



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:12 AM GMT

PDB ID : 3HKC  
Title : Tubulin-ABT751: RB3 stathmin-like domain complex  
Authors : Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.  
Deposited on : 2009-05-23  
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

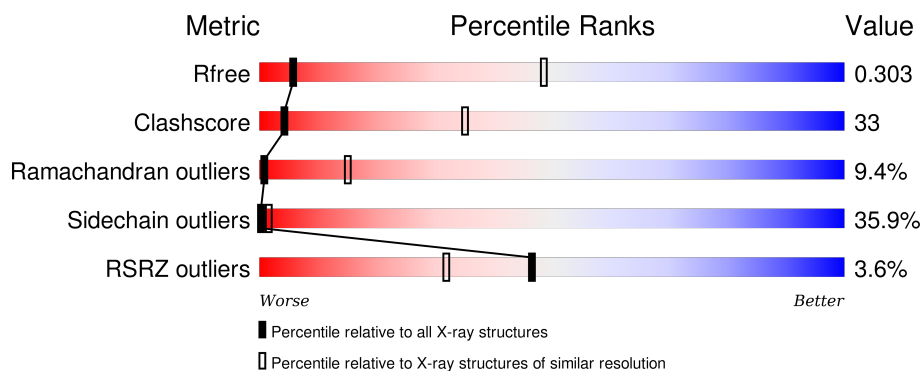
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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  $\geq 3$ , 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	451	<div> <div>4%</div> <div> <div></div> <div>39%</div> <div>39%</div> <div>14%</div> <div>5%</div> </div> </div>
1	C	451	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>35%</div> <div>15%</div> <div>5%</div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div></div> <div>29%</div> <div>40%</div> <div>23%</div> <div>6%</div> </div> </div>
2	D	445	<div> <div>3%</div> <div> <div></div> <div>29%</div> <div>42%</div> <div>20%</div> <div>6%</div> </div> </div>
3	E	142	<div> <div>0%</div> <div> <div></div> <div>35%</div> <div>37%</div> <div>13%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14145 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3300	2097	558	624	21			
1	C	428	Total	C	N	O	S	0	0	0
			3270	2078	553	619	20			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3240	2038	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3239	2038	545	632	24			

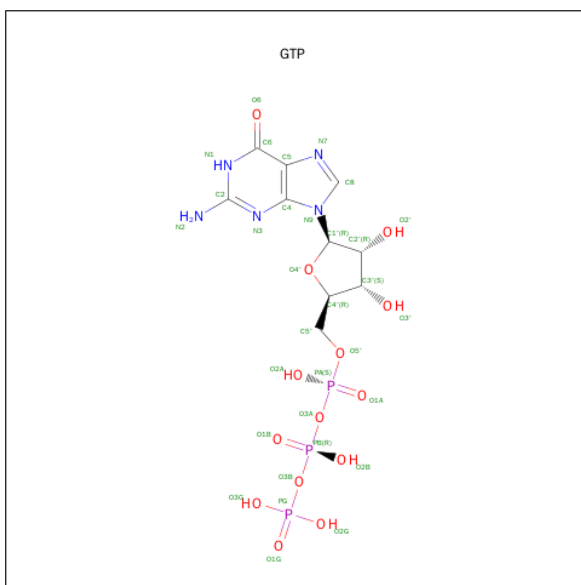
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			921	558	175	183	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

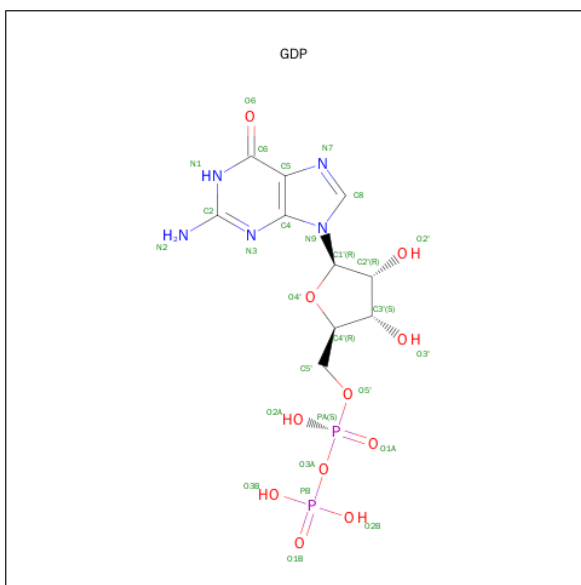


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

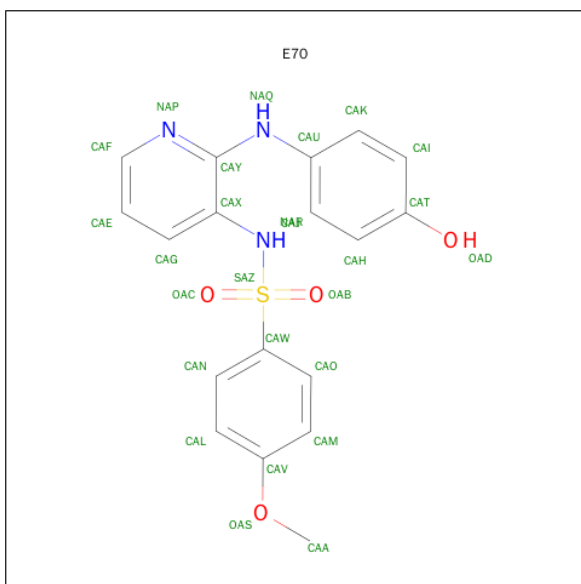
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 7 is N-{2-[4-HYDROXYPHENYL)AMINO]PYRIDIN-3-YL}-4-METHOXYBENZENESULFONAMIDE (three-letter code: E70) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>3</sub>O<sub>4</sub>S).



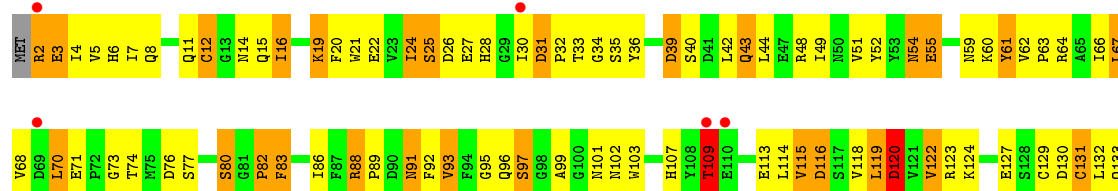
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			26	18	3	4	1		

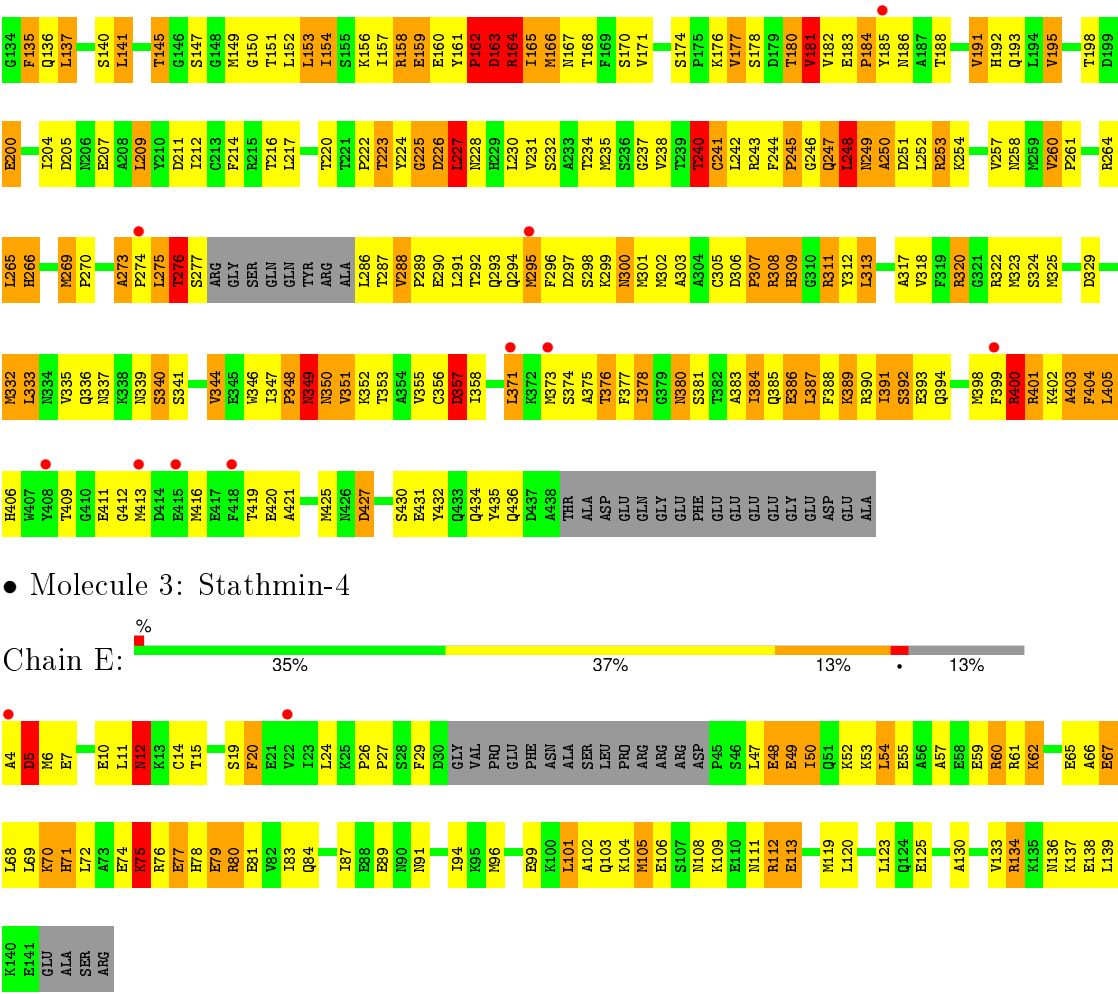
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			26	18	3	4	1		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	329.24Å 329.24Å 53.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 48.19 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-3.80) 97.6 (48.19-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.203 , 0.252 0.273 , 0.303	Depositor DCC
$R_{free}$ test set	1664 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	172.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 245.7	EDS
Estimated twinning fraction	0.068 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 33054 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GDP, GTP, MG, E70

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	0.79	0/3376	0.99	17/4588 (0.4%)
1	C	0.67	0/3344	0.91	11/4552 (0.2%)
2	B	0.68	0/3312	0.94	11/4498 (0.2%)
2	D	0.71	0/3311	0.95	10/4495 (0.2%)
3	E	0.75	0/929	0.92	2/1245 (0.2%)
All	All	0.72	0/14272	0.95	51/19378 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
2	D	0	2
3	E	0	2
All	All	0	8

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.56	126.00	118.30
1	C	211	ASP	CB-CG-OD2	8.46	125.91	118.30
1	A	76	ASP	CB-CG-OD2	8.07	125.56	118.30
1	A	120	ASP	CB-CG-OD2	7.62	125.16	118.30
1	C	120	ASP	CB-CG-OD2	7.48	125.03	118.30
2	B	205	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	397	LEU	CA-CB-CG	6.74	130.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	CB-CG-OD2	6.53	124.18	118.30
1	C	397	LEU	CA-CB-CG	6.52	130.31	115.30
1	A	266	HIS	CB-CA-C	-6.49	97.43	110.40
2	D	164	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	20	CYS	CA-CB-SG	6.45	125.61	114.00
2	D	120	ASP	CB-CG-OD2	6.35	124.02	118.30
2	B	116	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	160	ASP	CB-CG-OD2	6.24	123.92	118.30
2	B	39	ASP	CB-CG-OD2	6.19	123.87	118.30
2	D	427	ASP	CB-CG-OD2	6.18	123.86	118.30
2	D	226	ASP	CB-CG-OD2	6.11	123.80	118.30
2	D	163	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	266	HIS	CB-CA-C	-6.10	98.20	110.40
1	C	76	ASP	CB-CG-OD2	6.05	123.74	118.30
2	B	357	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	116	ASP	CB-CG-OD2	5.92	123.62	118.30
2	D	357	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	248	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	116	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	33	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	121	ARG	NE-CZ-NH1	5.77	123.19	120.30
2	D	39	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	160	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	297	ASP	CB-CG-OD2	5.61	123.35	118.30
3	E	54	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	269	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	127	ASP	CB-CG-OD2	5.48	123.23	118.30
2	D	164	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	251	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	322	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	392	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	269	LEU	CA-CB-CG	5.24	127.35	115.30
3	E	6	MET	N-CA-C	5.24	125.15	111.00
2	B	211	ASP	CB-CG-OD2	5.22	123.00	118.30
2	D	297	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	424	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	322	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	69	ASP	CB-CG-OD2	5.16	122.95	118.30
2	B	90	ASP	CB-CG-OD2	5.13	122.91	118.30
2	D	26	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	392	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	431	ASP	CB-CG-OD2	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	387	LEU	CA-CB-CG	5.08	126.98	115.30
2	B	306	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	HIS	Peptide
1	A	82	THR	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	D	162	PRO	Peptide
2	D	248	LEU	Peptide
3	E	5	ASP	Peptide
3	E	50	ILE	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	3169	185	0
1	C	3270	0	3122	180	0
2	B	3240	0	3056	269	0
2	D	3239	0	3058	269	0
3	E	921	0	814	41	0
4	A	32	0	12	4	0
4	C	32	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	3	0
6	D	28	0	12	4	0
7	B	26	0	17	5	0
7	D	26	0	17	5	0
All	All	14145	0	13301	912	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 33.

