



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:55 AM EDT

PDB ID : 4LNK / pdb_00004lnk
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of GS-glutamate-AMPPCP complex
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 2.87 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

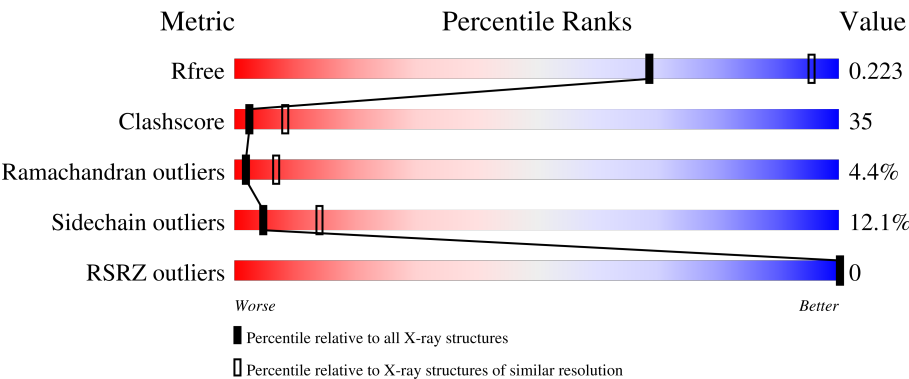
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.87 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.



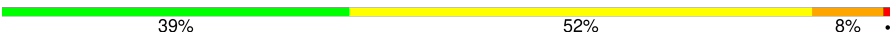
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	443	45%44%12%
1	B	443	42%48%9%
1	C	443	41%48%10%
1	D	443	42%46%11%

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Mol	Chain	Length	Quality of chain
1	E	443	
1	F	443	

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
2	GLU	C	501	-	-	X	-
2	GLU	D	501	-	-	X	-

2 Entry composition [i](#)

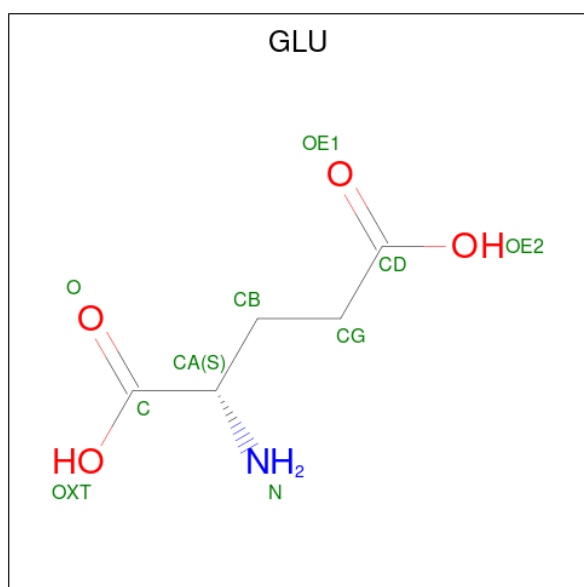
There are 6 unique types of molecules in this entry. The entry contains 21514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

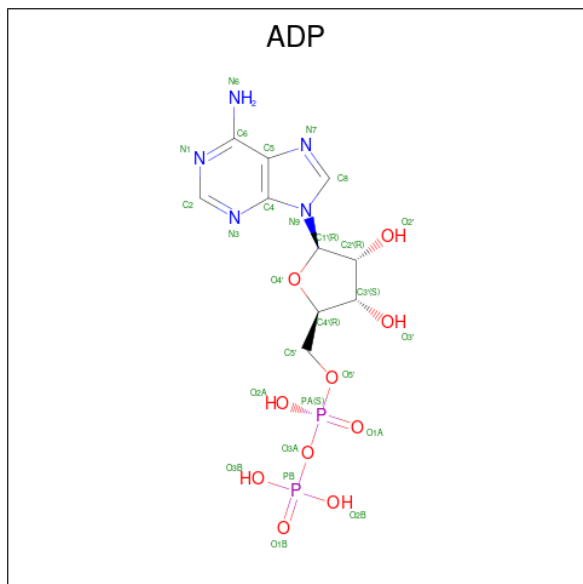
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			9	5	1	3		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

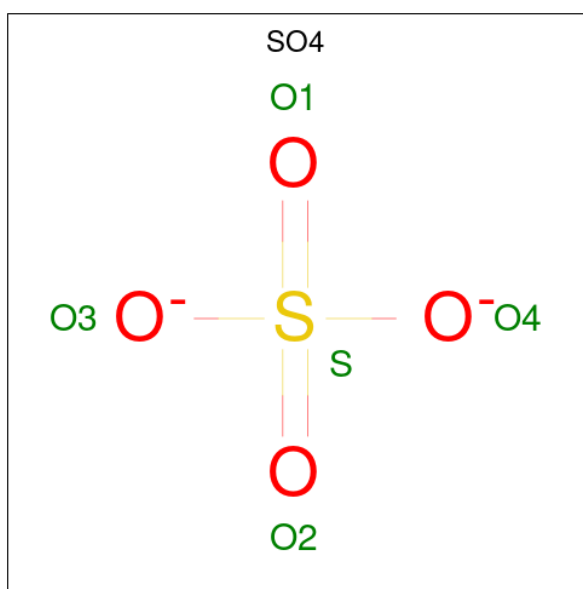


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0
4	B	2	Total 2	Mg 2	0	0
4	C	2	Total 2	Mg 2	0	0
4	D	2	Total 2	Mg 2	0	0
4	E	2	Total 2	Mg 2	0	0
4	F	2	Total 2	Mg 2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

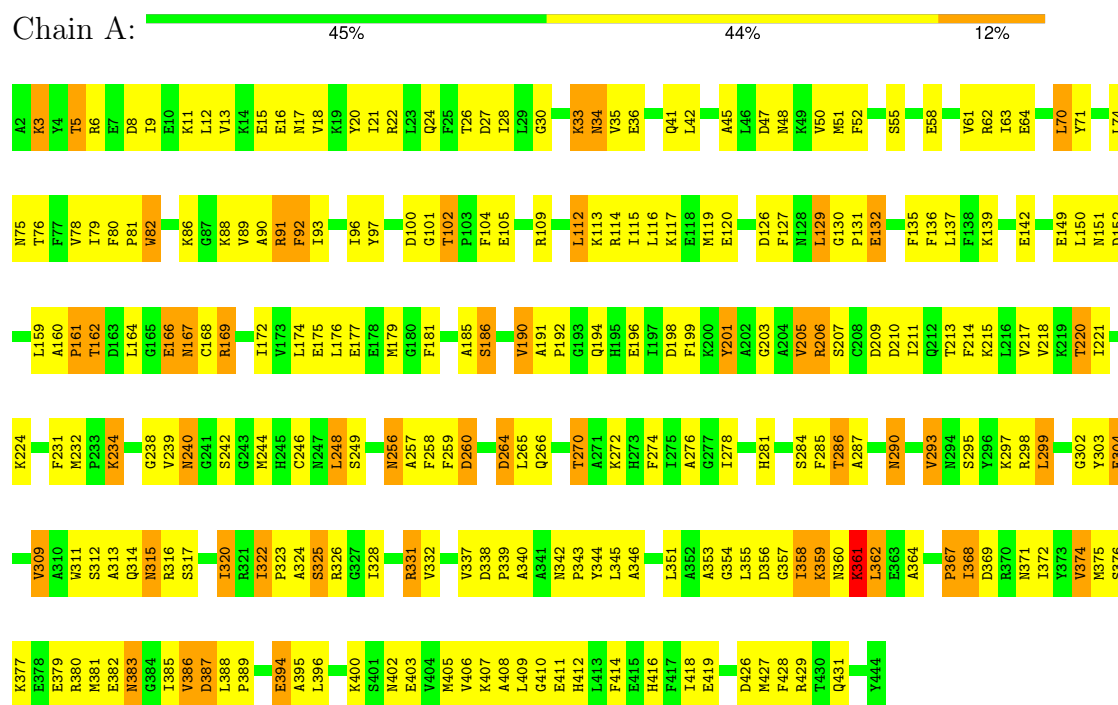
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	B	7	Total 7	O 7	0	0
6	C	6	Total 6	O 6	0	0
6	D	10	Total 10	O 10	0	0
6	E	11	Total 11	O 11	0	0
6	F	11	Total 11	O 11	0	0

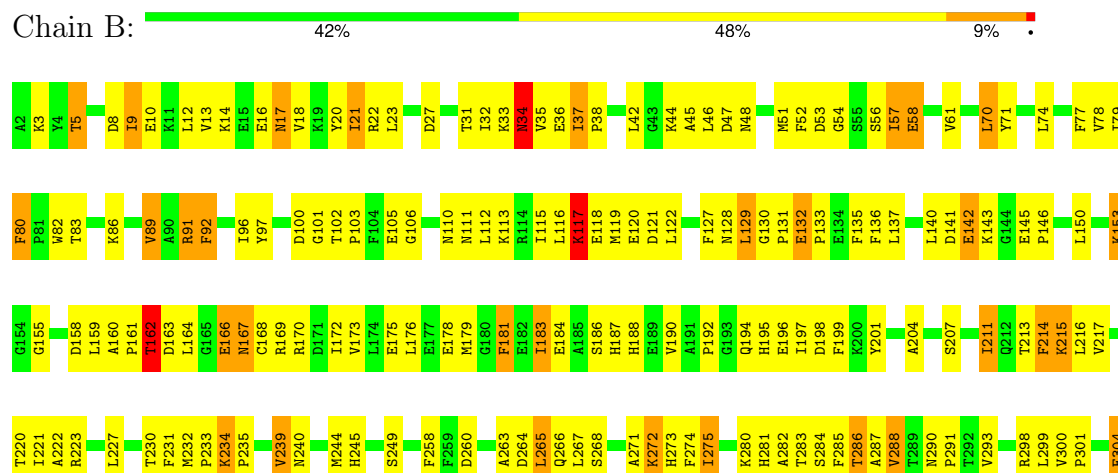
3 Residue-property plots

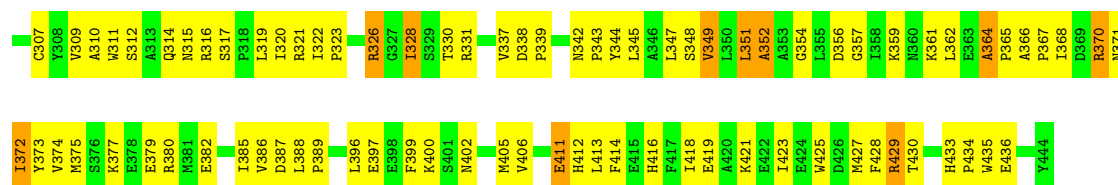
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



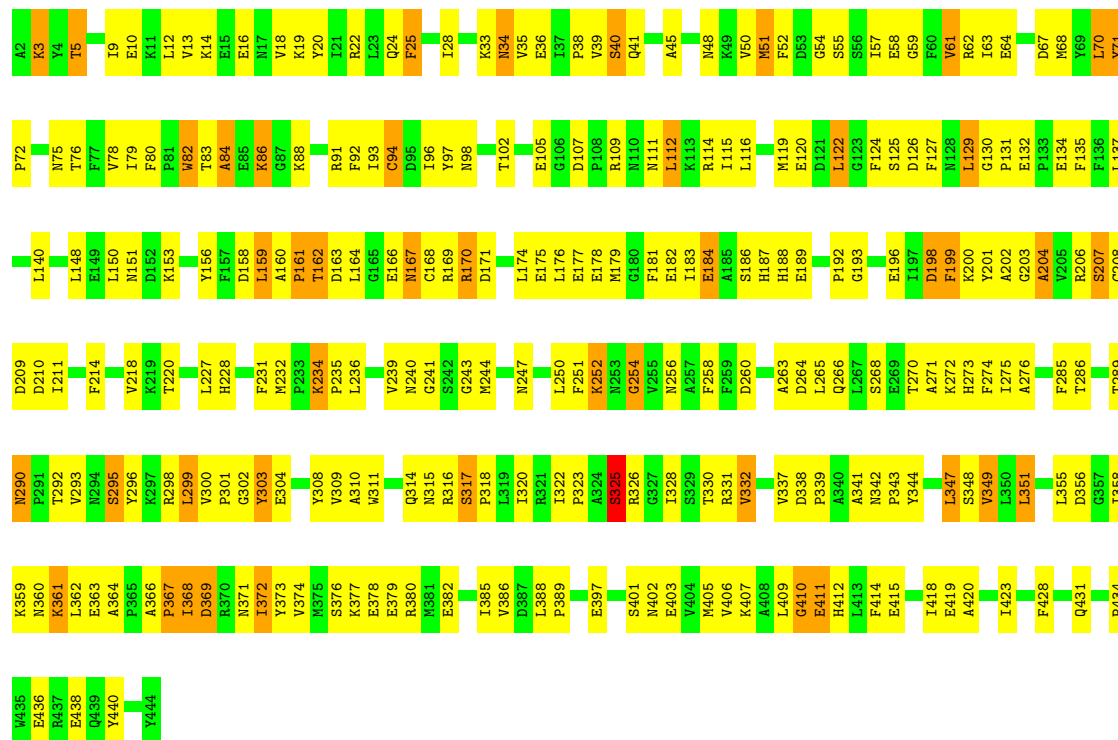
• Molecule 1: Glutamine synthetase





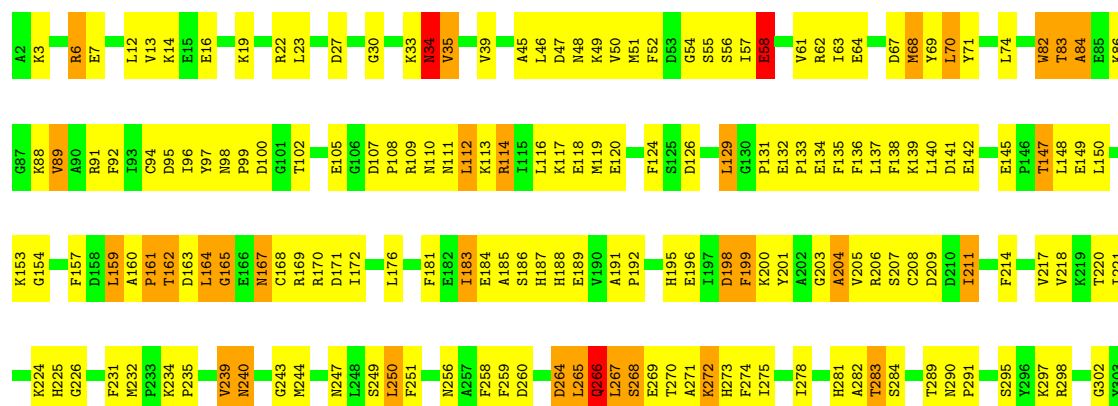
• Molecule 1: Glutamine synthetase

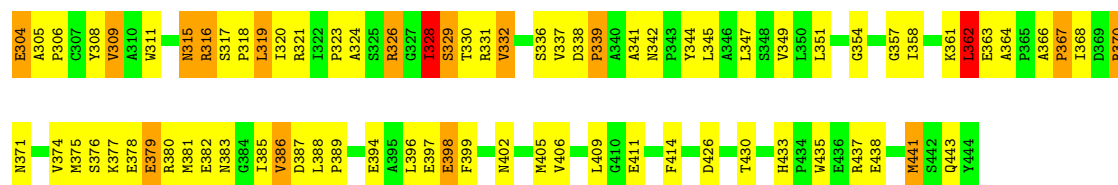
Chain C: 41% 48% 10%



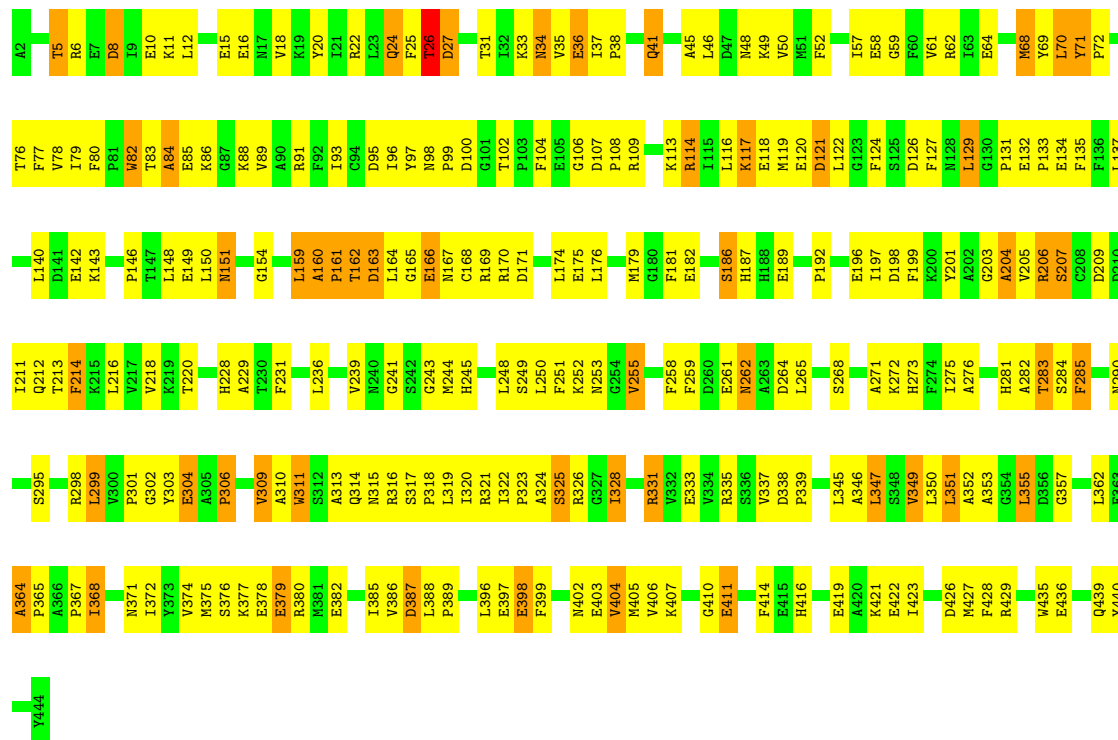
• Molecule 1: Glutamine synthetase

Chain D: 42% 46% 11%

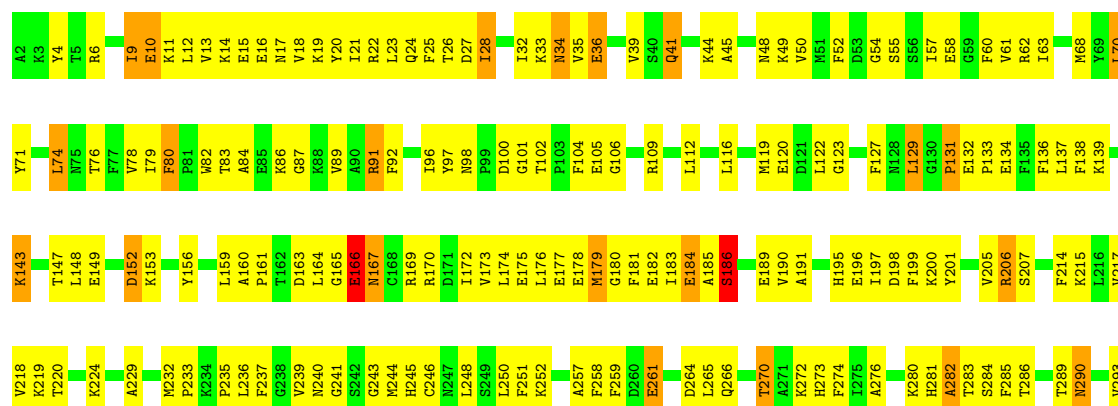


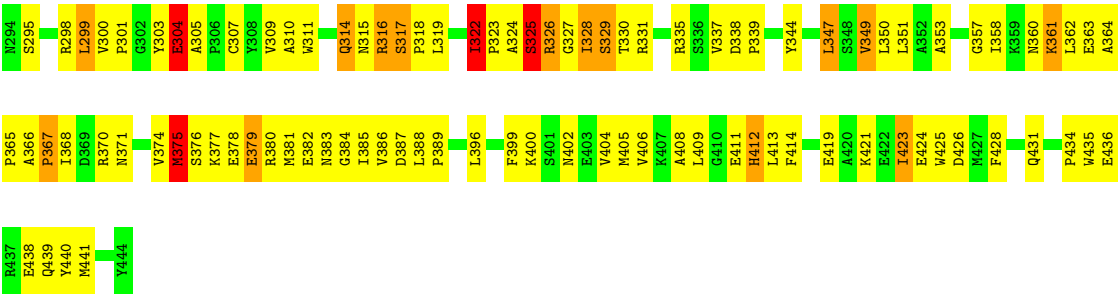


• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.50Å 240.86Å 207.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.06 – 2.87 120.06 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.8 (120.06-2.87) 90.8 (120.06-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.6.4_486, CNS 1.2	Depositor
R, R_{free}	0.195 , 0.236 0.192 , 0.223	Depositor DCC
R_{free} test set	9623 reflections (13.19%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.250 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.207 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.278 for -1/2*h+1/2*k,3/2*h+1/2*k,-l	Depositor
Outliers	2 of 72956 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21514	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5001e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, ADP, MG

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	0.62	0/3618	0.99	12/4895 (0.2%)
1	B	0.61	0/3618	0.99	14/4895 (0.3%)
1	C	0.61	0/3618	0.99	11/4895 (0.2%)
1	D	0.59	0/3618	0.99	12/4895 (0.2%)
1	E	0.61	0/3618	1.00	15/4895 (0.3%)
1	F	0.61	0/3618	1.02	12/4895 (0.2%)
All	All	0.61	0/21708	1.00	76/29370 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	305	ALA	CA-C-N	-11.49	109.05	120.31
1	F	305	ALA	C-N-CA	-11.49	109.05	120.31
1	B	234	LYS	CA-C-N	8.19	127.48	118.97
1	B	234	LYS	C-N-CA	8.19	127.48	118.97
1	C	80	PHE	CA-C-N	8.02	128.21	119.87
1	C	80	PHE	C-N-CA	8.02	128.21	119.87
1	A	290	ASN	CA-C-N	7.39	129.08	119.84
1	A	290	ASN	C-N-CA	7.39	129.08	119.84
1	E	160	ALA	N-CA-C	7.08	121.71	110.73
1	B	190	VAL	N-CA-C	6.51	117.26	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	290	ASN	CA-C-N	6.51	126.20	119.56
1	F	290	ASN	C-N-CA	6.51	126.20	119.56
1	E	160	ALA	CA-C-N	6.49	127.95	119.84
1	E	160	ALA	C-N-CA	6.49	127.95	119.84
1	A	309	VAL	N-CA-C	6.39	117.03	107.51
1	A	130	GLY	CA-C-N	6.37	126.34	119.78
1	A	130	GLY	C-N-CA	6.37	126.34	119.78
1	F	303	TYR	N-CA-C	-6.32	99.40	109.76
1	F	322	ILE	CA-C-N	6.29	126.25	120.21
1	F	322	ILE	C-N-CA	6.29	126.25	120.21
1	B	288	VAL	CB-CA-C	-6.20	105.53	111.05
1	E	132	GLU	CA-C-N	6.17	127.83	120.23
1	E	132	GLU	C-N-CA	6.17	127.83	120.23
1	D	132	GLU	CA-C-N	5.98	128.57	120.79
1	D	132	GLU	C-N-CA	5.98	128.57	120.79
1	A	191	ALA	CA-C-N	5.87	126.79	119.98
1	A	191	ALA	C-N-CA	5.87	126.79	119.98
1	E	290	ASN	CA-C-N	5.87	125.56	119.05
1	E	290	ASN	C-N-CA	5.87	125.56	119.05
1	C	71	TYR	CA-C-N	5.75	125.95	120.31
1	C	71	TYR	C-N-CA	5.75	125.95	120.31
1	E	71	TYR	CB-CA-C	-5.72	105.30	110.44
1	D	118	GLU	N-CA-C	-5.68	106.19	113.23
1	E	313	ALA	N-CA-C	-5.63	107.66	114.75
1	F	80	PHE	CA-C-N	5.63	126.87	119.84
1	F	80	PHE	C-N-CA	5.63	126.87	119.84
1	F	307	CYS	N-CA-C	-5.58	108.25	114.62
1	A	132	GLU	CA-C-N	5.58	127.09	120.23
1	A	132	GLU	C-N-CA	5.58	127.09	120.23
1	D	305	ALA	CA-C-N	5.47	126.68	119.84
1	D	305	ALA	C-N-CA	5.47	126.68	119.84
1	B	132	GLU	CA-C-N	5.45	126.65	119.84
1	B	132	GLU	C-N-CA	5.45	126.65	119.84
1	D	433	HIS	N-CA-C	5.42	118.01	110.20
1	D	58	GLU	N-CA-C	-5.39	106.71	113.28
1	C	12	LEU	N-CA-C	5.37	117.83	111.33
1	D	84	ALA	N-CA-C	-5.36	103.06	110.35
1	E	26	THR	N-CA-C	5.36	117.34	108.13
1	C	234	LYS	CA-C-N	5.26	124.44	118.97
1	C	234	LYS	C-N-CA	5.26	124.44	118.97
1	A	297	LYS	N-CA-C	-5.25	106.83	113.18
1	D	133	PRO	CB-CA-C	-5.23	107.48	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	328	ILE	N-CA-C	-5.22	105.31	111.00
1	B	80	PHE	CA-C-N	5.20	124.65	119.24
1	B	80	PHE	C-N-CA	5.20	124.65	119.24
1	C	107	ASP	CA-C-N	5.20	124.38	118.97
1	C	107	ASP	C-N-CA	5.20	124.38	118.97
1	B	9	ILE	CB-CA-C	-5.19	105.09	111.94
1	F	425	TRP	N-CA-C	-5.18	105.64	111.28
1	E	364	ALA	CA-C-N	5.16	126.29	119.84
1	E	364	ALA	C-N-CA	5.16	126.29	119.84
1	F	270	THR	N-CA-C	-5.15	104.59	111.24
1	C	290	ASN	CA-C-N	5.14	126.27	119.84
1	C	290	ASN	C-N-CA	5.14	126.27	119.84
1	D	34	ASN	N-CA-C	5.12	115.92	108.14
1	B	356	ASP	N-CA-C	-5.11	106.56	112.89
1	A	234	LYS	CA-C-N	5.10	125.17	119.87
1	A	234	LYS	C-N-CA	5.10	125.17	119.87
1	B	230	THR	N-CA-C	5.08	117.69	109.06
1	B	117	LYS	N-CA-C	-5.08	105.75	111.28
1	E	80	PHE	CA-C-N	5.07	125.14	119.87
1	E	80	PHE	C-N-CA	5.07	125.14	119.87
1	B	364	ALA	CA-C-N	5.06	125.04	120.03
1	B	364	ALA	C-N-CA	5.06	125.04	120.03
1	E	311	TRP	N-CA-C	5.06	118.42	107.49
1	D	13	VAL	CB-CA-C	-5.02	105.36	112.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	160	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	3535	0	3466	240	0
1	B	3535	0	3466	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3535	0	3466	250	0
1	D	3535	0	3466	250	0
1	E	3535	0	3466	286	0
1	F	3535	0	3466	271	0
2	A	10	0	5	0	0
2	B	9	0	5	0	0
2	C	10	0	5	4	0
2	D	10	0	5	4	0
2	E	10	0	5	3	0
2	F	9	0	5	1	0
3	A	27	0	12	3	0
3	B	27	0	12	4	0
3	C	27	0	12	5	0
3	D	27	0	12	1	0
3	E	27	0	12	4	0
3	F	27	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	10	0	0	0	0
5	E	5	0	0	1	0
6	A	12	0	0	0	0
6	B	7	0	0	0	0
6	C	6	0	0	1	0
6	D	10	0	0	1	0
6	E	11	0	0	0	0
6	F	11	0	0	0	0
All	All	21514	0	20898	1477	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 35.

