Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:28 PM EDT

PDB ID	:	2OOY
Title	:	Crystal structure of the adenylate sensor from AMP-activated protein kinase complexed with ATP
Authors	:	Townley, R.; Shapiro, L.
Deposited on	:	2007-01-26
Resolution	:	2.88 Å(reported)

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

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

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

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

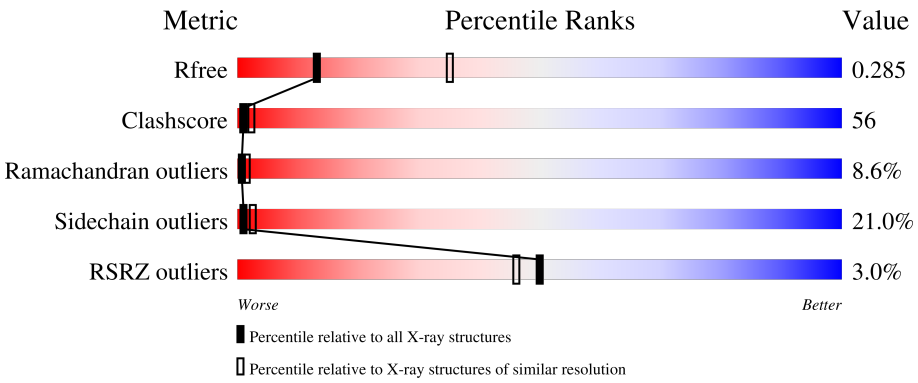
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (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 <=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	137	11% 25% 50% 17% • 6%
1	C	137	% 23% 44% 14% • 16%
2	B	97	3% 26% 41% 21% 7% 5%
2	D	97	4% 36% 36% 15% 6% 6%
3	E	333	2% 28% 53% 18% •

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Mol	Chain	Length	Quality of chain
3	G	333	31% 49% 15%

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
4	ATP	E	401	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9010 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1020	652	178	180	10	0	0	0
1	C	115	915	594	150	162	9	0	0	0

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	92	714	455	125	132	2	0	1	0
2	D	91	708	453	122	131	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	cloning artifact	UNP P78789
D	202	MET	-	cloning artifact	UNP P78789

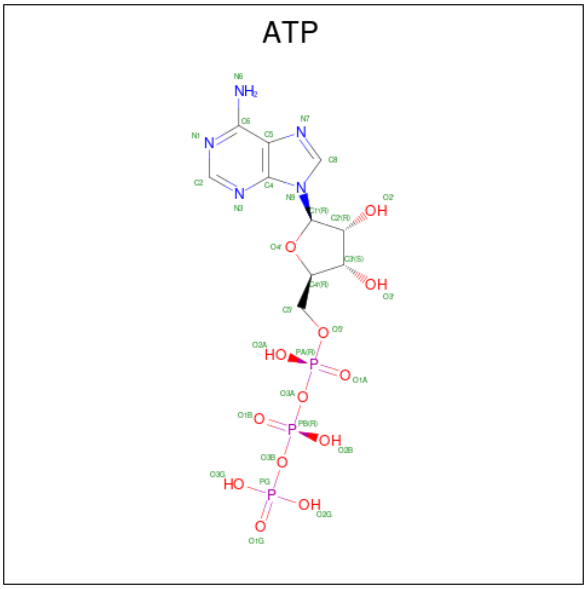
- Molecule 3 is a protein called Hypothetical protein C1556.08c in chromosome I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	324	2544	1627	421	481	15	0	1	0
3	E	333	2606	1663	432	496	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

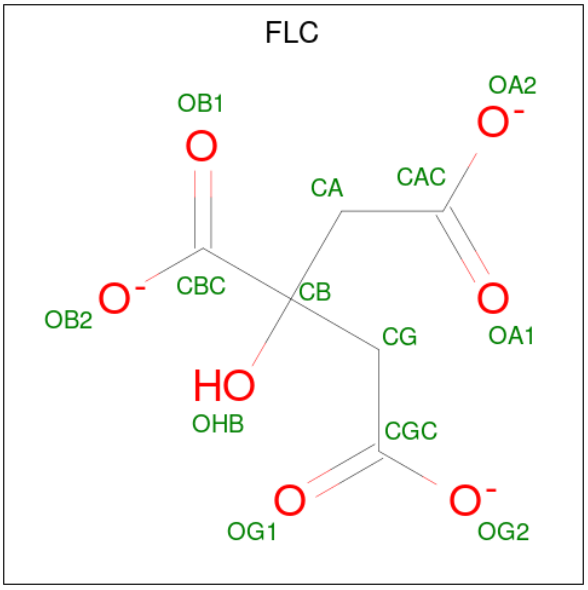
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	MET	-	cloning artifact	UNP Q10343
G	2	MET	-	cloning artifact	UNP Q10343

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	E	1	13	6	7	0	0

- Molecule 6 is water.

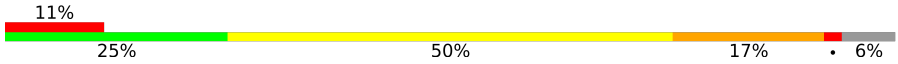
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	50	50	50	0	0
			Total	O		
6	B	41	41	41	0	0
			Total	O		
6	G	126	126	126	0	0
			Total	O		
6	C	50	50	50	0	0
			Total	O		
6	D	36	36	36	0	0
			Total	O		
6	E	125	125	125	0	0

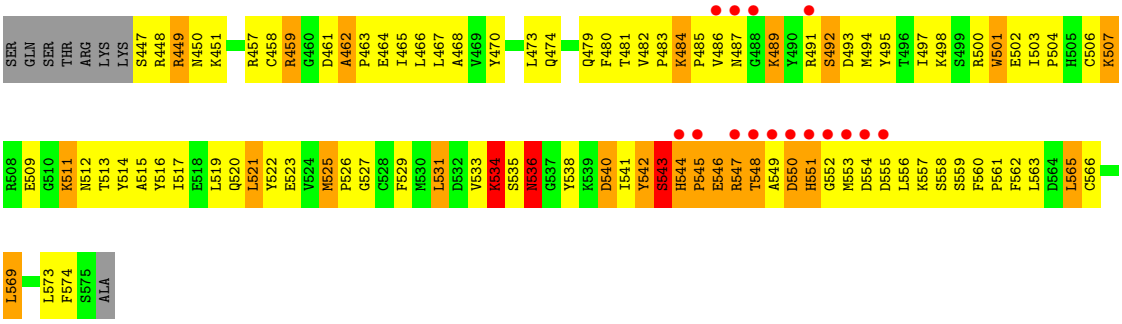
3 Residue-property plots (i)

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

- Molecule 1: SNF1-like protein kinase ssp2

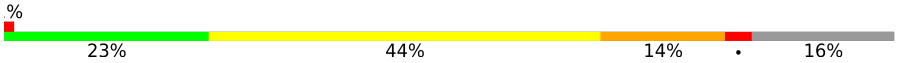
Chain A:

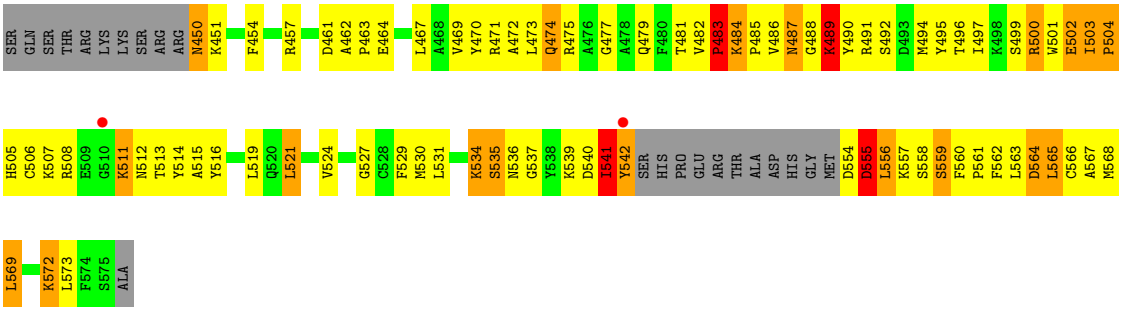




- Molecule 1: SNF1-like protein kinase ssp2

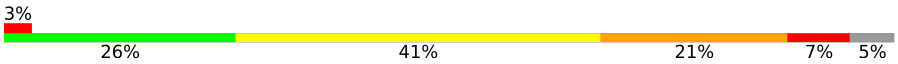
Chain C:

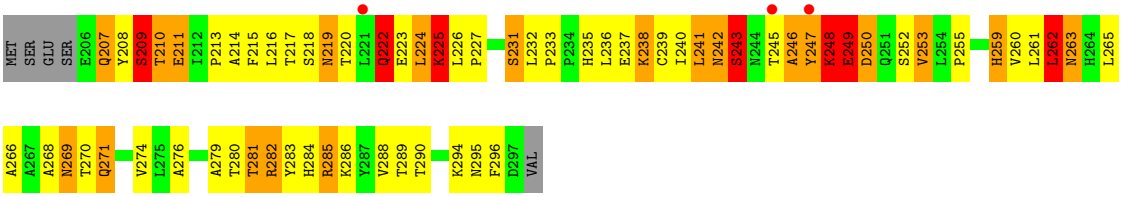




- Molecule 2: SPCC1919.03c protein

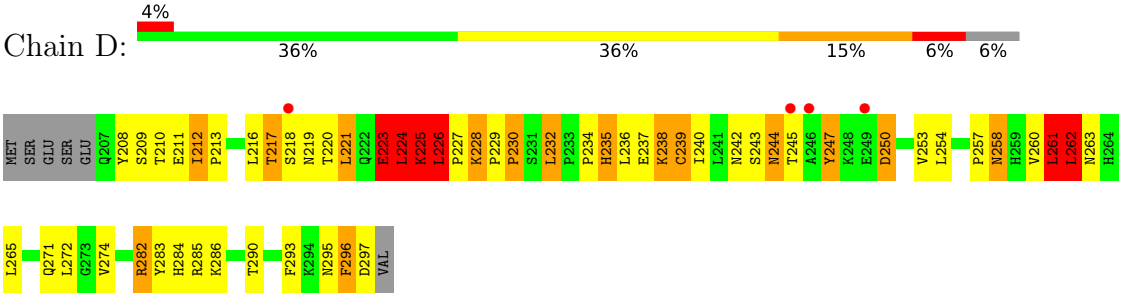
Chain B:





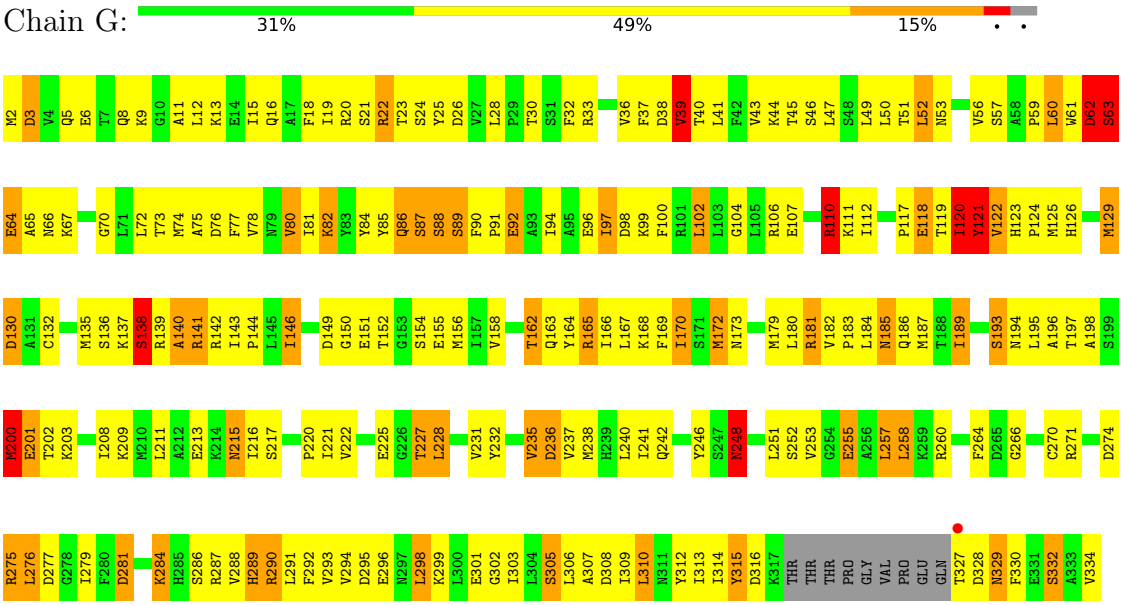
• Molecule 2: SPCC1919.03c protein

Chain D:



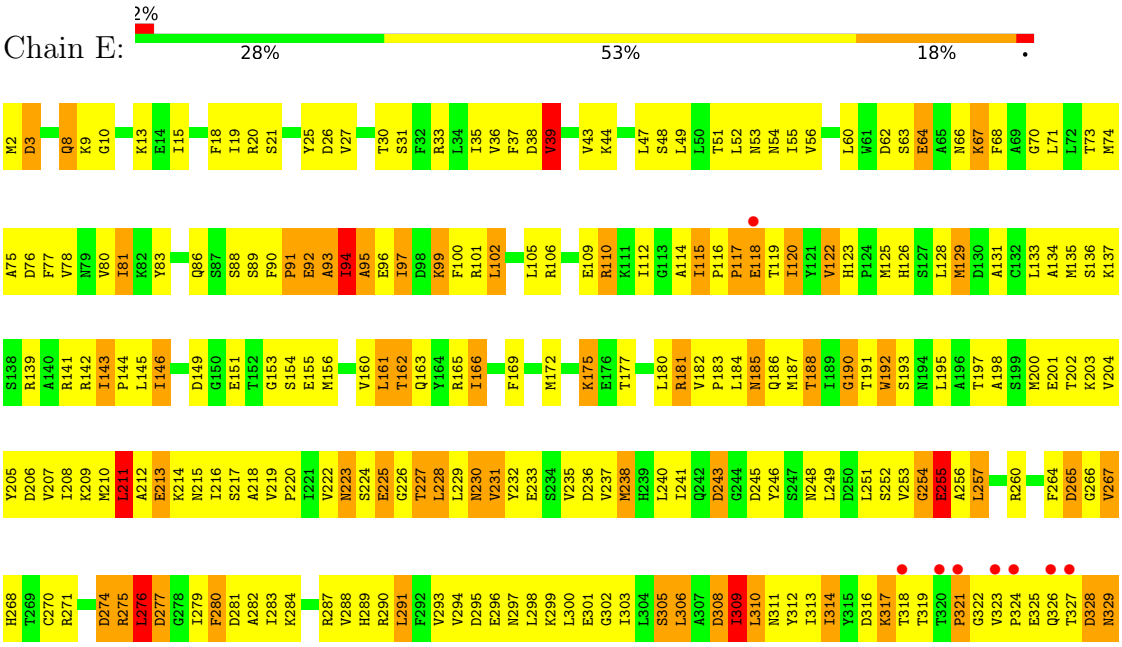
• Molecule 3: Hypothetical protein C1556.08c in chromosome I

Chain G:



• Molecule 3: Hypothetical protein C1556.08c in chromosome I

Chain E:



F330
E331
S332
A333
V334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.90Å 77.67Å 107.58Å 90.00° 123.99° 90.00°	Depositor
Resolution (Å)	50.00 – 2.88 19.83 – 2.88	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.88) 96.5 (19.83-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.298 0.187 , 0.285	Depositor DCC
R_{free} test set	1265 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	68.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.05	1/1047 (0.1%)	1.10	2/1415 (0.1%)
1	C	1.04	0/939	1.10	2/1269 (0.2%)
2	B	0.93	2/735 (0.3%)	1.10	2/1006 (0.2%)
2	D	1.02	2/726 (0.3%)	1.14	5/994 (0.5%)
3	E	1.04	6/2651 (0.2%)	1.13	6/3596 (0.2%)
3	G	1.09	2/2590 (0.1%)	1.12	10/3509 (0.3%)
All	All	1.05	13/8688 (0.1%)	1.12	27/11789 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	C	0	1
2	B	0	6
2	D	0	2
3	E	0	3
3	G	0	4
All	All	0	21

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	286	LYS	C-N	-9.06	1.13	1.34
2	D	239	CYS	CB-SG	-8.04	1.68	1.82
2	B	231	SER	CB-OG	6.08	1.50	1.42
3	E	267	VAL	CB-CG2	-5.92	1.40	1.52
3	E	118	GLU	CB-CG	5.84	1.63	1.52
2	B	286	LYS	C-N	-5.78	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	56	VAL	CB-CG2	-5.55	1.41	1.52
1	A	501	TRP	CB-CG	5.54	1.60	1.50
3	G	92	GLU	CG-CD	5.54	1.60	1.51
3	E	255	GLU	CG-CD	5.25	1.59	1.51
3	E	118	GLU	CG-CD	5.20	1.59	1.51
3	E	192	TRP	CB-CG	-5.07	1.41	1.50
3	E	33	ARG	CB-CG	-5.04	1.39	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	286	LYS	O-C-N	-7.90	110.06	122.70
3	E	94	ILE	N-CA-C	-7.39	91.04	111.00
2	B	209	SER	N-CA-C	7.15	130.32	111.00
3	G	257	LEU	CB-CG-CD2	-7.00	99.09	111.00
2	D	286	LYS	CA-C-N	6.84	132.25	117.20
3	G	122	VAL	N-CA-C	6.75	129.24	111.00
3	E	322	GLY	N-CA-C	-6.08	97.91	113.10
3	E	306	LEU	CB-CG-CD2	-6.05	100.71	111.00
2	D	261	LEU	CA-CB-CG	6.02	129.15	115.30
3	G	130	ASP	CB-CG-OD1	5.98	123.69	118.30
2	B	249	GLU	N-CA-C	-5.94	94.95	111.00
3	G	130	ASP	CB-CG-OD2	-5.94	112.96	118.30
3	G	72	LEU	CA-CB-CG	-5.94	101.65	115.30
3	E	243	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	A	531	LEU	CA-CB-CG	-5.86	101.81	115.30
2	D	226	LEU	CA-CB-CG	5.80	128.65	115.30
3	G	211	LEU	CB-CG-CD1	-5.70	101.31	111.00
3	G	315	TYR	N-CA-C	5.65	126.25	111.00
3	E	211	LEU	CB-CG-CD1	-5.60	101.48	111.00
1	C	521	LEU	CA-CB-CG	5.51	127.97	115.30
3	G	39	VAL	CB-CA-C	-5.50	100.96	111.40
3	G	60	LEU	CA-CB-CG	-5.30	103.11	115.30
2	D	254	LEU	CA-CB-CG	5.24	127.35	115.30
3	E	291	LEU	CA-CB-CG	-5.17	103.41	115.30
1	A	543	SER	C-N-CA	5.17	134.62	121.70
1	C	450	ASN	N-CA-C	5.09	124.75	111.00
3	G	121	TYR	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	ARG	Peptide
1	A	485	PRO	Peptide
1	A	536	ASN	Peptide
1	A	549	ALA	Peptide
1	A	550	ASP	Peptide
2	B	208	TYR	Peptide
2	B	209	SER	Peptide
2	B	242	ASN	Peptide
2	B	243	SER	Peptide
2	B	248	LYS	Peptide
2	B	250	ASP	Peptide
1	C	489	LYS	Peptide
2	D	219	ASN	Peptide
2	D	223	GLU	Peptide
3	E	266	GLY	Peptide
3	E	318	THR	Peptide
3	E	321	PRO	Peptide
3	G	120	ILE	Peptide
3	G	121	TYR	Peptide
3	G	62	ASP	Peptide
3	G	63	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1020	0	983	126	0
1	C	915	0	886	116	0
2	B	714	0	709	77	0
2	D	708	0	703	92	0
3	E	2606	0	2642	315	0
3	G	2544	0	2568	282	0
4	E	31	0	12	12	0
4	G	31	0	12	4	0
5	E	13	0	5	2	0
6	A	50	0	0	20	0
6	B	41	0	0	2	0
6	C	50	0	0	26	0
6	D	36	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	125	0	0	65	0
6	G	126	0	0	48	0
All	All	9010	0	8520	960	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 56.