All (912) 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:E:105:MET:SD	3:E:105:MET:CE	2.03	1.44
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.16
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.25	1.15
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.22	1.15
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.17	1.15
2:D:11:GLN:HG3	2:D:74:THR:CG2	1.77	1.13
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.18	1.12
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.77	1.11
2:B:11:GLN:HG3	2:B:74:THR:CG2	1.80	1.11
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.16	1.11
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.25	1.10
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.28	1.10
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.80	1.09
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.13	1.09
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.28	1.08
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.29	1.07
1:C:90:GLU:O	1:C:121:ARG:HD3	1.57	1.05
2:D:99:ALA:HB1	2:D:145:THR:CG2	1.86	1.04
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.04	1.03
2:D:151:THR:HB	2:D:193:GLN:HG2	1.37	1.03
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.91	1.01
2:B:250:ALA:HB1	7:B:700:E70:HAJ	1.44	1.00
2:D:11:GLN:CG	2:D:74:THR:HG21	1.91	0.99
2:B:223:THR:HB	2:B:225:GLY:H	1.27	0.99
2:D:250:ALA:HB1	7:D:700:E70:HAJ	1.45	0.98
1:A:90:GLU:O	1:A:121:ARG:HD3	1.62	0.98
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.46	0.97
2:D:223:THR:HB	2:D:225:GLY:H	1.30	0.96
2:D:251:ASP:HB2	2:D:254:LYS:H	1.31	0.95
1:A:247:ALA:HB1	3:E:19:SER:CB	1.97	0.95
2:B:251:ASP:HB2	2:B:254:LYS:H	1.32	0.95
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.15	0.94
2:D:11:GLN:HG3	2:D:74:THR:HG21	0.95	0.94
1:A:273:ALA:HB3	1:A:274:PRO:CD	1.99	0.93
1:A:181:VAL:H	2:B:258:ASN:HD21	1.16	0.93
1:C:206:ASN:HD21	4:C:600:GTP:HN22	1.08	0.93
2:D:412:GLY:O	3:E:133:VAL:HB	1.69	0.93
2:B:167:ASN:HD22	2:B:252:LEU:HD11	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.48	0.93
3:E:57:ALA:HA	3:E:60:ARG:NH1	1.84	0.91
1:C:99:ALA:HB2	1:C:145:THR:CG2	2.01	0.91
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.00	0.91
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.01	0.91
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.52	0.91
2:B:11:GLN:CG	2:B:74:THR:HG21	1.99	0.91
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.02	0.90
2:B:54:ASN:ND2	2:B:64:ARG:HD2	1.88	0.90
1:A:229:ARG:HH11	1:A:229:ARG:HG2	1.36	0.89
1:A:296:PHE:O	1:A:339:ARG:NH2	2.06	0.89
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.37	0.89
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.54	0.88
2:B:223:THR:HB	2:B:225:GLY:N	1.88	0.88
3:E:57:ALA:HA	3:E:60:ARG:HH12	1.39	0.88
2:B:179:ASP:HB2	1:C:248:LEU:HD21	1.55	0.88
1:C:273:ALA:CB	1:C:375:VAL:H	1.87	0.87
2:D:273:ALA:CB	2:D:274:PRO:CD	2.52	0.87
2:B:273:ALA:CB	2:B:274:PRO:CD	2.53	0.87
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.55	0.86
1:A:273:ALA:CB	1:A:375:VAL:H	1.88	0.86
2:B:401:ARG:NH2	1:C:434:GLU:O	2.09	0.86
2:B:165:ILE:CD1	2:B:252:LEU:HG	2.06	0.86
1:A:99:ALA:CB	1:A:145:THR:HG22	2.02	0.86
2:B:54:ASN:HD22	2:B:64:ARG:HD2	1.38	0.85
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.06	0.85
2:B:306:ASP:O	2:B:308:ARG:N	2.07	0.85
1:A:273:ALA:CB	1:A:274:PRO:CD	2.56	0.83
1:C:199:ASP:HB3	1:C:256:GLN:HE22	1.40	0.83
3:E:48:GLU:HG3	3:E:49:GLU:N	1.92	0.83
1:A:278:ALA:O	1:A:279:GLU:HB3	1.76	0.83
2:B:151:THR:HB	2:B:193:GLN:HG2	1.59	0.83
2:B:245:PRO:HG2	2:B:246:GLY:H	1.44	0.83
2:D:162:PRO:HD2	2:D:163:ASP:HB2	1.60	0.82
2:D:135:PHE:HB2	2:D:166:MET:CE	2.09	0.82
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.60	0.81
3:E:76:ARG:O	3:E:78:HIS:N	2.13	0.81
1:C:99:ALA:CB	1:C:145:THR:HG22	2.07	0.81
2:D:145:THR:HG23	6:D:600:GDP:O3B	1.81	0.81
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.63	0.81
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:LEU:O	2:B:276:THR:HB	1.80	0.81
2:D:165:ILE:CD1	2:D:252:LEU:HG	2.08	0.81
1:A:260:VAL:O	1:A:260:VAL:CG2	2.30	0.80
1:A:99:ALA:HB2	1:A:145:THR:CG2	2.07	0.80
2:D:223:THR:HB	2:D:225:GLY:N	1.96	0.80
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.80	0.79
2:D:350:ASN:H	2:D:350:ASN:HD22	1.26	0.79
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.64	0.79
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.64	0.78
2:D:273:ALA:HB1	2:D:274:PRO:HD3	1.64	0.78
2:B:114:LEU:O	2:B:116:ASP:N	2.17	0.78
1:A:181:VAL:H	2:B:258:ASN:ND2	1.82	0.78
1:A:315:CYS:SG	1:A:377:MET:CE	2.72	0.77
1:C:153:LEU:HD13	1:C:157:LEU:HD11	1.66	0.77
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.67	0.77
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.67	0.76
7:D:700:E70:NAP	7:D:700:E70:HAK	1.98	0.76
2:B:385:GLN:HE21	2:B:389:LYS:HD2	1.50	0.76
1:C:265:ILE:HD12	1:C:265:ILE:H	1.51	0.76
2:D:385:GLN:HE21	2:D:389:LYS:HD2	1.50	0.76
2:B:403:ALA:O	2:B:405:LEU:N	2.18	0.76
2:B:135:PHE:HZ	2:B:161:TYR:CD1	2.03	0.76
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.16	0.75
2:D:204:ILE:H	2:D:204:ILE:HD12	1.52	0.75
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.67	0.75
2:D:36:TYR:OH	2:D:40:SER:O	2.05	0.75
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.69	0.75
2:D:275:LEU:O	2:D:276:THR:HB	1.86	0.75
1:C:191:THR:HG23	1:C:425:MET:CE	2.17	0.75
2:B:2:ARG:O	2:B:3:GLU:HB2	1.85	0.75
2:B:251:ASP:C	2:B:253:ARG:H	1.89	0.75
1:A:266:HIS:O	1:A:268:PRO:HD3	1.87	0.75
2:D:306:ASP:O	2:D:308:ARG:N	2.14	0.74
2:D:245:PRO:HG2	2:D:246:GLY:H	1.53	0.74
2:D:135:PHE:HZ	2:D:161:TYR:CD1	2.04	0.74
2:D:114:LEU:O	2:D:116:ASP:N	2.19	0.74
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.03	0.74
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.70	0.74
1:A:34:GLY:O	1:A:61:HIS:HB2	1.88	0.74
1:C:182:VAL:CG2	1:C:408:TYR:OH	2.36	0.74
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:HD2	1:A:87:PHE:N	1.85	0.73
2:D:387:LEU:HD23	2:D:388:PHE:N	2.04	0.73
2:B:350:ASN:HD22	2:B:350:ASN:H	1.33	0.73
1:C:266:HIS:O	1:C:268:PRO:HD3	1.88	0.73
2:D:135:PHE:CZ	2:D:161:TYR:CD1	2.76	0.73
2:B:165:ILE:HD11	2:B:252:LEU:CG	2.13	0.72
1:A:190:THR:HG23	1:A:191:THR:H	1.54	0.72
1:C:181:VAL:H	2:D:258:ASN:HD21	1.34	0.72
2:B:135:PHE:CZ	2:B:161:TYR:CD1	2.77	0.72
2:B:391:ILE:HG13	2:B:392:SER:N	2.05	0.72
2:D:167:ASN:HD22	2:D:252:LEU:HD11	1.54	0.72
2:D:391:ILE:HG13	2:D:392:SER:N	2.03	0.72
2:B:251:ASP:O	2:B:253:ARG:N	2.23	0.72
1:C:90:GLU:O	1:C:121:ARG:CD	2.36	0.72
2:B:135:PHE:HB2	2:B:166:MET:CE	2.20	0.71
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.54	0.71
2:B:70:LEU:HD12	2:B:145:THR:HB	1.71	0.71
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.72	0.71
3:E:76:ARG:C	3:E:78:HIS:H	1.93	0.71
1:A:87:PHE:N	1:A:87:PHE:CD2	2.56	0.71
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.25	0.71
2:B:223:THR:CB	2:B:225:GLY:H	2.03	0.71
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.55	0.71
2:B:145:THR:HG23	6:B:600:GDP:O3B	1.90	0.71
3:E:48:GLU:O	3:E:50:ILE:N	2.23	0.71
3:E:10:GLU:HG3	3:E:20:PHE:HB3	1.71	0.71
2:D:20:PHE:O	2:D:24:ILE:HG23	1.90	0.71
2:D:145:THR:HG23	6:D:600:GDP:PB	2.31	0.70
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.73	0.70
1:A:265:ILE:H	1:A:265:ILE:HD12	1.55	0.70
1:C:341:ILE:HD13	1:C:341:ILE:H	1.55	0.70
2:D:241:CYS:HB3	2:D:247:GLN:HE21	1.55	0.70
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.71	0.70
1:A:182:VAL:CG2	1:A:408:TYR:OH	2.39	0.70
1:C:79:ARG:HH22	1:C:94:THR:CG2	2.04	0.70
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.74	0.70
1:A:315:CYS:SG	1:A:377:MET:HE2	2.32	0.70
1:C:79:ARG:NH2	1:C:94:THR:HG21	2.07	0.69
2:D:223:THR:CB	2:D:225:GLY:H	2.05	0.69
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.56	0.69
2:B:22:GLU:OE1	2:B:82:PRO:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:O	1:C:346:TRP:HE3	1.76	0.69
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.73	0.69
2:D:164:ARG:NH2	2:D:253:ARG:HH22	1.90	0.69
2:D:307:PRO:CB	2:D:312:TYR:OH	2.41	0.69
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.23	0.69
2:D:287:THR:CG2	2:D:290:GLU:HB2	2.22	0.69
1:A:339:ARG:HG3	1:A:340:THR:H	1.57	0.69
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.73	0.69
2:D:226:ASP:O	2:D:227:LEU:HB3	1.92	0.69
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.69
2:D:54:ASN:ND2	2:D:64:ARG:HD2	2.08	0.68
1:A:315:CYS:SG	1:A:377:MET:HE1	2.33	0.68
1:A:190:THR:HG23	1:A:191:THR:N	2.08	0.68
1:A:368:LEU:H	1:A:368:LEU:HD12	1.56	0.68
