



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:57 pm BST

PDB ID : 1SA1  
Title : Tubulin-podophyllotoxin: stathmin-like domain complex  
Authors : Ravelli, R.B.; Gigant, B.; Curmi, P.A.; Jourdain, I.; Lachkar, S.; Sobel, A.; Knossow, M.  
Deposited on : 2004-02-06  
Resolution : 4.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

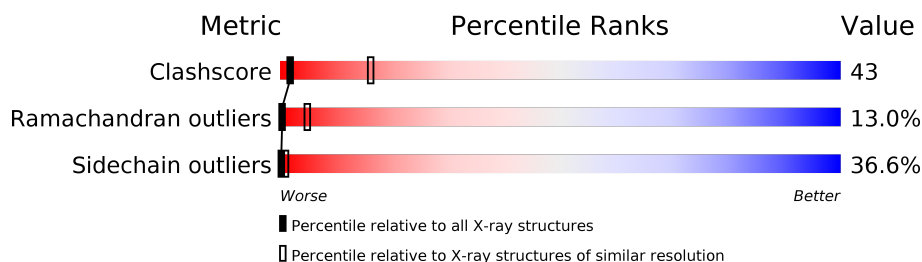
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

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
7	POD	B	700	X	-	-	-
7	POD	D	701	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14180 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	433	Total	C	N	O	S	0	0	0
			3299	2089	559	631	20			
1	C	430	Total	C	N	O	S	0	0	0
			3275	2072	555	628	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ILE	ALA	SEE REMARK 999	UNP P02550
C	265	ILE	ALA	SEE REMARK 999	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3241	2040	545	631	25			
2	D	426	Total	C	N	O	S	0	0	0
			3278	2059	556	638	25			

- Molecule 3 is a protein called Stathmin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	134	Total	C	N	O	S	0	0	0
			905	555	169	176	5			

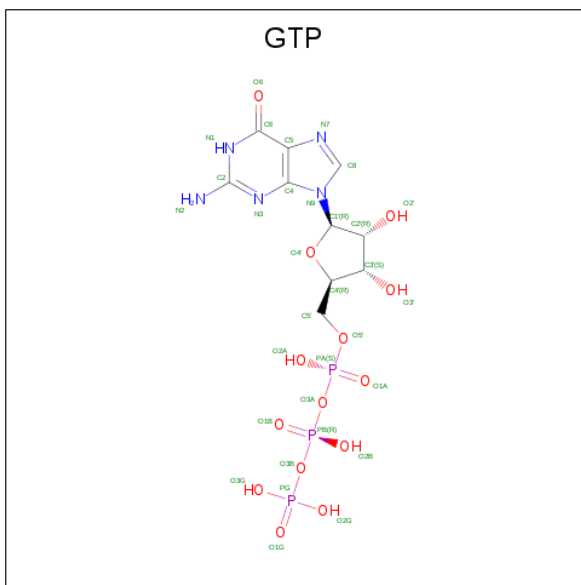
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P02554

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

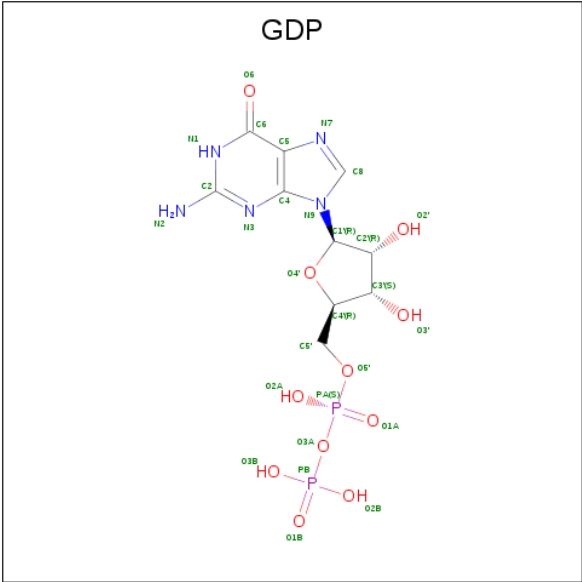
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



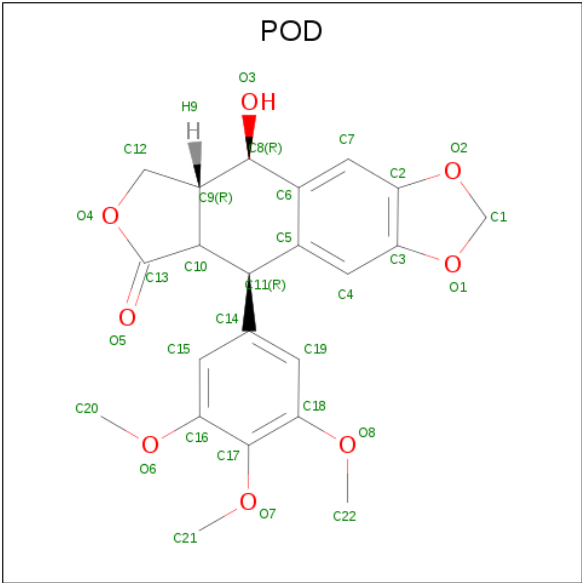
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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 9-HYDROXY-5-(3,4,5-TRIMETHOXYPHENYL)-5,8,8A,9-TETRAHYDR OFURO[3',4':6,7]NAPHTHO[2,3-D][1,3]DIOXOL-6(5AH)-ONE (three-letter code: POD) (formula: C<sub>22</sub>H<sub>22</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			30	22	8		

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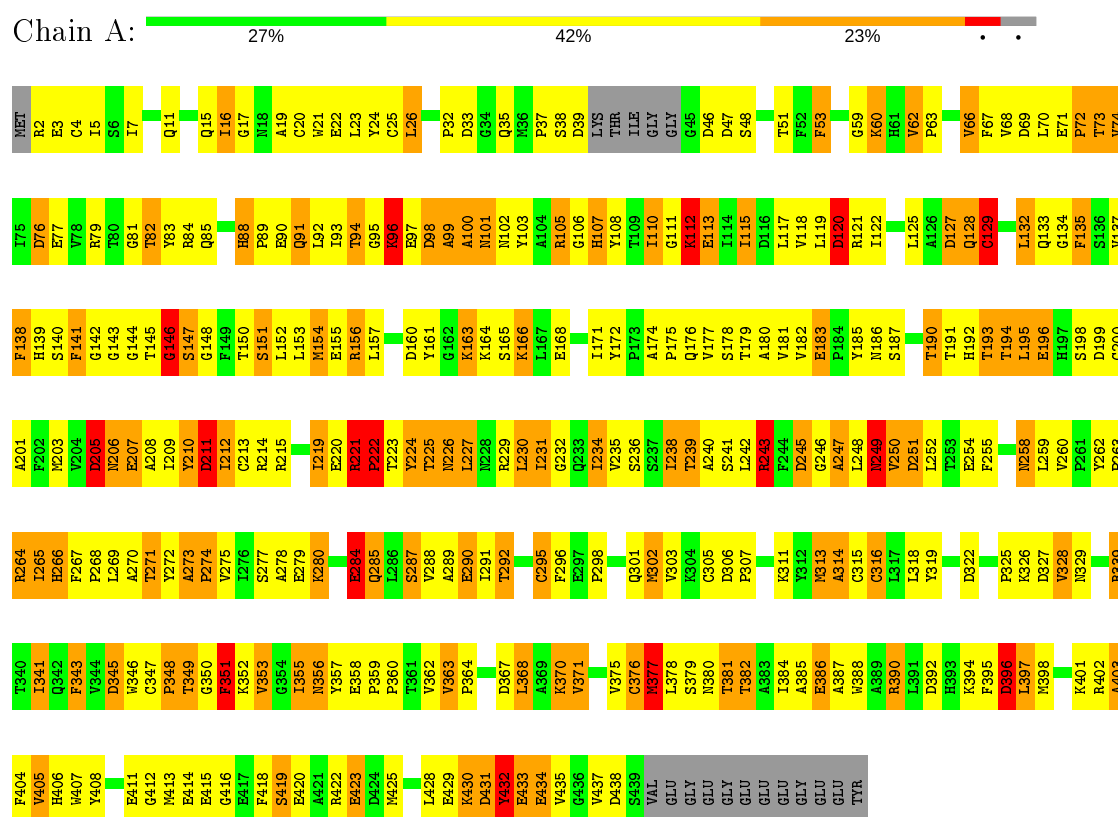
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			30	22	8		

