



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1Z7E
Title : Crystal structure of full length ArnA
Authors : Gatzeva-Topalova, P.Z.; May, A.P.; Sousa, M.C.
Deposited on : 2005-03-24
Resolution : 3.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

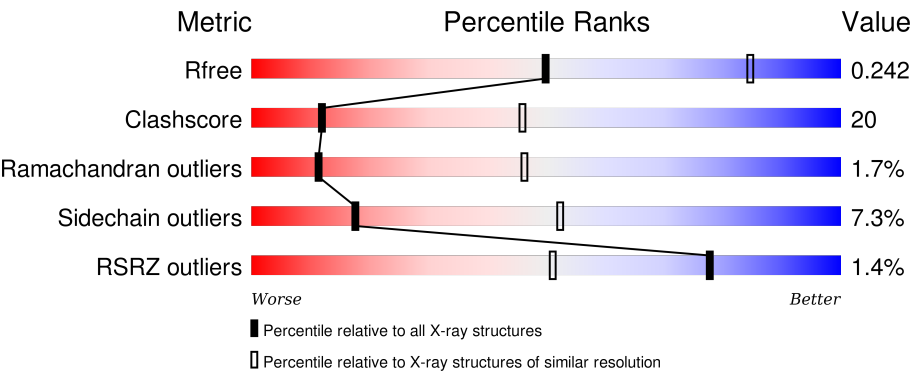
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	660	<div><div></div><div>59%34%. .</div></div>
1	B	660	<div><div>%</div><div>60%32%5%. .</div></div>
1	C	660	<div><div>%</div><div>60%33%. .</div></div>
1	D	660	<div><div>%</div><div>59%34%. .</div></div>
1	E	660	<div><div></div><div>60%32%5%. .</div></div>

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Mol	Chain	Length	Quality of chain
1	F	660	

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	ATP	E	1005	-	-	-	X
2	ATP	F	1006	-	-	-	X
3	UGA	A	1101	-	-	-	X
3	UGA	B	1102	-	-	-	X
3	UGA	D	1104	-	-	-	X
3	UGA	E	1105	-	-	-	X

2 Entry composition [i](#)

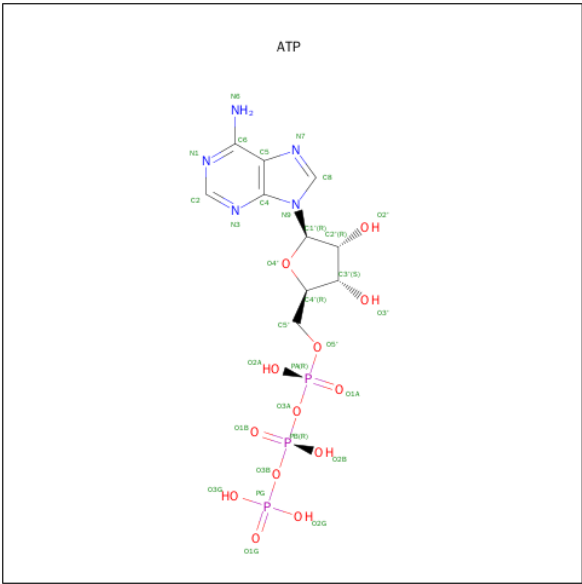
There are 3 unique types of molecules in this entry. The entry contains 30556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein ArnA.

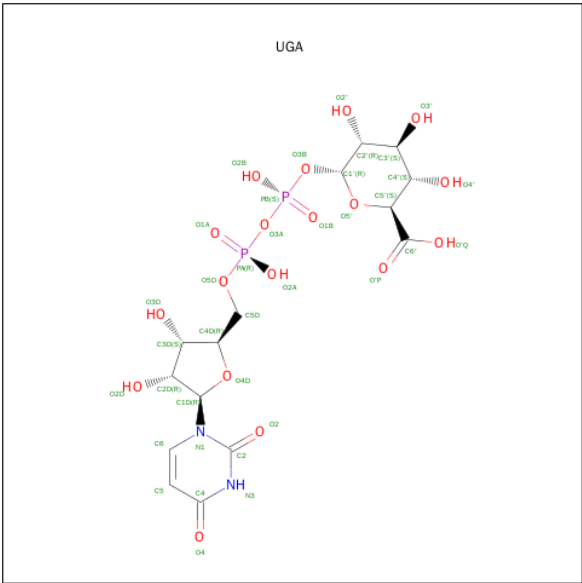
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	B	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	C	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	D	644	Total	C	N	O	S	0	0	0
			5048	3227	888	914	19			
1	E	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	F	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: C₁₅H₂₂N₂O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	E	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

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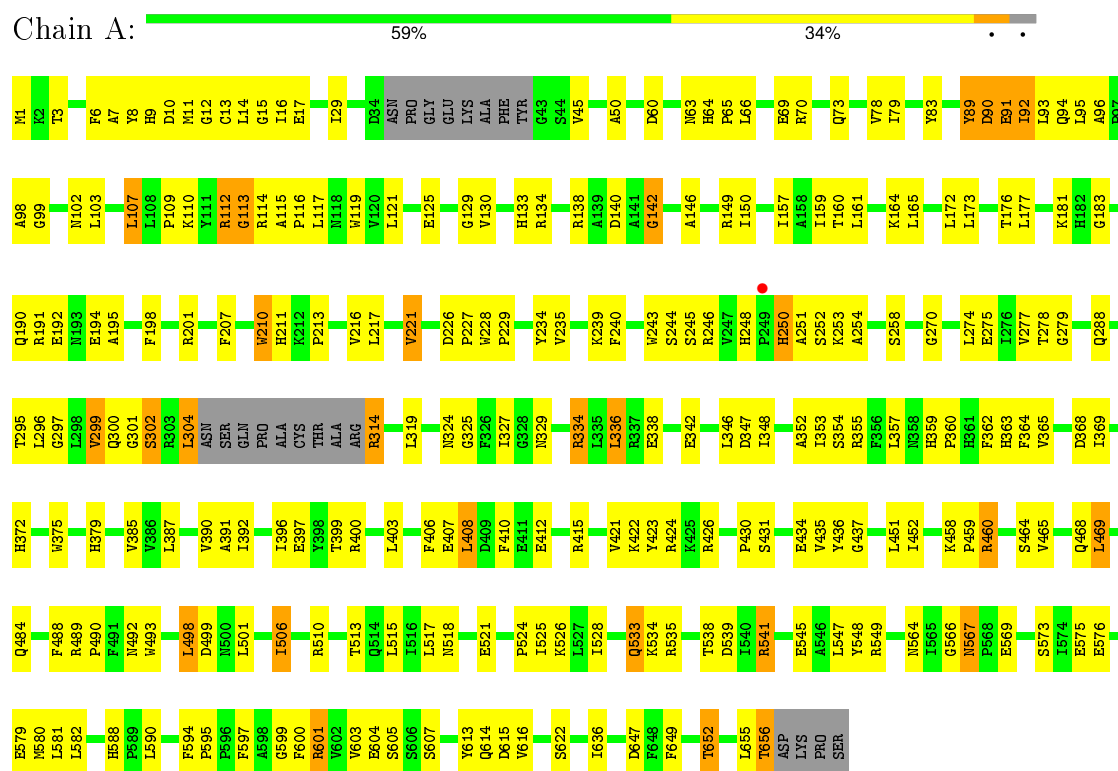
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

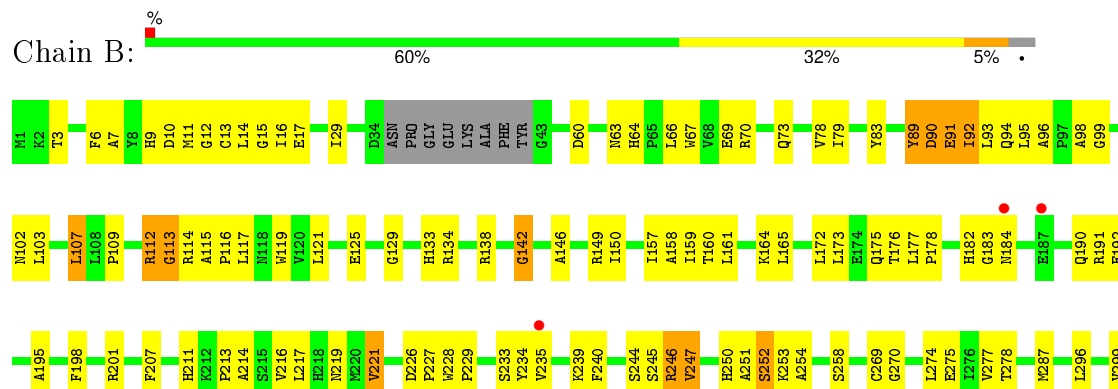
3 Residue-property plots

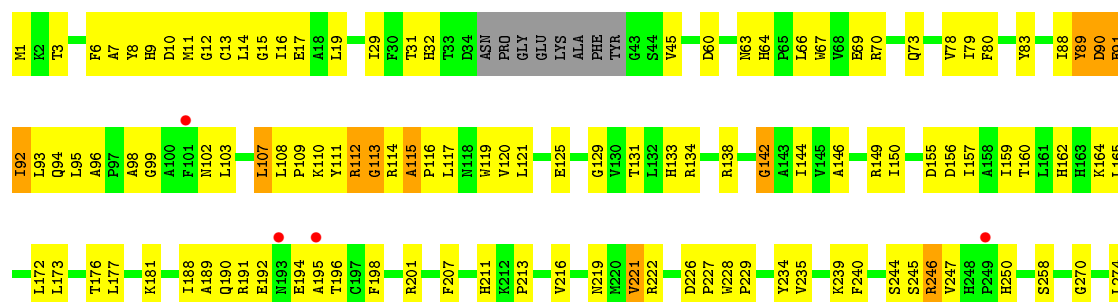
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

