



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:38 am BST

PDB ID : 4AUI
Title : STRUCTURE AND FUNCTION OF THE PORB PORIN FROM DISSEMINATING N. GONORRHOEAE
Authors : Zeth, K.; Kozjak-Pavlovic, V.; Faulstich, M.; Hurwitz, R.; Kepp, O.; Rudel, T.
Deposited on : 2012-05-17
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

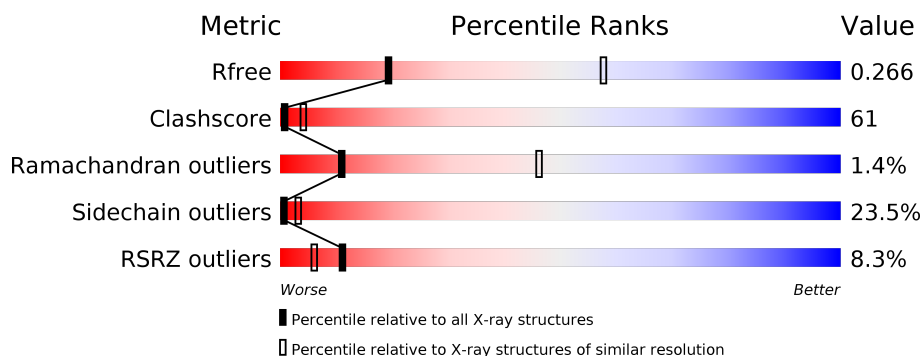
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>9%</div> <div>27%</div> <div>50%</div> <div>16%</div> <div>• 6%</div> </div>
1	B	327	<div> <div>7%</div> <div>28%</div> <div>49%</div> <div>15%</div> <div>• 6%</div> </div>
1	C	327	<div> <div>7%</div> <div>31%</div> <div>45%</div> <div>18%</div> <div>• 6%</div> </div>
2	D	8	<div> <div>38%</div> <div>13%</div> <div>63%</div> <div>25%</div> </div>
2	E	8	<div> <div>25%</div> <div>13%</div> <div>88%</div> </div>
2	F	8	<div> <div>25%</div> <div>63%</div> <div>13%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	400	-	-	X	-
4	PO4	A	402	-	-	X	-
4	PO4	B	401	-	-	X	-
4	PO4	B	402	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7329 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 PORIN (PORB).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	2	0	0
			2370	1481	427	462			
1	B	308	Total	C	N	O	2	0	0
			2360	1474	427	459			
1	C	308	Total	C	N	O	4	0	0
			2360	1474	427	459			

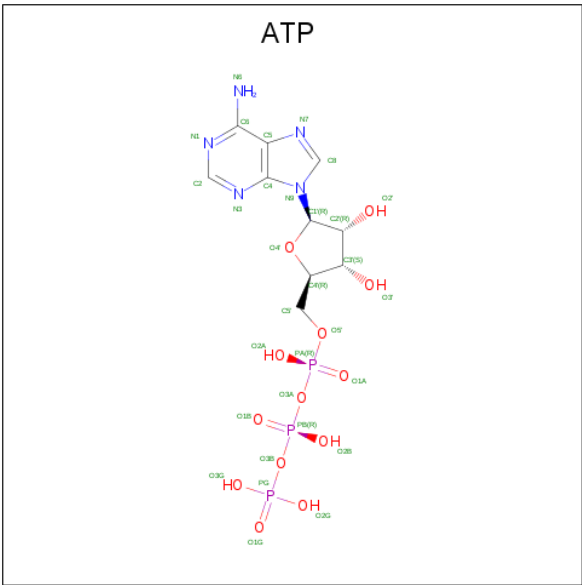
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASN	GLY	conflict	UNP Q51056
A	167	ASP	SER	conflict	UNP Q51056
B	102	ASN	GLY	conflict	UNP Q51056
B	167	ASP	SER	conflict	UNP Q51056
C	102	ASN	GLY	conflict	UNP Q51056
C	167	ASP	SER	conflict	UNP Q51056

- Molecule 2 is a protein called POLY ALA.

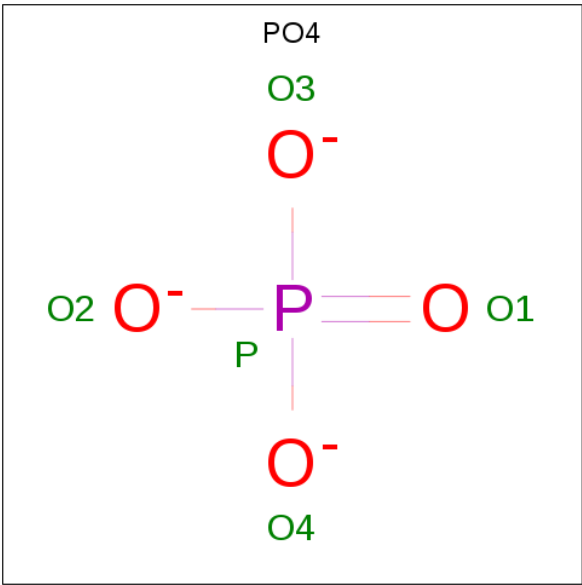
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	E	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	F	7	Total	C	N	O	0	0	0
			35	21	7	7			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

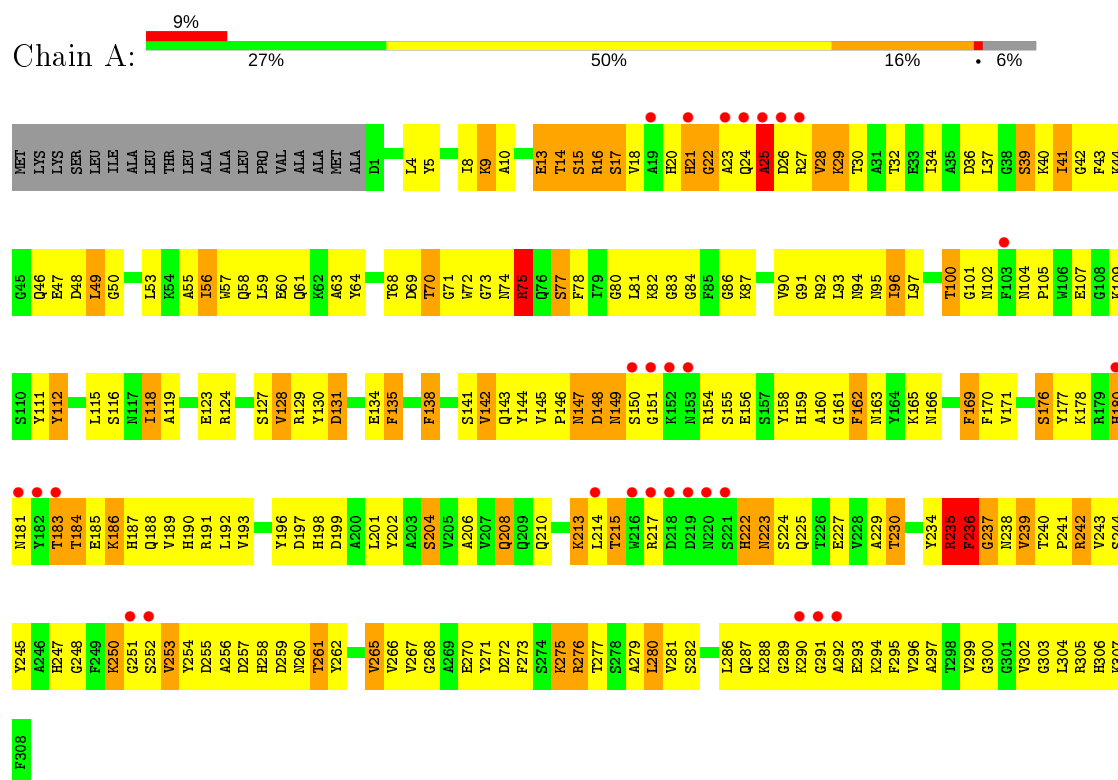
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

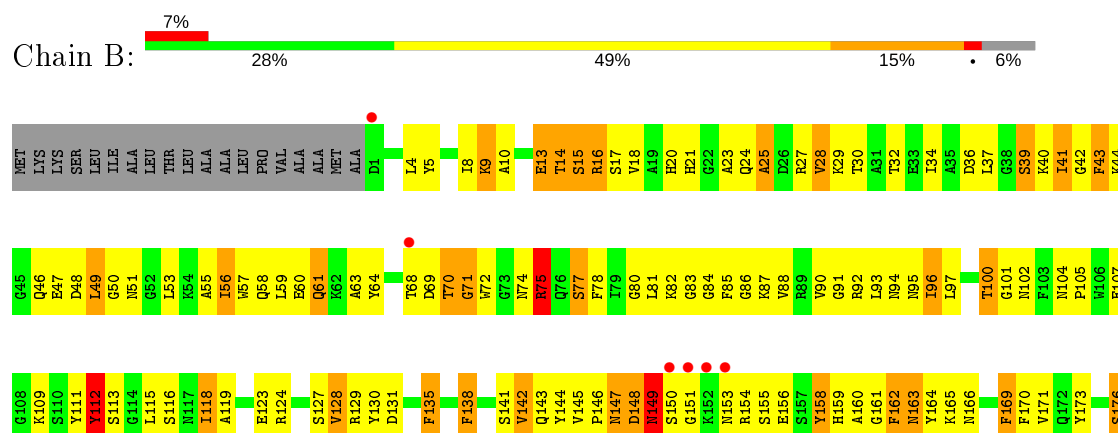
3 Residue-property plots

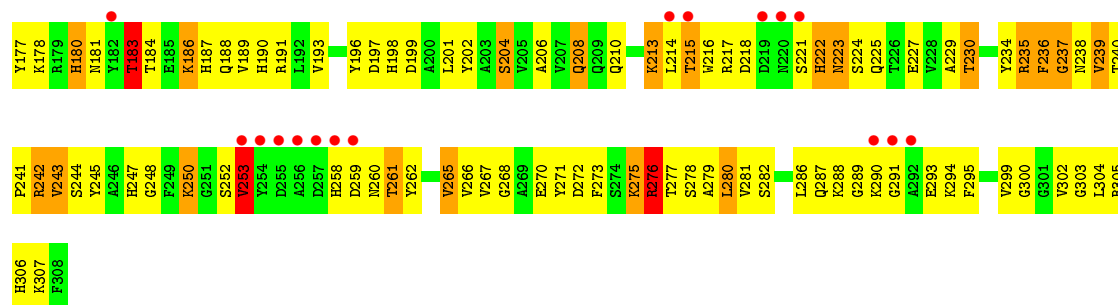
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: PORIN (PORB)

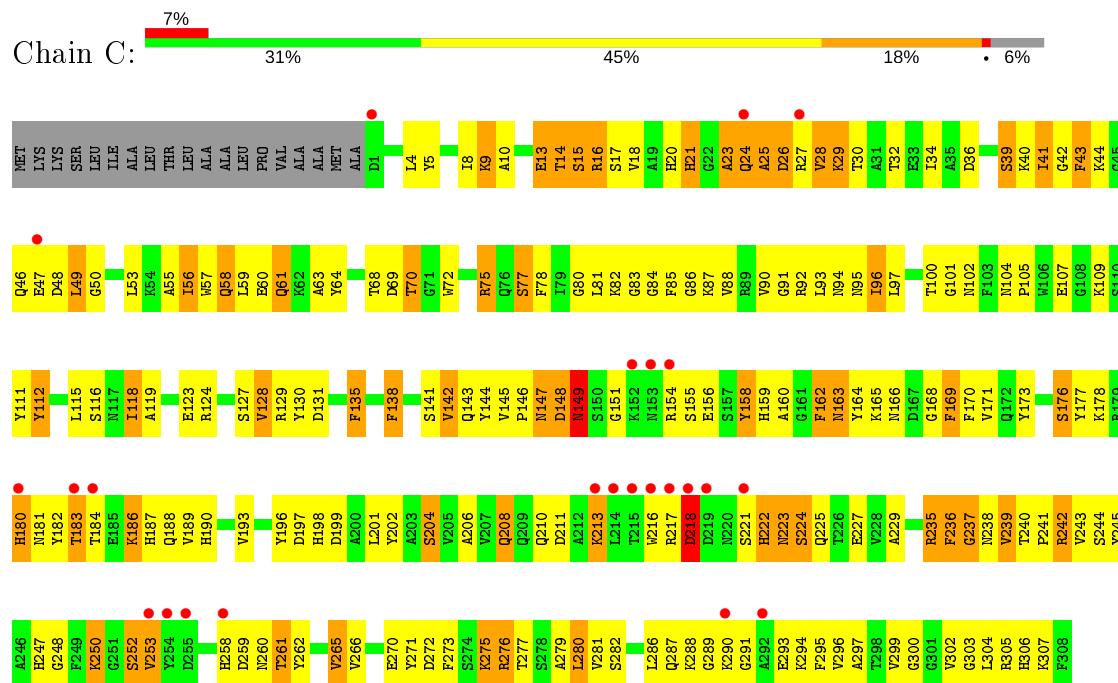


• Molecule 1: PORIN (PORB)

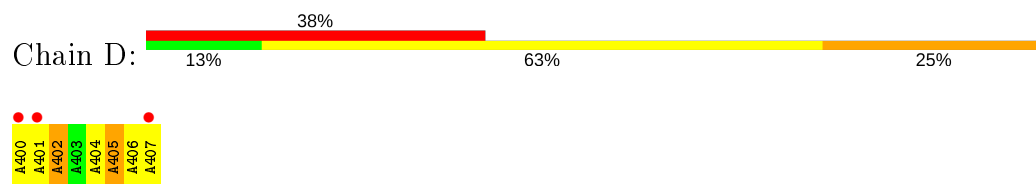




• Molecule 1: PORIN (PORB)



• Molecule 2: POLY ALA



• Molecule 2: POLY ALA



• Molecule 2: POLY ALA



A402
A403
A404
A405
A406
A407
A408
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.05Å 111.47Å 88.34Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	38.05 – 3.20 38.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	78.4 (38.05-3.20) 78.4 (38.05-3.20)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.268 0.221 , 0.266	Depositor DCC
R_{free} test set	702 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 134.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7329	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.87	8/2425 (0.3%)	0.94	10/3278 (0.3%)
1	B	0.78	7/2414 (0.3%)	0.95	8/3263 (0.2%)
1	C	0.82	9/2414 (0.4%)	0.90	3/3263 (0.1%)
2	D	0.72	0/39	1.31	0/53
2	E	0.75	0/39	1.12	0/53
2	F	0.59	0/34	1.20	0/46
All	All	0.82	24/7365 (0.3%)	0.93	21/9956 (0.2%)

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	3
1	B	0	4
1	C	0	6
2	D	0	2
2	E	0	1
All	All	0	16