### 3 Residue-property plots

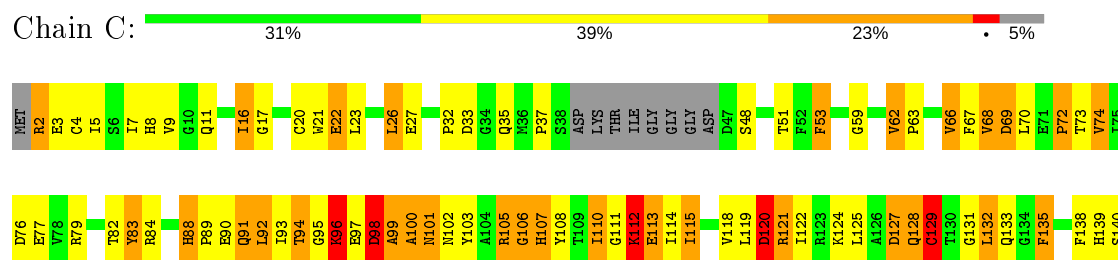
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

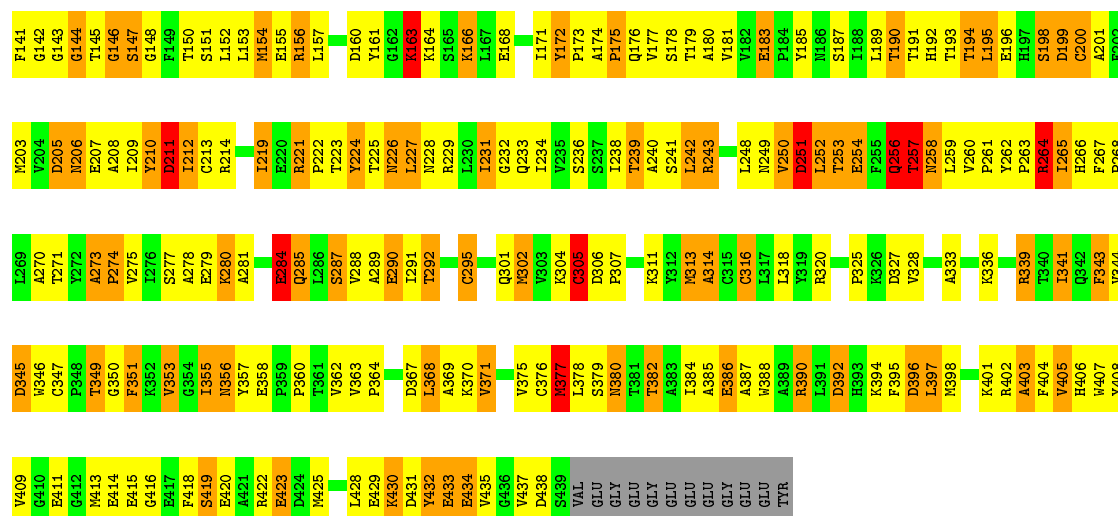
#### • Molecule 1: Tubulin alpha chain



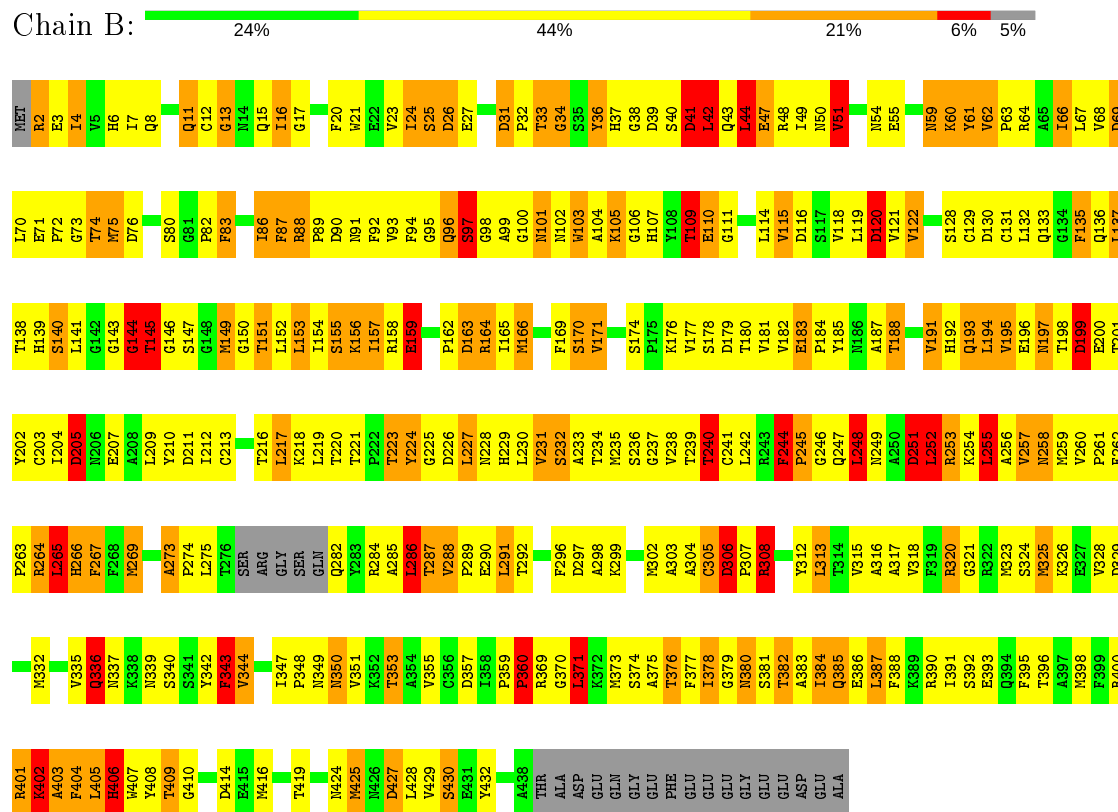
#### • Molecule 1: Tubulin alpha chain



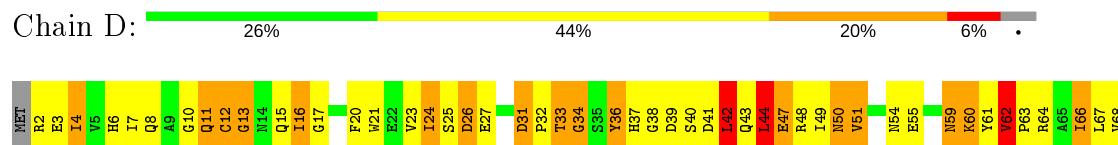


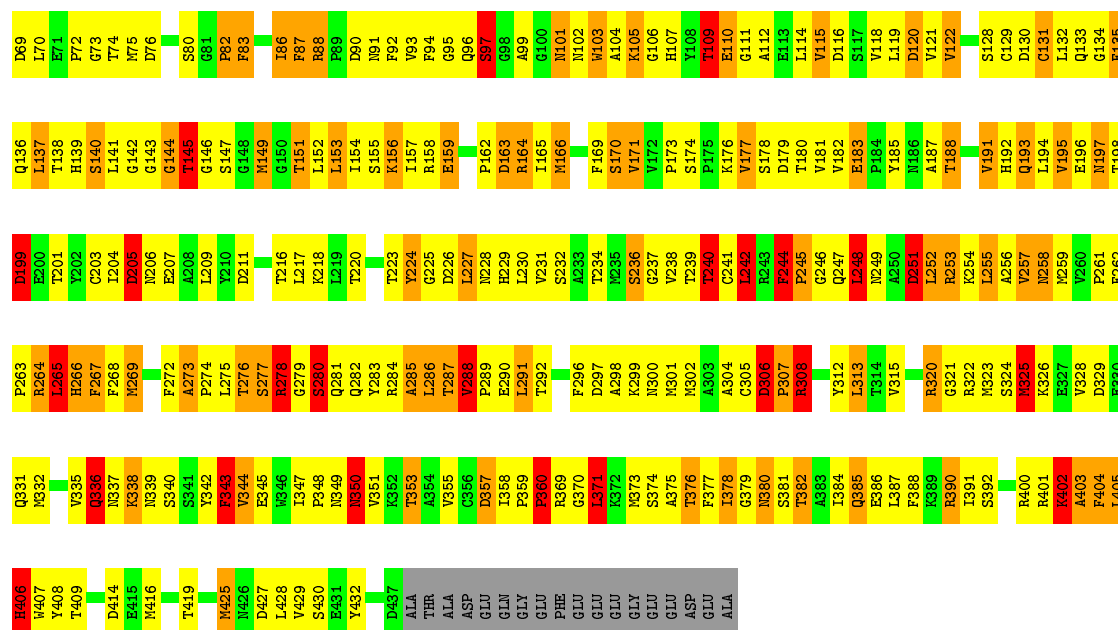


### • Molecule 2: Tubulin beta chain



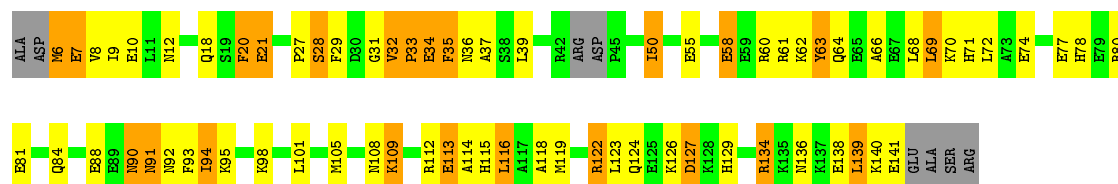
### • Molecule 2: Tubulin beta chain





### • Molecule 3: Stathmin 4

Chain E: 44% 34% 16% 6%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	328.06 Å   328.06 Å   54.30 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 4.20	Depositor
% Data completeness (in resolution range)	98.3 (20.00-4.20)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.204 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, POD

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	0.89	1/3374 (0.0%)	1.09	19/4593 (0.4%)
1	C	0.74	0/3349	1.00	11/4561 (0.2%)
2	B	0.86	3/3314 (0.1%)	1.08	25/4506 (0.6%)
2	D	0.76	2/3352 (0.1%)	1.04	20/4556 (0.4%)
3	E	0.87	0/914	0.95	2/1238 (0.2%)
All	All	0.82	6/14303 (0.0%)	1.05	77/19454 (0.4%)

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	4
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	15

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	44	LEU	C-N	11.14	1.59	1.34
2	B	44	LEU	C-N	9.19	1.55	1.34
2	B	360	PRO	C-N	8.02	1.52	1.34
2	D	360	PRO	C-N	6.55	1.49	1.34
2	B	2	ARG	NE-CZ	5.14	1.39	1.33
1	A	98	ASP	CB-CG	5.13	1.62	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	8.82	126.24	118.30
2	D	205	ASP	CB-CG-OD2	8.78	126.20	118.30
2	D	163	ASP	CB-CG-OD2	8.20	125.68	118.30
2	B	205	ASP	CB-CG-OD2	7.81	125.33	118.30
1	C	211	ASP	CB-CG-OD2	7.70	125.22	118.30
1	A	160	ASP	CB-CG-OD2	7.47	125.02	118.30
2	B	308	ARG	NE-CZ-NH1	7.45	124.03	120.30
2	B	306	ASP	CB-CG-OD2	7.29	124.86	118.30
2	B	199	ASP	CB-CG-OD2	7.26	124.84	118.30
1	C	160	ASP	CB-CG-OD2	7.26	124.83	118.30
2	D	360	PRO	CA-C-N	-7.19	101.38	117.20
1	A	211	ASP	CB-CG-OD2	7.17	124.76	118.30
2	B	163	ASP	CB-CG-OD2	7.12	124.71	118.30
1	C	392	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	69	ASP	CB-CG-OD2	7.02	124.62	118.30
1	A	243	ARG	NE-CZ-NH1	7.01	123.81	120.30
3	E	69	LEU	CA-CB-CG	6.73	130.78	115.30
2	B	211	ASP	CB-CG-OD2	6.72	124.35	118.30
2	B	130	ASP	CB-CG-OD2	6.62	124.25	118.30
2	D	427	ASP	CB-CG-OD2	6.62	124.25	118.30
2	D	306	ASP	CB-CG-OD2	6.55	124.19	118.30
2	B	251	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	199	ASP	CB-CG-OD2	6.39	124.06	118.30
2	D	199	ASP	CB-CG-OD2	6.38	124.05	118.30
2	B	2	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	D	211	ASP	CB-CG-OD2	6.38	124.04	118.30
2	D	308	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	76	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	120	ASP	CB-CG-OD2	6.27	123.94	118.30
2	B	179	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	297	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	162	PRO	N-CD-CG	-6.09	94.06	103.20