All (960) 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)
3:G:99:LYS:HE3	6:G:478:HOH:O	1.19	1.28
6:G:415:HOH:O	2:D:271:GLN:HG2	1.29	1.27
3:G:162:THR:HG21	6:G:516:HOH:O	1.29	1.27
2:D:210:THR:HB	6:D:322:HOH:O	1.26	1.25
3:E:290:ARG:HA	6:E:520:HOH:O	1.37	1.24
3:E:73:THR:HG22	3:E:75:ALA:H	1.04	1.21
1:A:458:CYS:HA	6:E:453:HOH:O	1.42	1.19
3:E:303:ILE:HG22	6:E:490:HOH:O	1.40	1.18
3:E:308:ASP:OD2	6:E:527:HOH:O	1.60	1.16
1:A:569:LEU:O	6:A:241:HOH:O	1.61	1.15
2:B:282:ARG:CB	2:B:282:ARG:HH11	1.62	1.13
2:D:235:HIS:HE1	2:D:258:ASN:CB	1.60	1.13
2:D:235:HIS:HE1	2:D:258:ASN:HB2	1.01	1.12
3:E:181:ARG:HE	3:E:275:ARG:NH2	1.47	1.12
2:D:225:LYS:HG2	2:D:226:LEU:H	1.15	1.11
3:E:215:ASN:HD22	3:E:331:GLU:HA	0.98	1.11
2:D:225:LYS:HG2	2:D:227:PRO:HD3	1.31	1.09
3:E:215:ASN:ND2	3:E:331:GLU:HA	1.68	1.08
3:E:215:ASN:HD21	3:E:332:SER:N	1.49	1.08
3:G:253:VAL:HG12	3:G:257:LEU:HD21	1.35	1.08
1:C:474:GLN:HG3	6:C:205:HOH:O	1.55	1.07
3:E:223:ASN:ND2	6:E:431:HOH:O	1.88	1.06
2:B:248:LYS:CB	2:B:249:GLU:HA	1.87	1.05
1:C:503:ILE:HD12	1:C:514:TYR:H	1.20	1.05
2:D:235:HIS:CE1	2:D:258:ASN:HB2	1.92	1.05
3:G:141:ARG:HD3	6:G:503:HOH:O	1.58	1.04
2:B:282:ARG:HH11	2:B:282:ARG:HB3	1.17	1.03
2:D:223:GLU:OE1	2:D:223:GLU:HA	1.51	1.03
3:E:184:LEU:HD12	3:E:187:MET:HE1	1.38	1.03
2:D:235:HIS:CE1	2:D:258:ASN:CB	2.43	1.02
2:D:236:LEU:O	2:D:237:GLU:HB3	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:249:LEU:HB3	6:E:519:HOH:O	1.59	1.01
3:G:39:VAL:HG21	3:G:62:ASP:HB2	1.41	1.00
4:E:401:ATP:C8	4:E:401:ATP:H5'1	1.95	1.00
3:G:43:VAL:HG12	6:G:485:HOH:O	1.61	0.99
2:B:249:GLU:OE2	3:G:165:ARG:HG2	1.62	0.98
2:B:282:ARG:NH1	2:B:282:ARG:HB2	1.78	0.97
2:D:282:ARG:HH11	2:D:282:ARG:HG3	1.28	0.97
3:G:220:PRO:O	6:G:482:HOH:O	1.83	0.96
1:C:482:VAL:HG13	2:D:213:PRO:HG3	1.46	0.96
1:C:503:ILE:HD13	1:C:503:ILE:N	1.79	0.96
3:G:139:ARG:O	3:G:141:ARG:N	1.98	0.95
3:E:215:ASN:ND2	3:E:332:SER:H	1.65	0.95
3:G:170:ILE:N	6:G:507:HOH:O	2.00	0.95
1:C:503:ILE:CD1	1:C:514:TYR:H	1.80	0.94
3:E:271:ARG:HH21	3:E:296:GLU:HA	1.32	0.94
2:B:282:ARG:CB	2:B:282:ARG:NH1	2.28	0.94
1:A:461:ASP:HB2	1:A:464:GLU:OE2	1.68	0.93
3:G:149:ASP:HB3	6:G:414:HOH:O	1.66	0.93
3:G:144:PRO:HB2	3:G:146:ILE:HD11	1.49	0.93
3:E:186:GLN:HB3	6:E:523:HOH:O	1.68	0.93
3:G:80:VAL:CG2	3:G:97:ILE:HD11	1.98	0.93
3:G:80:VAL:HG22	3:G:97:ILE:HD11	1.52	0.92
3:G:169:PHE:O	3:G:170:ILE:HG13	1.69	0.92
3:G:221:ILE:HA	6:G:482:HOH:O	1.69	0.92
3:G:141:ARG:O	6:G:493:HOH:O	1.87	0.92
3:E:92:GLU:O	3:E:93:ALA:CB	2.18	0.92
3:E:274:ASP:HB2	6:E:524:HOH:O	1.68	0.91
4:E:401:ATP:H5'1	4:E:401:ATP:H8	1.27	0.91
1:C:502:GLU:HG2	1:C:502:GLU:O	1.70	0.91
3:G:164[B]:TYR:H	3:G:164[B]:TYR:HD1	1.04	0.91
3:G:215:ASN:HD21	3:G:332:SER:HB2	1.35	0.91
2:D:296:PHE:O	2:D:297:ASP:HB2	1.69	0.91
3:G:279:ILE:HD13	3:G:291:LEU:HD22	1.50	0.90
1:C:503:ILE:HD12	1:C:514:TYR:N	1.86	0.90
3:E:185:ASN:HD22	3:E:186:GLN:N	1.69	0.90
3:G:88:SER:HB3	6:G:468:HOH:O	1.69	0.90
1:C:503:ILE:CD1	1:C:503:ILE:H	1.84	0.90
3:G:195:LEU:HD22	3:G:303:ILE:HD12	1.52	0.90
3:E:184:LEU:HA	3:E:187:MET:CE	2.03	0.89
1:C:500:ARG:HG2	1:C:500:ARG:HH11	1.37	0.89
3:G:96:GLU:OE2	6:G:411:HOH:O	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:144:PRO:HB2	3:E:146:ILE:HD11	1.53	0.88
3:E:184:LEU:HA	3:E:187:MET:HE2	1.56	0.88
1:C:561:PRO:HB3	6:E:447:HOH:O	1.72	0.88
3:E:90:PHE:HA	6:E:453:HOH:O	1.74	0.87
1:C:559:SER:HB3	6:D:324:HOH:O	1.73	0.87
3:E:215:ASN:HD21	3:E:332:SER:H	0.90	0.87
1:A:507:LYS:HD3	1:A:507:LYS:C	1.93	0.87
1:C:511:LYS:CB	6:C:211:HOH:O	2.21	0.87
2:D:223:GLU:OE1	2:D:223:GLU:CA	2.23	0.86
3:E:163:GLN:O	3:E:166:ILE:HG22	1.74	0.86
3:G:240:LEU:HD13	6:G:499:HOH:O	1.74	0.86
3:E:73:THR:HG22	3:E:75:ALA:N	1.89	0.86
1:A:503:ILE:HD12	1:A:561:PRO:HG3	1.55	0.86
1:A:457:ARG:HD3	6:A:420:HOH:O	1.74	0.85
1:C:473:LEU:O	6:C:208:HOH:O	1.95	0.85
1:C:503:ILE:N	1:C:503:ILE:CD1	2.37	0.85
2:D:258:ASN:HD22	2:D:260:VAL:H	1.24	0.85
1:C:463:PRO:HD2	6:C:200:HOH:O	1.76	0.85
2:D:296:PHE:O	2:D:297:ASP:CB	2.24	0.85
3:E:230:ASN:OD1	6:E:483:HOH:O	1.95	0.85
1:A:447:SER:CB	6:A:418:HOH:O	2.25	0.84
2:B:248:LYS:CB	2:B:249:GLU:CA	2.56	0.84
1:A:561:PRO:O	1:A:565:LEU:HD22	1.78	0.84
3:G:260:ARG:NH1	6:G:513:HOH:O	1.87	0.84
1:A:501:TRP:HA	6:A:2:HOH:O	1.78	0.84
3:G:140:ALA:O	3:G:142:ARG:N	2.10	0.84
3:E:215:ASN:ND2	3:E:332:SER:N	2.23	0.83
1:C:450:ASN:O	1:C:451:LYS:HG2	1.78	0.83
3:E:66:ASN:HB3	3:E:154:SER:OG	1.77	0.83
3:E:129:MET:HA	3:E:129:MET:HE2	1.60	0.83
3:E:241:ILE:HA	6:E:414:HOH:O	1.76	0.83
2:B:222:GLN:OE1	2:B:222:GLN:HA	1.78	0.83
3:G:185:ASN:ND2	3:G:186:GLN:HG3	1.95	0.82
2:D:225:LYS:CG	2:D:227:PRO:HD3	2.08	0.82
2:D:226:LEU:HD12	2:D:228:LYS:HE2	1.60	0.82
2:B:235:HIS:HA	6:B:317:HOH:O	1.80	0.82
3:E:77:PHE:O	3:E:81:ILE:HG22	1.80	0.82
6:G:469:HOH:O	1:C:450:ASN:CB	2.26	0.81
3:E:181:ARG:NE	3:E:275:ARG:NH2	2.28	0.81
3:E:129:MET:HE1	3:E:314:ILE:HG12	1.59	0.81
3:E:328:ASP:OD2	6:E:468:HOH:O	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:HG3	6:A:336:HOH:O	1.79	0.81
3:G:165:ARG:HD2	3:G:165:ARG:O	1.79	0.81
1:A:523:GLU:HA	1:A:529:PHE:CD2	2.14	0.81
1:C:479:GLN:OE1	1:C:500:ARG:NH1	2.11	0.81
3:E:10:GLY:HA2	3:E:13:LYS:HE2	1.59	0.81
3:E:237:VAL:O	3:E:240:LEU:N	2.14	0.81
3:E:305:SER:O	3:E:308:ASP:HB2	1.79	0.81
1:C:472:ALA:HB1	1:C:572:LYS:HB3	1.62	0.81
3:E:47:LEU:O	3:E:51:THR:HG22	1.80	0.81
2:B:250:ASP:HB2	2:B:253:VAL:HG12	1.61	0.80
3:G:279:ILE:CD1	3:G:291:LEU:HD22	2.09	0.80
3:G:63:SER:N	3:G:65:ALA:H	1.79	0.80
1:A:462:ALA:HB3	1:A:463:PRO:HD3	1.64	0.80
3:G:253:VAL:O	3:G:257:LEU:CD2	2.29	0.80
3:G:270:CYS:HB2	3:G:274:ASP:OD1	1.81	0.80
3:G:12:LEU:HD23	3:G:180:LEU:CD2	2.12	0.80
4:E:401:ATP:C2'	6:E:527:HOH:O	2.30	0.79
3:G:61:TRP:NE1	3:G:63:SER:HB2	1.96	0.79
3:G:279:ILE:HD13	3:G:291:LEU:CD2	2.12	0.79
1:A:509:GLU:OE1	6:A:240:HOH:O	1.99	0.79
3:E:271:ARG:NH2	3:E:296:GLU:HA	1.97	0.79
3:G:185:ASN:HD22	3:G:186:GLN:N	1.80	0.78
1:C:471:ARG:NH2	6:C:316:HOH:O	2.15	0.78
3:E:110:ARG:HH11	3:E:117:PRO:HA	1.46	0.78
1:A:525:MET:HB2	1:A:526:PRO:HD2	1.65	0.78
3:E:92:GLU:O	3:E:93:ALA:HB2	1.82	0.78
3:G:52:LEU:HD22	3:G:52:LEU:H	1.48	0.78
3:G:2:MET:HB2	6:G:464:HOH:O	1.83	0.78
3:G:104:GLY:O	3:G:107:GLU:HB3	1.84	0.78
3:G:221:ILE:CD1	3:G:253:VAL:HG11	2.14	0.78
2:D:225:LYS:CG	2:D:226:LEU:H	1.94	0.77
3:E:215:ASN:HD22	3:E:331:GLU:CA	1.90	0.77
3:G:251:LEU:HB3	3:G:255:GLU:HG3	1.65	0.77
1:C:516:TYR:OH	6:C:52:HOH:O	2.03	0.77
2:B:261:LEU:O	2:B:262:LEU:O	2.03	0.77
3:G:99:LYS:HD3	2:D:297:ASP:O	1.85	0.77
1:A:574:PHE:O	6:A:93:HOH:O	2.03	0.76
3:G:195:LEU:HD22	3:G:303:ILE:CD1	2.14	0.76
6:C:205:HOH:O	2:D:212:ILE:HG22	1.85	0.76
2:D:225:LYS:HZ3	2:D:227:PRO:HD2	1.50	0.76
3:E:212:ALA:O	3:E:213:GLU:HB3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:123:HIS:HB3	3:E:126:HIS:ND1	1.99	0.76
3:E:177:THR:HG21	3:E:280:PHE:CD2	2.21	0.76
3:G:253:VAL:O	3:G:257:LEU:HD22	1.84	0.76
1:C:500:ARG:HD2	1:C:514:TYR:CD2	2.21	0.76
2:D:225:LYS:HG2	2:D:227:PRO:CD	2.13	0.76
1:C:556:LEU:CD2	3:E:156:MET:SD	2.74	0.76
1:C:556:LEU:HD22	3:E:156:MET:SD	2.26	0.76
4:E:401:ATP:H2'	6:E:527:HOH:O	1.86	0.76
3:E:81:ILE:HD13	3:E:81:ILE:O	1.85	0.75
3:E:54:ASN:HA	6:E:515:HOH:O	1.86	0.75
1:A:573:LEU:N	6:A:241:HOH:O	1.76	0.75
3:E:290:ARG:HB3	6:E:442:HOH:O	1.87	0.75
1:C:521:LEU:HD12	2:D:229:PRO:HB3	1.68	0.75
3:E:204:VAL:HG11	3:E:240:LEU:CD2	2.16	0.75
3:E:243:ASP:HB2	6:E:414:HOH:O	1.86	0.75
3:E:270:CYS:SG	6:E:524:HOH:O	2.43	0.75
3:G:139:ARG:C	3:G:141:ARG:H	1.90	0.74
3:G:182:VAL:HB	3:G:187:MET:HE2	1.68	0.74
3:G:142:ARG:NE	3:G:334:VAL:O	2.19	0.74
1:C:503:ILE:HD11	6:C:212:HOH:O	1.88	0.74
3:E:62:ASP:OD2	3:E:64:GLU:HB2	1.87	0.73
3:E:73:THR:HG21	3:E:334:VAL:H	1.53	0.73
2:D:245:THR:N	6:D:302:HOH:O	2.22	0.73
3:G:61:TRP:HE1	3:G:63:SER:HB2	1.53	0.73
2:D:283:TYR:CE2	2:D:284:HIS:HD2	2.07	0.73
3:E:122:VAL:HG22	3:E:143:ILE:CD1	2.18	0.73
2:D:243:SER:OG	2:D:244:ASN:N	2.16	0.73
3:G:37:PHE:HB3	3:G:41:LEU:HD12	1.71	0.72
3:E:204:VAL:HG23	3:E:251:LEU:O	1.88	0.72
2:D:225:LYS:HG2	2:D:226:LEU:N	1.99	0.72
3:E:317:LYS:HE2	3:E:317:LYS:HA	1.72	0.72
3:E:2:MET:O	3:E:3:ASP:CB	2.38	0.72
3:G:21:SER:OG	3:G:22:ARG:NH1	2.22	0.72
3:G:221:ILE:HD13	3:G:253:VAL:HG11	1.70	0.72
3:G:61:TRP:CZ2	3:G:66:ASN:HA	2.25	0.72
3:G:6:GLU:CB	6:G:463:HOH:O	2.37	0.72
3:E:233:GLU:O	3:E:236:ASP:HB2	1.90	0.72
3:E:44:LYS:HD2	6:E:470:HOH:O	1.90	0.72
3:E:241:ILE:C	6:E:414:HOH:O	2.28	0.72
3:G:60:LEU:N	3:G:60:LEU:HD23	2.04	0.71
2:D:236:LEU:O	2:D:237:GLU:CB	2.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2:MET:O	3:E:3:ASP:HB3	1.89	0.71
3:E:163:GLN:OE1	6:E:444:HOH:O	2.08	0.71
3:E:205:TYR:HB3	6:E:519:HOH:O	1.90	0.71
3:E:310:LEU:O	3:E:314:ILE:HB	1.91	0.71
3:G:257:LEU:HD22	3:G:257:LEU:N	2.05	0.71
1:C:502:GLU:O	1:C:502:GLU:CG	2.38	0.71
3:G:162:THR:CG2	3:G:165:ARG:H	2.02	0.71
3:G:63:SER:CA	3:G:66:ASN:H	2.02	0.71
3:E:230:ASN:HB2	6:E:492:HOH:O	1.90	0.71
1:C:485:PRO:HG3	1:C:490:TYR:CE2	2.26	0.70
4:E:401:ATP:O1A	4:E:401:ATP:O3G	2.08	0.70
3:G:162:THR:CG2	6:G:516:HOH:O	2.03	0.70
1:C:461:ASP:HB3	6:C:200:HOH:O	1.91	0.70
3:E:202:THR:O	3:E:253:VAL:HG23	1.90	0.70
3:E:94:ILE:HG23	3:E:95:ALA:H	1.55	0.70
2:D:283:TYR:CE2	2:D:284:HIS:CD2	2.80	0.70
3:E:128:LEU:HD21	3:E:166:ILE:HD11	1.74	0.69
3:G:295:ASP:OD2	3:G:299:LYS:HB3	1.92	0.69
2:B:226:LEU:HB3	2:B:227:PRO:HD2	1.73	0.69
3:G:213:GLU:OE2	6:G:495:HOH:O	2.10	0.69
2:D:225:LYS:O	2:D:226:LEU:HB2	1.91	0.69
3:E:122:VAL:HG22	3:E:143:ILE:HD13	1.73	0.69
3:E:215:ASN:ND2	3:E:331:GLU:CA	2.52	0.69
3:E:289:HIS:HD2	6:E:409:HOH:O	1.75	0.69
1:A:538:TYR:CE1	1:A:561:PRO:HD2	2.29	0.69
1:A:503:ILE:HD12	1:A:561:PRO:CG	2.22	0.68
2:B:249:GLU:HB2	3:G:168:LYS:HZ2	1.58	0.68
3:G:288:VAL:HG12	3:G:289:HIS:O	1.92	0.68
3:E:96:GLU:OE1	6:E:403:HOH:O	2.10	0.68
3:E:241:ILE:CA	6:E:414:HOH:O	2.36	0.68
1:A:544:HIS:CE1	1:A:545:PRO:HG2	2.29	0.68
3:G:8:GLN:HE22	3:G:187:MET:CE	2.07	0.68
1:A:544:HIS:CG	1:A:545:PRO:HD2	2.28	0.68
3:G:328:ASP:HA	3:G:329:ASN:HB3	1.75	0.68
3:E:181:ARG:HB3	3:E:275:ARG:HH21	1.58	0.68
2:B:222:GLN:O	2:B:224:LEU:HG	1.94	0.68
3:G:182:VAL:O	3:G:187:MET:HE3	1.94	0.68
1:C:484:LYS:NZ	1:C:484:LYS:HB3	2.08	0.68
2:B:237:GLU:O	6:B:338:HOH:O	2.11	0.68
3:E:184:LEU:HD12	3:E:187:MET:CE	2.20	0.67
3:E:204:VAL:O	3:E:208:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PRO:HA	6:A:286:HOH:O	1.94	0.67
2:D:235:HIS:CE1	2:D:258:ASN:HB3	2.26	0.67
3:E:305:SER:HB3	6:E:527:HOH:O	1.93	0.67
3:E:324:PRO:HB2	6:E:436:HOH:O	1.95	0.67
2:B:239:CYS:O	2:B:242:ASN:HB2	1.95	0.67
2:B:285:ARG:HG3	6:G:437:HOH:O	1.93	0.67
3:G:220:PRO:HB3	3:G:292:PHE:CE2	2.30	0.67
1:C:554:ASP:N	6:C:216:HOH:O	2.27	0.67
1:A:562:PHE:CE1	1:A:566:CYS:SG	2.88	0.66
3:G:63:SER:HA	3:G:66:ASN:H	1.60	0.66
3:E:181:ARG:HE	3:E:275:ARG:HH22	1.38	0.66
3:E:75:ALA:HB3	6:E:451:HOH:O	1.93	0.66
3:E:181:ARG:HB3	3:E:275:ARG:NH2	2.09	0.66
2:B:269:ASN:OD1	2:B:269:ASN:N	2.28	0.66
3:G:67:LYS:HA	3:G:155:GLU:HG3	1.77	0.66
1:C:457:ARG:NH2	6:C:400:HOH:O	2.08	0.66
2:B:249:GLU:O	2:B:249:GLU:OE1	2.13	0.66
1:C:531:LEU:HB2	6:C:352:HOH:O	1.95	0.66
1:A:533:VAL:HG12	1:A:534:LYS:H	1.61	0.66
3:G:12:LEU:CD2	3:G:180:LEU:CD2	2.73	0.66
1:A:547:ARG:O	1:A:548:THR:HB	1.96	0.66
3:G:149:ASP:CB	6:G:414:HOH:O	2.35	0.66
3:E:110:ARG:NH1	3:E:117:PRO:HA	2.11	0.65
3:G:33:ARG:HD3	6:G:502:HOH:O	1.96	0.65
3:G:63:SER:O	3:G:66:ASN:OD1	2.14	0.65
3:E:73:THR:CG2	3:E:74:MET:N	2.58	0.65
3:E:289:HIS:CE1	6:E:491:HOH:O	2.48	0.65
3:G:86:GLN:HE22	3:G:327:THR:CB	2.09	0.65
1:A:492:SER:O	1:A:494:MET:N	2.30	0.65
2:D:245:THR:CA	6:D:302:HOH:O	2.44	0.65
2:B:213:PRO:HB2	2:B:216:LEU:HD12	1.78	0.65
3:G:52:LEU:HD22	3:G:52:LEU:N	2.12	0.65
2:B:249:GLU:HB3	3:G:168:LYS:HZ3	1.62	0.65
3:G:152:THR:HG22	3:G:152:THR:O	1.96	0.65
3:E:197:THR:HG22	3:E:220:PRO:HG2	1.77	0.65
3:E:223:ASN:OD1	6:E:466:HOH:O	2.14	0.65
3:E:231:VAL:O	6:E:486:HOH:O	2.14	0.65
3:E:251:LEU:HB3	3:E:255:GLU:HG3	1.78	0.65
1:A:491:ARG:HG2	1:A:492:SER:H	1.60	0.64
3:G:141:ARG:NH2	3:G:215:ASN:OD1	2.29	0.64
3:E:183:PRO:HA	3:E:274:ASP:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:HIS:NE2	1:A:545:PRO:HG2	2.12	0.64
2:D:240:ILE:HG23	6:D:307:HOH:O	1.97	0.64
3:E:231:VAL:HG12	3:E:267:VAL:HG22	1.79	0.64
3:G:12:LEU:HD23	3:G:180:LEU:HD21	1.79	0.64
3:G:166:ILE:O	3:G:169:PHE:O	2.14	0.64
3:E:232:TYR:CD2	3:E:253:VAL:HG13	2.32	0.64
6:C:42:HOH:O	3:E:156:MET:HE3	1.97	0.64
2:D:245:THR:CB	6:D:302:HOH:O	2.45	0.64
1:A:489:LYS:HA	6:A:91:HOH:O	1.97	0.64
3:G:81:ILE:HG12	3:G:94:ILE:HD11	1.80	0.64
3:G:182:VAL:O	3:G:187:MET:CE	2.46	0.64
2:B:223:GLU:C	2:B:225:LYS:H	2.00	0.64
3:E:232:TYR:HD2	3:E:253:VAL:HG13	1.62	0.64
3:G:87:SER:O	3:G:88:SER:HB3	1.98	0.64
3:E:141:ARG:O	3:E:163:GLN:HG3	1.98	0.64
3:E:223:ASN:O	3:E:226:GLY:N	2.22	0.64
3:E:319:THR:O	3:E:321:PRO:HD3	1.98	0.63
4:E:401:ATP:O2B	4:E:401:ATP:O5'	2.16	0.63
3:G:87:SER:O	3:G:88:SER:CB	2.46	0.63
2:B:271:GLN:N	2:B:271:GLN:OE1	2.31	0.63
3:E:129:MET:CE	3:E:314:ILE:HG12	2.27	0.63
3:G:111:LYS:HG3	3:G:111:LYS:O	1.97	0.63
3:E:144:PRO:HB2	3:E:146:ILE:CD1	2.27	0.63
2:D:230:PRO:HB2	6:D:317:HOH:O	1.99	0.63
3:G:168:LYS:O	3:G:172:MET:HG3	1.98	0.63
1:C:500:ARG:HD2	1:C:514:TYR:HD2	1.61	0.63
1:A:458:CYS:HB2	1:A:529:PHE:HB2	1.80	0.62
3:G:120:ILE:HG12	3:G:143:ILE:HG13	1.81	0.62
2:D:235:HIS:HB3	6:D:326:HOH:O	1.97	0.62
3:E:190:GLY:O	3:E:192:TRP:CD1	2.52	0.62
3:E:314:ILE:HG21	6:E:508:HOH:O	2.00	0.62
3:G:51:THR:HG21	3:G:242:GLN:OE1	1.99	0.62
3:G:129:MET:HE2	3:G:314:ILE:HG22	1.79	0.62
1:C:556:LEU:HD23	3:E:156:MET:SD	2.39	0.62
3:E:110:ARG:HE	3:E:110:ARG:HA	1.64	0.62
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.65	0.62
3:G:96:GLU:OE1	6:G:410:HOH:O	2.16	0.62
1:A:494:MET:CE	2:B:227:PRO:HG2	2.30	0.62
3:G:142:ARG:HE	3:G:334:VAL:C	2.03	0.62
3:G:5:GLN:HE21	3:G:9:LYS:HE2	1.64	0.62
1:A:523:GLU:HA	1:A:529:PHE:HD2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:PHE:CD2	3:E:93:ALA:HB2	2.35	0.62
2:D:282:ARG:HG3	2:D:282:ARG:NH1	2.08	0.62