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	PHE	CG-CD2	-12.64	1.19	1.38
1	A	236	PHE	CE1-CZ	-9.98	1.18	1.37
1	A	236	PHE	CG-CD1	-9.39	1.24	1.38
1	C	58	GLN	CD-NE2	-8.75	1.10	1.32
1	A	236	PHE	CE2-CZ	-8.48	1.21	1.37
1	C	58	GLN	CD-OE1	-7.76	1.06	1.24
1	C	236	PHE	CG-CD1	-7.51	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	PHE	CG-CD2	-7.35	1.27	1.38
1	B	236	PHE	CG-CD1	-7.25	1.27	1.38
1	A	149	ASN	CG-OD1	-7.19	1.08	1.24
1	B	236	PHE	CG-CD2	-7.15	1.28	1.38
1	A	236	PHE	CB-CG	-6.90	1.39	1.51
1	B	236	PHE	CE2-CZ	-6.65	1.24	1.37
1	A	149	ASN	CG-ND2	-6.26	1.17	1.32
1	C	149	ASN	CG-OD1	-6.22	1.10	1.24
1	C	236	PHE	CB-CG	-6.13	1.41	1.51
1	B	236	PHE	CB-CG	-5.86	1.41	1.51
1	B	149	ASN	CG-OD1	-5.76	1.11	1.24
1	C	149	ASN	CG-ND2	-5.50	1.19	1.32
1	C	236	PHE	CE2-CZ	-5.44	1.27	1.37
1	B	149	ASN	CG-ND2	-5.29	1.19	1.32
1	B	13	GLU	CB-CG	-5.25	1.42	1.52
1	A	75	ARG	CZ-NH1	5.17	1.39	1.33
1	C	13	GLU	CB-CG	-5.11	1.42	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ARG	NE-CZ-NH1	14.65	127.63	120.30
1	A	20	HIS	C-N-CA	8.25	142.33	121.70
1	C	236	PHE	CB-CA-C	-7.63	95.14	110.40
1	A	237	GLY	N-CA-C	-7.40	94.60	113.10
1	B	236	PHE	CB-CA-C	-7.05	96.30	110.40
1	B	75	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	237	GLY	N-CA-C	-6.84	95.99	113.10
1	A	22	GLY	N-CA-C	-6.45	96.97	113.10
1	A	25	ALA	N-CA-C	6.39	128.27	111.00
1	C	237	GLY	N-CA-C	-6.36	97.21	113.10
1	A	13	GLU	CB-CA-C	-6.09	98.21	110.40
1	C	13	GLU	CB-CA-C	-5.92	98.55	110.40
1	A	75	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	13	GLU	CB-CA-C	-5.63	99.15	110.40
1	A	13	GLU	OE1-CD-OE2	5.41	129.80	123.30
1	B	276	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	236	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	75	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	71	GLY	N-CA-C	5.12	125.91	113.10
1	B	183	THR	N-CA-CB	5.12	120.04	110.30
1	A	186	LYS	N-CA-CB	-5.05	101.52	110.60

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	THR	Peptide
1	A	235	ARG	Peptide
1	A	25	ALA	Peptide
1	B	100	THR	Peptide
1	B	20	HIS	Peptide
1	B	217	ARG	Peptide
1	B	25	ALA	Peptide
1	C	20	HIS	Peptide
1	C	21	HIS	Peptide
1	C	217	ARG	Peptide
1	C	23	ALA	Peptide
1	C	24	GLN	Peptide
1	C	25	ALA	Peptide
2	D	402	ALA	Peptide
2	D	405	ALA	Peptide
2	E	404	ALA	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	2370	0	2229	303	4
1	B	2360	0	2220	289	4
1	C	2360	0	2220	273	3
2	D	40	0	39	13	0
2	E	40	0	39	6	0
2	F	35	0	34	14	0
3	A	31	0	12	7	0
3	B	31	0	12	10	0
3	C	31	0	12	5	0
4	A	10	0	0	3	0
4	B	10	0	0	5	0
4	C	10	0	0	1	0
5	A	1	0	0	0	0
All	All	7329	0	6817	857	6

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 61.