2	D	297	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	196	GLU	CA-CB-CG	6.09	126.80	113.40
2	D	357	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	76	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	397	LEU	CA-CB-CG	5.92	128.92	115.30
2	D	26	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	245	ASP	CB-CG-OD2	5.87	123.59	118.30
3	E	127	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	397	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	322	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	264	ARG	C-N-CA	5.72	136.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CB-CG-OD2	5.69	123.42	118.30
2	D	179	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	431	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	264	ARG	C-N-CA	5.53	135.53	121.70
2	D	31	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	98	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	127	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	69	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	146	GLY	N-CA-C	-5.38	99.64	113.10
1	C	146	GLY	N-CA-C	-5.37	99.67	113.10
1	C	199	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	26	ASP	CB-CG-OD2	5.34	123.11	118.30
2	B	69	ASP	CB-CG-OD2	5.32	123.09	118.30
2	D	329	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	44	LEU	O-C-N	-5.31	114.21	122.70
2	D	282	GLN	CB-CA-C	5.30	121.00	110.40
2	B	120	ASP	CB-CG-OD2	5.29	123.06	118.30
2	B	360	PRO	CA-C-N	-5.28	105.58	117.20
1	C	127	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	41	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	120	ASP	CB-CG-OD2	5.27	123.04	118.30
2	D	130	ASP	CB-CG-OD2	5.24	123.02	118.30
2	D	276	THR	N-CA-C	5.24	125.15	111.00
2	B	31	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	387	LEU	CA-CB-CG	5.21	127.29	115.30
2	B	255	LEU	CA-CB-CG	5.13	127.10	115.30
2	B	329	ASP	CB-CG-OD2	5.10	122.89	118.30
2	D	162	PRO	N-CD-CG	-5.09	95.56	103.20
2	B	144	GLY	N-CA-C	5.07	125.78	113.10
1	A	269	LEU	CA-CB-CG	5.05	126.92	115.30
2	D	69	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	222	PRO	N-CD-CG	-5.03	95.66	103.20
2	D	242	LEU	CA-CB-CG	5.03	126.87	115.30
2	B	51	VAL	CB-CA-C	-5.02	101.87	111.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLY	Peptide
1	A	220	GLU	Peptide
1	A	221	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	339	ARG	Peptide
2	B	244	PHE	Peptide
2	B	286	LEU	Peptide
2	B	49	ILE	Peptide
1	C	221	ARG	Peptide
1	C	254	GLU	Peptide
1	C	339	ARG	Peptide
2	D	244	PHE	Peptide
2	D	288	VAL	Peptide
3	E	32	VAL	Peptide
3	E	39	LEU	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	3299	0	3129	275	0
1	C	3275	0	3104	271	0
2	B	3241	0	3033	321	0
2	D	3278	0	3074	297	0
3	E	905	0	730	59	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	3	0
5	C	32	0	12	2	0
6	B	28	0	12	1	0
6	D	28	0	12	2	0
7	B	30	0	19	5	0
7	D	30	0	19	4	0
All	All	14180	0	13156	1177	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 43.

