	A	534	SER
1	A	542	LYS
1	A	588	ILE
1	A	590	ILE

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Mol	Chain	Res	Type
1	A	606	MET
1	A	607	TRP
1	A	613	ASP
1	A	622	ASN
1	A	632	LYS
1	A	649	VAL
1	A	684	ASP
1	A	707	THR
1	A	714	GLU
1	A	715	ARG
1	A	719	THR
1	A	726	LEU
1	A	743	MET
1	A	750	LYS
1	A	761	SER
1	A	765	ASP
1	A	766	LEU
1	A	775	THR
1	A	784	LYS
1	A	798	VAL
1	A	811	ASN
1	A	828	ILE
1	A	843	THR
1	A	852	SER
1	A	855	LYS
1	A	858	ASN
1	A	861	ILE
1	A	863	GLN
1	A	871	TYR
1	A	880	SER
1	A	888	ASP
1	A	907	VAL
1	A	908	THR
1	A	917	MET
1	A	919	LEU
1	A	926	LEU
1	A	931	VAL
1	A	939	ASP
1	A	943	SER
1	A	944	VAL
1	A	977	ARG
1	A	999	GLN

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Mol	Chain	Res	Type
1	A	1002	VAL
1	A	1008	ILE
1	A	1015	LYS
1	A	1029	ASN
1	A	1043	ARG
1	A	1048	VAL
1	A	1077	TYR
1	A	1081	ASN
1	A	1083	GLN
1	A	1089	ILE
1	A	1090	LYS
1	A	1094	VAL
1	A	1097	ASN
1	A	1107	SER
1	A	1111	HIS
1	A	1115	GLN
1	A	1116	MET
1	A	1126	SER
1	A	1141	GLU
1	A	1145	MET
1	A	1148	THR
1	A	1153	PHE
1	A	1157	ILE
1	A	1167	THR
1	A	1176	GLU
1	A	1177	ILE
1	B	36	GLN
1	B	39	LYS
1	B	44	ASN
1	B	47	GLU
1	B	51	ARG
1	B	62	SER
1	B	69	ASN
1	B	75	LEU
1	B	77	ARG
1	B	83	SER
1	B	85	LEU
1	B	94	GLU
1	B	99	ILE
1	B	110	ASN
1	B	118	TYR
1	B	123	GLU

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Mol	Chain	Res	Type
1	B	125	GLU
1	B	129	ARG
1	B	139	ILE
1	B	144	GLU
1	B	147	ASP
1	B	152	LYS
1	B	160	ILE
1	B	164	LEU
1	B	166	VAL
1	B	257	ILE
1	B	270	ARG
1	B	284	SER
1	B	289	GLN
1	B	292	CYS
1	B	293	ASP
1	B	318	ASP
1	B	319	GLU
1	B	320	PHE
1	B	329	VAL
1	B	335	ILE
1	B	346	LYS
1	B	357	LEU
1	B	359	GLU
1	B	378	ILE
1	B	380	THR
1	B	434	ILE
1	B	437	LYS
1	B	451	ARG
1	B	469	LYS
1	B	481	ILE
1	B	482	GLU
1	B	487	LEU
1	B	488	PHE
1	B	489	ASP
1	B	490	ILE
1	B	493	SER
1	B	496	ARG
1	B	498	THR
1	B	506	ASN
1	B	517	GLU
1	B	518	LYS
1	B	523	ASP

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Mol	Chain	Res	Type
1	B	524	TYR
1	B	525	GLU
1	B	528	SER
1	B	531	THR
1	B	535	SER
1	B	538(A)	SER
1	B	542	LYS
1	B	555	GLU
1	B	565	LEU
1	B	575	GLN
1	B	580	THR
1	B	592	SER
1	B	606	MET
1	B	607	TRP
1	B	613	ASP
1	B	622	ASN
1	B	631	ARG
1	B	632	LYS
1	B	649	VAL
1	B	652	LYS
1	B	660	HIS
1	B	684	ASP
1	B	686	MET
1	B	687	LYS
1	B	707	THR
1	B	715	ARG
1	B	721	GLU
1	B	725	LYS
1	B	743	MET
1	B	766	LEU
1	B	775	THR
1	B	781	LEU
1	B	784	LYS
1	B	809	SER
1	B	811	ASN
1	B	828	ILE
1	B	831	MET
1	B	839	SER
1	B	843	THR
1	B	852	SER
1	B	856	SER
1	B	870	GLN