All (857) 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:B:75:ARG:NH2	3:B:400:ATP:C8	1.83	1.39
1:B:75:ARG:NH2	3:B:400:ATP:H8	1.22	1.19
2:F:404:ALA:HB1	2:F:405:ALA:HA	1.31	1.12
1:C:178:LYS:HD2	1:C:181:ASN:HB2	1.15	1.11
1:A:178:LYS:HD2	1:A:181:ASN:HB2	1.13	1.10
1:A:21:HIS:HB2	1:A:25:ALA:HA	1.20	1.10
1:B:178:LYS:HD2	1:B:181:ASN:HB2	1.12	1.08
1:A:21:HIS:HD2	1:A:25:ALA:HB1	1.19	1.07
1:A:21:HIS:HB2	1:A:25:ALA:CA	1.84	1.06
1:B:96:ILE:HD12	1:B:160:ALA:HA	1.35	1.05
2:D:401:ALA:N	2:F:407:ALA:HB3	1.73	1.04
2:D:401:ALA:H	2:F:407:ALA:HB3	0.92	1.03
2:D:404:ALA:HB1	2:D:405:ALA:HA	1.34	1.03
1:A:96:ILE:HG13	1:A:159:HIS:HB3	1.40	1.01
2:E:403:ALA:O	2:F:402:ALA:HB3	1.61	1.00
1:C:96:ILE:HD12	1:C:160:ALA:HA	1.44	1.00
1:A:96:ILE:HD12	1:A:160:ALA:HA	1.43	0.99
1:B:16:ARG:HH12	1:B:29:LYS:HA	1.27	0.99
1:C:96:ILE:HG13	1:C:159:HIS:HB3	1.44	0.98
1:A:198:HIS:HD2	1:A:199:ASP:H	1.10	0.97
2:D:402:ALA:O	2:F:406:ALA:HB3	1.63	0.97
1:B:13:GLU:OE2	1:B:109:LYS:CB	2.13	0.96
1:C:16:ARG:HH12	1:C:29:LYS:HA	1.26	0.96
1:A:21:HIS:CD2	1:A:25:ALA:HB1	1.99	0.96
1:C:198:HIS:HD2	1:C:199:ASP:CB	1.78	0.96
2:D:401:ALA:H	2:F:407:ALA:CB	1.78	0.96
1:A:16:ARG:HH12	1:A:29:LYS:HA	1.30	0.95
1:A:253:VAL:HG23	1:A:254:TYR:N	1.81	0.94
1:B:96:ILE:HG13	1:B:159:HIS:HB3	1.47	0.94
1:C:198:HIS:HD2	1:C:199:ASP:HB2	1.31	0.94
1:A:36:ASP:OD1	1:A:39:SER:HB2	1.68	0.93
1:A:44:LYS:HD2	1:A:58:GLN:HE21	1.29	0.93
1:B:178:LYS:HZ3	1:B:181:ASN:HD22	1.12	0.93
1:B:198:HIS:HD2	1:B:199:ASP:H	1.13	0.93
1:A:112:TYR:H	1:A:112:TYR:HD1	1.17	0.92
1:A:250:LYS:HB3	1:A:260:ASN:H	1.34	0.92
1:A:28:VAL:HG22	1:A:29:LYS:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HD3	1:C:151:GLY:H	1.34	0.92
1:C:46:GLN:HA	1:C:55:ALA:O	1.71	0.91
1:B:178:LYS:CD	1:B:181:ASN:HB2	1.99	0.91
1:B:28:VAL:HG22	1:B:29:LYS:H	1.36	0.91
1:B:75:ARG:NH2	3:B:400:ATP:N7	2.19	0.90
1:C:36:ASP:OD1	1:C:39:SER:HB2	1.71	0.90
1:C:13:GLU:OE2	1:C:109:LYS:CB	2.19	0.90
1:B:198:HIS:CD2	1:B:199:ASP:N	2.40	0.90
2:E:401:ALA:N	2:E:402:ALA:HA	1.86	0.89
1:A:198:HIS:CD2	1:A:199:ASP:N	2.39	0.89
1:B:63:ALA:HB1	1:C:59:LEU:HD21	1.54	0.89
1:B:16:ARG:NH1	1:B:29:LYS:HA	1.87	0.89
1:B:36:ASP:OD1	1:B:39:SER:HB2	1.72	0.89
1:A:253:VAL:HG23	1:A:254:TYR:H	1.38	0.88
1:A:63:ALA:HB1	1:B:59:LEU:HD21	1.56	0.88
1:C:112:TYR:HD1	1:C:112:TYR:H	1.22	0.88
1:C:16:ARG:NH1	1:C:29:LYS:HA	1.87	0.88
1:B:44:LYS:HD2	1:B:58:GLN:HE21	1.36	0.88
1:C:250:LYS:HB3	1:C:260:ASN:H	1.36	0.88
1:C:178:LYS:HZ3	1:C:181:ASN:HD22	1.19	0.87
1:B:198:HIS:HD2	1:B:199:ASP:N	1.72	0.87
1:B:276:ARG:HD2	1:C:47:GLU:OE1	1.74	0.87
1:B:149:ASN:OD1	1:B:155:SER:HB3	1.74	0.87
1:C:178:LYS:CD	1:C:181:ASN:HB2	2.03	0.87
1:C:28:VAL:HG22	1:C:29:LYS:H	1.37	0.87
1:A:49:LEU:N	1:A:50:GLY:HA3	1.90	0.86
1:C:49:LEU:N	1:C:50:GLY:HA3	1.90	0.86
1:A:46:GLN:HA	1:A:55:ALA:O	1.76	0.86
1:A:177:TYR:HD1	1:A:188:GLN:HG2	1.40	0.86
1:B:46:GLN:HA	1:B:55:ALA:O	1.75	0.86
1:A:127:SER:HB2	1:A:144:TYR:O	1.76	0.85
1:B:127:SER:HB2	1:B:144:TYR:O	1.76	0.85
1:A:178:LYS:CD	1:A:181:ASN:HB2	2.01	0.85
1:A:198:HIS:HD2	1:A:199:ASP:N	1.71	0.84
1:B:49:LEU:N	1:B:50:GLY:HA3	1.91	0.84
1:A:16:ARG:NH1	1:A:29:LYS:HA	1.93	0.83
1:C:177:TYR:HD1	1:C:188:GLN:HG2	1.41	0.83
1:A:178:LYS:HD2	1:A:181:ASN:CB	2.04	0.83
1:C:198:HIS:CD2	1:C:199:ASP:N	2.45	0.83
2:D:404:ALA:CB	2:D:405:ALA:HA	2.08	0.83
1:A:44:LYS:HD2	1:A:58:GLN:NE2	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LYS:NZ	1:B:181:ASN:HD22	1.77	0.82
1:B:178:LYS:O	1:B:186:LYS:HA	1.78	0.82
1:A:13:GLU:OE2	1:A:109:LYS:CB	2.27	0.82
1:A:198:HIS:CD2	1:A:199:ASP:H	1.97	0.81
1:C:291:GLY:O	1:C:294:LYS:HE2	1.79	0.81
1:A:9:LYS:HA	1:A:304:LEU:O	1.81	0.81
1:C:127:SER:HB2	1:C:144:TYR:O	1.80	0.81
1:B:60:GLU:O	1:B:75:ARG:HB2	1.81	0.81
1:B:177:TYR:HD1	1:B:188:GLN:HG2	1.45	0.80
1:C:178:LYS:O	1:C:186:LYS:HA	1.79	0.80
1:A:29:LYS:HD3	1:B:151:GLY:H	1.45	0.80
1:C:198:HIS:CD2	1:C:199:ASP:CB	2.65	0.80
1:A:178:LYS:O	1:A:186:LYS:HA	1.80	0.80
1:C:59:LEU:HA	1:C:77:SER:HB3	1.62	0.80
1:A:59:LEU:HA	1:A:77:SER:HB3	1.63	0.79
1:B:198:HIS:CD2	1:B:199:ASP:H	1.99	0.79
1:C:60:GLU:O	1:C:75:ARG:HB2	1.81	0.79
1:C:198:HIS:CD2	1:C:199:ASP:HB2	2.16	0.79
1:B:59:LEU:HA	1:B:77:SER:HB3	1.64	0.79
1:A:59:LEU:HD21	1:C:63:ALA:HB1	1.66	0.78
1:B:5:TYR:CE1	1:B:42:GLY:HA3	2.18	0.78
1:C:15:SER:O	1:C:30:THR:HA	1.83	0.78
1:A:15:SER:O	1:A:30:THR:HA	1.82	0.78
1:B:44:LYS:HD2	1:B:58:GLN:NE2	1.99	0.78
1:C:178:LYS:NZ	1:C:181:ASN:HD22	1.81	0.77
1:B:56:ILE:HD12	1:B:78:PHE:CE1	2.18	0.77
1:B:40:LYS:HE2	1:B:75:ARG:NH2	1.99	0.77
1:B:15:SER:O	1:B:30:THR:HA	1.85	0.77
1:B:250:LYS:HB3	1:B:260:ASN:H	1.48	0.77
1:C:60:GLU:C	1:C:75:ARG:HB2	2.04	0.77
1:C:143:GLN:HB2	1:C:159:HIS:HB2	1.66	0.77
2:E:407:ALA:O	2:F:402:ALA:HB1	1.85	0.77
1:B:36:ASP:OD2	1:B:64:TYR:HA	1.83	0.77
1:B:242:ARG:HG2	1:B:242:ARG:HH11	1.49	0.76
1:B:178:LYS:HD2	1:B:181:ASN:CB	2.05	0.75
1:B:302:VAL:HG12	1:B:303:GLY:N	2.01	0.75
1:C:178:LYS:HD2	1:C:181:ASN:CB	2.08	0.75
1:A:60:GLU:C	1:A:75:ARG:HB2	2.07	0.75
1:B:69:ASP:OD2	1:C:72:TRP:HB2	1.86	0.75
1:A:143:GLN:HB2	1:A:159:HIS:HB2	1.69	0.75
1:A:189:VAL:HG22	1:A:210:GLN:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:C	1:B:75:ARG:HB2	2.07	0.75
1:B:124:ARG:HH22	3:B:400:ATP:HN61	1.31	0.75
1:A:178:LYS:HE3	1:A:187:HIS:HB3	1.69	0.75
1:A:56:ILE:HD12	1:A:78:PHE:CE1	2.22	0.75
1:B:143:GLN:HB2	1:B:159:HIS:HB2	1.69	0.74
1:C:36:ASP:OD2	1:C:64:TYR:HA	1.87	0.74
1:A:36:ASP:OD2	1:A:64:TYR:HA	1.87	0.74
1:B:142:VAL:HG13	1:B:160:ALA:HB2	1.70	0.74
1:A:142:VAL:HG13	1:A:160:ALA:HB2	1.69	0.74
1:A:276:ARG:CG	1:A:276:ARG:HH11	2.00	0.74
1:C:252:SER:O	1:C:253:VAL:HG13	1.87	0.74
1:B:124:ARG:HH22	3:B:400:ATP:N6	1.85	0.74
1:C:21:HIS:HB2	1:C:23:ALA:HA	1.69	0.73
1:C:163:ASN:HD22	1:C:163:ASN:N	1.86	0.73
1:A:69:ASP:OD2	1:B:72:TRP:HB2	1.89	0.73
1:B:291:GLY:O	1:B:294:LYS:HE2	1.89	0.73
1:C:147:ASN:N	1:C:147:ASN:HD22	1.85	0.72
2:E:407:ALA:O	2:F:402:ALA:CB	2.37	0.72
1:A:291:GLY:O	1:A:294:LYS:HE2	1.90	0.72
1:A:47:GLU:OE1	1:C:276:ARG:HD2	1.89	0.72
1:B:302:VAL:HG12	1:B:303:GLY:H	1.54	0.72
1:A:181:ASN:HB3	1:A:184:THR:HG23	1.71	0.72
1:B:259:ASP:HB3	1:B:261:THR:HG22	1.72	0.72
1:B:9:LYS:HA	1:B:304:LEU:O	1.88	0.72
2:F:404:ALA:HB1	2:F:405:ALA:CA	2.17	0.72
1:A:21:HIS:HD2	1:A:25:ALA:CB	2.00	0.72
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.55	0.71
1:A:178:LYS:HZ3	1:A:181:ASN:HD22	1.38	0.71
1:A:252:SER:O	1:A:253:VAL:HG22	1.89	0.71
1:A:21:HIS:CD2	1:A:25:ALA:CB	2.73	0.71
1:A:242:ARG:HH11	1:A:242:ARG:HG2	1.56	0.71
1:A:259:ASP:HB3	1:A:261:THR:HG22	1.71	0.71
1:C:162:PHE:C	1:C:163:ASN:ND2	2.44	0.71
1:A:5:TYR:CE1	1:A:42:GLY:HA3	2.26	0.70
1:C:238:ASN:HB2	1:C:271:TYR:CE1	2.26	0.70
1:C:9:LYS:HA	1:C:304:LEU:O	1.91	0.70
1:B:187:HIS:CD2	1:B:188:GLN:N	2.60	0.70
1:A:27:ARG:HH11	1:A:27:ARG:HG2	1.57	0.70
1:C:44:LYS:HB3	1:C:58:GLN:HA	1.73	0.70
1:A:60:GLU:O	1:A:75:ARG:HB2	1.91	0.70
1:C:124:ARG:HH22	3:C:400:ATP:HN61	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ARG:HG2	1:C:242:ARG:HH11	1.56	0.70
1:C:27:ARG:HG2	1:C:27:ARG:HH11	1.56	0.69
1:C:259:ASP:HB3	1:C:261:THR:HG22	1.75	0.69
1:A:63:ALA:HB1	1:B:59:LEU:CD2	2.22	0.69
1:A:147:ASN:N	1:A:147:ASN:HD22	1.90	0.69
1:C:21:HIS:C	1:C:23:ALA:H	1.96	0.69
1:A:170:PHE:CE2	1:A:193:VAL:HG12	2.28	0.69
1:A:276:ARG:HD2	1:B:47:GLU:OE1	1.92	0.69
1:B:21:HIS:C	1:B:23:ALA:H	1.93	0.69
1:A:251:GLY:O	1:A:257:ASP:OD1	2.11	0.69
1:A:21:HIS:CB	1:A:25:ALA:HA	2.11	0.69
1:A:124:ARG:HH22	3:A:400:ATP:N6	1.91	0.69
1:A:162:PHE:O	1:A:163:ASN:ND2	2.24	0.69
1:B:28:VAL:HG22	1:B:29:LYS:N	2.08	0.68
1:A:162:PHE:C	1:A:163:ASN:ND2	2.46	0.68
1:A:276:ARG:HD3	1:A:307:LYS:O	1.91	0.68
1:A:28:VAL:HG22	1:A:29:LYS:N	2.07	0.68
1:A:276:ARG:HD3	1:A:306:HIS:CE1	2.28	0.68
1:B:128:VAL:O	1:B:143:GLN:HA	1.94	0.68
1:C:163:ASN:ND2	1:C:163:ASN:N	2.41	0.68
1:A:302:VAL:HG12	1:A:303:GLY:N	2.08	0.68
1:C:239:VAL:HG13	1:C:241:PRO:HD3	1.76	0.68
1:C:183:THR:O	1:C:184:THR:HG23	1.94	0.67
1:C:276:ARG:CG	1:C:276:ARG:HH11	2.05	0.67
1:A:112:TYR:N	1:A:112:TYR:HD1	1.92	0.67
1:B:276:ARG:CG	1:B:276:ARG:HH11	2.08	0.67
1:B:289:GLY:O	1:B:290:LYS:HG2	1.94	0.67
1:C:187:HIS:CD2	1:C:188:GLN:N	2.62	0.67
1:A:107:GLU:HG3	1:A:280:LEU:HD13	1.76	0.67
1:C:302:VAL:HG12	1:C:303:GLY:N	2.10	0.67
1:A:273:PHE:HZ	1:A:279:ALA:HB2	1.60	0.67
1:A:82:LYS:HA	1:A:86:GLY:O	1.93	0.67
1:B:147:ASN:HD22	1:B:147:ASN:N	1.92	0.67
1:B:24:GLN:HG3	1:B:24:GLN:O	1.94	0.67
1:C:9:LYS:HB3	1:C:305:ARG:HB2	1.76	0.66
1:B:63:ALA:HB1	1:C:59:LEU:CD2	2.25	0.66
1:C:128:VAL:O	1:C:143:GLN:HA	1.95	0.66
1:C:171:VAL:HA	1:C:193:VAL:O	1.95	0.66
1:B:166:ASN:O	1:B:169:PHE:HB2	1.95	0.66
1:B:242:ARG:NH1	1:B:242:ARG:HG2	2.08	0.66
1:A:238:ASN:HB2	1:A:271:TYR:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLY:O	1:A:290:LYS:HG2	1.95	0.66
1:A:242:ARG:NH1	1:A:242:ARG:HG2	2.10	0.66
1:C:198:HIS:HD2	1:C:199:ASP:N	1.94	0.66
1:A:9:LYS:HB3	1:A:305:ARG:HB2	1.79	0.65
1:C:142:VAL:HG13	1:C:160:ALA:HB2	1.79	0.65
1:A:202:TYR:CZ	1:A:204:SER:HB3	2.31	0.65
1:C:28:VAL:HG22	1:C:29:LYS:N	2.10	0.65
1:A:187:HIS:CD2	1:A:188:GLN:N	2.65	0.65
1:A:96:ILE:HG13	1:A:159:HIS:CB	2.22	0.65
1:C:189:VAL:HG22	1:C:210:GLN:HG2	1.78	0.65
1:B:252:SER:O	1:B:253:VAL:HG13	1.97	0.65
1:A:171:VAL:HA	1:A:193:VAL:O	1.97	0.65
1:B:124:ARG:NH2	3:B:400:ATP:N6	2.44	0.65
1:A:44:LYS:HB3	1:A:58:GLN:HG3	1.79	0.65
1:B:242:ARG:HH11	1:B:242:ARG:CG	2.08	0.65
1:C:222:HIS:O	1:C:253:VAL:HG21	1.96	0.65
1:A:135:PHE:O	1:A:138:PHE:HB2	1.97	0.65
1:A:215:THR:HG22	1:A:217:ARG:O	1.97	0.65
1:B:124:ARG:NH2	3:B:400:ATP:HN61	1.95	0.65
1:B:9:LYS:HB3	1:B:305:ARG:HB2	1.78	0.65
1:A:178:LYS:NZ	1:A:181:ASN:HD22	1.95	0.65
1:A:242:ARG:HH11	1:A:242:ARG:CG	2.10	0.64
1:A:44:LYS:HB3	1:A:58:GLN:HA	1.78	0.64
1:C:112:TYR:N	1:C:112:TYR:HD1	1.94	0.64
1:B:184:THR:CG2	1:B:187:HIS:HB2	2.27	0.64
1:B:44:LYS:HB3	1:B:58:GLN:HA	1.78	0.64
1:B:44:LYS:HB3	1:B:58:GLN:HG3	1.79	0.64
1:C:147:ASN:ND2	1:C:147:ASN:H	1.96	0.64
1:C:276:ARG:HD3	1:C:307:LYS:O	1.98	0.64
1:B:184:THR:HG21	1:B:187:HIS:HB2	1.80	0.64
1:C:75:ARG:HH22	3:C:400:ATP:H2'	1.63	0.64
1:C:273:PHE:HZ	1:C:279:ALA:HB2	1.63	0.64
3:A:400:ATP:O2B	3:A:400:ATP:H5'1	1.97	0.63
1:C:218:ASP:HB3	1:C:221:SER:HB2	1.79	0.63
1:C:289:GLY:O	1:C:290:LYS:HG2	1.98	0.63
1:C:5:TYR:CE1	1:C:42:GLY:HA3	2.33	0.63
1:B:197:ASP:O	1:B:198:HIS:HB2	1.97	0.63
1:A:128:VAL:O	1:A:143:GLN:HA	1.98	0.63
1:B:75:ARG:CZ	3:B:400:ATP:C8	2.78	0.63
1:C:55:ALA:HA	1:C:81:LEU:HD23	1.80	0.63
1:C:82:LYS:HA	1:C:86:GLY:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:404:ALA:CB	2:F:405:ALA:HA	2.19	0.63
1:B:171:VAL:HA	1:B:193:VAL:O	1.99	0.63
1:B:55:ALA:HA	1:B:81:LEU:HD23	1.81	0.63
1:C:41:ILE:HG22	1:C:63:ALA:HB2	1.81	0.63
1:B:170:PHE:CE2	1:B:193:VAL:HG12	2.33	0.62
1:B:273:PHE:HZ	1:B:279:ALA:HB2	1.64	0.62
1:C:95:ASN:HB2	1:C:123:GLU:H	1.63	0.62
1:B:276:ARG:HD3	1:B:307:LYS:O	1.98	0.62
1:A:242:ARG:NH2	1:A:270:GLU:HG3	2.14	0.62
1:C:242:ARG:NH1	1:C:242:ARG:HG2	2.12	0.62
1:A:273:PHE:CZ	1:A:279:ALA:HB2	2.35	0.62
1:A:55:ALA:HA	1:A:81:LEU:HD23	1.80	0.62
1:C:242:ARG:CG	1:C:242:ARG:HH11	2.11	0.62
1:C:147:ASN:N	1:C:147:ASN:ND2	2.47	0.62
1:C:197:ASP:O	1:C:198:HIS:HB2	1.98	0.62
1:A:14:THR:HG23	1:A:32:THR:OG1	1.99	0.62
1:B:149:ASN:OD1	1:B:155:SER:CB	2.47	0.62
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.64	0.62
1:C:165:LYS:HA	1:C:169:PHE:O	2.00	0.62
1:B:178:LYS:NZ	1:B:181:ASN:ND2	2.47	0.61
1:C:135:PHE:O	1:C:138:PHE:HB2	2.00	0.61
1:C:242:ARG:NH2	1:C:270:GLU:HG3	2.15	0.61
1:B:135:PHE:O	1:B:138:PHE:HB2	1.99	0.61
1:B:129:ARG:HB2	1:B:143:GLN:HG2	1.82	0.61
1:B:165:LYS:HA	1:B:169:PHE:O	2.01	0.61
1:C:202:TYR:CZ	1:C:204:SER:HB3	2.35	0.61
1:C:96:ILE:HG13	1:C:159:HIS:CB	2.27	0.61
1:B:147:ASN:ND2	1:B:147:ASN:H	1.99	0.61
1:C:198:HIS:CD2	1:C:199:ASP:CG	2.74	0.61
1:C:24:GLN:CG	1:C:24:GLN:O	2.48	0.61
1:A:142:VAL:HG13	1:A:160:ALA:CB	2.29	0.61
1:B:41:ILE:HG22	1:B:63:ALA:HB2	1.82	0.60
1:B:82:LYS:HA	1:B:86:GLY:O	1.99	0.60
1:C:273:PHE:CZ	1:C:279:ALA:HB2	2.36	0.60
1:A:162:PHE:C	1:A:163:ASN:HD22	2.04	0.60
1:B:141:SER:O	1:B:160:ALA:HB1	2.00	0.60
1:C:238:ASN:HB3	1:C:272:ASP:O	2.01	0.60
1:C:178:LYS:HE3	1:C:187:HIS:HB3	1.83	0.60
1:B:147:ASN:ND2	1:B:147:ASN:N	2.50	0.60
1:B:18:VAL:HG13	1:B:27:ARG:CD	2.31	0.60
1:B:238:ASN:HB2	1:B:271:TYR:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:PHE:CE2	1:C:193:VAL:HG12	2.36	0.60
1:B:94:ASN:OD1	1:B:124:ARG:HG2	2.02	0.60