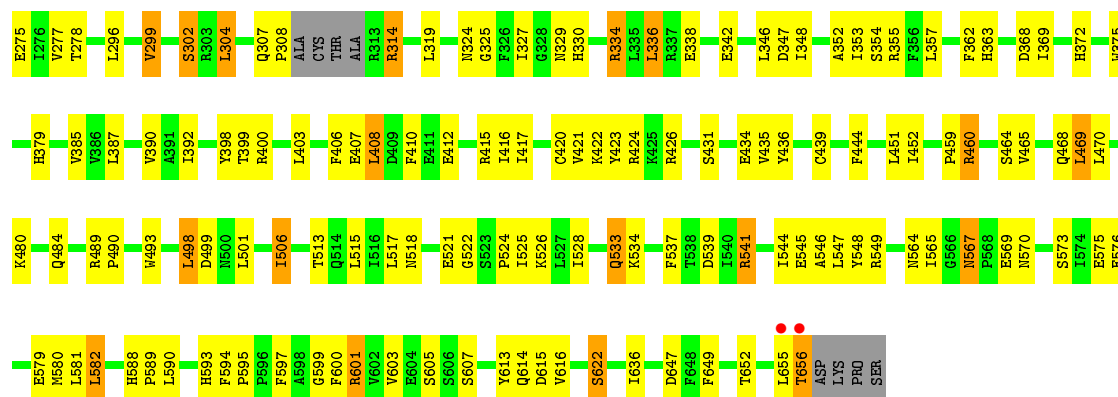
• Molecule 1: protein ArnA



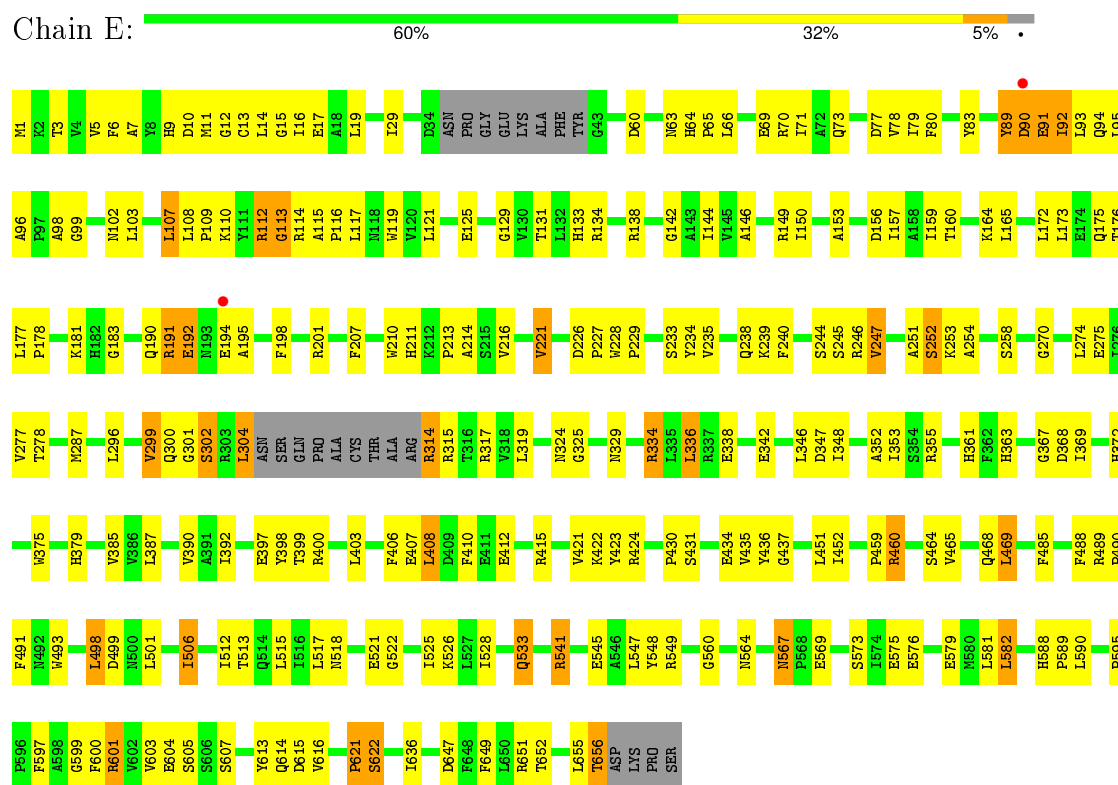
• Molecule 1: protein ArnA



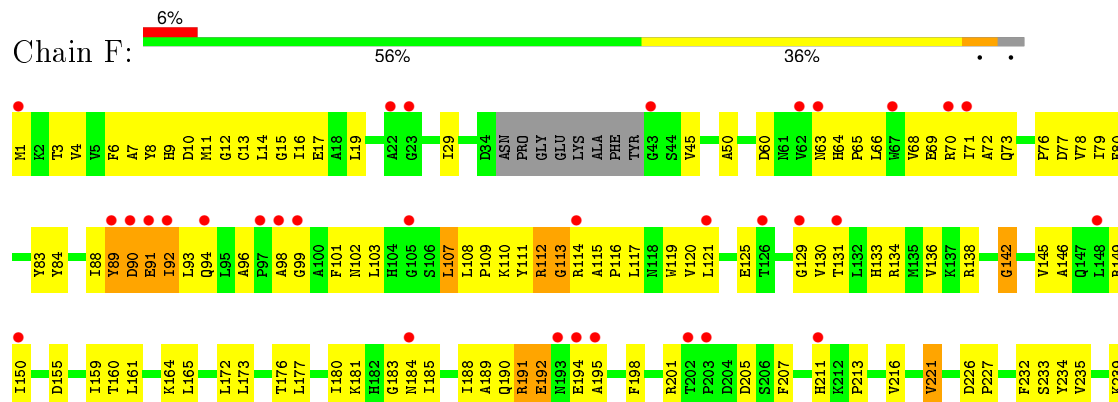


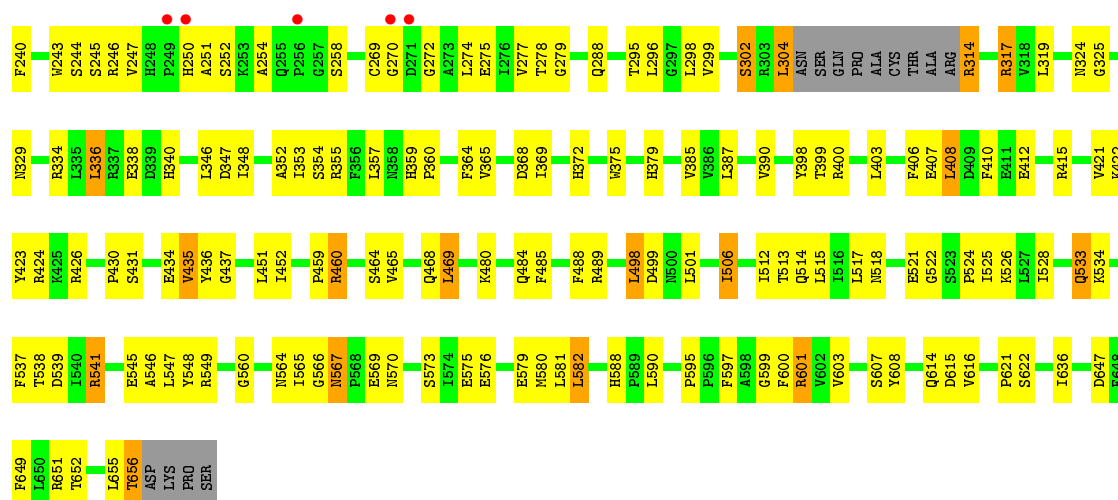


• Molecule 1: protein ArnA



• Molecule 1: protein ArnA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.69Å 166.23Å 261.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.65 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-3.00) 94.8 (49.65-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.247 0.222 , 0.242	Depositor DCC
R_{free} test set	12667 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	7 of 132564 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30556	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UGA, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/5143	0.64	1/6992 (0.0%)
1	B	0.42	0/5143	0.65	1/6992 (0.0%)
1	C	0.43	0/5143	0.66	1/6992 (0.0%)
1	D	0.42	0/5172	0.65	2/7033 (0.0%)
1	E	0.41	0/5143	0.65	2/6992 (0.0%)
1	F	0.44	0/5143	0.65	1/6992 (0.0%)
All	All	0.42	0/30887	0.65	8/41993 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	299	VAL	N-CA-C	-5.67	95.71	111.00
1	C	299	VAL	N-CA-C	-5.45	96.30	111.00
1	E	299	VAL	N-CA-C	-5.23	96.88	111.00
1	A	299	VAL	N-CA-C	-5.20	96.96	111.00
1	F	299	VAL	N-CA-C	-5.13	97.14	111.00
1	B	299	VAL	N-CA-C	-5.09	97.25	111.00
1	D	622	SER	N-CA-C	-5.05	97.37	111.00
1	E	622	SER	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5020	0	4924	206	0
1	B	5020	0	4924	202	2
1	C	5020	0	4924	201	2
1	D	5048	0	4942	199	0
1	E	5020	0	4924	202	0
1	F	5020	0	4924	219	0
2	A	31	0	12	5	0
2	B	31	0	12	4	0
2	C	31	0	12	4	0
2	D	31	0	12	4	0
2	E	31	0	12	2	0
2	F	31	0	12	3	0
3	A	37	0	19	1	0
3	B	37	0	19	1	0
3	C	37	0	19	1	0
3	D	37	0	19	1	0
3	E	37	0	19	1	0
3	F	37	0	19	1	0
All	All	30556	0	29748	1204	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1204) 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:E:533:GLN:NE2	1:E:533:GLN:H	1.56	1.03
1:A:533:GLN:NE2	1:A:533:GLN:H	1.58	1.01
1:C:533:GLN:H	1:C:533:GLN:NE2	1.59	1.00
1:F:533:GLN:NE2	1:F:533:GLN:H	1.61	0.97
1:D:533:GLN:NE2	1:D:533:GLN:H	1.61	0.97
1:B:533:GLN:NE2	1:B:533:GLN:H	1.61	0.96
1:D:112:ARG:HH12	1:D:190:GLN:HE22	1.04	0.96
1:D:368:ASP:H	1:D:372:HIS:HD2	1.05	0.96
1:C:112:ARG:HH12	1:C:190:GLN:HE22	0.96	0.96
1:D:533:GLN:HE21	1:D:533:GLN:H	0.96	0.95
1:B:112:ARG:NH1	1:B:190:GLN:HE22	1.65	0.94
1:C:368:ASP:H	1:C:372:HIS:HD2	1.14	0.93
1:F:112:ARG:HH12	1:F:190:GLN:HE22	1.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HH12	1:A:190:GLN:HE22	0.98	0.92
1:E:533:GLN:HE21	1:E:533:GLN:N	1.67	0.91
1:A:368:ASP:H	1:A:372:HIS:HD2	1.17	0.91
1:E:112:ARG:NH1	1:E:190:GLN:HE22	1.68	0.91
1:B:112:ARG:HH12	1:B:190:GLN:NE2	1.68	0.90
1:C:533:GLN:N	1:C:533:GLN:HE21	1.69	0.90
1:A:13:CYS:O	1:A:17:GLU:HG3	1.71	0.90
1:B:533:GLN:HE21	1:B:533:GLN:H	0.90	0.90
1:A:533:GLN:HE21	1:A:533:GLN:N	1.67	0.90
1:B:533:GLN:N	1:B:533:GLN:HE21	1.70	0.90
1:F:368:ASP:H	1:F:372:HIS:HD2	1.13	0.90
1:B:368:ASP:H	1:B:372:HIS:HD2	1.15	0.89
1:F:533:GLN:HE21	1:F:533:GLN:H	0.93	0.89
1:F:13:CYS:O	1:F:17:GLU:HG3	1.73	0.89
1:C:533:GLN:H	1:C:533:GLN:HE21	0.92	0.89
1:E:533:GLN:HE21	1:E:533:GLN:H	0.88	0.88
1:E:368:ASP:H	1:E:372:HIS:HD2	1.15	0.88
1:C:588:HIS:CD2	1:C:590:LEU:H	1.92	0.88
1:B:515:LEU:HA	1:B:518:ASN:HD22	1.37	0.88
1:C:258:SER:HA	1:C:302:SER:HA	1.56	0.87
1:F:533:GLN:HE21	1:F:533:GLN:N	1.73	0.87
1:C:515:LEU:HA	1:C:518:ASN:HD22	1.40	0.87
1:E:515:LEU:HA	1:E:518:ASN:HD22	1.39	0.87
1:E:112:ARG:HH12	1:E:190:GLN:NE2	1.72	0.86
1:C:588:HIS:HD2	1:C:590:LEU:H	1.20	0.86
1:B:13:CYS:O	1:B:17:GLU:HG3	1.76	0.86
1:A:533:GLN:HE21	1:A:533:GLN:H	0.90	0.85
1:D:533:GLN:N	1:D:533:GLN:HE21	1.73	0.85
1:F:258:SER:HA	1:F:302:SER:HA	1.55	0.85
1:A:515:LEU:HD22	1:A:525:ILE:HG23	1.60	0.84
1:D:588:HIS:CD2	1:D:590:LEU:H	1.95	0.83
1:E:601:ARG:CB	1:E:601:ARG:HH11	1.92	0.82
1:B:515:LEU:HD22	1:B:525:ILE:HG23	1.62	0.82
1:E:112:ARG:HH12	1:E:190:GLN:HE22	0.86	0.82
1:E:515:LEU:HD22	1:E:525:ILE:HG23	1.61	0.82
1:F:64:HIS:NE2	1:F:66:LEU:HD13	1.95	0.82
1:C:16:ILE:HD13	1:C:29:ILE:HD13	1.61	0.81
1:D:515:LEU:HA	1:D:518:ASN:HD22	1.46	0.81
1:B:601:ARG:CB	1:B:601:ARG:HH11	1.93	0.81
1:D:368:ASP:H	1:D:372:HIS:CD2	1.97	0.80
1:C:112:ARG:NH1	1:C:190:GLN:HE22	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:HD13	1:B:29:ILE:HD13	1.62	0.80
1:B:588:HIS:CD2	1:B:590:LEU:H	2.00	0.80
1:D:588:HIS:HD2	1:D:590:LEU:H	1.25	0.80
1:D:13:CYS:O	1:D:17:GLU:HG3	1.82	0.80
1:B:245:SER:HB2	1:B:274:LEU:HD11	1.63	0.79
1:A:258:SER:HA	1:A:302:SER:HA	1.64	0.79
1:F:207:PHE:CZ	1:F:304:LEU:HD11	2.18	0.79
1:A:245:SER:HB2	1:A:274:LEU:HD11	1.65	0.78
1:E:588:HIS:CD2	1:E:590:LEU:H	2.01	0.78
1:E:13:CYS:O	1:E:17:GLU:HG3	1.83	0.78
1:F:16:ILE:HD13	1:F:29:ILE:HD13	1.64	0.77
1:F:588:HIS:CD2	1:F:590:LEU:H	2.02	0.77
1:F:107:LEU:HD21	1:F:149:ARG:HG2	1.66	0.77
1:C:515:LEU:HD22	1:C:525:ILE:HG23	1.67	0.77
1:B:234:TYR:CE1	1:B:239:LYS:HB2	2.21	0.76
1:F:515:LEU:HD22	1:F:525:ILE:HG23	1.67	0.76
1:A:226:ASP:OD2	1:A:227:PRO:HA	1.85	0.76
1:A:112:ARG:NH1	1:A:190:GLN:HE22	1.78	0.75
1:A:588:HIS:CD2	1:A:590:LEU:H	2.04	0.75
1:C:601:ARG:HH11	1:C:601:ARG:CB	2.00	0.75
1:C:13:CYS:O	1:C:17:GLU:HG3	1.84	0.75
1:F:588:HIS:HD2	1:F:590:LEU:H	1.36	0.74
1:B:324:ASN:HD22	1:B:353:ILE:HG13	1.53	0.74
1:D:112:ARG:NH1	1:D:190:GLN:HE22	1.82	0.74
1:D:515:LEU:HD22	1:D:525:ILE:HG23	1.68	0.74
1:A:601:ARG:HH11	1:A:601:ARG:CB	2.01	0.74
1:A:460:ARG:HD3	1:A:614:GLN:O	1.87	0.73
1:F:112:ARG:NH1	1:F:190:GLN:HE22	1.82	0.73
1:C:173:LEU:O	1:C:177:LEU:HB2	1.88	0.73
1:B:258:SER:HA	1:B:302:SER:HA	1.71	0.73
1:D:460:ARG:HD3	1:D:614:GLN:O	1.87	0.73
1:D:636:ILE:H	1:D:636:ILE:HD12	1.54	0.73
1:E:258:SER:HA	1:E:302:SER:HA	1.71	0.73
1:A:16:ILE:HD13	1:A:29:ILE:HD13	1.70	0.72
1:E:655:LEU:O	1:E:656:THR:HG23	1.89	0.72
1:B:460:ARG:HD3	1:B:614:GLN:O	1.89	0.72
1:B:173:LEU:O	1:B:177:LEU:HB2	1.89	0.72
1:A:655:LEU:O	1:A:656:THR:HG23	1.90	0.72
1:A:213:PRO:HD2	1:A:216:VAL:HG21	1.71	0.72
1:C:3:THR:HG22	1:C:78:VAL:HG13	1.71	0.72
1:D:207:PHE:CZ	1:D:304:LEU:HD11	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:HG22	1:D:78:VAL:HG13	1.72	0.71
1:A:207:PHE:CZ	1:A:304:LEU:HD11	2.25	0.71
1:A:234:TYR:CE1	1:A:239:LYS:HB2	2.25	0.71
1:E:78:VAL:HB	1:E:98:ALA:HB3	1.71	0.71
1:F:14:LEU:HD12	1:F:15:GLY:N	2.05	0.71
1:F:636:ILE:H	1:F:636:ILE:HD12	1.55	0.71
1:D:63:ASN:HB3	1:D:89:TYR:CZ	2.25	0.71
1:F:601:ARG:HH11	1:F:601:ARG:CB	2.04	0.71
1:A:636:ILE:HD12	1:A:636:ILE:H	1.55	0.71
1:A:63:ASN:HB3	1:A:89:TYR:CZ	2.25	0.71
1:D:601:ARG:HH11	1:D:601:ARG:CB	2.04	0.71
1:A:434:GLU:CD	1:A:460:ARG:HH21	1.95	0.70
1:D:107:LEU:HD21	1:D:149:ARG:HG2	1.72	0.70
1:F:63:ASN:HB3	1:F:89:TYR:CZ	2.25	0.70
1:F:324:ASN:HD21	1:F:352:ALA:H	1.37	0.70
1:B:588:HIS:HD2	1:B:590:LEU:H	1.37	0.70
1:B:226:ASP:OD2	1:B:227:PRO:HA	1.92	0.70
1:C:460:ARG:HD3	1:C:614:GLN:O	1.91	0.70
1:D:226:ASP:OD2	1:D:227:PRO:HA	1.92	0.70
1:C:226:ASP:OD2	1:C:227:PRO:HA	1.92	0.70
1:C:324:ASN:HD22	1:C:353:ILE:HG13	1.56	0.70
1:B:11:MET:HG3	1:B:83:TYR:CE1	2.26	0.69
1:C:245:SER:HB2	1:C:274:LEU:HD11	1.73	0.69
1:C:517:LEU:O	1:C:521:GLU:HG2	1.91	0.69
1:B:636:ILE:HD12	1:B:636:ILE:H	1.57	0.69
1:A:515:LEU:HA	1:A:518:ASN:HD22	1.57	0.69
1:D:64:HIS:HD2	1:D:66:LEU:HB2	1.57	0.69
1:F:655:LEU:O	1:F:656:THR:HG23	1.92	0.69
1:B:63:ASN:HB3	1:B:89:TYR:CZ	2.28	0.69
1:F:19:LEU:HD11	1:F:80:PHE:CE2	2.28	0.69
1:E:16:ILE:HD13	1:E:29:ILE:HD13	1.72	0.69
1:B:112:ARG:HH12	1:B:190:GLN:HE22	0.82	0.69
1:C:636:ILE:HD12	1:C:636:ILE:H	1.58	0.69
1:F:173:LEU:O	1:F:177:LEU:HB2	1.93	0.69
1:B:134:ARG:O	1:B:142:GLY:HA3	1.92	0.68
1:A:1:MET:N	1:A:181:LYS:HE3	2.07	0.68
1:A:244:SER:CB	1:A:277:VAL:HB	2.23	0.68
1:B:422:LYS:HD3	1:B:423:TYR:CE2	2.27	0.68
1:E:517:LEU:O	1:E:521:GLU:HG2	1.93	0.68
1:A:517:LEU:O	1:A:521:GLU:HG2	1.94	0.68
1:C:235:VAL:HG21	1:C:296:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ASP:OD2	1:E:227:PRO:HA	1.93	0.68
1:E:369:ILE:HD11	1:E:408:LEU:HD21	1.75	0.67
1:F:11:MET:HG3	1:F:83:TYR:CE1	2.28	0.67
1:E:434:GLU:CD	1:E:460:ARG:HH21	1.97	0.67
1:C:112:ARG:HH12	1:C:190:GLN:NE2	1.81	0.67
1:B:3:THR:HG22	1:B:78:VAL:HG13	1.77	0.67
1:B:244:SER:CB	1:B:277:VAL:HB	2.25	0.67
1:C:526:LYS:HE3	1:C:603:VAL:HG21	1.77	0.67
1:E:173:LEU:O	1:E:177:LEU:HB2	1.93	0.67
1:C:3:THR:CG2	1:C:78:VAL:HG13	2.25	0.67
1:E:3:THR:HG22	1:E:78:VAL:HG13	1.77	0.67
1:C:63:ASN:HB3	1:C:89:TYR:CZ	2.30	0.67
1:E:11:MET:HG3	1:E:83:TYR:CE1	2.29	0.67
1:C:434:GLU:CD	1:C:460:ARG:HH21	1.98	0.67
1:E:329:ASN:HD22	1:E:355:ARG:NH2	1.92	0.67
1:C:329:ASN:HD22	1:C:355:ARG:NH2	1.92	0.67
1:E:368:ASP:H	1:E:372:HIS:CD2	2.05	0.67
1:A:369:ILE:HD11	1:A:408:LEU:HD21	1.76	0.67
1:F:422:LYS:HD3	1:F:423:TYR:CE2	2.30	0.67
1:F:460:ARG:HD3	1:F:614:GLN:O	1.94	0.67
1:F:3:THR:HG22	1:F:78:VAL:HG13	1.76	0.67
1:C:277:VAL:HG12	1:C:278:THR:HG23	1.78	0.66
1:F:515:LEU:HA	1:F:518:ASN:HD22	1.60	0.66
1:D:11:MET:HG3	1:D:83:TYR:CE1	2.31	0.66
1:C:368:ASP:H	1:C:372:HIS:CD2	2.05	0.66
1:E:107:LEU:HD21	1:E:149:ARG:HG2	1.77	0.66
1:B:515:LEU:HA	1:B:518:ASN:ND2	2.08	0.66
1:E:460:ARG:HD3	1:E:614:GLN:O	1.94	0.66
1:B:107:LEU:HD21	1:B:149:ARG:HG2	1.77	0.66
1:C:655:LEU:O	1:C:656:THR:HG23	1.96	0.66
1:F:245:SER:HB2	1:F:274:LEU:HD11	1.77	0.66
1:D:16:ILE:HD13	1:D:29:ILE:HD13	1.76	0.66
1:A:422:LYS:HD3	1:A:423:TYR:CE2	2.31	0.66
1:F:368:ASP:H	1:F:372:HIS:CD2	2.05	0.66
1:E:636:ILE:HD12	1:E:636:ILE:H	1.58	0.66
1:C:234:TYR:CE1	1:C:239:LYS:HB2	2.29	0.66
1:E:138:ARG:HH12	1:E:192:GLU:CD	1.99	0.66
1:E:134:ARG:O	1:E:142:GLY:HA3	1.94	0.66
1:C:244:SER:CB	1:C:277:VAL:HB	2.26	0.66
1:D:329:ASN:HD22	1:D:355:ARG:NH2	1.94	0.66
1:F:134:ARG:O	1:F:142:GLY:HA3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:GLU:CD	1:F:460:ARG:HH21	2.00	0.65
1:F:329:ASN:HD22	1:F:355:ARG:NH2	1.95	0.65
1:E:324:ASN:HD21	1:E:352:ALA:H	1.42	0.65
1:D:649:PHE:O	1:D:652:THR:HB	1.96	0.65
1:B:369:ILE:HD11	1:B:408:LEU:HD21	1.77	0.65
1:A:324:ASN:HD21	1:A:352:ALA:H	1.45	0.65
1:D:258:SER:HA	1:D:302:SER:HA	1.77	0.65
1:C:211:HIS:O	1:C:270:GLY:HA3	1.97	0.65
1:B:368:ASP:H	1:B:372:HIS:CD2	2.07	0.65
1:F:108:LEU:HD12	1:F:131:THR:HG21	1.79	0.65
1:F:211:HIS:O	1:F:270:GLY:HA3	1.97	0.65
1:F:213:PRO:HD2	1:F:216:VAL:HG21	1.77	0.65
1:A:11:MET:HG3	1:A:83:TYR:CE1	2.31	0.65
1:C:107:LEU:HD21	1:C:149:ARG:HG2	1.79	0.65
1:D:324:ASN:HD21	1:D:352:ALA:H	1.45	0.64
1:E:64:HIS:HD2	1:E:66:LEU:HB2	1.61	0.64
1:B:655:LEU:O	1:B:656:THR:HG23	1.96	0.64
1:A:588:HIS:HD2	1:A:590:LEU:H	1.44	0.64
1:D:138:ARG:HH12	1:D:192:GLU:CD	2.00	0.64
1:F:526:LYS:HE3	1:F:603:VAL:HG21	1.80	0.64
1:F:615:ASP:CG	1:F:616:VAL:H	2.00	0.64
1:A:329:ASN:HD22	1:A:355:ARG:NH2	1.96	0.64
1:B:207:PHE:CZ	1:B:304:LEU:HD11	2.33	0.64
1:F:422:LYS:HD3	1:F:423:TYR:CZ	2.33	0.64
1:B:517:LEU:O	1:B:521:GLU:HG2	1.98	0.64
1:B:64:HIS:HD2	1:B:66:LEU:HB2	1.63	0.64
1:B:347:ASP:OD1	1:B:348:ILE:N	2.31	0.64
1:F:64:HIS:HD2	1:F:66:LEU:HB2	1.61	0.64