1:A:246:GLY:O	1:A:247:ALA:O	2.11	0.68
1:A:346:TRP:O	1:A:346:TRP:HE3	1.76	0.68
1:C:34:GLY:O	1:C:61:HIS:HB2	1.93	0.68
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.28	0.68
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.76	0.68
1:A:229:ARG:HH11	1:A:229:ARG:CG	2.04	0.68
1:A:106:GLY:O	1:A:111:GLY:HA3	1.93	0.68
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.76	0.68
1:A:273:ALA:HB2	1:A:375:VAL:H	1.57	0.67
2:B:241:CYS:HB3	2:B:247:GLN:HE21	1.57	0.67
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.76	0.67
2:B:54:ASN:HD22	2:B:64:ARG:CD	2.07	0.67
2:B:20:PHE:O	2:B:24:ILE:HG23	1.94	0.67
2:D:158:ARG:O	2:D:159:GLU:HB3	1.93	0.67
2:B:21:TRP:O	2:B:25:SER:HB2	1.94	0.67
2:B:167:ASN:ND2	2:B:252:LEU:HD11	2.09	0.67
1:A:206:ASN:HD21	4:A:600:GTP:N2	1.89	0.67
3:E:133:VAL:HA	3:E:136:ASN:HB3	1.77	0.67
1:C:315:CYS:SG	1:C:377:MET:CE	2.82	0.67
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.60	0.67
1:C:190:THR:HG23	1:C:191:THR:H	1.59	0.67
1:A:87:PHE:H	1:A:87:PHE:HD2	1.41	0.67
2:D:226:ASP:O	2:D:227:LEU:CB	2.43	0.67
2:B:204:ILE:H	2:B:204:ILE:HD12	1.60	0.67
2:D:251:ASP:C	2:D:253:ARG:H	1.97	0.66
1:A:247:ALA:HA	3:E:12:ASN:OD1	1.94	0.66
1:A:398:MET:HG3	2:B:348:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.59	0.66
7:B:700:E70:NAP	7:B:700:E70:HAK	2.10	0.66
2:D:99:ALA:CB	2:D:145:THR:CG2	2.71	0.66
2:B:336:GLN:HE22	2:B:351:VAL:HG12	1.59	0.66
2:D:247:GLN:HG3	2:D:248:LEU:H	1.60	0.66
1:A:248:LEU:HD22	1:A:249:ASN:ND2	2.11	0.66
2:D:2:ARG:O	2:D:3:GLU:HB2	1.96	0.66
2:D:247:GLN:CG	2:D:248:LEU:H	2.08	0.66
2:D:51:VAL:HG12	2:D:52:TYR:CD1	2.31	0.66
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.76	0.66
2:D:307:PRO:HB2	2:D:312:TYR:OH	1.96	0.66
2:B:51:VAL:HG12	2:B:52:TYR:CD1	2.30	0.66
3:E:67:GLU:C	3:E:69:LEU:H	1.98	0.65
1:C:191:THR:HG23	1:C:425:MET:HE1	1.79	0.65
1:A:2:ARG:NH1	1:A:2:ARG:HA	2.12	0.65
2:B:265:LEU:HB3	2:B:432:TYR:CE2	2.32	0.65
2:D:306:ASP:C	2:D:308:ARG:H	2.00	0.65
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.77	0.65
3:E:130:ALA:O	3:E:134:ARG:HB3	1.96	0.65
1:C:261:PRO:HB2	1:C:262:TYR:CD1	2.32	0.65
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.79	0.64
2:D:205:ASP:OD1	2:D:207:GLU:HB3	1.97	0.64
2:D:336:GLN:HE22	2:D:351:VAL:HG12	1.62	0.64
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.90	0.64
2:D:403:ALA:O	2:D:405:LEU:N	2.31	0.64
1:C:87:PHE:HD2	1:C:87:PHE:N	1.96	0.64
2:B:36:TYR:OH	2:B:40:SER:O	2.13	0.64
2:B:251:ASP:C	2:B:253:ARG:N	2.50	0.64
2:B:404:PHE:CE1	1:C:261:PRO:HB3	2.33	0.64
1:C:430:LYS:O	1:C:434:GLU:HB2	1.97	0.63
3:E:70:LYS:HG2	3:E:70:LYS:O	1.97	0.63
1:A:246:GLY:HA2	3:E:14:CYS:SG	2.38	0.63
1:C:229:ARG:CG	1:C:229:ARG:HH11	2.10	0.63
1:C:251:ASP:OD1	1:C:252:LEU:N	2.30	0.63
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.39	0.63
2:B:140:SER:HA	2:B:171:VAL:HG23	1.80	0.63
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.80	0.63
2:D:54:ASN:HD22	2:D:64:ARG:HD2	1.61	0.63
2:D:298:SER:C	2:D:300:ASN:H	2.01	0.63
1:A:264:ARG:NH1	1:A:431:ASP:OD2	2.31	0.63
2:B:54:ASN:ND2	2:B:64:ARG:CD	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:O	2:D:25:SER:HB2	1.99	0.62
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.14	0.62
2:B:205:ASP:OD1	2:B:207:GLU:HB3	1.98	0.62
1:C:273:ALA:HB2	1:C:375:VAL:H	1.62	0.62
1:A:190:THR:CG2	1:A:191:THR:H	2.12	0.62
1:C:87:PHE:CD2	1:C:87:PHE:N	2.65	0.62
2:B:145:THR:HG23	6:B:600:GDP:PB	2.40	0.62
2:B:414:ASP:HB3	2:B:416:MET:HE3	1.82	0.62
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.64	0.62
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.82	0.62
2:D:191:VAL:CG1	2:D:425:MET:HG3	2.29	0.62
2:B:164:ARG:NH2	2:B:253:ARG:HH22	1.98	0.62
2:B:247:GLN:CG	2:B:248:LEU:H	2.13	0.62
1:A:153:LEU:HD13	1:A:157:LEU:HD11	1.81	0.62
2:D:251:ASP:HB2	2:D:254:LYS:HB2	1.81	0.61
2:D:311:ARG:HD3	2:D:436:GLN:HG2	1.81	0.61
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.82	0.61
2:B:312:TYR:HE2	2:B:377:PHE:HZ	1.47	0.61
2:B:350:ASN:HD22	2:B:350:ASN:N	1.97	0.61
1:C:405:VAL:CG1	1:C:406:HIS:N	2.62	0.61
3:E:76:ARG:O	3:E:79:GLU:N	2.33	0.61
2:B:162:PRO:HD2	2:B:163:ASP:HB2	1.81	0.61
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.81	0.61
2:D:165:ILE:HD11	2:D:252:LEU:CG	2.18	0.61
1:A:412:GLY:O	3:E:60:ARG:NH1	2.33	0.61
2:B:114:LEU:HB3	2:B:149:MET:HE2	1.83	0.61
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.82	0.61
2:B:251:ASP:HB2	2:B:254:LYS:HB2	1.81	0.61
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.83	0.60
1:C:315:CYS:SG	1:C:377:MET:HE2	2.41	0.60
1:A:248:LEU:HD12	1:A:354:GLY:HA3	1.83	0.60
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.28	0.60
3:E:80:ARG:HH21	3:E:84:GLN:HG2	1.65	0.60
2:D:70:LEU:HD12	2:D:145:THR:HB	1.83	0.60
1:A:260:VAL:O	1:A:260:VAL:HG23	2.01	0.60
1:A:190:THR:O	1:A:192:HIS:N	2.35	0.60
1:C:190:THR:HG23	1:C:191:THR:N	2.15	0.60
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.83	0.60
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.14	0.60
1:C:260:VAL:O	1:C:260:VAL:HG23	2.01	0.60
2:D:241:CYS:HB3	2:D:247:GLN:NE2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:83:ILE:O	3:E:87:ILE:HD12	2.01	0.60
2:D:158:ARG:O	2:D:159:GLU:CB	2.49	0.60
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.82	0.60
2:B:226:ASP:O	2:B:227:LEU:CB	2.50	0.60
1:C:190:THR:CG2	1:C:191:THR:H	2.15	0.60
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.66	0.60
2:B:88:ARG:HG3	2:B:89:PRO:HD2	1.84	0.60
2:D:337:ASN:HA	2:D:340:SER:HB3	1.84	0.59
1:C:368:LEU:H	1:C:368:LEU:HD12	1.67	0.59
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.37	0.59
1:A:71:GLU:OE2	4:A:600:GTP:O1G	2.20	0.59
2:D:251:ASP:O	2:D:253:ARG:N	2.33	0.59
2:D:150:GLY:O	2:D:154:ILE:HG23	2.01	0.59
2:D:251:ASP:C	2:D:253:ARG:N	2.55	0.59
1:C:199:ASP:HB3	1:C:256:GLN:NE2	2.14	0.59
2:B:403:ALA:C	2:B:405:LEU:H	2.06	0.58
2:D:204:ILE:N	2:D:204:ILE:HD12	2.17	0.58
1:A:217:LEU:O	1:A:218:ASP:HB3	2.03	0.58
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.02	0.58
3:E:101:LEU:O	3:E:103:GLN:N	2.27	0.58
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.69	0.58
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.67	0.58
1:A:86:LEU:HB3	1:A:87:PHE:HD2	1.67	0.58
2:D:298:SER:O	2:D:300:ASN:N	2.35	0.58
2:D:237:GLY:CA	2:D:376:THR:HG21	2.34	0.58
1:A:407:TRP:CG	2:B:257:VAL:HG23	2.38	0.58
1:A:2:ARG:HB2	1:A:131:GLY:O	2.03	0.58
1:A:77:GLU:O	1:A:80:THR:HG22	2.03	0.58
1:A:260:VAL:O	1:A:260:VAL:HG22	2.02	0.58
2:B:387:LEU:HD23	2:B:388:PHE:N	2.18	0.58
2:B:245:PRO:HG3	2:B:247:GLN:CD	2.23	0.58
2:B:357:ASP:OD2	2:B:357:ASP:N	2.35	0.58
2:B:336:GLN:NE2	2:B:351:VAL:CG1	2.67	0.58
2:D:435:TYR:O	2:D:436:GLN:HG3	2.02	0.58
2:B:298:SER:C	2:B:300:ASN:H	2.07	0.58
1:A:340:THR:HG22	1:A:340:THR:O	2.02	0.58
2:B:306:ASP:C	2:B:308:ARG:H	2.02	0.58
1:A:430:LYS:O	1:A:434:GLU:HB2	2.04	0.58
2:B:311:ARG:HD3	2:B:436:GLN:HG2	1.86	0.58
1:C:315:CYS:SG	1:C:377:MET:HE1	2.44	0.58
1:C:256:GLN:C	1:C:258:ASN:N	2.55	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:114:LEU:HB3	2:D:149:MET:HE2	1.85	0.57
1:C:270:ALA:O	1:C:302:MET:HB2	2.03	0.57
1:C:182:VAL:HG21	1:C:408:TYR:OH	2.03	0.57
2:B:237:GLY:CA	2:B:376:THR:HG21	2.33	0.57
1:C:108:TYR:O	1:C:112:LYS:HB2	2.04	0.57
1:C:139:HIS:CG	1:C:150:THR:HG21	2.40	0.57
2:D:273:ALA:CB	2:D:375:ALA:H	2.17	0.57
2:B:3:GLU:HG2	2:B:64:ARG:NH2	2.19	0.57
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.45	0.57
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.85	0.57
2:B:179:ASP:CB	1:C:248:LEU:HD21	2.31	0.57
1:C:105:ARG:NH2	2:D:253:ARG:HH21	2.02	0.57
2:B:115:VAL:HG12	2:B:116:ASP:N	2.19	0.57
1:C:313:MET:HG2	1:C:380:ASN:O	2.05	0.57
1:C:291:ILE:HD12	1:C:375:VAL:HG23	1.87	0.57
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.50	0.57
2:B:407:TRP:CE2	1:C:257:THR:HA	2.40	0.57
2:B:241:CYS:HB3	2:B:247:GLN:NE2	2.19	0.56
2:D:401:ARG:NH1	2:D:401:ARG:HG3	2.20	0.56
1:C:106:GLY:O	1:C:111:GLY:HA3	2.04	0.56
1:C:105:ARG:CZ	2:D:253:ARG:HH21	2.18	0.56
1:A:178:SER:OG	2:B:352:LYS:HE3	2.05	0.56
1:C:133:GLN:NE2	1:C:252:LEU:HB2	2.19	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.40	0.56
1:C:105:ARG:NH1	2:D:253:ARG:HH21	2.02	0.56
2:D:308:ARG:NH1	2:D:308:ARG:HG3	2.20	0.56
1:A:172:TYR:HE2	1:A:391:LEU:HD22	1.70	0.56
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.40	0.56
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.18	0.56
3:E:112:ARG:HG2	3:E:113:GLU:N	2.20	0.56
2:D:404:PHE:N	2:D:404:PHE:CD1	2.73	0.56
1:A:420:GLU:HG2	1:A:420:GLU:O	2.05	0.56