1:C:115:LEU:HD11	1:C:244:SER:HB3	1.83	0.60
1:C:75:ARG:NH2	3:C:400:ATP:C8	2.70	0.60
1:B:202:TYR:CZ	1:B:204:SER:HB3	2.37	0.60
1:C:8:ILE:HA	1:C:39:SER:OG	2.02	0.60
1:A:238:ASN:HB3	1:A:272:ASP:O	2.01	0.59
1:A:36:ASP:CG	1:A:39:SER:HB2	2.22	0.59
1:A:165:LYS:HA	1:A:169:PHE:O	2.02	0.59
1:A:223:ASN:OD1	1:A:223:ASN:C	2.40	0.59
1:A:197:ASP:O	1:A:198:HIS:HB2	2.01	0.59
1:B:273:PHE:CZ	1:B:279:ALA:HB2	2.37	0.59
1:C:56:ILE:HD12	1:C:78:PHE:CE1	2.38	0.59
1:C:178:LYS:NZ	1:C:181:ASN:ND2	2.50	0.59
1:A:107:GLU:OE2	1:A:305:ARG:HD3	2.02	0.59
1:C:302:VAL:HG12	1:C:303:GLY:H	1.68	0.59
1:B:18:VAL:HA	1:B:27:ARG:HG3	1.85	0.59
1:C:23:ALA:C	1:C:25:ALA:N	2.50	0.59
1:B:75:ARG:CZ	3:B:400:ATP:N7	2.65	0.59
1:C:18:VAL:HG13	1:C:27:ARG:CD	2.33	0.59
1:A:142:VAL:CG1	1:A:160:ALA:HB2	2.32	0.59
1:A:94:ASN:OD1	1:A:124:ARG:HG2	2.03	0.59
1:B:115:LEU:HD11	1:B:244:SER:HB3	1.84	0.59
1:B:5:TYR:CE1	1:B:42:GLY:CA	2.86	0.59
1:A:154:ARG:CB	1:A:156:GLU:CD	2.71	0.59
1:B:148:ASP:CG	1:B:149:ASN:H	2.06	0.59
1:B:189:VAL:HG22	1:B:210:GLN:HG2	1.85	0.59
1:C:154:ARG:CB	1:C:156:GLU:CD	2.71	0.59
1:C:97:LEU:HD12	1:C:97:LEU:H	1.67	0.59
1:A:129:ARG:HB2	1:A:143:GLN:HG2	1.85	0.58
1:A:235:ARG:O	1:A:236:PHE:CD1	2.56	0.58
1:C:166:ASN:O	1:C:169:PHE:HB2	2.03	0.58
1:C:94:ASN:OD1	1:C:124:ARG:HG2	2.03	0.58
1:B:142:VAL:HG13	1:B:160:ALA:CB	2.31	0.58
1:B:286:LEU:HD23	1:B:287:GLN:N	2.19	0.58
1:B:238:ASN:HB3	1:B:272:ASP:O	2.04	0.58
1:C:18:VAL:HA	1:C:27:ARG:HG3	1.84	0.58
1:A:239:VAL:HG13	1:A:241:PRO:HD3	1.86	0.58
1:B:302:VAL:CG1	1:B:303:GLY:H	2.16	0.58
1:A:95:ASN:HB2	1:A:123:GLU:H	1.68	0.58
1:B:142:VAL:CG1	1:B:160:ALA:HB2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASN:C	1:C:223:ASN:OD1	2.42	0.58
1:A:208:GLN:NE2	1:A:227:GLU:OE1	2.36	0.58
1:A:115:LEU:HD21	1:A:244:SER:HB2	1.86	0.58
1:A:8:ILE:HA	1:A:39:SER:OG	2.03	0.58
1:A:70:THR:CG2	1:B:70:THR:HG22	2.34	0.58
3:A:400:ATP:H5'1	3:A:400:ATP:PB	2.43	0.58
1:B:155:SER:HA	1:B:180:HIS:O	2.04	0.58
1:C:148:ASP:CG	1:C:149:ASN:H	2.07	0.58
1:A:270:GLU:OE2	1:A:280:LEU:HD22	2.04	0.57
1:C:107:GLU:OE2	1:C:305:ARG:HD3	2.04	0.57
1:A:115:LEU:HD11	1:A:244:SER:HB3	1.86	0.57
1:B:178:LYS:HE3	1:B:187:HIS:HB3	1.86	0.57
1:B:95:ASN:HB2	1:B:123:GLU:H	1.69	0.57
1:C:14:THR:HG23	1:C:32:THR:OG1	2.03	0.57
1:C:80:GLY:O	1:C:81:LEU:HD23	2.04	0.57
1:B:242:ARG:NH2	1:B:270:GLU:HG3	2.19	0.57
1:A:201:LEU:HD12	1:A:202:TYR:N	2.19	0.57
1:A:49:LEU:N	1:A:50:GLY:CA	2.66	0.57
1:B:223:ASN:OD1	1:B:223:ASN:C	2.42	0.57
1:A:253:VAL:CG2	1:A:254:TYR:N	2.56	0.57
1:A:18:VAL:HA	1:A:27:ARG:HG3	1.86	0.57
1:B:56:ILE:HD12	1:B:78:PHE:HE1	1.68	0.57
1:C:92:ARG:NH1	4:C:402:PO4:O1	2.37	0.57
1:B:247:HIS:HD2	1:B:262:TYR:O	1.87	0.57
1:C:181:ASN:O	1:C:184:THR:O	2.23	0.57
1:C:208:GLN:NE2	1:C:227:GLU:OE1	2.38	0.57
1:B:14:THR:HG23	1:B:32:THR:OG1	2.05	0.57
1:C:198:HIS:NE2	1:C:199:ASP:OD2	2.38	0.57
1:B:97:LEU:HD12	1:B:97:LEU:H	1.70	0.57
1:A:189:VAL:HG22	1:A:210:GLN:CG	2.35	0.56
1:B:154:ARG:CB	1:B:156:GLU:CD	2.73	0.56
1:A:250:LYS:HD2	1:A:251:GLY:O	2.05	0.56
1:B:8:ILE:HA	1:B:39:SER:OG	2.05	0.56
1:A:247:HIS:HD2	1:A:262:TYR:O	1.88	0.56
1:C:36:ASP:CG	1:C:39:SER:HB2	2.26	0.56
1:A:59:LEU:CD2	1:C:63:ALA:HB1	2.34	0.56
1:B:74:ASN:O	4:B:402:PO4:O3	2.23	0.56
1:C:21:HIS:HB2	1:C:23:ALA:H	1.71	0.56
1:C:44:LYS:HB3	1:C:58:GLN:HG3	1.86	0.56
1:A:112:TYR:N	1:A:112:TYR:CD1	2.60	0.56
1:A:18:VAL:HG13	1:A:27:ARG:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:TYR:OH	1:A:204:SER:HB3	2.05	0.56
1:B:111:TYR:HD1	1:B:299:VAL:HG21	1.71	0.56
1:B:210:GLN:NE2	1:B:225:GLN:HE21	2.04	0.56
1:C:182:TYR:O	1:C:183:THR:HB	2.06	0.56
1:A:55:ALA:HA	1:A:81:LEU:CD2	2.36	0.56
1:B:112:TYR:CD1	1:B:112:TYR:N	2.74	0.56
1:C:44:LYS:HA	1:C:57:TRP:CZ3	2.40	0.56
1:A:147:ASN:ND2	1:A:147:ASN:N	2.53	0.56
1:A:70:THR:HG22	1:B:70:THR:HG22	1.87	0.56
1:B:18:VAL:HG13	1:B:27:ARG:HD3	1.88	0.56
1:B:302:VAL:CG1	1:B:303:GLY:N	2.67	0.56
1:C:147:ASN:HD22	1:C:147:ASN:H	1.52	0.56
1:A:72:TRP:HB2	1:C:69:ASP:OD2	2.05	0.56
1:A:97:LEU:H	1:A:97:LEU:HD12	1.71	0.56
1:C:55:ALA:HA	1:C:81:LEU:CD2	2.35	0.56
1:B:163:ASN:ND2	1:B:163:ASN:N	2.54	0.56
1:C:155:SER:HA	1:C:180:HIS:O	2.05	0.55
1:A:302:VAL:HG12	1:A:303:GLY:H	1.71	0.55
1:B:4:LEU:HD11	1:B:41:ILE:HD11	1.87	0.55
1:B:5:TYR:CE1	1:B:42:GLY:C	2.80	0.55
1:C:286:LEU:HD23	1:C:287:GLN:N	2.22	0.55
1:C:124:ARG:NH2	3:C:400:ATP:HN61	2.04	0.55
1:C:49:LEU:N	1:C:50:GLY:CA	2.65	0.55
1:A:56:ILE:HD12	1:A:78:PHE:HE1	1.72	0.55
1:A:8:ILE:HD12	1:B:57:TRP:CE3	2.42	0.55
1:C:96:ILE:HD11	1:C:143:GLN:HG3	1.89	0.55
1:A:4:LEU:HD11	1:A:41:ILE:HD11	1.88	0.55
1:B:163:ASN:OD1	4:B:401:PO4:O2	2.25	0.55
1:B:187:HIS:HD2	1:B:188:GLN:H	1.53	0.55
1:B:23:ALA:O	1:B:24:GLN:HG2	2.07	0.55
1:A:155:SER:HA	1:A:180:HIS:O	2.07	0.55
1:A:40:LYS:HD2	1:A:60:GLU:OE2	2.07	0.55
1:A:41:ILE:HG22	1:A:63:ALA:HB2	1.88	0.55
1:A:75:ARG:O	1:A:92:ARG:HG2	2.07	0.55
1:B:148:ASP:CG	1:B:149:ASN:N	2.60	0.55
1:B:112:TYR:N	1:B:112:TYR:HD1	2.04	0.55
1:A:70:THR:HA	1:B:71:GLY:HA2	1.89	0.55
1:C:53:LEU:HD12	1:C:82:LYS:O	2.06	0.55
1:A:148:ASP:CG	1:A:149:ASN:H	2.09	0.54
1:A:80:GLY:O	1:A:81:LEU:HD23	2.07	0.54
1:B:115:LEU:HD21	1:B:244:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ILE:HG13	1:C:42:GLY:N	2.21	0.54
1:B:90:VAL:CG2	1:B:91:GLY:N	2.71	0.54
1:C:18:VAL:HG13	1:C:27:ARG:HD3	1.89	0.54
1:A:90:VAL:CG2	1:A:91:GLY:N	2.69	0.54
1:A:265:VAL:HG23	1:A:266:VAL:N	2.23	0.54
1:B:239:VAL:HG13	1:B:241:PRO:HD3	1.89	0.54
1:A:90:VAL:HG22	1:A:91:GLY:N	2.23	0.54
1:C:247:HIS:HD2	1:C:262:TYR:O	1.91	0.54
1:B:124:ARG:NH1	4:B:402:PO4:O2	2.41	0.54
1:C:182:TYR:O	1:C:183:THR:CB	2.56	0.54
1:C:27:ARG:CG	1:C:27:ARG:HH11	2.20	0.54
2:D:404:ALA:HB1	2:D:405:ALA:CA	2.22	0.54
1:B:44:LYS:HA	1:B:57:TRP:CZ3	2.43	0.54
1:C:4:LEU:HD11	1:C:41:ILE:HD11	1.90	0.54
1:A:181:ASN:HB3	1:A:184:THR:CG2	2.38	0.53
1:C:202:TYR:OH	1:C:204:SER:HB3	2.08	0.53
1:C:23:ALA:HA	1:C:25:ALA:C	2.27	0.53
1:B:27:ARG:HH11	1:B:27:ARG:CG	2.21	0.53
1:A:40:LYS:NZ	1:A:75:ARG:NH1	2.56	0.53
1:C:16:ARG:NH1	1:C:16:ARG:HG3	2.24	0.53
1:C:181:ASN:OD1	1:C:183:THR:HG22	2.08	0.53
1:C:148:ASP:CG	1:C:149:ASN:N	2.61	0.53
1:C:187:HIS:HD2	1:C:188:GLN:H	1.55	0.53
1:C:61:GLN:NE2	1:C:61:GLN:N	2.56	0.53
1:B:23:ALA:C	1:B:25:ALA:N	2.61	0.53
1:B:41:ILE:HG13	1:B:42:GLY:N	2.24	0.53
1:C:198:HIS:HD2	1:C:199:ASP:CA	2.22	0.53
1:B:306:HIS:CD2	1:C:57:TRP:CD1	2.97	0.53
1:C:60:GLU:HB3	1:C:75:ARG:HB3	1.91	0.53
1:C:75:ARG:O	1:C:92:ARG:HG2	2.09	0.53
1:A:16:ARG:HG3	1:A:16:ARG:HH11	1.73	0.53
1:C:116:SER:O	1:C:119:ALA:N	2.42	0.53
1:C:142:VAL:HG13	1:C:160:ALA:CB	2.39	0.53
1:C:235:ARG:NH2	1:C:272:ASP:OD2	2.40	0.53
1:A:177:TYR:OH	1:A:186:LYS:HD3	2.09	0.53
1:B:90:VAL:HG22	1:B:91:GLY:N	2.24	0.53
1:B:61:GLN:N	1:B:61:GLN:CD	2.63	0.52
1:C:16:ARG:HG3	1:C:16:ARG:HH11	1.73	0.52
1:A:183:THR:C	1:A:184:THR:HG22	2.30	0.52
1:B:162:PHE:C	1:B:163:ASN:ND2	2.62	0.52
1:B:60:GLU:CD	1:B:75:ARG:HG3	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:HD2	1:A:188:GLN:N	2.07	0.52
1:B:49:LEU:N	1:B:50:GLY:CA	2.67	0.52
1:C:142:VAL:CG1	1:C:160:ALA:HB2	2.39	0.52
1:C:162:PHE:C	1:C:163:ASN:HD22	2.09	0.52
1:C:61:GLN:CD	1:C:61:GLN:N	2.63	0.52
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.25	0.52
1:C:115:LEU:HD21	1:C:244:SER:HB2	1.91	0.52
1:A:57:TRP:CE3	1:C:8:ILE:HD12	2.43	0.52
1:A:21:HIS:HB2	1:A:25:ALA:CB	2.40	0.52
1:A:235:ARG:NH2	1:A:272:ASP:OD2	2.42	0.52
1:B:53:LEU:HD21	1:B:81:LEU:HD13	1.92	0.52
1:B:236:PHE:O	1:B:237:GLY:C	2.47	0.52
1:A:124:ARG:NH2	3:A:400:ATP:HN61	2.07	0.52
1:A:288:LYS:HB3	1:A:295:PHE:HB3	1.91	0.52
1:B:286:LEU:C	1:B:286:LEU:HD23	2.31	0.52
1:B:124:ARG:HH11	1:B:124:ARG:HB2	1.75	0.52
1:B:163:ASN:N	1:B:163:ASN:HD22	2.06	0.52
1:B:27:ARG:HB3	1:B:27:ARG:CZ	2.38	0.52
1:C:201:LEU:HD12	1:C:202:TYR:N	2.25	0.52
1:A:100:THR:O	1:A:102:ASN:N	2.43	0.51
1:A:183:THR:O	1:A:184:THR:HG22	2.10	0.51
1:A:302:VAL:CG1	1:A:303:GLY:N	2.72	0.51
1:B:193:VAL:HG22	1:B:206:ALA:HB2	1.92	0.51
1:A:148:ASP:CG	1:A:149:ASN:N	2.64	0.51
1:B:267:VAL:HG12	1:B:268:GLY:N	2.25	0.51
1:B:44:LYS:HD2	1:B:58:GLN:HG3	1.92	0.51
1:B:81:LEU:O	1:B:87:LYS:HA	2.10	0.51
1:A:44:LYS:HA	1:A:57:TRP:CZ3	2.45	0.51
1:A:71:GLY:O	1:B:72:TRP:NE1	2.39	0.51
1:B:129:ARG:NE	1:B:131:ASP:OD2	2.42	0.51
1:B:208:GLN:NE2	1:B:227:GLU:OE1	2.42	0.51
1:B:215:THR:O	1:B:216:TRP:C	2.49	0.51
2:D:405:ALA:O	2:D:407:ALA:N	2.43	0.51
1:B:107:GLU:HG3	1:B:280:LEU:HD13	1.92	0.51
1:B:112:TYR:HD1	1:B:112:TYR:H	1.58	0.51
1:C:27:ARG:CZ	1:C:27:ARG:HB3	2.39	0.51
1:C:53:LEU:HD21	1:C:81:LEU:HD13	1.93	0.51
1:B:74:ASN:HB2	4:B:402:PO4:O3	2.11	0.51
1:B:40:LYS:HD2	1:B:60:GLU:OE2	2.11	0.51
1:C:302:VAL:CG1	1:C:303:GLY:N	2.73	0.51
1:A:60:GLU:CD	1:A:75:ARG:HG3	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG22	1:B:206:ALA:CB	2.40	0.51
1:B:55:ALA:HA	1:B:81:LEU:CD2	2.40	0.51
1:C:21:HIS:HB2	1:C:23:ALA:CA	2.37	0.51
1:A:18:VAL:HG13	1:A:27:ARG:HD3	1.92	0.51
1:B:107:GLU:OE2	1:B:305:ARG:HD3	2.11	0.51
1:A:112:TYR:CD2	1:A:116:SER:HB2	2.46	0.50
1:A:124:ARG:NH2	3:A:400:ATP:N6	2.57	0.50
1:C:107:GLU:HG3	1:C:280:LEU:HD13	1.91	0.50
1:B:100:THR:OG1	1:B:101:GLY:N	2.44	0.50
1:B:53:LEU:HD12	1:B:82:LYS:O	2.11	0.50
1:B:93:LEU:O	1:B:124:ARG:HA	2.12	0.50
1:B:8:ILE:HD12	1:C:57:TRP:CE3	2.47	0.50
1:C:193:VAL:HG22	1:C:206:ALA:CB	2.41	0.50
1:A:124:ARG:HB2	1:A:124:ARG:HH11	1.76	0.50
1:A:5:TYR:CE1	1:A:42:GLY:C	2.85	0.50
1:A:61:GLN:N	1:A:61:GLN:CD	2.65	0.50
1:C:24:GLN:O	1:C:24:GLN:HG3	2.11	0.50
1:C:302:VAL:CG1	1:C:303:GLY:H	2.24	0.50
1:C:236:PHE:O	1:C:237:GLY:C	2.49	0.50
1:A:124:ARG:HH22	3:A:400:ATP:HN61	1.58	0.50
1:C:112:TYR:CD2	1:C:116:SER:HB2	2.46	0.50
1:A:96:ILE:HD11	1:A:143:GLN:HG3	1.94	0.50
1:B:145:VAL:O	1:B:145:VAL:HG12	2.11	0.50
1:B:29:LYS:HD3	1:C:151:GLY:N	2.17	0.50
1:B:276:ARG:HD3	1:B:306:HIS:CE1	2.46	0.50
1:A:235:ARG:O	1:A:236:PHE:HD1	1.93	0.50
1:B:36:ASP:CG	1:B:39:SER:HB2	2.31	0.50
1:C:129:ARG:NE	1:C:131:ASP:OD2	2.44	0.50
1:A:116:SER:O	1:A:119:ALA:N	2.44	0.49
1:A:5:TYR:CE1	1:A:42:GLY:CA	2.93	0.49
1:B:166:ASN:O	1:B:169:PHE:CB	2.60	0.49
1:B:10:ALA:O	1:B:303:GLY:HA2	2.12	0.49
1:B:278:SER:O	1:B:304:LEU:HD12	2.12	0.49
1:B:75:ARG:O	1:B:92:ARG:HG2	2.12	0.49
1:A:53:LEU:HD21	1:A:81:LEU:HD13	1.94	0.49
1:B:222:HIS:O	1:B:253:VAL:HG21	2.12	0.49
1:C:193:VAL:HG22	1:C:206:ALA:HB2	1.94	0.49
1:A:250:LYS:HB3	1:A:260:ASN:N	2.15	0.49
1:A:81:LEU:O	1:A:87:LYS:HA	2.11	0.49
1:A:181:ASN:CB	1:A:184:THR:HG23	2.42	0.49
1:A:40:LYS:HA	1:A:63:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:HA	1:C:63:ALA:H	1.78	0.49
1:A:34:ILE:HD12	1:B:127:SER:HA	1.93	0.49
1:B:96:ILE:HG13	1:B:159:HIS:CB	2.32	0.49
1:C:60:GLU:CD	1:C:75:ARG:HG3	2.33	0.49
1:C:265:VAL:HG23	1:C:266:VAL:N	2.27	0.49
1:A:276:ARG:HH22	2:D:406:ALA:HB2	1.78	0.49
1:B:100:THR:O	1:B:102:ASN:N	2.46	0.49
1:C:270:GLU:OE2	1:C:280:LEU:HD22	2.12	0.49
1:B:270:GLU:OE2	1:B:280:LEU:HD22	2.13	0.49
1:C:189:VAL:HG22	1:C:210:GLN:CG	2.43	0.49
1:A:253:VAL:O	1:A:256:ALA:N	2.45	0.49
1:C:177:TYR:OH	1:C:186:LYS:HD3	2.12	0.49
1:A:229:ALA:HA	1:A:245:TYR:O	2.13	0.48
1:A:275:LYS:CG	1:A:276:ARG:H	2.25	0.48
1:B:16:ARG:HH11	1:B:16:ARG:HG3	1.77	0.48
1:B:16:ARG:NH1	1:B:16:ARG:HG3	2.27	0.48
1:C:240:THR:HB	1:C:270:GLU:HB2	1.94	0.48
1:A:27:ARG:CG	1:A:27:ARG:HH11	2.23	0.48
1:A:10:ALA:O	1:A:303:GLY:HA2	2.14	0.48
1:A:184:THR:OG1	1:A:185:GLU:N	2.45	0.48
1:B:34:ILE:HD12	1:C:127:SER:HA	1.95	0.48
1:C:111:TYR:HD1	1:C:299:VAL:HG21	1.78	0.48
1:A:190:HIS:O	1:A:208:GLN:HA	2.13	0.48
1:A:39:SER:HB3	1:A:63:ALA:O	2.14	0.48
1:B:116:SER:O	1:B:119:ALA:N	2.45	0.48
1:B:202:TYR:OH	1:B:204:SER:HB3	2.13	0.48
1:C:304:LEU:HA	1:C:304:LEU:HD12	1.37	0.48
1:B:111:TYR:CD1	1:B:299:VAL:HG21	2.49	0.48
1:B:77:SER:O	1:B:92:ARG:O	2.32	0.48
1:A:222:HIS:C	1:A:222:HIS:ND1	2.67	0.48
1:B:40:LYS:CE	1:B:75:ARG:NH2	2.74	0.48
1:C:21:HIS:CB	1:C:23:ALA:H	2.27	0.48
1:A:138:PHE:HE1	1:A:162:PHE:CD2	2.32	0.48
1:A:282:SER:O	1:A:300:GLY:HA2	2.13	0.48
1:C:129:ARG:HD3	1:C:143:GLN:OE1	2.14	0.48
1:C:146:PRO:HD2	1:C:147:ASN:ND2	2.28	0.48
1:A:248:GLY:HA3	1:A:262:TYR:CE2	2.49	0.48
1:B:234:TYR:O	1:B:240:THR:HA	2.14	0.48
1:B:96:ILE:HG21	1:B:161:GLY:N	2.28	0.48
1:B:177:TYR:OH	1:B:186:LYS:HD3	2.13	0.48
1:B:190:HIS:O	1:B:208:GLN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:CD1	1:C:127:SER:HA	2.44	0.48
1:A:96:ILE:HG21	1:A:161:GLY:N	2.29	0.47
1:A:193:VAL:HG22	1:A:206:ALA:HB2	1.96	0.47
1:A:279:ALA:HA	1:A:304:LEU:CD1	2.44	0.47
1:B:243:VAL:HB	1:B:267:VAL:HG22	1.96	0.47