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Mol	Chain	Res	Type
1	B	874	LEU
1	B	875	SER
1	B	880	SER
1	B	881	LEU
1	B	885	GLU
1	B	886	ARG
1	B	907	VAL
1	B	919	LEU
1	B	926	LEU
1	B	930	SER
1	B	932	ILE
1	B	949	LYS
1	B	962	ASP
1	B	991	ARG
1	B	999	GLN
1	B	1009	SER
1	B	1011	VAL
1	B	1015	LYS
1	B	1022	GLN
1	B	1029	ASN
1	B	1048	VAL
1	B	1057	ARG
1	B	1085	ARG
1	B	1097	ASN
1	B	1111	HIS
1	B	1116	MET
1	B	1119	SER
1	B	1123	VAL
1	B	1143	MET
1	B	1147	THR
1	B	1153	PHE
1	B	1156	VAL
1	B	1167	THR
1	B	1177	ILE
1	C	44	ASN
1	C	77	ARG
1	C	79	LYS
1	C	90	LEU
1	C	94	GLU
1	C	95	SER
1	C	98	ASN
1	C	104	ASP

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Mol	Chain	Res	Type
1	C	108	GLN
1	C	110	ASN
1	C	126	GLN
1	C	129	ARG
1	C	147	ASP
1	C	151	ASP
1	C	156	ARG
1	C	161	LYS
1	C	163	ASP
1	C	167	ILE
1	C	168	PRO
1	C	175	LYS
1	C	189	PHE
1	C	193	ILE
1	C	194	LYS
1	C	202	LYS
1	C	205	ARG
1	C	206	ILE
1	C	207	VAL
1	C	208	ARG
1	C	212	GLU
1	C	213	LEU
1	C	227	SER
1	C	230	ASN
1	C	232	GLU
1	C	234	TYR
1	C	235	ILE
1	C	243	LYS
1	C	262	GLU
1	C	269	ARG
1	C	270	ARG
1	C	286	THR
1	C	287	LEU
1	C	288	ARG
1	C	289	GLN
1	C	313	LEU
1	C	323	ILE
1	C	329	VAL
1	C	334	THR
1	C	335	ILE
1	C	361	ASN
1	C	365	LYS

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Mol	Chain	Res	Type
1	C	377	ARG
1	C	386	ASP
1	C	388	MET
1	C	395	ILE
1	C	398	ARG
1	C	400	SER
1	C	406	ARG
1	C	408	ASP
1	C	414	GLN
1	C	417	GLU
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	444	VAL
1	C	445	ARG
1	C	456	LYS
1	C	464	ASN
1	C	469	LYS
1	C	472	THR
1	C	481	ILE
1	C	484	THR
1	C	489	ASP
1	C	494	LEU
1	C	496	ARG
1	C	510	ASN
1	C	515	ASN
1	C	518	LYS
1	C	526	LEU
1	C	531	THR
1	C	537	ILE
1	C	542	LYS
1	C	580	THR
1	C	588	ILE
1	C	606	MET
1	C	607	TRP
1	C	617	ASN
1	C	631	ARG
1	C	641	MET
1	C	649	VAL
1	C	652	LYS
1	C	668	LYS
1	C	685	GLN

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Mol	Chain	Res	Type
1	C	707	THR
1	C	714	GLU
1	C	717	ASN
1	C	719	THR
1	C	726	LEU
1	C	743	MET
1	C	756	ILE
1	C	760	LYS
1	C	766	LEU
1	C	781	LEU
1	C	784	LYS
1	C	807	GLN
1	C	828	ILE
1	C	839	SER
1	C	843	THR
1	C	853	ASP
1	C	854	ILE
1	C	855	LYS
1	C	861	ILE
1	C	875	SER
1	C	876	GLN
1	C	881	LEU
1	C	888	ASP
1	C	906	LYS
1	C	907	VAL
1	C	908	THR
1	C	931	VAL
1	C	946	SER
1	C	949	LYS
1	C	952	ILE
1	C	959	PHE
1	C	960	ASN
1	C	962	ASP
1	C	963	LEU
1	C	969	LYS
1	C	972	GLU
1	C	982	LEU
1	C	1008	ILE
1	C	1019	GLN
1	C	1029	ASN
1	C	1052	ILE
1	C	1054	LYS

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Mol	Chain	Res	Type
1	C	1062	LEU
1	C	1063	GLU
1	C	1070	GLU
1	C	1085	ARG
1	C	1090	LYS
1	C	1140	THR
1	C	1145	MET
1	C	1147	THR
1	D	38	LYS
1	D	44	ASN
1	D	70	GLU
1	D	72	LYS
1	D	77	ARG
1	D	88	SER
1	D	99	ILE
1	D	101	ARG
1	D	104	ASP
1	D	137	LYS
1	D	149	PHE
1	D	161	LYS
1	D	239	ILE
1	D	240	ASP
1	D	241	ASN
1	D	253	GLU
1	D	258	VAL
1	D	262	GLU
1	D	267	VAL
1	D	270	ARG
1	D	280	SER
1	D	283	LEU
1	D	289	GLN
1	D	296	ILE
1	D	315	SER
1	D	328	ARG
1	D	329	VAL
1	D	331	VAL
1	D	357	LEU
1	D	368	THR
1	D	370	LEU
1	D	386	ASP
1	D	400	SER
1	D	406	ARG