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.87	0.56
2:D:404:PHE:HD1	2:D:404:PHE:N	2.03	0.56
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.05	0.56
2:B:229:HIS:CE1	2:B:277:SER:HB3	2.40	0.56
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.35	0.56
2:D:135:PHE:CD1	2:D:135:PHE:N	2.74	0.56
2:D:312:TYR:HE2	2:D:377:PHE:HZ	1.54	0.56
1:C:71:GLU:OE2	4:C:600:GTP:O1G	2.23	0.56
2:D:245:PRO:HG3	2:D:247:GLN:CD	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.37	0.56
2:D:3:GLU:HG2	2:D:64:ARG:NH2	2.21	0.55
2:B:204:ILE:N	2:B:204:ILE:HD12	2.21	0.55
2:B:352:LYS:HG3	7:B:700:E70:HAM	1.89	0.55
2:D:401:ARG:HH11	2:D:401:ARG:HG3	1.72	0.55
2:B:102:ASN:OD1	2:B:102:ASN:O	2.24	0.55
7:D:700:E70:NAP	7:D:700:E70:CAK	2.67	0.55
1:A:105:ARG:NH2	2:B:253:ARG:HH21	2.04	0.55
1:A:3:GLU:HB2	1:A:132:LEU:HA	1.88	0.55
2:D:320:ARG:HA	2:D:356:CYS:O	2.06	0.55
2:B:435:TYR:O	2:B:436:GLN:HG3	2.06	0.55
1:A:312:TYR:HE2	1:A:379:SER:CB	2.18	0.55
1:C:105:ARG:HH22	2:D:253:ARG:NH2	2.04	0.55
2:B:8:GLN:HG2	2:B:14:ASN:HA	1.89	0.55
2:B:399:PHE:O	2:B:400:ARG:O	2.24	0.55
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.55
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.32	0.55
2:D:385:GLN:HE21	2:D:389:LYS:CD	2.20	0.55
2:B:171:VAL:HG12	2:B:204:ILE:HB	1.88	0.55
2:D:135:PHE:HB2	2:D:166:MET:HE2	1.87	0.55
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.54	0.55
2:B:348:PRO:O	2:B:350:ASN:N	2.39	0.55
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.42	0.55
1:C:103:TYR:O	1:C:104:ALA:C	2.41	0.55
2:B:337:ASN:HA	2:B:340:SER:HB3	1.89	0.55
2:B:344:VAL:HG22	2:B:346:TRP:NE1	2.22	0.55
1:C:107:HIS:HD2	1:C:108:TYR:CE2	2.25	0.55
2:D:16:ILE:HG23	2:D:235:MET:CE	2.37	0.54
2:D:164:ARG:HA	2:D:164:ARG:HE	1.71	0.54
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.29	0.54
2:B:247:GLN:HG3	2:B:248:LEU:H	1.72	0.54
2:B:226:ASP:O	2:B:227:LEU:HB3	2.06	0.54
1:A:12:ALA:O	1:A:13:GLY:C	2.46	0.54
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.89	0.54
1:A:182:VAL:HG21	1:A:408:TYR:OH	2.05	0.54
2:D:336:GLN:NE2	2:D:351:VAL:CG1	2.71	0.54
1:A:311:LYS:HD2	1:A:437:VAL:CB	2.37	0.54
1:C:273:ALA:CB	1:C:274:PRO:CD	2.65	0.54
2:B:407:TRP:NE1	1:C:257:THR:HA	2.22	0.54
2:B:308:ARG:HH11	2:B:308:ARG:HG3	1.73	0.54
2:B:22:GLU:OE1	2:B:82:PRO:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:O	1:A:396:ASP:C	2.46	0.54
2:B:167:ASN:HD22	2:B:252:LEU:CD1	2.14	0.54
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.43	0.54
2:B:308:ARG:NH1	2:B:308:ARG:HG3	2.22	0.54
2:D:151:THR:O	2:D:154:ILE:HD13	2.08	0.53
1:A:346:TRP:CE3	1:A:346:TRP:O	2.60	0.53
2:D:88:ARG:O	2:D:91:ASN:HB2	2.08	0.53
2:D:295:MET:CG	2:D:377:PHE:HB2	2.38	0.53
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.89	0.53
2:D:54:ASN:HD22	2:D:64:ARG:CD	2.21	0.53
2:B:7:ILE:O	2:B:137:LEU:HA	2.07	0.53
1:C:420:GLU:O	1:C:420:GLU:HG2	2.07	0.53
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.35	0.53
2:D:350:ASN:HD22	2:D:350:ASN:N	1.97	0.53
1:C:181:VAL:H	2:D:258:ASN:ND2	2.05	0.53
2:D:177:VAL:CG1	2:D:177:VAL:O	2.56	0.53
2:D:8:GLN:HG2	2:D:14:ASN:HA	1.91	0.53
2:B:385:GLN:HE21	2:B:389:LYS:CD	2.21	0.53
2:D:93:VAL:HG12	2:D:114:LEU:HD11	1.89	0.53
2:D:32:PRO:O	2:D:86:ILE:HD12	2.09	0.53
2:B:16:ILE:HG23	2:B:235:MET:CE	2.39	0.53
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.21	0.53
2:D:344:VAL:HG22	2:D:346:TRP:NE1	2.24	0.53
1:C:128:GLN:HG2	1:C:128:GLN:O	2.09	0.53
1:C:178:SER:OG	2:D:352:LYS:HE3	2.08	0.53
2:D:192:HIS:O	2:D:195:VAL:HG12	2.09	0.53
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.43	0.53
1:C:340:THR:HG22	1:C:340:THR:O	2.09	0.53
1:C:39:ASP:O	1:C:40:LYS:CB	2.57	0.53
3:E:19:SER:O	3:E:20:PHE:HB3	2.08	0.53
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.91	0.53
2:D:115:VAL:HG12	2:D:116:ASP:N	2.24	0.53
1:A:79:ARG:NH2	1:A:94:THR:HG21	2.24	0.53
2:D:181:VAL:HG21	2:D:404:PHE:HE2	1.74	0.53
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.44	0.52
1:C:239:THR:HB	1:C:243:ARG:HH11	1.74	0.52
2:D:140:SER:HA	2:D:171:VAL:HG23	1.91	0.52
2:B:177:VAL:CG1	2:B:177:VAL:O	2.57	0.52
2:B:251:ASP:HB2	2:B:254:LYS:N	2.14	0.52
2:B:151:THR:O	2:B:154:ILE:HD13	2.09	0.52
2:D:309:HIS:H	2:D:309:HIS:CD2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG13	1:A:93:ILE:HB	1.91	0.52
2:D:251:ASP:HB2	2:D:254:LYS:N	2.12	0.52
1:C:86:LEU:HB3	1:C:87:PHE:HD2	1.74	0.52
2:B:99:ALA:CB	2:B:145:THR:CG2	2.83	0.52
1:A:270:ALA:HB3	1:A:302:MET:CE	2.39	0.52
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.10	0.52
1:C:3:GLU:HB2	1:C:132:LEU:HA	1.92	0.52
1:C:384:ILE:O	1:C:384:ILE:CG1	2.58	0.52
2:D:225:GLY:O	2:D:228:ASN:N	2.40	0.52
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.40	0.52
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.90	0.52
1:C:49:PHE:H	1:C:49:PHE:HD2	1.57	0.52
1:C:87:PHE:HD2	1:C:87:PHE:H	1.55	0.52
2:D:251:ASP:O	2:D:252:LEU:HB3	2.10	0.52
2:B:245:PRO:CG	2:B:246:GLY:H	2.10	0.52
2:B:158:ARG:O	2:B:159:GLU:CB	2.57	0.52
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.51	0.51
2:B:404:PHE:N	2:B:404:PHE:CD1	2.77	0.51
2:D:88:ARG:HG3	2:D:89:PRO:HD2	1.92	0.51
2:D:22:GLU:OE1	2:D:82:PRO:HB2	2.11	0.51
1:A:191:THR:HG23	1:A:425:MET:CE	2.40	0.51
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.75	0.51
1:A:72:PRO:O	1:A:74:VAL:N	2.42	0.51
2:D:336:GLN:NE2	2:D:351:VAL:HG12	2.26	0.51
2:B:88:ARG:HG2	2:B:88:ARG:HH11	1.75	0.51
1:C:12:ALA:O	1:C:13:GLY:C	2.48	0.51
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.45	0.51
1:C:191:THR:HG23	1:C:425:MET:HE3	1.91	0.51
1:C:346:TRP:O	1:C:346:TRP:CE3	2.60	0.51
1:A:350:GLY:O	1:A:351:PHE:HB2	2.11	0.51
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.10	0.51
1:C:229:ARG:CG	1:C:229:ARG:NH1	2.72	0.51
1:A:190:THR:CG2	1:A:191:THR:N	2.71	0.51
1:A:310:GLY:HA3	1:A:383:ALA:HB2	1.92	0.51
2:B:229:HIS:ND1	2:B:277:SER:HB3	2.26	0.51
1:A:274:PRO:HG3	1:A:291:ILE:HG21	1.91	0.51
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.93	0.51
2:D:167:ASN:HD22	2:D:252:LEU:CD1	2.23	0.51
1:C:264:ARG:O	1:C:266:HIS:N	2.43	0.51
1:A:270:ALA:O	1:A:302:MET:HB2	2.11	0.51
2:B:309:HIS:CD2	2:B:309:HIS:H	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD22	1:A:110:ILE:HG23	1.93	0.51
3:E:74:GLU:C	3:E:76:ARG:H	2.14	0.51
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.92	0.51
1:A:297:GLU:HG3	1:A:299:ALA:H	1.75	0.51
2:B:401:ARG:HG3	2:B:401:ARG:NH1	2.25	0.51
2:D:24:ILE:O	2:D:28:HIS:HD2	1.94	0.51
1:A:139:HIS:CG	1:A:150:THR:HG21	2.46	0.51
2:B:158:ARG:O	2:B:159:GLU:HB3	2.11	0.51
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.76	0.50
1:A:36:MET:HG3	1:A:36:MET:O	2.09	0.50
1:A:223:THR:HB	1:A:226:ASN:H	1.77	0.50
2:B:318:VAL:HG13	2:B:376:THR:HG23	1.93	0.50
2:B:32:PRO:O	2:B:86:ILE:HD12	2.10	0.50
3:E:48:GLU:HG3	3:E:49:GLU:H	1.74	0.50
2:B:245:PRO:CG	2:B:246:GLY:N	2.75	0.50
2:B:93:VAL:HG12	2:B:114:LEU:HD11	1.93	0.50
2:B:350:ASN:ND2	2:B:350:ASN:H	2.04	0.50
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.42	0.50
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.46	0.50
1:A:335:ILE:O	1:A:339:ARG:HB3	2.12	0.50
2:D:384:ILE:HG22	2:D:432:TYR:CE1	2.47	0.50
2:B:336:GLN:NE2	2:B:351:VAL:HG11	2.27	0.50
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.46	0.50
2:B:307:PRO:CB	2:B:312:TYR:OH	2.60	0.50
1:C:191:THR:O	1:C:195:LEU:HB3	2.12	0.50
2:B:205:ASP:HB2	2:B:303:ALA:HA	1.94	0.50
1:C:72:PRO:O	1:C:74:VAL:N	2.44	0.50
1:C:217:LEU:O	1:C:218:ASP:HB3	2.11	0.50
1:A:86:LEU:HB3	1:A:87:PHE:CD2	2.45	0.50
1:C:213:CYS:HA	1:C:217:LEU:HB2	1.92	0.50
2:D:245:PRO:CG	2:D:246:GLY:H	2.15	0.49
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.30	0.49
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.30	0.49
2:D:54:ASN:ND2	2:D:64:ARG:CD	2.73	0.49
2:B:253:ARG:O	2:B:254:LYS:C	2.50	0.49
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.41	0.49
1:C:241:SER:OG	1:C:242:LEU:HD23	2.11	0.49
1:C:2:ARG:HA	1:C:2:ARG:NH1	2.26	0.49
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.85	0.49
1:C:191:THR:CG2	1:C:425:MET:CE	2.88	0.49
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:ILE:O	2:D:348:PRO:O	2.30	0.49
1:A:36:MET:HG2	1:A:61:HIS:NE2	2.27	0.49
2:D:381:SER:O	2:D:384:ILE:HB	2.12	0.49
2:B:88:ARG:O	2:B:91:ASN:HB2	2.12	0.49
2:B:135:PHE:CD1	2:B:135:PHE:N	2.80	0.49
2:B:404:PHE:HD1	2:B:404:PHE:N	2.10	0.49
2:B:320:ARG:HA	2:B:356:CYS:O	2.12	0.49
1:A:276:ILE:HD11	1:A:280:LYS:HD3	1.95	0.49
2:B:260:VAL:HG11	2:B:266:HIS:HA	1.95	0.49
2:D:183:GLU:N	2:D:184:PRO:HD2	2.28	0.49
1:C:267:PHE:CD1	1:C:267:PHE:N	2.81	0.49