1:C:81:LEU:O	1:C:87:LYS:HA	2.13	0.47
1:A:27:ARG:CZ	1:A:27:ARG:HB3	2.44	0.47
1:B:138:PHE:HE1	1:B:162:PHE:CD2	2.32	0.47
1:B:181:ASN:O	1:B:184:THR:O	2.32	0.47
1:B:230:THR:O	1:B:244:SER:HA	2.14	0.47
1:B:289:GLY:C	1:B:290:LYS:HG2	2.35	0.47
1:B:60:GLU:OE1	1:B:75:ARG:HG3	2.14	0.47
1:C:262:TYR:C	1:C:262:TYR:CD1	2.87	0.47
1:A:170:PHE:HE2	1:A:193:VAL:HG12	1.77	0.47
1:A:276:ARG:NH2	2:D:406:ALA:HB2	2.29	0.47
1:A:9:LYS:HG2	1:A:305:ARG:HG3	1.96	0.47
1:B:265:VAL:HG23	1:B:266:VAL:N	2.29	0.47
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.51	0.47
1:C:112:TYR:N	1:C:112:TYR:CD1	2.63	0.47
1:C:248:GLY:HA3	1:C:262:TYR:CE2	2.49	0.47
1:C:25:ALA:HA	1:C:26:ASP:CG	2.35	0.47
1:A:178:LYS:CE	1:A:187:HIS:HB3	2.42	0.47
1:B:248:GLY:HA3	1:B:262:TYR:CE2	2.49	0.47
1:C:138:PHE:HE1	1:C:162:PHE:CD2	2.32	0.47
1:B:146:PRO:HD2	1:B:147:ASN:ND2	2.29	0.47
1:C:115:LEU:HD21	1:C:244:SER:CB	2.44	0.47
1:A:187:HIS:HD2	1:A:188:GLN:H	1.62	0.47
1:C:145:VAL:O	1:C:156:GLU:HA	2.14	0.47
1:C:23:ALA:O	1:C:25:ALA:HB3	2.14	0.47
1:C:276:ARG:HG3	1:C:276:ARG:HH11	1.78	0.47
1:A:75:ARG:HA	1:A:75:ARG:HD3	1.17	0.47
1:B:177:TYR:CD1	1:B:188:GLN:HG2	2.37	0.47
1:B:235:ARG:NH2	1:B:272:ASP:OD2	2.47	0.47
1:C:275:LYS:HB3	1:C:275:LYS:HE2	1.44	0.47
1:A:252:SER:HA	1:A:257:ASP:OD1	2.15	0.47
1:A:267:VAL:HG12	1:A:268:GLY:N	2.30	0.47
1:B:147:ASN:HA	1:B:148:ASP:HA	1.43	0.47
1:C:218:ASP:HB3	1:C:221:SER:CB	2.45	0.47
1:A:16:ARG:HG3	1:A:17:SER:N	2.30	0.47
1:A:275:LYS:HB3	1:A:275:LYS:HE2	1.44	0.47
1:B:154:ARG:O	1:B:180:HIS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:TYR:OH	1:C:190:HIS:ND1	2.42	0.47
1:A:100:THR:OG1	1:A:101:GLY:N	2.47	0.46
1:B:184:THR:HG22	1:B:187:HIS:HB2	1.97	0.46
1:A:159:HIS:CE1	1:A:176:SER:HB2	2.49	0.46
1:A:115:LEU:HD21	1:A:244:SER:CB	2.45	0.46
1:B:96:ILE:HD11	1:B:143:GLN:HG3	1.97	0.46
1:A:240:THR:HB	1:A:270:GLU:HB2	1.97	0.46
1:B:130:TYR:O	1:B:141:SER:HA	2.14	0.46
1:C:222:HIS:ND1	1:C:222:HIS:C	2.68	0.46
1:C:40:LYS:HD2	1:C:60:GLU:OE2	2.15	0.46
2:D:402:ALA:O	2:F:406:ALA:CB	2.50	0.46
1:A:286:LEU:HD23	1:A:287:GLN:N	2.30	0.46
1:B:240:THR:HG22	1:B:242:ARG:HH12	1.81	0.46
1:C:129:ARG:HB2	1:C:143:GLN:HG2	1.97	0.46
1:C:16:ARG:HB2	1:C:30:THR:HG22	1.96	0.46
1:A:154:ARG:O	1:A:180:HIS:HB2	2.16	0.46
1:A:275:LYS:HG2	1:A:276:ARG:H	1.80	0.46
1:A:111:TYR:HD1	1:A:299:VAL:HG21	1.81	0.46
1:A:302:VAL:CG1	1:A:303:GLY:H	2.27	0.46
1:B:282:SER:O	1:B:300:GLY:HA2	2.15	0.46
1:B:43:PHE:C	1:B:44:LYS:HG2	2.36	0.46
1:C:93:LEU:O	1:C:124:ARG:HA	2.15	0.46
1:C:288:LYS:HB3	1:C:295:PHE:HB3	1.97	0.46
1:A:22:GLY:N	1:A:292:ALA:O	2.48	0.46
1:B:259:ASP:HB3	1:B:261:THR:CG2	2.43	0.46
1:B:276:ARG:HG3	1:B:276:ARG:HH11	1.79	0.46
1:A:147:ASN:ND2	1:A:147:ASN:H	2.14	0.46
1:B:213:LYS:HD2	1:B:213:LYS:HA	1.65	0.46
1:C:145:VAL:O	1:C:145:VAL:HG12	2.15	0.46
1:A:178:LYS:NZ	1:A:181:ASN:ND2	2.62	0.46
1:C:130:TYR:O	1:C:141:SER:HA	2.15	0.46
1:A:146:PRO:HD2	1:A:147:ASN:ND2	2.30	0.46
1:A:166:ASN:O	1:A:169:PHE:HB2	2.15	0.46
2:D:400:ALA:HA	2:D:401:ALA:C	2.35	0.46
1:A:21:HIS:HB2	1:A:26:ASP:N	2.31	0.45
1:A:289:GLY:C	1:A:290:LYS:HG2	2.36	0.45
1:B:222:HIS:ND1	1:B:222:HIS:C	2.69	0.45
1:C:23:ALA:C	1:C:25:ALA:HB3	2.37	0.45
1:C:289:GLY:C	1:C:290:LYS:HG2	2.35	0.45
1:C:40:LYS:NZ	1:C:75:ARG:NH1	2.65	0.45
1:A:46:GLN:CA	1:A:55:ALA:O	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TRP:CD1	1:C:306:HIS:CD2	3.04	0.45
1:B:29:LYS:HB3	1:B:29:LYS:HE3	1.77	0.45
1:B:97:LEU:HD21	1:B:189:VAL:HG12	1.98	0.45
1:C:213:LYS:HD2	1:C:213:LYS:HA	1.70	0.45
1:A:166:ASN:O	1:A:169:PHE:CB	2.64	0.45
1:A:250:LYS:CG	1:A:251:GLY:H	2.28	0.45
1:B:97:LEU:CD2	1:B:189:VAL:HG12	2.46	0.45
1:B:240:THR:HB	1:B:270:GLU:HB2	1.99	0.45
2:E:408:ALA:C	2:F:402:ALA:HB2	2.37	0.45
1:A:94:ASN:O	1:A:143:GLN:OE1	2.35	0.45
1:A:230:THR:O	1:A:244:SER:HA	2.16	0.45
1:A:262:TYR:CD1	1:A:262:TYR:C	2.89	0.45
1:A:276:ARG:CD	1:A:306:HIS:CE1	2.98	0.45
1:A:75:ARG:HH22	3:A:400:ATP:H2'	1.81	0.45
1:B:115:LEU:HD21	1:B:244:SER:CB	2.47	0.45
1:C:44:LYS:HD2	1:C:58:GLN:HG3	1.99	0.45
1:A:193:VAL:HG22	1:A:206:ALA:CB	2.47	0.45
1:B:145:VAL:O	1:B:156:GLU:HA	2.15	0.45
1:B:80:GLY:HA3	1:B:88:VAL:O	2.16	0.45
1:B:70:THR:CG2	1:C:70:THR:HG22	2.46	0.45
1:A:213:LYS:HD2	1:A:213:LYS:HA	1.64	0.45
1:B:218:ASP:HB3	1:B:221:SER:CB	2.47	0.45
1:C:48:ASP:OD1	1:C:49:LEU:N	2.43	0.45
1:C:5:TYR:CE1	1:C:42:GLY:CA	2.99	0.45
1:C:85:PHE:H	1:C:85:PHE:HD1	1.62	0.45
1:C:90:VAL:CG2	1:C:91:GLY:N	2.79	0.45
1:B:262:TYR:CD1	1:B:262:TYR:C	2.90	0.45
1:C:229:ALA:HA	1:C:245:TYR:O	2.17	0.45
1:C:171:VAL:HG23	1:C:193:VAL:O	2.17	0.45
1:C:21:HIS:HB2	1:C:23:ALA:N	2.30	0.45
1:C:5:TYR:CE1	1:C:42:GLY:C	2.90	0.45
1:B:27:ARG:NH1	1:B:27:ARG:CG	2.79	0.44
1:A:145:VAL:HG12	1:A:145:VAL:O	2.15	0.44
1:A:196:TYR:CE1	1:A:198:HIS:HB3	2.53	0.44
1:B:201:LEU:HD12	1:B:202:TYR:N	2.33	0.44
1:B:5:TYR:CD1	1:B:42:GLY:O	2.70	0.44
1:C:124:ARG:HB2	1:C:124:ARG:HH11	1.81	0.44
1:A:236:PHE:O	1:A:237:GLY:C	2.55	0.44
1:B:104:ASN:N	1:B:105:PRO:HD3	2.32	0.44
1:C:198:HIS:CD2	1:C:199:ASP:H	2.34	0.44
1:C:27:ARG:CG	1:C:27:ARG:NH1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:HG22	1:C:91:GLY:N	2.32	0.44
1:A:171:VAL:HG23	1:A:193:VAL:O	2.17	0.44
1:C:154:ARG:O	1:C:180:HIS:HB2	2.18	0.44
1:A:147:ASN:HA	1:A:148:ASP:HA	1.61	0.44
1:A:29:LYS:HD3	1:B:151:GLY:N	2.24	0.44
1:B:75:ARG:HH22	3:B:400:ATP:H8	0.50	0.44
1:C:100:THR:O	1:C:102:ASN:N	2.50	0.44
1:C:210:GLN:NE2	1:C:225:GLN:HE21	2.16	0.44
1:C:75:ARG:HA	1:C:75:ARG:HD3	1.18	0.44
1:A:129:ARG:NE	1:A:131:ASP:OD2	2.47	0.44
1:A:254:TYR:O	1:A:255:ASP:CB	2.65	0.44
1:A:90:VAL:CG2	1:A:91:GLY:H	2.30	0.44
1:A:9:LYS:HB3	1:A:305:ARG:CB	2.47	0.44
1:A:130:TYR:O	1:A:141:SER:HA	2.17	0.44
1:A:41:ILE:HG13	1:A:42:GLY:N	2.33	0.44
1:B:48:ASP:C	1:B:50:GLY:HA3	2.38	0.44
1:A:170:PHE:CE2	1:A:193:VAL:CG1	3.00	0.44
1:C:279:ALA:HA	1:C:304:LEU:CD1	2.48	0.44
1:C:48:ASP:C	1:C:50:GLY:HA3	2.35	0.44
1:A:145:VAL:O	1:A:156:GLU:HA	2.18	0.44
1:A:159:HIS:ND1	1:A:176:SER:HB2	2.32	0.44
1:A:259:ASP:HB3	1:A:261:THR:CG2	2.44	0.44
1:A:275:LYS:CG	1:A:276:ARG:N	2.81	0.44
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.44	0.44
1:B:159:HIS:CE1	1:B:176:SER:HB2	2.53	0.44
1:A:83:GLY:O	1:A:84:GLY:C	2.56	0.43
1:B:150:SER:HA	1:B:151:GLY:C	2.38	0.43
1:C:259:ASP:HB3	1:C:261:THR:CG2	2.47	0.43
1:C:43:PHE:C	1:C:44:LYS:HG2	2.37	0.43
1:C:44:LYS:HB3	1:C:58:GLN:CA	2.45	0.43
1:A:196:TYR:CZ	1:A:198:HIS:HB3	2.54	0.43
1:A:48:ASP:C	1:A:50:GLY:HA3	2.38	0.43
1:A:60:GLU:HB3	1:A:75:ARG:HB3	2.00	0.43
1:A:74:ASN:O	4:A:402:PO4:O2	2.36	0.43
1:B:146:PRO:O	1:B:148:ASP:HA	2.17	0.43
1:B:85:PHE:H	1:B:85:PHE:HD1	1.66	0.43
1:C:164:TYR:O	1:C:170:PHE:HA	2.17	0.43
1:C:43:PHE:N	1:C:43:PHE:CD1	2.85	0.43
1:A:96:ILE:HG21	1:A:160:ALA:C	2.39	0.43
1:A:48:ASP:OD1	1:A:49:LEU:N	2.48	0.43
1:A:53:LEU:HD12	1:A:82:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:N	1:B:61:GLN:NE2	2.65	0.43
1:C:80:GLY:HA3	1:C:88:VAL:O	2.19	0.43
1:A:118:ILE:HG13	1:A:227:GLU:HB3	2.00	0.43
1:A:146:PRO:O	1:A:148:ASP:HA	2.18	0.43
1:A:96:ILE:CG1	1:A:159:HIS:HB3	2.30	0.43
1:B:90:VAL:CG2	1:B:91:GLY:H	2.31	0.43
1:C:282:SER:O	1:C:300:GLY:HA2	2.18	0.43
1:C:296:VAL:HG12	1:C:297:ALA:N	2.32	0.43
1:C:97:LEU:HD21	1:C:189:VAL:HG12	2.01	0.43
1:A:9:LYS:HD2	1:A:37:LEU:O	2.19	0.43
1:B:275:LYS:HB3	1:B:275:LYS:HE2	1.44	0.43
1:B:279:ALA:HA	1:B:304:LEU:CD1	2.49	0.43
1:C:275:LYS:HG2	1:C:276:ARG:H	1.83	0.43
1:A:61:GLN:N	1:A:61:GLN:NE2	2.67	0.43
1:B:275:LYS:HG2	1:B:276:ARG:H	1.83	0.43
1:A:234:TYR:O	1:A:240:THR:HA	2.19	0.43
1:A:82:LYS:HB3	1:A:87:LYS:HG2	2.00	0.43
1:B:16:ARG:HB2	1:B:30:THR:HG22	2.00	0.43
1:B:40:LYS:HA	1:B:63:ALA:H	1.83	0.43
1:B:39:SER:HB3	1:B:63:ALA:O	2.19	0.43
1:B:158:TYR:HA	1:B:158:TYR:HD1	1.61	0.43
1:B:83:GLY:O	1:B:84:GLY:C	2.56	0.43
1:C:141:SER:O	1:C:160:ALA:HB1	2.18	0.43
1:C:275:LYS:CG	1:C:276:ARG:H	2.32	0.43
1:C:276:ARG:HD3	1:C:306:HIS:CE1	2.54	0.43
1:B:5:TYR:OH	1:B:60:GLU:HB2	2.18	0.43
1:C:46:GLN:CA	1:C:55:ALA:O	2.54	0.43
1:A:124:ARG:HH12	4:A:402:PO4:P	2.42	0.42
1:A:44:LYS:CD	1:A:58:GLN:HE21	2.16	0.42
1:A:187:HIS:CD2	1:A:187:HIS:C	2.93	0.42
1:C:159:HIS:CE1	1:C:176:SER:HB2	2.53	0.42
1:C:124:ARG:NH2	3:C:400:ATP:N7	2.60	0.42
1:B:82:LYS:HB3	1:B:87:LYS:HG2	2.01	0.42
1:C:211:ASP:OD1	1:C:224:SER:OG	2.34	0.42
1:A:129:ARG:HA	1:A:142:VAL:O	2.19	0.42
1:A:149:ASN:HB3	1:A:154:ARG:HA	2.02	0.42
1:A:170:PHE:HE2	1:A:193:VAL:CG1	2.31	0.42
1:A:21:HIS:CB	1:A:26:ASP:H	2.32	0.42
1:B:44:LYS:CD	1:B:58:GLN:HE21	2.20	0.42
1:C:15:SER:HB2	1:C:299:VAL:HG22	2.00	0.42
1:C:240:THR:HG22	1:C:242:ARG:HH12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:O	1:A:160:ALA:HB1	2.18	0.42
1:A:191:ARG:HE	1:A:191:ARG:HB2	1.63	0.42
1:B:46:GLN:CA	1:B:55:ALA:O	2.58	0.42
1:A:296:VAL:HG12	1:A:297:ALA:N	2.35	0.42
1:A:61:GLN:HB3	1:A:73:GLY:N	2.35	0.42
1:C:118:ILE:HG13	1:C:227:GLU:HB3	2.02	0.42
1:A:44:LYS:HD2	1:A:58:GLN:HG3	2.02	0.42
1:B:252:SER:C	1:B:253:VAL:HG22	2.39	0.42
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.83	0.42
1:B:34:ILE:HG13	1:C:146:PRO:HG2	2.02	0.42
1:C:60:GLU:OE1	1:C:75:ARG:HG3	2.20	0.42
1:A:41:ILE:HG23	1:A:61:GLN:HE21	1.85	0.42
1:B:118:ILE:HG13	1:B:227:GLU:HB3	2.02	0.42
1:B:28:VAL:CG2	1:B:29:LYS:N	2.77	0.42
1:A:44:LYS:HB3	1:A:58:GLN:CB	2.50	0.42
1:B:44:LYS:HD2	1:B:58:GLN:CG	2.50	0.42
1:C:165:LYS:HE3	1:C:168:GLY:HA2	2.02	0.42
1:B:164:TYR:O	1:B:170:PHE:HA	2.21	0.41
1:B:183:THR:O	1:B:214:LEU:CD2	2.68	0.41
1:B:191:ARG:HE	1:B:191:ARG:HB2	1.57	0.41
1:C:10:ALA:O	1:C:303:GLY:HA2	2.19	0.41
2:F:406:ALA:O	2:F:407:ALA:HB2	2.20	0.41
1:A:60:GLU:OE1	1:A:75:ARG:HG3	2.20	0.41
1:C:149:ASN:HB3	1:C:154:ARG:HA	2.02	0.41
1:A:44:LYS:HB3	1:A:58:GLN:CG	2.48	0.41
1:B:229:ALA:HA	1:B:245:TYR:O	2.20	0.41
1:C:158:TYR:HD1	1:C:158:TYR:HA	1.65	0.41
1:A:149:ASN:CB	1:A:155:SER:H	2.34	0.41
1:A:124:ARG:NH1	4:A:402:PO4:O2	2.53	0.41
2:D:401:ALA:CB	2:F:407:ALA:HB3	2.50	0.41
1:A:104:ASN:N	1:A:105:PRO:HD3	2.35	0.41
1:B:170:PHE:HE2	1:B:193:VAL:HG12	1.83	0.41
1:B:163:ASN:ND2	4:B:401:PO4:O4	2.51	0.41
1:B:129:ARG:HA	1:B:142:VAL:O	2.20	0.41
1:B:288:LYS:HB3	1:B:295:PHE:HB3	2.02	0.41
1:C:238:ASN:HB2	1:C:271:TYR:HE1	1.82	0.41
1:C:5:TYR:OH	1:C:58:GLN:NE2	2.54	0.41
1:A:178:LYS:HG2	1:A:178:LYS:O	2.21	0.41
1:A:185:GLU:O	1:A:186:LYS:C	2.59	0.41
1:A:23:ALA:HB1	1:A:24:GLN:OE1	2.21	0.41
1:B:275:LYS:CG	1:B:276:ARG:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:THR:HB	1:C:187:HIS:HB2	2.03	0.41
1:C:83:GLY:O	1:C:84:GLY:C	2.59	0.41
1:A:9:LYS:CA	1:A:304:LEU:O	2.61	0.41
1:A:40:LYS:HZ3	1:A:75:ARG:NH1	2.18	0.41
1:A:90:VAL:CG2	1:C:34:ILE:HG21	2.51	0.41
1:B:173:TYR:OH	1:B:190:HIS:ND1	2.40	0.41
1:C:190:HIS:O	1:C:208:GLN:HA	2.21	0.41
1:C:276:ARG:HG2	1:C:276:ARG:HH11	1.82	0.41
1:C:9:LYS:HB3	1:C:305:ARG:CB	2.46	0.41
1:B:10:ALA:HA	1:B:37:LEU:HG	2.03	0.41
1:B:10:ALA:O	1:B:303:GLY:CA	2.69	0.41
1:B:97:LEU:CD2	1:B:189:VAL:CG1	2.99	0.41
1:C:61:GLN:H	1:C:61:GLN:NE2	2.17	0.41
1:C:78:PHE:C	1:C:78:PHE:CD1	2.94	0.41
1:B:222:HIS:O	1:B:253:VAL:HG11	2.21	0.41
1:A:97:LEU:HD11	1:A:176:SER:CB	2.51	0.41
1:C:104:ASN:N	1:C:105:PRO:HD3	2.36	0.41
1:C:181:ASN:OD1	1:C:182:TYR:O	2.39	0.41
1:B:112:TYR:CD2	1:B:116:SER:HB2	2.56	0.40
1:B:189:VAL:HG22	1:B:210:GLN:CG	2.50	0.40
1:B:196:TYR:CZ	1:B:198:HIS:HB3	2.56	0.40
1:B:40:LYS:HE2	1:B:75:ARG:HH21	1.83	0.40
1:B:48:ASP:OD1	1:B:49:LEU:N	2.44	0.40
1:A:93:LEU:O	1:A:124:ARG:HA	2.21	0.40
1:A:150:SER:HA	1:A:151:GLY:C	2.41	0.40
1:A:210:GLN:NE2	1:A:225:GLN:HE21	2.19	0.40
2:E:407:ALA:O	2:E:408:ALA:C	2.60	0.40
1:A:276:ARG:NH1	1:A:276:ARG:CG	2.71	0.40
1:A:16:ARG:NH2	1:A:27:ARG:NH1	2.68	0.40
1:A:44:LYS:HB3	1:A:58:GLN:CA	2.47	0.40
1:A:40:LYS:HZ1	1:A:75:ARG:NH1	2.19	0.40
1:B:187:HIS:C	1:B:187:HIS:CD2	2.94	0.40
1:C:196:TYR:CZ	1:C:198:HIS:HB3	2.57	0.40
1:A:192:LEU:N	1:A:192:LEU:HD12	2.37	0.40
1:A:16:ARG:HH22	1:A:27:ARG:HH11	1.68	0.40
1:B:170:PHE:HE2	1:B:193:VAL:CG1	2.35	0.40
1:C:100:THR:OG1	1:C:101:GLY:N	2.53	0.40
1:C:147:ASN:HA	1:C:148:ASP:HA	1.49	0.40
1:A:134:GLU:HA	1:A:138:PHE:O	2.22	0.40
1:C:23:ALA:O	1:C:24:GLN:HB3	2.22	0.40
1:C:23:ALA:CB	1:C:25:ALA:O	2.69	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLY:O	1:B:112:TYR:OH[2_656]	1.86	0.34
1:A:255:ASP:O	1:C:147:ASN:O[2_656]	2.03	0.17
1:A:255:ASP:O	1:C:148:ASP:N[2_656]	2.09	0.11
1:A:84:GLY:O	1:B:158:TYR:OH[4_546]	2.11	0.09
1:B:153:ASN:ND2	1:B:180:HIS:CE1[2_656]	2.13	0.07
1:B:51:ASN:OD1	1:C:24:GLN:N[3_455]	2.17	0.03