All (1177) 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:33:PRO:HB3	3:E:35:PHE:CZ	1.64	1.33
1:C:240:ALA:HB2	1:C:243:ARG:NH1	1.39	1.33
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.18
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.22	1.15
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.22	1.14
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.78	1.13
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.24	1.11
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.02	1.10
1:C:240:ALA:HA	1:C:243:ARG:HG2	1.19	1.10
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.81	1.08
1:C:191:THR:HG23	1:C:425:MET:HE1	1.29	1.08
1:A:240:ALA:HA	1:A:243:ARG:CG	1.84	1.07
1:A:240:ALA:HA	1:A:243:ARG:HG3	1.09	1.07
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.30	1.07
2:D:332:MET:HG3	2:D:353:THR:HG21	1.34	1.07
1:C:240:ALA:CB	1:C:243:ARG:HH11	1.69	1.05
1:A:191:THR:HG23	1:A:425:MET:HE1	1.38	1.04
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.34	1.04
1:A:128:GLN:O	1:A:129:CYS:HB2	1.56	1.04
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.07	1.02
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	1.95	1.02
1:A:348:PRO:HG3	3:E:27:PRO:HD3	1.41	1.02
2:B:147:SER:O	2:B:151:THR:OG1	1.76	1.01
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.38	1.00
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.40	1.00
1:A:191:THR:HG23	1:A:425:MET:CE	1.92	1.00
2:D:191:VAL:HG11	2:D:425:MET:CE	1.93	0.98
2:B:251:ASP:O	2:B:253:ARG:N	1.96	0.97
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.44	0.97
1:A:24:TYR:CE2	1:A:243:ARG:NH2	2.31	0.97
3:E:33:PRO:HB3	3:E:35:PHE:CE2	1.98	0.97
1:A:353:VAL:HG21	3:E:20:PHE:CE2	1.99	0.97
2:B:158:ARG:O	2:B:159:GLU:HB2	1.63	0.96
1:C:209:ILE:HG22	1:C:227:LEU:HD12	1.44	0.96
1:A:273:ALA:HB3	1:A:274:PRO:CD	1.95	0.96
1:C:191:THR:HG23	1:C:425:MET:CE	1.96	0.96
2:D:291:LEU:HD21	2:D:375:ALA:CB	1.94	0.96
2:D:291:LEU:HD21	2:D:375:ALA:HB3	1.47	0.96
2:D:307:PRO:O	2:D:308:ARG:HB2	1.66	0.96
3:E:33:PRO:CB	3:E:35:PHE:CZ	2.48	0.96
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.96	0.95
1:A:347:CYS:O	1:A:348:PRO:O	1.85	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ASP:O	2:D:253:ARG:N	2.00	0.94
1:C:240:ALA:HA	1:C:243:ARG:CG	1.98	0.94
2:D:273:ALA:HB3	2:D:274:PRO:CD	1.97	0.94
3:E:88:GLU:O	3:E:92:ASN:HB2	1.68	0.94
1:A:209:ILE:HG22	1:A:227:LEU:HD12	1.48	0.94
1:C:240:ALA:HB2	1:C:243:ARG:HH11	0.79	0.93
1:C:301:GLN:HE22	1:C:307:PRO:HD3	1.34	0.93
2:B:403:ALA:O	2:B:405:LEU:N	2.01	0.93
2:D:247:GLN:C	2:D:248:LEU:HG	1.87	0.92
2:D:277:SER:O	2:D:278:ARG:HG3	1.68	0.92
2:D:273:ALA:CB	2:D:274:PRO:CD	2.47	0.92
2:B:244:PHE:HB3	2:B:245:PRO:HD3	1.52	0.91
2:B:332:MET:HG3	2:B:353:THR:HG21	1.50	0.91
1:C:128:GLN:O	1:C:129:CYS:HB2	1.67	0.90
2:D:147:SER:O	2:D:151:THR:OG1	1.90	0.90
2:D:32:PRO:O	2:D:86:ILE:HG13	1.72	0.89
1:A:273:ALA:CB	1:A:375:VAL:H	1.84	0.89
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.08	0.88
2:B:36:TYR:OH	2:B:40:SER:O	1.91	0.88
2:B:191:VAL:HG11	2:B:425:MET:CE	2.03	0.88
1:A:375:VAL:HG12	1:A:376:CYS:H	1.39	0.87
1:A:133:GLN:NE2	1:A:252:LEU:HG	1.88	0.87
2:D:405:LEU:O	2:D:407:TRP:N	2.07	0.87
2:B:68:VAL:HG13	2:B:118:VAL:HG21	1.56	0.87
2:B:247:GLN:OE1	2:B:247:GLN:HA	1.74	0.87
2:D:273:ALA:HB1	2:D:274:PRO:HD3	1.55	0.86
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.39	0.86
2:B:32:PRO:O	2:B:86:ILE:HG13	1.75	0.86
2:D:388:PHE:HD2	2:D:425:MET:HE1	1.40	0.86
2:D:158:ARG:O	2:D:159:GLU:HB2	1.72	0.86
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.05	0.85
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.58	0.85
1:C:240:ALA:CB	1:C:243:ARG:NH1	2.32	0.85
1:A:301:GLN:HE22	1:A:307:PRO:HD3	1.38	0.85
1:A:198:SER:OG	1:A:265:ILE:HD11	1.75	0.85
2:D:244:PHE:HB3	2:D:245:PRO:HD3	1.58	0.85
2:B:273:ALA:CB	2:B:274:PRO:CD	2.54	0.85
2:B:265:LEU:O	2:B:266:HIS:O	1.96	0.84
1:C:390:ARG:HH11	1:C:390:ARG:HG3	1.43	0.84
2:B:265:LEU:HD12	2:B:265:LEU:O	1.78	0.83
2:B:388:PHE:HD2	2:B:425:MET:HE1	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:VAL:O	2:D:351:VAL:HG13	1.76	0.83
2:B:247:GLN:C	2:B:248:LEU:HG	1.99	0.83
2:D:265:LEU:O	2:D:266:HIS:O	1.97	0.83
1:A:70:LEU:HD13	1:A:145:THR:HB	1.60	0.83
1:A:292:THR:O	1:A:295:CYS:HB2	1.78	0.82
2:B:244:PHE:CB	2:B:245:PRO:HD3	2.08	0.82
2:D:36:TYR:OH	2:D:40:SER:O	1.97	0.82
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.60	0.82
2:B:11:GLN:HG3	2:B:74:THR:CG2	2.09	0.82
1:C:70:LEU:HD13	1:C:145:THR:HB	1.63	0.81
2:D:205:ASP:OD2	2:D:207:GLU:HG3	1.81	0.81
2:D:247:GLN:O	2:D:248:LEU:HG	1.81	0.80
2:B:259:MET:HE1	2:B:378:ILE:HG22	1.64	0.80