All (1477) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:SER:HB2	1:F:62:ARG:HG3	1.32	1.10
1:C:182:GLU:HG3	1:C:200:LYS:HG3	1.32	1.08
1:C:162:THR:HG21	1:D:220:THR:OG1	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:MET:HE1	1:D:67:ASP:HB3	1.34	1.05
1:D:328:ILE:HD13	1:D:328:ILE:H	1.14	1.05
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.40	1.03
1:A:27:ASP:HB3	1:A:33:LYS:HD2	1.38	1.02
1:C:160:ALA:CB	1:C:169:ARG:HH22	1.74	1.00
1:C:274:PHE:HB2	1:C:358:ILE:HD11	1.45	0.95
1:F:34:ASN:HD22	1:F:34:ASN:C	1.73	0.95
1:F:265:LEU:HD12	1:F:272:LYS:HE2	1.47	0.94
1:C:234:LYS:HE3	1:C:239:VAL:O	1.68	0.93
1:A:119:MET:HE1	1:A:127:PHE:HB2	1.48	0.93
1:F:24:GLN:NE2	1:F:32:ILE:HD11	1.84	0.93
1:B:258:PHE:HA	1:B:271:ALA:HB2	1.47	0.93
1:F:74:LEU:HD22	1:F:74:LEU:H	1.33	0.91
1:D:57:ILE:HD11	1:D:96:ILE:HG12	1.53	0.91
1:B:78:VAL:HG11	1:B:179:MET:HE3	1.53	0.90
1:C:160:ALA:HB3	1:C:169:ARG:HH12	1.37	0.90
1:E:380:ARG:O	1:E:385:ILE:HB	1.71	0.90
1:E:315:ASN:HB3	1:E:318:PRO:HB3	1.52	0.90
1:F:24:GLN:HE21	1:F:32:ILE:HD11	1.36	0.90
1:A:169:ARG:HG3	1:A:169:ARG:HH21	1.36	0.89
1:C:160:ALA:HB1	1:C:161:PRO:HD2	1.54	0.88
1:D:63:ILE:HG22	1:D:64:GLU:HG3	1.54	0.88
1:A:325:SER:O	1:A:326:ARG:HD3	1.74	0.88
1:D:318:PRO:HG2	1:D:321:ARG:HB2	1.53	0.88
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.55	0.87
1:E:12:LEU:O	1:E:16:GLU:HB2	1.73	0.87
1:C:160:ALA:HB2	1:C:169:ARG:HH22	1.36	0.87
1:A:13:VAL:HG13	1:A:18:VAL:HB	1.58	0.85
1:B:160:ALA:CB	1:B:169:ARG:HH12	1.89	0.85
1:A:176:LEU:O	1:A:181:PHE:HB2	1.76	0.85
1:A:105:GLU:HG2	1:A:412:HIS:HB2	1.58	0.84
1:F:379:GLU:HA	1:F:379:GLU:OE1	1.76	0.84
1:B:160:ALA:HB3	1:B:169:ARG:HH12	1.42	0.83
1:A:9:ILE:HD12	1:A:74:LEU:HG	1.58	0.83
1:E:83:THR:HG22	1:E:88:LYS:HG2	1.60	0.83
1:C:130:GLY:HA3	3:C:502:ADP:O2'	1.79	0.83
1:B:164:LEU:HD12	1:C:220:THR:HG22	1.59	0.82
1:C:131:PRO:HG3	1:C:211:ILE:HD11	1.59	0.82
1:A:114:ARG:HH12	1:A:115:ILE:HD11	1.44	0.82
1:C:52:PHE:CD1	1:C:70:LEU:HD22	2.16	0.81
3:C:502:ADP:O2B	1:D:51:MET:HG3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.63	0.81
1:A:127:PHE:CD2	1:A:351:LEU:HD13	2.15	0.81
1:F:176:LEU:O	1:F:181:PHE:HB2	1.79	0.81
1:B:178:GLU:OE2	1:C:86:LYS:HD2	1.81	0.81
1:B:27:ASP:HB3	1:B:33:LYS:HE3	1.63	0.80
1:B:264:ASP:HB3	1:B:272:LYS:NZ	1.96	0.80
1:C:111:ASN:O	1:C:115:ILE:HD13	1.81	0.80
1:D:164:LEU:HD23	1:E:82:TRP:HB3	1.64	0.80
1:E:131:PRO:HD2	1:E:199:PHE:HB2	1.63	0.80
1:F:54:GLY:HA3	1:F:68:MET:HE3	1.63	0.80
1:B:80:PHE:HB3	1:B:82:TRP:CE3	2.17	0.80
1:E:121:ASP:O	1:E:122:LEU:HD23	1.82	0.80
1:F:325:SER:HB2	1:F:331:ARG:HH22	1.47	0.80
1:F:58:GLU:O	1:F:61:VAL:HG22	1.82	0.79
1:F:272:LYS:O	1:F:364:ALA:HB2	1.82	0.79
1:D:54:GLY:HA3	1:D:68:MET:HG3	1.64	0.79
1:D:243:GLY:HA3	1:D:298:ARG:NH1	1.98	0.79
1:E:206:ARG:O	1:E:206:ARG:HD3	1.81	0.79
1:F:368:ILE:HG12	1:F:385:ILE:HD11	1.63	0.79
1:E:58:GLU:HG2	1:E:416:HIS:CD2	2.18	0.79
1:F:329:SER:HB3	3:F:502:ADP:O1B	1.83	0.79
1:C:371:ASN:HB3	1:C:374:VAL:HG22	1.62	0.79
1:A:162:THR:HG21	1:B:220:THR:OG1	1.83	0.78
1:A:406:VAL:HG22	1:A:414:PHE:CE1	2.19	0.78
1:C:236:LEU:O	1:C:239:VAL:HG22	1.84	0.78
1:E:161:PRO:HG2	1:E:167:ASN:CG	2.07	0.78
1:A:311:TRP:HB3	1:A:320:ILE:HB	1.64	0.78
1:E:243:GLY:HA2	1:E:298:ARG:NH1	1.97	0.78
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.20	0.77
1:B:131:PRO:HG3	1:B:211:ILE:HD11	1.65	0.77
1:C:52:PHE:HE1	1:C:70:LEU:HD13	1.48	0.77
1:C:236:LEU:HB2	1:C:239:VAL:CG2	2.14	0.77
1:E:167:ASN:HB3	1:E:170:ARG:HB3	1.66	0.77
1:D:55:SER:O	1:D:62:ARG:HB3	1.84	0.76
1:C:406:VAL:HG22	1:C:414:PHE:CE1	2.20	0.76
1:A:293:VAL:HG11	1:A:428:PHE:CD1	2.21	0.76
1:A:115:ILE:HG22	1:A:351:LEU:HD23	1.67	0.76
1:B:372:ILE:HD13	1:B:385:ILE:HD13	1.68	0.76
1:A:206:ARG:HH11	1:A:206:ARG:CG	1.98	0.76
1:F:34:ASN:C	1:F:34:ASN:ND2	2.41	0.76
1:B:258:PHE:CA	1:B:271:ALA:HB2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HD2	1:C:92:PHE:N	2.01	0.75
1:C:93:ILE:HD12	1:C:209:ASP:HB3	1.66	0.75
1:C:367:PRO:O	1:C:369:ASP:N	2.19	0.75
1:F:357:GLY:HA2	1:F:362:LEU:HD22	1.67	0.75
1:E:272:LYS:HA	1:E:275:ILE:HD12	1.67	0.75
1:F:11:LYS:O	1:F:15:GLU:HG3	1.86	0.75
1:F:184:GLU:HG2	1:F:200:LYS:HE3	1.66	0.75
3:B:502:ADP:O3B	1:C:51:MET:HG3	1.85	0.75
1:D:160:ALA:HB1	1:D:161:PRO:CD	2.16	0.75
1:F:377:LYS:HG3	1:F:380:ARG:HH21	1.50	0.75
1:A:131:PRO:HD2	1:A:199:PHE:HB2	1.67	0.75
1:B:5:THR:HG23	1:B:8:ASP:CG	2.11	0.75
1:E:375:MET:HG3	1:E:380:ARG:HG2	1.67	0.75
1:A:150:LEU:HD13	1:A:192:PRO:O	1.86	0.75
1:C:150:LEU:HD13	1:C:192:PRO:O	1.86	0.75
1:A:309:VAL:HG23	1:A:386:VAL:O	1.87	0.75
1:D:134:GLU:OE1	2:D:501:GLU:N	2.20	0.75
1:D:406:VAL:HG22	1:D:414:PHE:HE1	1.51	0.75
1:E:20:TYR:HB3	1:E:89:VAL:HG22	1.69	0.75
1:B:80:PHE:CD2	1:B:82:TRP:HZ3	2.04	0.75
1:C:411:GLU:HG3	1:C:415:GLU:OE1	1.87	0.75
1:A:357:GLY:HA2	1:A:362:LEU:HD22	1.67	0.74
1:B:116:LEU:HD23	1:B:351:LEU:HD11	1.67	0.74
1:C:182:GLU:HG3	1:C:200:LYS:CG	2.13	0.74
1:F:13:VAL:HG13	1:F:18:VAL:HB	1.69	0.74
1:F:405:MET:O	1:F:408:ALA:HB3	1.88	0.74
1:D:290:ASN:HB3	1:D:295:SER:HB3	1.70	0.74
1:B:22:ARG:HG2	1:B:34:ASN:OD1	1.88	0.74
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.22	0.73
1:A:26:THR:HG22	1:A:27:ASP:O	1.88	0.73
1:B:97:TYR:CE2	1:B:103:PRO:HG3	2.24	0.73
1:C:271:ALA:O	1:C:275:ILE:HG12	1.87	0.73
1:F:374:VAL:HG23	1:F:375:MET:H	1.54	0.73
1:C:295:SER:O	1:C:299:LEU:HD23	1.89	0.73
1:D:167:ASN:ND2	1:E:22:ARG:HH22	1.86	0.73
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.54	0.72
1:A:160:ALA:O	1:A:161:PRO:C	2.32	0.72
1:A:287:ALA:HB2	1:A:395:ALA:O	1.88	0.72
1:E:303:TYR:O	1:E:304:GLU:HG3	1.89	0.72
1:E:116:LEU:O	1:E:119:MET:HB3	1.90	0.72
1:A:164:LEU:HD13	1:B:82:TRP:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ILE:HG22	1:D:320:ILE:HD11	1.70	0.72
1:D:207:SER:O	1:D:211:ILE:HG12	1.89	0.71
1:F:6:ARG:O	1:F:10:GLU:HB2	1.89	0.71
1:E:243:GLY:CA	1:E:298:ARG:NH1	2.53	0.71
1:F:183:ILE:HG23	1:F:198:ASP:O	1.90	0.71
1:F:129:LEU:HG	1:F:347:LEU:HD21	1.73	0.71
1:A:55:SER:O	1:A:62:ARG:HB3	1.90	0.71
1:C:13:VAL:HG13	1:C:18:VAL:HB	1.71	0.71
1:D:169:ARG:HH22	1:D:188:HIS:HB2	1.55	0.71
1:D:302:GLY:N	1:D:316:ARG:HH22	1.88	0.71
1:E:315:ASN:HB3	1:E:318:PRO:CB	2.20	0.71
1:C:236:LEU:HB2	1:C:239:VAL:HG21	1.73	0.70
1:B:290:ASN:ND2	1:B:299:LEU:HD21	2.06	0.70
1:E:243:GLY:CA	1:E:298:ARG:HH12	2.03	0.70
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.72	0.70
1:C:71:TYR:CE1	1:C:97:TYR:HB2	2.25	0.70
1:E:186:SER:O	1:F:36:GLU:HG2	1.91	0.70
1:F:178:GLU:C	1:F:180:GLY:H	1.96	0.70
1:F:160:ALA:O	1:F:169:ARG:NH2	2.25	0.70
1:A:160:ALA:CB	1:A:169:ARG:HH12	2.04	0.70
1:E:25:PHE:CE1	1:E:57:ILE:HD11	2.27	0.70
1:A:176:LEU:HD11	1:A:214:PHE:HD1	1.57	0.69
1:D:375:MET:HB3	1:D:379:GLU:HB3	1.74	0.69
1:A:377:LYS:HD3	1:A:380:ARG:HH12	1.57	0.69
1:C:52:PHE:HD1	1:C:70:LEU:HD22	1.57	0.69
1:B:52:PHE:CD1	1:B:70:LEU:HD22	2.27	0.69
1:B:115:ILE:HG22	1:B:351:LEU:HD13	1.75	0.69
1:B:264:ASP:HB3	1:B:272:LYS:HZ2	1.58	0.69
1:E:58:GLU:O	1:E:61:VAL:HG22	1.92	0.69
1:F:57:ILE:HD11	1:F:96:ILE:HG13	1.75	0.69
1:B:160:ALA:HB1	1:B:161:PRO:CD	2.23	0.69
1:C:300:VAL:HG13	1:C:301:PRO:HD2	1.73	0.69
1:D:274:PHE:HB2	1:D:358:ILE:HD11	1.75	0.69
1:E:27:ASP:OD1	1:E:33:LYS:HE3	1.93	0.69
1:E:27:ASP:HB3	1:E:33:LYS:HE3	1.75	0.69
1:F:58:GLU:HB3	1:F:61:VAL:HG23	1.75	0.69
1:F:405:MET:HE2	1:F:405:MET:HA	1.75	0.69
1:D:6:ARG:HG3	1:D:6:ARG:HH11	1.58	0.69
1:B:347:LEU:O	1:B:351:LEU:HB2	1.92	0.69
1:D:176:LEU:O	1:D:181:PHE:HB2	1.94	0.68
1:D:129:LEU:HD12	1:D:347:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:PRO:HD3	1:E:169:ARG:NH1	2.09	0.68
1:C:160:ALA:CB	1:C:169:ARG:NH2	2.52	0.68
1:A:127:PHE:HZ	1:A:248:LEU:HD22	1.57	0.68
1:B:111:ASN:O	1:B:115:ILE:HD13	1.93	0.68
1:E:120:GLU:C	1:E:122:LEU:H	2.02	0.68
1:B:143:LYS:NZ	1:B:143:LYS:HB3	2.08	0.68
1:B:20:TYR:HB3	1:B:89:VAL:HG13	1.76	0.68
1:C:356:ASP:O	1:C:360:ASN:HB2	1.94	0.68
1:A:100:ASP:O	1:A:102:THR:N	2.27	0.68
1:A:114:ARG:NH1	1:A:115:ILE:HD11	2.09	0.68
1:B:77:PHE:CZ	1:B:79:ILE:HD11	2.29	0.67
1:B:77:PHE:HZ	1:B:79:ILE:HD11	1.58	0.67
1:C:207:SER:O	1:C:211:ILE:HG12	1.94	0.67
1:B:80:PHE:HB3	1:B:82:TRP:HE3	1.60	0.67
1:F:91:ARG:HD2	1:F:91:ARG:C	2.18	0.67
1:F:328:ILE:HD13	1:F:328:ILE:N	2.09	0.67
1:A:388:LEU:HB3	1:A:389:PRO:HD2	1.75	0.67
1:C:5:THR:O	1:C:9:ILE:HG12	1.94	0.67
1:C:403:GLU:O	1:C:407:LYS:HG3	1.95	0.67
1:A:224:LYS:HB2	1:F:164:LEU:HD21	1.75	0.67
1:D:83:THR:HG22	1:D:88:LYS:HG2	1.77	0.67
1:F:241:GLY:HA3	1:F:298:ARG:HG2	1.77	0.67
1:E:140:LEU:HD21	1:E:228:HIS:HB2	1.76	0.67
1:E:331:ARG:HH11	3:E:502:ADP:H5'1	1.58	0.67
1:D:105:GLU:CD	1:D:105:GLU:H	2.03	0.67
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.77	0.67
1:E:159:LEU:HD13	1:F:22:ARG:HH11	1.59	0.67
1:F:406:VAL:HG22	1:F:414:PHE:CE1	2.30	0.67
1:B:260:ASP:O	1:B:266:GLN:HA	1.95	0.66
1:E:351:LEU:CD2	1:E:355:LEU:HG	2.26	0.66
1:A:13:VAL:CG1	1:A:18:VAL:HB	2.25	0.66
1:B:10:GLU:O	1:B:14:LYS:HG2	1.94	0.66
1:A:376:SER:O	1:A:380:ARG:N	2.29	0.66
1:B:371:ASN:O	1:B:374:VAL:HG22	1.95	0.66
1:C:309:VAL:HG23	1:C:386:VAL:O	1.96	0.66
1:E:248:LEU:O	1:E:331:ARG:HB2	1.96	0.66
1:E:323:PRO:HB2	1:E:331:ARG:HH12	1.60	0.66
1:E:206:ARG:HD3	1:E:206:ARG:C	2.20	0.66
1:A:234:LYS:HE3	1:A:239:VAL:O	1.95	0.66
1:D:167:ASN:HD21	1:E:22:ARG:HH22	1.44	0.66
1:A:214:PHE:O	1:A:218:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:GLU:HB3	1:F:196:GLU:OE1	1.96	0.66
1:F:423:ILE:C	1:F:423:ILE:HD12	2.21	0.66
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.60	0.66
1:D:83:THR:CG2	1:D:88:LYS:HG2	2.26	0.66
1:F:374:VAL:HG23	1:F:375:MET:N	2.10	0.66
1:B:143:LYS:HB3	1:B:143:LYS:HZ2	1.62	0.66
1:F:322:ILE:HG23	1:F:331:ARG:O	1.96	0.66
1:A:177:GLU:OE1	1:B:38:PRO:HG2	1.96	0.65
1:C:175:GLU:O	1:C:179:MET:HB2	1.95	0.65
1:B:131:PRO:HD2	1:B:199:PHE:HB2	1.77	0.65
1:E:5:THR:HG23	1:E:8:ASP:OD1	1.96	0.65
1:A:30:GLY:HA2	1:A:342:ASN:OD1	1.97	0.65
1:B:181:PHE:HE2	1:B:199:PHE:HE2	1.43	0.65
1:D:375:MET:HE2	1:D:379:GLU:O	1.97	0.65
1:F:27:ASP:HB3	1:F:33:LYS:HE3	1.77	0.65
1:D:315:ASN:HB3	1:D:318:PRO:HG3	1.78	0.65
1:B:140:LEU:HD23	1:B:146:PRO:HA	1.79	0.65
1:B:309:VAL:HA	1:B:319:LEU:HD23	1.79	0.65
1:A:270:THR:HG22	1:A:358:ILE:HD12	1.78	0.65
1:A:3:LYS:HB2	1:A:75:ASN:CG	2.22	0.65
1:E:68:MET:HG2	1:E:96:ILE:HG22	1.77	0.65
1:E:315:ASN:C	1:E:318:PRO:HD3	2.22	0.65
1:E:380:ARG:HB3	1:E:385:ILE:HG21	1.79	0.64
1:A:45:ALA:HA	1:A:50:VAL:HG23	1.79	0.64
1:B:71:TYR:CD2	1:B:97:TYR:CE1	2.84	0.64
1:B:411:GLU:HA	1:B:411:GLU:OE2	1.96	0.64
1:F:371:ASN:O	1:F:374:VAL:HG22	1.98	0.64
1:B:187:HIS:HE1	1:B:196:GLU:OE1	1.80	0.64
1:B:323:PRO:HG2	1:B:331:ARG:HG3	1.79	0.64
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.80	0.64
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.33	0.64
1:D:183:ILE:HA	1:D:199:PHE:HA	1.79	0.64
1:E:315:ASN:CB	1:E:318:PRO:HB3	2.28	0.64
1:B:293:VAL:HG11	1:B:428:PHE:CD1	2.33	0.64
1:E:162:THR:HG23	1:F:220:THR:HG23	1.80	0.64
1:E:378:GLU:O	1:E:382:GLU:HG2	1.97	0.64
1:A:127:PHE:CZ	1:A:248:LEU:HD22	2.33	0.64
1:C:162:THR:HG21	1:D:220:THR:HG1	1.63	0.64
1:C:310:ALA:CB	1:C:368:ILE:HD13	2.28	0.64
1:E:323:PRO:HD2	1:E:331:ARG:NH2	2.13	0.64
1:A:342:ASN:HD22	1:A:345:LEU:HG	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:HD22	1:A:409:LEU:HD22	1.79	0.64
1:C:160:ALA:HB3	1:C:169:ARG:NH1	2.10	0.64
1:F:74:LEU:H	1:F:74:LEU:CD2	2.08	0.64
1:C:311:TRP:CH2	1:C:367:PRO:HB3	2.33	0.64
1:D:328:ILE:H	1:D:328:ILE:CD1	1.93	0.64
1:C:135:PHE:HB3	1:C:231:PHE:CE1	2.33	0.63
1:D:224:LYS:HE2	1:D:225:HIS:CE1	2.33	0.63
1:E:371:ASN:O	1:E:374:VAL:HG22	1.98	0.63
1:F:259:PHE:CD2	1:F:327:GLY:HA2	2.33	0.63
1:B:54:GLY:O	1:B:57:ILE:HG12	1.98	0.63
1:F:377:LYS:HG3	1:F:380:ARG:NH2	2.13	0.63
1:B:181:PHE:CE2	1:B:199:PHE:HE2	2.15	0.63
1:C:160:ALA:CB	1:C:188:HIS:HD2	2.11	0.63
1:E:406:VAL:HG13	1:E:414:PHE:CD1	2.32	0.63
1:A:224:LYS:HB2	1:F:164:LEU:CD2	2.29	0.63
1:C:372:ILE:HD12	1:C:373:TYR:N	2.12	0.63
1:D:311:TRP:CZ2	1:D:367:PRO:HD3	2.33	0.63
1:D:138:PHE:HA	1:D:149:GLU:O	1.99	0.63
1:D:370:ARG:HG3	1:D:371:ASN:N	2.13	0.63
1:F:273:HIS:O	1:F:276:ALA:HB3	1.99	0.63
1:F:368:ILE:HG12	1:F:385:ILE:CD1	2.29	0.63
1:A:169:ARG:HH21	1:A:169:ARG:CG	2.11	0.63
1:A:264:ASP:HB3	1:A:265:LEU:HD12	1.81	0.63
1:B:160:ALA:HB3	1:B:169:ARG:NH1	2.14	0.63
1:F:434:PRO:O	1:F:438:GLU:HG3	1.98	0.63
1:B:187:HIS:CE1	1:B:196:GLU:OE1	2.52	0.62
1:E:252:LYS:HG2	1:E:253:ASN:OD1	1.99	0.62
1:E:131:PRO:CG	1:E:199:PHE:HD1	2.13	0.62
1:F:172:ILE:O	1:F:176:LEU:HG	1.98	0.62
1:A:312:SER:OG	1:A:369:ASP:HA	1.99	0.62
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.81	0.62
1:D:328:ILE:HD13	1:D:328:ILE:N	2.00	0.62
1:E:281:HIS:CE1	1:E:404:VAL:HG11	2.34	0.62
1:E:396:LEU:HD11	1:E:421:LYS:HB3	1.81	0.62
1:B:127:PHE:CE2	1:B:351:LEU:HG	2.34	0.62
1:D:91:ARG:HD2	1:D:92:PHE:N	2.14	0.62
1:F:11:LYS:HA	1:F:14:LYS:HE2	1.80	0.62
1:D:375:MET:HB2	1:D:380:ARG:HG2	1.81	0.62
1:A:176:LEU:HD11	1:A:214:PHE:CD1	2.34	0.62
1:E:241:GLY:HA3	1:E:298:ARG:HG3	1.82	0.62
1:E:310:ALA:CB	1:E:368:ILE:HD12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ALA:HB1	1:E:347:LEU:HD13	1.79	0.62
1:A:127:PHE:CE2	1:A:351:LEU:HD13	2.34	0.62
1:E:162:THR:CG2	1:F:220:THR:HG23	2.30	0.62
1:E:306:PRO:HA	1:E:317:SER:HB3	1.80	0.62
1:E:371:ASN:HB3	1:E:374:VAL:HG13	1.80	0.62
1:F:76:THR:O	1:F:78:VAL:HG23	2.00	0.62
1:C:323:PRO:HG2	1:C:331:ARG:CZ	2.30	0.61
1:F:322:ILE:HD12	1:F:322:ILE:N	2.15	0.61
1:E:48:ASN:HB3	1:E:71:TYR:CD1	2.35	0.61
1:E:159:LEU:HD13	1:F:22:ARG:NH1	2.16	0.61
1:E:283:THR:HB	1:E:398:GLU:OE1	2.00	0.61
1:E:351:LEU:HD23	1:E:355:LEU:HG	1.81	0.61
1:C:57:ILE:HG13	1:C:96:ILE:HD13	1.80	0.61
1:F:137:LEU:HD12	1:F:195:HIS:CD2	2.35	0.61
1:D:320:ILE:HG22	1:D:320:ILE:O	1.99	0.61
1:F:133:PRO:HD2	1:F:197:ILE:O	2.01	0.61
1:F:435:TRP:O	1:F:439:GLN:HG2	2.00	0.61
1:C:236:LEU:HB2	1:C:239:VAL:HG22	1.83	0.61
1:E:406:VAL:HG22	1:E:414:PHE:CE1	2.35	0.61
1:F:26:THR:HG22	1:F:27:ASP:O	2.00	0.61
1:A:377:LYS:CD	1:A:380:ARG:HH12	2.13	0.61
1:B:153:LYS:HA	1:B:192:PRO:HB3	1.81	0.61
1:B:309:VAL:HG23	1:B:386:VAL:O	2.00	0.61
1:E:68:MET:HG2	1:E:96:ILE:CG2	2.31	0.61
1:F:152:ASP:C	1:F:153:LYS:HD2	2.25	0.61
1:B:175:GLU:OE1	1:C:86:LYS:HE3	2.00	0.61
1:C:315:ASN:ND2	1:C:371:ASN:HA	2.15	0.61
1:D:399:PHE:HE1	1:D:405:MET:HB3	1.65	0.61
1:F:381:MET:HA	1:F:385:ILE:O	2.01	0.61
1:C:351:LEU:O	1:C:355:LEU:HG	2.00	0.61
1:D:71:TYR:CD2	1:D:97:TYR:CD1	2.89	0.61
1:F:384:GLY:O	1:F:385:ILE:HG13	2.00	0.61
1:A:160:ALA:HB3	1:A:169:ARG:NH1	2.16	0.61
1:B:167:ASN:HD22	1:B:170:ARG:H	1.47	0.61
1:D:185:ALA:HB2	1:E:37:ILE:HG22	1.83	0.61
1:C:310:ALA:HB1	1:C:368:ILE:HD13	1.82	0.60
1:F:104:PHE:HZ	1:F:412:HIS:CE1	2.19	0.60
1:C:93:ILE:CD1	1:C:209:ASP:HB3	2.31	0.60
1:F:91:ARG:HD2	1:F:92:PHE:N	2.17	0.60
1:D:243:GLY:HA3	1:D:298:ARG:HH12	1.65	0.60
1:E:154:GLY:O	1:E:192:PRO:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:HIS:O	1:E:276:ALA:HB3	2.01	0.60
1:E:377:LYS:HE2	1:E:387:ASP:OD2	2.02	0.60
1:F:274:PHE:HB2	1:F:358:ILE:HD11	1.83	0.60
1:A:160:ALA:HB1	1:A:161:PRO:CD	2.31	0.60
1:A:160:ALA:HB3	1:A:169:ARG:HH12	1.65	0.60
1:B:27:ASP:CB	1:B:33:LYS:HE3	2.29	0.60
1:B:145:GLU:OE1	1:B:145:GLU:HA	2.02	0.60
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.83	0.60
1:D:217:VAL:O	1:D:221:ILE:HD13	2.01	0.60
1:A:105:GLU:HG2	1:A:412:HIS:CB	2.29	0.60
1:C:290:ASN:O	1:C:296:TYR:HE1	1.84	0.60
1:D:23:LEU:HB2	1:D:35:VAL:HG13	1.83	0.60
1:F:178:GLU:C	1:F:180:GLY:N	2.60	0.60
1:A:136:PHE:CE2	1:A:194:GLN:HB2	2.36	0.60
1:E:27:ASP:OD2	1:E:27:ASP:C	2.44	0.60
1:E:380:ARG:HB3	1:E:385:ILE:CG2	2.31	0.60
1:F:175:GLU:O	1:F:179:MET:HG3	2.02	0.60
1:F:261:GLU:HA	1:F:266:GLN:HG2	1.84	0.60
1:B:396:LEU:O	1:B:400:LYS:HB2	2.01	0.59
1:C:39:VAL:C	1:C:41:GLN:H	2.09	0.59
1:D:426:ASP:O	1:D:430:THR:HG23	2.02	0.59
1:F:104:PHE:CZ	1:F:412:HIS:CE1	2.90	0.59
1:B:372:ILE:HD11	1:B:385:ILE:HG21	1.83	0.59
1:C:61:VAL:HB	1:C:419:GLU:OE1	2.01	0.59
1:F:404:VAL:HG13	1:F:405:MET:HE3	1.85	0.59
1:B:80:PHE:CD2	1:B:82:TRP:CZ3	2.89	0.59
3:B:502:ADP:O1B	1:C:51:MET:HE2	2.02	0.59
1:C:316:ARG:HD3	1:C:317:SER:OG	2.02	0.59
1:E:124:PHE:CD2	1:E:250:LEU:HD13	2.37	0.59
1:E:403:GLU:OE2	1:E:407:LYS:HE3	2.02	0.59
1:F:55:SER:CB	1:F:62:ARG:HG3	2.21	0.59
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.82	0.59
1:B:141:ASP:OD2	1:B:145:GLU:HB2	2.02	0.59
1:B:217:VAL:O	1:B:221:ILE:HG12	2.03	0.59
1:D:51:MET:HE1	1:D:67:ASP:CB	2.21	0.59
1:D:131:PRO:HG3	1:D:211:ILE:HD11	1.84	0.59
1:F:250:LEU:O	1:F:257:ALA:HB3	2.02	0.59
1:C:160:ALA:O	1:C:161:PRO:C	2.45	0.59
1:C:371:ASN:HB3	1:C:374:VAL:CG2	2.30	0.59
1:A:5:THR:HG23	1:A:8:ASP:CG	2.27	0.59
1:B:164:LEU:HB2	1:C:220:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:MET:HA	1:D:385:ILE:O	2.02	0.59
1:A:325:SER:OG	1:B:51:MET:HE1	2.02	0.59
1:C:310:ALA:HB1	1:C:368:ILE:HB	1.85	0.59
1:B:131:PRO:CG	1:B:211:ILE:HD11	2.31	0.59
1:C:160:ALA:HB2	1:C:169:ARG:NH2	2.13	0.59
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.36	0.59
1:A:161:PRO:O	1:A:167:ASN:ND2	2.36	0.59
1:B:168:CYS:SG	1:B:222:ALA:HA	2.42	0.59
1:B:414:PHE:O	1:B:418:ILE:HG12	2.03	0.59
1:E:131:PRO:C	1:E:133:PRO:HD3	2.28	0.59
1:A:52:PHE:CD1	1:A:70:LEU:HD13	2.38	0.59
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.85	0.59
1:C:174:LEU:HD13	1:D:86:LYS:HB2	1.83	0.59
1:E:315:ASN:O	1:E:318:PRO:HD3	2.03	0.58
1:C:292:THR:OG1	1:C:295:SER:HB2	2.03	0.58
1:D:186:SER:HB2	1:D:196:GLU:O	2.02	0.58
1:E:161:PRO:HD3	1:E:169:ARG:HH11	1.66	0.58
1:A:142:GLU:CD	1:A:142:GLU:H	2.11	0.58
1:C:167:ASN:HD21	1:D:22:ARG:HH22	1.51	0.58
1:C:137:LEU:HD13	1:C:227:LEU:HD13	1.86	0.58
1:D:264:ASP:O	1:D:265:LEU:HB2	2.03	0.58
1:E:161:PRO:HG2	1:E:167:ASN:ND2	2.17	0.58
1:F:250:LEU:HB2	1:F:258:PHE:CZ	2.39	0.58
1:B:176:LEU:O	1:B:181:PHE:HB2	2.04	0.58
1:E:272:LYS:CA	1:E:275:ILE:HD12	2.32	0.58
1:E:388:LEU:HB3	1:E:389:PRO:HD2	1.84	0.58
1:B:264:ASP:HB3	1:B:272:LYS:HZ1	1.67	0.58
1:C:167:ASN:HD21	1:D:22:ARG:NH2	2.01	0.58
1:A:63:ILE:HD12	1:F:316:ARG:NH2	2.19	0.58
1:D:278:ILE:CG2	1:D:320:ILE:HD11	2.34	0.58
1:E:375:MET:HB2	1:E:379:GLU:HB3	1.85	0.58
1:A:169:ARG:HG3	1:A:169:ARG:NH2	2.14	0.58
1:A:325:SER:O	1:A:326:ARG:CD	2.49	0.58
1:C:164:LEU:HD12	1:D:220:THR:HG22	1.86	0.58
1:E:134:GLU:OE2	2:E:501:GLU:HG2	2.04	0.58
1:F:240:ASN:HD21	2:F:501:GLU:HB2	1.68	0.58
1:D:34:ASN:C	1:D:34:ASN:ND2	2.60	0.57
1:E:148:LEU:HD12	1:E:236:LEU:HD21	1.86	0.57
1:F:131:PRO:O	1:F:133:PRO:HD3	2.03	0.57
1:A:86:LYS:HD2	1:F:178:GLU:OE1	2.05	0.57
1:A:418:ILE:O	1:A:419:GLU:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ASN:HB3	1:C:318:PRO:HD3	1.85	0.57
1:E:310:ALA:HB2	1:E:368:ILE:HD12	1.85	0.57
1:B:160:ALA:CB	1:B:169:ARG:HH22	2.17	0.57
1:C:28:ILE:HD11	1:C:58:GLU:OE2	2.03	0.57
1:F:28:ILE:HB	1:F:57:ILE:O	2.04	0.57
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.69	0.57
1:B:406:VAL:HG12	1:B:406:VAL:O	2.04	0.57
1:B:425:TRP:O	1:B:429:ARG:HG3	2.05	0.57
1:C:366:ALA:O	1:C:368:ILE:N	2.37	0.57
1:D:267:LEU:HB3	1:D:271:ALA:HB3	1.87	0.57
1:D:320:ILE:HG23	1:D:332:VAL:HG23	1.87	0.57
1:D:402:ASN:O	1:D:406:VAL:HG23	2.05	0.57
1:E:124:PHE:CE2	1:E:250:LEU:HD13	2.39	0.57
1:A:354:GLY:O	1:A:358:ILE:HG12	2.04	0.57
1:A:372:ILE:HA	1:A:375:MET:SD	2.45	0.57
1:A:402:ASN:O	1:A:406:VAL:HG23	2.05	0.57
1:C:115:ILE:HG22	1:C:351:LEU:HD13	1.85	0.57
1:D:142:GLU:H	1:D:142:GLU:CD	2.13	0.57
1:D:167:ASN:ND2	1:E:22:ARG:NH2	2.52	0.57
1:E:323:PRO:HG2	1:E:331:ARG:NH1	2.20	0.57
1:A:135:PHE:HB3	1:A:231:PHE:CE1	2.39	0.57
1:F:309:VAL:HG13	1:F:319:LEU:HD23	1.87	0.57
1:D:159:LEU:CD1	1:E:22:ARG:HH11	2.17	0.57
1:E:350:LEU:O	1:E:353:ALA:HB3	2.04	0.57
1:D:112:LEU:HD23	1:D:116:LEU:HG	1.87	0.56
1:E:199:PHE:HZ	1:E:214:PHE:HB2	1.70	0.56
1:E:315:ASN:OD1	1:E:371:ASN:HA	2.05	0.56
1:F:378:GLU:C	1:F:380:ARG:H	2.11	0.56
1:A:381:MET:HE3	1:A:381:MET:HA	1.86	0.56
1:C:130:GLY:CA	3:C:502:ADP:O2'	2.52	0.56
1:B:47:ASP:O	1:B:48:ASN:HB2	2.06	0.56
1:B:244:MET:H	1:B:338:ASP:HA	1.70	0.56
1:C:129:LEU:O	1:C:201:TYR:HA	2.06	0.56
1:C:270:THR:CG2	1:C:358:ILE:HD12	2.35	0.56
1:E:204:ALA:HB1	1:E:347:LEU:CD1	2.34	0.56
1:F:191:ALA:HB1	1:F:239:VAL:CG2	2.35	0.56
1:A:11:LYS:HE2	1:A:15:GLU:OE2	2.05	0.56
1:B:181:PHE:HE2	1:B:199:PHE:CE2	2.23	0.56
1:E:399:PHE:HE1	1:E:405:MET:HB3	1.69	0.56
1:E:27:ASP:CB	1:E:33:LYS:HE3	2.35	0.56
1:E:265:LEU:HD13	1:E:272:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:TYR:HB3	1:F:89:VAL:HG22	1.87	0.56
1:A:388:LEU:HB3	1:A:389:PRO:CD	2.35	0.56
1:B:160:ALA:HB2	1:B:188:HIS:HD2	1.69	0.56
1:B:402:ASN:O	1:B:406:VAL:HG23	2.05	0.56
1:C:202:ALA:HB1	1:C:206:ARG:HD3	1.88	0.56
1:D:247:ASN:HB3	1:D:331:ARG:HD2	1.87	0.56
1:F:293:VAL:HG11	1:F:428:PHE:CG	2.40	0.56
1:F:311:TRP:CD1	1:F:311:TRP:H	2.23	0.56
1:C:207:SER:HA	1:C:210:ASP:HB2	1.88	0.56
1:D:283:THR:HB	1:D:398:GLU:OE1	2.05	0.56
1:A:396:LEU:O	1:A:400:LYS:HG3	2.05	0.56
1:B:91:ARG:HD2	1:B:92:PHE:N	2.21	0.56
1:B:271:ALA:O	1:B:275:ILE:HG12	2.06	0.56
1:C:273:HIS:HA	1:C:362:LEU:O	2.05	0.56
1:A:377:LYS:HD3	1:A:380:ARG:NH1	2.20	0.56
1:C:160:ALA:CB	1:C:169:ARG:HH12	2.13	0.56
1:A:64:GLU:OE2	1:F:371:ASN:OD1	2.24	0.55
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.87	0.55
1:A:119:MET:CE	1:A:127:PHE:HB2	2.31	0.55
1:B:5:THR:HG23	1:B:8:ASP:OD2	2.07	0.55
1:B:52:PHE:HD1	1:B:70:LEU:HD22	1.71	0.55
1:D:138:PHE:CD2	1:D:148:LEU:HA	2.42	0.55
1:A:86:LYS:HG3	1:F:174:LEU:HB3	1.88	0.55
1:B:249:SER:HA	1:B:258:PHE:CE1	2.41	0.55
1:C:28:ILE:HG13	1:C:57:ILE:O	2.05	0.55
1:C:91:ARG:HD2	1:C:91:ARG:C	2.30	0.55
1:F:317:SER:HB3	1:F:335:ARG:HH22	1.70	0.55
1:A:338:ASP:OD2	1:A:340:ALA:HB3	2.06	0.55
1:B:137:LEU:HD13	1:B:227:LEU:HD13	1.89	0.55
1:D:316:ARG:HG2	1:D:317:SER:N	2.20	0.55
1:A:79:ILE:HD13	1:A:90:ALA:HB2	1.88	0.55
1:A:116:LEU:HD23	1:A:351:LEU:CD2	2.37	0.55
1:B:160:ALA:HB2	1:B:169:ARG:HH12	1.69	0.55