1:E:567:ASN:ND2	1:E:569:GLU:H	1.94	0.64
1:E:541:ARG:NH1	1:E:636:ILE:HG12	2.13	0.64
1:B:403:LEU:O	1:B:407:GLU:HG3	1.98	0.64
1:C:431:SER:HB3	1:C:489:ARG:HG2	1.79	0.64
1:C:515:LEU:HA	1:C:518:ASN:ND2	2.13	0.64
1:C:649:PHE:O	1:C:652:THR:HB	1.98	0.64
1:D:3:THR:CG2	1:D:78:VAL:HG13	2.29	0.63
1:D:541:ARG:NH1	1:D:636:ILE:HG12	2.13	0.63
1:A:597:PHE:CE2	1:A:599:GLY:HA2	2.33	0.63
1:E:422:LYS:HD3	1:E:423:TYR:CE2	2.33	0.63
1:E:588:HIS:HD2	1:E:590:LEU:H	1.44	0.63
1:A:324:ASN:HD22	1:A:353:ILE:HG13	1.62	0.63
1:F:235:VAL:HG21	1:F:296:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LEU:O	1:D:407:GLU:HG3	1.98	0.63
1:D:1:MET:N	1:D:181:LYS:HE3	2.14	0.63
1:C:134:ARG:O	1:C:142:GLY:HA3	1.99	0.63
1:E:63:ASN:HB3	1:E:89:TYR:CZ	2.34	0.63
1:C:6:PHE:HZ	1:C:92:ILE:HD11	1.64	0.63
1:D:573:SER:OG	1:D:576:GLU:HG3	1.99	0.62
1:A:173:LEU:O	1:A:177:LEU:HB2	1.99	0.62
1:F:324:ASN:HD21	1:F:352:ALA:N	1.96	0.62
1:A:107:LEU:HD21	1:A:149:ARG:HG2	1.80	0.62
1:D:134:ARG:O	1:D:142:GLY:HA3	1.98	0.62
1:D:593:HIS:CG	1:D:655:LEU:HD13	2.34	0.62
1:F:244:SER:CB	1:F:277:VAL:HB	2.29	0.62
1:F:277:VAL:HG12	1:F:278:THR:HG23	1.80	0.62
1:C:615:ASP:CG	1:C:616:VAL:H	2.03	0.62
1:D:14:LEU:HD12	1:D:15:GLY:N	2.14	0.62
1:F:226:ASP:OD2	1:F:227:PRO:HA	2.00	0.62
1:D:369:ILE:HD12	1:D:412:GLU:HB3	1.82	0.62
1:A:524:PRO:HD3	1:C:297:GLY:HA3	1.80	0.62
1:B:434:GLU:CD	1:B:460:ARG:HH21	2.02	0.62
1:A:277:VAL:HG12	1:A:278:THR:HG23	1.81	0.62
1:D:368:ASP:N	1:D:372:HIS:HD2	1.88	0.62
1:A:526:LYS:HE3	1:A:603:VAL:HG21	1.81	0.62
1:E:573:SER:OG	1:E:576:GLU:HG3	2.00	0.62
1:D:588:HIS:HE1	1:D:647:ASP:OD1	1.83	0.62
1:E:588:HIS:HE1	1:E:647:ASP:OD1	1.83	0.62
1:F:138:ARG:HH12	1:F:192:GLU:CD	2.03	0.61
1:A:213:PRO:HD2	1:A:216:VAL:CG2	2.29	0.61
1:C:573:SER:OG	1:C:576:GLU:HG3	1.99	0.61
1:F:369:ILE:HD11	1:F:408:LEU:HD21	1.82	0.61
1:C:11:MET:HG3	1:C:83:TYR:CE1	2.34	0.61
1:B:338:GLU:HG3	1:B:548:TYR:OH	2.00	0.61
1:D:517:LEU:O	1:D:521:GLU:HG2	2.00	0.61
1:E:234:TYR:CE1	1:E:239:LYS:HB2	2.35	0.61
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.65	0.61
1:C:368:ASP:N	1:C:372:HIS:HD2	1.94	0.61
1:C:369:ILE:HD11	1:C:408:LEU:HD21	1.82	0.61
1:A:244:SER:HB3	1:A:277:VAL:HB	1.83	0.61
1:E:567:ASN:HD21	1:E:569:GLU:HB2	1.65	0.61
1:A:3:THR:HG22	1:A:78:VAL:HG13	1.82	0.61
1:C:207:PHE:CZ	1:C:304:LEU:HD11	2.34	0.61
1:E:245:SER:HB2	1:E:274:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:HD3	1:B:423:TYR:CZ	2.35	0.61
1:D:64:HIS:CD2	1:D:66:LEU:HB2	2.36	0.61
1:C:64:HIS:HD2	1:C:66:LEU:HB2	1.65	0.61
1:F:573:SER:OG	1:F:576:GLU:HG3	2.00	0.61
1:E:150:ILE:HD12	1:E:165:LEU:HD23	1.82	0.61
1:B:501:LEU:H	1:B:501:LEU:HD22	1.64	0.61
1:D:434:GLU:CD	1:D:460:ARG:HH21	2.03	0.61
1:B:244:SER:HB2	1:B:277:VAL:HB	1.81	0.61
1:B:573:SER:OG	1:B:576:GLU:HG3	2.00	0.61
1:F:244:SER:HB3	1:F:277:VAL:HB	1.82	0.61
1:E:277:VAL:HG12	1:E:278:THR:HG23	1.83	0.61
1:B:431:SER:HB3	1:B:489:ARG:HG2	1.83	0.61
1:C:588:HIS:HE1	1:C:647:ASP:OD1	1.84	0.60
1:A:460:ARG:O	1:A:460:ARG:HG3	1.98	0.60
1:D:78:VAL:HB	1:D:98:ALA:HB3	1.83	0.60
1:D:567:ASN:HD21	1:D:569:GLU:HB2	1.66	0.60
1:C:469:LEU:HD12	1:F:469:LEU:HD12	1.82	0.60
1:F:575:GLU:O	1:F:579:GLU:HG3	2.00	0.60
1:A:64:HIS:HD2	1:A:66:LEU:HB2	1.65	0.60
1:D:424:ARG:HG2	1:D:424:ARG:HH11	1.66	0.60
1:E:422:LYS:HD3	1:E:423:TYR:CZ	2.36	0.60
1:B:575:GLU:O	1:B:579:GLU:HG3	2.01	0.60
1:E:64:HIS:NE2	1:E:66:LEU:HD13	2.16	0.60
1:C:6:PHE:CZ	1:C:92:ILE:HD11	2.36	0.60
1:A:134:ARG:O	1:A:142:GLY:HA3	2.00	0.60
1:F:517:LEU:O	1:F:521:GLU:HG2	2.01	0.60
1:C:113:GLY:HA3	1:C:198:PHE:H	1.67	0.60
1:F:234:TYR:CE1	1:F:239:LYS:HB2	2.37	0.60
1:D:515:LEU:HA	1:D:518:ASN:ND2	2.17	0.60
1:D:460:ARG:HG3	1:D:460:ARG:O	1.98	0.60
1:E:207:PHE:CZ	1:E:304:LEU:HD11	2.36	0.60
1:B:424:ARG:HG2	1:B:424:ARG:HH11	1.66	0.60
1:D:434:GLU:HG2	1:D:464:SER:HB2	1.84	0.59
1:C:593:HIS:CG	1:C:655:LEU:HD13	2.37	0.59
1:F:99:GLY:HA3	1:F:134:ARG:HH12	1.67	0.59
1:A:615:ASP:CG	1:A:616:VAL:H	2.06	0.59
1:F:107:LEU:HD13	1:F:129:GLY:HA3	1.84	0.59
1:A:369:ILE:HD11	1:A:408:LEU:CD2	2.33	0.59
1:F:567:ASN:ND2	1:F:569:GLU:H	2.00	0.59
1:B:329:ASN:HD22	1:B:355:ARG:NH2	2.00	0.59
1:E:102:ASN:HD22	1:E:133:HIS:CE1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:SER:HB2	1:A:277:VAL:HB	1.85	0.59
1:A:64:HIS:NE2	1:A:66:LEU:HD13	2.17	0.59
1:D:245:SER:HB2	1:D:274:LEU:HD11	1.83	0.59
1:C:588:HIS:HD2	1:C:590:LEU:N	1.97	0.59
1:F:541:ARG:NH1	1:F:636:ILE:HG12	2.17	0.59
1:C:244:SER:HB2	1:C:277:VAL:HB	1.84	0.59
1:E:324:ASN:HD21	1:E:352:ALA:N	2.00	0.59
1:B:64:HIS:NE2	1:B:66:LEU:HD13	2.18	0.59
1:D:347:ASP:OD1	1:D:348:ILE:N	2.36	0.59
1:F:108:LEU:HD12	1:F:131:THR:CG2	2.32	0.59
1:B:369:ILE:HD11	1:B:408:LEU:CD2	2.33	0.59
1:C:107:LEU:HD13	1:C:129:GLY:HA3	1.83	0.59
1:C:403:LEU:O	1:C:407:GLU:HG3	2.03	0.59
1:B:138:ARG:HH12	1:B:192:GLU:CD	2.06	0.59
1:B:601:ARG:HB2	1:B:601:ARG:HH11	1.68	0.58
1:C:434:GLU:HG2	1:C:464:SER:HB2	1.85	0.58
1:C:597:PHE:CE2	1:C:599:GLY:HA2	2.38	0.58
1:A:431:SER:HB3	1:A:489:ARG:HG2	1.85	0.58
1:F:1:MET:N	1:F:181:LYS:HE3	2.18	0.58
1:D:615:ASP:CG	1:D:616:VAL:H	2.06	0.58
1:D:526:LYS:HE3	1:D:603:VAL:HG21	1.85	0.58
1:A:422:LYS:HD3	1:A:423:TYR:CZ	2.37	0.58
1:C:347:ASP:OD1	1:C:348:ILE:N	2.37	0.58
1:F:109:PRO:HB2	1:F:195:ALA:HB2	1.85	0.58
1:F:6:PHE:HZ	1:F:92:ILE:HD11	1.68	0.58
1:B:369:ILE:HD12	1:B:412:GLU:HB3	1.84	0.58
1:E:649:PHE:O	1:E:652:THR:HB	2.03	0.58
1:B:615:ASP:CG	1:B:616:VAL:H	2.06	0.58
1:F:70:ARG:O	1:F:73:GLN:HB2	2.03	0.58
1:F:324:ASN:HD22	1:F:353:ILE:HG13	1.69	0.58
1:B:368:ASP:N	1:B:372:HIS:HD2	1.95	0.58
1:A:588:HIS:HE1	1:A:647:ASP:OD1	1.85	0.58
1:A:70:ARG:O	1:A:73:GLN:HB2	2.04	0.58
1:E:515:LEU:HA	1:E:518:ASN:ND2	2.15	0.58
1:C:541:ARG:NH1	1:C:636:ILE:HG12	2.19	0.58
1:E:369:ILE:HD11	1:E:408:LEU:CD2	2.33	0.58
1:C:369:ILE:CD1	1:C:390:VAL:HG11	2.34	0.58
1:D:113:GLY:HA3	1:D:198:PHE:H	1.69	0.58
1:D:234:TYR:CE1	1:D:239:LYS:HB2	2.39	0.58
1:A:78:VAL:HB	1:A:98:ALA:HB3	1.83	0.58
1:A:501:LEU:HD22	1:A:501:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASP:H	1:A:372:HIS:CD2	2.09	0.58
1:D:324:ASN:HD22	1:D:353:ILE:HG13	1.69	0.58
1:D:499:ASP:HB2	1:D:513:THR:HG21	1.85	0.58
1:B:113:GLY:HA3	1:B:198:PHE:H	1.67	0.58
1:A:541:ARG:NH1	1:A:636:ILE:HG12	2.18	0.57
1:D:64:HIS:NE2	1:D:66:LEU:HD13	2.18	0.57
1:B:3:THR:HG22	1:B:78:VAL:CG1	2.33	0.57
1:E:244:SER:HB2	1:E:277:VAL:HB	1.85	0.57
1:E:6:PHE:CZ	1:E:92:ILE:HD11	2.39	0.57
1:F:346:LEU:C	1:F:346:LEU:HD23	2.25	0.57
1:E:1:MET:N	1:E:181:LYS:HE3	2.19	0.57
1:A:89:TYR:C	1:A:93:LEU:HD23	2.25	0.57
1:A:369:ILE:HD12	1:A:412:GLU:HB3	1.84	0.57
1:F:499:ASP:HB2	1:F:513:THR:HG21	1.86	0.57
1:D:99:GLY:HA3	1:D:134:ARG:HH12	1.69	0.57
1:E:567:ASN:HD22	1:E:567:ASN:C	2.07	0.57
1:F:588:HIS:HE1	1:F:647:ASP:OD1	1.88	0.57
1:E:64:HIS:CD2	1:E:66:LEU:HB2	2.40	0.57
1:F:567:ASN:HD21	1:F:569:GLU:HB2	1.69	0.57
1:A:465:VAL:HG21	1:D:468:GLN:OE1	2.04	0.57
1:D:655:LEU:O	1:D:656:THR:HG23	2.04	0.57
1:C:64:HIS:NE2	1:C:66:LEU:HD13	2.20	0.57
1:C:575:GLU:O	1:C:579:GLU:HG3	2.04	0.57
1:B:526:LYS:HE3	1:B:603:VAL:HG21	1.86	0.57
1:F:375:TRP:O	1:F:379:HIS:HD2	1.88	0.57
1:D:213:PRO:HD2	1:D:216:VAL:HG21	1.86	0.57
1:A:649:PHE:O	1:A:652:THR:HB	2.05	0.57
1:E:347:ASP:OD1	1:E:348:ILE:N	2.37	0.57
1:E:434:GLU:HG2	1:E:464:SER:HB2	1.86	0.57
1:D:324:ASN:HD21	1:D:352:ALA:N	2.02	0.57
1:E:6:PHE:HZ	1:E:92:ILE:HD11	1.70	0.57
1:E:368:ASP:N	1:E:372:HIS:HD2	1.93	0.57
1:C:324:ASN:HD21	1:C:352:ALA:H	1.52	0.57
1:D:567:ASN:ND2	1:D:569:GLU:H	2.02	0.57
1:A:107:LEU:HD13	1:A:129:GLY:HA3	1.86	0.57
1:F:369:ILE:HD12	1:F:412:GLU:HB3	1.87	0.57
1:B:235:VAL:HG21	1:B:296:LEU:HD13	1.87	0.57
1:E:369:ILE:CD1	1:E:390:VAL:HG11	2.35	0.56
1:A:299:VAL:O	1:A:301:GLY:N	2.38	0.56
1:E:424:ARG:HG2	1:E:424:ARG:HH11	1.68	0.56
1:C:70:ARG:O	1:C:73:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TRP:NE1	1:E:604:GLU:OE2	2.30	0.56
1:E:324:ASN:HD22	1:E:353:ILE:HG13	1.69	0.56
1:C:338:GLU:HG3	1:C:548:TYR:OH	2.05	0.56
1:E:235:VAL:HG21	1:E:296:LEU:HD13	1.86	0.56
1:C:138:ARG:HH12	1:C:192:GLU:CD	2.08	0.56
1:A:346:LEU:HD23	1:A:346:LEU:C	2.26	0.56
1:E:601:ARG:HB2	1:E:601:ARG:HH11	1.68	0.56
1:F:460:ARG:HG3	1:F:460:ARG:O	2.01	0.56
1:F:3:THR:CG2	1:F:78:VAL:HG13	2.35	0.56
1:D:369:ILE:HD11	1:D:408:LEU:HD21	1.87	0.56
1:E:244:SER:CB	1:E:277:VAL:HB	2.34	0.56
1:F:146:ALA:CB	1:F:176:THR:HG21	2.36	0.56
1:B:649:PHE:O	1:B:652:THR:HB	2.05	0.56
1:F:347:ASP:OD1	1:F:348:ILE:N	2.38	0.56
1:B:121:LEU:O	1:B:219:ASN:HB3	2.05	0.56
1:C:213:PRO:HD2	1:C:216:VAL:HG21	1.88	0.56
1:E:615:ASP:CG	1:E:616:VAL:H	2.09	0.56
1:B:499:ASP:HB2	1:B:513:THR:HG21	1.88	0.56
1:A:515:LEU:HA	1:A:518:ASN:ND2	2.21	0.55
1:E:567:ASN:HD22	1:E:569:GLU:H	1.54	0.55
1:E:150:ILE:CD1	1:E:165:LEU:HD23	2.36	0.55
1:C:422:LYS:HD3	1:C:423:TYR:CE2	2.42	0.55
1:C:422:LYS:HD3	1:C:423:TYR:CZ	2.41	0.55
1:D:92:ILE:O	1:D:95:LEU:HG	2.06	0.55
1:C:92:ILE:O	1:C:95:LEU:HG	2.06	0.55
1:C:1:MET:N	1:C:181:LYS:HE3	2.21	0.55
1:B:246:ARG:HB3	1:B:275:GLU:HB3	1.87	0.55
1:F:424:ARG:HG2	1:F:424:ARG:HH11	1.71	0.55
1:A:138:ARG:HH12	1:A:192:GLU:CD	2.09	0.55
1:F:90:ASP:O	1:F:94:GLN:HG2	2.06	0.55
1:D:3:THR:HG22	1:D:78:VAL:CG1	2.36	0.55
1:B:244:SER:HB3	1:B:277:VAL:HB	1.89	0.55
1:A:347:ASP:OD1	1:A:348:ILE:N	2.39	0.55
1:C:465:VAL:HG21	1:F:468:GLN:OE1	2.06	0.55
1:E:252:SER:C	1:E:254:ALA:H	2.10	0.55
1:F:368:ASP:N	1:F:372:HIS:HD2	1.94	0.55
1:E:601:ARG:HB3	1:E:601:ARG:HH11	1.68	0.55
1:B:324:ASN:HD21	1:B:352:ALA:H	1.54	0.55
1:D:235:VAL:HG21	1:D:296:LEU:HD13	1.89	0.55
1:C:567:ASN:HD21	1:C:569:GLU:HB2	1.72	0.55
1:D:431:SER:HB3	1:D:489:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:O	1:A:95:LEU:HG	2.07	0.55
1:A:325:GLY:HA3	2:A:1001:ATP:H5'2	1.89	0.55
1:C:115:ALA:N	1:C:116:PRO:CD	2.70	0.55
1:A:573:SER:OG	1:A:576:GLU:HG3	2.07	0.55
1:F:501:LEU:H	1:F:501:LEU:HD22	1.71	0.55
1:E:460:ARG:HG3	1:E:460:ARG:O	2.01	0.55
1:F:6:PHE:CZ	1:F:92:ILE:HD11	2.42	0.55
1:C:499:ASP:HB2	1:C:513:THR:HG21	1.88	0.55
1:E:14:LEU:HD12	1:E:15:GLY:N	2.22	0.55
1:A:600:PHE:O	1:A:601:ARG:HG3	2.07	0.55
1:D:369:ILE:HD11	1:D:408:LEU:CD2	2.37	0.55
1:E:545:GLU:O	1:E:549:ARG:HG2	2.07	0.55
1:A:150:ILE:HD12	1:A:165:LEU:HD23	1.88	0.55
1:A:150:ILE:CD1	1:A:165:LEU:HD23	2.37	0.55
1:A:114:ARG:O	1:A:115:ALA:HB3	2.07	0.55
1:D:277:VAL:HG12	1:D:278:THR:HG23	1.88	0.55
1:A:109:PRO:O	1:A:195:ALA:HA	2.07	0.54
1:B:324:ASN:HD21	1:B:352:ALA:N	2.05	0.54
1:F:434:GLU:HG2	1:F:464:SER:HB2	1.89	0.54
1:F:71:ILE:HD12	1:F:92:ILE:HD12	1.89	0.54
1:E:436:TYR:HA	1:E:451:LEU:HD22	1.89	0.54
1:B:567:ASN:ND2	1:B:569:GLU:H	2.05	0.54
1:A:601:ARG:NH2	1:C:294:GLN:O	2.37	0.54
1:C:324:ASN:HD21	1:C:352:ALA:N	2.06	0.54
1:B:3:THR:CG2	1:B:78:VAL:HG13	2.36	0.54
1:B:369:ILE:CD1	1:B:390:VAL:HG11	2.37	0.54
1:D:422:LYS:HD3	1:D:423:TYR:CE2	2.42	0.54
1:E:3:THR:CG2	1:E:78:VAL:HG13	2.37	0.54
1:D:173:LEU:O	1:D:177:LEU:HB2	2.08	0.54
1:B:469:LEU:HD12	1:E:469:LEU:HD12	1.89	0.54
1:D:115:ALA:N	1:D:116:PRO:CD	2.69	0.54
1:D:69:GLU:O	1:D:73:GLN:HG2	2.08	0.54