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Mol	Chain	Res	Type
1	D	414	GLN
1	D	417	GLU
1	D	427	VAL
1	D	428	LYS
1	D	434	ILE
1	D	451	ARG
1	D	467	LYS
1	D	469	LYS
1	D	487	LEU
1	D	490	ILE
1	D	494	LEU
1	D	506	ASN
1	D	519	ARG
1	D	525	GLU
1	D	528	SER
1	D	531	THR
1	D	535	SER
1	D	539	SER
1	D	542	LYS
1	D	551	LYS
1	D	580	THR
1	D	590	ILE
1	D	607	TRP
1	D	613	ASP
1	D	622	ASN
1	D	631	ARG
1	D	647	ASN
1	D	649	VAL
1	D	652	LYS
1	D	664	GLN
1	D	707	THR
1	D	715	ARG
1	D	743	MET
1	D	756	ILE
1	D	775	THR
1	D	781	LEU
1	D	784	LYS
1	D	791	VAL
1	D	807	GLN
1	D	828	ILE
1	D	831	MET
1	D	835	SER

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Mol	Chain	Res	Type
1	D	839	SER
1	D	843	THR
1	D	853	ASP
1	D	856	SER
1	D	863	GLN
1	D	873	ASN
1	D	881	LEU
1	D	886	ARG
1	D	907	VAL
1	D	908	THR
1	D	912	LYS
1	D	917	MET
1	D	925	ASP
1	D	926	LEU
1	D	931	VAL
1	D	949	LYS
1	D	952	ILE
1	D	961	LYS
1	D	962	ASP
1	D	996	GLU
1	D	999	GLN
1	D	1043	ARG
1	D	1048	VAL
1	D	1052	ILE
1	D	1054	LYS
1	D	1056	LYS
1	D	1057	ARG
1	D	1064	THR
1	D	1069	ASP
1	D	1070	GLU
1	D	1085	ARG
1	D	1090	LYS
1	D	1093	ASN
1	D	1103	LYS
1	D	1105	ASP
1	D	1110	SER
1	D	1123	VAL
1	D	1141	GLU
1	D	1147	THR
1	D	1148	THR
1	D	1153	PHE
1	D	1161	THR

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Mol	Chain	Res	Type
1	D	1162	VAL
1	D	1167	THR
1	D	1174	LEU
1	D	1175	ILE
1	D	1177	ILE
1	D	1178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	98	ASN
1	A	108	GLN
1	A	145	HIS
1	A	241	ASN
1	A	254	HIS
1	A	256	ASN
1	A	326	ASN
1	A	330	GLN
1	A	333	HIS
1	A	414	GLN
1	A	432	HIS
1	A	491	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	898	ASN
1	A	1005	GLN
1	A	1019	GLN
1	A	1025	ASN
1	A	1026	GLN
1	A	1029	ASN

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Mol	Chain	Res	Type
1	A	1044	ASN
1	A	1071	ASN
1	A	1083	GLN
1	A	1093	ASN
1	A	1097	ASN
1	A	1099	ASN
1	A	1111	HIS
1	B	44	ASN
1	B	98	ASN
1	B	108	GLN
1	B	110	ASN
1	B	145	HIS
1	B	241	ASN
1	B	256	ASN
1	B	272	GLN
1	B	326	ASN
1	B	330	GLN
1	B	432	HIS
1	B	506	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	736	HIS
1	B	778	ASN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	898	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1022	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1073	ASN
1	B	1097	ASN
1	B	1111	HIS
1	C	44	ASN

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Mol	Chain	Res	Type
1	C	108	GLN
1	C	145	HIS
1	C	256	ASN
1	C	326	ASN
1	C	330	GLN
1	C	361	ASN
1	C	432	HIS
1	C	464	ASN
1	C	574	HIS
1	C	575	GLN
1	C	589	ASN
1	C	617	ASN
1	C	622	ASN
1	C	653	ASN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN
1	C	863	GLN
1	C	898	ASN
1	C	924	ASN
1	C	1005	GLN
1	C	1019	GLN
1	C	1025	ASN
1	C	1029	ASN
1	D	44	ASN
1	D	142	HIS
1	D	145	HIS
1	D	241	ASN
1	D	259	HIS
1	D	272	GLN
1	D	289	GLN
1	D	301	ASN
1	D	330	GLN
1	D	364	GLN
1	D	432	HIS
1	D	506	ASN
1	D	515	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN

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Mol	Chain	Res	Type
1	D	589	ASN
1	D	617	ASN
1	D	622	ASN
1	D	647	ASN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN
1	D	863	GLN
1	D	864	HIS
1	D	873	ASN
1	D	898	ASN
1	D	960	ASN
1	D	999	GLN
1	D	1005	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1071	ASN
1	D	1083	GLN
1	D	1111	HIS
1	D	1115	GLN
1	D	1150	GLN
1	D	1164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
4	BTI	D	1202	-	16,16,16	1.76	2 (12%)	21,21,21	2.10	4 (19%)
4	BTI	C	1203	-	16,16,16	1.68	2 (12%)	21,21,21	2.31	5 (23%)
4	BTI	B	1201	-	16,16,16	1.72	2 (12%)	21,21,21	2.65	5 (23%)
2	ADP	A	1201	-	24,29,29	0.99	1 (4%)	29,45,45	1.46	4 (13%)
4	BTI	B	1202	-	16,16,16	1.74	2 (12%)	21,21,21	2.30	4 (19%)
5	ATP	C	1202	-	26,33,33	0.95	1 (3%)	31,52,52	1.38	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTI	D	1202	-	-	3/5/27/27	0/2/2/2
4	BTI	C	1203	-	-	3/5/27/27	0/2/2/2
4	BTI	B	1201	-	-	2/5/27/27	0/2/2/2
2	ADP	A	1201	-	-	3/12/32/32	0/3/3/3
4	BTI	B	1202	-	-	3/5/27/27	0/2/2/2
5	ATP	C	1202	-	-	4/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1201	BTI	O3-C3	5.52	1.35	1.23
4	B	1202	BTI	O3-C3	4.72	1.33	1.23
4	C	1203	BTI	O3-C3	4.66	1.33	1.23
4	D	1202	BTI	O3-C3	4.61	1.33	1.23
4	D	1202	BTI	C2-S1	-4.24	1.75	1.82
4	B	1202	BTI	C2-S1	-4.05	1.76	1.82
4	C	1203	BTI	C2-S1	-3.65	1.76	1.82
4	B	1201	BTI	C2-S1	-2.97	1.77	1.82
2	A	1201	ADP	C5-C4	2.47	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1202	ATP	C5-C4	2.47	1.47	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1201	BTI	C2-C4-N2	-9.35	104.75	113.13
4	D	1202	BTI	C2-C4-N2	-7.30	106.59	113.13
4	C	1203	BTI	C2-C4-N2	-6.76	107.07	113.13
4	B	1202	BTI	C2-C4-N2	-6.18	107.59	113.13
4	C	1203	BTI	C6-C5-N3	-5.84	105.61	113.03
4	B	1202	BTI	C6-C5-N3	-5.50	106.04	113.03
4	B	1201	BTI	C6-C5-N3	-4.82	106.90	113.03
2	A	1201	ADP	PA-O3A-PB	-4.09	118.80	132.83
4	D	1202	BTI	C6-C5-N3	-3.65	108.39	113.03
4	B	1202	BTI	C8-C7-C2	-3.41	106.95	113.86
5	C	1202	ATP	N3-C2-N1	-3.39	123.38	128.68
4	B	1201	BTI	C5-C6-S1	3.31	109.14	106.31
2	A	1201	ADP	N3-C2-N1	-3.18	123.72	128.68
4	B	1202	BTI	N2-C3-N3	3.04	111.61	108.76
4	C	1203	BTI	C4-C2-S1	2.96	108.03	105.20
5	C	1202	ATP	PA-O3A-PB	-2.93	122.77	132.83
4	D	1202	BTI	C8-C7-C2	-2.92	107.93	113.86
5	C	1202	ATP	PB-O3B-PG	-2.86	123.03	132.83
2	A	1201	ADP	C4-C5-N7	-2.65	106.63	109.40
4	B	1201	BTI	C4-C2-S1	2.46	107.55	105.20
2	A	1201	ADP	O3B-PB-O2B	2.35	116.63	107.64
4	D	1202	BTI	N2-C3-N3	2.28	110.90	108.76
4	B	1201	BTI	C8-C7-C2	-2.16	109.47	113.86
4	C	1203	BTI	C6-C5-C4	2.13	110.51	108.66
4	C	1203	BTI	N2-C3-N3	2.03	110.67	108.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1202	BTI	S1-C2-C7-C8
4	D	1202	BTI	C4-C2-C7-C8
4	C	1203	BTI	S1-C2-C7-C8
4	C	1203	BTI	C4-C2-C7-C8
2	A	1201	ADP	C5'-O5'-PA-O2A
2	A	1201	ADP	C5'-O5'-PA-O3A
4	B	1202	BTI	S1-C2-C7-C8

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Mol	Chain	Res	Type	Atoms
4	B	1202	BTI	C4-C2-C7-C8
5	C	1202	ATP	O4'-C4'-C5'-O5'
5	C	1202	ATP	C3'-C4'-C5'-O5'
4	B	1201	BTI	S1-C2-C7-C8
4	B	1201	BTI	C4-C2-C7-C8
5	C	1202	ATP	PB-O3B-PG-O2G
2	A	1201	ADP	C5'-O5'-PA-O1A
4	B	1202	BTI	C11-C10-C9-C8
4	D	1202	BTI	C7-C8-C9-C10
5	C	1202	ATP	PG-O3B-PB-O3A
4	C	1203	BTI	C7-C8-C9-C10