1:B:265:LEU:O	1:B:266:GLN:HB2	2.06	0.55
1:B:419:GLU:O	1:B:423:ILE:HG12	2.06	0.55
1:D:111:ASN:OD1	1:D:114:ARG:NH1	2.39	0.55
1:E:302:GLY:H	1:E:316:ARG:NH1	2.05	0.55
1:F:24:GLN:OE1	1:F:91:ARG:HD3	2.07	0.55
1:A:91:ARG:CD	1:A:91:ARG:C	2.80	0.55
1:A:351:LEU:O	1:A:355:LEU:HG	2.06	0.55
1:B:71:TYR:CD2	1:B:97:TYR:CD1	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ALA:HA	1:D:50:VAL:HG23	1.89	0.55
1:F:325:SER:HB2	1:F:331:ARG:NH2	2.21	0.55
1:E:25:PHE:CD1	1:E:57:ILE:HD11	2.41	0.55
1:A:164:LEU:HD22	1:B:82:TRP:CD1	2.41	0.55
1:D:159:LEU:CD1	1:E:22:ARG:NH1	2.70	0.55
1:D:298:ARG:NH1	2:D:501:GLU:O	2.40	0.55
1:A:302:GLY:H	1:A:316:ARG:NH2	2.05	0.55
1:C:308:TYR:HE2	1:C:380:ARG:NH1	2.05	0.55
1:E:20:TYR:OH	1:E:36:GLU:HG3	2.07	0.55
1:E:163:ASP:OD2	1:F:89:VAL:HG11	2.07	0.55
1:E:419:GLU:O	1:E:423:ILE:HG12	2.07	0.55
1:F:311:TRP:CZ2	1:F:367:PRO:HD3	2.42	0.55
1:F:375:MET:HE2	1:F:380:ARG:HG2	1.88	0.55
1:A:356:ASP:HA	1:A:359:LYS:HD3	1.89	0.55
1:D:239:VAL:HG23	1:D:240:ASN:N	2.20	0.55
1:E:83:THR:HB	5:E:505:SO4:O4	2.07	0.55
1:A:287:ALA:HB2	1:A:395:ALA:C	2.31	0.54
3:A:502:ADP:O1A	1:B:44:LYS:NZ	2.40	0.54
1:D:394:GLU:O	1:D:398:GLU:HB2	2.07	0.54
1:F:9:ILE:CD1	1:F:74:LEU:HB3	2.37	0.54
1:F:161:PRO:HG2	1:F:166:GLU:OE1	2.07	0.54
1:F:236:LEU:HB2	1:F:239:VAL:CG1	2.37	0.54
1:B:244:MET:CB	1:B:339:PRO:HD3	2.37	0.54
1:B:371:ASN:OD1	1:B:374:VAL:HG13	2.07	0.54
1:C:293:VAL:HG11	1:C:428:PHE:CG	2.43	0.54
1:D:95:ASP:OD1	1:D:113:LYS:NZ	2.38	0.54
1:D:282:ALA:O	1:D:283:THR:C	2.49	0.54
1:E:379:GLU:HA	1:E:382:GLU:HG3	1.90	0.54
1:C:126:ASP:HB2	1:C:251:PHE:HB2	1.88	0.54
1:C:177:GLU:C	1:C:179:MET:H	2.15	0.54
1:C:178:GLU:O	1:C:178:GLU:HG3	2.07	0.54
1:D:109:ARG:HG3	1:D:344:TYR:CE2	2.42	0.54
1:B:52:PHE:CE1	1:B:70:LEU:HD13	2.43	0.54
1:D:311:TRP:CE3	1:D:367:PRO:HB3	2.43	0.54
1:E:27:ASP:OD1	1:E:31:THR:HB	2.07	0.54
1:C:54:GLY:HA3	1:C:68:MET:HE3	1.90	0.54
1:C:311:TRP:HB3	1:C:320:ILE:HB	1.90	0.54
1:E:131:PRO:HG3	1:E:199:PHE:HD1	1.73	0.54
1:F:138:PHE:HB3	1:F:147:THR:O	2.07	0.54
1:C:301:PRO:HA	1:C:316:ARG:HH22	1.73	0.54
1:D:69:TYR:HD1	1:D:99:PRO:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:LEU:HB2	1:F:239:VAL:HG12	1.89	0.54
1:B:244:MET:HB2	1:B:339:PRO:HD3	1.90	0.54
1:B:304:GLU:HA	1:B:317:SER:OG	2.07	0.54
1:C:402:ASN:O	1:C:406:VAL:HG23	2.08	0.54
1:E:120:GLU:C	1:E:122:LEU:N	2.65	0.54
1:E:386:VAL:HG23	1:E:386:VAL:O	2.08	0.54
1:A:274:PHE:O	1:A:278:ILE:HG12	2.08	0.54
1:A:403:GLU:O	1:A:407:LYS:HG3	2.08	0.54
1:E:285:PHE:CD1	1:E:285:PHE:C	2.86	0.54
1:F:68:MET:HG2	1:F:97:TYR:O	2.07	0.54
1:B:321:ARG:C	1:B:322:ILE:HD12	2.32	0.53
1:C:25:PHE:N	1:C:25:PHE:CD2	2.76	0.53
1:A:270:THR:HG22	1:A:358:ILE:CD1	2.38	0.53
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.21	0.53
1:C:25:PHE:CE1	1:C:33:LYS:HB2	2.43	0.53
1:D:136:PHE:CD1	1:D:235:PRO:HG2	2.43	0.53
1:D:203:GLY:O	1:D:204:ALA:C	2.52	0.53
1:E:243:GLY:HA3	1:E:298:ARG:HH12	1.71	0.53
1:F:165:GLY:O	1:F:166:GLU:C	2.52	0.53
1:A:323:PRO:HB2	1:A:331:ARG:NH1	2.23	0.53
1:C:58:GLU:OE2	1:C:58:GLU:HA	2.08	0.53
1:E:322:ILE:HD12	1:E:322:ILE:H	1.73	0.53
1:F:215:LYS:O	1:F:219:LYS:HG3	2.08	0.53
1:F:233:PRO:O	1:F:298:ARG:HG3	2.08	0.53
1:A:160:ALA:HB2	1:A:169:ARG:HH12	1.72	0.53
1:A:238:GLY:HA2	1:A:303:TYR:CZ	2.43	0.53
1:D:332:VAL:HG22	1:D:332:VAL:O	2.08	0.53
1:B:164:LEU:HB2	1:C:220:THR:HG22	1.91	0.53
1:C:78:VAL:HG12	1:C:79:ILE:N	2.23	0.53
1:C:260:ASP:OD1	1:C:263:ALA:HB2	2.09	0.53
1:D:271:ALA:O	1:D:275:ILE:HG13	2.09	0.53
1:F:57:ILE:CD1	1:F:96:ILE:HG13	2.38	0.53
1:A:41:GLN:HE22	1:F:200:LYS:HD2	1.74	0.53
1:E:175:GLU:O	1:E:179:MET:HG3	2.09	0.53
1:F:205:VAL:C	1:F:207:SER:N	2.63	0.53
1:B:129:LEU:O	1:B:201:TYR:HA	2.09	0.53
1:C:51:MET:HE1	1:C:67:ASP:HB3	1.89	0.53
1:D:160:ALA:HB3	1:D:169:ARG:NH1	2.22	0.53
1:B:375:MET:HB3	1:B:379:GLU:HG3	1.91	0.53
1:D:304:GLU:HB3	2:D:501:GLU:HB3	1.90	0.53
1:F:127:PHE:CD1	1:F:351:LEU:HD12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.91	0.53
1:C:379:GLU:HA	1:C:382:GLU:HB2	1.91	0.53
1:E:187:HIS:CE1	1:E:196:GLU:CD	2.86	0.53
1:F:17:ASN:O	1:F:19:LYS:HG2	2.08	0.53
1:A:356:ASP:O	1:A:360:ASN:HB2	2.09	0.52
1:B:127:PHE:CD2	1:B:351:LEU:HG	2.43	0.52
1:C:420:ALA:O	1:C:423:ILE:HB	2.10	0.52
1:D:124:PHE:HB3	1:D:251:PHE:O	2.09	0.52
1:D:159:LEU:HD11	1:E:22:ARG:HH11	1.73	0.52
1:B:266:GLN:HB3	1:B:326:ARG:HG2	1.90	0.52
1:C:111:ASN:HD21	1:C:409:LEU:HD23	1.75	0.52
1:D:328:ILE:C	1:D:330:THR:H	2.18	0.52
1:E:45:ALA:HA	1:E:50:VAL:HG23	1.91	0.52
1:E:57:ILE:HG13	1:E:96:ILE:HD13	1.90	0.52
1:E:85:GLU:HG3	1:E:86:LYS:HG2	1.92	0.52
1:E:252:LYS:O	1:E:255:VAL:HG22	2.09	0.52
1:E:376:SER:O	1:E:380:ARG:HG3	2.10	0.52
1:F:295:SER:O	1:F:299:LEU:HD22	2.08	0.52
1:B:27:ASP:CG	1:B:33:LYS:HE3	2.35	0.52
1:C:51:MET:HE1	1:C:67:ASP:CG	2.34	0.52
1:C:160:ALA:HB1	1:C:161:PRO:CD	2.32	0.52
1:F:281:HIS:CE1	1:F:404:VAL:HG11	2.44	0.52
1:F:290:ASN:ND2	1:F:299:LEU:HD21	2.25	0.52
1:E:68:MET:HE2	1:E:98:ASN:HA	1.90	0.52
1:F:274:PHE:C	1:F:274:PHE:CD2	2.87	0.52
1:F:315:ASN:O	1:F:318:PRO:HD3	2.09	0.52
1:F:351:LEU:C	1:F:351:LEU:HD23	2.34	0.52
1:E:164:LEU:HD21	1:F:224:LYS:HB2	1.92	0.52
1:E:372:ILE:HG23	1:E:385:ILE:HD13	1.91	0.52
1:F:281:HIS:CD2	1:F:353:ALA:HB1	2.45	0.52
1:A:80:PHE:CZ	1:A:91:ARG:HG2	2.44	0.52
1:A:389:PRO:HB3	1:A:394:GLU:HB3	1.91	0.52
1:D:184:GLU:HG3	1:D:200:LYS:HG2	1.91	0.52
1:E:402:ASN:O	1:E:406:VAL:HG23	2.10	0.52
1:A:3:LYS:HB2	1:A:75:ASN:ND2	2.25	0.52
1:A:96:ILE:HG22	1:A:104:PHE:CB	2.40	0.52
1:B:323:PRO:O	1:B:326:ARG:NH2	2.43	0.52
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.91	0.52
1:D:19:LYS:HA	1:D:39:VAL:HG11	1.91	0.52
1:D:160:ALA:HB2	1:D:188:HIS:HB2	1.91	0.52
1:E:25:PHE:CE1	1:E:57:ILE:CD1	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ASP:O	1:F:265:LEU:HB2	2.10	0.52
1:A:9:ILE:O	1:A:13:VAL:HG23	2.09	0.52
1:B:34:ASN:C	1:B:34:ASN:ND2	2.67	0.52
1:B:52:PHE:CE2	1:B:54:GLY:HA2	2.44	0.52
1:B:414:PHE:CE1	1:B:418:ILE:HD11	2.44	0.52
1:C:285:PHE:HB2	1:C:349:VAL:HG13	1.90	0.52
1:D:243:GLY:CA	1:D:298:ARG:NH1	2.72	0.52
1:E:243:GLY:HA2	1:E:298:ARG:HH12	1.62	0.52
1:E:423:ILE:O	1:E:427:MET:HG3	2.10	0.52
1:F:281:HIS:O	1:F:284:SER:N	2.26	0.52
1:B:349:VAL:O	1:B:352:ALA:HB3	2.10	0.52
1:C:160:ALA:HB2	1:C:188:HIS:HD2	1.74	0.52
1:D:68:MET:CE	1:D:98:ASN:HA	2.40	0.52
1:E:170:ARG:NH1	1:F:84:ALA:HB2	2.25	0.52
1:E:212:GLN:HA	1:E:212:GLN:OE1	2.10	0.52
1:E:435:TRP:O	1:E:439:GLN:HB2	2.10	0.52
1:E:161:PRO:HG2	1:E:167:ASN:OD1	2.09	0.51
1:B:160:ALA:O	1:B:161:PRO:C	2.53	0.51
1:E:176:LEU:O	1:E:181:PHE:HB2	2.10	0.51
1:A:177:GLU:OE2	1:A:177:GLU:HA	2.10	0.51
1:A:270:THR:CG2	1:A:358:ILE:HD12	2.41	0.51
1:B:136:PHE:CE2	1:B:194:GLN:HB2	2.45	0.51
1:F:282:ALA:HA	1:F:285:PHE:CZ	2.45	0.51
1:F:329:SER:CB	3:F:502:ADP:O1B	2.54	0.51
1:A:5:THR:O	1:A:8:ASP:HB2	2.11	0.51
1:A:185:ALA:O	1:A:186:SER:HB3	2.10	0.51
1:B:97:TYR:HE2	1:B:103:PRO:HG3	1.75	0.51
1:C:163:ASP:HB2	1:D:82:TRP:HE3	1.75	0.51
1:E:259:PHE:CZ	1:E:261:GLU:HB2	2.46	0.51
1:E:309:VAL:HG23	1:E:386:VAL:O	2.10	0.51
1:B:117:LYS:HG2	1:B:118:GLU:N	2.25	0.51
1:E:6:ARG:O	1:E:10:GLU:HG3	2.09	0.51
1:E:34:ASN:ND2	1:E:34:ASN:O	2.43	0.51
1:A:21:ILE:HD13	1:A:42:LEU:HD13	1.92	0.51
1:A:80:PHE:C	1:A:82:TRP:H	2.18	0.51
1:A:91:ARG:C	1:A:92:PHE:CD1	2.88	0.51
1:A:314:GLN:O	1:A:315:ASN:ND2	2.26	0.51
1:B:286:THR:C	1:B:288:VAL:H	2.19	0.51
1:D:139:LYS:O	1:D:147:THR:HG23	2.10	0.51
1:E:303:TYR:C	1:E:304:GLU:HG3	2.35	0.51
1:B:234:LYS:HE3	1:B:239:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASP:HB3	1:C:263:ALA:HB3	1.93	0.51
1:C:322:ILE:HG23	1:C:331:ARG:O	2.10	0.51
1:D:48:ASN:HB3	1:D:71:TYR:CD1	2.46	0.51
1:D:160:ALA:O	1:D:161:PRO:C	2.54	0.51
1:D:383:ASN:C	1:D:385:ILE:H	2.19	0.51
1:E:12:LEU:O	1:E:16:GLU:CB	2.55	0.51
1:F:106:GLY:HA2	1:F:413:LEU:HG	1.93	0.51
1:F:323:PRO:O	1:F:326:ARG:NH2	2.42	0.51
1:A:265:LEU:O	1:A:266:GLN:HB2	2.11	0.51
1:B:372:ILE:CD1	1:B:385:ILE:HD13	2.38	0.51
1:E:196:GLU:OE1	1:E:198:ASP:OD1	2.27	0.51
1:E:281:HIS:HE1	1:E:404:VAL:HG11	1.75	0.51
1:F:317:SER:HB3	1:F:335:ARG:NH2	2.26	0.51
1:A:137:LEU:HB2	1:A:151:ASN:OD1	2.11	0.51
1:B:96:ILE:N	1:B:96:ILE:HD12	2.26	0.51
1:F:402:ASN:OD1	1:F:404:VAL:HG12	2.11	0.51
1:C:112:LEU:HA	1:C:348:SER:OG	2.11	0.51
1:C:160:ALA:HB2	1:C:188:HIS:CD2	2.46	0.51
1:C:302:GLY:H	1:C:316:ARG:HH21	1.58	0.51
1:C:410:GLY:O	1:C:411:GLU:C	2.54	0.51
1:D:159:LEU:HD13	1:E:34:ASN:ND2	2.25	0.51
1:E:134:GLU:CD	2:E:501:GLU:HG2	2.36	0.51
1:F:285:PHE:HB2	1:F:349:VAL:HG13	1.91	0.51
1:B:286:THR:O	1:B:288:VAL:N	2.44	0.50
1:C:232:MET:HE3	1:C:235:PRO:HA	1.91	0.50
1:E:189:GLU:OE1	1:E:196:GLU:OE2	2.30	0.50
1:E:379:GLU:HA	1:E:382:GLU:CG	2.41	0.50
1:F:402:ASN:HB3	1:F:405:MET:CG	2.41	0.50
1:D:170:ARG:HH11	1:E:84:ALA:HB2	1.75	0.50
1:F:377:LYS:O	1:F:381:MET:HE2	2.11	0.50
1:C:3:LYS:HB3	1:C:75:ASN:OD1	2.11	0.50
1:D:19:LYS:HA	1:D:39:VAL:CG1	2.41	0.50
1:F:375:MET:HB2	1:F:380:ARG:HG2	1.92	0.50
1:A:13:VAL:HG13	1:A:18:VAL:CB	2.37	0.50
1:A:34:ASN:CG	1:F:159:LEU:HG	2.36	0.50
1:C:232:MET:HE3	1:C:235:PRO:HB3	1.94	0.50
1:D:331:ARG:NH1	3:D:502:ADP:O2A	2.43	0.50
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.93	0.50
1:F:23:LEU:HD23	1:F:92:PHE:HB2	1.93	0.50
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.47	0.50
1:C:202:ALA:HB3	1:C:207:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:TYR:CE2	1:D:97:TYR:CG	3.00	0.50
1:E:52:PHE:CE1	1:E:70:LEU:HD13	2.46	0.50
1:F:45:ALA:HA	1:F:50:VAL:HG23	1.94	0.50
1:A:26:THR:HG21	1:A:342:ASN:OD1	2.11	0.50
1:A:91:ARG:NH2	1:A:213:THR:OG1	2.45	0.50
1:A:152:ASP:OD1	1:A:161:PRO:HD3	2.11	0.50
1:B:21:ILE:HG21	1:B:37:ILE:HD11	1.93	0.50
1:B:396:LEU:HD11	1:B:421:LYS:HB3	1.93	0.50
1:E:48:ASN:OD1	1:E:72:PRO:HD2	2.12	0.50
1:E:159:LEU:CD1	1:F:22:ARG:NH1	2.75	0.50
1:F:251:PHE:HD1	1:F:251:PHE:N	2.10	0.50
1:B:110:ASN:O	1:B:113:LYS:N	2.45	0.50
1:B:258:PHE:O	1:B:267:LEU:HA	2.12	0.50
1:D:119:MET:SD	1:D:250:LEU:HD21	2.52	0.50
1:E:322:ILE:HD12	1:E:322:ILE:N	2.26	0.50
1:C:71:TYR:CD1	1:C:97:TYR:CD1	3.00	0.50
1:C:290:ASN:ND2	1:C:299:LEU:HD21	2.27	0.50
1:F:251:PHE:N	1:F:251:PHE:CD1	2.79	0.50
1:A:58:GLU:O	1:A:61:VAL:HG22	2.11	0.50
1:E:164:LEU:HD23	1:E:164:LEU:O	2.12	0.50
1:E:236:LEU:HB2	1:E:239:VAL:CG2	2.42	0.50
1:F:265:LEU:HD12	1:F:272:LYS:CE	2.31	0.50
1:C:300:VAL:CG1	1:C:301:PRO:HD2	2.42	0.49
1:C:372:ILE:HD12	1:C:373:TYR:H	1.75	0.49
1:D:315:ASN:HB3	1:D:318:PRO:CG	2.43	0.49
1:F:80:PHE:HB3	1:F:82:TRP:CE3	2.47	0.49
1:A:16:GLU:HG3	1:A:88:LYS:NZ	2.27	0.49
1:C:25:PHE:CD1	1:C:33:LYS:HB2	2.47	0.49
1:D:47:ASP:O	1:D:49:LYS:HD2	2.12	0.49
1:D:58:GLU:O	1:D:61:VAL:HG22	2.12	0.49
1:D:96:ILE:N	1:D:96:ILE:HD12	2.27	0.49
1:F:322:ILE:HD12	1:F:322:ILE:H	1.77	0.49
1:A:160:ALA:O	1:A:161:PRO:O	2.30	0.49
1:A:244:MET:O	1:A:337:VAL:HB	2.12	0.49
1:A:264:ASP:C	1:A:265:LEU:HD12	2.38	0.49
1:B:131:PRO:CB	1:B:211:ILE:HD11	2.42	0.49
1:B:169:ARG:HD3	1:B:195:HIS:HB3	1.94	0.49
1:D:52:PHE:CE1	1:D:70:LEU:HD13	2.47	0.49
1:D:159:LEU:HD11	1:E:22:ARG:NH1	2.27	0.49
1:D:249:SER:HA	1:D:258:PHE:CE1	2.48	0.49
1:E:93:ILE:HD12	1:E:209:ASP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:PRO:HD2	1:E:335:ARG:NH2	2.27	0.49
1:B:155:GLY:O	1:B:158:ASP:HB2	2.12	0.49
1:D:47:ASP:O	1:D:48:ASN:HB2	2.12	0.49
1:D:98:ASN:HB2	1:D:102:THR:O	2.12	0.49
1:C:111:ASN:ND2	1:C:409:LEU:HD23	2.28	0.49
1:C:127:PHE:HE2	1:C:347:LEU:HD12	1.78	0.49
1:D:54:GLY:CA	1:D:68:MET:HG3	2.40	0.49
1:D:187:HIS:NE2	1:D:196:GLU:OE1	2.45	0.49
1:D:203:GLY:O	1:D:205:VAL:N	2.46	0.49
1:D:244:MET:HE2	1:D:339:PRO:HA	1.93	0.49
1:F:48:ASN:ND2	1:F:71:TYR:CD2	2.81	0.49
1:F:191:ALA:HB1	1:F:239:VAL:HG22	1.93	0.49
1:A:58:GLU:OE2	1:A:416:HIS:CD2	2.66	0.49
1:F:285:PHE:HB3	1:F:405:MET:SD	2.52	0.49
1:F:325:SER:CB	1:F:331:ARG:HH22	2.21	0.49
1:A:249:SER:OG	3:A:502:ADP:N1	2.40	0.49
1:B:368:ILE:N	1:B:368:ILE:HD12	2.27	0.49
1:D:394:GLU:OE1	6:D:601:HOH:O	2.20	0.49
1:E:323:PRO:HD2	1:E:331:ARG:HH22	1.77	0.49
1:A:256:ASN:ND2	1:A:328:ILE:O	2.36	0.49
1:B:244:MET:O	1:B:244:MET:HG2	2.12	0.49
1:B:291:PRO:HB2	1:B:421:LYS:NZ	2.28	0.49
1:D:51:MET:HE3	1:D:51:MET:HB3	1.66	0.49
1:F:19:LYS:HD2	1:F:39:VAL:HG11	1.94	0.49
1:A:78:VAL:HG13	1:A:91:ARG:HG3	1.93	0.49
1:A:217:VAL:O	1:A:221:ILE:HG12	2.12	0.49
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.95	0.49
1:D:291:PRO:HG3	1:D:341:ALA:HA	1.95	0.49
1:F:134:GLU:HG2	1:F:189:GLU:HG3	1.94	0.49
1:A:172:ILE:CD1	1:A:218:VAL:HA	2.42	0.49
1:B:78:VAL:CG1	1:B:179:MET:HE3	2.36	0.49
1:B:168:CYS:O	1:B:172:ILE:HG13	2.13	0.49
1:C:170:ARG:O	1:C:171:ASP:C	2.56	0.49
1:E:159:LEU:CD1	1:F:22:ARG:HH11	2.24	0.49
1:E:306:PRO:HG2	1:E:335:ARG:C	2.37	0.49
1:E:371:ASN:HB3	1:E:374:VAL:CG1	2.42	0.49
1:F:402:ASN:O	1:F:406:VAL:HG23	2.12	0.49
1:A:304:GLU:HG3	1:A:304:GLU:O	2.13	0.48
1:B:119:MET:HE3	1:B:120:GLU:HG3	1.94	0.48
1:C:378:GLU:OE2	1:C:378:GLU:N	2.44	0.48
1:D:46:LEU:HD23	1:D:74:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:TYR:CE1	1:E:99:PRO:HA	2.48	0.48
1:B:21:ILE:O	1:B:21:ILE:HG22	2.13	0.48
1:C:16:GLU:O	1:C:88:LYS:HD2	2.13	0.48
1:C:414:PHE:O	1:C:418:ILE:HG12	2.14	0.48
1:F:80:PHE:C	1:F:82:TRP:H	2.19	0.48
1:A:127:PHE:CZ	1:A:248:LEU:CD2	2.96	0.48
1:F:78:VAL:HB	1:F:91:ARG:HG3	1.95	0.48
1:A:383:ASN:N	1:A:383:ASN:OD1	2.47	0.48
1:C:376:SER:OG	1:C:378:GLU:CD	2.56	0.48
1:E:159:LEU:C	1:E:159:LEU:HD12	2.38	0.48
1:A:76:THR:O	1:A:91:ARG:NH1	2.46	0.48
1:B:58:GLU:O	1:B:61:VAL:HG22	2.13	0.48
1:C:58:GLU:O	1:C:61:VAL:HG22	2.14	0.48
1:C:270:THR:HG22	1:C:358:ILE:HD12	1.94	0.48
1:C:285:PHE:HB3	1:C:405:MET:SD	2.54	0.48
1:D:170:ARG:HH11	1:E:84:ALA:CB	2.27	0.48
1:E:142:GLU:CD	1:E:142:GLU:H	2.20	0.48
1:E:161:PRO:O	1:E:162:THR:C	2.56	0.48
1:E:323:PRO:HG2	1:E:331:ARG:CZ	2.43	0.48
1:A:181:PHE:HZ	1:A:210:ASP:HA	1.78	0.48
1:A:207:SER:O	1:A:211:ILE:HG13	2.13	0.48
1:A:311:TRP:CB	1:A:320:ILE:HB	2.39	0.48
1:B:311:TRP:HB3	1:B:320:ILE:HB	1.96	0.48
1:B:319:LEU:HD12	1:B:319:LEU:O	2.14	0.48
1:C:290:ASN:O	1:C:296:TYR:CE1	2.65	0.48
1:E:211:ILE:HG22	1:E:211:ILE:O	2.13	0.48
1:F:259:PHE:CG	1:F:327:GLY:HA2	2.49	0.48
1:F:388:LEU:HB3	1:F:389:PRO:CD	2.44	0.48
1:C:10:GLU:O	1:C:14:LYS:HD3	2.14	0.48
1:C:22:ARG:HB3	1:C:34:ASN:HD22	1.79	0.48
1:D:302:GLY:HA2	1:D:316:ARG:HH12	1.78	0.48
1:E:104:PHE:CZ	1:E:106:GLY:HA3	2.49	0.48
1:F:131:PRO:HG2	1:F:199:PHE:HD1	1.79	0.48
1:F:139:LYS:N	1:F:149:GLU:O	2.46	0.48
1:C:169:ARG:HH21	1:C:188:HIS:HA	1.79	0.48
1:D:266:GLN:O	1:D:267:LEU:HD13	2.13	0.48
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.49	0.48
1:A:324:ALA:O	1:A:325:SER:O	2.32	0.48
1:B:131:PRO:C	1:B:133:PRO:HD3	2.38	0.48
1:C:285:PHE:HB2	1:C:349:VAL:CG1	2.43	0.48
1:E:68:MET:HG3	1:E:97:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:PHE:C	1:E:414:PHE:CD2	2.91	0.48
1:F:54:GLY:HA3	1:F:68:MET:CE	2.41	0.48
1:F:265:LEU:CD1	1:F:272:LYS:HE2	2.30	0.48
1:F:384:GLY:C	1:F:385:ILE:HG13	2.39	0.48
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.43	0.47
1:C:240:ASN:HD21	2:C:501:GLU:HA	1.78	0.47
1:D:27:ASP:OD2	1:D:27:ASP:C	2.57	0.47
1:D:134:GLU:HG2	1:D:196:GLU:HB2	1.95	0.47
1:E:131:PRO:HG2	1:E:199:PHE:CD1	2.49	0.47
1:E:251:PHE:HE1	3:E:502:ADP:HN62	1.60	0.47
1:A:360:ASN:O	1:A:361:LYS:C	2.57	0.47
1:E:243:GLY:HA3	2:E:501:GLU:HB3	1.96	0.47
1:F:98:ASN:OD1	1:F:104:PHE:HA	2.14	0.47
1:F:284:SER:O	1:F:399:PHE:HB2	2.14	0.47
1:A:314:GLN:C	1:A:315:ASN:HD22	2.17	0.47
1:A:376:SER:H	1:A:379:GLU:HB3	1.79	0.47
1:E:174:LEU:HD13	1:F:86:LYS:HB2	1.95	0.47
1:F:52:PHE:CZ	1:F:96:ILE:HD12	2.50	0.47
1:F:100:ASP:O	1:F:102:THR:N	2.47	0.47
1:F:311:TRP:H	1:F:311:TRP:HD1	1.60	0.47
1:A:239:VAL:O	1:A:240:ASN:C	2.57	0.47
1:C:161:PRO:HB2	1:C:167:ASN:HA	1.97	0.47
1:D:117:LYS:HA	1:D:120:GLU:HB2	1.96	0.47
1:A:256:ASN:OD1	1:A:258:PHE:HB2	2.14	0.47
1:E:285:PHE:HB3	1:E:405:MET:SD	2.55	0.47
1:F:205:VAL:HG13	1:F:206:ARG:N	2.28	0.47
1:C:214:PHE:O	1:C:218:VAL:HG23	2.14	0.47
1:E:11:LYS:O	1:E:15:GLU:HG2	2.13	0.47
1:E:175:GLU:OE1	1:F:86:LYS:HE3	2.14	0.47
1:F:191:ALA:CB	1:F:239:VAL:HG22	2.44	0.47
1:A:129:LEU:O	1:A:201:TYR:HA	2.15	0.47
1:A:172:ILE:HD13	1:A:218:VAL:HA	1.95	0.47
1:A:190:VAL:HG21	1:A:304:GLU:OE1	2.14	0.47
1:A:286:THR:OG1	1:A:388:LEU:HD22	2.15	0.47
1:B:379:GLU:HA	1:B:382:GLU:HG3	1.96	0.47
1:C:25:PHE:CE1	1:C:33:LYS:CB	2.98	0.47
1:C:83:THR:C	1:C:84:ALA:O	2.58	0.47
1:C:129:LEU:HD22	1:C:131:PRO:N	2.29	0.47
1:C:187:HIS:CE1	1:C:196:GLU:OE1	2.68	0.47
1:C:247:ASN:HB3	1:C:331:ARG:HD2	1.97	0.47
1:D:135:PHE:HB3	1:D:231:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:LEU:HD13	1:D:192:PRO:HB2	1.97	0.47
1:D:396:LEU:O	1:D:399:PHE:N	2.48	0.47
1:F:78:VAL:HG21	1:F:91:ARG:NH2	2.30	0.47
1:F:250:LEU:HB2	1:F:258:PHE:CE2	2.49	0.47
1:F:316:ARG:HD2	1:F:371:ASN:ND2	2.29	0.47
1:B:328:ILE:C	1:B:330:THR:H	2.22	0.47
1:B:429:ARG:HD3	1:B:430:THR:HG23	1.97	0.47
1:D:221:ILE:O	1:D:225:HIS:ND1	2.48	0.47
1:A:51:MET:HE1	1:F:325:SER:OG	2.15	0.47
1:B:342:ASN:OD1	1:B:343:PRO:HD2	2.15	0.47
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.74	0.47
1:D:388:LEU:HB3	1:D:389:PRO:HD2	1.97	0.47
1:E:137:LEU:HD23	1:E:229:ALA:HA	1.97	0.47
1:E:187:HIS:HE1	1:E:196:GLU:CD	2.23	0.47
1:E:315:ASN:ND2	1:E:372:ILE:HD12	2.30	0.47
1:F:60:PHE:CE1	1:F:423:ILE:HD11	2.50	0.47
1:F:134:GLU:HB2	1:F:243:GLY:H	1.80	0.47
1:F:205:VAL:C	1:F:207:SER:H	2.22	0.47
1:A:17:ASN:OD1	1:A:17:ASN:O	2.33	0.47
1:A:93:ILE:HD12	1:A:209:ASP:CG	2.40	0.47
1:A:139:LYS:HB2	1:A:149:GLU:HB2	1.96	0.47
1:B:118:GLU:O	1:B:121:ASP:HB2	2.15	0.47
1:B:160:ALA:CB	1:B:188:HIS:HD2	2.28	0.47
1:C:372:ILE:HG22	1:C:385:ILE:HD13	1.97	0.47
1:D:49:LYS:HA	1:D:69:TYR:CE2	2.49	0.47
1:D:140:LEU:HD12	1:D:226:GLY:C	2.40	0.47
1:D:376:SER:OG	1:D:379:GLU:HB2	2.15	0.47
1:E:24:GLN:HE21	1:E:24:GLN:HB2	1.47	0.47
1:B:298:ARG:C	1:B:300:VAL:H	2.23	0.46
1:B:315:ASN:HD21	1:B:372:ILE:H	1.63	0.46
1:D:58:GLU:HB3	1:D:61:VAL:HG23	1.98	0.46
1:D:309:VAL:HG23	1:D:386:VAL:HB	1.97	0.46
1:E:357:GLY:HA2	1:E:362:LEU:HD12	1.96	0.46
1:A:116:LEU:HD23	1:A:351:LEU:HD22	1.96	0.46
1:A:206:ARG:HH11	1:A:206:ARG:HG3	1.79	0.46
1:B:184:GLU:HG3	3:B:502:ADP:H3'	1.98	0.46
1:B:315:ASN:ND2	1:B:372:ILE:HG22	2.30	0.46
1:C:314:GLN:HE21	1:D:64:GLU:HB2	1.79	0.46
1:D:131:PRO:HG2	1:D:199:PHE:CD1	2.51	0.46
1:E:124:PHE:CD1	1:E:124:PHE:N	2.83	0.46
1:E:124:PHE:HD1	1:E:124:PHE:H	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:MET:HB2	1:F:380:ARG:CG	2.45	0.46
1:F:399:PHE:CE1	1:F:405:MET:HB3	2.49	0.46
1:F:402:ASN:HB3	1:F:405:MET:HG3	1.98	0.46
1:B:48:ASN:HB3	1:B:71:TYR:CD1	2.50	0.46
1:B:164:LEU:HD11	1:C:82:TRP:CD1	2.51	0.46
1:B:176:LEU:HD13	1:B:183:ILE:HD11	1.98	0.46
1:D:211:ILE:O	1:D:214:PHE:N	2.47	0.46
1:F:131:PRO:C	1:F:133:PRO:HD3	2.40	0.46
1:F:289:THR:HB	1:F:337:VAL:HG22	1.98	0.46
1:F:326:ARG:HD3	1:F:326:ARG:HA	1.64	0.46
1:A:374:VAL:HG23	1:A:374:VAL:O	2.14	0.46
1:A:379:GLU:O	1:A:382:GLU:HG2	2.15	0.46
1:C:131:PRO:HG2	1:C:199:PHE:CE1	2.50	0.46
1:C:260:ASP:HB2	1:C:268:SER:HB3	1.98	0.46
1:C:414:PHE:C	1:C:414:PHE:CD2	2.93	0.46
1:F:300:VAL:CG1	1:F:301:PRO:HD2	2.45	0.46
1:A:64:GLU:OE1	1:F:314:GLN:OE1	2.34	0.46
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.76	0.46
1:D:160:ALA:HB1	1:D:161:PRO:HD3	1.96	0.46
1:D:311:TRP:CZ3	1:D:367:PRO:HB3	2.50	0.46
1:D:323:PRO:HG3	1:D:331:ARG:NE	2.30	0.46
1:E:131:PRO:CG	1:E:199:PHE:CD1	2.96	0.46
1:F:189:GLU:OE2	1:F:190:VAL:HG23	2.16	0.46
1:F:323:PRO:HD2	1:F:331:ARG:O	2.15	0.46
1:A:132:GLU:HB3	1:A:196:GLU:OE2	2.15	0.46
1:E:71:TYR:CD2	1:E:97:TYR:CD1	3.03	0.46
1:E:71:TYR:CD2	1:E:97:TYR:CE1	3.03	0.46
1:E:315:ASN:HB3	1:E:318:PRO:CG	2.45	0.46
1:F:19:LYS:HB2	1:F:87:GLY:HA3	1.97	0.46
1:F:48:ASN:ND2	1:F:71:TYR:CG	2.83	0.46
1:F:259:PHE:HB2	1:F:330:THR:OG1	2.15	0.46
1:A:345:LEU:HD22	1:A:409:LEU:CD2	2.44	0.46
1:B:121:ASP:O	1:B:122:LEU:HD23	2.16	0.46
1:C:125:SER:O	1:C:126:ASP:OD1	2.34	0.46
1:D:185:ALA:CB	1:E:37:ILE:HG22	2.44	0.46
1:E:57:ILE:HG13	1:E:96:ILE:CD1	2.45	0.46
1:E:120:GLU:O	1:E:122:LEU:N	2.48	0.46
1:A:45:ALA:HA	1:A:50:VAL:CG2	2.44	0.46
1:A:109:ARG:HG3	1:A:344:TYR:CE2	2.51	0.46
1:A:112:LEU:HD13	1:A:205:VAL:HG12	1.98	0.46
1:A:427:MET:O	1:A:431:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PHE:CE1	1:B:405:MET:HB3	2.51	0.46
1:B:433:HIS:HB3	1:B:434:PRO:HD2	1.98	0.46
1:C:71:TYR:C	1:C:94:CYS:HB3	2.41	0.46
1:C:241:GLY:HA3	1:C:298:ARG:HG3	1.98	0.46
1:C:411:GLU:O	1:C:415:GLU:HG3	2.15	0.46
1:D:318:PRO:CG	1:D:321:ARG:HB2	2.36	0.46
1:B:53:ASP:OD2	1:B:53:ASP:C	2.59	0.46
1:C:48:ASN:OD1	1:C:72:PRO:HD2	2.16	0.46
1:E:129:LEU:HD12	1:E:207:SER:HB3	1.97	0.46
1:B:397:GLU:OE1	1:B:400:LYS:HE3	2.16	0.46
1:C:132:GLU:HB3	1:C:198:ASP:OD1	2.16	0.46
1:D:161:PRO:HB2	1:D:167:ASN:H	1.81	0.46
1:E:285:PHE:C	1:E:285:PHE:HD1	2.23	0.46
1:A:20:TYR:HB3	1:A:89:VAL:HG22	1.98	0.45
1:A:114:ARG:NH1	1:A:115:ILE:CD1	2.78	0.45
1:A:164:LEU:HB2	1:B:220:THR:HG23	1.97	0.45
1:A:207:SER:O	1:A:210:ASP:HB2	2.16	0.45
1:A:220:THR:HG23	1:F:164:LEU:HB3	1.97	0.45
1:B:285:PHE:CD1	1:B:285:PHE:C	2.94	0.45
1:B:435:TRP:O	1:B:436:GLU:C	2.59	0.45
1:C:22:ARG:HB3	1:C:34:ASN:ND2	2.31	0.45
1:C:98:ASN:OD1	1:C:102:THR:HG23	2.16	0.45
1:D:112:LEU:HD23	1:D:112:LEU:O	2.17	0.45
1:D:256:ASN:ND2	1:D:330:THR:O	2.50	0.45
1:F:281:HIS:O	1:F:282:ALA:C	2.58	0.45
1:A:12:LEU:O	1:A:16:GLU:HB2	2.16	0.45
1:B:128:ASN:HB3	1:B:201:TYR:HD1	1.80	0.45
1:B:164:LEU:CD1	1:C:220:THR:HG22	2.39	0.45
1:B:370:ARG:NH2	1:B:379:GLU:OE1	2.49	0.45
1:C:164:LEU:HB2	1:D:220:THR:HG23	1.98	0.45
1:C:187:HIS:C	1:C:187:HIS:CD2	2.94	0.45
1:C:203:GLY:O	1:C:204:ALA:C	2.59	0.45
1:C:260:ASP:CG	1:C:263:ALA:HB2	2.41	0.45
1:D:137:LEU:HD12	1:D:195:HIS:NE2	2.31	0.45
1:E:48:ASN:HB3	1:E:71:TYR:CE1	2.50	0.45
1:F:309:VAL:HG23	1:F:386:VAL:O	2.16	0.45
1:C:256:ASN:OD1	1:C:258:PHE:HB2	2.16	0.45
1:E:85:GLU:OE1	1:E:86:LYS:HE2	2.16	0.45
1:E:338:ASP:HB2	1:E:339:PRO:HD2	1.98	0.45