1:A:405:VAL:CG1	1:A:406:HIS:N	2.76	0.49
1:C:133:GLN:CD	1:C:252:LEU:HB2	2.32	0.49
1:A:395:PHE:O	1:A:397:LEU:N	2.45	0.49
2:B:408:TYR:O	2:B:409:THR:C	2.50	0.49
1:C:265:ILE:HG22	1:C:265:ILE:O	2.12	0.49
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.48	0.49
1:C:248:LEU:O	1:C:249:ASN:HB2	2.12	0.49
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.95	0.49
2:D:253:ARG:O	2:D:254:LYS:C	2.49	0.49
2:D:2:ARG:N	2:D:133:GLN:OE1	2.46	0.49
1:A:404:PHE:O	1:A:405:VAL:C	2.50	0.49
1:A:347:CYS:O	1:A:348:PRO:C	2.51	0.49
3:E:137:LYS:C	3:E:139:LEU:H	2.16	0.49
2:D:307:PRO:HB3	2:D:312:TYR:OH	2.13	0.48
1:A:229:ARG:NH1	1:A:229:ARG:CG	2.69	0.48
2:D:31:ASP:HB3	2:D:32:PRO:HD2	1.96	0.48
2:B:240:THR:HG21	2:B:320:ARG:CZ	2.42	0.48
2:D:48:ARG:HB3	2:D:243:ARG:HA	1.95	0.48
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.13	0.48
2:B:242:LEU:HG	7:B:700:E70:HAH	1.96	0.48
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.78	0.48
1:C:190:THR:CG2	1:C:191:THR:N	2.76	0.48
2:B:295:MET:CG	2:B:377:PHE:HB2	2.44	0.48
2:B:181:VAL:HG21	2:B:404:PHE:HE2	1.78	0.48
1:A:273:ALA:HB2	1:A:375:VAL:O	2.13	0.48
1:C:111:GLY:O	1:C:113:GLU:N	2.47	0.48
2:D:180:THR:C	2:D:182:VAL:H	2.17	0.48
1:A:119:LEU:HD22	1:A:156:ARG:HH21	1.79	0.48
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.96	0.48
1:A:249:ASN:HD22	1:A:249:ASN:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:357:ASP:N	2:D:357:ASP:OD2	2.46	0.48
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.96	0.48
2:D:273:ALA:HB2	2:D:375:ALA:N	2.29	0.48
2:B:70:LEU:C	2:B:95:GLY:HA3	2.34	0.48
2:D:403:ALA:C	2:D:405:LEU:H	2.18	0.48
2:B:406:HIS:HA	2:B:409:THR:HB	1.95	0.48
2:B:108:TYR:O	2:B:112:ALA:HB3	2.14	0.48
2:B:150:GLY:O	2:B:154:ILE:HG23	2.13	0.48
1:C:190:THR:O	1:C:192:HIS:N	2.47	0.48
1:A:249:ASN:ND2	1:A:249:ASN:N	2.61	0.48
1:A:66:VAL:HG11	1:A:122:ILE:HG13	1.96	0.48
2:D:240:THR:HG21	2:D:320:ARG:CZ	2.43	0.47
2:B:400:ARG:C	2:B:402:LYS:H	2.17	0.47
1:A:280:LYS:O	1:A:282:TYR:N	2.47	0.47
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.96	0.47
2:B:70:LEU:CD1	2:B:145:THR:HB	2.43	0.47
1:C:271:THR:HG23	1:C:301:GLN:HA	1.95	0.47
1:C:273:ALA:HB2	1:C:375:VAL:O	2.13	0.47
2:B:192:HIS:O	2:B:195:VAL:HG12	2.14	0.47
1:A:277:SER:O	1:A:280:LYS:HB2	2.15	0.47
2:B:200:GLU:HA	2:B:266:HIS:HB2	1.96	0.47
1:A:419:SER:O	1:A:423:GLU:HG3	2.13	0.47
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.29	0.47
2:D:76:ASP:O	2:D:80:SER:HB2	2.15	0.47
2:B:83:PHE:HA	2:B:83:PHE:HD2	1.64	0.47
2:B:336:GLN:NE2	2:B:351:VAL:HG12	2.25	0.47
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.78	0.47
2:D:344:VAL:HG22	2:D:346:TRP:HE1	1.80	0.47
2:D:177:VAL:O	2:D:177:VAL:HG12	2.14	0.47
2:B:177:VAL:HG12	2:B:177:VAL:O	2.15	0.47
1:C:310:GLY:HA3	1:C:383:ALA:HB2	1.97	0.47
2:B:264:ARG:HD3	2:B:431:GLU:OE1	2.14	0.47
1:C:309:HIS:ND1	1:C:310:GLY:N	2.62	0.47
2:D:399:PHE:O	2:D:400:ARG:O	2.32	0.47
1:A:271:THR:HG23	1:A:301:GLN:HA	1.96	0.47
2:D:51:VAL:CG1	2:D:52:TYR:CD1	2.97	0.47
1:A:265:ILE:HG22	1:A:265:ILE:O	2.14	0.47
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.68	0.47
2:B:120:ASP:HA	2:B:123:ARG:NH1	2.30	0.47
2:D:107:HIS:O	2:D:152:LEU:HD22	2.15	0.47
2:B:156:LYS:HG2	3:E:76:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ARG:HH22	2:D:253:ARG:HH22	1.61	0.47
1:A:181:VAL:N	2:B:258:ASN:HD21	1.97	0.47
3:E:76:ARG:C	3:E:78:HIS:N	2.63	0.47
2:B:261:PRO:HG2	2:B:262:PHE:H	1.79	0.47
2:D:383:ALA:O	2:D:386:GLU:HB2	2.15	0.47
2:B:220:THR:O	2:B:222:PRO:HD3	2.14	0.47
2:D:51:VAL:O	2:D:64:ARG:NH2	2.47	0.46
2:B:30:ILE:HG22	2:B:31:ASP:O	2.15	0.46
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.50	0.46
2:D:224:TYR:OH	6:D:600:GDP:H2'	2.15	0.46
2:B:287:THR:CG2	2:B:290:GLU:H	2.28	0.46
1:A:244:PHE:O	1:A:245:ASP:HB3	2.16	0.46
1:A:154:MET:O	1:A:158:SER:HB2	2.15	0.46
1:C:273:ALA:HB2	1:C:375:VAL:N	2.29	0.46
2:D:225:GLY:O	2:D:228:ASN:HB2	2.14	0.46
3:E:74:GLU:O	3:E:76:ARG:N	2.48	0.46
2:D:348:PRO:O	2:D:350:ASN:N	2.48	0.46
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.50	0.46
2:B:178:SER:HB2	2:B:183:GLU:OE1	2.14	0.46
2:D:273:ALA:HB2	2:D:375:ALA:H	1.80	0.46
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.56	0.46
1:A:345:ASP:HB3	1:A:346:TRP:CD1	2.50	0.46
2:B:198:THR:OG1	2:B:266:HIS:HE1	1.97	0.46
2:D:180:THR:C	2:D:182:VAL:N	2.68	0.46
1:C:223:THR:HB	1:C:226:ASN:H	1.80	0.46
1:C:77:GLU:O	1:C:80:THR:HG22	2.16	0.46
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.51	0.46
2:D:30:ILE:HG22	2:D:31:ASP:O	2.16	0.46
2:D:260:VAL:HG11	2:D:266:HIS:HA	1.98	0.46
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.81	0.46
2:D:352:LYS:HG3	7:D:700:E70:HAM	1.96	0.46
2:D:171:VAL:HG12	2:D:204:ILE:HB	1.96	0.46
2:D:261:PRO:HG3	2:D:313:LEU:HG	1.97	0.46
1:A:234:ILE:CG1	1:A:272:TYR:HB2	2.46	0.46
1:C:273:ALA:HB3	1:C:375:VAL:H	1.73	0.46
1:A:344:VAL:O	1:A:346:TRP:N	2.49	0.46
2:B:306:ASP:C	2:B:308:ARG:N	2.63	0.46
2:D:209:LEU:HA	2:D:209:LEU:HD12	1.79	0.46
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.96	0.46
2:D:292:THR:HA	2:D:295:MET:HE3	1.98	0.46
3:E:101:LEU:O	3:E:104:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.46	0.46
1:A:252:LEU:O	1:A:255:PHE:HB2	2.16	0.46
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.45
2:D:242:LEU:HD21	2:D:252:LEU:HB2	1.97	0.45
1:C:86:LEU:HB3	1:C:87:PHE:CD2	2.51	0.45
1:C:70:LEU:HD13	1:C:145:THR:HB	1.97	0.45
1:A:278:ALA:HA	1:A:281:ALA:HB2	1.98	0.45
1:A:267:PHE:CD1	1:A:267:PHE:N	2.85	0.45
1:A:88:HIS:CD2	1:A:90:GLU:OE1	2.69	0.45
1:C:264:ARG:O	1:C:266:HIS:CD2	2.69	0.45
3:E:69:LEU:C	3:E:71:HIS:H	2.19	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.51	0.45
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.44	0.45
1:C:344:VAL:O	1:C:346:TRP:N	2.50	0.45
2:D:298:SER:C	2:D:300:ASN:N	2.69	0.45
2:D:5:VAL:HG21	2:D:135:PHE:HD2	1.80	0.45
1:C:32:PRO:C	1:C:34:GLY:H	2.20	0.45
1:A:273:ALA:HB3	1:A:375:VAL:H	1.74	0.45
1:C:31:GLN:HA	1:C:32:PRO:HD2	1.82	0.45
1:A:317:LEU:HA	1:A:317:LEU:HD23	1.80	0.45
2:D:224:TYR:O	2:D:228:ASN:ND2	2.50	0.45
2:D:350:ASN:H	2:D:350:ASN:ND2	2.04	0.45
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.52	0.45
3:E:4:ALA:O	3:E:5:ASP:HB3	2.16	0.45
2:D:349:ASN:OD1	2:D:349:ASN:N	2.47	0.45
2:D:264:ARG:HD3	2:D:431:GLU:OE1	2.17	0.45
1:A:99:ALA:CB	1:A:145:THR:CG2	2.81	0.45
2:B:273:ALA:HB2	2:B:375:ALA:O	2.17	0.45
1:C:256:GLN:O	1:C:259:LEU:N	2.48	0.45
2:D:133:GLN:NE2	2:D:252:LEU:HB3	2.30	0.45
2:B:307:PRO:HB2	2:B:312:TYR:OH	2.17	0.45
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.98	0.45
1:C:190:THR:O	1:C:194:THR:HB	2.17	0.45
2:D:313:LEU:HB2	2:D:380:ASN:O	2.17	0.45
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.45
2:B:180:THR:C	2:B:182:VAL:H	2.21	0.45
7:B:700:E70:CAK	7:B:700:E70:NAP	2.76	0.44
1:C:341:ILE:H	1:C:341:ILE:CD1	2.23	0.44
3:E:65:GLU:C	3:E:67:GLU:H	2.20	0.44
1:A:171:ILE:O	1:A:171:ILE:HG22	2.17	0.44
1:C:99:ALA:CB	1:C:145:THR:CG2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HH22	2:B:253:ARG:NH2	2.15	0.44
2:B:111:GLY:HA2	2:B:149:MET:HE3	1.99	0.44
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.91	0.44
1:C:312:TYR:HE2	1:C:379:SER:CB	2.30	0.44
2:B:313:LEU:HD13	2:B:313:LEU:HA	1.80	0.44
1:C:404:PHE:O	1:C:405:VAL:C	2.55	0.44
2:B:262:PHE:HA	2:B:263:PRO:HD3	1.85	0.44
2:B:19:LYS:HA	2:B:19:LYS:HD3	1.61	0.44
2:D:83:PHE:HD2	2:D:83:PHE:HA	1.63	0.44
2:D:141:LEU:HA	2:D:141:LEU:HD12	1.87	0.44
2:B:274:PRO:C	2:B:275:LEU:HG	2.38	0.44
2:D:378:ILE:CD1	7:D:700:E70:HAI	2.47	0.44
2:B:306:ASP:HA	2:B:307:PRO:HD2	1.82	0.44
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.00	0.44
1:C:202:PHE:CE1	1:C:238:ILE:HG21	2.52	0.44
2:D:318:VAL:HG13	2:D:376:THR:HG23	1.98	0.44
1:C:223:THR:N	1:C:226:ASN:HB2	2.33	0.44
2:D:406:HIS:HA	2:D:409:THR:HB	2.00	0.44
3:E:79:GLU:O	3:E:80:ARG:C	2.56	0.44
2:B:351:VAL:O	2:B:351:VAL:CG1	2.66	0.44
2:B:381:SER:O	2:B:384:ILE:HB	2.17	0.44
2:D:180:THR:O	2:D:182:VAL:N	2.51	0.44
2:D:401:ARG:CG	2:D:401:ARG:HH11	2.30	0.44
3:E:112:ARG:CG	3:E:113:GLU:N	2.79	0.44
2:B:198:THR:OG1	2:B:266:HIS:CE1	2.70	0.44
2:B:107:HIS:O	2:B:152:LEU:HD22	2.17	0.44
2:B:216:THR:O	2:B:217:LEU:HG	2.17	0.44
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.00	0.44
2:D:191:VAL:HG11	2:D:425:MET:CG	2.45	0.44
2:B:174:SER:CB	2:B:207:GLU:HB2	2.47	0.44
1:A:273:ALA:HB2	1:A:375:VAL:N	2.28	0.44
2:D:224:TYR:CD2	6:D:600:GDP:C5	3.06	0.44
2:D:253:ARG:HB2	2:D:253:ARG:HH11	1.83	0.44
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.31	0.44
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.83	0.44