3:G:162:THR:HG23	3:G:165:ARG:H	1.64	0.61
3:E:165:ARG:HG3	6:E:489:HOH:O	1.99	0.61
3:E:245:ASP:OD1	3:E:245:ASP:C	2.35	0.61
3:G:8:GLN:HE22	3:G:187:MET:HE1	1.66	0.61
3:G:80:VAL:HG21	3:G:97:ILE:HD11	1.80	0.61
1:A:520:GLN:HG2	1:A:522:TYR:CZ	2.35	0.61
3:E:81:ILE:HD13	3:E:81:ILE:C	2.20	0.61
3:E:94:ILE:HG23	3:E:95:ALA:N	2.15	0.61
3:G:156:MET:O	3:G:158:VAL:HG23	2.01	0.61
3:G:44:LYS:NZ	2:D:272:LEU:HA	2.15	0.61
3:G:78:VAL:N	6:G:477:HOH:O	2.06	0.61
1:A:466:LEU:CD1	1:A:497:ILE:HD11	2.31	0.61
3:E:200:MET:HG3	3:E:254:GLY:HA2	1.82	0.61
3:G:197:THR:HG22	3:G:220:PRO:HG2	1.82	0.61
3:E:62:ASP:OD2	3:E:62:ASP:C	2.39	0.61
3:E:303:ILE:CG2	6:E:490:HOH:O	2.18	0.61
3:G:189:ILE:HD13	3:G:312:TYR:CD2	2.36	0.60
1:A:500:ARG:HD3	1:A:516:TYR:CE1	2.36	0.60
3:G:187:MET:SD	3:G:189:ILE:HD11	2.41	0.60
2:B:268:ALA:O	2:B:276:ALA:HB3	2.01	0.60
2:D:250:ASP:O	2:D:253:VAL:HG12	1.99	0.60
3:E:275:ARG:O	3:E:277:ASP:N	2.34	0.60
3:G:162:THR:HG23	3:G:164[B]:TYR:CD1	2.36	0.60
3:E:129:MET:HE1	6:E:508:HOH:O	2.01	0.60
3:E:129:MET:CE	3:E:314:ILE:CG1	2.80	0.60
1:A:533:VAL:HG12	1:A:534:LYS:N	2.16	0.60
3:G:135:MET:O	3:G:138:SER:O	2.19	0.60
1:A:459:ARG:HA	1:A:527:GLY:O	2.01	0.60
2:B:249:GLU:CB	3:G:168:LYS:NZ	2.65	0.60
1:C:477:GLY:N	6:C:208:HOH:O	2.32	0.60
3:E:128:LEU:HD11	3:E:166:ILE:HG13	1.84	0.60
3:E:268:HIS:O	3:E:291:LEU:HD23	2.02	0.60
1:A:502:GLU:HG3	6:A:239:HOH:O	2.02	0.60
3:G:74:MET:SD	3:G:238:MET:HB2	2.41	0.60
3:E:63:SER:O	3:E:64:GLU:C	2.40	0.60
3:E:66:ASN:ND2	6:E:447:HOH:O	2.34	0.60
3:E:185:ASN:HD22	3:E:186:GLN:H	1.49	0.59
1:A:502:GLU:O	1:A:504:PRO:HD3	2.03	0.59
1:C:486:VAL:N	1:C:489:LYS:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:217:SER:OG	3:E:290:ARG:NH1	2.36	0.59
2:B:249:GLU:HB2	3:G:168:LYS:NZ	2.16	0.59
2:D:224:LEU:O	2:D:225:LYS:HB3	2.01	0.59
2:D:240:ILE:HG21	2:D:257:PRO:HA	1.82	0.59
3:E:81:ILE:C	3:E:81:ILE:CD1	2.71	0.59
2:B:250:ASP:C	2:B:252:SER:H	2.04	0.59
2:D:225:LYS:HZ3	2:D:227:PRO:CD	2.14	0.59
3:E:131:ALA:O	3:E:135:MET:HG3	2.02	0.59
3:E:306:LEU:HB2	4:E:401:ATP:O1G	2.00	0.59
2:B:288:VAL:HG22	3:G:32:PHE:CZ	2.38	0.59
3:G:215:ASN:ND2	3:G:332:SER:HB2	2.13	0.59
1:A:574:PHE:CD2	3:E:93:ALA:CB	2.86	0.59
3:G:305:SER:O	3:G:308:ASP:HB2	2.03	0.59
3:G:181:ARG:HA	3:G:275:ARG:HG3	1.84	0.59
1:C:558:SER:HB2	3:E:156:MET:SD	2.42	0.59
3:G:37:PHE:HB3	3:G:41:LEU:CD1	2.33	0.58
3:E:73:THR:HG22	3:E:74:MET:N	2.14	0.58
3:E:181:ARG:HH21	3:E:275:ARG:HH22	1.49	0.58
1:A:557:LYS:O	2:B:281:THR:HG21	2.03	0.58
3:E:193:SER:HA	6:E:463:HOH:O	2.02	0.58
2:B:270:THR:O	2:B:271:GLN:HB2	2.04	0.58
3:E:166:ILE:C	3:E:166:ILE:HD13	2.22	0.58
1:A:520:GLN:HG2	1:A:522:TYR:CE2	2.38	0.58
3:G:12:LEU:CD2	3:G:180:LEU:HD22	2.33	0.58
3:G:63:SER:C	3:G:66:ASN:H	2.05	0.58
3:G:74:MET:HG3	3:G:235:VAL:HA	1.84	0.58
1:C:503:ILE:HD13	1:C:503:ILE:H	1.48	0.58
3:E:53:ASN:O	3:E:55:ILE:HG23	2.03	0.58
3:E:145:LEU:HD11	3:E:161:LEU:HD13	1.84	0.58
2:B:283:TYR:OH	3:G:124:PRO:HG2	2.04	0.58
3:G:88:SER:O	3:G:89:SER:HB2	2.03	0.58
3:G:144:PRO:HB2	3:G:146:ILE:CD1	2.27	0.58
2:D:282:ARG:HH11	2:D:282:ARG:CG	2.07	0.58
2:D:272:LEU:O	2:D:274:VAL:HG13	2.03	0.58
1:A:466:LEU:HD22	1:A:495:TYR:CD2	2.39	0.57
3:G:39:VAL:HG22	3:G:61:TRP:O	2.02	0.57
3:E:77:PHE:O	3:E:81:ILE:CG2	2.51	0.57
3:E:86:GLN:O	3:E:86:GLN:HG3	2.05	0.57
3:E:110:ARG:HA	3:E:110:ARG:NE	2.19	0.57
1:A:459:ARG:HH21	3:E:91:PRO:HG2	1.69	0.57
2:B:209:SER:OG	2:B:210:THR:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:227:THR:HA	3:E:298:LEU:O	2.05	0.57
3:G:163:GLN:HE22	3:G:307:ALA:HB2	1.69	0.57
1:C:561:PRO:CB	6:E:447:HOH:O	2.42	0.57
3:E:191:THR:HG22	3:E:192:TRP:N	2.19	0.57
3:E:296:GLU:CB	6:E:488:HOH:O	2.53	0.57
1:A:574:PHE:CE2	3:E:93:ALA:HB2	2.39	0.57
3:E:94:ILE:O	3:E:97:ILE:N	2.28	0.57
3:E:275:ARG:HG3	3:E:277:ASP:OD2	2.05	0.57
1:C:513:THR:HA	1:C:540:ASP:HA	1.86	0.57
3:E:305:SER:HA	6:E:520:HOH:O	2.05	0.57
2:B:240:ILE:HB	2:B:255:PRO:HG2	1.86	0.56
3:E:73:THR:HB	6:E:451:HOH:O	2.04	0.56
3:G:86:GLN:HB3	3:G:209:LYS:NZ	2.20	0.56
3:G:162:THR:HG22	3:G:165:ARG:H	1.70	0.56
3:G:236:ASP:OD2	3:G:260:ARG:HD3	2.06	0.56
1:C:472:ALA:CB	1:C:572:LYS:HB3	2.34	0.56
3:E:102:LEU:O	3:E:106:ARG:HG2	2.06	0.56
1:A:544:HIS:ND1	1:A:545:PRO:HD2	2.20	0.56
3:G:179:MET:HA	3:G:181:ARG:HD3	1.87	0.56
3:E:66:ASN:HB3	3:E:154:SER:HG	1.66	0.56
3:E:141:ARG:HB2	3:E:333:ALA:O	2.06	0.56
3:E:185:ASN:HD22	3:E:185:ASN:C	2.06	0.56
3:E:245:ASP:O	3:E:248:ASN:HB2	2.05	0.56
1:A:509:GLU:O	1:A:509:GLU:HG3	2.06	0.56
3:E:68:PHE:CE1	3:E:70:GLY:O	2.58	0.56
1:A:502:GLU:CG	6:A:239:HOH:O	2.53	0.56
3:G:162:THR:HA	6:G:493:HOH:O	2.04	0.56
3:G:183:PRO:HB2	3:G:185:ASN:HD21	1.71	0.56
1:C:505:HIS:CD2	3:E:66:ASN:HB2	2.40	0.56
1:C:560:PHE:HD2	1:C:564:ASP:OD2	1.87	0.56
1:A:465:ILE:O	1:A:466:LEU:C	2.44	0.56
3:G:90:PHE:CZ	1:C:573:LEU:HD22	2.41	0.56
3:G:92:GLU:HB3	6:C:400:HOH:O	2.05	0.56
1:A:500:ARG:HD3	1:A:516:TYR:HE1	1.70	0.56
3:G:295:ASP:OD2	3:G:299:LYS:CB	2.54	0.56
2:D:212:ILE:CG1	2:D:217:THR:HG22	2.36	0.56
3:E:8:GLN:NE2	3:E:182:VAL:HB	2.21	0.56
3:E:81:ILE:HG23	3:E:208:ILE:HG21	1.88	0.56
3:E:81:ILE:HG12	3:E:94:ILE:HD11	1.87	0.56
3:G:9:LYS:O	3:G:13:LYS:HG3	2.05	0.56
1:C:504:PRO:HG2	6:E:456:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:92:GLU:O	3:E:93:ALA:HB3	2.02	0.56
1:A:517:ILE:HG22	1:A:519:LEU:HD11	1.88	0.56
2:D:234:PRO:O	2:D:236:LEU:O	2.23	0.56
3:E:116:PRO:HB2	6:E:476:HOH:O	2.06	0.56
3:G:290:ARG:HE	4:G:401:ATP:PG	2.29	0.55
3:E:25:TYR:O	3:E:27:VAL:N	2.40	0.55
3:E:71:LEU:HD22	3:E:144:PRO:HD3	1.89	0.55
2:B:215:PHE:O	2:B:216:LEU:HB2	2.06	0.55
1:C:481:THR:HG23	6:C:315:HOH:O	2.06	0.55
1:C:561:PRO:CA	6:E:447:HOH:O	2.53	0.55
1:C:470:TYR:O	1:C:474:GLN:N	2.40	0.55
3:E:212:ALA:O	3:E:213:GLU:CB	2.51	0.55
3:G:39:VAL:HG21	3:G:62:ASP:CB	2.26	0.55
3:G:62:ASP:O	3:G:67:LYS:O	2.25	0.55
1:C:500:ARG:HH11	1:C:500:ARG:CG	2.16	0.55
1:C:511:LYS:CA	6:C:211:HOH:O	2.54	0.55
3:G:63:SER:C	3:G:65:ALA:N	2.59	0.55
3:G:215:ASN:O	3:G:216:ILE:HD13	2.07	0.55
1:C:464:GLU:O	1:C:467:LEU:HB3	2.07	0.55
1:C:475:ARG:HG3	1:C:572:LYS:HG3	1.89	0.55
2:D:237:GLU:O	2:D:237:GLU:HG2	2.07	0.55
2:D:293:PHE:CG	3:E:49:LEU:HD13	2.42	0.55
3:E:181:ARG:HH21	3:E:275:ARG:NH2	2.05	0.55
3:E:177:THR:O	3:E:180:LEU:HG	2.07	0.55
1:A:546:GLU:O	1:A:547:ARG:HB2	2.07	0.54
2:B:259[B]:HIS:CD2	2:B:259[B]:HIS:H	2.25	0.54
3:G:106:ARG:O	3:G:110:ARG:HB2	2.07	0.54
3:G:169:PHE:C	6:G:507:HOH:O	2.40	0.54
3:G:295:ASP:OD1	3:G:295:ASP:C	2.45	0.54
3:E:188:THR:N	6:E:462:HOH:O	2.33	0.54
3:E:255:GLU:O	3:E:257:LEU:N	2.41	0.54
3:G:257:LEU:CD1	6:G:513:HOH:O	2.56	0.54
3:E:265:ASP:OD1	3:E:287:ARG:HD3	2.07	0.54
3:G:169:PHE:O	3:G:170:ILE:CG1	2.49	0.54
3:G:231:VAL:HG22	3:G:232:TYR:N	2.23	0.54
3:E:19:ILE:HG21	3:E:129:MET:CE	2.37	0.54
3:G:193:SER:O	3:G:194:ASN:HB2	2.07	0.54
3:G:291:LEU:HD12	3:G:291:LEU:N	2.23	0.54
1:C:500:ARG:CG	1:C:514:TYR:HD2	2.20	0.54
1:C:503:ILE:HG12	1:C:506:CYS:HB2	1.88	0.54
1:C:540:ASP:O	1:C:542:TYR:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:73:THR:CG2	3:E:334:VAL:H	2.20	0.54
3:E:94:ILE:CG2	3:E:95:ALA:H	2.19	0.54
3:E:252:SER:OG	3:E:255:GLU:HG2	2.06	0.54
3:E:311:ASN:HA	3:E:314:ILE:HG22	1.89	0.54
2:D:239:CYS:HB2	2:D:242:ASN:ND2	2.22	0.54
3:E:36:VAL:HG12	3:E:37:PHE:N	2.21	0.54
3:E:222:VAL:HG23	3:E:223:ASN:N	2.23	0.54
3:E:312:TYR:C	3:E:314:ILE:H	2.11	0.54
3:E:255:GLU:O	3:E:256:ALA:C	2.43	0.53
2:B:249:GLU:O	2:B:249:GLU:CD	2.47	0.53
2:B:274:VAL:HB	2:B:294:LYS:O	2.08	0.53
6:C:205:HOH:O	2:D:212:ILE:CG2	2.50	0.53
3:E:192:TRP:CH2	3:E:293:VAL:HG11	2.44	0.53
1:A:574:PHE:CG	3:E:93:ALA:CB	2.92	0.53
1:C:500:ARG:CD	1:C:514:TYR:HD2	2.21	0.53
1:A:503:ILE:HG23	1:A:561:PRO:HG3	1.90	0.53
3:G:70:GLY:HA3	3:G:106:ARG:NH2	2.23	0.53
3:E:200:MET:HG3	3:E:254:GLY:CA	2.38	0.53
3:G:39:VAL:CG2	3:G:62:ASP:HB2	2.26	0.53
2:D:221:LEU:HB3	6:D:312:HOH:O	2.08	0.53
1:A:522:TYR:CE1	2:B:233:PRO:HD3	2.43	0.53
3:G:117:PRO:O	6:G:419:HOH:O	2.19	0.53
1:C:561:PRO:HA	6:E:447:HOH:O	2.07	0.53
1:C:503:ILE:HD12	1:C:503:ILE:H	1.69	0.53
1:A:462:ALA:HB3	1:A:463:PRO:CD	2.38	0.53
3:G:126:HIS:ND1	6:G:453:HOH:O	2.34	0.53
1:A:494:MET:HE1	2:B:226:LEU:HB3	1.91	0.53
2:D:258:ASN:ND2	2:D:260:VAL:H	2.00	0.53
3:E:319:THR:C	3:E:321:PRO:HD3	2.29	0.53
2:B:250:ASP:C	2:B:252:SER:N	2.58	0.53
3:E:175:LYS:HD2	3:E:175:LYS:C	2.29	0.53
3:E:235:VAL:HG23	3:E:235:VAL:O	2.08	0.53
1:A:540:ASP:N	3:G:151:GLU:OE1	2.24	0.52
3:G:44:LYS:HD2	6:G:412:HOH:O	2.09	0.52
3:G:198:ALA:HB1	3:G:202:THR:OG1	2.09	0.52
3:E:110:ARG:NH1	3:E:117:PRO:CA	2.71	0.52
3:E:254:GLY:HA3	6:E:418:HOH:O	2.08	0.52
1:A:500:ARG:NH1	1:A:514:TYR:CE2	2.78	0.52
1:C:503:ILE:CG1	1:C:506:CYS:HB2	2.40	0.52
3:E:328:ASP:CG	3:E:328:ASP:O	2.48	0.52
1:A:466:LEU:HD12	1:A:497:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:28:LEU:HD13	3:G:32:PHE:CZ	2.45	0.52
3:E:165:ARG:HH22	5:E:402:FLC:HG1	1.74	0.52
3:G:11:ALA:O	3:G:15:ILE:HG12	2.09	0.52
3:E:314:ILE:HG23	3:E:314:ILE:O	2.10	0.52
1:A:541:ILE:HG22	1:A:541:ILE:O	2.09	0.52
3:G:85:TYR:O	3:G:86:GLN:CG	2.57	0.52
3:G:203:LYS:NZ	6:G:501:HOH:O	2.43	0.52
3:E:96:GLU:O	3:E:97:ILE:C	2.47	0.52
1:C:484:LYS:HB3	1:C:484:LYS:HZ2	1.73	0.51
1:A:489:LYS:CB	6:A:91:HOH:O	2.57	0.51
1:A:533:VAL:HB	2:B:265:LEU:HB3	1.92	0.51
1:A:573:LEU:HD22	3:E:90:PHE:CZ	2.44	0.51
2:B:249:GLU:OE2	3:G:165:ARG:CG	2.49	0.51
1:C:479:GLN:CD	1:C:500:ARG:HH12	2.07	0.51
1:C:500:ARG:CD	1:C:514:TYR:CD2	2.93	0.51
1:C:568:MET:O	1:C:569:LEU:C	2.47	0.51
1:A:503:ILE:HB	1:A:506:CYS:HB2	1.93	0.51
3:E:172:MET:HA	3:E:284:LYS:HE3	1.92	0.51
3:G:215:ASN:HD21	3:G:332:SER:CB	2.14	0.51
3:E:216:ILE:HG22	4:E:401:ATP:H5'2	1.92	0.51
1:A:544:HIS:CG	1:A:545:PRO:CD	2.93	0.51
2:D:226:LEU:CD1	2:D:228:LYS:HE2	2.34	0.51
3:E:47:LEU:HD12	6:E:470:HOH:O	2.11	0.51
3:G:33:ARG:NH1	6:G:448:HOH:O	2.42	0.51
3:E:195:LEU:HA	4:E:401:ATP:C2	2.45	0.51
3:E:309:ILE:O	3:E:313:ILE:HG12	2.10	0.51
3:G:44:LYS:HZ1	2:D:272:LEU:HA	1.75	0.51
3:G:169:PHE:CE1	3:G:173:ASN:ND2	2.79	0.51
3:G:222:VAL:HA	3:G:227:THR:O	2.11	0.51
3:G:258:LEU:HB2	6:G:514:HOH:O	2.11	0.51
3:G:293:VAL:HB	3:G:302:GLY:H	1.75	0.51
3:G:329:ASN:ND2	3:G:330:PHE:H	2.09	0.51
3:G:33:ARG:NH2	6:G:484:HOH:O	2.44	0.51
3:G:139:ARG:C	3:G:141:ARG:N	2.56	0.51
1:A:562:PHE:O	1:A:565:LEU:HD23	2.11	0.50
2:D:216:LEU:HA	2:D:221:LEU:HD23	1.93	0.50
2:D:296:PHE:O	2:D:297:ASP:CG	2.50	0.50
1:A:523:GLU:HG3	1:A:529:PHE:CE2	2.46	0.50
3:G:63:SER:HA	3:G:66:ASN:N	2.24	0.50
2:D:223:GLU:OE1	2:D:223:GLU:C	2.50	0.50
1:A:551:HIS:HB3	6:A:353:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:222:VAL:HG12	3:G:228:LEU:HA	1.93	0.50
3:G:80:VAL:CG2	3:G:97:ILE:CD1	2.83	0.50
1:C:502:GLU:O	1:C:503:ILE:C	2.49	0.50
3:E:223:ASN:O	3:E:224:SER:C	2.50	0.50
1:A:458:CYS:N	1:A:529:PHE:O	2.39	0.50
1:A:500:ARG:NE	6:A:56:HOH:O	2.44	0.50
2:B:222:GLN:OE1	2:B:222:GLN:CA	2.57	0.50
3:G:24:SER:O	3:G:26:ASP:N	2.44	0.50
2:B:282:ARG:HB2	2:B:282:ARG:CZ	2.39	0.50
3:E:21:SER:O	6:E:450:HOH:O	2.20	0.50
3:E:314:ILE:CG2	6:E:508:HOH:O	2.58	0.50
1:A:520:GLN:CG	1:A:522:TYR:CE2	2.94	0.50
2:B:265:LEU:HD12	2:B:266:ALA:N	2.26	0.50
3:G:257:LEU:HD22	3:G:257:LEU:H	1.75	0.50
1:C:561:PRO:HB2	1:C:565:LEU:HD22	1.92	0.50
3:E:177:THR:CG2	3:E:280:PHE:CD2	2.92	0.50
1:A:517:ILE:HG22	1:A:519:LEU:CD1	2.41	0.50
3:G:16:GLN:HG2	3:G:313:ILE:O	2.12	0.49
3:G:167:LEU:O	3:G:170:ILE:HB	2.12	0.49
3:E:181:ARG:NH2	3:E:275:ARG:HH22	2.10	0.49
3:G:5:GLN:O	3:G:9:LYS:HG2	2.12	0.49
1:C:471:ARG:O	1:C:475:ARG:HG2	2.12	0.49
2:D:213:PRO:O	2:D:217:THR:HG23	2.12	0.49
3:E:149:ASP:O	3:E:153:GLY:N	2.40	0.49
3:E:166:ILE:HD13	3:E:166:ILE:O	2.12	0.49
3:E:248:ASN:O	3:E:251:LEU:HD12	2.12	0.49
3:E:295:ASP:HB3	3:E:301:GLU:OE1	2.12	0.49
1:C:454:PHE:O	1:C:530:MET:HE2	2.11	0.49
1:C:479:GLN:CG	2:D:210:THR:HG22	2.42	0.49
6:C:77:HOH:O	2:D:230:PRO:HD3	2.12	0.49
3:E:270:CYS:SG	3:E:293:VAL:HG22	2.52	0.49
1:A:543:SER:H	1:A:544:HIS:HA	1.77	0.49
1:A:560:PHE:HA	1:A:562:PHE:N	2.27	0.49
3:G:139:ARG:CB	3:G:332:SER:CB	2.90	0.49
3:G:162:THR:HG22	3:G:165:ARG:HB2	1.94	0.49
1:C:524:VAL:HG22	2:D:232:LEU:HD23	1.95	0.49
3:E:198:ALA:HB1	3:E:202:THR:CB	2.43	0.49
3:E:207:VAL:O	3:E:211:LEU:HG	2.12	0.49
3:G:76:ASP:O	3:G:80:VAL:HG12	2.12	0.49
3:G:12:LEU:HD21	3:G:180:LEU:HD22	1.95	0.49
3:G:51:THR:CG2	3:G:242:GLN:OE1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:ILE:HG23	1:C:541:ILE:O	2.12	0.49
3:E:67:LYS:HA	3:E:155:GLU:HG3	1.93	0.49
3:E:123:HIS:HD2	3:E:125:MET:H	1.61	0.49
1:A:495:TYR:HE1	2:B:227:PRO:O	1.95	0.49
1:C:519:LEU:HD23	1:C:531:LEU:HD21	1.94	0.49
3:G:149:ASP:OD1	3:G:149:ASP:O	2.31	0.49
3:G:294:VAL:HA	3:G:299:LYS:O	2.13	0.49
3:E:204:VAL:HG11	3:E:240:LEU:HD22	1.95	0.48
1:A:494:MET:HE2	2:B:227:PRO:HG2	1.93	0.48
2:B:247:TYR:O	2:B:248:LYS:C	2.50	0.48
3:G:163:GLN:N	6:G:493:HOH:O	1.60	0.48
3:G:217:SER:N	4:G:401:ATP:O1B	2.44	0.48
3:E:43:VAL:HG21	3:E:105:LEU:HD13	1.95	0.48
3:G:86:GLN:CB	3:G:209:LYS:NZ	2.77	0.48
2:D:221:LEU:O	2:D:221:LEU:HD22	2.13	0.48
2:D:225:LYS:CG	2:D:226:LEU:N	2.66	0.48
3:E:274:ASP:O	3:E:275:ARG:HB3	2.13	0.48
2:D:212:ILE:HG13	2:D:217:THR:HG22	1.94	0.48
3:E:282:ALA:O	3:E:283:ILE:C	2.51	0.48
1:A:535:SER:HB2	1:A:562:PHE:CG	2.47	0.48
2:B:246:ALA:O	2:B:248:LYS:N	2.46	0.48
2:B:249:GLU:CD	2:B:249:GLU:C	2.71	0.48
3:G:85:TYR:O	3:G:86:GLN:HG3	2.12	0.48
3:G:241:ILE:HD12	3:G:246:TYR:CE2	2.49	0.48
3:G:97:ILE:HA	3:G:100:PHE:HD1	1.78	0.48
1:A:503:ILE:CD1	1:A:515:ALA:HB2	2.43	0.48
1:A:503:ILE:HD11	1:A:515:ALA:HB2	1.95	0.48
1:A:544:HIS:C	1:A:546:GLU:H	2.17	0.48
2:B:250:ASP:HB3	2:B:252:SER:H	1.79	0.48
3:E:240:LEU:HD23	3:E:249:LEU:HD23	1.95	0.48
3:G:45:THR:O	3:G:49:LEU:HG	2.13	0.48
2:D:226:LEU:H	2:D:227:PRO:HD3	1.78	0.48
3:E:75:ALA:O	3:E:76:ASP:C	2.52	0.48
1:A:552:GLY:HA2	1:A:553:MET:HA	1.54	0.48
3:E:122:VAL:HG22	3:E:143:ILE:HD11	1.94	0.48
3:E:141:ARG:HH12	3:E:217:SER:N	2.12	0.48
3:E:200:MET:CE	6:E:492:HOH:O	2.61	0.48
3:E:218:ALA:HB1	3:E:231:VAL:CG2	2.43	0.48