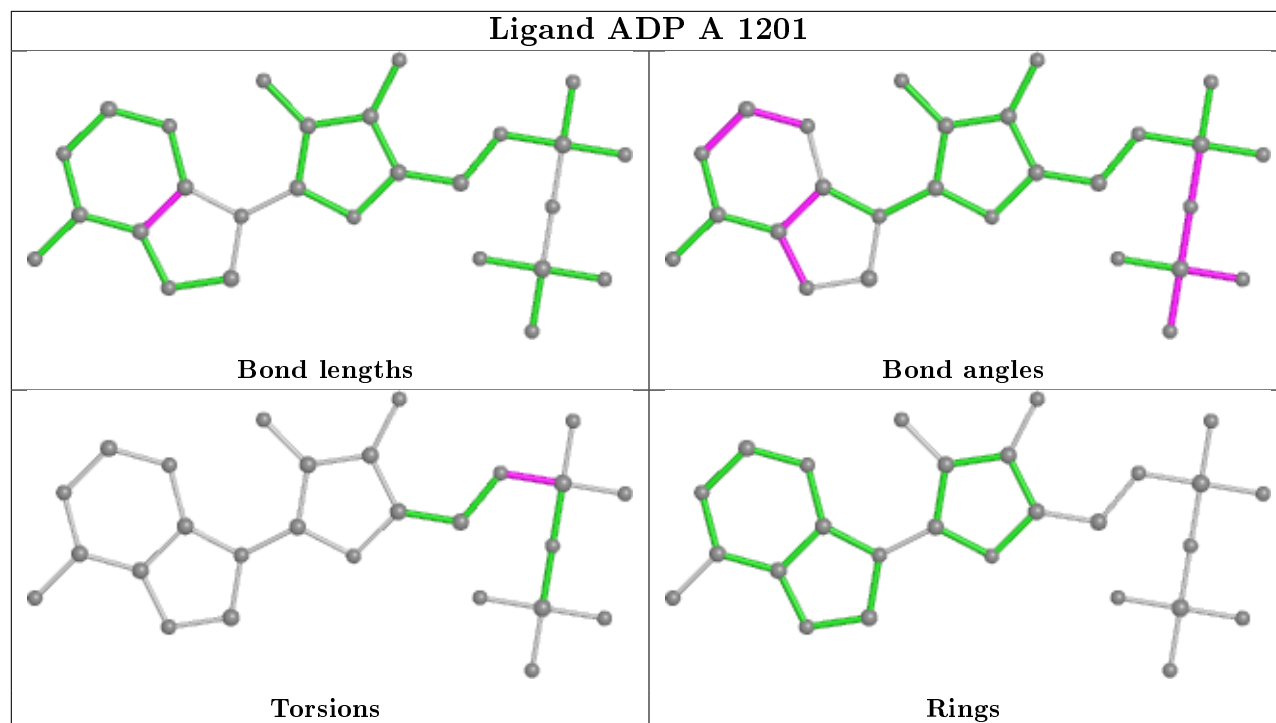
There are no ring outliers.

6 monomers are involved in 31 short contacts:

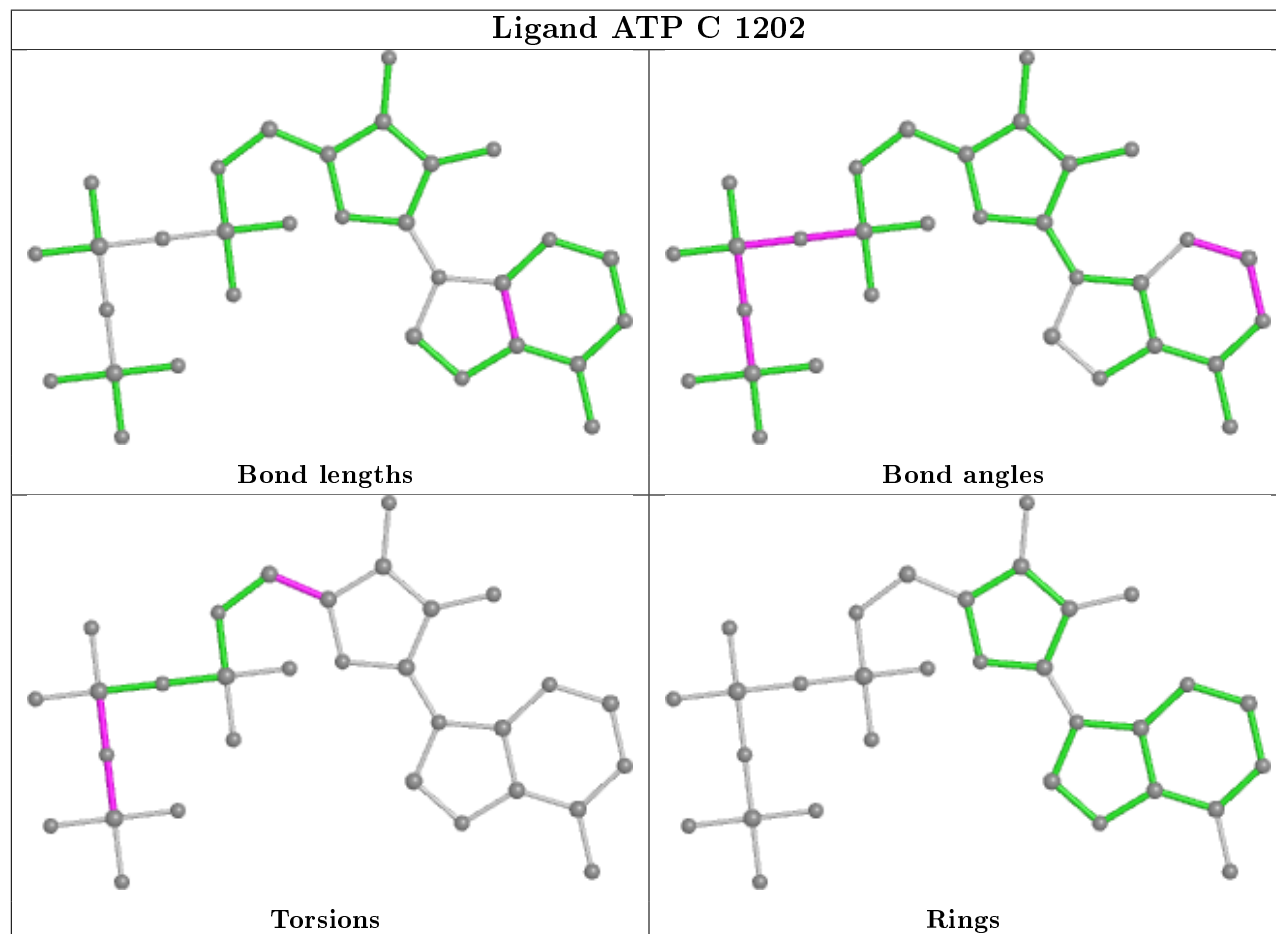
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1202	BTI	5	0
4	C	1203	BTI	1	0
4	B	1201	BTI	8	0
2	A	1201	ADP	2	0
4	B	1202	BTI	9	0
5	C	1202	ATP	6	0