1:F:403:LEU:O	1:F:407:GLU:HG3	2.07	0.54
1:C:489:ARG:HB2	1:C:564:ASN:HD22	1.72	0.54
1:F:112:ARG:HH12	1:F:190:GLN:NE2	1.86	0.54
1:B:541:ARG:NH1	1:B:636:ILE:HG12	2.23	0.54
1:A:399:THR:HG22	1:A:459:PRO:HG2	1.89	0.54
1:A:78:VAL:HG23	1:A:99:GLY:O	2.07	0.54
1:E:211:HIS:O	1:E:270:GLY:HA3	2.08	0.54
1:D:346:LEU:HD23	1:D:346:LEU:C	2.28	0.54
1:B:324:ASN:ND2	1:B:353:ILE:HG13	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:SER:HB3	1:C:277:VAL:HB	1.89	0.54
1:F:180:ILE:HG12	1:F:185:ILE:HG21	1.90	0.54
1:F:64:HIS:CD2	1:F:66:LEU:HB2	2.41	0.54
1:B:434:GLU:HG2	1:B:464:SER:HB2	1.89	0.54
1:C:369:ILE:HD12	1:C:412:GLU:HB3	1.90	0.54
1:F:649:PHE:O	1:F:652:THR:HB	2.08	0.54
1:F:9:HIS:CG	1:F:10:ASP:H	2.26	0.54
1:C:78:VAL:HB	1:C:98:ALA:HB3	1.89	0.54
1:C:99:GLY:HA3	1:C:134:ARG:HH12	1.73	0.54
1:F:1:MET:CE	1:F:77:ASP:HB3	2.38	0.54
1:A:172:LEU:HD23	1:A:172:LEU:C	2.29	0.54
1:B:252:SER:C	1:B:254:ALA:H	2.10	0.54
1:F:489:ARG:HB2	1:F:564:ASN:HD22	1.73	0.54
1:E:115:ALA:N	1:E:116:PRO:CD	2.70	0.54
1:E:499:ASP:HB2	1:E:513:THR:HG21	1.89	0.54
1:A:113:GLY:HA3	1:A:198:PHE:H	1.72	0.54
1:A:113:GLY:HA3	1:A:198:PHE:O	2.06	0.54
1:C:14:LEU:HD12	1:C:15:GLY:N	2.23	0.53
1:F:597:PHE:CE2	1:F:599:GLY:HA2	2.43	0.53
1:F:506:ILE:O	1:F:506:ILE:HG23	2.08	0.53
1:B:601:ARG:HH11	1:B:601:ARG:HB3	1.71	0.53
1:C:89:TYR:C	1:C:93:LEU:HD23	2.28	0.53
1:A:211:HIS:O	1:A:270:GLY:HA3	2.08	0.53
1:B:346:LEU:C	1:B:346:LEU:HD23	2.28	0.53
1:B:600:PHE:O	1:B:601:ARG:HG3	2.08	0.53
1:F:213:PRO:HD2	1:F:216:VAL:CG2	2.38	0.53
1:E:213:PRO:HD2	1:E:216:VAL:HG21	1.91	0.53
1:C:424:ARG:HH11	1:C:424:ARG:HG2	1.73	0.53
1:C:3:THR:HG22	1:C:78:VAL:CG1	2.38	0.53
1:D:79:ILE:HG13	1:D:96:ALA:HB2	1.89	0.53
1:F:369:ILE:HD11	1:F:408:LEU:CD2	2.38	0.53
1:A:3:THR:CG2	1:A:78:VAL:HG13	2.38	0.53
1:A:338:GLU:HG3	1:A:548:TYR:OH	2.09	0.53
1:F:545:GLU:O	1:F:549:ARG:HG2	2.08	0.53
1:F:636:ILE:N	1:F:636:ILE:HD12	2.21	0.53
1:A:324:ASN:HD21	1:A:352:ALA:N	2.06	0.53
1:D:567:ASN:ND2	1:D:569:GLU:HB2	2.23	0.53
1:C:567:ASN:C	1:C:567:ASN:HD22	2.11	0.53
1:F:117:LEU:HD13	1:F:165:LEU:HD12	1.89	0.53
1:A:9:HIS:CG	1:A:10:ASP:H	2.27	0.53
1:F:426:ARG:HG3	1:F:484:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ILE:HD12	1:F:165:LEU:HD23	1.90	0.53
1:A:368:ASP:N	1:A:372:HIS:HD2	1.97	0.53
1:A:575:GLU:O	1:A:579:GLU:HG3	2.09	0.53
1:D:172:LEU:C	1:D:172:LEU:HD23	2.29	0.53
1:B:109:PRO:HB2	1:B:195:ALA:HB2	1.91	0.53
1:F:159:ILE:HG23	1:F:160:THR:N	2.24	0.53
1:D:244:SER:CB	1:D:277:VAL:HB	2.39	0.53
1:B:92:ILE:O	1:B:95:LEU:HG	2.09	0.53
1:E:346:LEU:HD23	1:E:346:LEU:C	2.29	0.53
1:F:338:GLU:HG3	1:F:548:TYR:OH	2.09	0.53
1:F:112:ARG:CB	1:F:112:ARG:HH11	2.21	0.53
1:B:588:HIS:HD2	1:B:590:LEU:N	2.06	0.53
1:F:567:ASN:HD22	1:F:567:ASN:C	2.12	0.53
1:E:19:LEU:HD11	1:E:80:PHE:CE2	2.44	0.53
1:C:600:PHE:O	1:C:601:ARG:HG3	2.09	0.52
1:E:14:LEU:HD12	1:E:14:LEU:C	2.29	0.52
1:A:295:THR:HA	1:B:601:ARG:NH2	2.24	0.52
1:E:78:VAL:HA	1:E:96:ALA:HB1	1.90	0.52
1:E:107:LEU:HD13	1:E:129:GLY:HA3	1.91	0.52
1:B:576:GLU:O	1:B:580:MET:HG3	2.10	0.52
1:D:567:ASN:HD22	1:D:569:GLU:H	1.57	0.52
1:A:499:ASP:HB2	1:A:513:THR:HG21	1.91	0.52
1:D:588:HIS:HD2	1:D:590:LEU:N	2.02	0.52
1:B:588:HIS:HE1	1:B:647:ASP:OD1	1.93	0.52
1:F:89:TYR:C	1:F:93:LEU:HD23	2.30	0.52
1:E:369:ILE:HD12	1:E:412:GLU:HB3	1.90	0.52
1:F:11:MET:HG3	1:F:83:TYR:CZ	2.44	0.52
1:B:498:LEU:O	1:B:499:ASP:HB2	2.10	0.52
1:D:597:PHE:CE2	1:D:599:GLY:HA2	2.45	0.52
1:F:246:ARG:HB3	1:F:275:GLU:HB3	1.90	0.52
1:C:636:ILE:N	1:C:636:ILE:HD12	2.23	0.52
1:B:121:LEU:HD21	1:B:161:LEU:HD22	1.91	0.52
1:C:567:ASN:ND2	1:C:569:GLU:H	2.07	0.52
1:A:235:VAL:HG21	1:A:296:LEU:HD13	1.90	0.52
1:A:102:ASN:HD22	1:A:133:HIS:CE1	2.28	0.52
1:D:244:SER:HB2	1:D:277:VAL:HB	1.91	0.52
1:D:114:ARG:O	1:D:115:ALA:HB3	2.09	0.52
1:D:575:GLU:O	1:D:579:GLU:HG3	2.10	0.52
1:A:452:ILE:HG12	1:D:452:ILE:HG12	1.91	0.52
1:B:172:LEU:HD23	1:B:172:LEU:C	2.29	0.52
1:B:460:ARG:HG3	1:B:460:ARG:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:HIS:CD2	1:C:66:LEU:H	2.28	0.52
1:D:567:ASN:HD22	1:D:567:ASN:C	2.11	0.52
1:B:528:ILE:HD13	3:B:1102:UGA:C2	2.39	0.52
1:C:16:ILE:CD1	1:C:29:ILE:HD13	2.37	0.52
1:B:78:VAL:HB	1:B:98:ALA:HB3	1.91	0.52
1:B:69:GLU:O	1:B:73:GLN:HG2	2.09	0.52
1:A:11:MET:HG3	1:A:83:TYR:CZ	2.45	0.52
1:F:348:ILE:HG12	2:F:1006:ATP:C2	2.44	0.52
1:E:399:THR:HG22	1:E:459:PRO:HG2	1.92	0.52
1:E:119:TRP:CZ2	1:E:201:ARG:HG2	2.45	0.52
1:E:567:ASN:ND2	1:E:569:GLU:HB2	2.24	0.51
1:B:78:VAL:HA	1:B:96:ALA:HB1	1.90	0.51
1:B:159:ILE:HB	1:B:227:PRO:HD2	1.91	0.51
1:F:576:GLU:O	1:F:580:MET:HG3	2.11	0.51
1:E:102:ASN:HD22	1:E:133:HIS:HE1	1.56	0.51
1:F:431:SER:HB3	1:F:489:ARG:HG2	1.93	0.51
1:D:78:VAL:HG23	1:D:99:GLY:O	2.10	0.51
1:D:107:LEU:HD13	1:D:129:GLY:HA3	1.93	0.51
1:C:369:ILE:HD11	1:C:408:LEU:CD2	2.40	0.51
1:D:498:LEU:O	1:D:499:ASP:HB2	2.10	0.51
1:D:19:LEU:HD11	1:D:80:PHE:CE2	2.45	0.51
1:D:506:ILE:O	1:D:506:ILE:HG23	2.09	0.51
1:E:108:LEU:HD12	1:E:131:THR:HG21	1.90	0.51
1:E:214:ALA:HB1	1:E:247:VAL:HG12	1.92	0.51
1:B:99:GLY:HA3	1:B:134:ARG:HH12	1.75	0.51
1:A:6:PHE:HZ	1:A:92:ILE:HD11	1.76	0.51
1:C:498:LEU:O	1:C:499:ASP:HB2	2.09	0.51
1:A:434:GLU:HG2	1:A:464:SER:HB2	1.93	0.51
1:A:246:ARG:HB3	1:A:275:GLU:HB3	1.93	0.51
1:C:90:ASP:O	1:C:91:GLU:C	2.48	0.51
1:A:506:ILE:O	1:A:506:ILE:HG23	2.10	0.51
1:C:102:ASN:HD22	1:C:133:HIS:CE1	2.28	0.51
1:B:567:ASN:HD21	1:B:569:GLU:HB2	1.76	0.51
1:A:604:GLU:OE2	1:D:67:TRP:NE1	2.40	0.51
1:C:468:GLN:OE1	1:F:465:VAL:HG21	2.10	0.51
1:B:107:LEU:HD13	1:B:129:GLY:HA3	1.92	0.51
1:B:597:PHE:CE2	1:B:599:GLY:HA2	2.46	0.51
1:B:14:LEU:HD12	1:B:15:GLY:N	2.25	0.51
1:C:342:GLU:OE2	1:C:363:HIS:HE1	1.94	0.51
1:E:172:LEU:HD23	1:E:172:LEU:C	2.31	0.51
1:B:115:ALA:N	1:B:116:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:TYR:C	1:D:93:LEU:HD23	2.31	0.51
1:C:64:HIS:CD2	1:C:66:LEU:HB2	2.46	0.51
1:F:113:GLY:HA3	1:F:198:PHE:H	1.76	0.51
1:E:597:PHE:CE2	1:E:599:GLY:HA2	2.46	0.51
1:B:452:ILE:HG12	1:E:452:ILE:HG12	1.92	0.51
1:E:99:GLY:HA3	1:E:134:ARG:HH12	1.76	0.50
1:D:636:ILE:N	1:D:636:ILE:HD12	2.24	0.50
1:C:369:ILE:HD11	1:C:390:VAL:HG11	1.92	0.50
1:A:117:LEU:HD13	1:A:165:LEU:HD12	1.93	0.50
1:B:146:ALA:CB	1:B:176:THR:HG21	2.42	0.50
1:E:575:GLU:O	1:E:579:GLU:HG3	2.10	0.50
1:A:567:ASN:ND2	1:A:569:GLU:H	2.10	0.50
1:A:115:ALA:N	1:A:116:PRO:CD	2.74	0.50
1:E:338:GLU:HG3	1:E:548:TYR:OH	2.11	0.50
1:D:90:ASP:O	1:D:94:GLN:HG2	2.11	0.50
1:C:324:ASN:ND2	1:C:353:ILE:HG13	2.25	0.50
1:F:79:ILE:HG13	1:F:96:ALA:HB2	1.93	0.50
1:F:1:MET:HE2	1:F:77:ASP:HB3	1.93	0.50
1:B:70:ARG:O	1:B:73:GLN:HB2	2.11	0.50
1:F:269:CYS:HB2	1:F:272:GLY:O	2.11	0.50
1:E:113:GLY:HA3	1:E:198:PHE:H	1.75	0.50
1:C:615:ASP:CG	1:C:616:VAL:N	2.65	0.50
1:C:346:LEU:HD23	1:C:346:LEU:C	2.32	0.50
1:B:11:MET:HG3	1:B:83:TYR:CZ	2.46	0.50
1:A:297:GLY:HA3	1:B:524:PRO:HD3	1.93	0.50
1:F:115:ALA:N	1:F:116:PRO:CD	2.74	0.50
1:E:501:LEU:H	1:E:501:LEU:HD22	1.76	0.50
1:D:600:PHE:O	1:D:601:ARG:HG3	2.12	0.50
1:A:64:HIS:CD2	1:A:66:LEU:HB2	2.45	0.50
1:D:6:PHE:CZ	1:D:92:ILE:HD11	2.46	0.50
1:B:400:ARG:HH12	1:B:506:ILE:HG23	1.76	0.50
1:E:109:PRO:HB2	1:E:195:ALA:HB2	1.92	0.50
1:F:539:ASP:OD1	1:F:541:ARG:HG3	2.10	0.50
1:A:636:ILE:HD12	1:A:636:ILE:N	2.26	0.50
1:B:347:ASP:OD1	2:B:1002:ATP:O2'	2.30	0.50
1:D:400:ARG:HH12	1:D:506:ILE:HG23	1.77	0.50
1:A:567:ASN:C	1:A:567:ASN:HD22	2.15	0.50
1:E:489:ARG:HB2	1:E:564:ASN:HD22	1.76	0.50
1:C:9:HIS:CG	1:C:10:ASP:H	2.29	0.50
1:F:64:HIS:O	1:F:68:VAL:HG23	2.12	0.50
1:B:601:ARG:CB	1:B:601:ARG:NH1	2.71	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLN:NE2	1:C:239:LYS:N	2.60	0.50
1:E:431:SER:HB3	1:E:489:ARG:HG2	1.94	0.50
1:D:109:PRO:HB2	1:D:195:ALA:HB2	1.94	0.50
1:A:545:GLU:O	1:A:549:ARG:HG2	2.12	0.50
1:C:601:ARG:HH11	1:C:601:ARG:HB3	1.77	0.49
1:D:102:ASN:HD22	1:D:133:HIS:CE1	2.30	0.49
1:B:468:GLN:OE1	1:E:465:VAL:HG21	2.12	0.49
1:A:436:TYR:HA	1:A:451:LEU:HD22	1.95	0.49
1:A:336:LEU:HG	1:A:359:HIS:CD2	2.47	0.49
1:E:533:GLN:NE2	1:E:533:GLN:N	2.40	0.49
1:B:465:VAL:HG21	1:E:468:GLN:OE1	2.11	0.49
1:C:452:ILE:HG12	1:F:452:ILE:HG12	1.94	0.49
1:A:375:TRP:O	1:A:379:HIS:HD2	1.95	0.49
1:E:601:ARG:CB	1:E:601:ARG:NH1	2.70	0.49
1:F:221:VAL:HG21	1:F:245:SER:CB	2.42	0.49
1:E:89:TYR:C	1:E:93:LEU:HD23	2.33	0.49
1:A:252:SER:C	1:A:254:ALA:H	2.16	0.49
1:B:233:SER:HB3	1:B:240:PHE:CZ	2.47	0.49
1:E:506:ILE:HG23	1:E:506:ILE:O	2.12	0.49
1:F:78:VAL:HA	1:F:96:ALA:HB1	1.95	0.49
1:F:99:GLY:HA3	1:F:134:ARG:NH1	2.27	0.49
1:D:14:LEU:HD12	1:D:14:LEU:C	2.33	0.49
1:C:114:ARG:O	1:C:115:ALA:HB3	2.11	0.49
1:D:70:ARG:O	1:D:73:GLN:HB2	2.13	0.49
1:B:506:ILE:O	1:B:506:ILE:HG23	2.12	0.49
1:E:131:THR:HG23	1:E:144:ILE:HG23	1.93	0.49
1:F:615:ASP:CG	1:F:616:VAL:N	2.65	0.49
1:F:146:ALA:HB1	1:F:176:THR:HG21	1.93	0.49
1:A:347:ASP:OD1	2:A:1001:ATP:O2'	2.31	0.49
1:D:422:LYS:HD3	1:D:423:TYR:CZ	2.47	0.49
1:E:498:LEU:O	1:E:499:ASP:HB2	2.12	0.49
1:D:375:TRP:O	1:D:379:HIS:HD2	1.95	0.49
1:C:99:GLY:HA3	1:C:134:ARG:NH1	2.28	0.49
1:F:221:VAL:HG21	1:F:245:SER:HB3	1.94	0.49
1:C:431:SER:HB3	1:C:489:ARG:CG	2.43	0.49
1:B:6:PHE:HZ	1:B:92:ILE:HD11	1.78	0.49
1:A:79:ILE:HG13	1:A:96:ALA:HB2	1.95	0.49
1:B:567:ASN:HD22	1:B:567:ASN:C	2.14	0.49
1:F:252:SER:C	1:F:254:ALA:H	2.16	0.49
1:D:426:ARG:HG3	1:D:484:GLN:HG2	1.95	0.49
1:E:3:THR:HG22	1:E:78:VAL:CG1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TYR:C	1:B:93:LEU:HD23	2.33	0.48
1:C:238:GLN:NE2	1:C:239:LYS:H	2.10	0.48
1:B:325:GLY:HA3	2:B:1002:ATP:H5'2	1.95	0.48
1:F:244:SER:HB2	1:F:277:VAL:HB	1.94	0.48
1:C:567:ASN:ND2	1:C:569:GLU:HB2	2.28	0.48
1:A:601:ARG:HH21	1:C:294:GLN:C	2.17	0.48
1:A:324:ASN:ND2	1:A:353:ILE:HG13	2.26	0.48
1:A:3:THR:HG22	1:A:78:VAL:CG1	2.42	0.48
1:B:603:VAL:CG1	1:B:607:SER:OG	2.62	0.48
1:D:6:PHE:HZ	1:D:92:ILE:HD11	1.78	0.48
1:B:252:SER:C	1:B:254:ALA:N	2.67	0.48
1:B:545:GLU:O	1:B:549:ARG:HG2	2.13	0.48
1:C:528:ILE:HD13	3:C:1103:UGA:C2	2.43	0.48
1:D:324:ASN:ND2	1:D:353:ILE:HG13	2.28	0.48
1:A:78:VAL:HA	1:A:96:ALA:HB1	1.94	0.48
1:F:369:ILE:CD1	1:F:390:VAL:HG11	2.43	0.48
1:F:109:PRO:O	1:F:195:ALA:HA	2.12	0.48
1:E:92:ILE:O	1:E:95:LEU:HG	2.13	0.48
1:C:397:GLU:OE2	1:C:400:ARG:NH1	2.46	0.48
1:A:109:PRO:HB2	1:A:195:ALA:HB2	1.96	0.48
1:B:150:ILE:CD1	1:B:165:LEU:HD23	2.44	0.48
1:B:64:HIS:CD2	1:B:66:LEU:H	2.31	0.48
1:E:109:PRO:O	1:E:195:ALA:HA	2.14	0.48
1:D:159:ILE:HB	1:D:227:PRO:HD2	1.96	0.48
1:B:431:SER:HB3	1:B:489:ARG:CG	2.44	0.48
1:A:498:LEU:O	1:A:499:ASP:HB2	2.13	0.48
1:A:437:GLY:HA3	1:A:452:ILE:O	2.14	0.48
1:A:533:GLN:NE2	1:A:533:GLN:N	2.41	0.48
1:A:601:ARG:HH11	1:A:601:ARG:HB3	1.77	0.48
1:A:576:GLU:O	1:A:580:MET:HG3	2.14	0.48
1:F:437:GLY:HA3	1:F:452:ILE:O	2.13	0.48
1:F:7:ALA:HB1	1:F:12:GLY:CA	2.43	0.48
1:C:11:MET:HG3	1:C:83:TYR:CZ	2.47	0.48
1:C:348:ILE:HG12	2:C:1003:ATP:C2	2.49	0.48
1:A:146:ALA:CB	1:A:176:THR:HG21	2.43	0.48
1:D:605:SER:HB2	1:D:613:TYR:CD2	2.49	0.48
1:D:342:GLU:OE2	1:D:363:HIS:HE1	1.97	0.48
1:A:228:TRP:HB3	1:A:229:PRO:HD2	1.95	0.48