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.80	0.80
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.62	0.80
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.45	0.80
1:A:191:THR:CG2	1:A:425:MET:HE3	2.12	0.79
1:A:191:THR:CG2	1:A:425:MET:CE	2.60	0.79
2:B:401:ARG:O	1:C:262:TYR:OH	2.00	0.79
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.65	0.79
2:D:320:ARG:HG2	2:D:360:PRO:HD3	1.64	0.79
2:B:244:PHE:HB3	2:B:245:PRO:CD	2.12	0.79
2:D:405:LEU:C	2:D:407:TRP:H	1.84	0.79
2:B:287:THR:CG2	2:B:289:PRO:HD2	2.14	0.78
1:A:240:ALA:HB2	1:A:243:ARG:NH1	1.98	0.78
2:B:351:VAL:HG13	2:B:351:VAL:O	1.82	0.78
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.13	0.78
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.48	0.78
1:A:98:ASP:HB3	1:A:105:ARG:HH21	1.47	0.78
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.23	0.78
1:C:16:ILE:HD13	1:C:171:ILE:HD11	1.66	0.78
2:D:244:PHE:CB	2:D:245:PRO:HD3	2.15	0.77
1:A:99:ALA:O	1:A:100:ALA:HB2	1.84	0.77
2:B:102:ASN:OD1	2:B:105:LYS:HB2	1.84	0.77
2:D:205:ASP:OD1	2:D:207:GLU:HB2	1.85	0.77
2:D:279:GLY:O	2:D:280:SER:HB2	1.83	0.77
1:C:209:ILE:CG2	1:C:227:LEU:HD12	2.14	0.77
1:C:273:ALA:HB3	1:C:375:VAL:H	1.49	0.77
1:C:273:ALA:CB	1:C:375:VAL:H	1.97	0.77
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.24	0.77
1:C:95:GLY:O	1:C:97:GLU:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.00	0.76
1:A:419:SER:O	1:A:423:GLU:HB2	1.86	0.76
2:B:320:ARG:HG2	2:B:360:PRO:HD3	1.67	0.76
1:C:405:VAL:HG13	1:C:406:HIS:N	1.99	0.76
2:D:140:SER:HA	2:D:171:VAL:HG23	1.67	0.76
1:A:198:SER:OG	1:A:265:ILE:CD1	2.33	0.76
1:A:249:ASN:HB2	1:A:254:GLU:HB3	1.68	0.76
2:B:234:THR:O	2:B:238:VAL:HG23	1.86	0.75
1:C:132:LEU:HG	1:C:133:GLN:N	2.01	0.75
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.68	0.75
2:B:259:MET:CE	2:B:378:ILE:HG22	2.16	0.75
2:D:11:GLN:HG3	2:D:74:THR:CG2	2.15	0.75
2:D:382:THR:HA	2:D:432:TYR:HD2	1.51	0.75
1:A:191:THR:HA	1:A:194:THR:HG22	1.67	0.75
1:A:273:ALA:HB2	1:A:375:VAL:H	1.50	0.75
1:A:273:ALA:CB	1:A:274:PRO:CD	2.54	0.74
2:B:4:ILE:HG23	2:B:51:VAL:HG12	1.69	0.74
1:A:132:LEU:HG	1:A:133:GLN:N	2.02	0.74
1:A:239:THR:O	1:A:241:SER:N	2.19	0.74
2:B:405:LEU:C	2:B:407:TRP:H	1.91	0.74
1:A:70:LEU:HD13	1:A:145:THR:CB	2.17	0.74
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.12	0.74
1:A:355:ILE:HD11	3:E:18:GLN:HB3	1.70	0.74
1:A:210:TYR:HE1	1:A:214:ARG:HE	1.34	0.74
1:C:171:ILE:CG2	1:C:206:ASN:HD21	2.01	0.74
2:B:312:TYR:HD2	2:B:381:SER:HB3	1.53	0.73
1:A:353:VAL:HG21	3:E:20:PHE:HE2	1.49	0.73
1:C:108:TYR:HD2	3:E:108:ASN:CG	1.91	0.73
1:C:205:ASP:C	1:C:205:ASP:OD1	2.24	0.73
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.02	0.73
2:B:312:TYR:CD2	2:B:381:SER:HB3	2.24	0.73
1:A:265:ILE:HG23	1:A:267:PHE:CZ	2.24	0.72
1:A:240:ALA:CA	1:A:243:ARG:HG3	2.05	0.72
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.53	0.72
1:A:273:ALA:HB3	1:A:375:VAL:H	1.54	0.72
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.72	0.72
1:A:16:ILE:HD13	1:A:171:ILE:CD1	2.18	0.72
2:B:93:VAL:HG11	2:B:118:VAL:HG23	1.72	0.72
2:D:287:THR:HB	2:D:290:GLU:HG3	1.71	0.72
1:A:5:ILE:HD12	1:A:132:LEU:HD13	1.70	0.72
2:B:140:SER:HA	2:B:171:VAL:HG23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:SER:O	1:C:243:ARG:O	2.07	0.71
2:D:68:VAL:HG13	2:D:118:VAL:HG21	1.72	0.71
1:C:265:ILE:HG23	1:C:267:PHE:CZ	2.24	0.71
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.24	0.71
2:B:68:VAL:CG1	2:B:118:VAL:HG21	2.19	0.71
2:D:291:LEU:CD2	2:D:375:ALA:HB3	2.21	0.71
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.39	0.71
1:A:223:THR:O	1:A:226:ASN:HB2	1.91	0.71
1:C:98:ASP:HB3	1:C:105:ARG:HH21	1.55	0.71
2:B:287:THR:O	2:B:288:VAL:HB	1.89	0.71
2:D:312:TYR:CD2	2:D:381:SER:HB3	2.26	0.71
2:B:405:LEU:O	2:B:407:TRP:N	2.23	0.70
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.72	0.70
2:D:247:GLN:OE1	2:D:247:GLN:HA	1.91	0.70
2:D:336:GLN:OE1	2:D:351:VAL:HG11	1.91	0.70
1:A:95:GLY:O	1:A:97:GLU:N	2.24	0.70
1:C:208:ALA:O	1:C:212:ILE:HD12	1.91	0.70
2:B:59:ASN:O	2:B:60:LYS:O	2.10	0.70
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.73	0.70
1:C:339:ARG:CB	1:C:341:ILE:HG22	2.22	0.70
1:C:405:VAL:CG1	1:C:406:HIS:N	2.53	0.70
1:C:191:THR:CG2	1:C:425:MET:CE	2.69	0.70
1:A:209:ILE:CG2	1:A:227:LEU:HD12	2.22	0.70
1:A:185:TYR:OH	1:A:403:ALA:HB3	1.91	0.70
1:A:405:VAL:HG13	1:A:406:HIS:N	2.05	0.70
2:B:404:PHE:CD2	1:C:261:PRO:HA	2.25	0.70
2:D:312:TYR:HD2	2:D:381:SER:HB3	1.56	0.70
2:B:7:ILE:O	2:B:137:LEU:HA	1.92	0.70
2:D:244:PHE:HB3	2:D:245:PRO:CD	2.20	0.69
1:C:107:HIS:HD2	1:C:108:TYR:CE1	2.10	0.69