1:A:461:ASP:HB2	6:A:234:HOH:O	2.14	0.48
3:G:235:VAL:C	3:G:237:VAL:H	2.16	0.48
3:E:19:ILE:HG21	3:E:129:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:HD22	1:A:495:TYR:CE2	2.49	0.47
3:G:118:GLU:H	3:G:118:GLU:CD	2.18	0.47
2:B:238:LYS:CG	2:B:238:LYS:O	2.62	0.47
3:G:82:LYS:O	3:G:85:TYR:O	2.32	0.47
3:G:149:ASP:OD1	3:G:149:ASP:C	2.53	0.47
3:E:142:ARG:HB2	3:E:161:LEU:O	2.14	0.47
3:E:175:LYS:CB	6:E:429:HOH:O	2.61	0.47
2:B:249:GLU:HB3	3:G:168:LYS:NZ	2.27	0.47
3:G:80:VAL:HG23	3:G:84:TYR:CE1	2.50	0.47
1:C:561:PRO:HB2	1:C:565:LEU:CD2	2.45	0.47
3:E:297:ASN:HB3	3:E:299:LYS:NZ	2.28	0.47
1:A:491:ARG:HG2	1:A:492:SER:N	2.29	0.47
3:G:189:ILE:HG23	3:G:312:TYR:CD2	2.49	0.47
3:G:276:LEU:O	3:G:277:ASP:C	2.51	0.47
1:C:521:LEU:HD12	2:D:229:PRO:CB	2.42	0.47
3:E:68:PHE:CE1	3:E:70:GLY:C	2.88	0.47
3:E:329:ASN:HB3	3:E:330:PHE:H	1.42	0.47
3:G:75:ALA:HB1	6:G:521:HOH:O	2.13	0.47
3:G:200:MET:O	3:G:252:SER:HB2	2.15	0.47
1:A:525:MET:HE3	1:A:525:MET:HB3	1.82	0.47
3:E:83:TYR:CE2	3:E:112:ILE:HG21	2.50	0.47
3:G:3:ASP:HB3	3:G:6:GLU:CB	2.45	0.47
1:C:511:LYS:HA	6:C:211:HOH:O	2.13	0.47
1:A:482:VAL:HG13	2:B:213:PRO:HG3	1.96	0.47
1:C:567:ALA:HB3	6:C:264:HOH:O	2.14	0.47
3:E:191:THR:CG2	3:E:192:TRP:N	2.78	0.47
1:A:449:ARG:HA	1:A:451:LYS:HG2	1.97	0.47
3:G:96:GLU:O	3:G:98:ASP:N	2.48	0.47
3:E:181:ARG:NE	3:E:275:ARG:HH22	2.04	0.47
3:E:265:ASP:OD2	3:E:289:HIS:CE1	2.68	0.47
1:A:561:PRO:HB3	3:G:66:ASN:HD21	1.80	0.46
3:G:43:VAL:CG1	6:G:485:HOH:O	2.39	0.46
3:G:59:PRO:C	3:G:60:LEU:HD23	2.36	0.46
3:G:235:VAL:C	3:G:237:VAL:N	2.68	0.46
3:G:252:SER:O	3:G:253:VAL:C	2.53	0.46
1:C:561:PRO:O	1:C:564:ASP:N	2.48	0.46
2:B:224:LEU:O	2:B:226:LEU:HD23	2.15	0.46
3:G:2:MET:CB	6:G:464:HOH:O	2.54	0.46
3:G:63:SER:H	3:G:65:ALA:H	1.58	0.46
3:G:184:LEU:C	3:G:186:GLN:N	2.69	0.46
3:E:216:ILE:HD13	3:E:216:ILE:HG21	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ASN:C	1:A:536:ASN:HD22	2.19	0.46
3:G:39:VAL:HG13	3:G:60:LEU:HB3	1.97	0.46
3:G:271:ARG:NH1	3:G:296:GLU:HA	2.31	0.46
3:E:74:MET:HG2	6:E:497:HOH:O	2.14	0.46
3:E:257:LEU:HA	3:E:257:LEU:HD12	1.51	0.46
1:A:465:ILE:HG12	6:E:454:HOH:O	2.15	0.46
1:C:563:LEU:O	1:C:566:CYS:HB2	2.15	0.46
3:E:187:MET:HE2	3:E:187:MET:HB2	1.71	0.46
1:A:506:CYS:O	1:A:507:LYS:C	2.53	0.46
3:G:237:VAL:O	3:G:238:MET:C	2.54	0.46
1:C:556:LEU:HD11	3:E:149:ASP:HA	1.98	0.46
3:E:129:MET:HE3	3:E:314:ILE:CG1	2.46	0.46
1:A:574:PHE:CG	3:E:93:ALA:HB1	2.51	0.46
3:G:96:GLU:C	3:G:98:ASP:N	2.67	0.46
3:G:195:LEU:CD2	3:G:303:ILE:HD12	2.36	0.46
1:C:535:SER:HB2	1:C:562:PHE:CD1	2.51	0.46
1:C:561:PRO:O	1:C:562:PHE:C	2.54	0.46
1:A:465:ILE:O	1:A:468:ALA:N	2.48	0.46
3:G:306:LEU:HD23	3:G:306:LEU:HA	1.61	0.46
2:D:285:ARG:HD2	2:D:285:ARG:HA	1.60	0.46
2:B:240:ILE:C	2:B:242:ASN:N	2.68	0.46
3:G:185:ASN:HD22	3:G:186:GLN:HG3	1.75	0.46
3:E:47:LEU:O	3:E:48:SER:C	2.50	0.46
1:A:507:LYS:HD3	1:A:507:LYS:O	2.16	0.46
3:G:60:LEU:N	3:G:60:LEU:CD2	2.66	0.46
3:G:102:LEU:HD12	3:G:102:LEU:HA	1.79	0.46
3:E:67:LYS:NZ	6:E:459:HOH:O	2.49	0.46
1:A:531:LEU:HD12	1:A:531:LEU:HA	1.75	0.46
2:B:214:ALA:C	2:B:215:PHE:O	2.54	0.46
2:B:241:LEU:C	2:B:243:SER:H	2.19	0.46
3:G:185:ASN:HD22	3:G:186:GLN:H	1.63	0.46
3:G:281:ASP:OD2	3:G:281:ASP:C	2.55	0.46
3:E:288:VAL:HG12	3:E:290:ARG:H	1.81	0.46
3:G:47:LEU:HA	3:G:50:LEU:HD12	1.97	0.45
1:C:462:ALA:HB1	1:C:495:TYR:CE2	2.51	0.45
3:E:142:ARG:NE	3:E:334:VAL:O	2.35	0.45
1:A:458:CYS:HB3	6:E:454:HOH:O	2.16	0.45
1:A:520:GLN:O	1:A:531:LEU:HD12	2.17	0.45
1:A:573:LEU:HG	6:A:241:HOH:O	2.16	0.45
3:G:169:PHE:CA	6:G:507:HOH:O	2.64	0.45
2:D:247:TYR:CD1	2:D:247:TYR:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:264:PHE:CD2	3:E:265:ASP:O	2.68	0.45
1:C:505:HIS:O	1:C:508:ARG:HB3	2.17	0.45
1:C:506:CYS:C	1:C:508:ARG:H	2.19	0.45
3:E:8:GLN:OE1	3:E:180:LEU:HA	2.16	0.45
3:E:90:PHE:HA	3:E:91:PRO:HD3	1.72	0.45
3:E:190:GLY:HA2	3:E:308:ASP:OD2	2.16	0.45
3:G:49:LEU:O	3:G:53:ASN:HB2	2.17	0.45
1:C:535:SER:HB2	1:C:562:PHE:CG	2.51	0.45
3:E:229:LEU:HD23	3:E:229:LEU:HA	1.54	0.45
3:E:237:VAL:O	3:E:238:MET:C	2.54	0.45
3:E:317:LYS:HA	3:E:317:LYS:CE	2.44	0.45
3:E:225:GLU:H	3:E:225:GLU:HG2	1.49	0.45
1:A:481:THR:HG22	6:A:285:HOH:O	2.16	0.45
3:E:241:ILE:HG21	3:E:246:TYR:CD2	2.52	0.45
3:E:288:VAL:CG1	3:E:290:ARG:O	2.64	0.45
1:A:559:SER:O	1:A:562:PHE:HB3	2.16	0.45
3:G:80:VAL:HG21	3:G:97:ILE:CD1	2.45	0.45
3:E:123:HIS:CD2	3:E:125:MET:H	2.34	0.45
3:E:165:ARG:NH1	5:E:402:FLC:OG2	2.49	0.45
3:E:181:ARG:HE	3:E:181:ARG:HB3	1.71	0.45
3:E:279:ILE:HG23	3:E:291:LEU:CD1	2.47	0.45
1:A:463:PRO:HB2	6:A:234:HOH:O	2.16	0.45
2:B:290:THR:HG23	3:G:36:VAL:HG21	1.99	0.45
3:G:62:ASP:O	3:G:67:LYS:N	2.44	0.45
3:G:138:SER:O	3:G:139:ARG:C	2.53	0.45
1:C:529:PHE:N	1:C:529:PHE:CD1	2.85	0.45
3:E:81:ILE:O	3:E:81:ILE:CD1	2.62	0.45
3:E:144:PRO:HA	3:E:160:VAL:HG22	1.99	0.45
2:B:211:GLU:H	2:B:211:GLU:HG3	1.33	0.45
1:C:497:ILE:O	1:C:519:LEU:N	2.37	0.45
1:A:533:VAL:CG1	1:A:534:LYS:N	2.80	0.45
3:G:6:GLU:CB	6:G:464:HOH:O	2.65	0.45
3:G:184:LEU:C	3:G:186:GLN:H	2.19	0.45
3:G:203:LYS:HA	3:G:203:LYS:HD3	1.68	0.45
3:E:253:VAL:O	3:E:254:GLY:C	2.55	0.45
3:G:135:MET:O	3:G:136:SER:C	2.55	0.44
2:D:232:LEU:HD11	2:D:236:LEU:HB2	1.97	0.44
3:E:20:ARG:HG2	3:E:129:MET:HG3	1.99	0.44
3:E:133:LEU:O	3:E:136:SER:N	2.50	0.44
3:G:38:ASP:C	3:G:40:THR:N	2.71	0.44
3:G:126:HIS:HB3	6:G:453:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:LEU:O	3:G:186:GLN:N	2.50	0.44
2:D:232:LEU:CD1	2:D:236:LEU:HB2	2.47	0.44
3:E:327:THR:O	3:E:329:ASN:N	2.51	0.44
1:A:533:VAL:CG1	1:A:534:LYS:H	2.26	0.44
2:D:208:TYR:OH	6:D:323:HOH:O	2.21	0.44
3:E:306:LEU:N	4:E:401:ATP:O1G	2.45	0.44
1:A:550:ASP:CG	1:A:551:HIS:H	2.20	0.44
1:C:519:LEU:N	1:C:519:LEU:HD12	2.32	0.44
2:D:283:TYR:HE2	2:D:284:HIS:HD2	1.58	0.44
3:E:15:ILE:O	3:E:18:PHE:HB3	2.18	0.44
3:E:314:ILE:HG12	6:E:508:HOH:O	2.17	0.44
1:A:470:TYR:O	1:A:473:LEU:HB2	2.18	0.44
1:C:537:GLY:N	6:C:27:HOH:O	2.44	0.44
3:E:19:ILE:HG21	3:E:129:MET:HE2	1.99	0.44
3:G:182:VAL:O	3:G:187:MET:HE2	2.17	0.44
3:G:307:ALA:HB3	4:G:401:ATP:O1A	2.18	0.44
1:C:469:VAL:O	1:C:473:LEU:HB2	2.17	0.44
3:E:209:LYS:O	3:E:212:ALA:O	2.36	0.44
1:A:574:PHE:CD2	3:E:93:ALA:HB1	2.52	0.44
1:C:542:TYR:CD1	1:C:542:TYR:C	2.90	0.44
1:C:572:LYS:HD2	1:C:572:LYS:HA	1.58	0.44
3:E:78:VAL:CA	3:E:81:ILE:HG22	2.48	0.44
3:E:133:LEU:O	3:E:134:ALA:C	2.55	0.44
1:A:459:ARG:HG3	1:A:459:ARG:NH1	2.32	0.44
3:G:310:LEU:HA	3:G:310:LEU:HD23	1.80	0.44
2:D:295:ASN:ND2	3:E:101:ARG:HH12	2.16	0.44
3:E:305:SER:HB2	4:E:401:ATP:O2B	2.18	0.44
1:A:523:GLU:CA	1:A:529:PHE:CD2	2.96	0.43
1:A:550:ASP:CG	1:A:551:HIS:N	2.71	0.43
3:G:185:ASN:HD22	3:G:185:ASN:C	2.17	0.43
1:A:521:LEU:HD23	1:A:531:LEU:HA	2.00	0.43
2:B:223:GLU:C	2:B:225:LYS:N	2.70	0.43
1:C:542:TYR:N	1:C:542:TYR:CD1	2.86	0.43
2:D:210:THR:CB	6:D:322:HOH:O	2.11	0.43
2:D:216:LEU:O	2:D:217:THR:O	2.36	0.43
3:E:99:LYS:HG2	3:E:100:PHE:N	2.33	0.43
3:E:210:MET:O	3:E:214:LYS:HB2	2.18	0.43
2:D:220:THR:HG22	2:D:220:THR:O	2.19	0.43
2:D:282:ARG:NH1	2:D:282:ARG:CG	2.74	0.43
3:E:80:VAL:HG12	3:E:109:GLU:HG2	2.01	0.43
2:B:296:PHE:CB	3:E:99:LYS:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:96:GLU:O	3:G:97:ILE:C	2.53	0.43
3:G:132:CYS:HB3	3:G:314:ILE:HD13	1.99	0.43
1:C:482:VAL:HG13	1:C:483:PRO:HD2	1.99	0.43
1:C:503:ILE:HD11	1:C:514:TYR:H	1.74	0.43
3:E:166:ILE:HG23	3:E:166:ILE:HD12	1.58	0.43
2:B:280:THR:OG1	2:B:289:THR:HG23	2.18	0.43
3:G:22:ARG:HD3	3:G:22:ARG:HA	1.48	0.43
3:G:73:THR:HG23	3:G:75:ALA:H	1.84	0.43
2:D:265:LEU:HA	2:D:265:LEU:HD12	1.73	0.43
3:E:231:VAL:HG11	6:E:505:HOH:O	2.17	0.43
2:D:283:TYR:C	2:D:283:TYR:CD2	2.92	0.43
3:E:309:ILE:O	3:E:310:LEU:C	2.57	0.43
2:B:222:GLN:O	2:B:223:GLU:C	2.57	0.43
2:D:237:GLU:O	2:D:237:GLU:CG	2.66	0.43
3:E:255:GLU:HG2	3:E:255:GLU:H	1.60	0.43
1:A:466:LEU:HD11	1:A:497:ILE:HD11	2.00	0.43
3:G:129:MET:CE	3:G:314:ILE:HG22	2.47	0.43
1:C:569:LEU:HD22	1:C:573:LEU:HG	2.01	0.43
3:E:228:LEU:HD23	3:E:228:LEU:HA	1.79	0.43
3:E:231:VAL:C	6:E:486:HOH:O	2.54	0.43
3:E:243:ASP:N	6:E:414:HOH:O	2.42	0.43
3:G:276:LEU:HA	3:G:276:LEU:HD12	1.72	0.43
3:E:136:SER:OG	3:E:311:ASN:ND2	2.52	0.43
2:B:220:THR:OG1	2:B:224:LEU:HD13	2.19	0.43
3:G:20:ARG:HG2	3:G:129:MET:HG3	2.00	0.43
1:C:508:ARG:HD2	6:C:376:HOH:O	2.19	0.43
3:E:276:LEU:O	3:E:280:PHE:HB2	2.19	0.43
3:G:112:ILE:HD12	3:G:330:PHE:CZ	2.54	0.42
2:D:262:LEU:HD13	2:D:262:LEU:HA	1.68	0.42
3:E:97:ILE:HA	3:E:97:ILE:HD13	1.57	0.42
3:E:288:VAL:HG12	3:E:290:ARG:O	2.18	0.42
3:E:312:TYR:C	3:E:314:ILE:N	2.69	0.42
3:G:23:THR:O	3:G:26:ASP:HB2	2.19	0.42
3:G:185:ASN:HD21	3:G:186:GLN:HG3	1.82	0.42
3:E:128:LEU:HD11	3:E:166:ILE:CG1	2.48	0.42
3:E:141:ARG:HH11	3:E:217:SER:HB3	1.84	0.42
1:A:500:ARG:HG2	1:A:514:TYR:CD2	2.54	0.42
3:G:2:MET:CG	6:G:464:HOH:O	2.66	0.42
3:G:120:ILE:HD13	3:G:120:ILE:H	1.84	0.42
1:C:541:ILE:HD12	1:C:541:ILE:HA	1.81	0.42
2:D:212:ILE:HD12	2:D:213:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:110:ARG:HE	3:E:110:ARG:CA	2.32	0.42
3:E:218:ALA:O	3:E:219:VAL:HG23	2.19	0.42
1:A:461:ASP:O	1:A:464:GLU:N	2.53	0.42
1:A:489:LYS:CA	6:A:91:HOH:O	2.61	0.42
2:B:296:PHE:HB3	3:E:99:LYS:HD2	2.00	0.42
3:G:149:ASP:O	3:G:151:GLU:N	2.53	0.42
3:G:305:SER:OG	3:G:306:LEU:N	2.51	0.42
3:G:306:LEU:HD12	6:G:526:HOH:O	2.18	0.42
1:C:501:TRP:HB2	6:C:213:HOH:O	2.19	0.42
3:E:302:GLY:C	3:E:303:ILE:HG13	2.40	0.42
3:G:201:GLU:HA	3:G:252:SER:HB2	2.01	0.42
3:G:295:ASP:HB3	3:G:301:GLU:OE1	2.19	0.42
1:C:491:ARG:O	1:C:494:MET:HG2	2.18	0.42
1:C:515:ALA:HA	1:C:537:GLY:O	2.19	0.42
1:C:555:ASP:OD2	1:C:555:ASP:N	2.53	0.42
2:D:272:LEU:HD12	3:E:49:LEU:CD2	2.50	0.42
3:G:123:HIS:CD2	3:G:125:MET:H	2.37	0.42
3:E:37:PHE:HB2	3:E:60:LEU:HD23	2.00	0.42
4:E:401:ATP:C8	4:E:401:ATP:C5'	2.85	0.42
3:E:255:GLU:C	3:E:257:LEU:N	2.73	0.42
3:E:294:VAL:HG12	3:E:300:LEU:HA	2.01	0.42
2:B:236:LEU:HD23	2:B:261:LEU:HD22	2.01	0.42
1:C:454:PHE:HB2	1:C:530:MET:CE	2.50	0.42
1:A:540:ASP:HB3	3:G:151:GLU:OE1	2.19	0.41
2:B:218:SER:O	2:B:219:ASN:HB3	2.20	0.41
2:B:263:ASN:ND2	2:B:279:ALA:HB1	2.34	0.41
3:G:80:VAL:HG22	3:G:97:ILE:CD1	2.37	0.41
3:G:91:PRO:HD2	6:C:17:HOH:O	2.20	0.41
3:G:120:ILE:H	3:G:120:ILE:CD1	2.33	0.41
3:G:294:VAL:HB	3:G:298:LEU:HA	2.01	0.41
2:D:261:LEU:HD21	6:D:307:HOH:O	2.19	0.41
3:E:115:ILE:HG13	3:E:116:PRO:HD2	2.00	0.41
3:E:162:THR:HG21	6:E:460:HOH:O	2.20	0.41
3:E:240:LEU:HA	3:E:240:LEU:HD12	1.80	0.41
3:E:275:ARG:O	3:E:276:LEU:C	2.58	0.41
3:E:323:VAL:HA	3:E:324:PRO:HA	1.85	0.41
3:G:78:VAL:HG13	3:G:208:ILE:HG23	2.02	0.41
1:C:479:GLN:NE2	1:C:500:ARG:HH22	2.18	0.41
1:C:484:LYS:NZ	1:C:484:LYS:CB	2.79	0.41
3:E:186:GLN:CB	6:E:523:HOH:O	2.47	0.41
1:A:561:PRO:O	1:A:565:LEU:CD2	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:PRO:CA	3:G:66:ASN:HD21	2.34	0.41
3:G:164[B]:TYR:HE1	6:G:493:HOH:O	2.04	0.41
1:C:487:ASN:O	1:C:489:LYS:N	2.43	0.41
3:E:56:VAL:HB	6:E:497:HOH:O	2.19	0.41
3:E:206:ASP:O	3:E:209:LYS:HB3	2.19	0.41
3:E:290:ARG:CZ	3:E:290:ARG:HB2	2.50	0.41
1:A:484:LYS:HE3	1:A:484:LYS:HA	2.03	0.41
2:B:250:ASP:CA	2:B:252:SER:H	2.33	0.41
1:C:472:ALA:CB	1:C:573:LEU:HD23	2.49	0.41
1:C:499:SER:HG	1:C:501:TRP:HE1	1.67	0.41
1:C:506:CYS:HB3	1:C:511:LYS:CB	2.50	0.41
3:E:38:ASP:O	3:E:39:VAL:C	2.57	0.41
1:A:464:GLU:O	1:A:467:LEU:HB3	2.20	0.41
2:B:224:LEU:HB3	2:B:226:LEU:HD21	2.02	0.41
3:G:86:GLN:HB3	3:G:209:LYS:HZ1	1.84	0.41
3:G:168:LYS:O	3:G:172:MET:CG	2.66	0.41
6:C:77:HOH:O	2:D:229:PRO:HA	2.20	0.41
1:A:542:TYR:HA	1:A:543:SER:CB	2.50	0.41
3:G:90:PHE:HA	3:G:91:PRO:HD3	1.82	0.41
3:G:130:ASP:OD2	6:G:453:HOH:O	2.22	0.41
1:C:534:LYS:O	1:C:534:LYS:HG2	2.19	0.41
2:D:295:ASN:ND2	3:E:101:ARG:NH1	2.68	0.41
1:A:495:TYR:CE1	2:B:227:PRO:O	2.74	0.41
3:G:309:ILE:O	3:G:313:ILE:HG12	2.20	0.41
2:B:265:LEU:HD12	2:B:266:ALA:H	1.85	0.41
3:G:23:THR:O	3:G:24:SER:C	2.59	0.41
3:G:39:VAL:CG2	3:G:61:TRP:O	2.68	0.41
3:G:77:PHE:N	6:G:477:HOH:O	2.53	0.41
3:G:129:MET:HE1	3:G:314:ILE:HB	2.01	0.41
3:G:248:ASN:O	3:G:251:LEU:HD12	2.20	0.41
3:G:329:ASN:N	3:G:329:ASN:HD22	2.18	0.41
1:C:454:PHE:HE1	2:D:238:LYS:O	2.03	0.41
3:E:27:VAL:HG13	3:E:169:PHE:HB2	2.03	0.41
3:E:102:LEU:HD12	3:E:102:LEU:HA	1.87	0.41
3:E:209:LYS:HG2	3:E:213:GLU:OE1	2.20	0.41
3:G:80:VAL:HG23	3:G:84:TYR:CD1	2.56	0.41
3:E:68:PHE:CZ	3:E:70:GLY:C	2.95	0.41
1:A:479:GLN:NE2	1:A:500:ARG:NH2	2.69	0.40
1:A:563:LEU:HA	1:A:566:CYS:HB2	2.03	0.40
2:B:238:LYS:O	2:B:238:LYS:HG2	2.21	0.40
3:G:193:SER:O	3:G:194:ASN:CB	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:SER:OG	2:D:210:THR:N	2.54	0.40
3:E:120:ILE:HG23	3:E:143:ILE:HG13	2.03	0.40
3:E:181:ARG:NH2	3:E:275:ARG:NH2	2.68	0.40
3:E:265:ASP:HB2	3:E:289:HIS:CE1	2.56	0.40
1:A:466:LEU:HD21	1:A:494:MET:O	2.21	0.40
3:G:18:PHE:O	3:G:19:ILE:C	2.59	0.40
3:G:77:PHE:CA	6:G:477:HOH:O	2.69	0.40
3:G:236:ASP:CG	3:G:260:ARG:HH11	2.25	0.40
1:C:505:HIS:CE1	1:C:506:CYS:SG	3.14	0.40
3:E:114:ALA:HA	3:E:330:PHE:CD1	2.55	0.40
3:E:309:ILE:H	3:E:309:ILE:HG12	1.45	0.40
2:B:283:TYR:O	2:B:284:HIS:C	2.59	0.40
1:C:495:TYR:CZ	2:D:229:PRO:HD3	2.56	0.40
3:E:283:ILE:HD13	3:E:283:ILE:HG21	1.83	0.40
3:G:65:ALA:C	3:G:67:LYS:N	2.71	0.40
1:C:494:MET:C	1:C:496:THR:H	2.25	0.40
1:C:521:LEU:CD1	2:D:229:PRO:HB3	2.47	0.40
3:G:44:LYS:CD	6:G:412:HOH:O	2.69	0.40
3:G:196:ALA:O	3:G:220:PRO:HD2	2.22	0.40
3:G:307:ALA:CB	4:G:401:ATP:O1A	2.70	0.40
1:C:500:ARG:HG2	1:C:500:ARG:NH1	2.18	0.40
2:D:228:LYS:HA	2:D:228:LYS:HD3	1.82	0.40
3:E:74:MET:HE2	3:E:238:MET:H	1.87	0.40
3:E:203:LYS:HD3	3:E:203:LYS:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	127/137 (93%)	90 (71%)	20 (16%)	17 (13%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	111/137 (81%)	84 (76%)	18 (16%)	9 (8%)	1 2
2	B	91/97 (94%)	60 (66%)	17 (19%)	14 (15%)	0 0
2	D	89/97 (92%)	71 (80%)	11 (12%)	7 (8%)	1 2
3	E	331/333 (99%)	256 (77%)	49 (15%)	26 (8%)	1 2
3	G	321/333 (96%)	265 (83%)	36 (11%)	20 (6%)	1 4
All	All	1070/1134 (94%)	826 (77%)	151 (14%)	93 (9%)	1 1