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	306/327 (94%)	277 (90%)	27 (9%)	2 (1%)	22	61
1	B	306/327 (94%)	276 (90%)	26 (8%)	4 (1%)	12	47
1	C	306/327 (94%)	281 (92%)	19 (6%)	6 (2%)	7	38
2	D	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	E	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
2	F	5/8 (62%)	4 (80%)	1 (20%)	0	100	100
All	All	935/1005 (93%)	847 (91%)	75 (8%)	13 (1%)	11	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	TYR
1	B	253	VAL
1	C	253	VAL
1	A	253	VAL
1	C	218	ASP
1	B	186	LYS
1	C	186	LYS

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Mol	Chain	Res	Type
2	E	406	ALA
1	B	28	VAL
1	C	26	ASP
1	C	28	VAL
1	C	216	TRP
1	A	28	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/259 (93%)	183 (76%)	57 (24%)	0	3
1	B	238/259 (92%)	182 (76%)	56 (24%)	1	3
1	C	238/259 (92%)	183 (77%)	55 (23%)	1	3
All	All	716/777 (92%)	548 (76%)	168 (24%)	1	3

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	14	THR
1	A	15	SER
1	A	16	ARG
1	A	17	SER
1	A	21	HIS
1	A	29	LYS
1	A	39	SER
1	A	41	ILE
1	A	43	PHE
1	A	49	LEU
1	A	56	ILE
1	A	68	THR
1	A	70	THR
1	A	75	ARG
1	A	77	SER