2:B:308:ARG:HH11	2:B:308:ARG:CA	2.06	0.69
1:C:179:THR:HG22	1:C:180:ALA:N	2.06	0.69
2:D:107:HIS:CE1	2:D:193:GLN:NE2	2.61	0.69
1:A:67:PHE:HB2	1:A:92:LEU:CD2	2.23	0.69
2:B:347:ILE:O	2:B:347:ILE:HG22	1.92	0.69
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.73	0.69
2:B:221:THR:HG21	1:C:325:PRO:HG2	1.75	0.69
2:D:321:GLY:HA2	2:D:359:PRO:HD3	1.73	0.69
1:C:99:ALA:O	1:C:100:ALA:HB2	1.93	0.69
1:C:115:ILE:HG13	1:C:152:LEU:HG	1.75	0.69
1:A:99:ALA:O	1:A:100:ALA:CB	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:HB3	1:A:267:PHE:HD2	1.59	0.68
1:A:353:VAL:CG2	3:E:20:PHE:CE2	2.76	0.68
2:B:88:ARG:O	2:B:91:ASN:HB2	1.94	0.68
1:A:405:VAL:CG1	1:A:406:HIS:N	2.56	0.68
2:D:143:GLY:O	2:D:147:SER:HB3	1.93	0.68
2:D:234:THR:O	2:D:238:VAL:HG23	1.93	0.68
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.75	0.68
1:C:70:LEU:N	1:C:70:LEU:HD12	2.09	0.68
1:C:70:LEU:HD13	1:C:145:THR:CB	2.24	0.68
2:D:351:VAL:CG1	2:D:351:VAL:O	2.42	0.68
1:C:288:VAL:HA	1:C:291:ILE:HD11	1.76	0.68
2:B:404:PHE:HD2	1:C:261:PRO:HA	1.58	0.68
2:D:13:GLY:O	2:D:16:ILE:HG22	1.94	0.68
3:E:60:ARG:O	3:E:63:TYR:HB3	1.94	0.68
1:C:240:ALA:CA	1:C:243:ARG:HG2	2.10	0.68
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.76	0.68
1:A:205:ASP:C	1:A:205:ASP:OD1	2.33	0.67
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.75	0.67
2:D:67:LEU:HD12	2:D:92:PHE:CD2	2.29	0.67
2:D:102:ASN:HB2	2:D:408:TYR:CE2	2.30	0.67
1:A:105:ARG:HD2	1:A:411:GLU:OE1	1.94	0.67
2:B:225:GLY:O	2:B:227:LEU:N	2.27	0.67
1:C:79:ARG:HH22	1:C:94:THR:CG2	2.07	0.67
2:B:158:ARG:HD2	2:B:197:ASN:HB3	1.75	0.67
1:C:180:ALA:CB	2:D:258:ASN:HD21	2.07	0.67
1:A:375:VAL:HG12	1:A:376:CYS:N	2.09	0.67
2:B:33:THR:O	2:B:34:GLY:O	2.13	0.67
2:B:11:GLN:CG	2:B:74:THR:HG21	2.19	0.67
1:C:128:GLN:O	1:C:129:CYS:CB	2.41	0.67
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.76	0.67
2:D:347:ILE:O	2:D:347:ILE:HG22	1.95	0.67
1:A:107:HIS:HD2	1:A:108:TYR:CE1	2.12	0.66
1:A:288:VAL:HA	1:A:291:ILE:HD11	1.77	0.66
2:D:16:ILE:HD11	2:D:231:VAL:HG11	1.78	0.66
2:D:287:THR:CG2	2:D:289:PRO:HD2	2.25	0.66
1:A:102:ASN:OD1	1:A:105:ARG:HB2	1.96	0.66
2:B:107:HIS:CE1	2:B:193:GLN:NE2	2.64	0.66
1:C:100:ALA:O	1:C:101:ASN:HB2	1.94	0.66
2:B:70:LEU:HD13	2:B:145:THR:HB	1.78	0.66
2:B:239:THR:O	2:B:240:THR:C	2.34	0.66
1:C:67:PHE:HB2	1:C:92:LEU:HD22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:O	1:A:129:CYS:CB	2.36	0.66
1:C:191:THR:HA	1:C:194:THR:HG22	1.78	0.66
1:C:375:VAL:HG12	1:C:376:CYS:H	1.59	0.66
1:A:147:SER:O	1:A:190:THR:OG1	2.12	0.66
2:D:225:GLY:O	2:D:227:LEU:N	2.29	0.66
1:C:105:ARG:NH2	2:D:2:ARG:HH21	1.93	0.66
2:B:247:GLN:O	2:B:248:LEU:HG	1.96	0.66
2:B:158:ARG:O	2:B:159:GLU:CB	2.39	0.65
1:A:67:PHE:HB2	1:A:92:LEU:HD22	1.77	0.65
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.32	0.65
1:A:271:THR:HG23	1:A:301:GLN:HA	1.78	0.65
2:B:349:ASN:O	2:B:351:VAL:N	2.28	0.65
2:D:298:ALA:HB1	2:D:306:ASP:HB3	1.79	0.65
1:A:115:ILE:HG13	1:A:152:LEU:HG	1.79	0.65
2:B:238:VAL:CG1	2:B:378:ILE:HD11	2.27	0.65
2:D:269:MET:HE1	2:D:301:MET:HG3	1.78	0.65
2:D:180:THR:HB	2:D:183:GLU:OE2	1.96	0.65
2:D:33:THR:O	2:D:34:GLY:O	2.15	0.64
2:D:4:ILE:HG23	2:D:51:VAL:HG12	1.77	0.64
2:B:87:PHE:H	2:B:87:PHE:HD2	1.46	0.64
1:C:336:LYS:HE3	1:C:341:ILE:HD12	1.79	0.64
2:D:204:ILE:HG21	2:D:231:VAL:HG13	1.77	0.64
2:D:238:VAL:CG1	2:D:378:ILE:HD11	2.27	0.64
1:A:368:LEU:H	1:A:368:LEU:HD12	1.63	0.64
2:B:387:LEU:O	2:B:390:ARG:HG2	1.98	0.64
2:B:221:THR:CG2	1:C:325:PRO:HG2	2.27	0.64
2:B:287:THR:HG22	2:B:289:PRO:HD2	1.79	0.64
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.16	0.64
2:D:59:ASN:O	2:D:60:LYS:O	2.16	0.64
1:A:236:SER:HA	1:A:243:ARG:HH22	1.62	0.64
1:C:252:LEU:O	1:C:254:GLU:N	2.31	0.64
2:D:141:LEU:HD13	2:D:170:SER:HB3	1.78	0.64
2:B:336:GLN:CD	2:B:351:VAL:HG11	2.18	0.64
2:B:406:HIS:CE1	2:B:407:TRP:CD1	2.86	0.64
1:C:5:ILE:HD12	1:C:132:LEU:HD13	1.80	0.64
1:A:412:GLY:O	3:E:60:ARG:NH1	2.31	0.63
2:B:115:VAL:HG12	2:B:116:ASP:N	2.13	0.63
2:B:180:THR:HB	2:B:183:GLU:OE2	1.97	0.63
2:B:16:ILE:HD11	2:B:231:VAL:HG11	1.79	0.63
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.32	0.63
1:C:238:ILE:HD13	1:C:378:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:O	1:A:251:ASP:HB3	1.98	0.63
2:B:141:LEU:HD13	2:B:170:SER:HB3	1.79	0.63
2:D:336:GLN:CD	2:D:351:VAL:HG11	2.19	0.63
1:A:339:ARG:CB	1:A:341:ILE:HG22	2.28	0.63
1:C:265:ILE:HG12	1:C:265:ILE:O	1.99	0.63
1:A:24:TYR:CD2	1:A:243:ARG:NH2	2.66	0.63
2:B:287:THR:HB	2:B:290:GLU:HG3	1.79	0.63
2:B:403:ALA:C	2:B:405:LEU:H	2.01	0.63
2:D:165:ILE:HG13	2:D:252:LEU:HD23	1.80	0.63