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	LYS
1	A	542	TYR
1	A	543	SER
1	A	545	PRO
1	A	548	THR
1	A	554	ASP
1	A	555	ASP
2	B	209	SER
2	B	219	ASN
2	B	222	GLN
2	B	243	SER
2	B	247	TYR
2	B	259[A]	HIS
2	B	259[B]	HIS
2	B	262	LEU
3	G	64	GLU
3	G	88	SER
3	G	140	ALA
3	G	141	ARG
3	G	170	ILE
3	G	264	PHE
3	G	316	ASP
1	C	511	LYS
2	D	217	THR
2	D	224	LEU
2	D	225	LYS
2	D	226	LEU
3	E	64	GLU
3	E	93	ALA
1	A	448	ARG

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Mol	Chain	Res	Type
1	A	493	ASP
1	A	534	LYS
1	A	551	HIS
2	B	225	LYS
2	B	245	THR
3	G	89	SER
3	G	110	ARG
3	G	121	TYR
3	G	150	GLY
3	G	200	MET
3	G	215	ASN
3	G	284	LYS
1	C	488	GLY
1	C	502	GLU
1	C	555	ASP
2	D	218	SER
3	E	3	ASP
3	E	26	ASP
3	E	88	SER
3	E	94	ILE
3	E	274	ASP
3	E	309	ILE
3	E	329	ASN
3	E	333	ALA
1	A	511	LYS
2	B	207	GLN
2	B	248	LYS
3	G	138	SER
1	C	483	PRO
1	C	489	LYS
3	E	95	ALA
3	E	97	ILE
3	E	117	PRO
3	E	213	GLU
3	E	254	GLY
3	E	328	ASP
1	A	487	ASN
1	A	556	LEU
3	G	3	ASP
3	G	25	TYR
3	G	248	ASN
1	C	527	GLY