1:E:175:GLN:O	1:E:178:PRO:HD2	2.14	0.48
1:C:221:VAL:HG21	1:C:245:SER:OG	2.14	0.48
1:B:636:ILE:N	1:B:636:ILE:HD12	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:SER:HB2	1:B:613:TYR:CD2	2.49	0.48
1:B:491:PHE:CZ	1:B:621:PRO:HB3	2.49	0.48
1:D:99:GLY:HA3	1:D:134:ARG:NH1	2.29	0.48
1:F:601:ARG:HB2	1:F:601:ARG:HH11	1.78	0.48
1:C:325:GLY:HA3	2:C:1003:ATP:H5'2	1.95	0.48
1:F:325:GLY:HA3	2:F:1006:ATP:H5'2	1.95	0.48
1:A:426:ARG:HG3	1:A:484:GLN:HG2	1.96	0.48
1:C:157:ILE:HG13	1:C:159:ILE:HG22	1.96	0.48
1:F:399:THR:HG22	1:F:459:PRO:HG2	1.96	0.48
1:B:7:ALA:HB1	1:B:12:GLY:HA2	1.96	0.48
1:E:600:PHE:O	1:E:601:ARG:HG3	2.14	0.47
1:F:78:VAL:HB	1:F:98:ALA:HB3	1.96	0.47
1:A:431:SER:HB3	1:A:489:ARG:CG	2.43	0.47
1:A:130:VAL:HG23	1:A:172:LEU:HD13	1.95	0.47
1:D:64:HIS:CD2	1:D:66:LEU:H	2.32	0.47
1:E:153:ALA:O	1:E:156:ASP:HB2	2.14	0.47
1:F:3:THR:HG22	1:F:78:VAL:CG1	2.42	0.47
1:C:347:ASP:OD1	2:C:1003:ATP:O2'	2.31	0.47
1:E:117:LEU:HD13	1:E:165:LEU:HD12	1.97	0.47
1:A:6:PHE:CZ	1:A:92:ILE:HD11	2.48	0.47
1:D:108:LEU:HD12	1:D:131:THR:HG21	1.96	0.47
1:D:545:GLU:O	1:D:549:ARG:HG2	2.15	0.47
1:C:460:ARG:O	1:C:460:ARG:HG3	2.08	0.47
1:B:6:PHE:CZ	1:B:92:ILE:HD11	2.49	0.47
1:B:228:TRP:HB3	1:B:229:PRO:HD2	1.95	0.47
1:E:375:TRP:O	1:E:379:HIS:HD2	1.96	0.47
1:A:528:ILE:HD13	3:A:1101:UGA:C2	2.45	0.47
1:C:539:ASP:OD1	1:C:541:ARG:HG3	2.15	0.47
1:E:252:SER:C	1:E:254:ALA:N	2.67	0.47
1:C:14:LEU:HD12	1:C:14:LEU:C	2.35	0.47
1:B:538:THR:OG1	1:B:566:GLY:HA2	2.14	0.47
1:D:112:ARG:HH11	1:D:112:ARG:CB	2.28	0.47
1:F:64:HIS:CD2	1:F:66:LEU:H	2.32	0.47
1:B:277:VAL:HG12	1:B:278:THR:HG23	1.96	0.47
1:E:11:MET:HG3	1:E:83:TYR:CZ	2.49	0.47
1:E:150:ILE:HD12	1:E:165:LEU:CD2	2.45	0.47
1:A:64:HIS:CD2	1:A:66:LEU:H	2.33	0.47
1:A:64:HIS:ND1	1:A:65:PRO:HD2	2.29	0.47
1:F:512:ILE:HG23	1:F:513:THR:N	2.30	0.47
1:D:117:LEU:HD13	1:D:165:LEU:HD12	1.96	0.47
1:D:9:HIS:CG	1:D:10:ASP:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD12	1:A:15:GLY:N	2.29	0.47
1:E:430:PRO:HB3	1:E:488:PHE:CZ	2.50	0.47
1:D:109:PRO:O	1:D:195:ALA:HA	2.14	0.47
1:B:7:ALA:HB1	1:B:12:GLY:CA	2.45	0.47
1:A:354:SER:HA	1:A:357:LEU:HG	1.97	0.47
1:D:334:ARG:NH1	1:D:338:GLU:OE2	2.47	0.47
1:E:526:LYS:HE3	1:E:603:VAL:HG21	1.96	0.47
1:D:501:LEU:H	1:D:501:LEU:HD22	1.80	0.47
1:B:109:PRO:HB3	1:B:190:GLN:NE2	2.30	0.47
1:A:603:VAL:CG1	1:A:607:SER:OG	2.63	0.47
1:F:567:ASN:ND2	1:F:569:GLU:HB2	2.28	0.47
1:F:512:ILE:HG23	1:F:513:THR:H	1.80	0.47
1:F:150:ILE:CD1	1:F:165:LEU:HD23	2.45	0.47
1:A:121:LEU:HD21	1:A:161:LEU:HD22	1.97	0.47
1:A:469:LEU:HD12	1:D:469:LEU:HD12	1.97	0.47
1:B:336:LEU:HG	1:B:359:HIS:CD2	2.50	0.47
1:F:119:TRP:CZ2	1:F:201:ARG:HG2	2.50	0.47
1:B:553:ASN:OD1	1:B:558:CYS:HB2	2.15	0.47
1:C:8:TYR:HA	1:C:45:VAL:HG21	1.96	0.47
1:C:79:ILE:HG13	1:C:96:ALA:HB2	1.97	0.47
1:B:9:HIS:CG	1:B:10:ASP:H	2.33	0.47
1:D:533:GLN:N	1:D:533:GLN:NE2	2.44	0.46
1:F:64:HIS:ND1	1:F:65:PRO:HD2	2.30	0.46
1:F:16:ILE:CD1	1:F:29:ILE:HD13	2.40	0.46
1:F:107:LEU:HD13	1:F:129:GLY:CA	2.45	0.46
1:A:601:ARG:HB2	1:A:601:ARG:HH11	1.76	0.46
1:C:334:ARG:NH1	1:C:338:GLU:OE2	2.48	0.46
1:E:512:ILE:HG23	1:E:513:THR:N	2.30	0.46
1:B:14:LEU:HD12	1:B:14:LEU:C	2.36	0.46
1:B:396:ILE:HD13	1:B:400:ARG:NH2	2.29	0.46
1:F:537:PHE:O	1:F:570:ASN:HB2	2.16	0.46
1:C:130:VAL:HG23	1:C:172:LEU:HD13	1.98	0.46
1:B:175:GLN:O	1:B:178:PRO:HD2	2.14	0.46
1:D:439:CYS:HB3	1:D:444:PHE:CE2	2.50	0.46
1:E:588:HIS:HD2	1:E:590:LEU:N	2.12	0.46
1:D:369:ILE:CD1	1:D:390:VAL:HG11	2.46	0.46
1:C:150:ILE:HD12	1:C:165:LEU:HD23	1.98	0.46
1:E:329:ASN:HD22	1:E:355:ARG:HH22	1.61	0.46
1:A:369:ILE:CD1	1:A:390:VAL:HG11	2.45	0.46
1:E:64:HIS:ND1	1:E:65:PRO:HD2	2.30	0.46
1:A:615:ASP:CG	1:A:616:VAL:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ASP:CG	1:B:616:VAL:N	2.69	0.46
1:E:108:LEU:HD12	1:E:131:THR:CG2	2.46	0.46
1:B:211:HIS:O	1:B:270:GLY:HA3	2.14	0.46
1:C:426:ARG:HG3	1:C:484:GLN:HG2	1.96	0.46
1:D:417:ILE:O	1:D:420:CYS:HB2	2.15	0.46
1:D:7:ALA:HB1	1:D:12:GLY:HA2	1.98	0.46
1:E:324:ASN:ND2	1:E:353:ILE:HG13	2.29	0.46
1:E:603:VAL:CG1	1:E:607:SER:OG	2.64	0.46
1:C:480:LYS:HE2	1:F:400:ARG:O	2.15	0.46
1:E:159:ILE:HG23	1:E:160:THR:N	2.29	0.46
1:B:64:HIS:CD2	1:B:66:LEU:HB2	2.45	0.46
1:D:121:LEU:O	1:D:219:ASN:HB3	2.16	0.46
1:A:406:PHE:O	1:A:410:PHE:HB3	2.16	0.46
1:B:150:ILE:HD12	1:B:165:LEU:HD23	1.97	0.46
1:D:7:ALA:HB1	1:D:12:GLY:CA	2.45	0.46
1:E:114:ARG:O	1:E:115:ALA:HB3	2.15	0.46
1:F:522:GLY:CA	1:F:595:PRO:HG2	2.46	0.46
1:E:605:SER:HB2	1:E:613:TYR:CD2	2.50	0.46
1:A:99:GLY:HA3	1:A:134:ARG:HH12	1.81	0.46
1:F:431:SER:HB3	1:F:489:ARG:CG	2.45	0.46
1:E:437:GLY:HA3	1:E:452:ILE:O	2.16	0.46
1:C:172:LEU:C	1:C:172:LEU:HD23	2.36	0.46
1:E:7:ALA:HB1	1:E:12:GLY:HA2	1.98	0.46
1:D:314:ARG:HH11	1:D:314:ARG:HG2	1.81	0.46
1:B:533:GLN:N	1:B:533:GLN:NE2	2.44	0.46
1:F:114:ARG:O	1:F:115:ALA:HB3	2.16	0.46
1:B:213:PRO:HD2	1:B:216:VAL:HG21	1.98	0.46
1:A:8:TYR:HA	1:A:45:VAL:HG21	1.98	0.46
1:C:537:PHE:O	1:C:570:ASN:HB2	2.16	0.46
1:B:490:PRO:HB3	1:B:493:TRP:CE2	2.50	0.46
1:E:348:ILE:HG12	2:E:1005:ATP:C2	2.51	0.46
1:A:588:HIS:CD2	1:A:590:LEU:HB2	2.50	0.46
1:B:78:VAL:HG23	1:B:99:GLY:O	2.16	0.46
1:E:79:ILE:HG13	1:E:96:ALA:HB2	1.98	0.46
1:B:157:ILE:HG13	1:B:159:ILE:HG22	1.98	0.46
1:D:157:ILE:HG13	1:D:159:ILE:HG22	1.98	0.46
1:F:109:PRO:HB2	1:F:195:ALA:CB	2.46	0.46
1:F:582:LEU:HD11	1:F:597:PHE:CE2	2.51	0.46
1:C:553:ASN:OD1	1:C:558:CYS:HB2	2.15	0.46
1:A:605:SER:HB2	1:A:613:TYR:CD2	2.51	0.46
1:A:159:ILE:HB	1:A:227:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:GLY:HA3	2:D:1004:ATP:H5'2	1.98	0.45
1:D:615:ASP:CG	1:D:616:VAL:N	2.69	0.45
1:D:150:ILE:HD12	1:D:165:LEU:HD23	1.98	0.45
1:A:210:TRP:HA	1:A:217:LEU:HD11	1.97	0.45
1:C:213:PRO:HD2	1:C:216:VAL:CG2	2.46	0.45
1:D:506:ILE:O	1:D:506:ILE:CG2	2.64	0.45
1:A:396:ILE:HD13	1:A:400:ARG:NH2	2.31	0.45
1:F:7:ALA:HB1	1:F:12:GLY:HA2	1.98	0.45
1:B:90:ASP:O	1:B:91:GLU:C	2.53	0.45
1:B:287:MET:HA	1:F:50:ALA:HB2	1.99	0.45
1:C:336:LEU:HD21	1:C:362:PHE:HB2	1.97	0.45
1:B:375:TRP:O	1:B:379:HIS:HD2	1.98	0.45
1:F:88:ILE:HG22	1:F:93:LEU:CD2	2.46	0.45
1:E:392:ILE:HG13	1:E:408:LEU:HD12	1.98	0.45
1:A:392:ILE:HG13	1:A:408:LEU:HD12	1.98	0.45
1:F:6:PHE:O	1:F:84:TYR:HB2	2.16	0.45
1:D:8:TYR:HA	1:D:45:VAL:HG21	1.97	0.45
1:D:110:LYS:NZ	1:D:194:GLU:HB3	2.31	0.45
1:D:211:HIS:O	1:D:270:GLY:HA3	2.17	0.45
1:A:468:GLN:OE1	1:D:465:VAL:HG21	2.16	0.45
1:F:636:ILE:CD1	1:F:636:ILE:H	2.28	0.45
1:D:107:LEU:HD13	1:D:129:GLY:CA	2.47	0.45
1:C:314:ARG:HG2	1:C:314:ARG:HH11	1.82	0.45
1:C:19:LEU:HD11	1:C:80:PHE:CE2	2.51	0.45
1:E:406:PHE:O	1:E:410:PHE:HB3	2.16	0.45
1:C:399:THR:HG22	1:C:459:PRO:HG2	1.99	0.45
1:A:90:ASP:O	1:A:94:GLN:HG2	2.16	0.45
1:E:348:ILE:HD13	1:E:367:GLY:O	2.17	0.45
1:E:615:ASP:CG	1:E:616:VAL:N	2.70	0.45
1:C:400:ARG:O	1:F:480:LYS:HE2	2.16	0.45
1:A:50:ALA:HB2	1:E:287:MET:HA	1.99	0.45
1:D:228:TRP:HB3	1:D:229:PRO:HD2	1.97	0.45
1:B:530:GLY:H	1:B:602:VAL:HG13	1.81	0.45
1:D:528:ILE:HD13	3:D:1104:UGA:C2	2.45	0.45
1:F:514:GLN:NE2	1:F:608:TYR:OH	2.41	0.45
1:D:601:ARG:HH11	1:D:601:ARG:HB2	1.80	0.45
1:E:159:ILE:HB	1:E:227:PRO:HD2	1.99	0.45
1:F:567:ASN:HD22	1:F:569:GLU:H	1.65	0.45
1:E:252:SER:O	1:E:254:ALA:N	2.50	0.45
1:D:489:ARG:HB2	1:D:564:ASN:HD22	1.81	0.45
1:B:114:ARG:O	1:B:115:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HD12	1:D:131:THR:CG2	2.47	0.45
1:B:102:ASN:HD22	1:B:133:HIS:CE1	2.35	0.45
1:C:109:PRO:O	1:C:195:ALA:HA	2.16	0.45
1:A:539:ASP:OD1	1:A:541:ARG:HG3	2.17	0.45
1:F:498:LEU:O	1:F:499:ASP:HB2	2.17	0.45
1:E:512:ILE:HG23	1:E:513:THR:H	1.81	0.45
1:D:338:GLU:HG3	1:D:548:TYR:OH	2.16	0.45
1:D:119:TRP:CZ2	1:D:201:ARG:HG2	2.51	0.45
1:F:102:ASN:HD22	1:F:133:HIS:CE1	2.34	0.45
1:F:515:LEU:HA	1:F:518:ASN:ND2	2.28	0.45
1:F:434:GLU:OE2	1:F:460:ARG:NH2	2.50	0.45
1:D:348:ILE:HG12	2:D:1004:ATP:C2	2.52	0.45
1:D:90:ASP:O	1:D:91:GLU:C	2.55	0.45
1:D:436:TYR:HA	1:D:451:LEU:HD22	1.98	0.45
1:A:403:LEU:O	1:A:407:GLU:HG3	2.17	0.45
1:B:107:LEU:HD13	1:B:129:GLY:CA	2.47	0.45
1:A:348:ILE:HG12	2:A:1001:ATP:C2	2.51	0.45
1:C:512:ILE:HG23	1:C:513:THR:N	2.32	0.45
1:F:538:THR:OG1	1:F:566:GLY:HA2	2.17	0.45
1:E:9:HIS:CG	1:E:10:ASP:H	2.34	0.45
1:F:347:ASP:OD1	2:F:1006:ATP:O2'	2.33	0.44
1:B:582:LEU:HD11	1:B:597:PHE:CE2	2.52	0.44
1:C:252:SER:C	1:C:254:ALA:H	2.20	0.44
1:E:325:GLY:HA3	2:E:1005:ATP:H5'2	1.99	0.44
1:C:16:ILE:HD13	1:C:29:ILE:CD1	2.39	0.44
1:D:235:VAL:HG23	1:D:240:PHE:CE1	2.53	0.44
1:C:396:ILE:HD13	1:C:400:ARG:NH2	2.32	0.44
1:C:359:HIS:HA	1:C:360:PRO:HD3	1.87	0.44
1:F:121:LEU:HD21	1:F:161:LEU:HD22	1.98	0.44
1:F:233:SER:HB3	1:F:240:PHE:CZ	2.51	0.44
1:F:8:TYR:HA	1:F:45:VAL:HG21	1.99	0.44
1:D:146:ALA:CB	1:D:176:THR:HG21	2.47	0.44
1:C:12:GLY:O	1:C:16:ILE:HG13	2.17	0.44
1:A:567:ASN:HD21	1:A:569:GLU:HB2	1.83	0.44
1:C:146:ALA:CB	1:C:176:THR:HG21	2.47	0.44
1:A:119:TRP:CZ2	1:A:201:ARG:HG2	2.51	0.44
1:B:78:VAL:HG22	1:B:79:ILE:N	2.32	0.44
1:F:252:SER:C	1:F:254:ALA:N	2.71	0.44
1:A:90:ASP:O	1:A:91:GLU:C	2.55	0.44
1:E:110:LYS:NZ	1:E:194:GLU:HB3	2.33	0.44
1:E:235:VAL:HG23	1:E:240:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:NH1	1:A:338:GLU:OE2	2.51	0.44
1:C:146:ALA:HB1	1:C:176:THR:HG21	2.00	0.44
1:F:364:PHE:CG	1:F:365:VAL:N	2.86	0.44
1:D:539:ASP:OD1	1:D:541:ARG:HG3	2.17	0.44
1:C:113:GLY:HA3	1:C:198:PHE:O	2.18	0.44
1:E:334:ARG:NH1	1:E:338:GLU:OE2	2.51	0.44
1:E:70:ARG:O	1:E:73:GLN:HB2	2.17	0.44
1:B:326:PHE:CZ	1:B:540:ILE:HD13	2.52	0.44
1:D:399:THR:HG22	1:D:459:PRO:HG2	2.00	0.44
1:C:299:VAL:O	1:C:301:GLY:N	2.46	0.44
1:C:436:TYR:HA	1:C:451:LEU:HD22	1.99	0.44
1:C:501:LEU:H	1:C:501:LEU:HD22	1.81	0.44
1:D:11:MET:HG3	1:D:83:TYR:CZ	2.52	0.44
1:D:12:GLY:O	1:D:16:ILE:HG13	2.18	0.44
1:C:534:LYS:HA	1:C:573:SER:HA	1.99	0.44
1:A:510:ARG:NH1	2:A:1001:ATP:O3G	2.51	0.44
1:F:436:TYR:HA	1:F:451:LEU:HD22	1.99	0.44
1:F:243:TRP:CD1	1:F:279:GLY:HA2	2.53	0.44
1:C:524:PRO:HB2	1:C:601:ARG:HD3	2.00	0.44
1:F:603:VAL:CG1	1:F:607:SER:OG	2.65	0.44
1:A:235:VAL:HG23	1:A:240:PHE:CE1	2.53	0.44
1:B:594:PHE:HB3	1:B:595:PRO:HD2	2.00	0.44
1:B:485:PHE:CZ	1:B:560:GLY:HA2	2.52	0.44
1:D:522:GLY:CA	1:D:595:PRO:HG2	2.48	0.44
1:E:403:LEU:O	1:E:407:GLU:HG3	2.18	0.44
1:C:545:GLU:O	1:C:549:ARG:HG2	2.16	0.44
1:A:157:ILE:HG13	1:A:159:ILE:HG22	1.99	0.43
1:A:159:ILE:HG23	1:A:160:THR:N	2.33	0.43
1:D:78:VAL:HA	1:D:96:ALA:HB1	1.99	0.43
1:E:107:LEU:HD13	1:E:129:GLY:CA	2.48	0.43
1:A:424:ARG:NH1	1:A:424:ARG:HG2	2.32	0.43
1:C:392:ILE:HG13	1:C:408:LEU:HD12	2.00	0.43
1:B:424:ARG:HG2	1:B:424:ARG:NH1	2.33	0.43
1:A:489:ARG:HB2	1:A:564:ASN:HD22	1.83	0.43
1:B:146:ALA:HB1	1:B:176:THR:HG21	2.00	0.43
1:B:359:HIS:HA	1:B:360:PRO:HD3	1.88	0.43
1:F:172:LEU:HD23	1:F:172:LEU:C	2.39	0.43
1:B:399:THR:HG22	1:B:459:PRO:HG2	2.00	0.43
1:D:156:ASP:O	1:D:222:ARG:HD2	2.18	0.43
1:F:369:ILE:HD11	1:F:390:VAL:HG11	1.99	0.43
1:B:338:GLU:HB3	1:B:340:HIS:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLY:CA	1:B:595:PRO:HG2	2.48	0.43