1:A:7:ILE:HA	1:A:66:VAL:HG23	1.79	0.63
1:A:70:LEU:HD12	1:A:70:LEU:N	2.14	0.63
2:B:116:ASP:O	2:B:120:ASP:HB3	1.98	0.63
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.80	0.63
1:C:145:THR:N	5:C:601:GTP:O2B	2.32	0.63
2:D:265:LEU:HD12	2:D:265:LEU:O	1.99	0.63
2:D:382:THR:HA	2:D:432:TYR:CD2	2.34	0.63
2:B:102:ASN:HB2	2:B:408:TYR:CE2	2.34	0.62
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.34	0.62
1:C:210:TYR:HE1	1:C:214:ARG:HE	1.44	0.62
2:D:291:LEU:CD2	2:D:375:ALA:CB	2.75	0.62
1:C:171:ILE:HG23	1:C:206:ASN:HD21	1.63	0.62
1:C:356:ASN:O	1:C:358:GLU:N	2.28	0.62
1:C:191:THR:CG2	1:C:425:MET:HE1	2.17	0.62
2:D:118:VAL:O	2:D:122:VAL:HG13	1.99	0.62
2:D:387:LEU:O	2:D:390:ARG:HG2	1.99	0.62
1:A:201:ALA:HB3	1:A:267:PHE:CD2	2.33	0.62
1:A:396:ASP:OD1	1:A:422:ARG:NE	2.30	0.62
1:C:271:THR:HG23	1:C:301:GLN:HA	1.82	0.62
1:A:292:THR:O	1:A:295:CYS:CB	2.46	0.62
1:A:265:ILE:CG2	1:A:267:PHE:CZ	2.82	0.62
2:D:349:ASN:O	2:D:351:VAL:N	2.33	0.62
2:B:255:LEU:HD22	2:B:259:MET:HG3	1.81	0.62
2:D:388:PHE:HD2	2:D:425:MET:CE	2.13	0.62
2:B:267:PHE:CD1	2:B:267:PHE:N	2.67	0.62
2:D:115:VAL:HG12	2:D:116:ASP:N	2.14	0.62
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.81	0.62
2:B:388:PHE:HD2	2:B:425:MET:CE	2.12	0.62
1:A:346:TRP:CE3	1:A:347:CYS:HB2	2.35	0.61
1:C:368:LEU:H	1:C:368:LEU:HD12	1.64	0.61
3:E:77:GLU:OE2	3:E:80:ARG:CB	2.47	0.61
1:A:265:ILE:HG12	1:A:265:ILE:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HB2	1:A:375:VAL:N	2.15	0.61
1:C:180:ALA:HB2	2:D:258:ASN:HD21	1.65	0.61
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.83	0.61
1:A:119:LEU:HD22	1:A:156:ARG:HE	1.65	0.61
1:C:185:TYR:OH	1:C:403:ALA:HB3	2.00	0.61
1:C:99:ALA:O	1:C:100:ALA:CB	2.48	0.61
1:A:145:THR:N	5:A:600:GTP:O2B	2.34	0.61
1:C:390:ARG:NH1	1:C:390:ARG:HG3	2.09	0.61
1:C:419:SER:O	1:C:423:GLU:HB2	1.99	0.61
1:A:385:ALA:O	1:A:388:TRP:N	2.34	0.61
2:D:93:VAL:HG11	2:D:118:VAL:HG23	1.82	0.61
2:D:67:LEU:HD12	2:D:92:PHE:CE2	2.35	0.60
2:B:351:VAL:O	2:B:351:VAL:CG1	2.48	0.60
2:D:70:LEU:HD13	2:D:145:THR:HB	1.82	0.60
1:C:265:ILE:CG2	1:C:267:PHE:CZ	2.83	0.60
1:C:377:MET:HG3	1:C:377:MET:O	2.00	0.60
2:D:287:THR:O	2:D:288:VAL:HB	2.00	0.60
3:E:90:ASN:O	3:E:92:ASN:N	2.35	0.60
1:C:266:HIS:O	1:C:268:PRO:HD3	2.01	0.60
2:D:191:VAL:CG1	2:D:425:MET:CE	2.76	0.60
2:B:102:ASN:O	2:B:105:LYS:N	2.34	0.60
2:D:259:MET:CE	2:D:378:ILE:HG22	2.31	0.60
1:A:348:PRO:HG3	3:E:27:PRO:CD	2.24	0.60
2:B:259:MET:CE	2:B:378:ILE:CG2	2.79	0.60
1:C:252:LEU:C	1:C:254:GLU:N	2.54	0.60
7:D:701:POD:O6	7:D:701:POD:C21	2.50	0.60
1:A:250:VAL:O	1:A:251:ASP:CB	2.49	0.60
1:A:48:SER:O	1:A:243:ARG:O	2.20	0.60
2:B:114:LEU:O	2:B:115:VAL:C	2.40	0.60
1:C:240:ALA:CA	1:C:243:ARG:HD3	2.31	0.60
1:A:407:TRP:CE3	2:B:257:VAL:HB	2.37	0.59
1:A:273:ALA:CB	1:A:375:VAL:N	2.63	0.59
2:B:265:LEU:O	2:B:266:HIS:C	2.40	0.59
2:B:255:LEU:CD2	2:B:259:MET:HG3	2.31	0.59
1:C:147:SER:O	1:C:190:THR:OG1	2.15	0.59
2:B:181:VAL:O	2:B:181:VAL:HG12	2.01	0.59
2:B:251:ASP:C	2:B:253:ARG:N	2.56	0.59
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.67	0.59
1:A:171:ILE:CG2	1:A:206:ASN:HD21	2.15	0.59
1:A:76:ASP:O	1:A:79:ARG:N	2.35	0.59
2:D:239:THR:O	2:D:240:THR:C	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:CB	2:B:258:ASN:HD21	2.16	0.59
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.84	0.59
2:D:185:TYR:HD1	2:D:408:TYR:HE1	1.50	0.59
2:D:241:CYS:HB2	7:D:701:POD:H203	1.85	0.59
2:D:165:ILE:CG1	2:D:252:LEU:HD23	2.32	0.59
2:B:165:ILE:HG13	2:B:252:LEU:HD23	1.85	0.59
1:C:207:GLU:O	1:C:211:ASP:HB2	2.03	0.59
2:D:255:LEU:HD22	2:D:259:MET:CG	2.33	0.59
2:D:88:ARG:O	2:D:91:ASN:HB2	2.02	0.59
1:A:133:GLN:HE21	1:A:252:LEU:CG	1.95	0.59
1:C:316:CYS:O	1:C:377:MET:HA	2.03	0.59
2:B:264:ARG:O	2:B:266:HIS:CD2	2.56	0.59
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.37	0.59
2:D:116:ASP:O	2:D:120:ASP:HB3	2.03	0.59
2:D:207:GLU:HB2	2:D:304:ALA:HB2	1.83	0.59
1:C:273:ALA:CB	1:C:274:PRO:CD	2.70	0.58
1:C:385:ALA:O	1:C:388:TRP:N	2.35	0.58
1:C:7:ILE:HG12	1:C:66:VAL:CG2	2.33	0.58
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.36	0.58
2:D:259:MET:HE1	2:D:378:ILE:HG22	1.83	0.58
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.37	0.58
2:D:36:TYR:HD1	2:D:37:HIS:N	2.01	0.58
2:D:177:VAL:CG1	2:D:177:VAL:O	2.50	0.58
1:A:356:ASN:O	1:A:358:GLU:N	2.31	0.58
2:D:101:ASN:HA	2:D:144:GLY:H	1.68	0.58
2:D:404:PHE:O	2:D:407:TRP:HB2	2.04	0.58
1:A:252:LEU:O	1:A:255:PHE:HB2	2.02	0.58
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.68	0.58
2:D:7:ILE:O	2:D:137:LEU:HA	2.03	0.58
1:A:247:ALA:HB2	3:E:12:ASN:CB	2.34	0.58
2:B:174:SER:OG	2:B:176:LYS:O	2.18	0.58