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Mol	Chain	Res	Type
1	C	541	ILE
2	D	262	LEU
3	E	52	LEU
3	E	91	PRO
3	E	211	LEU
3	E	276	LEU
1	A	547	ARG
2	B	241	LEU
2	B	246	ALA
1	C	504	PRO
3	E	139	ARG
3	E	238	MET
3	E	308	ASP
3	E	332	SER
1	A	462	ALA
1	A	544	HIS
3	G	266	GLY
3	G	97	ILE
2	D	230	PRO
3	E	190	GLY
3	E	39	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	106/120 (88%)	85 (80%)	21 (20%)	1 3
1	C	96/120 (80%)	73 (76%)	23 (24%)	0 1
2	B	80/88 (91%)	59 (74%)	21 (26%)	0 1
2	D	79/88 (90%)	58 (73%)	21 (27%)	0 1
3	E	293/296 (99%)	238 (81%)	55 (19%)	1 4
3	G	283/296 (96%)	228 (81%)	55 (19%)	1 3
All	All	937/1008 (93%)	741 (79%)	196 (21%)	1 2

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	459	ARG
1	A	474	GLN
1	A	480	PHE
1	A	484	LYS
1	A	486	VAL
1	A	492	SER
1	A	507	LYS
1	A	511	LYS
1	A	512	ASN
1	A	513	THR
1	A	521	LEU
1	A	525	MET
1	A	534	LYS
1	A	536	ASN
1	A	540	ASP
1	A	543	SER
1	A	546	GLU
1	A	558	SER
1	A	565	LEU
1	A	569	LEU
2	B	207	GLN
2	B	210	THR
2	B	211	GLU
2	B	217	THR
2	B	222	GLN
2	B	224	LEU
2	B	225	LYS
2	B	231	SER
2	B	232	LEU
2	B	238	LYS
2	B	249	GLU
2	B	253	VAL
2	B	260	VAL
2	B	262	LEU
2	B	263	ASN
2	B	269	ASN
2	B	271	GLN
2	B	281	THR
2	B	282	ARG
2	B	285	ARG
2	B	295	ASN

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Mol	Chain	Res	Type
3	G	22	ARG
3	G	30	THR
3	G	39	VAL
3	G	46	SER
3	G	52	LEU
3	G	57	SER
3	G	62	ASP
3	G	63	SER
3	G	64	GLU
3	G	80	VAL
3	G	82	LYS
3	G	86	GLN
3	G	87	SER
3	G	102	LEU
3	G	110	ARG
3	G	118	GLU
3	G	119	THR
3	G	120	ILE
3	G	122	VAL
3	G	129	MET
3	G	137	LYS
3	G	138	SER
3	G	146	ILE
3	G	154	SER
3	G	162	THR
3	G	165	ARG
3	G	172	MET
3	G	181	ARG
3	G	185	ASN
3	G	189	ILE
3	G	193	SER
3	G	200	MET
3	G	201	GLU
3	G	225	GLU
3	G	227	THR
3	G	228	LEU
3	G	235	VAL
3	G	236	ASP
3	G	248	ASN
3	G	255	GLU
3	G	258	LEU
3	G	275	ARG

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Mol	Chain	Res	Type
3	G	276	LEU
3	G	281	ASP
3	G	284	LYS
3	G	286	SER
3	G	287	ARG
3	G	289	HIS
3	G	290	ARG
3	G	298	LEU
3	G	305	SER
3	G	310	LEU
3	G	315	TYR
3	G	329	ASN
3	G	332	SER
1	C	474	GLN
1	C	483	PRO
1	C	484	LYS
1	C	487	ASN
1	C	492	SER
1	C	500	ARG
1	C	503	ILE
1	C	507	LYS
1	C	512	ASN
1	C	534	LYS
1	C	535	SER
1	C	536	ASN
1	C	539	LYS
1	C	541	ILE
1	C	542	TYR
1	C	555	ASP
1	C	556	LEU
1	C	557	LYS
1	C	559	SER
1	C	564	ASP
1	C	565	LEU
1	C	569	LEU
1	C	572	LYS
2	D	211	GLU
2	D	212	ILE
2	D	221	LEU
2	D	223	GLU
2	D	224	LEU
2	D	225	LYS

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Mol	Chain	Res	Type
2	D	226	LEU
2	D	228	LYS
2	D	232	LEU
2	D	235	HIS
2	D	238	LYS
2	D	244	ASN
2	D	247	TYR
2	D	250	ASP
2	D	258	ASN
2	D	261	LEU
2	D	262	LEU
2	D	263	ASN
2	D	282	ARG
2	D	290	THR
2	D	296	PHE
3	E	8	GLN
3	E	9	LYS
3	E	30	THR
3	E	31	SER
3	E	35	ILE
3	E	39	VAL
3	E	67	LYS
3	E	81	ILE
3	E	89	SER
3	E	92	GLU
3	E	94	ILE
3	E	99	LYS
3	E	102	LEU
3	E	110	ARG
3	E	115	ILE
3	E	118	GLU
3	E	119	THR
3	E	120	ILE
3	E	122	VAL
3	E	129	MET
3	E	137	LYS
3	E	143	ILE
3	E	146	ILE
3	E	151	GLU
3	E	161	LEU
3	E	162	THR
3	E	166	ILE

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Mol	Chain	Res	Type
3	E	175	LYS
3	E	181	ARG
3	E	185	ASN
3	E	188	THR
3	E	201	GLU
3	E	223	ASN
3	E	225	GLU
3	E	227	THR
3	E	228	LEU
3	E	230	ASN
3	E	231	VAL
3	E	255	GLU
3	E	257	LEU
3	E	260	ARG
3	E	265	ASP
3	E	275	ARG
3	E	276	LEU
3	E	277	ASP
3	E	280	PHE
3	E	281	ASP
3	E	305	SER
3	E	309	ILE
3	E	310	LEU
3	E	314	ILE
3	E	316	ASP
3	E	317	LYS
3	E	325	GLU
3	E	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	A	479	GLN
1	A	520	GLN
1	A	536	ASN
2	B	207	GLN
2	B	263	ASN
2	B	284	HIS
3	G	5	GLN
3	G	8	GLN
3	G	66	ASN

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Mol	Chain	Res	Type
3	G	86	GLN
3	G	123	HIS
3	G	163	GLN
3	G	173	ASN
3	G	185	ASN
3	G	248	ASN
3	G	329	ASN
1	C	474	GLN
1	C	505	HIS
1	C	512	ASN
1	C	536	ASN
2	D	235	HIS
2	D	242	ASN
2	D	258	ASN
2	D	284	HIS
2	D	295	ASN
3	E	123	HIS
3	E	185	ASN
3	E	186	GLN
3	E	215	ASN
3	E	242	GLN
3	E	289	HIS
3	E	311	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FLC	E	402	-	12,12,12	1.14	0	17,17,17	1.49	3 (17%)
4	ATP	E	401	-	26,33,33	1.06	2 (7%)	31,52,52	1.69	6 (19%)
4	ATP	G	401	-	26,33,33	1.29	3 (11%)	31,52,52	1.84	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FLC	E	402	-	-	6/16/16/16	-
4	ATP	E	401	-	-	3/18/38/38	0/3/3/3
4	ATP	G	401	-	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	401	ATP	C5-C4	3.26	1.49	1.40
4	E	401	ATP	C5-C4	2.49	1.47	1.40
4	G	401	ATP	C2-N3	2.44	1.36	1.32
4	G	401	ATP	O4'-C1'	2.41	1.44	1.41
4	E	401	ATP	C2-N3	2.07	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	401	ATP	PA-O3A-PB	-5.53	113.84	132.83
4	E	401	ATP	PA-O3A-PB	-4.62	116.96	132.83
4	G	401	ATP	C4-C5-N7	-3.42	105.84	109.40
4	E	401	ATP	C4-C5-N7	-3.31	105.95	109.40
5	E	402	FLC	OB2-CBC-CB	3.29	118.77	113.05
4	G	401	ATP	PB-O3B-PG	-3.20	121.83	132.83
4	E	401	ATP	N3-C2-N1	-3.09	123.85	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	401	ATP	O5'-C5'-C4'	3.04	119.47	108.99
4	E	401	ATP	C3'-C2'-C1'	2.95	105.42	100.98
4	E	401	ATP	C5'-C4'-C3'	-2.94	104.17	115.18
4	G	401	ATP	C2'-C3'-C4'	2.71	107.90	102.64
5	E	402	FLC	OB1-CBC-CB	-2.62	118.55	122.25
4	E	401	ATP	PA-O5'-C5'	-2.09	109.41	121.68
5	E	402	FLC	CB-CA-CAC	-2.04	108.88	113.81