1:F:285:PHE:HB2	1:F:349:VAL:CG1	2.46	0.45
1:A:96:ILE:HG22	1:A:104:PHE:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:CB	1:A:169:ARG:NH1	2.72	0.45
1:A:405:MET:O	1:A:408:ALA:HB3	2.17	0.45
1:B:56:SER:C	1:B:58:GLU:H	2.24	0.45
1:B:161:PRO:O	1:B:167:ASN:OD1	2.35	0.45
1:B:204:ALA:O	1:B:207:SER:N	2.50	0.45
1:C:38:PRO:O	1:C:41:GLN:HB2	2.16	0.45
1:D:138:PHE:HB3	1:D:147:THR:O	2.17	0.45
1:D:232:MET:O	1:D:235:PRO:HD3	2.17	0.45
1:E:5:THR:H	1:E:8:ASP:HB2	1.82	0.45
1:E:95:ASP:OD1	1:E:109:ARG:HG2	2.17	0.45
1:E:236:LEU:O	1:E:239:VAL:HG22	2.15	0.45
1:A:285:PHE:CD1	1:A:285:PHE:C	2.95	0.45
1:B:162:THR:HG21	1:C:220:THR:OG1	2.16	0.45
1:C:122:LEU:HD11	1:C:359:LYS:HB2	1.99	0.45
1:C:388:LEU:HB3	1:C:389:PRO:HD2	1.97	0.45
1:D:396:LEU:O	1:D:397:GLU:C	2.59	0.45
1:E:249:SER:OG	3:E:502:ADP:N1	2.43	0.45
1:F:27:ASP:CB	1:F:33:LYS:HE3	2.46	0.45
1:F:127:PHE:CG	1:F:351:LEU:HD12	2.52	0.45
1:A:105:GLU:O	1:A:105:GLU:HG3	2.16	0.45
1:A:315:ASN:OD1	1:A:371:ASN:HA	2.16	0.45
1:A:379:GLU:C	1:A:382:GLU:HG2	2.42	0.45
1:B:214:PHE:O	1:B:216:LEU:N	2.49	0.45
1:B:285:PHE:HB3	1:B:405:MET:SD	2.57	0.45
1:B:309:VAL:O	1:B:310:ALA:HB2	2.17	0.45
1:B:388:LEU:HB3	1:B:389:PRO:HD2	1.99	0.45
1:D:147:THR:OG1	1:D:149:GLU:HB2	2.16	0.45
1:D:159:LEU:HD13	1:E:34:ASN:CG	2.42	0.45
1:D:361:LYS:O	1:D:362:LEU:O	2.34	0.45
1:E:310:ALA:HB1	1:E:368:ILE:HD12	1.98	0.45
1:E:410:GLY:O	1:E:411:GLU:C	2.60	0.45
1:A:34:ASN:C	1:A:34:ASN:ND2	2.74	0.45
1:A:104:PHE:CD1	1:A:104:PHE:C	2.93	0.45
1:B:282:ALA:HA	1:B:285:PHE:CE2	2.52	0.45
1:B:373:TYR:CD1	1:B:373:TYR:C	2.95	0.45
1:C:120:GLU:HA	1:C:124:PHE:O	2.17	0.45
1:C:160:ALA:O	1:C:161:PRO:O	2.35	0.45
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.98	0.45
1:C:368:ILE:O	1:C:368:ILE:HG22	2.16	0.45
1:D:54:GLY:C	1:D:56:SER:N	2.74	0.45
1:D:69:TYR:CD1	1:D:99:PRO:HA	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:LEU:HD13	1:D:192:PRO:O	2.16	0.45
1:E:5:THR:N	1:E:8:ASP:HB2	2.32	0.45
1:E:59:GLY:O	1:E:62:ARG:HG3	2.17	0.45
1:E:68:MET:HE3	1:E:68:MET:HB2	1.74	0.45
1:E:271:ALA:O	1:E:275:ILE:HD12	2.16	0.45
1:E:285:PHE:HB2	1:E:349:VAL:HG13	1.98	0.45
1:F:311:TRP:CE2	1:F:367:PRO:HB3	2.52	0.45
1:F:421:LYS:O	1:F:424:GLU:HB3	2.16	0.45
1:B:136:PHE:CD1	1:B:235:PRO:HG2	2.52	0.45
1:B:311:TRP:CE2	1:B:367:PRO:HB3	2.51	0.45
1:C:57:ILE:C	1:C:59:GLY:H	2.25	0.45
1:C:276:ALA:HB2	1:C:364:ALA:CA	2.47	0.45
1:C:293:VAL:HG11	1:C:428:PHE:CD1	2.52	0.45
1:D:161:PRO:O	1:D:162:THR:C	2.60	0.45
1:D:272:LYS:O	1:D:364:ALA:HB2	2.17	0.45
1:E:135:PHE:HB3	1:E:231:PHE:CE1	2.52	0.45
1:F:370:ARG:HH21	1:F:375:MET:HG2	1.82	0.45
1:A:92:PHE:CD1	1:A:92:PHE:N	2.85	0.45
1:A:206:ARG:CG	1:A:206:ARG:NH1	2.67	0.45
1:E:37:ILE:HD12	1:E:41:GLN:HB2	1.99	0.45
1:E:249:SER:HA	1:E:258:PHE:CE1	2.52	0.45
1:E:331:ARG:HD2	3:E:502:ADP:C4	2.52	0.45
1:F:116:LEU:O	1:F:119:MET:HB3	2.17	0.45
1:F:315:ASN:C	1:F:318:PRO:HD3	2.41	0.45
1:A:259:PHE:O	1:A:260:ASP:HB2	2.17	0.45
1:B:20:TYR:HE2	1:B:22:ARG:NH1	2.14	0.45
1:B:21:ILE:CG2	1:B:37:ILE:HD11	2.46	0.45
1:B:106:GLY:HA2	1:B:413:LEU:HG	1.99	0.45
1:B:368:ILE:HG12	1:B:385:ILE:HD11	1.99	0.45
1:C:410:GLY:O	1:C:412:HIS:N	2.50	0.45
1:D:30:GLY:N	1:D:342:ASN:ND2	2.64	0.45
1:D:171:ASP:OD1	1:D:225:HIS:NE2	2.40	0.45
1:E:281:HIS:O	1:E:282:ALA:C	2.60	0.45
1:E:310:ALA:CB	1:E:372:ILE:HD11	2.47	0.45
1:F:214:PHE:O	1:F:218:VAL:HG23	2.17	0.45
1:A:410:GLY:O	1:A:411:GLU:C	2.59	0.44
1:C:176:LEU:O	1:C:181:PHE:HB2	2.17	0.44
1:C:181:PHE:HB3	1:C:183:ILE:HG13	1.98	0.44
1:D:172:ILE:HG21	1:D:218:VAL:HG22	1.98	0.44
1:E:301:PRO:HA	1:E:316:ARG:HH12	1.82	0.44
1:F:41:GLN:HE22	1:F:44:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:GLU:O	1:F:167:ASN:C	2.60	0.44
1:A:105:GLU:O	1:A:105:GLU:CG	2.65	0.44
1:B:142:GLU:OE2	1:B:143:LYS:HG3	2.18	0.44
1:B:160:ALA:CB	1:B:169:ARG:NH1	2.68	0.44
1:C:289:THR:O	1:C:341:ALA:HB2	2.17	0.44
1:D:201:TYR:CD1	1:D:201:TYR:C	2.95	0.44
1:D:239:VAL:CG2	1:D:240:ASN:N	2.78	0.44
1:E:164:LEU:CD2	1:F:224:LYS:HB2	2.46	0.44
1:E:170:ARG:NH1	1:E:171:ASP:OD2	2.50	0.44
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.48	0.44
1:E:379:GLU:OE1	1:E:382:GLU:HG3	2.18	0.44
1:F:9:ILE:HD11	1:F:74:LEU:HB3	1.98	0.44
1:F:20:TYR:CZ	1:F:36:GLU:HB2	2.52	0.44
1:F:374:VAL:CG2	1:F:375:MET:H	2.27	0.44
1:A:281:HIS:HD2	1:A:353:ALA:HA	1.81	0.44
1:B:46:LEU:HD22	1:B:74:LEU:HD21	1.98	0.44
1:B:213:THR:O	1:B:217:VAL:HG23	2.17	0.44
1:D:141:ASP:HB3	1:D:147:THR:CG2	2.48	0.44
1:E:231:PHE:CD1	1:E:339:PRO:HB3	2.52	0.44
1:E:372:ILE:HA	1:E:375:MET:CE	2.47	0.44
1:F:52:PHE:HZ	1:F:96:ILE:HD12	1.81	0.44
1:F:137:LEU:HD23	1:F:229:ALA:HA	1.98	0.44
1:A:131:PRO:HD2	1:A:199:PHE:CB	2.44	0.44
1:A:274:PHE:CE1	1:A:354:GLY:HA3	2.52	0.44
1:B:280:LYS:HD2	1:B:362:LEU:HD21	1.98	0.44
1:B:372:ILE:CD1	1:B:385:ILE:HG21	2.48	0.44
1:C:243:GLY:HA3	2:C:501:GLU:OXT	2.18	0.44
1:D:164:LEU:O	1:D:165:GLY:O	2.34	0.44
1:D:326:ARG:HA	1:D:326:ARG:HD3	1.68	0.44
1:D:371:ASN:O	1:D:374:VAL:HG22	2.17	0.44
1:E:37:ILE:HB	1:E:38:PRO:HD2	2.00	0.44
1:E:197:ILE:HD12	1:E:214:PHE:HE1	1.82	0.44
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.99	0.44
1:F:9:ILE:O	1:F:13:VAL:HG23	2.18	0.44
1:F:134:GLU:OE2	1:F:189:GLU:OE1	2.35	0.44
1:F:423:ILE:HA	1:F:426:ASP:HB2	1.99	0.44
1:D:91:ARG:HD2	1:D:91:ARG:C	2.43	0.44
1:E:25:PHE:HE1	1:E:57:ILE:CD1	2.30	0.44
1:E:203:GLY:O	1:E:204:ALA:C	2.60	0.44
1:E:364:ALA:HA	1:E:365:PRO:HD3	1.79	0.44
1:F:4:TYR:HB3	1:F:9:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:SER:OG	1:B:51:MET:CE	2.65	0.44
1:B:167:ASN:ND2	1:B:170:ARG:H	2.13	0.44
1:B:425:TRP:NE1	1:B:429:ARG:HG2	2.33	0.44
1:B:433:HIS:HB3	1:B:434:PRO:CD	2.47	0.44
1:C:182:GLU:OE2	1:C:182:GLU:HA	2.17	0.44
1:D:188:HIS:HE1	1:D:191:ALA:O	2.01	0.44
1:D:208:CYS:O	1:D:209:ASP:C	2.60	0.44
1:D:268:SER:O	1:D:272:LYS:HG2	2.17	0.44
1:E:140:LEU:CD2	1:E:228:HIS:HB2	2.46	0.44
1:E:150:LEU:HD13	1:E:192:PRO:HG2	1.99	0.44
1:E:372:ILE:HA	1:E:375:MET:HE3	1.99	0.44
1:F:370:ARG:NH2	1:F:375:MET:HG2	2.33	0.44
1:F:419:GLU:O	1:F:423:ILE:HG23	2.18	0.44
1:A:96:ILE:HG21	1:A:104:PHE:HD2	1.83	0.44
1:B:162:THR:HG22	1:B:163:ASP:H	1.83	0.44
1:D:269:GLU:O	1:D:273:HIS:CG	2.70	0.44
1:D:289:THR:HB	1:D:337:VAL:HG22	2.00	0.44
1:E:68:MET:CG	1:E:96:ILE:HG22	2.45	0.44
1:E:119:MET:HA	1:E:355:LEU:HD11	2.00	0.44
1:F:131:PRO:HG2	1:F:199:PHE:CD1	2.53	0.44
1:A:22:ARG:NH2	1:F:163:ASP:OD1	2.39	0.44
1:A:179:MET:HE3	1:A:179:MET:HB3	1.81	0.44
1:A:276:ALA:HB1	1:A:362:LEU:HB3	2.00	0.44
1:B:48:ASN:HB3	1:B:71:TYR:CE1	2.53	0.44
1:C:39:VAL:C	1:C:41:GLN:N	2.76	0.44
1:C:150:LEU:HD22	1:C:193:GLY:HA3	1.99	0.44
1:C:308:TYR:CD1	1:C:372:ILE:HD13	2.53	0.44
1:C:311:TRP:CE2	1:C:367:PRO:HA	2.52	0.44
1:D:377:LYS:HG2	1:D:381:MET:HE2	1.99	0.44
1:D:405:MET:HE2	1:D:405:MET:HA	1.99	0.44
1:E:76:THR:HG21	1:E:93:ILE:HB	1.99	0.44
1:E:351:LEU:C	1:E:353:ALA:N	2.75	0.44
1:E:406:VAL:HG22	1:E:414:PHE:CD1	2.52	0.44
1:F:379:GLU:OE1	1:F:379:GLU:CA	2.57	0.44
1:A:325:SER:HB2	1:A:331:ARG:HH11	1.83	0.44
1:B:56:SER:C	1:B:58:GLU:N	2.75	0.44
1:B:249:SER:HA	1:B:258:PHE:HE1	1.83	0.44
1:C:124:PHE:CD2	1:C:250:LEU:HD22	2.53	0.44
1:D:154:GLY:HA3	1:D:188:HIS:NE2	2.33	0.44
1:E:16:GLU:HB3	1:E:18:VAL:HG23	2.00	0.44
1:F:205:VAL:O	1:F:206:ARG:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:VAL:O	1:F:207:SER:N	2.51	0.44
1:A:331:ARG:NH2	3:A:502:ADP:O4'	2.51	0.43
1:A:376:SER:O	1:A:379:GLU:N	2.51	0.43
1:B:116:LEU:CD2	1:B:351:LEU:HD11	2.45	0.43
1:C:14:LYS:HD2	1:C:14:LYS:N	2.33	0.43
1:D:84:ALA:C	1:D:86:LYS:H	2.25	0.43
1:D:141:ASP:C	1:D:141:ASP:OD2	2.60	0.43
1:E:321:ARG:HD3	1:E:335:ARG:HD2	1.99	0.43
1:E:426:ASP:HA	1:E:429:ARG:HG2	1.99	0.43
1:F:182:GLU:HB2	1:F:200:LYS:HG3	2.00	0.43
1:B:135:PHE:CE1	1:B:195:HIS:HB2	2.53	0.43
1:C:270:THR:HG23	1:C:358:ILE:HD12	1.98	0.43
1:D:49:LYS:HA	1:D:69:TYR:HE2	1.84	0.43
1:D:134:GLU:HG2	1:D:189:GLU:HG3	2.00	0.43
1:D:183:ILE:HG22	1:D:198:ASP:O	2.17	0.43
1:D:269:GLU:OE1	1:D:272:LYS:HG3	2.18	0.43
1:E:76:THR:O	1:E:77:PHE:C	2.61	0.43
1:E:165:GLY:O	1:E:166:GLU:C	2.61	0.43
1:E:284:SER:HA	1:E:398:GLU:HB3	1.99	0.43
1:E:347:LEU:HA	1:E:347:LEU:HD23	1.55	0.43
1:F:52:PHE:CD1	1:F:70:LEU:HD22	2.52	0.43
1:F:120:GLU:C	1:F:122:LEU:H	2.26	0.43
1:F:123:GLY:C	1:F:252:LYS:HE2	2.42	0.43
1:F:399:PHE:HE1	1:F:405:MET:HB3	1.81	0.43
1:B:23:LEU:HD23	1:B:92:PHE:HB2	2.01	0.43
1:B:112:LEU:O	1:B:116:LEU:HB2	2.17	0.43
1:C:68:MET:HE3	1:C:68:MET:HB2	1.64	0.43
1:C:367:PRO:O	1:C:368:ILE:C	2.61	0.43
1:C:436:GLU:O	1:C:440:TYR:CD2	2.71	0.43
1:D:27:ASP:OD1	1:D:33:LYS:CE	2.66	0.43
1:D:234:LYS:NZ	1:D:239:VAL:O	2.42	0.43
1:D:354:GLY:O	1:D:357:GLY:N	2.51	0.43
1:D:435:TRP:O	1:D:438:GLU:HG2	2.17	0.43
1:E:27:ASP:CG	1:E:33:LYS:HE3	2.43	0.43
1:E:406:VAL:O	1:E:410:GLY:N	2.48	0.43
1:F:185:ALA:O	1:F:186:SER:CB	2.65	0.43
1:A:342:ASN:ND2	1:A:345:LEU:HG	2.31	0.43
1:A:375:MET:HE2	1:A:380:ARG:HA	2.00	0.43
1:B:130:GLY:HA3	3:B:502:ADP:O2'	2.18	0.43
1:B:288:VAL:HG11	1:B:345:LEU:O	2.19	0.43
1:C:51:MET:HE1	1:C:67:ASP:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ILE:CG2	1:D:332:VAL:HG23	2.47	0.43
1:E:325:SER:O	1:E:326:ARG:NE	2.51	0.43
1:F:360:ASN:O	1:F:361:LYS:C	2.61	0.43
1:F:378:GLU:C	1:F:380:ARG:N	2.76	0.43
1:A:48:ASN:OD1	1:A:71:TYR:HA	2.18	0.43
1:A:246:CYS:SG	1:A:337:VAL:HG21	2.58	0.43
1:C:434:PRO:O	1:C:438:GLU:HG3	2.18	0.43
1:D:266:GLN:HG2	1:D:326:ARG:HG3	2.00	0.43
1:D:376:SER:C	1:D:378:GLU:N	2.75	0.43
1:E:16:GLU:O	1:E:88:LYS:HD2	2.17	0.43
1:E:117:LYS:O	1:E:118:GLU:C	2.62	0.43
1:E:345:LEU:O	1:E:346:ALA:C	2.61	0.43
1:F:261:GLU:HA	1:F:266:GLN:CG	2.49	0.43
1:A:27:ASP:HB3	1:A:33:LYS:CD	2.27	0.43
1:A:426:ASP:HA	1:A:429:ARG:HG2	2.00	0.43
1:E:170:ARG:O	1:E:174:LEU:HG	2.18	0.43
1:A:175:GLU:OE2	1:B:86:LYS:HE3	2.19	0.43
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.86	0.43
1:B:343:PRO:O	1:B:347:LEU:HD23	2.18	0.43
1:C:265:LEU:O	1:C:266:GLN:HB2	2.19	0.43
1:A:295:SER:O	1:A:299:LEU:HD23	2.19	0.43
1:A:298:ARG:HH21	1:A:338:ASP:HB3	1.84	0.43
1:A:368:ILE:HG13	1:A:385:ILE:HD11	2.01	0.43
1:A:387:ASP:OD2	1:A:387:ASP:N	2.43	0.43
1:C:20:TYR:CE2	1:C:36:GLU:HB3	2.54	0.43
1:E:100:ASP:OD2	1:E:102:THR:OG1	2.32	0.43
1:E:181:PHE:HZ	1:E:213:THR:HB	1.84	0.43
1:F:304:GLU:H	1:F:304:GLU:HG2	1.39	0.43
1:F:309:VAL:O	1:F:310:ALA:HB2	2.19	0.43
1:A:33:LYS:HE2	1:F:156:TYR:O	2.18	0.43
1:A:91:ARG:C	1:A:91:ARG:HD2	2.44	0.43
1:A:406:VAL:C	1:A:408:ALA:H	2.27	0.43
1:C:161:PRO:O	1:C:167:ASN:ND2	2.52	0.43
1:D:54:GLY:C	1:D:56:SER:H	2.27	0.43
1:D:153:LYS:HA	1:D:192:PRO:HB3	2.00	0.43
1:D:168:CYS:O	1:D:172:ILE:HG13	2.18	0.43
1:D:282:ALA:O	1:D:284:SER:N	2.52	0.43
1:F:374:VAL:CG2	1:F:375:MET:N	2.80	0.43
1:A:302:GLY:C	1:A:304:GLU:H	2.27	0.43
1:C:184:GLU:H	1:C:199:PHE:HA	1.83	0.43
1:D:380:ARG:C	1:D:382:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:VAL:HA	1:D:414:PHE:CD1	2.53	0.43
1:E:271:ALA:C	1:E:275:ILE:HD12	2.44	0.43
1:E:272:LYS:HA	1:E:275:ILE:CD1	2.43	0.43
1:E:281:HIS:O	1:E:284:SER:N	2.52	0.43
1:F:364:ALA:HA	1:F:365:PRO:HD2	1.93	0.43
1:A:164:LEU:CB	1:B:220:THR:HG23	2.49	0.42
1:B:10:GLU:HG2	1:B:42:LEU:HD21	2.01	0.42
1:B:48:ASN:ND2	1:B:71:TYR:CG	2.86	0.42
1:B:377:LYS:NZ	1:B:380:ARG:HH12	2.17	0.42
1:C:134:GLU:HG2	1:C:189:GLU:HG3	2.00	0.42
1:D:100:ASP:OD1	1:D:100:ASP:C	2.62	0.42
1:D:141:ASP:OD1	1:D:145:GLU:HB2	2.20	0.42
1:E:436:GLU:O	1:E:440:TYR:HB2	2.19	0.42
1:F:366:ALA:HA	1:F:367:PRO:HD2	1.78	0.42
1:B:31:THR:HG22	1:B:32:ILE:N	2.34	0.42
1:D:244:MET:HE2	1:D:244:MET:HB3	1.86	0.42
1:D:328:ILE:C	1:D:330:THR:N	2.77	0.42
1:D:345:LEU:O	1:D:349:VAL:HG22	2.19	0.42
1:D:406:VAL:HG13	1:D:414:PHE:CE1	2.54	0.42
1:F:41:GLN:NE2	1:F:44:LYS:HD3	2.33	0.42
1:A:169:ARG:CG	1:A:169:ARG:NH2	2.73	0.42
1:B:286:THR:C	1:B:288:VAL:N	2.77	0.42
1:B:301:PRO:HA	1:B:307:CYS:SG	2.59	0.42
1:D:396:LEU:C	1:D:398:GLU:N	2.75	0.42
1:F:376:SER:O	1:F:378:GLU:N	2.52	0.42
1:A:34:ASN:ND2	1:A:34:ASN:O	2.52	0.42
1:A:311:TRP:CZ2	1:A:367:PRO:HD3	2.55	0.42
1:B:166:GLU:O	1:B:167:ASN:C	2.61	0.42
1:C:72:PRO:HA	1:C:94:CYS:HB3	2.01	0.42
1:C:114:ARG:NH2	1:C:407:LYS:O	2.53	0.42
1:C:325:SER:HB2	3:C:502:ADP:O3B	2.19	0.42
1:D:6:ARG:HG3	1:D:6:ARG:NH1	2.29	0.42
1:D:107:ASP:HA	1:D:108:PRO:HD3	1.88	0.42
1:D:258:PHE:HB2	1:D:330:THR:HG22	2.02	0.42
1:D:366:ALA:HA	1:D:367:PRO:HD2	1.86	0.42
1:E:78:VAL:CG1	1:E:79:ILE:N	2.82	0.42
1:F:385:ILE:O	1:F:385:ILE:HG22	2.19	0.42
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.80	0.42
1:B:140:LEU:HD23	1:B:146:PRO:CA	2.47	0.42
1:B:427:MET:HE2	1:B:427:MET:HB3	1.94	0.42
1:D:112:LEU:HD23	1:D:112:LEU:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:GLN:HE21	1:E:41:GLN:HB3	1.63	0.42
1:E:244:MET:O	1:E:244:MET:HG2	2.20	0.42
1:D:234:LYS:HG2	1:D:297:LYS:O	2.19	0.42
1:D:266:GLN:HB3	1:D:326:ARG:HH11	1.85	0.42
1:F:360:ASN:O	1:F:361:LYS:O	2.38	0.42
1:F:377:LYS:HD3	1:F:387:ASP:OD2	2.20	0.42
1:A:274:PHE:CE2	1:A:278:ILE:HD11	2.54	0.42
1:C:129:LEU:HD22	1:C:131:PRO:CD	2.49	0.42
1:D:71:TYR:CD2	1:D:97:TYR:CG	3.08	0.42
1:D:304:GLU:CG	2:D:501:GLU:HG2	2.50	0.42
1:D:324:ALA:O	1:D:326:ARG:NE	2.52	0.42
1:F:178:GLU:O	1:F:180:GLY:N	2.52	0.42
1:F:273:HIS:CD2	1:F:361:LYS:HG2	2.55	0.42
1:A:9:ILE:CD1	1:A:74:LEU:HG	2.41	0.42
1:B:16:GLU:O	1:B:17:ASN:HB3	2.20	0.42
1:B:160:ALA:HB2	1:B:188:HIS:CD2	2.51	0.42
1:C:55:SER:O	1:C:62:ARG:HB3	2.20	0.42
1:F:280:LYS:HE3	1:F:280:LYS:HB2	1.66	0.42
1:B:372:ILE:HD12	1:B:372:ILE:O	2.20	0.42
1:C:232:MET:HE3	1:C:235:PRO:CB	2.50	0.42
1:D:131:PRO:HG2	1:D:199:PHE:HD1	1.84	0.42
1:D:349:VAL:HG13	1:D:409:LEU:HD21	2.02	0.42
1:E:109:ARG:NH1	1:E:209:ASP:OD1	2.53	0.42
1:E:134:GLU:OE2	1:E:196:GLU:OE2	2.37	0.42
1:A:113:LYS:O	1:A:117:LYS:HG3	2.20	0.42
1:A:312:SER:OG	1:A:313:ALA:N	2.52	0.42
1:A:405:MET:O	1:A:406:VAL:C	2.63	0.42
1:B:285:PHE:HB2	1:B:349:VAL:HG11	2.00	0.42
1:B:386:VAL:HG22	1:B:387:ASP:O	2.19	0.42
1:C:302:GLY:C	1:C:304:GLU:H	2.28	0.42
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.54	0.42
1:E:399:PHE:CE1	1:E:405:MET:HB3	2.53	0.42
1:A:311:TRP:O	1:A:311:TRP:CD2	2.73	0.41
1:B:412:HIS:CD2	1:B:416:HIS:CD2	3.08	0.41
1:C:39:VAL:O	1:C:39:VAL:HG22	2.19	0.41
1:C:125:SER:C	1:C:126:ASP:CG	2.87	0.41
1:C:163:ASP:HB2	1:D:82:TRP:CE3	2.54	0.41
1:D:380:ARG:HB3	1:D:385:ILE:HG21	2.02	0.41
1:E:146:PRO:HB3	1:E:228:HIS:CG	2.55	0.41
1:E:258:PHE:C	1:E:268:SER:OG	2.63	0.41
1:E:321:ARG:O	1:E:321:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ARG:HG3	1:F:344:TYR:CE2	2.55	0.41
1:B:16:GLU:O	1:B:17:ASN:CB	2.68	0.41
1:B:18:VAL:CG2	1:B:79:ILE:HD12	2.51	0.41
1:B:42:LEU:O	1:B:45:ALA:HB3	2.20	0.41
1:B:160:ALA:HB1	1:B:161:PRO:HD3	1.99	0.41
1:B:260:ASP:HB2	1:B:268:SER:HB3	2.01	0.41
1:C:326:ARG:HD3	1:C:330:THR:OG1	2.20	0.41
1:D:309:VAL:HG23	1:D:386:VAL:O	2.20	0.41
1:E:6:ARG:NE	1:E:46:LEU:HD13	2.35	0.41
1:E:387:ASP:OD2	1:E:387:ASP:N	2.49	0.41
1:E:428:PHE:CD2	1:E:428:PHE:C	2.98	0.41
1:F:119:MET:SD	1:F:127:PHE:HB2	2.61	0.41
1:A:164:LEU:HD13	1:B:82:TRP:CB	2.47	0.41
1:A:174:LEU:O	1:A:177:GLU:HB2	2.20	0.41
1:B:173:VAL:HG22	1:B:197:ILE:HD13	2.01	0.41
1:C:342:ASN:HA	1:C:343:PRO:HD2	1.94	0.41
1:D:55:SER:O	1:D:62:ARG:CB	2.61	0.41
1:E:321:ARG:O	1:E:333:GLU:HB3	2.20	0.41
1:E:328:ILE:H	1:E:328:ILE:HG12	1.44	0.41
1:F:176:LEU:HD23	1:F:217:VAL:HG11	2.00	0.41
1:A:272:LYS:O	1:A:364:ALA:HB2	2.21	0.41
1:C:135:PHE:HB3	1:C:231:PHE:CD1	2.55	0.41
1:C:140:LEU:HD21	1:C:228:HIS:HB2	2.01	0.41
1:C:160:ALA:HB1	1:C:169:ARG:HH22	1.71	0.41
1:D:52:PHE:CD1	1:D:70:LEU:HD13	2.55	0.41
1:E:24:GLN:OE1	1:E:91:ARG:HD3	2.21	0.41
1:E:46:LEU:C	1:E:48:ASN:H	2.28	0.41
1:F:259:PHE:CE2	1:F:327:GLY:HA2	2.54	0.41
1:F:290:ASN:HB3	1:F:295:SER:HB3	2.01	0.41
1:F:399:PHE:HZ	1:F:409:LEU:HD12	1.86	0.41
1:A:196:GLU:OE2	1:A:198:ASP:OD1	2.38	0.41
1:A:311:TRP:O	1:A:311:TRP:CG	2.73	0.41
1:B:167:ASN:ND2	1:B:170:ARG:HB2	2.35	0.41
1:B:239:VAL:HG23	1:B:240:ASN:O	2.20	0.41
1:C:45:ALA:HA	1:C:50:VAL:HG23	2.03	0.41
1:C:131:PRO:CG	1:C:211:ILE:HD11	2.41	0.41
1:C:206:ARG:HG3	1:C:206:ARG:NH1	2.35	0.41
1:C:264:ASP:HB3	1:C:272:LYS:HZ1	1.85	0.41
1:E:27:ASP:HB3	1:E:33:LYS:HG3	2.01	0.41
1:F:293:VAL:HG11	1:F:428:PHE:CD2	2.55	0.41
1:F:414:PHE:CD2	1:F:414:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:O	1:C:361:LYS:C	2.63	0.41
1:C:377:LYS:HA	1:C:380:ARG:HG3	2.01	0.41
1:D:308:TYR:HA	1:D:386:VAL:O	2.20	0.41
1:E:236:LEU:HB2	1:E:239:VAL:HG21	2.02	0.41
1:F:143:LYS:H	1:F:143:LYS:HG2	1.55	0.41
1:F:161:PRO:CG	1:F:166:GLU:OE1	2.69	0.41
1:F:351:LEU:O	1:F:351:LEU:HG	2.21	0.41
1:A:284:SER:CB	1:A:402:ASN:HD22	2.34	0.41
1:A:311:TRP:HE3	1:A:322:ILE:HD11	1.85	0.41
1:B:113:LYS:O	1:B:117:LYS:N	2.51	0.41
1:B:131:PRO:HG2	1:B:199:PHE:CD1	2.56	0.41
1:B:232:MET:HA	1:B:233:PRO:HD3	1.93	0.41
1:B:304:GLU:OE1	1:C:63:ILE:O	2.39	0.41
1:C:303:TYR:HB2	6:C:605:HOH:O	2.19	0.41
1:D:282:ALA:C	1:D:284:SER:N	2.78	0.41
1:E:129:LEU:C	1:E:129:LEU:HD22	2.45	0.41
1:E:137:LEU:CD2	1:E:229:ALA:HB2	2.50	0.41
1:B:244:MET:O	1:B:337:VAL:HB	2.21	0.41
1:B:268:SER:O	1:B:272:LYS:HB2	2.21	0.41
1:C:116:LEU:O	1:C:119:MET:HE2	2.21	0.41
1:C:351:LEU:CD2	1:C:355:LEU:HG	2.51	0.41
1:C:376:SER:O	1:C:380:ARG:HG3	2.21	0.41
1:D:82:TRP:O	1:D:89:VAL:HG23	2.21	0.41
1:F:244:MET:O	1:F:245:HIS:C	2.60	0.41
1:A:20:TYR:CZ	1:F:170:ARG:HG3	2.56	0.41
1:A:186:SER:O	1:B:36:GLU:HG2	2.20	0.41
1:B:132:GLU:HB3	1:B:198:ASP:OD1	2.21	0.41
1:B:280:LYS:HD3	1:B:281:HIS:CE1	2.56	0.41
1:B:366:ALA:HA	1:B:367:PRO:HD2	1.93	0.41
1:B:370:ARG:O	1:B:371:ASN:C	2.64	0.41
1:C:109:ARG:HG3	1:C:344:TYR:CE2	2.56	0.41
1:C:134:GLU:OE2	2:C:501:GLU:OE2	2.39	0.41
1:C:169:ARG:HD3	1:C:186:SER:HB2	2.03	0.41
1:C:187:HIS:HD2	1:C:188:HIS:O	2.04	0.41
1:C:308:TYR:HE2	1:C:380:ARG:CZ	2.33	0.41
1:D:34:ASN:C	1:D:34:ASN:HD22	2.28	0.41
1:E:71:TYR:HA	1:E:72:PRO:HD2	1.89	0.41
1:E:126:ASP:HB2	1:E:251:PHE:HB2	2.03	0.41
1:E:295:SER:O	1:E:299:LEU:HD22	2.21	0.41
1:F:16:GLU:HG2	1:F:79:ILE:HD13	2.03	0.41
1:F:232:MET:HA	1:F:233:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:THR:HG21	1:F:389:PRO:HD2	2.03	0.41
1:F:375:MET:H	1:F:375:MET:HG3	1.53	0.41
1:F:396:LEU:O	1:F:400:LYS:HB2	2.21	0.41
1:A:116:LEU:HD23	1:A:351:LEU:HD21	2.03	0.41
1:B:312:SER:CB	1:B:315:ASN:HB2	2.51	0.41
1:D:6:ARG:HD3	1:D:6:ARG:O	2.20	0.41
1:D:62:ARG:O	1:D:63:ILE:HD13	2.21	0.41
1:D:281:HIS:O	1:D:282:ALA:C	2.64	0.41
1:E:151:ASN:ND2	1:E:166:GLU:OE2	2.54	0.41
1:F:62:ARG:HG2	1:F:63:ILE:N	2.35	0.41
1:A:20:TYR:C	1:A:21:ILE:HG13	2.46	0.40
1:A:214:PHE:O	1:A:215:LYS:C	2.65	0.40
1:B:214:PHE:O	1:B:215:LYS:C	2.64	0.40
1:B:260:ASP:OD1	1:B:260:ASP:C	2.64	0.40
1:B:282:ALA:O	1:B:283:THR:C	2.64	0.40
1:B:364:ALA:HA	1:B:365:PRO:HD2	1.77	0.40
1:B:399:PHE:HE1	1:B:405:MET:HB3	1.85	0.40
1:C:116:LEU:O	1:C:120:GLU:HG2	2.21	0.40
1:C:244:MET:HE2	1:C:338:ASP:O	2.22	0.40
1:C:258:PHE:CE1	1:C:332:VAL:HG12	2.56	0.40
1:C:289:THR:HB	1:C:337:VAL:HG22	2.04	0.40
1:D:67:ASP:C	1:D:68:MET:HG2	2.45	0.40
1:D:259:PHE:N	1:D:330:THR:HG21	2.36	0.40
1:D:380:ARG:O	1:D:385:ILE:HB	2.21	0.40
1:E:236:LEU:HB2	1:E:239:VAL:HG22	2.03	0.40
1:E:245:HIS:CD2	1:E:245:HIS:H	2.38	0.40
1:E:311:TRP:CZ2	1:E:367:PRO:HD3	2.56	0.40
1:F:170:ARG:O	1:F:173:VAL:HB	2.20	0.40
1:F:237:PHE:CD2	1:F:237:PHE:C	2.99	0.40
1:F:347:LEU:HD13	1:F:347:LEU:HA	1.69	0.40
1:F:436:GLU:O	1:F:440:TYR:HD2	2.03	0.40
1:A:6:ARG:HH12	1:A:47:ASP:CG	2.29	0.40
1:A:201:TYR:HD2	1:A:201:TYR:H	1.69	0.40
1:C:76:THR:O	1:C:78:VAL:HG23	2.21	0.40
1:C:285:PHE:CD1	1:C:285:PHE:C	3.00	0.40
1:D:437:ARG:O	1:D:441:MET:N	2.47	0.40
1:E:114:ARG:O	1:E:114:ARG:HG3	2.22	0.40
1:E:250:LEU:HD23	1:E:250:LEU:HA	1.84	0.40
1:A:97:TYR:HD2	1:A:102:THR:C	2.29	0.40
1:B:265:LEU:HD13	1:B:265:LEU:HA	1.84	0.40
1:B:273:HIS:ND1	1:B:361:LYS:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:LEU:O	1:C:326:ARG:NH1	2.54	0.40
1:C:315:ASN:HB3	1:C:318:PRO:HG3	2.03	0.40
1:E:69:TYR:HE1	1:E:99:PRO:HA	1.87	0.40
1:E:406:VAL:HG13	1:E:414:PHE:CG	2.57	0.40
1:B:54:GLY:C	1:B:56:SER:N	2.80	0.40
1:B:344:TYR:O	1:B:348:SER:OG	2.27	0.40
1:C:51:MET:HE3	1:C:51:MET:HB3	1.86	0.40
1:C:232:MET:HE3	1:C:235:PRO:CA	2.51	0.40
1:C:240:ASN:ND2	2:C:501:GLU:HA	2.37	0.40
1:C:252:LYS:C	1:C:254:GLY:H	2.29	0.40
1:C:325:SER:CB	3:C:502:ADP:O3B	2.69	0.40
1:D:12:LEU:O	1:D:16:GLU:HB2	2.22	0.40
1:D:159:LEU:HD11	1:E:22:ARG:HD3	2.03	0.40
1:D:328:ILE:HG12	1:D:329:SER:N	2.37	0.40
1:D:402:ASN:OD1	1:D:405:MET:HG2	2.21	0.40
1:E:26:THR:O	1:E:26:THR:HG22	2.21	0.40
1:E:34:ASN:ND2	1:E:34:ASN:C	2.79	0.40
1:F:25:PHE:CD2	1:F:25:PHE:N	2.89	0.40
1:F:127:PHE:HE2	1:F:347:LEU:CD1	2.34	0.40
1:F:248:LEU:HD11	1:F:350:LEU:HD13	2.04	0.40
1:F:405:MET:HE2	1:F:405:MET:CA	2.48	0.40
1:A:64:GLU:HG2	1:F:316:ARG:HA	2.03	0.40
1:A:78:VAL:CG1	1:A:91:ARG:HG3	2.51	0.40
1:A:258:PHE:CE1	1:A:332:VAL:HG23	2.57	0.40
1:A:402:ASN:CG	1:A:405:MET:HG2	2.46	0.40
1:A:428:PHE:CD2	1:A:428:PHE:C	2.99	0.40
1:B:128:ASN:HB3	1:B:201:TYR:CD1	2.56	0.40
1:B:357:GLY:HA2	1:B:362:LEU:HD13	2.04	0.40
1:B:412:HIS:O	1:B:416:HIS:HD2	2.03	0.40
1:C:129:LEU:HD22	1:C:131:PRO:HD3	2.03	0.40
1:D:27:ASP:OD1	1:D:33:LYS:HE3	2.22	0.40
1:D:169:ARG:NH2	1:D:188:HIS:CA	2.84	0.40
1:D:270:THR:HG23	1:D:358:ILE:HD12	2.02	0.40
1:D:319:LEU:HD11	1:D:388:LEU:HD11	2.03	0.40
1:E:107:ASP:OD1	1:E:108:PRO:HD2	2.22	0.40
1:E:264:ASP:O	1:E:265:LEU:HB2	2.21	0.40
1:E:302:GLY:N	1:E:316:ARG:NH1	2.69	0.40
1:F:120:GLU:C	1:F:122:LEU:N	2.80	0.40
1:F:250:LEU:HD12	1:F:274:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	441/443 (100%)	362 (82%)	57 (13%)	22 (5%)	1	5
1	B	441/443 (100%)	348 (79%)	76 (17%)	17 (4%)	2	8
1	C	441/443 (100%)	359 (81%)	60 (14%)	22 (5%)	1	5
1	D	441/443 (100%)	360 (82%)	59 (13%)	22 (5%)	1	5
1	E	441/443 (100%)	364 (82%)	61 (14%)	16 (4%)	2	10
1	F	441/443 (100%)	369 (84%)	55 (12%)	17 (4%)	2	8
All	All	2646/2658 (100%)	2162 (82%)	368 (14%)	116 (4%)	2	7