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.66	0.44
2:D:220:THR:O	2:D:222:PRO:HD3	2.18	0.44
2:D:19:LYS:HB3	2:D:232:SER:HB3	2.00	0.44
1:A:70:LEU:HD13	1:A:145:THR:HB	1.99	0.44
2:D:276:THR:HG23	2:D:277:SER:N	2.33	0.44
1:A:191:THR:O	1:A:195:LEU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:243:ARG:O	2.36	0.44
1:C:405:VAL:HG12	1:C:406:HIS:N	2.33	0.44
2:D:270:PRO:HD2	2:D:302:MET:HB2	2.00	0.44
2:D:119:LEU:HD11	2:D:156:LYS:HB3	1.99	0.44
2:B:427:ASP:O	2:B:430:SER:N	2.51	0.43
2:B:19:LYS:O	2:B:23:VAL:HG23	2.18	0.43
1:C:82:THR:O	1:C:83:TYR:HB2	2.18	0.43
1:C:96:LYS:HD3	2:D:131:CYS:HB2	2.01	0.43
2:B:24:ILE:O	2:B:28:HIS:HD2	2.01	0.43
2:D:351:VAL:CG1	2:D:351:VAL:O	2.66	0.43
2:D:89:PRO:O	2:D:92:PHE:HD1	2.01	0.43
2:D:198:THR:OG1	2:D:266:HIS:CE1	2.71	0.43
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.32	0.43
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.48	0.43
2:D:133:GLN:HE21	2:D:252:LEU:HD23	1.84	0.43
2:D:311:ARG:HE	2:D:344:VAL:HG23	1.83	0.43
2:D:44:LEU:HA	2:D:49:ILE:HB	1.98	0.43
1:A:341:ILE:H	1:A:341:ILE:HD13	1.82	0.43
2:B:51:VAL:CG1	2:B:52:TYR:CD1	3.00	0.43
2:B:339:ASN:O	2:B:341:SER:N	2.51	0.43
1:C:154:MET:O	1:C:158:SER:HB2	2.18	0.43
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.53	0.43
1:A:85:GLN:HA	1:A:85:GLN:HE21	1.83	0.43
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.92	0.43
2:D:188:THR:HG23	2:D:425:MET:SD	2.59	0.43
2:B:44:LEU:HA	2:B:49:ILE:HB	2.01	0.43
2:B:380:ASN:C	2:B:380:ASN:HD22	2.21	0.43
2:B:424:ASN:O	2:B:427:ASP:HB2	2.18	0.43
2:D:109:THR:OG1	2:D:411:GLU:OE1	2.31	0.43
1:C:50:ASN:HD22	1:C:50:ASN:HA	1.66	0.43
2:B:2:ARG:N	2:B:133:GLN:OE1	2.52	0.43
1:A:206:ASN:ND2	4:A:600:GTP:HN22	1.99	0.43
2:D:308:ARG:CG	2:D:308:ARG:HH11	2.30	0.43
2:D:247:GLN:CG	2:D:248:LEU:N	2.77	0.43
2:D:336:GLN:NE2	2:D:351:VAL:HG11	2.33	0.43
1:C:405:VAL:HG13	1:C:406:HIS:N	2.33	0.43
1:C:128:GLN:CG	1:C:128:GLN:O	2.66	0.43
2:D:269:MET:HB3	2:D:303:ALA:HB3	1.99	0.43
2:D:427:ASP:O	2:D:430:SER:N	2.52	0.43
1:A:50:ASN:HA	1:A:50:ASN:HD22	1.65	0.43
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:THR:HA	2:D:154:ILE:HD13	2.00	0.43
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.18	0.43
2:B:14:ASN:ND2	2:B:67:LEU:HD23	2.34	0.43
2:B:183:GLU:N	2:B:184:PRO:HD2	2.34	0.43
2:B:48:ARG:HB3	2:B:243:ARG:HA	2.00	0.43
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.54	0.43
1:A:108:TYR:CE1	1:A:413:MET:HG3	2.53	0.43
2:D:273:ALA:HB3	2:D:375:ALA:H	1.84	0.43
1:A:278:ALA:O	1:A:279:GLU:CB	2.57	0.43
2:D:226:ASP:N	2:D:226:ASP:OD1	2.52	0.43
2:B:294:GLN:O	2:B:294:GLN:HG3	2.19	0.43
1:A:375:VAL:HG12	1:A:376:CYS:H	1.84	0.42
2:D:384:ILE:CG2	2:D:432:TYR:CE1	3.02	0.42
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.54	0.42
2:D:16:ILE:HG23	2:D:235:MET:HE1	1.99	0.42
2:B:131:CYS:O	2:B:131:CYS:SG	2.76	0.42
2:D:11:GLN:CG	2:D:74:THR:CG2	2.71	0.42
1:A:223:THR:N	1:A:226:ASN:HB2	2.34	0.42
2:D:123:ARG:HG2	2:D:127:GLU:OE1	2.19	0.42
2:B:59:ASN:O	2:B:60:LYS:O	2.36	0.42
3:E:75:LYS:HB3	3:E:75:LYS:HE2	1.42	0.42
2:B:225:GLY:O	2:B:228:ASN:HB2	2.19	0.42
1:C:239:THR:CB	1:C:243:ARG:HH11	2.32	0.42
1:A:244:PHE:CZ	1:A:358:GLN:HG2	2.53	0.42
2:B:180:THR:C	2:B:182:VAL:N	2.71	0.42
2:B:313:LEU:HB2	2:B:380:ASN:O	2.19	0.42
2:B:192:HIS:HD2	2:B:421:ALA:CA	2.20	0.42
2:D:140:SER:O	2:D:147:SER:HB3	2.19	0.42
1:A:183:GLU:CB	1:A:184:PRO:HD3	2.45	0.42
1:C:139:HIS:HD2	1:C:146:GLY:O	2.02	0.42
2:B:16:ILE:HG22	2:B:17:GLY:N	2.34	0.42
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.75	0.42
1:A:195:LEU:O	1:A:266:HIS:HE1	2.02	0.42
1:A:231:ILE:O	1:A:232:GLY:C	2.58	0.42
2:B:358:ILE:HA	2:B:359:PRO:HD3	1.84	0.42
1:A:280:LYS:HA	1:A:283:HIS:CE1	2.54	0.42
1:C:82:THR:O	1:C:83:TYR:CB	2.68	0.42
1:C:347:CYS:O	1:C:348:PRO:C	2.58	0.42
2:B:229:HIS:CE1	2:B:276:THR:O	2.73	0.42
1:A:340:THR:CG2	1:A:340:THR:O	2.67	0.42
1:A:217:LEU:O	1:A:218:ASP:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:O	2:D:157:ILE:HG12	2.20	0.42
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.83	0.42
2:B:153:LEU:O	2:B:157:ILE:HG12	2.19	0.42
1:C:66:VAL:HG11	1:C:122:ILE:HG13	2.01	0.42
2:D:5:VAL:HG13	2:D:132:LEU:HD13	2.00	0.42
1:A:218:ASP:OD1	1:A:218:ASP:O	2.37	0.42
2:D:380:ASN:HD22	2:D:380:ASN:C	2.22	0.42
1:C:79:ARG:HH22	1:C:94:THR:HG22	1.83	0.42
1:C:2:ARG:HB2	1:C:131:GLY:O	2.20	0.42
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.75	0.42
1:A:210:TYR:O	1:A:214:ARG:HG3	2.20	0.42
1:C:97:GLU:OE2	2:D:164:ARG:NH2	2.50	0.42
1:C:202:PHE:CE2	1:C:268:PRO:HG2	2.55	0.42
1:A:223:THR:H	1:A:226:ASN:HB2	1.84	0.42
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.34	0.42
2:D:245:PRO:CG	2:D:246:GLY:N	2.78	0.42
2:B:19:LYS:HB3	2:B:232:SER:HB3	2.02	0.42
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.20	0.42
2:D:339:ASN:HD22	2:D:339:ASN:HA	1.72	0.42
1:C:231:ILE:O	1:C:232:GLY:C	2.57	0.41
2:B:16:ILE:HG23	2:B:235:MET:HE3	2.00	0.41
2:D:48:ARG:HH22	2:D:249:ASN:HB3	1.84	0.41
1:A:234:ILE:HG13	1:A:272:TYR:HB2	2.01	0.41
3:E:60:ARG:C	3:E:62:LYS:N	2.73	0.41
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.32	0.41
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.67	0.41
1:A:297:GLU:HA	1:A:298:PRO:HD2	1.75	0.41
1:C:312:TYR:HB2	1:C:342:GLN:O	2.21	0.41
2:D:296:PHE:HE1	2:D:332:MET:HE3	1.85	0.41
2:D:99:ALA:CB	2:D:145:THR:HG21	2.50	0.41
2:B:312:TYR:HB2	2:B:343:PHE:CD2	2.55	0.41
1:A:265:ILE:N	1:A:265:ILE:HD12	2.29	0.41
2:B:416:MET:O	2:B:420:GLU:HB2	2.19	0.41
1:A:223:THR:O	1:A:227:LEU:HD13	2.19	0.41
2:B:180:THR:O	2:B:182:VAL:N	2.53	0.41
1:C:234:ILE:CG1	1:C:272:TYR:HB2	2.50	0.41
2:D:234:THR:O	2:D:238:VAL:HG23	2.20	0.41
1:A:249:ASN:H	1:A:254:GLU:HG2	1.85	0.41
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.90	0.41
1:A:287:SER:O	1:A:290:GLU:N	2.53	0.41
2:B:209:LEU:HB3	2:B:227:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:C	1:A:192:HIS:N	2.72	0.41
2:B:16:ILE:HG23	2:B:235:MET:HE1	2.02	0.41
1:C:262:TYR:HB2	1:C:265:ILE:HD13	2.02	0.41
1:A:191:THR:HG23	1:A:425:MET:HE1	2.03	0.41
2:B:89:PRO:O	2:B:92:PHE:HD1	2.03	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.72	0.41
2:B:292:THR:HA	2:B:295:MET:HE3	2.02	0.41
2:B:247:GLN:CG	2:B:248:LEU:N	2.83	0.41
3:E:67:GLU:C	3:E:69:LEU:N	2.70	0.41
2:B:298:SER:O	2:B:300:ASN:N	2.53	0.41
2:D:14:ASN:ND2	2:D:67:LEU:HD23	2.36	0.41
1:A:258:ASN:O	1:A:259:LEU:HD23	2.21	0.41
2:B:167:ASN:O	2:B:168:THR:HG22	2.20	0.41
2:D:132:LEU:HD23	2:D:164:ARG:HG3	2.02	0.41
1:C:251:ASP:O	1:C:255:PHE:HB3	2.21	0.41
1:C:260:VAL:O	1:C:260:VAL:CG2	2.67	0.41
2:D:204:ILE:N	2:D:204:ILE:CD1	2.82	0.41
1:A:249:ASN:H	1:A:254:GLU:CD	2.24	0.41
3:E:67:GLU:HG3	3:E:68:LEU:N	2.36	0.41
2:D:237:GLY:O	2:D:240:THR:OG1	2.39	0.41
1:C:108:TYR:HE1	1:C:413:MET:HG3	1.86	0.41
2:D:313:LEU:HA	2:D:313:LEU:HD13	1.85	0.41
2:B:48:ARG:HH22	2:B:249:ASN:HB3	1.86	0.41
2:D:120:ASP:HA	2:D:123:ARG:NH1	2.36	0.41
2:B:33:THR:O	2:B:34:GLY:O	2.38	0.41
1:A:384:ILE:O	1:A:384:ILE:CG1	2.69	0.41
1:C:305:CYS:SG	1:C:306:ASP:N	2.94	0.41
1:C:36:MET:C	1:C:38:SER:H	2.23	0.41
2:B:350:ASN:N	2:B:350:ASN:ND2	2.67	0.41
1:A:182:VAL:CG2	1:A:182:VAL:O	2.68	0.41
2:B:30:ILE:HA	2:B:35:SER:O	2.21	0.41
2:D:329:ASP:O	2:D:333:LEU:HB2	2.21	0.41
2:B:226:ASP:N	2:B:226:ASP:OD1	2.54	0.40
2:D:15:GLN:HA	2:D:15:GLN:NE2	2.36	0.40
2:D:273:ALA:CB	2:D:375:ALA:N	2.82	0.40
1:A:70:LEU:HB2	1:A:145:THR:HG21	2.03	0.40
1:C:108:TYR:CE1	1:C:413:MET:HG3	2.56	0.40
2:D:182:VAL:O	2:D:185:TYR:HB2	2.21	0.40
1:C:174:ALA:O	1:C:175:PRO:C	2.59	0.40
1:C:208:ALA:O	1:C:212:ILE:HD13	2.21	0.40
2:B:5:VAL:HG21	2:B:135:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:THR:CG2	1:C:61:HIS:HE1	2.35	0.40
1:C:40:LYS:O	1:C:41:THR:HB	2.21	0.40
3:E:65:GLU:O	3:E:67:GLU:N	2.55	0.40
2:B:356:CYS:SG	2:B:358:ILE:HG22	2.62	0.40
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.56	0.40
1:A:103:TYR:O	1:A:104:ALA:C	2.59	0.40
1:A:399:TYR:CE2	1:A:402:ARG:NH2	2.89	0.40
1:C:182:VAL:O	1:C:182:VAL:CG2	2.68	0.40
2:D:287:THR:CG2	2:D:290:GLU:H	2.34	0.40
2:B:401:ARG:HH11	2:B:401:ARG:CG	2.35	0.40
1:C:187:SER:O	1:C:191:THR:HB	2.22	0.40
1:A:202:PHE:CE2	1:A:268:PRO:HG2	2.57	0.40
2:D:20:PHE:CD1	2:D:20:PHE:C	2.94	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	422/451 (94%)	319 (76%)	70 (17%)	33 (8%)	1	20
1	C	422/451 (94%)	316 (75%)	70 (17%)	36 (8%)	1	17
2	B	415/445 (93%)	315 (76%)	58 (14%)	42 (10%)	1	13
2	D	415/445 (93%)	308 (74%)	64 (15%)	43 (10%)	1	12
3	E	120/142 (84%)	82 (68%)	24 (20%)	14 (12%)	0	9
All	All	1794/1934 (93%)	1340 (75%)	286 (16%)	168 (9%)	1	15