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

Ligand ADP A 1201



Ligand ATP C 1202



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1133/1173 (96%)	-0.32	37 (3%)	46	36	23, 51, 104, 136	0
1	B	1033/1173 (88%)	-0.23	34 (3%)	46	36	31, 65, 130, 216	0
1	C	1067/1173 (90%)	-0.19	29 (2%)	54	44	36, 62, 108, 133	0
1	D	1067/1173 (90%)	-0.32	28 (2%)	56	46	21, 57, 115, 174	0
All	All	4300/4692 (91%)	-0.26	128 (2%)	50	40	21, 59, 114, 216	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1095	HIS	8.3
1	C	933	THR	8.2
1	C	932	ILE	6.1
1	B	271	HIS	5.9
1	A	218	HIS	5.1
1	B	89	ASP	5.1
1	B	526	LEU	4.8
1	B	88	SER	4.7
1	A	177	TYR	4.7
1	A	421	TYR	4.4
1	B	524	TYR	4.3
1	A	388	MET	4.3
1	C	1147	THR	4.2
1	D	1128	GLY	4.2
1	C	88	SER	4.2
1	B	424	SER	4.2
1	A	219	ARG	4.1
1	C	92	PRO	3.9
1	C	492	PRO	3.7
1	D	282	GLY	3.7
1	B	492	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	241	ASN	3.6
1	B	493	SER	3.5
1	A	1094	VAL	3.5
1	A	215	ASP	3.4
1	C	89	ASP	3.4
1	A	227	SER	3.4
1	A	999	GLN	3.4
1	B	454	GLY	3.4
1	D	1107	SER	3.3
1	A	1178	GLU	3.3
1	A	1128	GLY	3.3
1	A	399	SER	3.2
1	D	1154	ASP	3.2
1	D	1177	ILE	3.2
1	C	1140	THR	3.1
1	D	152	LYS	3.1
1	D	168	PRO	3.1
1	B	315	SER	3.0
1	C	416	ALA	3.0
1	B	455	VAL	3.0
1	B	1094	VAL	2.9
1	C	180	ALA	2.9
1	A	271	HIS	2.9
1	A	1095	HIS	2.9
1	C	415	GLY	2.9
1	B	425	LEU	2.9
1	B	91	GLY	2.9
1	C	1146	GLU	2.9
1	A	224	ALA	2.9
1	C	388	MET	2.8
1	B	380	THR	2.8
1	B	240	ASP	2.8
1	A	208	ARG	2.8
1	B	153	VAL	2.8
1	A	180	ALA	2.8
1	C	421	TYR	2.8
1	C	1142	ALA	2.7
1	D	1153	PHE	2.7
1	D	1053	ASP	2.7
1	B	270	ARG	2.7
1	B	282	GLY	2.7
1	B	90	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	205	ARG	2.7
1	C	395	ILE	2.7
1	C	282	GLY	2.7
1	A	88	SER	2.7
1	A	384	LEU	2.7
1	B	381	GLU	2.7
1	A	232	GLU	2.6
1	D	879	LYS	2.6
1	D	1126	SER	2.6
1	A	213	LEU	2.6
1	B	457	THR	2.6
1	A	1138	LEU	2.6
1	C	972	GLU	2.6
1	D	88	SER	2.6
1	C	384	LEU	2.5
1	D	314	VAL	2.5
1	C	936	TYR	2.5
1	D	386	ASP	2.5
1	D	1127	VAL	2.5
1	A	175	LYS	2.5
1	B	494	LEU	2.4
1	D	151	ASP	2.4
1	D	87	GLY	2.4
1	A	89	ASP	2.4
1	C	934	ASP	2.4
1	A	494	LEU	2.3
1	D	310	VAL	2.3
1	A	176	SER	2.3
1	A	1156	VAL	2.3
1	A	174	ILE	2.3
1	C	937	LYS	2.3
1	A	1159	GLN	2.3
1	C	417	GLU	2.3
1	A	221	LYS	2.3
1	B	527	ALA	2.3
1	B	157	THR	2.3
1	D	285	PRO	2.3
1	C	490	ILE	2.2
1	D	1155	GLY	2.2
1	B	382	ASP	2.2
1	B	1096	THR	2.2
1	D	271	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	452	ILE	2.2
1	B	975	THR	2.2
1	D	242	PRO	2.2
1	C	970	GLY	2.2
1	C	1070	GLU	2.2
1	A	1151	ALA	2.2
1	B	1097	ASN	2.2
1	D	488	PHE	2.2
1	C	197	SER	2.2
1	D	1130	THR	2.2
1	A	420	PRO	2.1
1	B	283	LEU	2.1
1	D	321	PHE	2.1
1	B	269	ARG	2.1
1	C	491	GLN	2.1
1	A	493	SER	2.1
1	A	523	ASP	2.1
1	C	385	ASN	2.1
1	A	70	GLU	2.1
1	D	309	THR	2.0
1	B	92	PRO	2.0
1	A	185	GLU	2.0
1	D	92	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