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	190	VAL
1	A	325	SER
1	B	316	ARG
1	C	84	ALA
1	C	86	LYS
1	C	184	GLU
1	C	368	ILE
1	D	165	GLY
1	D	204	ALA
1	D	362	LEU
1	D	368	ILE
1	E	161	PRO
1	F	282	ALA
1	F	316	ARG
1	F	361	LYS
1	F	411	GLU
1	A	260	ASP
1	A	304	GLU
1	B	100	ASP

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Mol	Chain	Res	Type
1	B	162	THR
1	B	214	PHE
1	B	215	LYS
1	C	159	LEU
1	C	161	PRO
1	C	166	GLU
1	C	170	ARG
1	C	325	SER
1	C	369	ASP
1	C	410	GLY
1	C	411	GLU
1	D	157	PHE
1	D	162	THR
1	D	167	ASN
1	D	260	ASP
1	E	121	ASP
1	E	166	GLU
1	E	204	ALA
1	E	324	ALA
1	E	325	SER
1	E	411	GLU
1	F	167	ASN
1	F	186	SER
1	F	304	GLU
1	A	167	ASN
1	A	186	SER
1	A	203	GLY
1	A	256	ASN
1	A	317	SER
1	A	368	ILE
1	B	101	GLY
1	B	287	ALA
1	B	314	GLN
1	C	158	ASP
1	C	167	ASN
1	D	240	ASN
1	D	266	GLN
1	D	268	SER
1	D	315	ASN
1	D	411	GLU
1	E	186	SER
1	E	262	ASN