1:F:314:ARG:HG2	1:F:314:ARG:HH11	1.83	0.43
1:F:190:GLN:O	1:F:192:GLU:N	2.51	0.43
1:B:16:ILE:CD1	1:B:29:ILE:HD13	2.40	0.43
1:F:590:LEU:HD11	1:F:651:ARG:NH1	2.33	0.43
1:F:600:PHE:O	1:F:601:ARG:HG3	2.18	0.43
1:D:159:ILE:HG23	1:D:160:THR:N	2.33	0.43
1:E:221:VAL:HG21	1:E:245:SER:HB3	2.01	0.43
1:B:252:SER:O	1:B:254:ALA:N	2.50	0.43
1:E:582:LEU:HD11	1:E:597:PHE:CE2	2.54	0.43
1:B:437:GLY:HA3	1:B:452:ILE:O	2.19	0.43
1:F:130:VAL:HG23	1:F:172:LEU:HD13	1.99	0.43
1:A:364:PHE:CG	1:A:365:VAL:N	2.86	0.43
1:C:601:ARG:HB2	1:C:601:ARG:HH11	1.78	0.43
1:B:348:ILE:HD13	1:B:367:GLY:O	2.19	0.43
1:B:567:ASN:ND2	1:B:569:GLU:HB2	2.33	0.43
1:A:400:ARG:HH12	1:A:506:ILE:HG23	1.83	0.43
1:C:259:VAL:HG22	1:C:267:ILE:CD1	2.48	0.43
1:C:354:SER:HA	1:C:357:LEU:HG	2.00	0.43
1:B:119:TRP:CZ2	1:B:201:ARG:HG2	2.54	0.43
1:E:157:ILE:HG13	1:E:159:ILE:HG22	1.99	0.43
1:D:246:ARG:HB3	1:D:275:GLU:HB3	2.01	0.43
1:A:314:ARG:HG2	1:A:314:ARG:HH11	1.84	0.43
1:A:109:PRO:HB3	1:A:190:GLN:NE2	2.33	0.43
1:A:16:ILE:CD1	1:A:29:ILE:HD13	2.44	0.43
1:E:1:MET:HE1	1:E:77:ASP:HB3	2.00	0.43
1:F:324:ASN:ND2	1:F:353:ILE:HG13	2.31	0.43
1:A:580:MET:HE2	1:A:580:MET:HB3	1.87	0.43
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.88	0.43
1:C:87:LEU:HD12	1:C:88:ILE:N	2.34	0.43
1:C:78:VAL:HA	1:C:96:ALA:HB1	2.00	0.43
1:B:392:ILE:HG13	1:B:408:LEU:HD12	2.00	0.43
1:B:348:ILE:HG12	2:B:1002:ATP:C2	2.54	0.43
1:C:576:GLU:O	1:C:580:MET:HG3	2.18	0.43
1:C:64:HIS:ND1	1:C:65:PRO:HD2	2.33	0.43
1:F:546:ALA:HB3	1:F:565:ILE:HD13	2.00	0.43
1:C:522:GLY:CA	1:C:595:PRO:HG2	2.49	0.43
1:B:99:GLY:HA3	1:B:134:ARG:NH1	2.33	0.43
1:F:213:PRO:HB2	1:F:216:VAL:HG23	2.00	0.43
1:D:150:ILE:CD1	1:D:165:LEU:HD23	2.49	0.43
1:C:492:ASN:OD1	1:C:535:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:THR:OG1	1:A:566:GLY:HA2	2.19	0.43
1:B:539:ASP:OD1	1:B:541:ARG:HG3	2.19	0.43
1:B:369:ILE:HD11	1:B:390:VAL:HG11	2.00	0.43
1:D:347:ASP:OD1	2:D:1004:ATP:O2'	2.35	0.43
1:B:601:ARG:HB3	1:B:601:ARG:NH1	2.34	0.43
1:C:221:VAL:HG21	1:C:245:SER:CB	2.49	0.43
1:C:636:ILE:CD1	1:C:636:ILE:H	2.30	0.43
1:E:369:ILE:HD11	1:E:390:VAL:HG11	2.00	0.43
1:E:221:VAL:HG21	1:E:245:SER:CB	2.49	0.43
1:E:233:SER:HB3	1:E:240:PHE:CZ	2.54	0.43
1:D:582:LEU:HD11	1:D:597:PHE:CE2	2.53	0.43
1:A:252:SER:C	1:A:254:ALA:N	2.72	0.43
1:F:354:SER:HA	1:F:357:LEU:HG	2.01	0.43
1:F:110:LYS:NZ	1:F:194:GLU:HB3	2.33	0.43
1:F:15:GLY:O	1:F:19:LEU:HB2	2.19	0.42
1:A:506:ILE:O	1:A:506:ILE:CG2	2.66	0.42
1:F:430:PRO:HB3	1:F:488:PHE:CZ	2.54	0.42
1:A:490:PRO:HB3	1:A:493:TRP:CE2	2.53	0.42
1:B:117:LEU:HD13	1:B:165:LEU:HD12	2.01	0.42
1:B:510:ARG:NH1	2:B:1002:ATP:O3G	2.52	0.42
1:C:375:TRP:O	1:C:379:HIS:HD2	2.01	0.42
1:D:307:GLN:O	1:D:308:PRO:C	2.57	0.42
1:A:524:PRO:HB2	1:A:601:ARG:HD3	2.00	0.42
1:C:133:HIS:HD2	1:C:134:ARG:O	2.01	0.42
1:F:221:VAL:HG21	1:F:245:SER:OG	2.19	0.42
1:D:329:ASN:HD22	1:D:355:ARG:HH22	1.64	0.42
1:A:78:VAL:HG22	1:A:79:ILE:N	2.35	0.42
1:A:362:PHE:CE2	1:A:364:PHE:HB2	2.55	0.42
1:D:588:HIS:CG	1:D:589:PRO:HD2	2.54	0.42
1:C:78:VAL:HG23	1:C:99:GLY:O	2.19	0.42
1:E:99:GLY:HA3	1:E:134:ARG:NH1	2.35	0.42
1:F:90:ASP:O	1:F:91:GLU:C	2.57	0.42
1:A:248:HIS:C	1:A:250:HIS:N	2.72	0.42
1:D:490:PRO:HB3	1:D:493:TRP:CE2	2.54	0.42
1:E:315:ARG:CZ	1:E:361:HIS:NE2	2.83	0.42
1:B:159:ILE:HG23	1:B:160:THR:N	2.34	0.42
1:B:107:LEU:CD1	1:B:129:GLY:HA3	2.50	0.42
1:F:528:ILE:HD13	3:F:1106:UGA:C2	2.49	0.42
1:C:111:TYR:H	1:C:196:THR:HB	1.85	0.42
1:C:533:GLN:N	1:C:533:GLN:NE2	2.42	0.42
1:F:524:PRO:HB2	1:F:601:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:GLU:O	1:F:72:ALA:HB3	2.20	0.42
1:D:330:HIS:HB3	1:D:544:ILE:HG12	2.02	0.42
1:C:109:PRO:HB3	1:C:190:GLN:NE2	2.34	0.42
1:E:109:PRO:HB3	1:E:190:GLN:NE2	2.35	0.42
1:C:177:LEU:HD12	1:C:177:LEU:HA	1.92	0.42
1:A:329:ASN:ND2	1:A:355:ARG:NH2	2.66	0.42
1:A:107:LEU:HD13	1:A:129:GLY:CA	2.49	0.42
1:D:221:VAL:HG21	1:D:245:SER:CB	2.49	0.42
1:D:431:SER:HB3	1:D:489:ARG:CG	2.50	0.42
1:C:150:ILE:CD1	1:C:165:LEU:HD23	2.49	0.42
1:E:342:GLU:OE2	1:E:363:HIS:HE1	2.01	0.42
1:D:336:LEU:HD21	1:D:362:PHE:HB2	2.02	0.42
1:A:7:ALA:HB1	1:A:12:GLY:CA	2.50	0.42
1:C:540:ILE:CD1	1:C:544:ILE:HD13	2.50	0.42
1:F:155:ASP:OD1	1:F:155:ASP:N	2.52	0.42
1:E:336:LEU:HA	1:E:336:LEU:HD12	1.90	0.42
1:D:112:ARG:HH22	1:D:190:GLN:NE2	2.18	0.42
1:B:489:ARG:HB2	1:B:564:ASN:HD22	1.84	0.42
1:E:485:PHE:CZ	1:E:560:GLY:HA2	2.54	0.42
1:D:636:ILE:H	1:D:636:ILE:CD1	2.28	0.42
1:A:534:LYS:HA	1:A:573:SER:HA	2.02	0.42
1:A:228:TRP:CB	1:A:229:PRO:HD2	2.50	0.42
1:C:131:THR:HG23	1:C:144:ILE:HG23	2.02	0.42
1:E:491:PHE:CE2	1:E:621:PRO:HB3	2.55	0.42
1:B:362:PHE:CE2	1:B:364:PHE:HB2	2.55	0.42
1:E:228:TRP:HB3	1:E:229:PRO:HD2	2.00	0.42
1:F:336:LEU:HA	1:F:336:LEU:HD12	1.85	0.42
1:C:416:ILE:N	1:C:416:ILE:HD12	2.35	0.42
1:E:146:ALA:CB	1:E:176:THR:HG21	2.49	0.42
1:E:112:ARG:CB	1:E:112:ARG:HH11	2.33	0.42
1:F:159:ILE:HB	1:F:227:PRO:HD2	2.01	0.42
1:D:327:ILE:HD11	2:D:1004:ATP:O2G	2.20	0.42
1:F:435:VAL:HG22	1:F:468:GLN:HB2	2.01	0.42
1:C:567:ASN:HD22	1:C:569:GLU:H	1.66	0.42
1:E:7:ALA:HB1	1:E:12:GLY:CA	2.50	0.42
1:F:406:PHE:O	1:F:410:PHE:HB3	2.20	0.42
1:E:314:ARG:HG2	1:E:314:ARG:HH11	1.83	0.42
1:D:603:VAL:CG1	1:D:607:SER:OG	2.68	0.41
1:E:246:ARG:HB3	1:E:275:GLU:HB3	2.02	0.41
1:B:436:TYR:HA	1:B:451:LEU:HD22	2.02	0.41
1:A:430:PRO:HB3	1:A:488:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:HA	1:A:458:LYS:HD3	1.92	0.41
1:F:398:TYR:N	1:F:398:TYR:CD1	2.87	0.41
1:F:601:ARG:HB3	1:F:601:ARG:HH11	1.84	0.41
1:E:71:ILE:HD12	1:E:92:ILE:HD12	2.02	0.41
1:D:213:PRO:HB2	1:D:216:VAL:HG23	2.02	0.41
1:A:400:ARG:O	1:D:480:LYS:HE2	2.19	0.41
1:C:252:SER:C	1:C:254:ALA:N	2.73	0.41
1:B:314:ARG:NH1	1:B:315:ARG:O	2.52	0.41
1:C:605:SER:HB2	1:C:613:TYR:CD2	2.56	0.41
1:F:4:VAL:HG23	1:F:76:PRO:HB3	2.02	0.41
1:D:155:ASP:N	1:D:155:ASP:OD1	2.49	0.41
1:D:31:THR:HG23	1:D:32:HIS:N	2.35	0.41
1:E:190:GLN:O	1:E:192:GLU:N	2.53	0.41
1:E:541:ARG:HH12	1:E:636:ILE:HG12	1.85	0.41
1:E:238:GLN:NE2	1:E:239:LYS:H	2.18	0.41
1:D:228:TRP:CB	1:D:229:PRO:HD2	2.51	0.41
1:E:69:GLU:O	1:E:73:GLN:HG2	2.20	0.41
1:D:111:TYR:CE2	1:D:120:VAL:HG12	2.55	0.41
1:E:528:ILE:HD13	3:E:1105:UGA:C2	2.50	0.41
1:E:90:ASP:O	1:E:91:GLU:C	2.58	0.41
1:D:354:SER:HA	1:D:357:LEU:HG	2.01	0.41
1:F:588:HIS:HD2	1:F:590:LEU:N	2.11	0.41
1:D:524:PRO:HB2	1:D:601:ARG:HD3	2.00	0.41
1:F:582:LEU:HD11	1:F:597:PHE:CD2	2.56	0.41
1:F:113:GLY:HA3	1:F:198:PHE:O	2.21	0.41
1:C:506:ILE:O	1:C:506:ILE:HG23	2.19	0.41
1:B:221:VAL:HG21	1:B:245:SER:CB	2.50	0.41
1:E:588:HIS:HA	1:E:589:PRO:HD3	1.94	0.41
1:F:296:LEU:CB	1:F:298:LEU:HD13	2.50	0.41
1:C:121:LEU:O	1:C:219:ASN:HB3	2.21	0.41
1:F:485:PHE:CZ	1:F:560:GLY:HA2	2.55	0.41
1:A:110:LYS:NZ	1:A:194:GLU:HB3	2.35	0.41
1:E:522:GLY:CA	1:E:595:PRO:HG2	2.50	0.41
1:F:111:TYR:CE2	1:F:120:VAL:HG12	2.55	0.41
1:B:129:GLY:HA2	1:B:150:ILE:HD12	2.02	0.41
1:E:567:ASN:C	1:E:567:ASN:ND2	2.72	0.41
1:A:327:ILE:HD11	2:A:1001:ATP:O2G	2.21	0.41
1:F:435:VAL:CG2	1:F:468:GLN:HB2	2.51	0.41
1:E:400:ARG:HH12	1:E:506:ILE:HG23	1.86	0.41
1:D:594:PHE:HB3	1:D:595:PRO:HD2	2.03	0.41
1:B:430:PRO:HB3	1:B:488:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:PHE:O	1:D:410:PHE:HB3	2.20	0.41
1:D:159:ILE:O	1:D:162:HIS:HB3	2.21	0.41
1:F:534:LYS:HA	1:F:573:SER:HA	2.03	0.41
1:B:113:GLY:HA3	1:B:198:PHE:O	2.20	0.41
1:C:437:GLY:HA3	1:C:452:ILE:O	2.21	0.41
1:F:130:VAL:HG23	1:F:172:LEU:CD1	2.50	0.41
1:A:342:GLU:OE2	1:A:363:HIS:HE1	2.02	0.41
1:D:546:ALA:HB3	1:D:565:ILE:HD13	2.03	0.41
1:A:221:VAL:HG21	1:A:245:SER:CB	2.51	0.41
1:E:77:ASP:O	1:E:98:ALA:HB3	2.21	0.41
1:C:512:ILE:HG23	1:C:513:THR:H	1.85	0.41
1:E:5:VAL:HG21	1:E:19:LEU:HD23	2.01	0.41
1:E:90:ASP:O	1:E:94:GLN:HG2	2.20	0.41
1:B:217:LEU:HD12	1:B:269:CYS:SG	2.61	0.41
1:A:243:TRP:CD1	1:A:279:GLY:HA2	2.55	0.41
1:B:157:ILE:O	1:B:158:ALA:C	2.60	0.41
1:E:636:ILE:N	1:E:636:ILE:HD12	2.29	0.41
1:C:107:LEU:HD13	1:C:129:GLY:CA	2.50	0.41
1:A:69:GLU:O	1:A:73:GLN:HG2	2.21	0.41
1:F:338:GLU:HB3	1:F:340:HIS:CE1	2.56	0.41
1:E:113:GLY:HA3	1:E:198:PHE:O	2.20	0.41
1:B:506:ILE:O	1:B:506:ILE:CG2	2.69	0.41
1:B:491:PHE:CE1	1:B:621:PRO:HB3	2.55	0.41
1:D:131:THR:HG23	1:D:144:ILE:HG23	2.02	0.41
1:F:522:GLY:HA3	1:F:595:PRO:CG	2.50	0.41
1:A:112:ARG:NH1	1:A:140:ASP:O	2.54	0.41
1:B:431:SER:CB	1:B:489:ARG:HG2	2.51	0.41
1:B:506:ILE:HD12	1:B:506:ILE:HA	1.89	0.41
1:C:159:ILE:HG23	1:C:160:THR:N	2.36	0.41
1:B:90:ASP:O	1:B:94:GLN:HG2	2.21	0.41
1:C:336:LEU:HG	1:C:359:HIS:CD2	2.56	0.41
1:B:214:ALA:HB1	1:B:247:VAL:HG12	2.03	0.41
1:C:233:SER:HB3	1:C:240:PHE:CZ	2.56	0.41
1:A:492:ASN:OD1	1:A:535:ARG:HD2	2.21	0.41
1:E:398:TYR:N	1:E:398:TYR:CD1	2.88	0.41
1:D:88:ILE:H	1:D:88:ILE:HG13	1.76	0.41
1:E:601:ARG:NH2	1:F:295:THR:HA	2.36	0.40
1:E:590:LEU:HD11	1:E:651:ARG:NH1	2.35	0.40
1:D:392:ILE:HG13	1:D:408:LEU:HD12	2.03	0.40
1:F:8:TYR:CA	1:F:45:VAL:HG21	2.51	0.40
1:F:359:HIS:HA	1:F:360:PRO:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:THR:OG1	1:C:566:GLY:HA2	2.21	0.40
1:B:588:HIS:HA	1:B:589:PRO:HD3	1.98	0.40
1:A:588:HIS:HD2	1:A:590:LEU:HB2	1.85	0.40
1:A:1:MET:H3	1:A:181:LYS:HE3	1.85	0.40
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.89	0.40
1:A:397:GLU:OE2	1:A:400:ARG:NH1	2.54	0.40
1:B:435:VAL:CG2	1:B:468:GLN:HB2	2.51	0.40
1:D:8:TYR:CA	1:D:45:VAL:HG21	2.52	0.40
1:A:94:GLN:HG2	1:A:94:GLN:H	1.63	0.40
1:D:111:TYR:H	1:D:196:THR:HB	1.86	0.40
1:F:101:PHE:CE2	1:F:145:VAL:HG21	2.56	0.40
1:D:537:PHE:O	1:D:570:ASN:HB2	2.21	0.40
1:D:398:TYR:CD1	1:D:398:TYR:N	2.90	0.40
1:F:317:ARG:HG3	1:F:317:ARG:NH1	2.37	0.40
1:C:109:PRO:HB2	1:C:195:ALA:HB2	2.04	0.40
1:E:353:ILE:HD12	1:E:353:ILE:C	2.42	0.40
1:F:232:PHE:CG	1:F:239:LYS:HE3	2.56	0.40
1:B:375:TRP:CE2	1:B:379:HIS:CD2	3.09	0.40
1:B:364:PHE:CG	1:B:365:VAL:N	2.89	0.40
1:B:315:ARG:CZ	1:B:361:HIS:NE2	2.84	0.40
1:D:580:MET:HE2	1:D:580:MET:HB3	1.91	0.40
1:E:367:GLY:HA2	1:E:372:HIS:CD2	2.57	0.40
1:C:434:GLU:OE2	1:C:460:ARG:NH2	2.55	0.40
1:C:603:VAL:CG1	1:C:607:SER:OG	2.69	0.40
1:F:136:VAL:HG22	1:F:142:GLY:H	1.85	0.40
1:F:567:ASN:ND2	1:F:567:ASN:C	2.74	0.40
1:E:424:ARG:HG2	1:E:424:ARG:NH1	2.36	0.40
1:A:359:HIS:HA	1:A:360:PRO:HD3	1.89	0.40
1:E:397:GLU:OE2	1:E:400:ARG:NH1	2.53	0.40
1:F:121:LEU:HA	1:F:121:LEU:HD13	1.95	0.40
1:E:490:PRO:HB3	1:E:493:TRP:CE2	2.57	0.40
1:D:470:LEU:HD23	1:D:470:LEU:HA	1.97	0.40
1:D:416:ILE:N	1:D:416:ILE:HD12	2.37	0.40
1:C:367:GLY:HA2	1:C:372:HIS:CD2	2.56	0.40
1:A:112:ARG:HH11	1:A:112:ARG:CB	2.34	0.40
1:A:391:ALA:HA	1:A:408:LEU:HD13	2.04	0.40
1:C:390:VAL:HG13	2:C:1003:ATP:C4	2.57	0.40
1:D:102:ASN:HD22	1:D:133:HIS:HE1	1.69	0.40
1:C:336:LEU:HA	1:C:336:LEU:HD12	1.76	0.40
1:C:314:ARG:NH1	1:C:315:ARG:O	2.51	0.40
1:A:7:ALA:HB1	1:A:12:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:VAL:O	1:E:301:GLY:N	2.54	0.40
1:A:594:PHE:HB3	1:A:595:PRO:HD2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:ND2	1:C:171:GLN:OE1[1_655]	2.03	0.17
1:B:182:HIS:O	1:C:167:HIS:NE2[1_655]	2.13	0.07