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER

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Mol	Chain	Res	Type
1	A	73	THR
1	A	164	LYS
1	A	191	THR
1	A	247	ALA
1	A	248	LEU
1	A	273	ALA
1	A	341	ILE
1	A	345	ASP
1	A	348	PRO
2	B	3	GLU
2	B	34	GLY
2	B	43	GLN
2	B	60	LYS
2	B	62	VAL
2	B	73	GLY
2	B	97	SER
2	B	115	VAL
2	B	163	ASP
2	B	245	PRO
2	B	273	ALA
2	B	276	THR
2	B	288	VAL
2	B	299	LYS
2	B	348	PRO
2	B	349	ASN
2	B	400	ARG
1	C	40	LYS
1	C	73	THR
1	C	164	LYS
1	C	191	THR
1	C	247	ALA
1	C	265	ILE
1	C	273	ALA
1	C	341	ILE
1	C	345	ASP
1	C	348	PRO
2	D	3	GLU
2	D	43	GLN
2	D	60	LYS
2	D	62	VAL
2	D	73	GLY
2	D	97	SER

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Mol	Chain	Res	Type
2	D	115	VAL
2	D	163	ASP
2	D	181	VAL
2	D	217	LEU
2	D	240	THR
2	D	245	PRO
2	D	273	ALA
2	D	276	THR
2	D	288	VAL
2	D	299	LYS
2	D	344	VAL
2	D	348	PRO
2	D	400	ARG
3	E	5	ASP
3	E	47	LEU
3	E	49	GLU
3	E	77	GLU
3	E	102	ALA
1	A	72	PRO
1	A	83	TYR
1	A	112	LYS
1	A	265	ILE
1	A	279	GLU
1	A	326	LYS
1	A	377	MET
1	A	405	VAL
2	B	35	SER
2	B	82	PRO
2	B	113	GLU
2	B	159	GLU
2	B	181	VAL
2	B	217	LEU
2	B	227	LEU
2	B	240	THR
2	B	250	ALA
2	B	340	SER
2	B	344	VAL
2	B	371	LEU
2	B	404	PHE
1	C	48	SER
1	C	72	PRO
1	C	112	LYS

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Mol	Chain	Res	Type
1	C	162	GLY
1	C	249	ASN
1	C	257	THR
1	C	377	MET
1	C	405	VAL
1	C	432	TYR
2	D	34	GLY
2	D	82	PRO
2	D	113	GLU
2	D	159	GLU
2	D	227	LEU
2	D	307	PRO
2	D	340	SER
2	D	349	ASN
2	D	371	LEU
2	D	403	ALA
2	D	404	PHE
3	E	7	GLU
3	E	20	PHE
3	E	29	PHE
3	E	75	LYS
3	E	105	MET
1	A	32	PRO
1	A	281	ALA
1	A	314	ALA
1	A	366	GLY
1	A	396	ASP
1	A	432	TYR
2	B	109	THR
2	B	162	PRO
2	B	225	GLY
2	B	244	PHE
2	B	307	PRO
2	B	322	ARG
2	B	403	ALA
1	C	18	ASN
1	C	33	ASP
1	C	41	THR
1	C	82	THR
1	C	83	TYR
1	C	264	ARG
1	C	433	GLU

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Mol	Chain	Res	Type
2	D	35	SER
2	D	109	THR
2	D	162	PRO
2	D	244	PHE
2	D	250	ALA
2	D	266	HIS
2	D	322	ARG
2	D	402	LYS
3	E	12	ASN
1	A	18	ASN
1	A	245	ASP
1	A	304	LYS
1	A	351	PHE
2	B	59	ASN
1	C	163	LYS
1	C	304	LYS
2	D	59	ASN
2	D	247	GLN
2	D	248	LEU
3	E	66	ALA
3	E	138	GLU
1	A	175	PRO
2	B	248	LEU
2	B	402	LYS
1	C	32	PRO
1	C	175	PRO
1	C	339	ARG
1	C	351	PHE
1	C	396	ASP
3	E	26	PRO
2	D	225	GLY
1	A	162	GLY
2	B	72	PRO
1	C	34	GLY
1	A	13	GLY
1	A	274	PRO
2	B	89	PRO
1	C	274	PRO
2	D	31	ASP
1	A	306	ASP
1	C	306	ASP

### 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	347/378 (92%)	229 (66%)	118 (34%)	0	2
1	C	340/378 (90%)	228 (67%)	112 (33%)	0	3
2	B	348/383 (91%)	221 (64%)	127 (36%)	0	1
2	D	348/383 (91%)	220 (63%)	128 (37%)	0	1
3	E	81/126 (64%)	41 (51%)	40 (49%)	0	0
All	All	1464/1648 (89%)	939 (64%)	525 (36%)	0	1

All (525) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	9	VAL
1	A	11	GLN
1	A	15	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	48	SER
1	A	49	PHE
1	A	50	ASN
1	A	60	LYS
1	A	61	HIS
1	A	64	ARG
1	A	66	VAL
1	A	68	VAL
1	A	76	ASP
1	A	79	ARG
1	A	80	THR
1	A	82	THR
1	A	84	ARG
1	A	87	PHE

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Mol	Chain	Res	Type
1	A	88	HIS
1	A	90	GLU
1	A	94	THR
1	A	96	LYS
1	A	105	ARG
1	A	115	ILE
1	A	116	ASP
1	A	119	LEU
1	A	121	ARG
1	A	122	ILE
1	A	123	ARG
1	A	124	LYS
1	A	128	GLN
1	A	140	SER
1	A	141	PHE
1	A	153	LEU
1	A	155	GLU
1	A	158	SER
1	A	163	LYS
1	A	165	SER
1	A	167	LEU
1	A	176	GLN
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	191	THR
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	200	CYS
1	A	206	ASN
1	A	217	LEU
1	A	220	GLU
1	A	223	THR
1	A	226	ASN
1	A	230	LEU
1	A	234	ILE
1	A	236	SER
1	A	237	SER
1	A	239	THR
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	245	ASP
1	A	248	LEU
1	A	252	LEU
1	A	253	THR
1	A	256	GLN
1	A	260	VAL
1	A	264	ARG
1	A	268	PRO
1	A	269	LEU
1	A	275	VAL
1	A	277	SER
1	A	279	GLU
1	A	288	VAL
1	A	301	GLN
1	A	302	MET
1	A	304	LYS
1	A	306	ASP
1	A	309	HIS
1	A	311	LYS
1	A	315	CYS
1	A	316	CYS
1	A	318	LEU
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	340	THR
1	A	341	ILE
1	A	343	PHE
1	A	345	ASP
1	A	347	CYS
1	A	349	THR
1	A	356	ASN
1	A	361	THR
1	A	362	VAL
1	A	363	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	386	GLU

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Mol	Chain	Res	Type
1	A	394	LYS
1	A	397	LEU
1	A	401	LYS
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	420	GLU
1	A	433	GLU
1	A	434	GLU
2	B	2	ARG
2	B	4	ILE
2	B	12	CYS
2	B	16	ILE
2	B	19	LYS
2	B	24	ILE
2	B	25	SER
2	B	27	GLU
2	B	33	THR
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	44	LEU
2	B	54	ASN
2	B	55	GLU
2	B	61	TYR
2	B	67	LEU
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	77	SER
2	B	83	PHE
2	B	88	ARG
2	B	93	VAL
2	B	96	GLN
2	B	97	SER
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	116	ASP
2	B	119	LEU

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Mol	Chain	Res	Type
2	B	120	ASP
2	B	122	VAL
2	B	129	CYS
2	B	130	ASP
2	B	131	CYS
2	B	135	PHE
2	B	141	LEU
2	B	145	THR
2	B	153	LEU
2	B	154	ILE
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG
2	B	165	ILE
2	B	166	MET
2	B	168	THR
2	B	170	SER
2	B	174	SER
2	B	176	LYS
2	B	177	VAL
2	B	178	SER
2	B	180	THR
2	B	181	VAL
2	B	191	VAL
2	B	195	VAL
2	B	200	GLU
2	B	209	LEU
2	B	211	ASP
2	B	212	ILE
2	B	214	PHE
2	B	215	ARG
2	B	216	THR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	240	THR
2	B	241	CYS
2	B	248	LEU
2	B	249	ASN
2	B	253	ARG
2	B	258	ASN
2	B	260	VAL

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Mol	Chain	Res	Type
2	B	265	LEU
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	301	MET
2	B	305	CYS
2	B	308	ARG
2	B	309	HIS
2	B	311	ARG
2	B	313	LEU
2	B	320	ARG
2	B	323	MET
2	B	324	SER
2	B	325	MET
2	B	332	MET
2	B	333	LEU
2	B	335	VAL
2	B	336	GLN
2	B	341	SER
2	B	349	ASN
2	B	350	ASN
2	B	351	VAL
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	378	ILE
2	B	380	ASN
2	B	384	ILE
2	B	386	GLU
2	B	387	LEU
2	B	389	LYS
2	B	390	ARG
2	B	391	ILE
2	B	392	SER

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Mol	Chain	Res	Type
2	B	393	GLU
2	B	394	GLN
2	B	398	MET
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	413	MET
2	B	416	MET
2	B	419	THR
2	B	420	GLU
2	B	423	SER
2	B	434	GLN
1	C	2	ARG
1	C	4	CYS
1	C	9	VAL
1	C	11	GLN
1	C	15	GLN
1	C	16	ILE
1	C	22	GLU
1	C	23	LEU
1	C	26	LEU
1	C	49	PHE
1	C	50	ASN
1	C	51	THR
1	C	60	LYS
1	C	61	HIS
1	C	66	VAL
1	C	68	VAL
1	C	76	ASP
1	C	78	VAL
1	C	79	ARG
1	C	80	THR
1	C	82	THR
1	C	84	ARG
1	C	87	PHE
1	C	88	HIS
1	C	94	THR
1	C	96	LYS
1	C	105	ARG
1	C	114	ILE
1	C	115	ILE
1	C	116	ASP

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Mol	Chain	Res	Type
1	C	119	LEU
1	C	121	ARG
1	C	122	ILE
1	C	123	ARG
1	C	124	LYS
1	C	128	GLN
1	C	140	SER
1	C	141	PHE
1	C	153	LEU
1	C	155	GLU
1	C	158	SER
1	C	160	ASP
1	C	163	LYS
1	C	165	SER
1	C	167	LEU
1	C	176	GLN
1	C	182	VAL
1	C	183	GLU
1	C	187	SER
1	C	191	THR
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	200	CYS
1	C	206	ASN
1	C	217	LEU
1	C	220	GLU
1	C	223	THR
1	C	226	ASN
1	C	230	LEU
1	C	234	ILE
1	C	236	SER
1	C	237	SER
1	C	239	THR
1	C	242	LEU
1	C	248	LEU
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	255	PHE
1	C	257	THR

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Mol	Chain	Res	Type
1	C	269	LEU
1	C	275	VAL
1	C	288	VAL
1	C	301	GLN
1	C	302	MET
1	C	304	LYS
1	C	306	ASP
1	C	309	HIS
1	C	311	LYS
1	C	315	CYS
1	C	316	CYS
1	C	318	LEU
1	C	329	ASN
1	C	334	THR
1	C	340	THR
1	C	341	ILE
1	C	343	PHE
1	C	347	CYS
1	C	349	THR
1	C	356	ASN
1	C	362	VAL
1	C	363	VAL
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	386	GLU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	405	VAL
1	C	409	VAL
1	C	413	MET
1	C	415	GLU
1	C	419	SER
1	C	420	GLU
1	C	433	GLU
1	C	434	GLU
2	D	2	ARG
2	D	4	ILE

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Mol	Chain	Res	Type
2	D	12	CYS
2	D	16	ILE
2	D	19	LYS
2	D	24	ILE
2	D	25	SER
2	D	27	GLU
2	D	33	THR
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	54	ASN
2	D	55	GLU
2	D	61	TYR
2	D	67	LEU
2	D	68	VAL
2	D	70	LEU
2	D	71	GLU
2	D	77	SER
2	D	80	SER
2	D	83	PHE
2	D	88	ARG
2	D	91	ASN
2	D	93	VAL
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	116	ASP
2	D	119	LEU
2	D	120	ASP
2	D	122	VAL
2	D	124	LYS
2	D	129	CYS
2	D	130	ASP
2	D	131	CYS
2	D	135	PHE
2	D	137	LEU
2	D	141	LEU
2	D	145	THR
2	D	153	LEU
2	D	154	ILE