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	401	ATP	O4'-C4'-C5'-O5'
4	E	401	ATP	PB-O3A-PA-O5'
5	E	402	FLC	CG-CB-CBC-OB1
5	E	402	FLC	CG-CB-CBC-OB2
5	E	402	FLC	OHB-CB-CBC-OB1
5	E	402	FLC	OHB-CB-CBC-OB2
4	G	401	ATP	C3'-C4'-C5'-O5'
4	G	401	ATP	PB-O3A-PA-O5'
4	G	401	ATP	PB-O3A-PA-O1A
5	E	402	FLC	CA-CB-CBC-OB1
5	E	402	FLC	CA-CB-CBC-OB2
4	G	401	ATP	PB-O3B-PG-O1G
4	E	401	ATP	C4'-C5'-O5'-PA
4	E	401	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

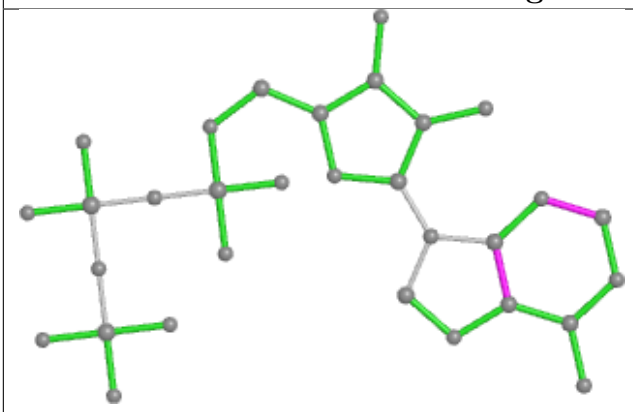
3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	402	FLC	2	0
4	E	401	ATP	12	0
4	G	401	ATP	4	0

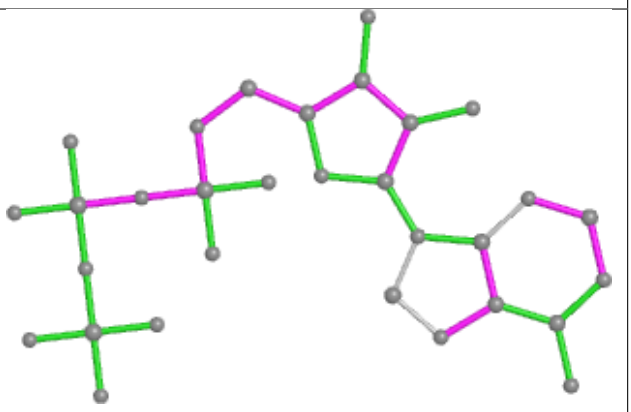
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

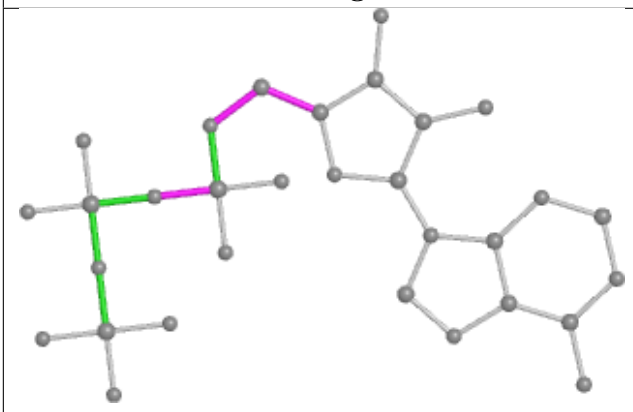
Ligand ATP E 401



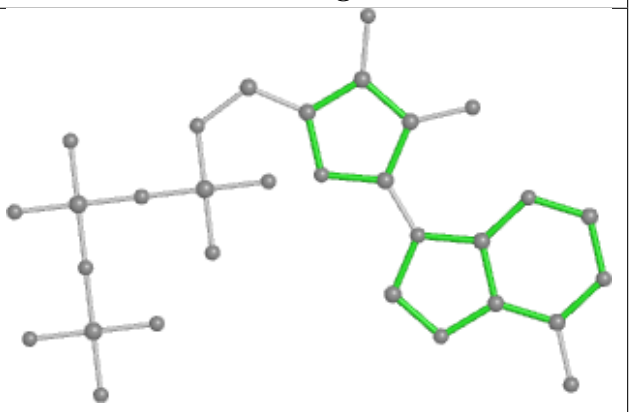
Bond lengths



Bond angles

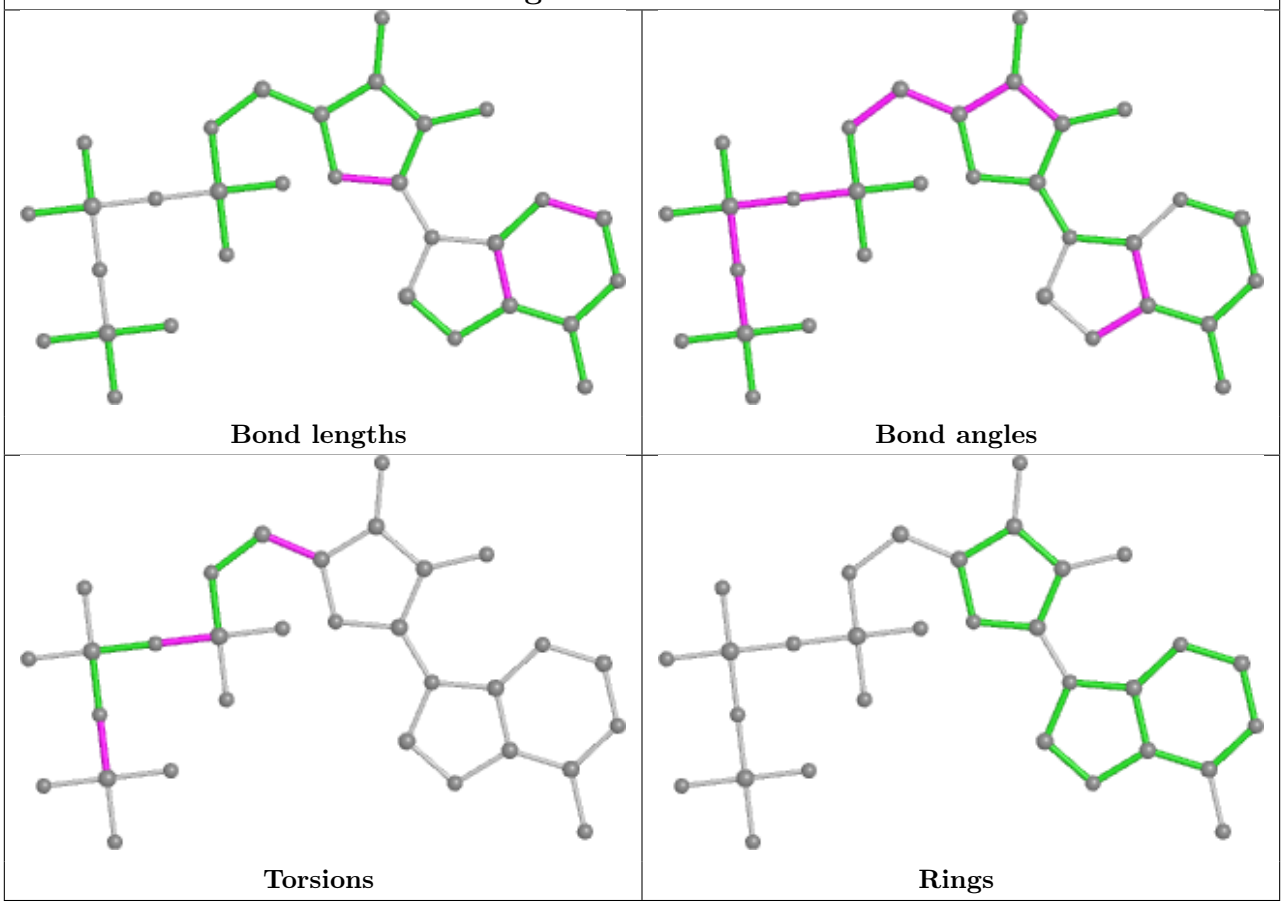


Torsions



Rings

Ligand ATP G 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	286:LYS	C	287:TYR	N	1.13

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	129/137 (94%)	0.01	15 (11%)	4	3	30, 54, 113, 128	0
1	C	115/137 (83%)	-0.37	2 (1%)	70	70	38, 55, 88, 102	0
2	B	92/97 (94%)	-0.23	3 (3%)	46	41	23, 64, 94, 100	0
2	D	91/97 (93%)	-0.10	4 (4%)	34	30	23, 63, 100, 103	0
3	E	333/333 (100%)	-0.53	8 (2%)	59	57	25, 49, 84, 128	0
3	G	324/333 (97%)	-0.61	1 (0%)	94	94	26, 44, 69, 80	0
All	All	1084/1134 (95%)	-0.41	33 (3%)	50	46	23, 50, 91, 128	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	320	THR	6.7
1	A	552	GLY	5.2
1	A	544	HIS	4.6
2	D	246	ALA	4.6
3	E	327	THR	4.2
3	E	318	THR	3.9
1	A	551	HIS	3.9
2	D	245	THR	3.4
3	G	327	THR	3.4
1	C	542	TYR	3.4
1	A	553	MET	3.3
1	A	545	PRO	3.2
1	A	547	ARG	3.2
1	A	488	GLY	3.1
3	E	324	PRO	3.0
2	B	245	THR	2.9
1	A	550	ASP	2.9
2	D	249	GLU	2.8
2	B	221	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	323	VAL	2.6
1	A	554	ASP	2.5
3	E	326	GLN	2.5
1	A	487	ASN	2.5
2	D	218	SER	2.4
1	A	548	THR	2.4
2	B	247	TYR	2.3
1	A	486	VAL	2.3
3	E	321	PRO	2.2
1	A	549	ALA	2.2
3	E	118	GLU	2.2
1	A	555	ASP	2.1
1	A	491	ARG	2.1
1	C	510	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

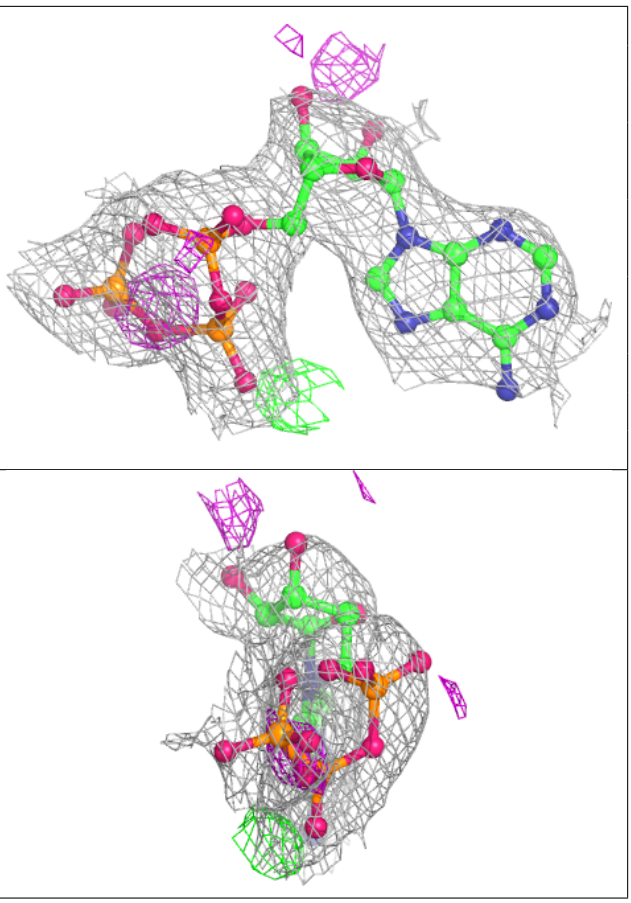
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

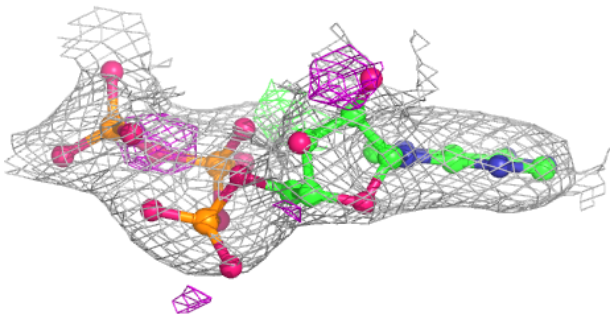
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FLC	E	402	13/13	0.92	0.23	99,101,102,102	0
4	ATP	E	401	31/31	0.93	0.16	55,60,90,92	0
4	ATP	G	401	31/31	0.94	0.15	50,54,98,99	0

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

Electron density around ATP E 401:

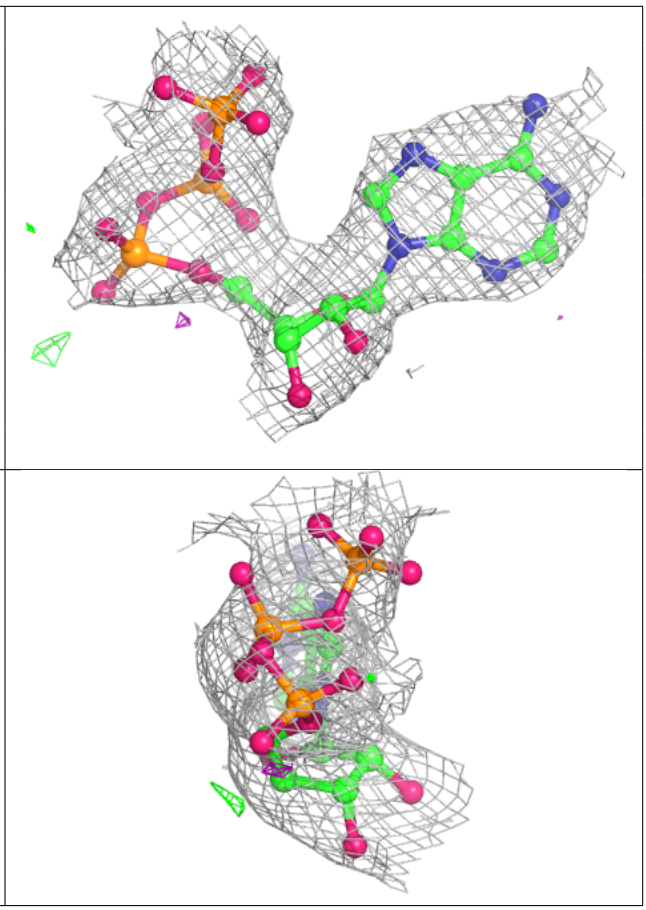
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around ATP G 401:

$2mF_o$-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.