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	633/660 (96%)	581 (92%)	42 (7%)	10 (2%)	12	48
1	B	633/660 (96%)	578 (91%)	43 (7%)	12 (2%)	10	43
1	C	633/660 (96%)	573 (90%)	50 (8%)	10 (2%)	12	48
1	D	638/660 (97%)	584 (92%)	44 (7%)	10 (2%)	12	48
1	E	633/660 (96%)	580 (92%)	42 (7%)	11 (2%)	11	46
1	F	633/660 (96%)	577 (91%)	45 (7%)	11 (2%)	11	46
All	All	3803/3960 (96%)	3473 (91%)	266 (7%)	64 (2%)	11	46

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	300	GLN
1	A	302	SER
1	B	90	ASP
1	B	251	ALA

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Mol	Chain	Res	Type
1	B	302	SER
1	C	90	ASP
1	D	90	ASP
1	E	90	ASP
1	F	90	ASP
1	F	142	GLY
1	F	302	SER
1	A	142	GLY
1	B	250	HIS
1	C	142	GLY
1	C	302	SER
1	D	142	GLY
1	D	189	ALA
1	F	189	ALA
1	A	210	TRP
1	A	250	HIS
1	B	142	GLY
1	C	250	HIS
1	C	251	ALA
1	C	300	GLN
1	D	250	HIS
1	D	302	SER
1	E	253	LYS
1	E	300	GLN
1	E	302	SER
1	F	191	ARG
1	F	250	HIS
1	A	183	GLY
1	A	251	ALA
1	B	253	LYS
1	E	192	GLU
1	E	251	ALA
1	E	252	SER
1	F	192	GLU
1	F	251	ALA
1	A	253	LYS
1	B	246	ARG
1	B	252	SER
1	B	300	GLN
1	C	91	GLU
1	C	192	GLU
1	D	188	ILE

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Mol	Chain	Res	Type
1	D	246	ARG
1	E	183	GLY
1	E	191	ARG
1	F	113	GLY
1	F	188	ILE
1	A	113	GLY
1	B	431	SER
1	D	113	GLY
1	E	210	TRP
1	F	183	GLY
1	B	183	GLY
1	C	113	GLY
1	D	115	ALA
1	E	113	GLY
1	B	113	GLY
1	C	183	GLY
1	D	299	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/559 (94%)	489 (93%)	37 (7%)	19	55
1	B	526/559 (94%)	488 (93%)	38 (7%)	18	53
1	C	526/559 (94%)	489 (93%)	37 (7%)	19	55
1	D	528/559 (94%)	491 (93%)	37 (7%)	19	55
1	E	526/559 (94%)	487 (93%)	39 (7%)	17	52
1	F	526/559 (94%)	485 (92%)	41 (8%)	16	49
All	All	3158/3354 (94%)	2929 (93%)	229 (7%)	17	52

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP

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Mol	Chain	Res	Type
1	A	89	TYR
1	A	91	GLU
1	A	92	ILE
1	A	103	LEU
1	A	107	LEU
1	A	112	ARG
1	A	125	GLU
1	A	164	LYS
1	A	191	ARG
1	A	221	VAL
1	A	288	GLN
1	A	304	LEU
1	A	314	ARG
1	A	319	LEU
1	A	334	ARG
1	A	336	LEU
1	A	385	VAL
1	A	387	LEU
1	A	408	LEU
1	A	415	ARG
1	A	421	VAL
1	A	435	VAL
1	A	460	ARG
1	A	469	LEU
1	A	498	LEU
1	A	506	ILE
1	A	533	GLN
1	A	541	ARG
1	A	547	LEU
1	A	567	ASN
1	A	581	LEU
1	A	582	LEU
1	A	601	ARG
1	A	622	SER
1	A	652	THR
1	A	656	THR
1	B	60	ASP
1	B	89	TYR
1	B	91	GLU
1	B	92	ILE
1	B	103	LEU
1	B	107	LEU

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Mol	Chain	Res	Type
1	B	112	ARG
1	B	125	GLU
1	B	164	LYS
1	B	191	ARG
1	B	221	VAL
1	B	247	VAL
1	B	304	LEU
1	B	314	ARG
1	B	319	LEU
1	B	334	ARG
1	B	336	LEU
1	B	355	ARG
1	B	365	VAL
1	B	385	VAL
1	B	387	LEU
1	B	408	LEU
1	B	415	ARG
1	B	421	VAL
1	B	435	VAL
1	B	460	ARG
1	B	469	LEU
1	B	498	LEU
1	B	506	ILE
1	B	533	GLN
1	B	541	ARG
1	B	547	LEU
1	B	567	ASN
1	B	581	LEU
1	B	582	LEU
1	B	601	ARG
1	B	621	PRO
1	B	656	THR
1	C	89	TYR
1	C	91	GLU
1	C	92	ILE
1	C	103	LEU
1	C	107	LEU
1	C	112	ARG
1	C	125	GLU
1	C	164	LYS
1	C	191	ARG
1	C	221	VAL