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Mol	Chain	Res	Type
2	D	158	ARG
2	D	160	GLU
2	D	164	ARG
2	D	165	ILE
2	D	166	MET
2	D	168	THR
2	D	170	SER
2	D	174	SER
2	D	176	LYS
2	D	177	VAL
2	D	178	SER
2	D	180	THR
2	D	181	VAL
2	D	184	PRO
2	D	191	VAL
2	D	195	VAL
2	D	200	GLU
2	D	209	LEU
2	D	211	ASP
2	D	212	ILE
2	D	214	PHE
2	D	216	THR
2	D	223	THR
2	D	227	LEU
2	D	230	LEU
2	D	240	THR
2	D	241	CYS
2	D	248	LEU
2	D	249	ASN
2	D	253	ARG
2	D	260	VAL
2	D	265	LEU
2	D	269	MET
2	D	275	LEU
2	D	276	THR
2	D	286	LEU
2	D	293	GLN
2	D	294	GLN
2	D	295	MET
2	D	300	ASN
2	D	301	MET
2	D	305	CYS

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Mol	Chain	Res	Type
2	D	308	ARG
2	D	309	HIS
2	D	311	ARG
2	D	313	LEU
2	D	320	ARG
2	D	323	MET
2	D	324	SER
2	D	325	MET
2	D	332	MET
2	D	333	LEU
2	D	335	VAL
2	D	341	SER
2	D	349	ASN
2	D	350	ASN
2	D	351	VAL
2	D	355	VAL
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	378	ILE
2	D	380	ASN
2	D	384	ILE
2	D	386	GLU
2	D	387	LEU
2	D	389	LYS
2	D	390	ARG
2	D	391	ILE
2	D	392	SER
2	D	393	GLU
2	D	394	GLN
2	D	398	MET
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	413	MET
2	D	416	MET
2	D	419	THR
2	D	420	GLU
2	D	434	GLN

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Mol	Chain	Res	Type
3	E	5	ASP
3	E	11	LEU
3	E	12	ASN
3	E	15	THR
3	E	24	LEU
3	E	27	PRO
3	E	48	GLU
3	E	52	LYS
3	E	53	LYS
3	E	54	LEU
3	E	55	GLU
3	E	59	GLU
3	E	60	ARG
3	E	61	ARG
3	E	62	LYS
3	E	67	GLU
3	E	70	LYS
3	E	71	HIS
3	E	72	LEU
3	E	75	LYS
3	E	77	GLU
3	E	79	GLU
3	E	80	ARG
3	E	81	GLU
3	E	89	GLU
3	E	91	ASN
3	E	94	ILE
3	E	96	MET
3	E	99	GLU
3	E	101	LEU
3	E	106	GLU
3	E	109	LYS
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	119	MET
3	E	120	LEU
3	E	123	LEU
3	E	125	GLU
3	E	134	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	85	GLN
1	A	88	HIS
1	A	91	GLN
1	A	107	HIS
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	ASN
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	329	ASN
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	54	ASN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	192	HIS
2	B	193	GLN
2	B	197	ASN
2	B	206	ASN
2	B	247	GLN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	331	GLN
2	B	336	GLN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	436	GLN
1	C	50	ASN
1	C	61	HIS
1	C	85	GLN
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS

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Mol	Chain	Res	Type
1	C	176	GLN
1	C	206	ASN
1	C	216	ASN
1	C	256	GLN
1	C	266	HIS
1	C	329	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	15	GLN
2	D	28	HIS
2	D	43	GLN
2	D	54	ASN
2	D	133	GLN
2	D	136	GLN
2	D	192	HIS
2	D	193	GLN
2	D	206	ASN
2	D	247	GLN
2	D	249	ASN
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	309	HIS
2	D	331	GLN
2	D	336	GLN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	436	GLN
3	E	111	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GTP	A	600	-	25,34,34	0.95	2 (8%)	34,54,54	1.44	6 (17%)
6	GDP	B	600	-	23,30,30	1.13	2 (8%)	30,47,47	1.88	7 (23%)
7	E70	B	700	-	27,28,28	2.71	5 (18%)	37,39,39	1.90	6 (16%)
4	GTP	C	600	-	25,34,34	1.00	2 (8%)	34,54,54	1.93	9 (26%)
6	GDP	D	600	-	23,30,30	0.97	1 (4%)	30,47,47	1.97	6 (20%)
7	E70	D	700	-	27,28,28	3.54	7 (25%)	37,39,39	2.05	6 (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
4	GTP	A	600	-	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
7	E70	B	700	-	-	0/17/17/17	0/3/3/3
4	GTP	C	600	-	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3
7	E70	D	700	-	-	0/17/17/17	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	700	E70	CAX-NAR	-4.69	1.34	1.42
7	B	700	E70	CAX-NAR	-3.08	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	E70	CAU-NAQ	-3.00	1.34	1.40
7	D	700	E70	CAU-NAQ	-2.47	1.35	1.40
4	C	600	GTP	O4'-C4'	-2.31	1.39	1.45
4	A	600	GTP	O4'-C4'	-2.06	1.40	1.45
6	B	600	GDP	C2-N1	2.01	1.39	1.35
7	D	700	E70	CAY-NAP	2.15	1.38	1.35
4	C	600	GTP	C6-N1	2.88	1.38	1.33
4	A	600	GTP	C6-N1	3.05	1.38	1.33
6	D	600	GDP	C6-N1	3.18	1.39	1.33
7	D	700	E70	SAZ-NAR	3.19	1.68	1.63
7	B	700	E70	SAZ-NAR	3.41	1.69	1.63
7	D	700	E70	CAW-SAZ	3.56	1.81	1.76
6	B	600	GDP	C6-N1	3.73	1.40	1.33
7	B	700	E70	OAC-SAZ	6.69	1.50	1.43
7	D	700	E70	OAC-SAZ	8.75	1.53	1.43
7	B	700	E70	OAB-SAZ	10.34	1.54	1.43
7	D	700	E70	OAB-SAZ	13.66	1.58	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	E70	OAC-SAZ-OAB	-7.76	109.25	119.54
7	D	700	E70	OAC-SAZ-OAB	-7.15	110.06	119.54
6	D	600	GDP	N3-C2-N1	-5.50	119.06	127.44
6	B	600	GDP	N3-C2-N1	-5.47	119.11	127.44
4	C	600	GTP	N3-C2-N1	-5.36	119.28	127.44
6	D	600	GDP	C2'-C1'-N9	-4.42	107.54	114.29
4	C	600	GTP	PB-O3B-PG	-4.16	118.72	132.67
6	D	600	GDP	C5-C6-N1	-4.14	117.93	123.59
6	B	600	GDP	PA-O3A-PB	-3.89	119.63	132.67
4	A	600	GTP	N3-C2-N1	-3.84	121.60	127.44
4	C	600	GTP	C4-C5-N7	-3.83	105.95	109.48
6	B	600	GDP	C2'-C1'-N9	-3.81	108.48	114.29
4	C	600	GTP	PA-O3A-PB	-3.62	122.58	132.73
6	D	600	GDP	PA-O3A-PB	-3.57	120.68	132.67
4	A	600	GTP	PB-O3B-PG	-3.23	121.83	132.67
4	C	600	GTP	C1'-N9-C4	-3.16	122.18	126.94
7	D	700	E70	CAE-CAF-NAP	-2.98	118.46	123.44
6	B	600	GDP	C5-C6-N1	-2.91	119.61	123.59
4	A	600	GTP	PA-O3A-PB	-2.56	125.54	132.73
4	A	600	GTP	C1'-N9-C4	-2.45	123.24	126.94
4	A	600	GTP	C6-C5-C4	-2.15	118.32	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	GTP	C5-C6-N1	-2.15	120.65	123.59
4	C	600	GTP	C6-C5-C4	-2.08	118.41	120.90
4	A	600	GTP	C5-C6-N1	-2.00	120.85	123.59
7	B	700	E70	CAX-NAR-SAZ	2.04	130.00	123.49
6	B	600	GDP	C2'-C3'-C4'	2.13	106.99	102.61
6	D	600	GDP	O4'-C4'-C3'	2.20	109.57	105.15
7	B	700	E70	CAW-SAZ-NAR	2.20	109.71	106.87
7	B	700	E70	CAF-NAP-CAY	2.22	121.40	116.75
6	B	600	GDP	C4'-O4'-C1'	2.34	112.30	109.72
7	D	700	E70	CAF-NAP-CAY	2.51	122.00	116.75
4	C	600	GTP	C6-N1-C2	2.59	119.53	115.94
4	C	600	GTP	N2-C2-N1	2.92	122.03	117.20
6	B	600	GDP	C6-N1-C2	3.25	120.44	115.94
7	D	700	E70	CAW-SAZ-NAR	3.35	111.19	106.87
7	B	700	E70	NAQ-CAY-NAP	3.80	121.23	118.34
6	D	600	GDP	C6-N1-C2	3.86	121.30	115.94
7	D	700	E70	NAQ-CAY-NAP	4.67	121.89	118.34
7	D	700	E70	OAB-SAZ-CAW	4.94	114.21	107.96
7	B	700	E70	OAB-SAZ-CAW	5.07	114.37	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	4	0
6	B	600	GDP	3	0
7	B	700	E70	5	0
4	C	600	GTP	4	0
6	D	600	GDP	4	0
7	D	700	E70	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	427/451 (94%)	0.10	17 (3%) 42 28	46, 51, 52, 57	0
1	C	428/451 (94%)	0.17	18 (4%) 40 26	44, 51, 52, 62	0
2	B	419/445 (94%)	0.18	14 (3%) 50 34	49, 51, 52, 54	0
2	D	419/445 (94%)	0.12	15 (3%) 46 32	48, 51, 52, 54	0
3	E	124/142 (87%)	-0.34	2 (1%) 74 60	41, 50, 56, 59	0
All	All	1817/1934 (93%)	0.11	66 (3%) 46 32	41, 51, 52, 62	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	4.7
2	D	418	PHE	4.2
2	D	399	PHE	3.8
1	A	315	CYS	3.7
1	C	30	ILE	3.6
3	E	4	ALA	3.6
1	A	351	PHE	3.6
2	D	408	TYR	3.4
1	C	245	ASP	3.3
1	A	346	TRP	3.3
2	B	35	SER	3.3
1	A	350	GLY	3.2
2	B	101	ASN	3.1
2	B	98	GLY	3.0
3	E	22	VAL	3.0
2	B	349	ASN	3.0
1	C	370	LYS	2.9
2	D	413	MET	2.9
1	A	313	MET	2.8
1	A	178	SER	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	415	GLU	2.8
2	B	61	TYR	2.8
1	C	302	MET	2.7
2	D	185	TYR	2.7
2	D	371	LEU	2.7
1	C	367	ASP	2.7
1	C	346	TRP	2.6
2	B	312	TYR	2.6
2	B	65	ALA	2.6
2	B	353	THR	2.5
2	D	109	THR	2.5
1	C	276	ILE	2.5
1	C	303	VAL	2.5
1	C	363	VAL	2.4
2	B	33	THR	2.4
1	C	247	ALA	2.4
1	C	295	CYS	2.3
2	B	244	PHE	2.3
1	C	272	TYR	2.3
2	D	274	PRO	2.3
2	B	53	TYR	2.3
2	D	373	MET	2.2
2	D	30	ILE	2.2
1	A	413	MET	2.2
1	A	345	ASP	2.2
1	A	87	PHE	2.2
2	B	49	ILE	2.2
2	D	2	ARG	2.2
2	D	69	ASP	2.2
2	D	110	GLU	2.2
1	C	296	PHE	2.1
1	C	203	MET	2.1
1	A	435	VAL	2.1
2	D	295	MET	2.1
1	A	432	TYR	2.1
1	C	60	LYS	2.1
2	B	57	THR	2.1
1	A	4	CYS	2.1
1	A	347	CYS	2.1
1	C	371	VAL	2.1
1	C	388	TRP	2.1
1	C	319	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	316	CYS	2.0
1	A	311	LYS	2.0
2	B	60	LYS	2.0
1	A	317	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	E70	D	700	26/26	0.92	0.36	1.48	52,53,57,59	0
7	E70	B	700	26/26	0.93	0.40	0.95	52,52,57,59	0
6	GDP	D	600	28/28	0.95	0.19	-0.78	48,51,52,52	0
6	GDP	B	600	28/28	0.86	0.22	-0.78	48,51,52,52	0
4	GTP	C	600	32/32	0.92	0.20	-1.07	48,49,50,51	0
4	GTP	A	600	32/32	0.95	0.13	-1.92	47,49,51,51	0
5	MG	C	601	1/1	0.97	0.06	-4.82	41,41,41,41	0
5	MG	A	601	1/1	0.98	0.10	-5.48	40,40,40,40	0
5	MG	B	601	1/1	0.82	0.90	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.