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Mol	Chain	Res	Type
1	A	96	ILE
1	A	112	TYR
1	A	118	ILE
1	A	128	VAL
1	A	131	ASP
1	A	135	PHE
1	A	138	PHE
1	A	142	VAL
1	A	147	ASN
1	A	148	ASP
1	A	158	TYR
1	A	162	PHE
1	A	169	PHE
1	A	176	SER
1	A	180	HIS
1	A	183	THR
1	A	184	THR
1	A	204	SER
1	A	208	GLN
1	A	213	LYS
1	A	214	LEU
1	A	215	THR
1	A	222	HIS
1	A	223	ASN
1	A	224	SER
1	A	230	THR
1	A	235	ARG
1	A	236	PHE
1	A	239	VAL
1	A	242	ARG
1	A	243	VAL
1	A	250	LYS
1	A	258	HIS
1	A	261	THR
1	A	265	VAL
1	A	275	LYS
1	A	276	ARG
1	A	277	THR
1	A	280	LEU
1	A	281	VAL
1	A	293	GLU
1	B	9	LYS

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Mol	Chain	Res	Type
1	B	14	THR
1	B	15	SER
1	B	16	ARG
1	B	17	SER
1	B	39	SER
1	B	41	ILE
1	B	43	PHE
1	B	49	LEU
1	B	56	ILE
1	B	61	GLN
1	B	68	THR
1	B	70	THR
1	B	75	ARG
1	B	77	SER
1	B	96	ILE
1	B	112	TYR
1	B	113	SER
1	B	118	ILE
1	B	128	VAL
1	B	135	PHE
1	B	138	PHE
1	B	142	VAL
1	B	147	ASN
1	B	148	ASP
1	B	149	ASN
1	B	158	TYR
1	B	162	PHE
1	B	163	ASN
1	B	169	PHE
1	B	176	SER
1	B	180	HIS
1	B	183	THR
1	B	204	SER
1	B	208	GLN
1	B	213	LYS
1	B	215	THR
1	B	222	HIS
1	B	223	ASN
1	B	224	SER
1	B	230	THR
1	B	235	ARG
1	B	239	VAL

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Mol	Chain	Res	Type
1	B	242	ARG
1	B	243	VAL
1	B	250	LYS
1	B	253	VAL
1	B	258	HIS
1	B	261	THR
1	B	265	VAL
1	B	275	LYS
1	B	276	ARG
1	B	277	THR
1	B	280	LEU
1	B	281	VAL
1	B	293	GLU
1	C	9	LYS
1	C	14	THR
1	C	15	SER
1	C	16	ARG
1	C	17	SER
1	C	29	LYS
1	C	39	SER
1	C	41	ILE
1	C	43	PHE
1	C	49	LEU
1	C	56	ILE
1	C	61	GLN
1	C	68	THR
1	C	70	THR
1	C	75	ARG
1	C	77	SER
1	C	96	ILE
1	C	112	TYR
1	C	118	ILE
1	C	128	VAL
1	C	135	PHE
1	C	138	PHE
1	C	142	VAL
1	C	147	ASN
1	C	148	ASP
1	C	149	ASN
1	C	158	TYR
1	C	162	PHE
1	C	163	ASN

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Mol	Chain	Res	Type
1	C	169	PHE
1	C	176	SER
1	C	180	HIS
1	C	183	THR
1	C	204	SER
1	C	208	GLN
1	C	213	LYS
1	C	218	ASP
1	C	222	HIS
1	C	223	ASN
1	C	224	SER
1	C	235	ARG
1	C	239	VAL
1	C	242	ARG
1	C	243	VAL
1	C	250	LYS
1	C	252	SER
1	C	258	HIS
1	C	261	THR
1	C	265	VAL
1	C	275	LYS
1	C	276	ARG
1	C	277	THR
1	C	280	LEU
1	C	281	VAL
1	C	293	GLU

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	147	ASN
1	A	181	ASN
1	A	187	HIS
1	A	198	HIS
1	A	225	GLN
1	A	264	GLN
1	B	58	GLN
1	B	147	ASN
1	B	181	ASN
1	B	187	HIS
1	B	198	HIS

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Mol	Chain	Res	Type
1	B	225	GLN
1	B	306	HIS
1	C	58	GLN
1	C	147	ASN
1	C	163	ASN
1	C	181	ASN
1	C	187	HIS
1	C	198	HIS
1	C	225	GLN
1	C	264	GLN
1	C	306	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	PO4	B	402	-	4,4,4	0.97	0	6,6,6	0.56	0
4	PO4	C	401	-	4,4,4	0.85	0	6,6,6	0.55	0
3	ATP	C	400	-	26,33,33	1.04	3 (11%)	31,52,52	1.47	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	A	401	-	4,4,4	0.85	0	6,6,6	0.39	0
3	ATP	A	400	5	26,33,33	0.95	2 (7%)	31,52,52	1.64	4 (12%)
3	ATP	B	400	-	26,33,33	1.08	2 (7%)	31,52,52	1.58	8 (25%)
4	PO4	B	401	-	4,4,4	0.90	0	6,6,6	0.67	0
4	PO4	C	402	-	4,4,4	0.88	0	6,6,6	0.56	0
4	PO4	A	402	-	4,4,4	0.91	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	400	-	-	9/18/38/38	0/3/3/3
3	ATP	A	400	5	-	5/18/38/38	0/3/3/3
3	ATP	B	400	-	-	6/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	ATP	C5-C4	2.97	1.48	1.40
3	C	400	ATP	C5-C4	2.69	1.48	1.40
3	A	400	ATP	C5-C4	2.50	1.47	1.40
3	B	400	ATP	C2-N3	2.39	1.35	1.32
3	C	400	ATP	C2-N3	2.17	1.35	1.32
3	A	400	ATP	C2-N3	2.09	1.35	1.32
3	C	400	ATP	O4'-C1'	2.03	1.43	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ATP	PB-O3B-PG	-4.39	117.78	132.83
3	B	400	ATP	C1'-N9-C4	3.87	133.45	126.64
3	A	400	ATP	C3'-C2'-C1'	3.54	106.31	100.98
3	A	400	ATP	C4-C5-N7	-3.48	105.78	109.40
3	C	400	ATP	C3'-C2'-C1'	3.27	105.90	100.98
3	C	400	ATP	C4-C5-N7	-3.13	106.14	109.40
3	A	400	ATP	N3-C2-N1	-3.03	123.95	128.68
3	B	400	ATP	N3-C2-N1	-2.94	124.08	128.68
3	B	400	ATP	N6-C6-N1	2.88	124.56	118.57
3	C	400	ATP	N3-C2-N1	-2.87	124.20	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	ATP	C3'-C2'-C1'	2.78	105.16	100.98
3	B	400	ATP	C4-C5-N7	-2.46	106.83	109.40
3	C	400	ATP	PB-O3B-PG	-2.44	124.44	132.83
3	B	400	ATP	C5-C6-N1	-2.30	115.14	120.35
3	B	400	ATP	C2-N1-C6	2.17	122.47	118.75
3	B	400	ATP	O4'-C1'-C2'	-2.11	103.85	106.93

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	400	ATP	C5'-O5'-PA-O1A
3	C	400	ATP	C5'-O5'-PA-O2A
3	C	400	ATP	C5'-O5'-PA-O3A
3	A	400	ATP	C5'-O5'-PA-O2A
3	A	400	ATP	C5'-O5'-PA-O3A
3	A	400	ATP	O4'-C4'-C5'-O5'
3	A	400	ATP	C3'-C4'-C5'-O5'
3	B	400	ATP	O4'-C4'-C5'-O5'
3	B	400	ATP	PB-O3B-PG-O2G
3	B	400	ATP	C5'-O5'-PA-O3A
3	C	400	ATP	PG-O3B-PB-O1B
3	A	400	ATP	C5'-O5'-PA-O1A
3	B	400	ATP	PB-O3A-PA-O1A
3	B	400	ATP	PB-O3A-PA-O2A
3	C	400	ATP	PB-O3A-PA-O1A
3	B	400	ATP	PB-O3B-PG-O3G
3	C	400	ATP	O4'-C4'-C5'-O5'
3	C	400	ATP	PG-O3B-PB-O2B
3	C	400	ATP	PA-O3A-PB-O2B
3	C	400	ATP	PB-O3A-PA-O2A

There are no ring outliers.

7 monomers are involved in 31 short contacts:

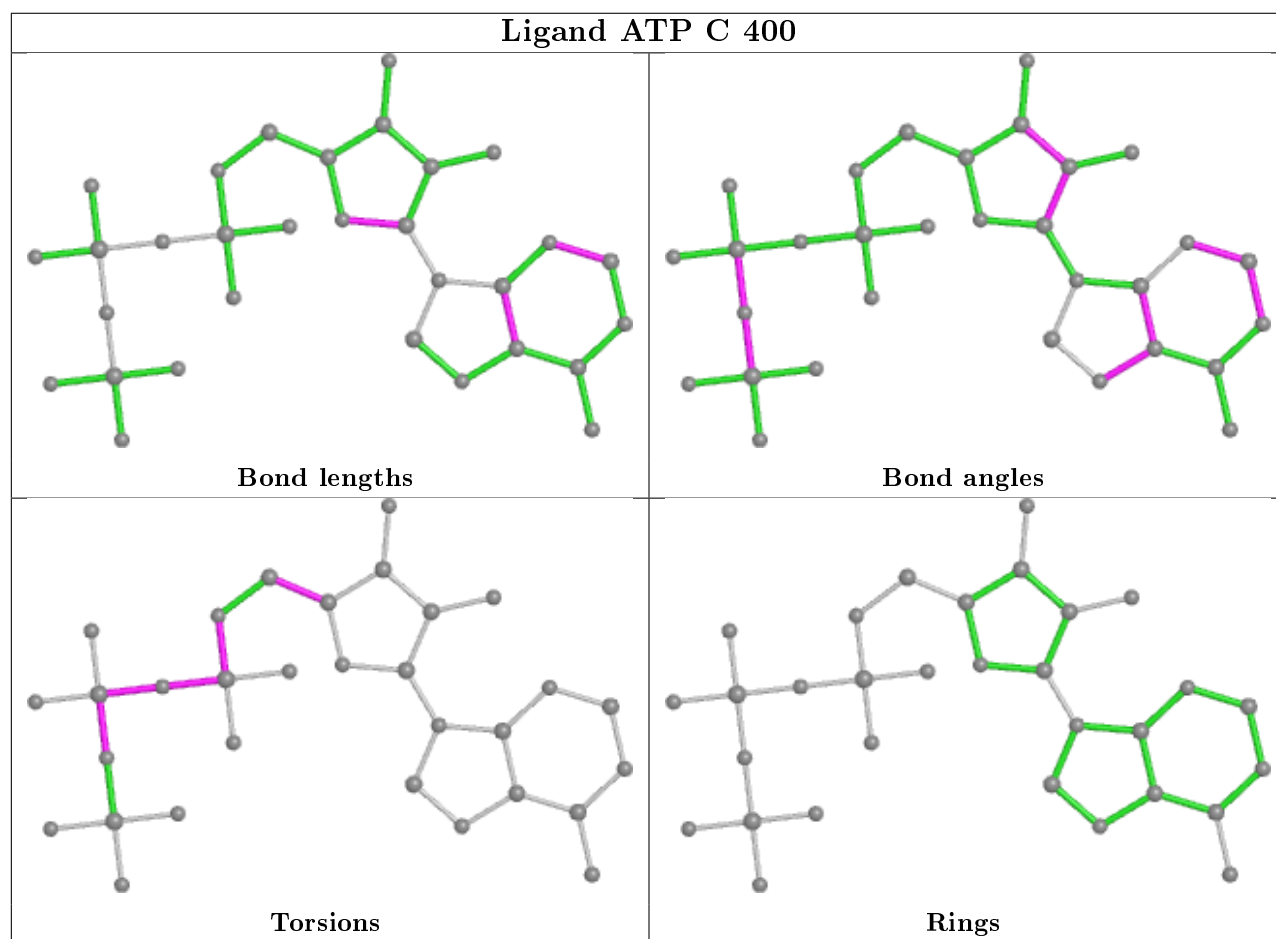
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	PO4	3	0
3	C	400	ATP	5	0
3	A	400	ATP	7	0
3	B	400	ATP	10	0
4	B	401	PO4	2	0