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Mol	Chain	Res	Type
1	C	247	VAL
1	C	288	GLN
1	C	304	LEU
1	C	314	ARG
1	C	317	ARG
1	C	319	LEU
1	C	334	ARG
1	C	336	LEU
1	C	385	VAL
1	C	387	LEU
1	C	408	LEU
1	C	415	ARG
1	C	421	VAL
1	C	435	VAL
1	C	460	ARG
1	C	469	LEU
1	C	498	LEU
1	C	506	ILE
1	C	533	GLN
1	C	541	ARG
1	C	547	LEU
1	C	567	ASN
1	C	581	LEU
1	C	582	LEU
1	C	601	ARG
1	C	622	SER
1	C	656	THR
1	D	60	ASP
1	D	89	TYR
1	D	91	GLU
1	D	92	ILE
1	D	103	LEU
1	D	107	LEU
1	D	112	ARG
1	D	125	GLU
1	D	164	LYS
1	D	191	ARG
1	D	221	VAL
1	D	247	VAL
1	D	304	LEU
1	D	314	ARG
1	D	319	LEU

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Mol	Chain	Res	Type
1	D	334	ARG
1	D	336	LEU
1	D	385	VAL
1	D	387	LEU
1	D	408	LEU
1	D	415	ARG
1	D	421	VAL
1	D	435	VAL
1	D	460	ARG
1	D	469	LEU
1	D	498	LEU
1	D	506	ILE
1	D	533	GLN
1	D	534	LYS
1	D	541	ARG
1	D	547	LEU
1	D	567	ASN
1	D	581	LEU
1	D	582	LEU
1	D	601	ARG
1	D	622	SER
1	D	656	THR
1	E	60	ASP
1	E	89	TYR
1	E	91	GLU
1	E	92	ILE
1	E	103	LEU
1	E	107	LEU
1	E	112	ARG
1	E	121	LEU
1	E	125	GLU
1	E	164	LYS
1	E	191	ARG
1	E	221	VAL
1	E	247	VAL
1	E	304	LEU
1	E	314	ARG
1	E	317	ARG
1	E	319	LEU
1	E	334	ARG
1	E	336	LEU
1	E	385	VAL

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Mol	Chain	Res	Type
1	E	387	LEU
1	E	408	LEU
1	E	415	ARG
1	E	421	VAL
1	E	435	VAL
1	E	460	ARG
1	E	469	LEU
1	E	498	LEU
1	E	506	ILE
1	E	533	GLN
1	E	541	ARG
1	E	547	LEU
1	E	567	ASN
1	E	581	LEU
1	E	582	LEU
1	E	601	ARG
1	E	621	PRO
1	E	622	SER
1	E	656	THR
1	F	60	ASP
1	F	89	TYR
1	F	91	GLU
1	F	92	ILE
1	F	103	LEU
1	F	107	LEU
1	F	112	ARG
1	F	125	GLU
1	F	164	LYS
1	F	184	ASN
1	F	191	ARG
1	F	205	ASP
1	F	221	VAL
1	F	247	VAL
1	F	288	GLN
1	F	304	LEU
1	F	314	ARG
1	F	317	ARG
1	F	319	LEU
1	F	334	ARG
1	F	336	LEU
1	F	385	VAL
1	F	387	LEU

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Mol	Chain	Res	Type
1	F	408	LEU
1	F	415	ARG
1	F	421	VAL
1	F	435	VAL
1	F	460	ARG
1	F	469	LEU
1	F	498	LEU
1	F	506	ILE
1	F	533	GLN
1	F	541	ARG
1	F	547	LEU
1	F	567	ASN
1	F	581	LEU
1	F	582	LEU
1	F	601	ARG
1	F	621	PRO
1	F	622	SER
1	F	656	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	133	HIS
1	A	147	GLN
1	A	175	GLN
1	A	190	GLN
1	A	248	HIS
1	A	288	GLN
1	A	324	ASN
1	A	329	ASN
1	A	363	HIS
1	A	372	HIS
1	A	379	HIS
1	A	514	GLN
1	A	518	ASN
1	A	533	GLN
1	A	564	ASN
1	A	567	ASN
1	A	588	HIS
1	A	639	GLN
1	B	118	ASN

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Mol	Chain	Res	Type
1	B	133	HIS
1	B	175	GLN
1	B	190	GLN
1	B	218	HIS
1	B	248	HIS
1	B	288	GLN
1	B	324	ASN
1	B	329	ASN
1	B	363	HIS
1	B	372	HIS
1	B	379	HIS
1	B	514	GLN
1	B	518	ASN
1	B	533	GLN
1	B	564	ASN
1	B	567	ASN
1	B	588	HIS
1	B	639	GLN
1	C	64	HIS
1	C	118	ASN
1	C	133	HIS
1	C	147	GLN
1	C	171	GLN
1	C	175	GLN
1	C	190	GLN
1	C	238	GLN
1	C	288	GLN
1	C	324	ASN
1	C	329	ASN
1	C	363	HIS
1	C	372	HIS
1	C	379	HIS
1	C	514	GLN
1	C	518	ASN
1	C	533	GLN
1	C	564	ASN
1	C	567	ASN
1	C	588	HIS
1	C	639	GLN
1	D	118	ASN
1	D	133	HIS
1	D	147	GLN

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Mol	Chain	Res	Type
1	D	175	GLN
1	D	190	GLN
1	D	218	HIS
1	D	288	GLN
1	D	324	ASN
1	D	329	ASN
1	D	363	HIS
1	D	372	HIS
1	D	379	HIS
1	D	514	GLN
1	D	518	ASN
1	D	533	GLN
1	D	564	ASN
1	D	567	ASN
1	D	588	HIS
1	D	639	GLN
1	E	118	ASN
1	E	133	HIS
1	E	147	GLN
1	E	175	GLN
1	E	190	GLN
1	E	218	HIS
1	E	238	GLN
1	E	248	HIS
1	E	288	GLN
1	E	324	ASN
1	E	329	ASN
1	E	363	HIS
1	E	372	HIS
1	E	379	HIS
1	E	514	GLN
1	E	518	ASN
1	E	533	GLN
1	E	564	ASN
1	E	567	ASN
1	E	588	HIS
1	E	639	GLN
1	F	102	ASN
1	F	118	ASN
1	F	147	GLN
1	F	175	GLN
1	F	190	GLN

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Mol	Chain	Res	Type
1	F	218	HIS
1	F	288	GLN
1	F	324	ASN
1	F	329	ASN
1	F	363	HIS
1	F	372	HIS
1	F	379	HIS
1	F	514	GLN
1	F	518	ASN
1	F	533	GLN
1	F	564	ASN
1	F	567	ASN
1	F	588	HIS
1	F	639	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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
2	ATP	A	1001	-	24,33,33	0.61	0	31,52,52	1.37	4 (12%)
3	UGA	A	1101	-	27,39,39	0.91	1 (3%)	41,60,60	2.36	4 (9%)
2	ATP	B	1002	-	24,33,33	0.59	0	31,52,52	1.34	5 (16%)
3	UGA	B	1102	-	27,39,39	0.86	1 (3%)	41,60,60	2.34	4 (9%)
2	ATP	C	1003	-	24,33,33	0.59	0	31,52,52	1.34	5 (16%)
3	UGA	C	1103	-	27,39,39	0.91	1 (3%)	41,60,60	2.36	4 (9%)
2	ATP	D	1004	-	24,33,33	0.60	0	31,52,52	1.33	5 (16%)
3	UGA	D	1104	-	27,39,39	0.87	1 (3%)	41,60,60	2.32	4 (9%)
2	ATP	E	1005	-	24,33,33	0.59	0	31,52,52	1.34	5 (16%)
3	UGA	E	1105	-	27,39,39	0.93	1 (3%)	41,60,60	2.36	4 (9%)
2	ATP	F	1006	-	24,33,33	0.63	0	31,52,52	1.40	4 (12%)
3	UGA	F	1106	-	27,39,39	0.84	1 (3%)	41,60,60	2.33	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	1001	-	-	0/18/38/38	0/3/3/3
3	UGA	A	1101	-	-	0/17/61/61	0/3/3/3
2	ATP	B	1002	-	-	0/18/38/38	0/3/3/3
3	UGA	B	1102	-	-	0/17/61/61	0/3/3/3
2	ATP	C	1003	-	-	0/18/38/38	0/3/3/3
3	UGA	C	1103	-	-	0/17/61/61	0/3/3/3
2	ATP	D	1004	-	-	0/18/38/38	0/3/3/3
3	UGA	D	1104	-	-	0/17/61/61	0/3/3/3
2	ATP	E	1005	-	-	0/18/38/38	0/3/3/3
3	UGA	E	1105	-	-	0/17/61/61	0/3/3/3
2	ATP	F	1006	-	-	0/18/38/38	0/3/3/3
3	UGA	F	1106	-	-	0/17/61/61	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1106	UGA	C4-N3	2.59	1.37	1.33
3	C	1103	UGA	C4-N3	2.82	1.38	1.33
3	D	1104	UGA	C4-N3	2.83	1.38	1.33
3	B	1102	UGA	C4-N3	2.89	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	UGA	C4-N3	2.90	1.38	1.33
3	E	1105	UGA	C4-N3	2.96	1.38	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1006	ATP	C4'-O4'-C1'	-3.48	105.89	109.72
3	B	1102	UGA	C5-C4-N3	-3.45	114.27	123.12
3	D	1104	UGA	C5-C4-N3	-3.40	114.40	123.12
3	C	1103	UGA	C5-C4-N3	-3.37	114.47	123.12
3	E	1105	UGA	C5-C4-N3	-3.34	114.55	123.12
2	A	1001	ATP	C4'-O4'-C1'	-3.34	106.05	109.72
3	F	1106	UGA	C5-C4-N3	-3.32	114.59	123.12
3	A	1101	UGA	C5-C4-N3	-3.32	114.61	123.12
2	D	1004	ATP	C4'-O4'-C1'	-3.29	106.11	109.72
2	B	1002	ATP	C4'-O4'-C1'	-3.20	106.20	109.72
2	E	1005	ATP	C4'-O4'-C1'	-3.15	106.26	109.72
2	C	1003	ATP	C1'-N9-C4	-3.09	122.28	126.94
2	C	1003	ATP	C4'-O4'-C1'	-2.97	106.45	109.72
2	A	1001	ATP	C1'-N9-C4	-2.85	122.65	126.94
2	F	1006	ATP	C1'-N9-C4	-2.81	122.70	126.94
2	E	1005	ATP	C1'-N9-C4	-2.79	122.73	126.94
2	B	1002	ATP	C1'-N9-C4	-2.77	122.76	126.94
2	D	1004	ATP	C1'-N9-C4	-2.65	122.95	126.94
3	E	1105	UGA	C1'-O5'-C5'	2.01	115.29	112.17
2	D	1004	ATP	C2'-C1'-N9	2.06	117.44	114.29
2	E	1005	ATP	C2'-C1'-N9	2.07	117.45	114.29
3	F	1106	UGA	C1'-O5'-C5'	2.08	115.40	112.17
2	B	1002	ATP	O4'-C1'-N9	2.08	112.46	108.10
2	E	1005	ATP	O4'-C1'-N9	2.10	112.50	108.10
2	C	1003	ATP	O4'-C1'-N9	2.10	112.50	108.10
3	C	1103	UGA	C1'-O5'-C5'	2.15	115.50	112.17
2	E	1005	ATP	O3G-PG-O2G	2.15	115.57	107.38
2	F	1006	ATP	O3G-PG-O2G	2.17	115.66	107.38
2	C	1003	ATP	O3G-PG-O2G	2.18	115.67	107.38
3	A	1101	UGA	C1'-O5'-C5'	2.18	115.56	112.17
2	D	1004	ATP	O3G-PG-O2G	2.19	115.72	107.38
2	C	1003	ATP	O3A-PA-O5'	2.19	108.75	102.94
3	D	1104	UGA	C1'-O5'-C5'	2.19	115.57	112.17
2	A	1001	ATP	O3G-PG-O2G	2.21	115.78	107.38
2	B	1002	ATP	O3G-PG-O2G	2.23	115.87	107.38
3	B	1102	UGA	C1'-O5'-C5'	2.27	115.69	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1004	ATP	O4'-C1'-N9	2.29	112.89	108.10
2	B	1002	ATP	C2'-C1'-N9	2.30	117.80	114.29
2	A	1001	ATP	O4'-C1'-N9	2.35	113.02	108.10
2	F	1006	ATP	C2'-C1'-N9	2.70	118.42	114.29
3	E	1105	UGA	O5'-C1'-O3B	4.50	117.30	111.36
3	C	1103	UGA	O5'-C1'-O3B	4.56	117.38	111.36
3	D	1104	UGA	O5'-C1'-O3B	4.57	117.39	111.36
3	A	1101	UGA	O5'-C1'-O3B	4.76	117.64	111.36
3	F	1106	UGA	O5'-C1'-O3B	4.79	117.68	111.36
3	B	1102	UGA	O5'-C1'-O3B	4.81	117.71	111.36
3	F	1106	UGA	C4-N3-C2	12.70	126.72	114.14
3	B	1102	UGA	C4-N3-C2	12.76	126.78	114.14
3	D	1104	UGA	C4-N3-C2	12.83	126.84	114.14
3	C	1103	UGA	C4-N3-C2	13.01	127.02	114.14
3	E	1105	UGA	C4-N3-C2	13.03	127.05	114.14
3	A	1101	UGA	C4-N3-C2	13.06	127.07	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ATP	5	0
3	A	1101	UGA	1	0
2	B	1002	ATP	4	0
3	B	1102	UGA	1	0
2	C	1003	ATP	4	0
3	C	1103	UGA	1	0
2	D	1004	ATP	4	0
3	D	1104	UGA	1	0
2	E	1005	ATP	2	0
3	E	1105	UGA	1	0
2	F	1006	ATP	3	0
3	F	1106	UGA	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	639/660 (96%)	-0.15	1 (0%)	95 87	20, 43, 74, 90	0
1	B	639/660 (96%)	-0.15	4 (0%)	90 73	19, 43, 73, 90	0
1	C	639/660 (96%)	-0.14	5 (0%)	87 67	20, 43, 73, 90	0
1	D	644/660 (97%)	-0.11	6 (0%)	85 64	20, 44, 74, 90	0
1	E	639/660 (96%)	-0.16	2 (0%)	94 84	20, 44, 73, 90	0
1	F	639/660 (96%)	0.14	37 (5%)	26 10	19, 43, 75, 91	0
All	All	3839/3960 (96%)	-0.10	55 (1%)	78 51	19, 43, 74, 91	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	656	THR	5.9
1	D	656	THR	4.3
1	F	195	ALA	4.3
1	F	193	ASN	3.9
1	F	99	GLY	3.6
1	C	655	LEU	3.6
1	D	655	LEU	3.3
1	F	1	MET	3.3
1	F	91	GLU	3.2
1	F	203	PRO	3.1
1	F	194	GLU	3.1
1	F	90	ASP	3.1
1	F	97	PRO	2.9
1	F	43	GLY	2.9
1	F	256	PRO	2.9
1	F	105	GLY	2.8
1	F	250	HIS	2.8
1	F	121	LEU	2.8
1	D	249	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	22	ALA	2.7
1	F	211	HIS	2.7
1	B	235	VAL	2.7
1	F	131	THR	2.6
1	F	150	ILE	2.6
1	F	249	PRO	2.6
1	D	193	ASN	2.5
1	F	62	VAL	2.5
1	F	129	GLY	2.5
1	F	114	ARG	2.5
1	F	184	ASN	2.5
1	F	63	ASN	2.5
1	F	94	GLN	2.4
1	F	89	TYR	2.4
1	F	23	GLY	2.4
1	B	184	ASN	2.3
1	E	90	ASP	2.3
1	F	98	ALA	2.3
1	D	195	ALA	2.3
1	B	187	GLU	2.3
1	F	70	ARG	2.2
1	E	194	GLU	2.2
1	D	101	PHE	2.2
1	C	43	GLY	2.2
1	F	71	ILE	2.2
1	A	249	PRO	2.2
1	F	92	ILE	2.2
1	F	148	LEU	2.1
1	C	249	PRO	2.1
1	F	67	TRP	2.1
1	C	256	PRO	2.1
1	F	202	THR	2.1
1	F	271	ASP	2.0
1	F	126	THR	2.0
1	B	656	THR	2.0
1	F	270	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	UGA	B	1102	37/37	0.94	0.25	2.26	27,36,59,60	0
2	ATP	E	1005	31/31	0.91	0.25	2.26	30,42,83,83	0
3	UGA	A	1101	37/37	0.94	0.26	2.26	27,36,61,61	0
3	UGA	E	1105	37/37	0.94	0.24	2.17	30,36,60,61	0
3	UGA	D	1104	37/37	0.93	0.25	2.02	31,36,61,62	0
2	ATP	F	1006	31/31	0.92	0.23	2.00	27,40,81,82	0
2	ATP	D	1004	31/31	0.90	0.23	1.85	30,40,81,82	0
2	ATP	A	1001	31/31	0.92	0.24	1.58	28,39,82,83	0
2	ATP	B	1002	31/31	0.91	0.24	1.52	30,39,81,82	0
3	UGA	F	1106	37/37	0.93	0.24	1.43	30,36,61,61	0
3	UGA	C	1103	37/37	0.94	0.23	1.32	31,38,61,62	0
2	ATP	C	1003	31/31	0.91	0.21	1.15	32,41,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.