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Mol	Chain	Res	Type
1	E	352	ALA
1	F	101	GLY
1	F	166	GLU
1	F	179	MET
1	F	324	ALA
1	F	325	SER
1	F	412	HIS
1	A	166	GLU
1	A	240	ASN
1	A	361	LYS
1	B	17	ASN
1	B	263	ALA
1	C	204	ALA
1	C	367	PRO
1	D	283	THR
1	D	306	PRO
1	D	329	SER
1	E	306	PRO
1	E	368	ILE
1	A	161	PRO
1	A	346	ALA
1	A	367	PRO
1	B	166	GLU
1	B	245	HIS
1	B	284	SER
1	B	352	ALA
1	C	40	SER
1	C	303	TYR
1	C	361	LYS
1	D	161	PRO
1	D	316	ARG
1	E	309	VAL
1	F	375	MET
1	A	257	ALA
1	A	358	ILE
1	B	34	ASN
1	D	3	LYS
1	E	84	ALA
1	E	214	PHE
1	F	383	ASN
1	C	317	SER
1	D	211	ILE

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Mol	Chain	Res	Type
1	D	367	PRO
1	A	343	PRO
1	C	254	GLY
1	F	367	PRO
1	A	374	VAL
1	B	275	ILE
1	B	57	ILE
1	C	61	VAL
1	D	339	PRO
1	A	81	PRO
1	E	218	VAL
1	F	131	PRO

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	382/382 (100%)	337 (88%)	45 (12%)	5	15
1	B	382/382 (100%)	341 (89%)	41 (11%)	6	19
1	C	382/382 (100%)	339 (89%)	43 (11%)	5	17
1	D	382/382 (100%)	333 (87%)	49 (13%)	4	12
1	E	382/382 (100%)	329 (86%)	53 (14%)	3	10
1	F	382/382 (100%)	334 (87%)	48 (13%)	4	12
All	All	2292/2292 (100%)	2013 (88%)	279 (12%)	5	14

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	THR
1	A	24	GLN
1	A	28	ILE
1	A	33	LYS
1	A	34	ASN

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Mol	Chain	Res	Type
1	A	35	VAL
1	A	36	GLU
1	A	70	LEU
1	A	82	TRP
1	A	91	ARG
1	A	92	PHE
1	A	102	THR
1	A	112	LEU
1	A	120	GLU
1	A	126	ASP
1	A	129	LEU
1	A	159	LEU
1	A	162	THR
1	A	166	GLU
1	A	168	CYS
1	A	169	ARG
1	A	201	TYR
1	A	205	VAL
1	A	206	ARG
1	A	220	THR
1	A	232	MET
1	A	242	SER
1	A	248	LEU
1	A	264	ASP
1	A	270	THR
1	A	286	THR
1	A	293	VAL
1	A	299	LEU
1	A	315	ASN
1	A	320	ILE
1	A	322	ILE
1	A	331	ARG
1	A	359	LYS
1	A	361	LYS
1	A	362	LEU
1	A	383	ASN
1	A	386	VAL
1	A	387	ASP
1	A	394	GLU
1	B	3	LYS
1	B	5	THR
1	B	9	ILE