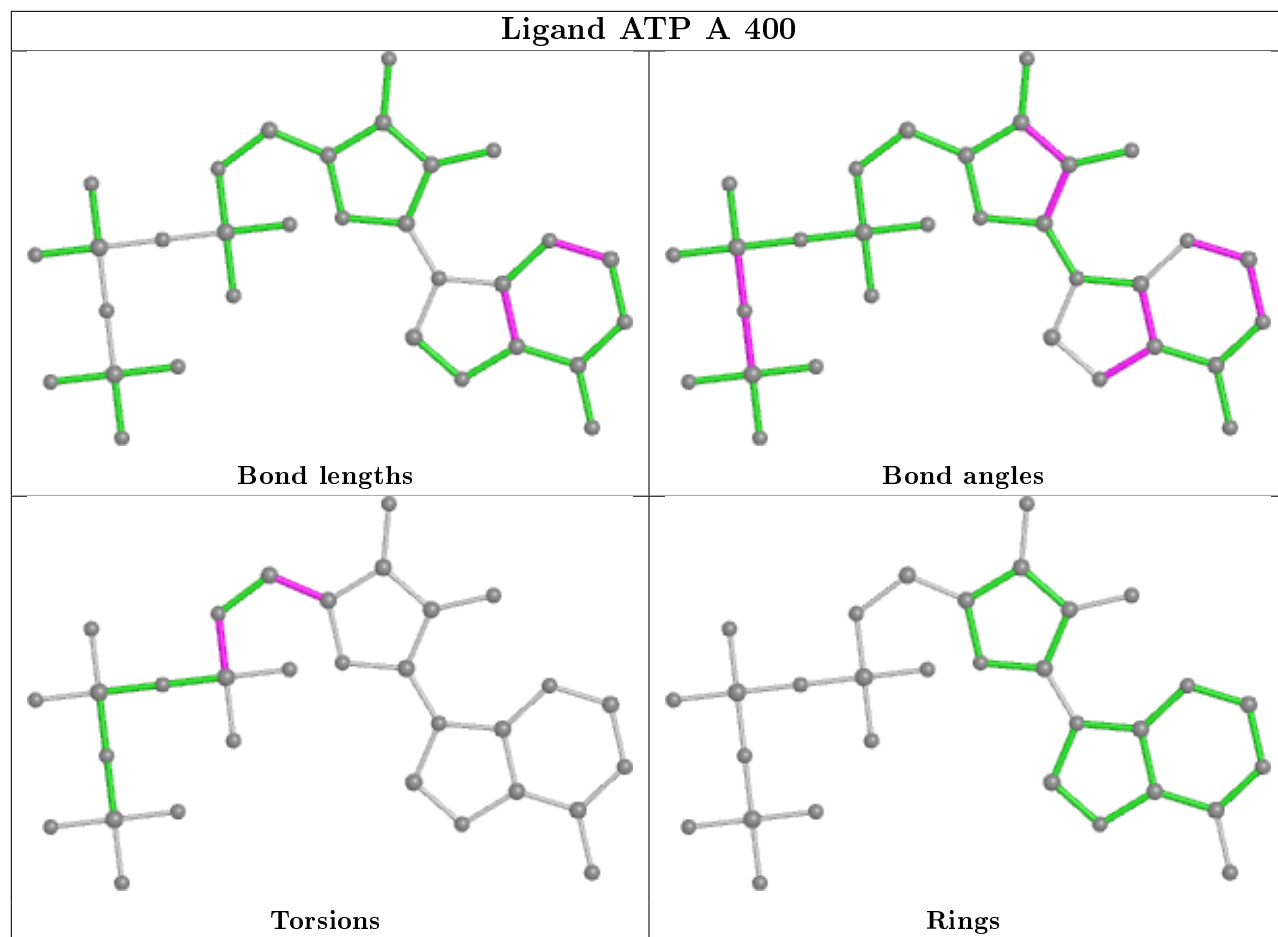
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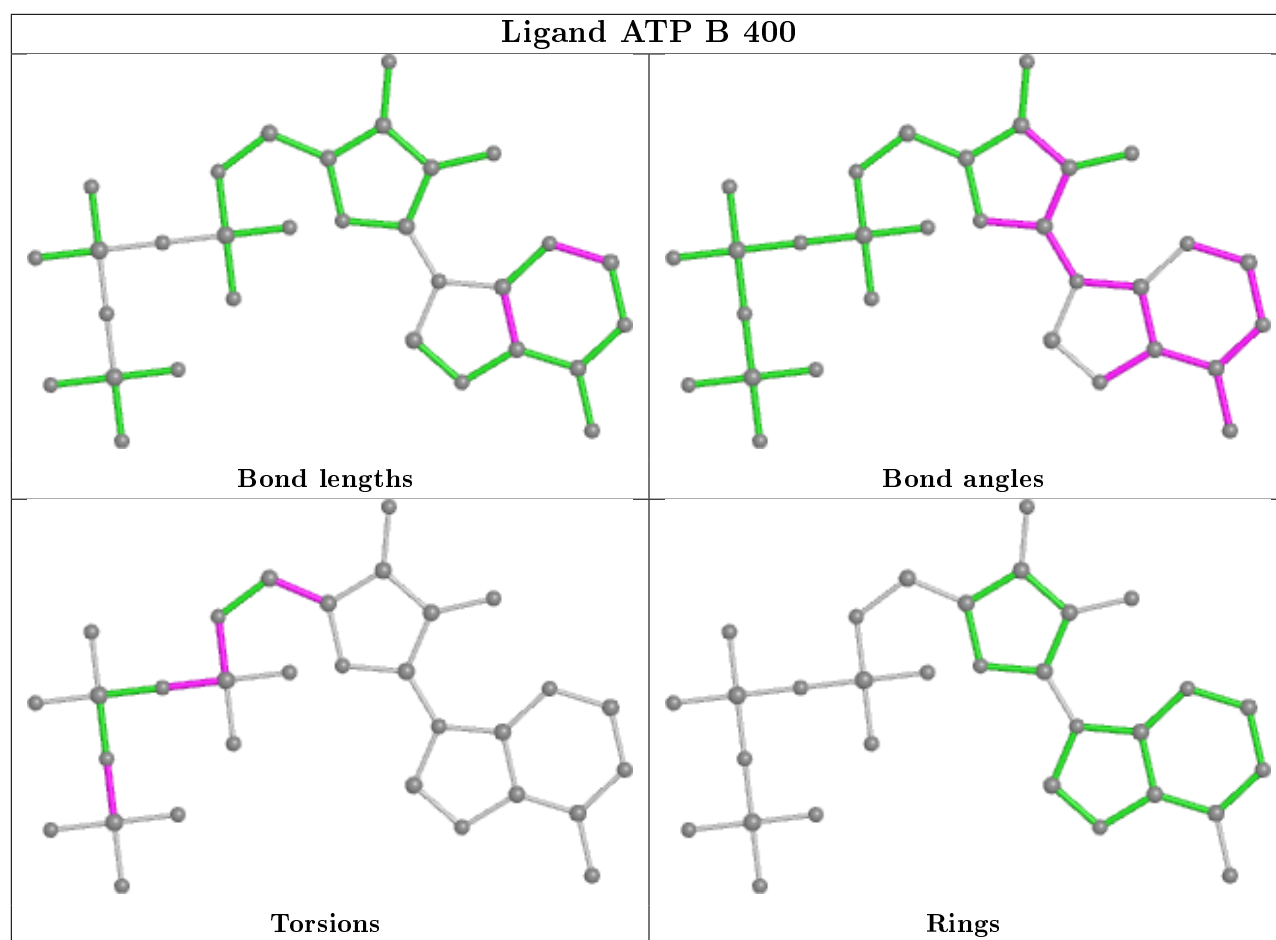
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	PO4	1	0
4	A	402	PO4	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/327 (94%)	0.27	28 (9%) 9 5	43, 89, 236, 293	2 (0%)
1	B	308/327 (94%)	0.07	22 (7%) 16 9	45, 87, 231, 281	1 (0%)
1	C	308/327 (94%)	0.10	24 (7%) 13 7	40, 88, 234, 270	1 (0%)
2	D	8/8 (100%)	1.59	3 (37%) 0 0	110, 146, 197, 201	0
2	E	8/8 (100%)	1.79	2 (25%) 0 0	77, 135, 163, 164	0
2	F	7/8 (87%)	0.38	0 100 100	68, 96, 174, 186	0
All	All	947/1005 (94%)	0.17	79 (8%) 11 6	40, 89, 235, 293	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	GLY	10.9
1	A	26	ASP	10.3
1	A	251	GLY	8.5
1	A	183	THR	8.3
1	A	25	ALA	8.1
1	B	254	TYR	7.5
1	A	291	GLY	7.4
1	A	151	GLY	7.2
1	B	1	ASP	6.9
1	A	218	ASP	6.9
1	A	290	LYS	6.7
1	C	153	ASN	6.2
2	E	401	ALA	6.2
1	A	220	ASN	6.2
1	A	152	LYS	6.1
1	C	255	ASP	6.1
1	B	258	HIS	6.0
1	C	183	THR	5.9
1	C	1	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	219	ASP	5.5
1	B	257	ASP	5.4
1	A	182	TYR	5.4
1	A	221	SER	5.2
2	D	401	ALA	5.1
1	C	214	LEU	5.1
1	A	27	ARG	4.7
1	B	253	VAL	4.7
1	A	219	ASP	4.6
1	A	24	GLN	4.2
1	C	215	THR	4.2
1	C	180	HIS	4.2
1	C	221	SER	4.2
1	B	150	SER	4.1
2	E	406	ALA	4.1
1	B	255	ASP	4.0
1	A	252	SER	3.9
1	A	23	ALA	3.9
1	B	214	LEU	3.8
1	B	291	GLY	3.8
1	A	216	TRP	3.8
1	B	220	ASN	3.7
1	C	254	TYR	3.7
1	C	216	TRP	3.7
1	A	180	HIS	3.6
1	B	256	ALA	3.6
1	B	215	THR	3.6
1	B	290	LYS	3.5
1	B	153	ASN	3.5
1	B	221	SER	3.5
1	A	153	ASN	3.3
1	C	213	LYS	3.2
1	A	103	PHE	3.1
2	D	407	ALA	3.1
1	C	290	LYS	3.1
1	A	19	ALA	3.0
1	A	214	LEU	3.0
1	C	253	VAL	2.9
1	C	154	ARG	2.9
1	C	258	HIS	2.8
1	C	47	GLU	2.8
1	B	259	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	292	ALA	2.7
1	C	218	ASP	2.7
1	B	292	ALA	2.7
1	B	182	TYR	2.6
2	D	400	ALA	2.6
1	C	184	THR	2.6
1	A	21	HIS	2.6
1	C	217	ARG	2.4
1	C	292	ALA	2.4
1	C	27	ARG	2.2
1	A	217	ARG	2.2
1	B	152	LYS	2.1
1	C	152	LYS	2.1
1	C	24	GLN	2.1
1	A	150	SER	2.1
1	A	181	ASN	2.1
1	B	219	ASP	2.1
1	B	68	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	B	401	5/5	0.77	0.37	197,209,215,216	0
3	ATP	C	400	31/31	0.79	0.35	95,177,292,361	0
3	ATP	B	400	31/31	0.81	0.27	44,153,308,407	0
4	PO4	A	401	5/5	0.83	0.30	171,178,188,188	0
4	PO4	C	401	5/5	0.83	0.48	165,178,183,184	0

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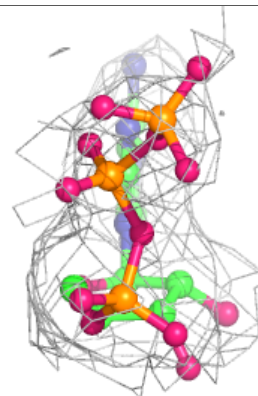
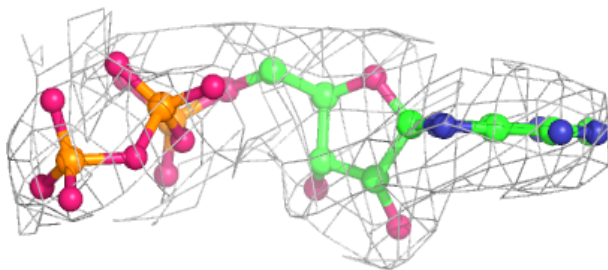
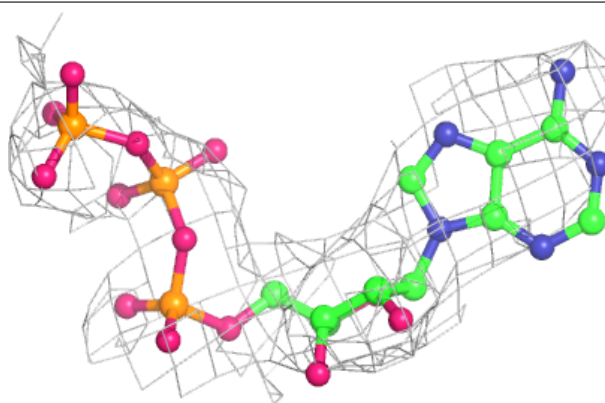
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	B	402	5/5	0.83	0.29	173,176,179,183	0
4	PO4	C	402	5/5	0.86	0.36	153,165,168,178	0
3	ATP	A	400	31/31	0.87	0.27	103,135,212,302	0
5	MG	A	403	1/1	0.93	0.20	39,39,39,39	0
4	PO4	A	402	5/5	0.93	0.12	99,103,119,129	0

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

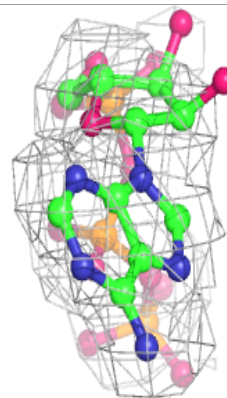
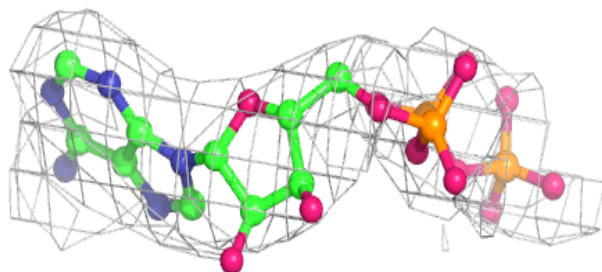
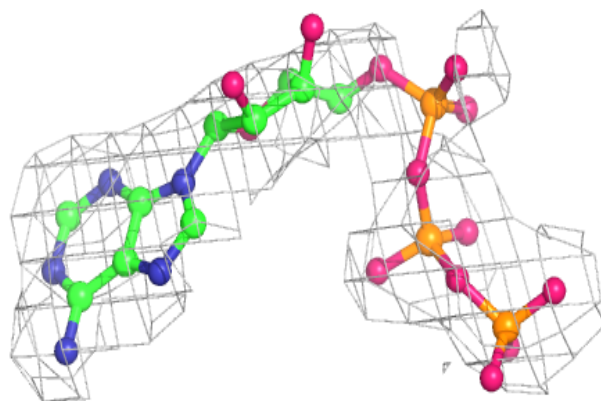
Electron density around ATP C 400:

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

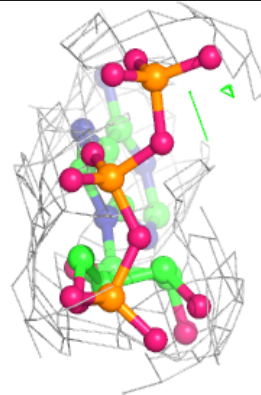
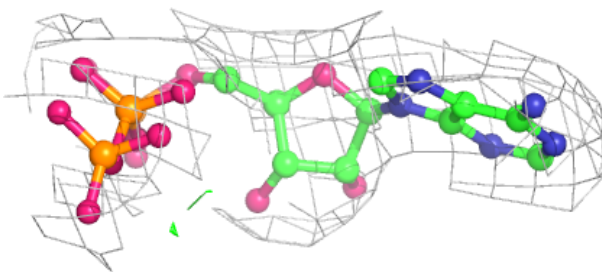
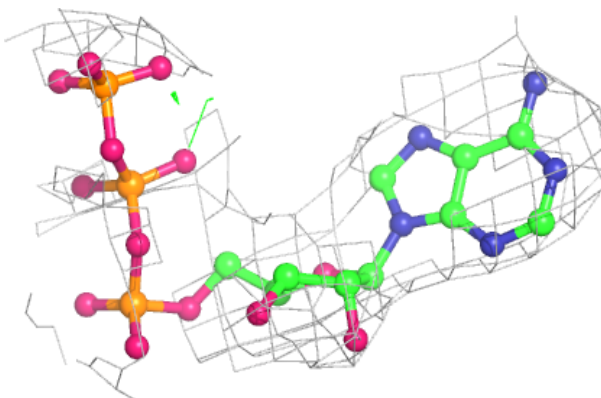


Electron density around ATP B 400:

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

**Electron density around ATP A 400:**

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



6.5 Other polymers

There are no such residues in this entry.