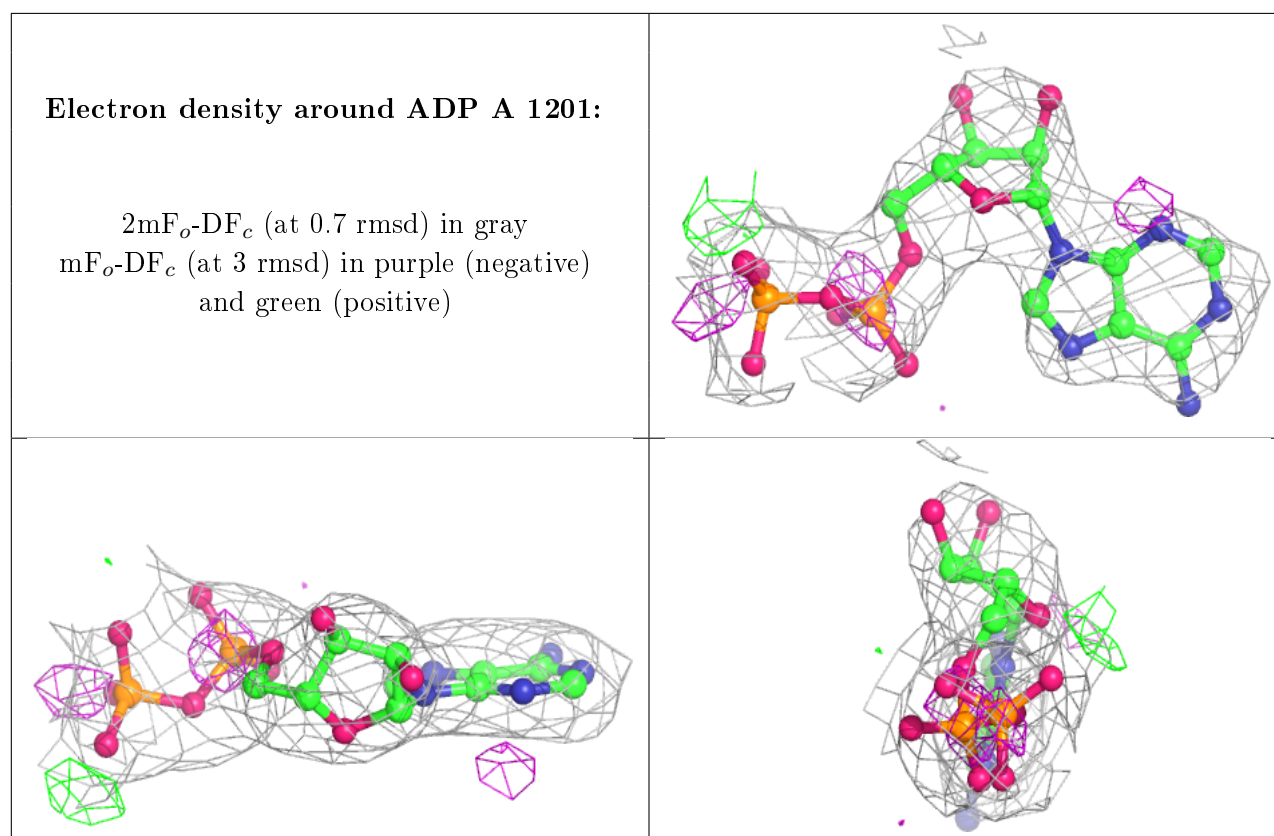
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