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Mol	Chain	Res	Type
1	B	12	LEU
1	B	21	ILE
1	B	34	ASN
1	B	35	VAL
1	B	37	ILE
1	B	58	GLU
1	B	70	LEU
1	B	83	THR
1	B	89	VAL
1	B	91	ARG
1	B	92	PHE
1	B	102	THR
1	B	105	GLU
1	B	117	LYS
1	B	129	LEU
1	B	142	GLU
1	B	153	LYS
1	B	159	LEU
1	B	162	THR
1	B	167	ASN
1	B	181	PHE
1	B	183	ILE
1	B	186	SER
1	B	211	ILE
1	B	239	VAL
1	B	265	LEU
1	B	272	LYS
1	B	286	THR
1	B	304	GLU
1	B	326	ARG
1	B	328	ILE
1	B	349	VAL
1	B	351	LEU
1	B	359	LYS
1	B	370	ARG
1	B	372	ILE
1	B	411	GLU
1	B	429	ARG
1	C	3	LYS
1	C	5	THR
1	C	19	LYS
1	C	24	GLN

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Mol	Chain	Res	Type
1	C	25	PHE
1	C	34	ASN
1	C	35	VAL
1	C	40	SER
1	C	51	MET
1	C	64	GLU
1	C	70	LEU
1	C	82	TRP
1	C	94	CYS
1	C	105	GLU
1	C	112	LEU
1	C	122	LEU
1	C	129	LEU
1	C	148	LEU
1	C	151	ASN
1	C	153	LYS
1	C	156	TYR
1	C	159	LEU
1	C	162	THR
1	C	168	CYS
1	C	198	ASP
1	C	199	PHE
1	C	207	SER
1	C	208	CYS
1	C	252	LYS
1	C	286	THR
1	C	295	SER
1	C	299	LEU
1	C	325	SER
1	C	328	ILE
1	C	332	VAL
1	C	347	LEU
1	C	349	VAL
1	C	351	LEU
1	C	363	GLU
1	C	372	ILE
1	C	397	GLU
1	C	401	SER
1	C	431	GLN
1	D	6	ARG
1	D	7	GLU
1	D	14	LYS

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Mol	Chain	Res	Type
1	D	34	ASN
1	D	35	VAL
1	D	58	GLU
1	D	68	MET
1	D	70	LEU
1	D	82	TRP
1	D	83	THR
1	D	89	VAL
1	D	94	CYS
1	D	110	ASN
1	D	112	LEU
1	D	114	ARG
1	D	126	ASP
1	D	129	LEU
1	D	147	THR
1	D	159	LEU
1	D	163	ASP
1	D	164	LEU
1	D	183	ILE
1	D	198	ASP
1	D	199	PHE
1	D	206	ARG
1	D	239	VAL
1	D	250	LEU
1	D	264	ASP
1	D	265	LEU
1	D	266	GLN
1	D	267	LEU
1	D	272	LYS
1	D	304	GLU
1	D	309	VAL
1	D	319	LEU
1	D	326	ARG
1	D	328	ILE
1	D	332	VAL
1	D	336	SER
1	D	351	LEU
1	D	362	LEU
1	D	363	GLU
1	D	370	ARG
1	D	379	GLU
1	D	386	VAL

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Mol	Chain	Res	Type
1	D	387	ASP
1	D	398	GLU
1	D	441	MET
1	D	443	GLN
1	E	5	THR
1	E	8	ASP
1	E	24	GLN
1	E	26	THR
1	E	27	ASP
1	E	34	ASN
1	E	35	VAL
1	E	36	GLU
1	E	41	GLN
1	E	49	LYS
1	E	64	GLU
1	E	68	MET
1	E	70	LEU
1	E	82	TRP
1	E	113	LYS
1	E	114	ARG
1	E	117	LYS
1	E	129	LEU
1	E	143	LYS
1	E	149	GLU
1	E	151	ASN
1	E	159	LEU
1	E	162	THR
1	E	163	ASP
1	E	168	CYS
1	E	182	GLU
1	E	201	TYR
1	E	205	VAL
1	E	206	ARG
1	E	207	SER
1	E	216	LEU
1	E	220	THR
1	E	255	VAL
1	E	262	ASN
1	E	283	THR
1	E	285	PHE
1	E	299	LEU
1	E	304	GLU

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Mol	Chain	Res	Type
1	E	314	GLN
1	E	320	ILE
1	E	328	ILE
1	E	331	ARG
1	E	337	VAL
1	E	347	LEU
1	E	349	VAL
1	E	351	LEU
1	E	355	LEU
1	E	379	GLU
1	E	387	ASP
1	E	397	GLU
1	E	398	GLU
1	E	404	VAL
1	E	422	GLU
1	F	9	ILE
1	F	10	GLU
1	F	12	LEU
1	F	21	ILE
1	F	28	ILE
1	F	34	ASN
1	F	35	VAL
1	F	36	GLU
1	F	41	GLN
1	F	49	LYS
1	F	70	LEU
1	F	74	LEU
1	F	83	THR
1	F	91	ARG
1	F	105	GLU
1	F	112	LEU
1	F	129	LEU
1	F	143	LYS
1	F	148	LEU
1	F	152	ASP
1	F	166	GLU
1	F	177	GLU
1	F	184	GLU
1	F	186	SER
1	F	201	TYR
1	F	206	ARG
1	F	246	CYS

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Mol	Chain	Res	Type
1	F	261	GLU
1	F	270	THR
1	F	283	THR
1	F	299	LEU
1	F	304	GLU
1	F	314	GLN
1	F	317	SER
1	F	322	ILE
1	F	325	SER
1	F	326	ARG
1	F	328	ILE
1	F	329	SER
1	F	347	LEU
1	F	349	VAL
1	F	363	GLU
1	F	375	MET
1	F	379	GLU
1	F	382	GLU
1	F	423	ILE
1	F	431	GLN
1	F	441	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	41	GLN
1	A	245	HIS
1	A	443	GLN
1	B	24	GLN
1	B	187	HIS
1	B	194	GLN
1	B	240	ASN
1	B	315	ASN
1	B	431	GLN
1	B	443	GLN
1	C	110	ASN
1	C	167	ASN
1	C	290	ASN
1	C	371	ASN
1	D	75	ASN
1	D	151	ASN

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Mol	Chain	Res	Type
1	D	240	ASN
1	D	342	ASN
1	D	431	GLN
1	D	433	HIS
1	E	34	ASN
1	E	41	GLN
1	E	75	ASN
1	E	247	ASN
1	E	281	HIS
1	E	314	GLN
1	E	360	ASN
1	E	371	ASN
1	E	416	HIS
1	F	24	GLN
1	F	110	ASN
1	F	194	GLN
1	F	240	ASN
1	F	371	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\# Z > 2$
2	GLU	A	501	4	8,9,9	1.16	1 (12%)	8,11,11	1.23	1 (12%)
3	ADP	F	502	-	28,29,29	1.49	5 (17%)	43,45,45	1.84	8 (18%)
3	ADP	A	502	-	28,29,29	1.72	5 (17%)	43,45,45	1.94	8 (18%)
2	GLU	B	501	4	7,8,9	0.96	0	4,9,11	1.12	0
3	ADP	B	502	-	28,29,29	1.72	4 (14%)	43,45,45	1.81	8 (18%)
3	ADP	E	502	-	28,29,29	1.67	4 (14%)	43,45,45	1.91	10 (23%)
5	SO4	A	505	-	4,4,4	0.30	0	6,6,6	0.17	0
2	GLU	E	501	4	8,9,9	1.18	0	8,11,11	1.37	1 (12%)
2	GLU	D	501	4	8,9,9	0.95	0	8,11,11	1.40	2 (25%)
2	GLU	F	501	-	7,8,9	0.99	0	4,9,11	1.41	1 (25%)
5	SO4	A	506	-	4,4,4	0.28	0	6,6,6	0.30	0
3	ADP	D	502	-	28,29,29	1.72	4 (14%)	43,45,45	1.83	8 (18%)
5	SO4	E	505	-	4,4,4	0.24	0	6,6,6	0.16	0
3	ADP	C	502	-	28,29,29	1.61	4 (14%)	43,45,45	1.72	8 (18%)
2	GLU	C	501	4	8,9,9	1.00	0	8,11,11	1.34	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	501	4	-	1/9/9/9	-
3	ADP	F	502	-	-	0/16/32/32	0/3/3/3
3	ADP	A	502	-	-	3/16/32/32	0/3/3/3
2	GLU	B	501	4	-	3/6/7/9	-
3	ADP	B	502	-	-	2/16/32/32	0/3/3/3
3	ADP	E	502	-	-	3/16/32/32	0/3/3/3
2	GLU	E	501	4	-	2/9/9/9	-
2	GLU	D	501	4	-	5/9/9/9	-
2	GLU	F	501	-	-	2/6/7/9	-
3	ADP	D	502	-	-	5/16/32/32	0/3/3/3
3	ADP	C	502	-	-	2/16/32/32	0/3/3/3
2	GLU	C	501	4	-	2/9/9/9	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	ADP	C5-C4	5.42	1.48	1.39
3	A	502	ADP	C5-C4	5.32	1.48	1.39
3	B	502	ADP	C5-C4	5.16	1.48	1.39
3	C	502	ADP	C5-C4	5.01	1.48	1.39
3	F	502	ADP	C5-C4	4.91	1.47	1.39
3	E	502	ADP	C5-C4	4.88	1.47	1.39
3	B	502	ADP	PA-O3A	4.61	1.64	1.59
3	E	502	ADP	PA-O3A	4.52	1.64	1.59
3	A	502	ADP	PA-O3A	4.09	1.63	1.59
3	C	502	ADP	PA-O3A	3.97	1.63	1.59
3	D	502	ADP	PA-O3A	3.93	1.63	1.59
3	B	502	ADP	C5-C6	3.30	1.50	1.41
3	E	502	ADP	C5-C6	3.25	1.50	1.41
3	A	502	ADP	C5-C6	3.11	1.49	1.41
3	F	502	ADP	C5-C6	2.98	1.49	1.41
3	D	502	ADP	C5-C6	2.97	1.49	1.41
3	C	502	ADP	C5-C6	2.88	1.49	1.41
3	E	502	ADP	C8-N7	2.76	1.37	1.31
3	D	502	ADP	C8-N7	2.73	1.36	1.31
3	A	502	ADP	C8-N7	2.73	1.36	1.31
3	B	502	ADP	C8-N7	2.61	1.36	1.31
3	F	502	ADP	C8-N7	2.45	1.36	1.31
3	C	502	ADP	C8-N7	2.38	1.36	1.31
3	F	502	ADP	PA-O3A	2.38	1.62	1.59
3	A	502	ADP	C5-N7	-2.19	1.35	1.39
2	A	501	GLU	OXT-C	-2.11	1.23	1.30
3	F	502	ADP	C5-N7	-2.02	1.35	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ADP	C5-C4-N3	-7.02	117.05	126.72
3	B	502	ADP	C5-C4-N3	-5.99	118.47	126.72
3	F	502	ADP	C5-C4-N3	-5.87	118.64	126.72
3	D	502	ADP	C5-C4-N3	-5.81	118.72	126.72
3	E	502	ADP	C5-C4-N3	-5.58	119.03	126.72
3	C	502	ADP	C5-C4-N3	-5.54	119.08	126.72
3	A	502	ADP	N3-C4-N9	4.79	135.31	127.17
3	F	502	ADP	N3-C4-N9	4.60	135.00	127.17
3	C	502	ADP	N3-C4-N9	4.53	134.88	127.17
3	D	502	ADP	N3-C4-N9	4.50	134.81	127.17
3	E	502	ADP	N3-C4-N9	4.28	134.45	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	ADP	C4-C5-N7	-4.23	105.74	110.58
3	A	502	ADP	C4-C5-N7	-4.11	105.88	110.58
3	B	502	ADP	N3-C4-N9	4.10	134.14	127.17
3	E	502	ADP	C2-N3-C4	3.92	121.41	111.83
3	A	502	ADP	C2-N3-C4	3.89	121.33	111.83
3	E	502	ADP	C4-C5-N7	-3.87	106.16	110.58
3	F	502	ADP	C2-N3-C4	3.83	121.18	111.83
3	C	502	ADP	C2-N3-C4	3.66	120.78	111.83
3	B	502	ADP	C2-N3-C4	3.65	120.75	111.83
3	D	502	ADP	C4-C5-N7	-3.65	106.41	110.58
3	D	502	ADP	C2-N3-C4	3.42	120.18	111.83
3	E	502	ADP	N3-C2-N1	-3.42	123.41	128.58
3	F	502	ADP	C4-C5-N7	-3.39	106.71	110.58
3	E	502	ADP	C4-N9-C8	3.37	109.28	105.74
2	E	501	GLU	OXT-C-O	-3.35	116.47	124.08
3	F	502	ADP	N3-C2-N1	-3.31	123.57	128.58
3	C	502	ADP	N3-C2-N1	-3.29	123.61	128.58
3	C	502	ADP	C4-C5-N7	-3.03	107.11	110.58
3	E	502	ADP	C6-C5-N7	2.94	137.76	132.09
2	A	501	GLU	OXT-C-O	-2.88	117.54	124.08
3	D	502	ADP	N3-C2-N1	-2.86	124.25	128.58
3	E	502	ADP	C5-N7-C8	2.73	107.75	103.45
3	B	502	ADP	N3-C2-N1	-2.72	124.46	128.58
3	A	502	ADP	C5-N7-C8	2.69	107.67	103.45
3	A	502	ADP	O4'-C1'-N9	2.68	113.25	108.09
3	B	502	ADP	C5-N7-C8	2.67	107.65	103.45
3	D	502	ADP	C5-N7-C8	2.67	107.64	103.45
3	A	502	ADP	N3-C2-N1	-2.61	124.63	128.58
3	E	502	ADP	N9-C8-N7	-2.56	110.30	113.94
3	C	502	ADP	C4-N9-C8	2.56	108.43	105.74
3	B	502	ADP	C6-C5-N7	2.53	136.97	132.09
2	D	501	GLU	OE1-CD-CG	-2.52	115.10	123.09
3	F	502	ADP	C5-N7-C8	2.51	107.40	103.45
3	A	502	ADP	C3'-C2'-C1'	2.48	106.16	101.46
2	C	501	GLU	OE1-CD-CG	-2.43	115.38	123.09
3	D	502	ADP	C3'-C2'-C1'	2.42	106.05	101.46
3	F	502	ADP	C4-N9-C8	2.41	108.27	105.74
3	D	502	ADP	C4-N9-C8	2.27	108.13	105.74
2	D	501	GLU	OXT-C-O	-2.26	118.95	124.08
2	C	501	GLU	OE2-CD-CG	2.18	120.89	114.00
3	C	502	ADP	C6-C5-N7	2.15	136.23	132.09
3	E	502	ADP	C2'-C3'-C4'	2.13	106.72	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	ADP	C5-N7-C8	2.11	106.77	103.45
3	F	502	ADP	C6-C5-N7	2.06	136.06	132.09
2	F	501	GLU	OE1-CD-CG	-2.01	116.71	123.09
3	B	502	ADP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (30) torsion outliers are listed below:

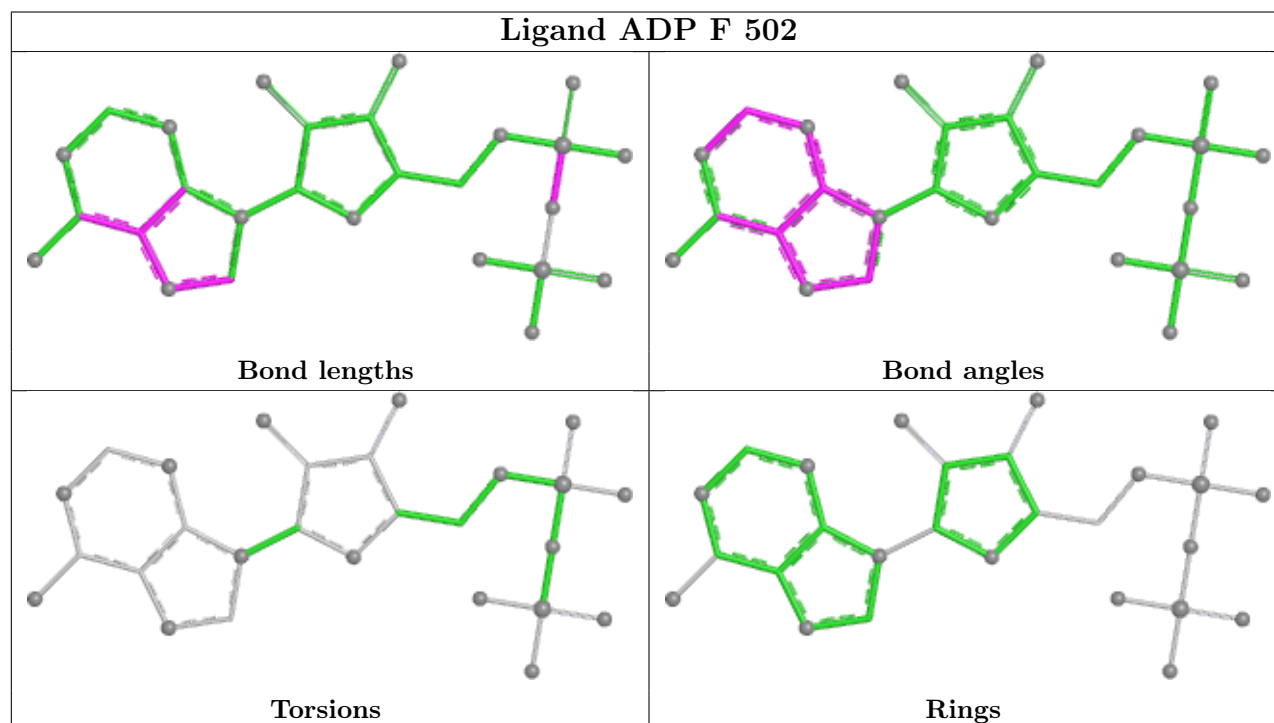
Mol	Chain	Res	Type	Atoms
2	D	501	GLU	O-C-CA-N
2	F	501	GLU	O-C-CA-CB
3	A	502	ADP	C5'-O5'-PA-O1A
3	A	502	ADP	C5'-O5'-PA-O2A
3	A	502	ADP	C5'-O5'-PA-O3A
3	D	502	ADP	C5'-O5'-PA-O2A
3	E	502	ADP	C5'-O5'-PA-O2A
3	B	502	ADP	O4'-C4'-C5'-O5'
3	C	502	ADP	O4'-C4'-C5'-O5'
3	E	502	ADP	O4'-C4'-C5'-O5'
3	E	502	ADP	C3'-C4'-C5'-O5'
2	D	501	GLU	OXT-C-CA-N
3	C	502	ADP	C3'-C4'-C5'-O5'
3	D	502	ADP	O4'-C4'-C5'-O5'
3	B	502	ADP	C3'-C4'-C5'-O5'
3	D	502	ADP	C3'-C4'-C5'-O5'
2	D	501	GLU	CA-CB-CG-CD
2	E	501	GLU	OXT-C-CA-N
2	B	501	GLU	CA-CB-CG-CD
3	D	502	ADP	C2'-C1'-N9-C8
2	F	501	GLU	CA-CB-CG-CD
2	A	501	GLU	CA-CB-CG-CD
2	C	501	GLU	O-C-CA-N
2	E	501	GLU	O-C-CA-N
2	C	501	GLU	OXT-C-CA-N
2	D	501	GLU	OXT-C-CA-CB
2	B	501	GLU	OE2-CD-CG-CB
3	D	502	ADP	O4'-C1'-N9-C8
2	B	501	GLU	OE1-CD-CG-CB
2	D	501	GLU	OE2-CD-CG-CB

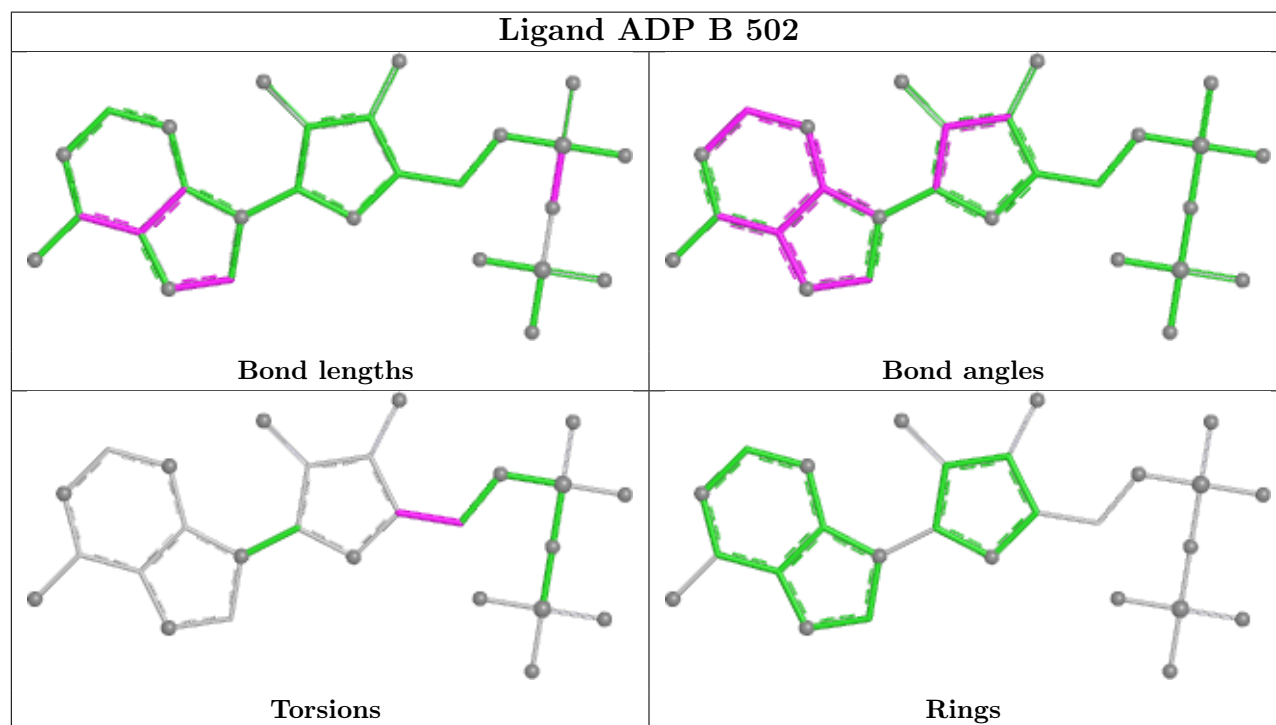
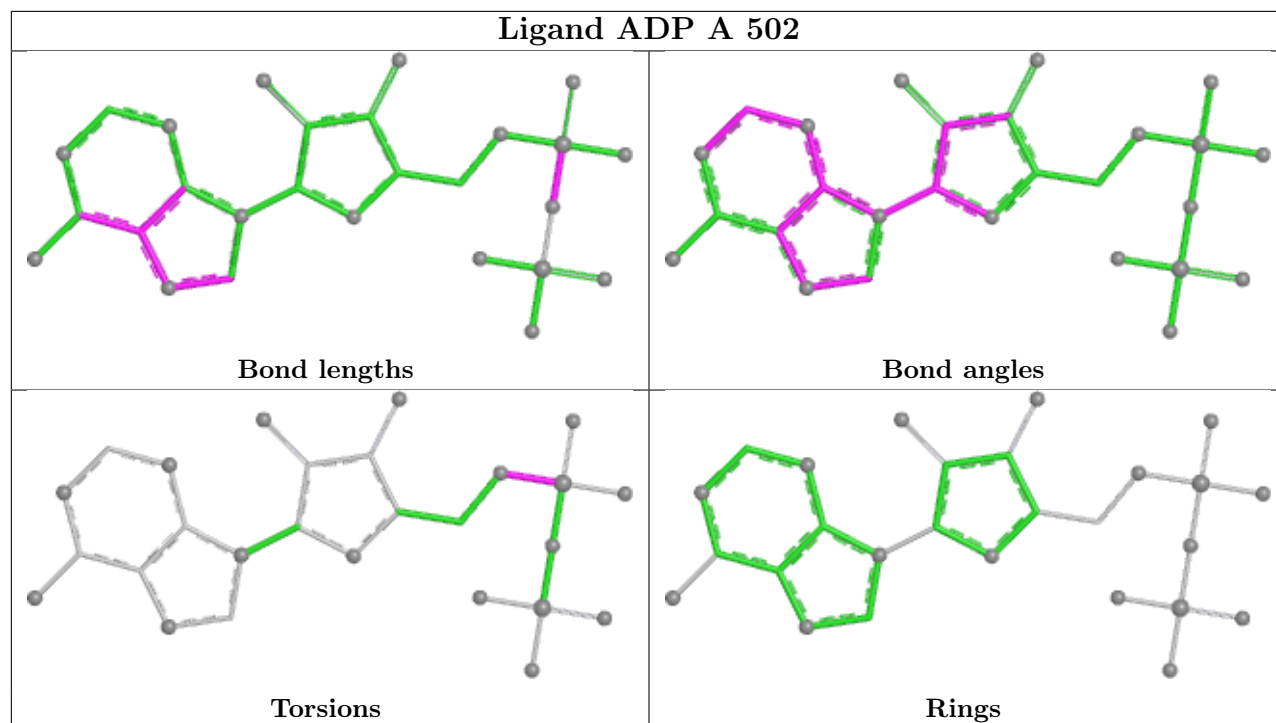
There are no ring outliers.

11 monomers are involved in 32 short contacts:

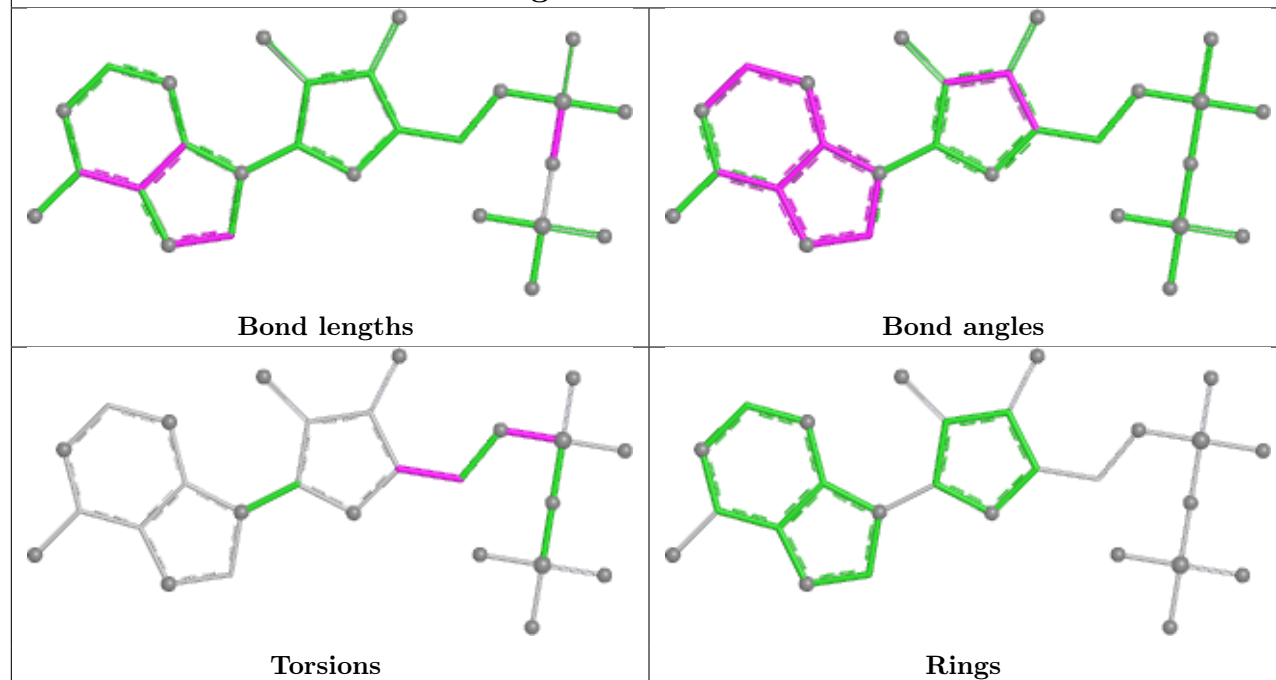
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502	ADP	2	0
3	A	502	ADP	3	0
3	B	502	ADP	4	0
3	E	502	ADP	4	0
2	E	501	GLU	3	0
2	D	501	GLU	4	0
2	F	501	GLU	1	0
3	D	502	ADP	1	0
5	E	505	SO4	1	0
3	C	502	ADP	5	0
2	C	501	GLU	4	0

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.

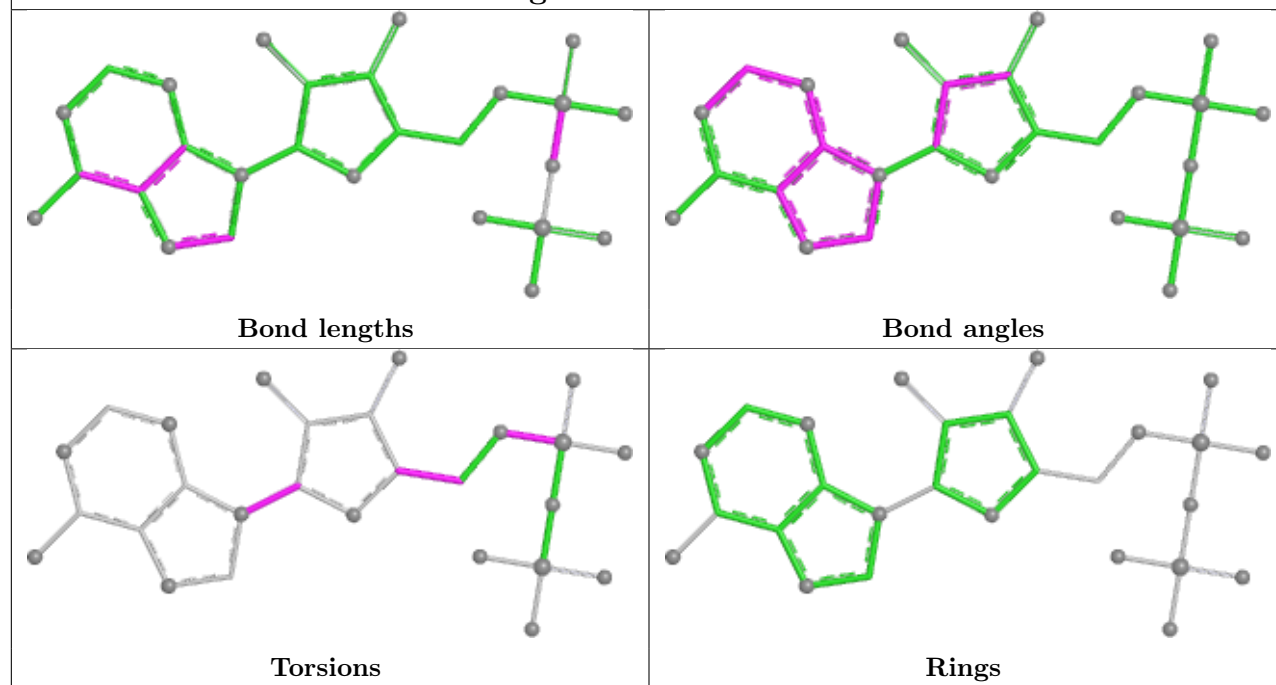


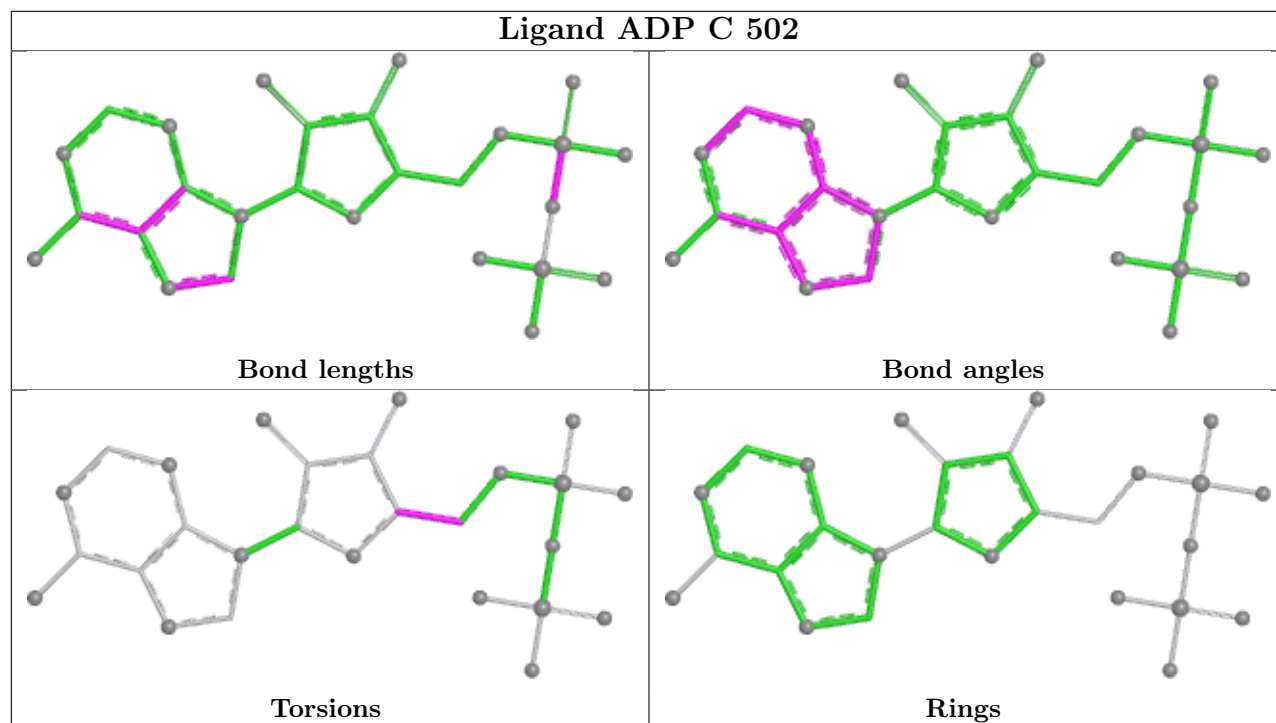


Ligand ADP E 502



Ligand ADP D 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/443 (100%)	-1.25	0 100 100	41, 61, 97, 127	1 (0%)
1	B	443/443 (100%)	-1.22	0 100 100	32, 62, 95, 118	1 (0%)
1	C	443/443 (100%)	-1.23	0 100 100	39, 63, 94, 120	1 (0%)
1	D	443/443 (100%)	-1.25	0 100 100	45, 63, 98, 128	0
1	E	443/443 (100%)	-1.26	0 100 100	36, 61, 96, 122	1 (0%)
1	F	443/443 (100%)	-1.24	0 100 100	39, 63, 96, 136	2 (0%)
All	All	2658/2658 (100%)	-1.24	0 100 100	32, 62, 97, 136	6 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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
5	SO4	E	505	5/5	0.95	0.07	93,98,100,104	0

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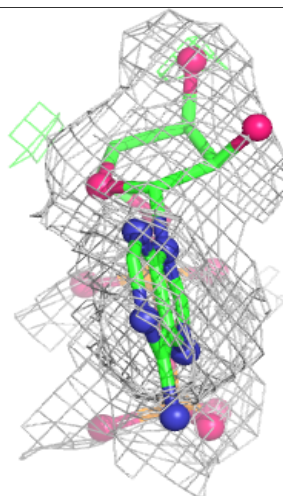
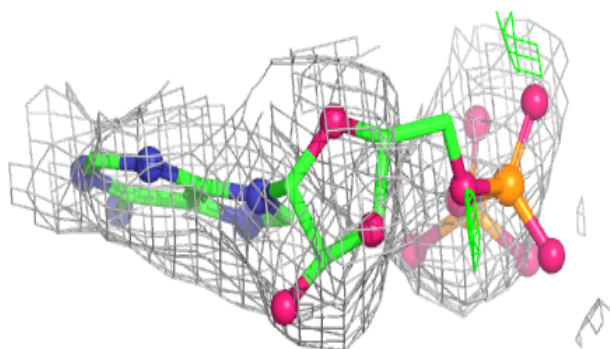
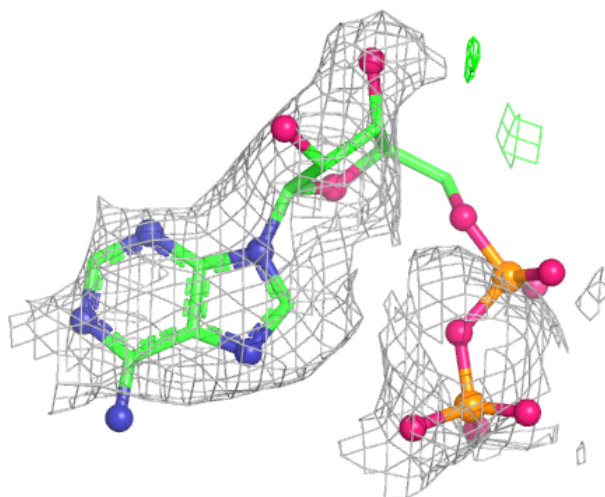
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	A	505	5/5	0.96	0.06	90,93,99,108	0
4	MG	B	504	1/1	0.97	0.07	64,64,64,64	0
3	ADP	A	502	27/27	0.97	0.08	83,106,152,159	0
3	ADP	F	502	27/27	0.97	0.09	81,108,134,135	0
3	ADP	E	502	27/27	0.98	0.06	79,97,130,141	0
2	GLU	E	501	10/10	0.98	0.06	57,63,68,68	0
4	MG	A	503	1/1	0.98	0.06	64,64,64,64	0
2	GLU	F	501	9/10	0.98	0.08	55,68,71,72	0
2	GLU	B	501	9/10	0.98	0.10	65,71,75,76	0
5	SO4	A	506	5/5	0.98	0.09	73,74,82,90	0
3	ADP	D	502	27/27	0.98	0.06	75,93,114,131	0
3	ADP	B	502	27/27	0.99	0.05	71,83,114,117	0
4	MG	A	504	1/1	0.99	0.04	50,50,50,50	0
4	MG	B	503	1/1	0.99	0.04	51,51,51,51	0
3	ADP	C	502	27/27	0.99	0.05	70,85,98,108	0
4	MG	C	503	1/1	0.99	0.04	60,60,60,60	0
4	MG	C	504	1/1	0.99	0.04	51,51,51,51	0
4	MG	D	504	1/1	0.99	0.03	61,61,61,61	0
4	MG	E	503	1/1	0.99	0.06	61,61,61,61	0
4	MG	E	504	1/1	0.99	0.04	49,49,49,49	0
4	MG	F	504	1/1	0.99	0.06	53,53,53,53	0
2	GLU	A	501	10/10	0.99	0.07	64,70,75,78	0
2	GLU	C	501	10/10	0.99	0.05	57,62,68,68	0
2	GLU	D	501	10/10	0.99	0.06	58,71,76,79	0
4	MG	D	503	1/1	1.00	0.04	49,49,49,49	0
4	MG	F	503	1/1	1.00	0.06	59,59,59,59	0

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

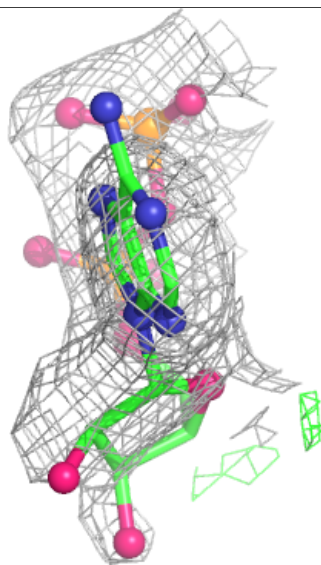
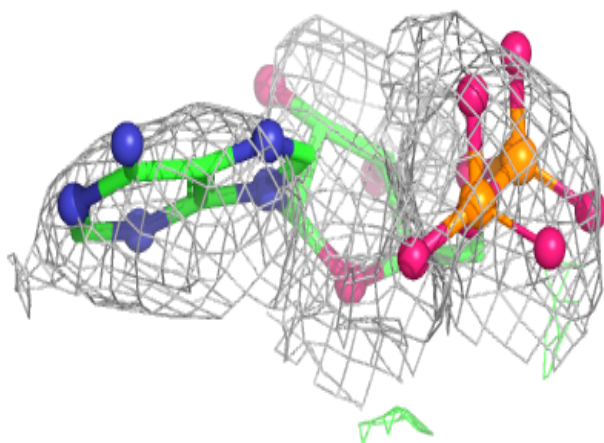
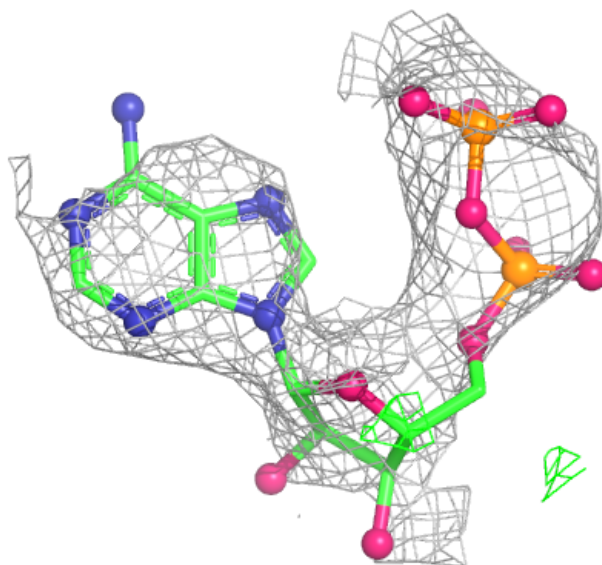
Electron density around ADP A 502:

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



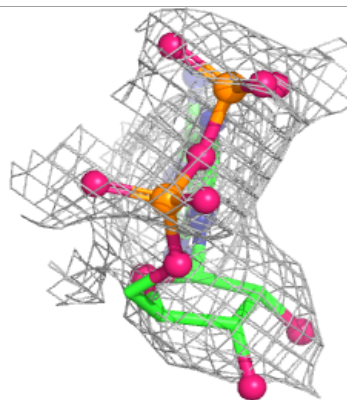
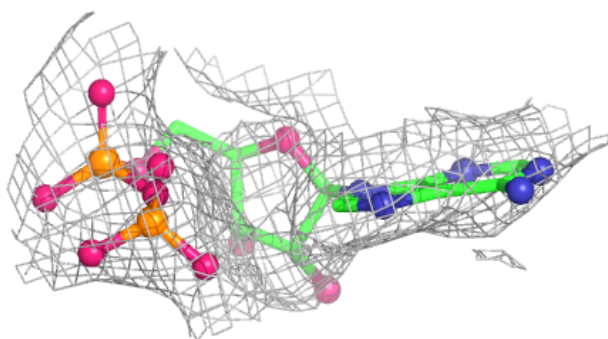
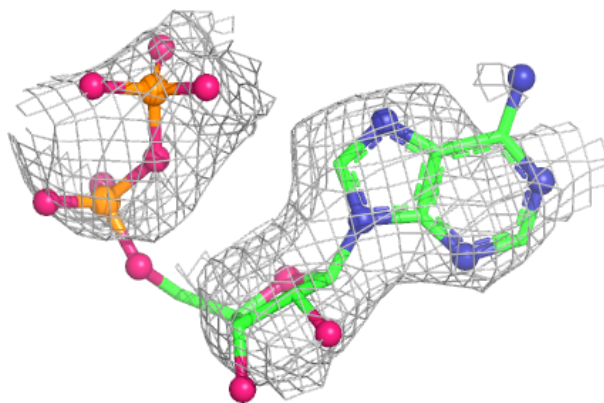
Electron density around ADP F 502:

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



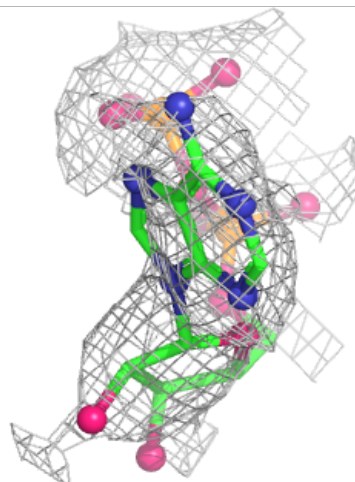
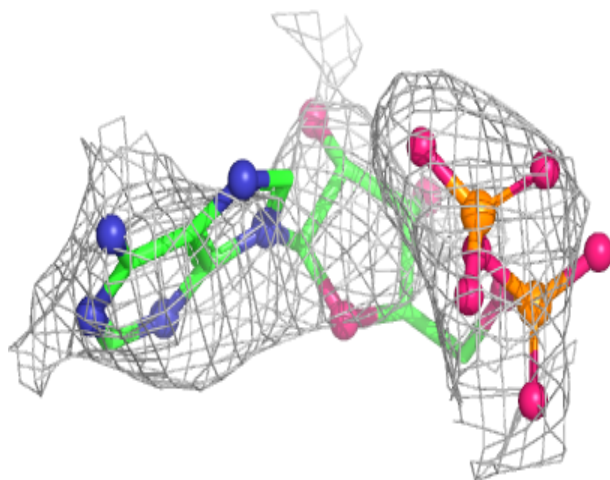
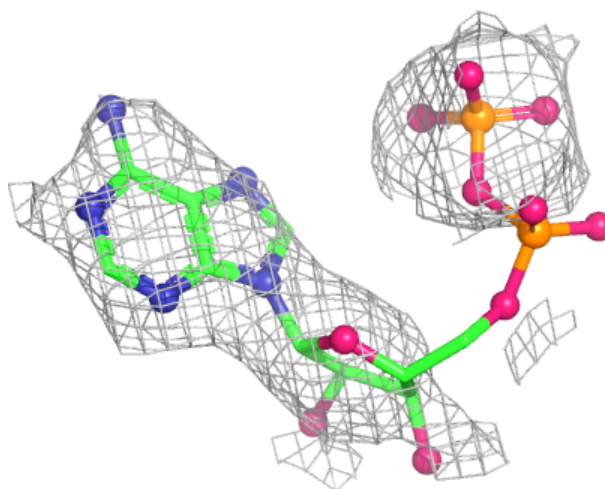
Electron density around ADP E 502:

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



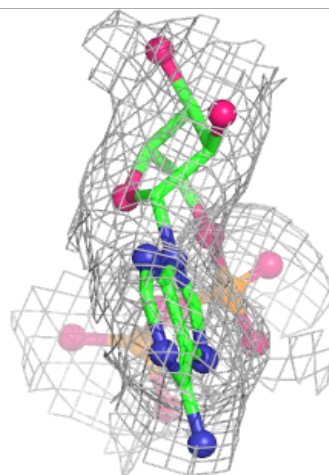
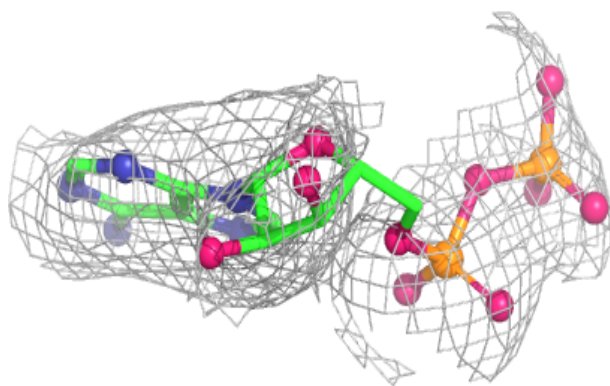
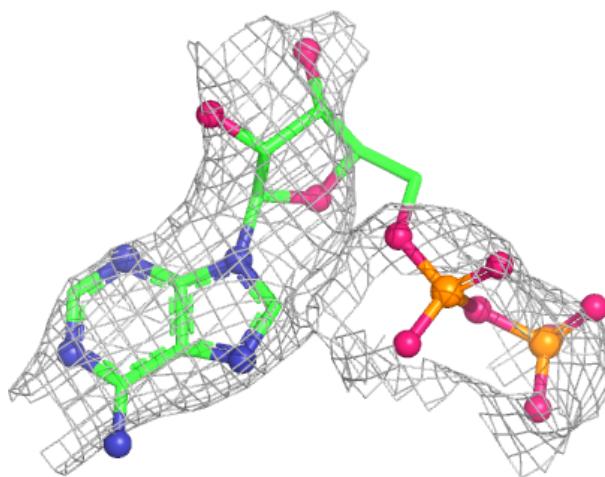
Electron density around ADP D 502:

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



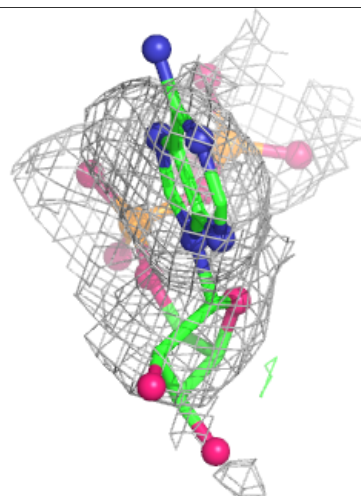
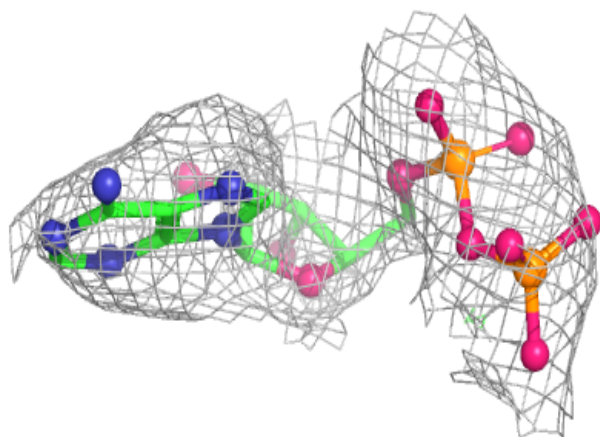
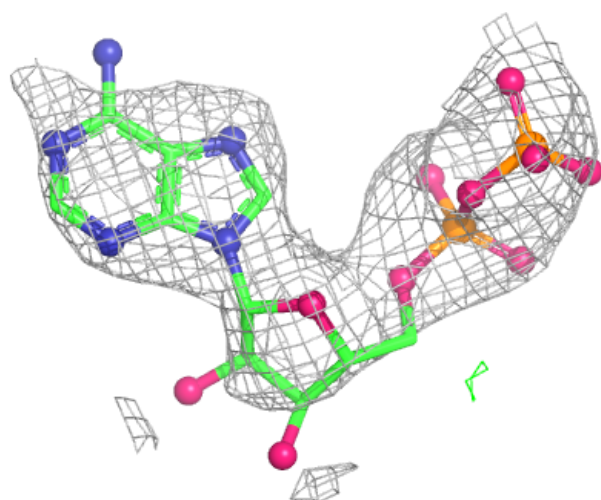
Electron density around ADP B 502:

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



Electron density around ADP C 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.