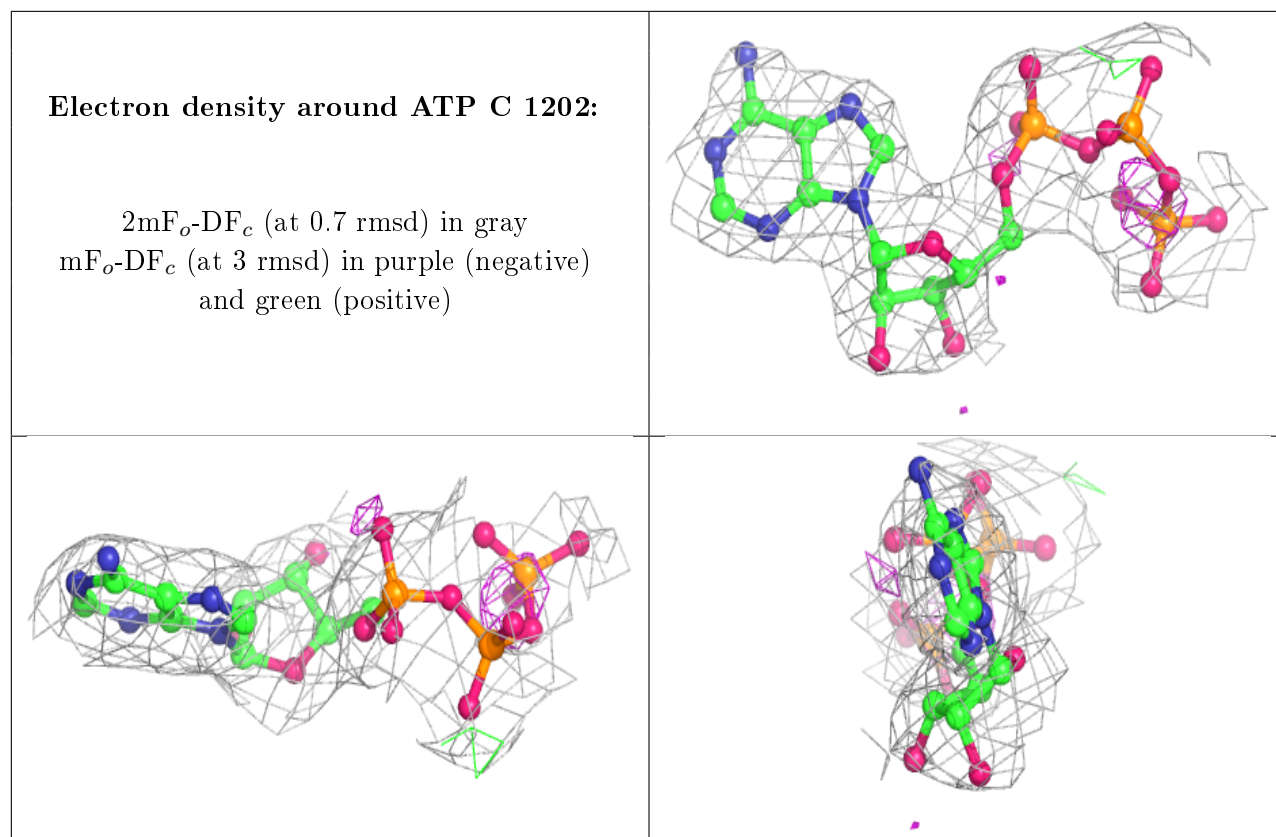
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	A	1201	27/27	0.91	0.16	75,82,96,97	0
3	MN	A	1202	1/1	0.92	0.20	94,94,94,94	0
5	ATP	C	1202	31/31	0.93	0.17	69,72,104,105	0
4	BTI	B	1201	15/15	0.94	0.20	56,59,61,64	0
3	MN	B	1203	1/1	0.97	0.15	83,83,83,83	0
3	MN	D	1203	1/1	0.97	0.13	85,85,85,85	0
4	BTI	B	1202	15/15	0.97	0.12	31,40,44,50	0
4	BTI	C	1203	15/15	0.97	0.14	55,59,61,63	0
4	BTI	D	1202	15/15	0.98	0.14	46,50,51,52	0
3	MN	C	1201	1/1	0.99	0.25	55,55,55,55	0
6	CL	D	1201	1/1	0.99	0.07	45,45,45,45	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.