2:D:102:ASN:OD1	2:D:105:LYS:HB2	2.04	0.58
2:D:195:VAL:HG21	2:D:428:LEU:HD13	1.86	0.58
1:A:298:PRO:O	1:A:301:GLN:HG3	2.03	0.58
2:B:255:LEU:HD22	2:B:259:MET:CG	2.34	0.58
1:A:395:PHE:HD2	1:A:396:ASP:N	2.02	0.58
2:B:44:LEU:O	2:B:47:GLU:C	2.42	0.58
7:D:701:POD:O6	7:D:701:POD:H213	2.03	0.58
1:A:392:ASP:OD1	1:A:429:GLU:OE1	2.22	0.58
1:C:223:THR:O	1:C:226:ASN:HB2	2.04	0.58
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:TRP:CE3	2:D:257:VAL:HB	2.39	0.58
2:D:158:ARG:HD2	2:D:197:ASN:HB3	1.84	0.58
2:D:405:LEU:C	2:D:407:TRP:N	2.50	0.58
2:B:296:PHE:CE2	2:B:377:PHE:HE1	2.21	0.57
2:B:382:THR:HA	2:B:432:TYR:HD2	1.69	0.57
2:B:337:ASN:HA	2:B:340:SER:HB3	1.86	0.57
2:D:133:GLN:HE21	2:D:252:LEU:HB2	1.68	0.57
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.39	0.57
1:C:119:LEU:CD1	1:C:156:ARG:HB3	2.35	0.57
2:D:44:LEU:O	2:D:47:GLU:C	2.41	0.57
1:A:346:TRP:O	1:A:346:TRP:HE3	1.88	0.57
2:B:118:VAL:O	2:B:122:VAL:HG13	2.05	0.57
2:B:204:ILE:HG21	2:B:231:VAL:HG13	1.87	0.57
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.85	0.57
1:C:260:VAL:O	1:C:260:VAL:HG23	2.04	0.57
2:D:133:GLN:NE2	2:D:252:LEU:HB2	2.19	0.57
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.87	0.57
1:A:435:VAL:HG22	3:E:35:PHE:CE1	2.39	0.57
1:C:7:ILE:HA	1:C:66:VAL:HG23	1.87	0.57
2:B:6:HIS:CE1	2:B:21:TRP:HE1	2.22	0.57
2:D:68:VAL:CG1	2:D:118:VAL:HG21	2.33	0.57
1:C:16:ILE:HD13	1:C:171:ILE:CD1	2.34	0.57
2:B:337:ASN:C	2:B:339:ASN:H	2.06	0.57
1:C:213:CYS:HB3	1:C:219:ILE:HD11	1.86	0.57
1:C:266:HIS:HB3	1:C:380:ASN:OD1	2.04	0.57
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.85	0.57
1:A:206:ASN:HD22	1:A:206:ASN:N	2.03	0.57
2:B:312:TYR:HD1	2:B:343:PHE:CE2	2.23	0.57
1:C:168:GLU:HG2	1:C:201:ALA:HB2	1.86	0.57
1:C:252:LEU:C	1:C:254:GLU:H	2.08	0.57
1:A:238:ILE:HD13	1:A:378:LEU:HD11	1.85	0.56
2:B:154:ILE:C	2:B:156:LYS:H	2.08	0.56
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.87	0.56
1:A:407:TRP:CG	2:B:257:VAL:HG23	2.39	0.56
1:C:264:ARG:O	1:C:266:HIS:CD2	2.58	0.56
2:B:244:PHE:CB	2:B:245:PRO:CD	2.78	0.56
1:C:100:ALA:HB2	1:C:105:ARG:HG2	1.88	0.56
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.87	0.56
2:D:185:TYR:HD1	2:D:408:TYR:CE1	2.24	0.56
3:E:119:MET:HA	3:E:122:ARG:NH2	2.20	0.56
2:B:151:THR:HG22	2:B:193:GLN:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:GLU:OE2	2:B:255:LEU:HD13	2.05	0.56
2:B:87:PHE:CD2	2:B:87:PHE:N	2.73	0.56
1:C:292:THR:O	1:C:295:CYS:HB2	2.06	0.56
2:B:388:PHE:CD2	2:B:425:MET:HE1	2.33	0.56
2:D:283:TYR:HD2	2:D:285:ALA:HB3	1.71	0.56
2:D:388:PHE:CD2	2:D:425:MET:HE1	2.30	0.56
1:C:67:PHE:HB2	1:C:92:LEU:CD2	2.36	0.56
1:A:263:PRO:HG3	3:E:37:ALA:HA	1.88	0.56
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.86	0.56
7:B:700:POD:H213	7:B:700:POD:O6	2.06	0.56
1:A:246:GLY:O	1:A:247:ALA:O	2.23	0.56
1:C:368:LEU:H	1:C:368:LEU:CD1	2.19	0.56
2:D:119:LEU:HD11	2:D:156:LYS:HB3	1.86	0.56
2:B:111:GLY:HA2	2:B:149:MET:HE1	1.88	0.55
1:C:240:ALA:HA	1:C:243:ARG:CD	2.36	0.55
2:D:256:ALA:C	2:D:258:ASN:H	2.09	0.55
2:D:388:PHE:CD2	2:D:425:MET:CE	2.89	0.55
1:A:24:TYR:HE2	1:A:243:ARG:NH2	1.97	0.55
2:B:101:ASN:HA	2:B:144:GLY:H	1.71	0.55
1:C:213:CYS:HB3	1:C:219:ILE:CD1	2.36	0.55
2:D:287:THR:HG22	2:D:289:PRO:HD2	1.87	0.55
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.88	0.55
1:C:206:ASN:N	1:C:206:ASN:HD22	2.05	0.55
1:C:198:SER:HB2	1:C:265:ILE:CD1	2.37	0.55
1:A:143:GLY:O	1:A:147:SER:HB3	2.05	0.55
1:A:213:CYS:HB3	1:A:219:ILE:HD11	1.88	0.55
1:A:7:ILE:HG12	1:A:66:VAL:CG2	2.37	0.55
2:B:263:PRO:C	2:B:265:LEU:H	2.08	0.55
2:D:145:THR:HG23	6:D:603:GDP:O3B	2.06	0.55
2:D:265:LEU:O	2:D:266:HIS:C	2.45	0.55
2:B:136:GLN:HG3	2:B:136:GLN:O	2.06	0.55
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.55	0.55
2:D:195:VAL:HA	2:D:265:LEU:HD23	1.88	0.55
3:E:114:ALA:C	3:E:116:LEU:H	2.10	0.55
2:B:205:ASP:OD2	2:B:207:GLU:HG3	2.07	0.55
2:B:255:LEU:CD2	2:B:259:MET:CG	2.85	0.55
1:C:100:ALA:CB	1:C:105:ARG:HG2	2.37	0.55
2:D:107:HIS:CE1	2:D:193:GLN:HE22	2.25	0.55
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.89	0.55
1:A:430:LYS:O	1:A:434:GLU:HB2	2.07	0.55
2:B:119:LEU:O	2:B:122:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:GLY:O	2:B:16:ILE:HG22	2.07	0.55
2:B:321:GLY:HA2	2:B:359:PRO:HD3	1.89	0.55
1:C:260:VAL:O	1:C:260:VAL:CG2	2.55	0.54
2:D:11:GLN:CG	2:D:74:THR:HG21	2.26	0.54
1:C:95:GLY:C	1:C:97:GLU:H	2.11	0.54
2:D:165:ILE:HD11	2:D:252:LEU:HD23	1.89	0.54
1:A:219:ILE:C	1:A:221:ARG:H	2.11	0.54
1:A:213:CYS:HB3	1:A:219:ILE:CD1	2.37	0.54
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.89	0.54
2:B:165:ILE:CG1	2:B:252:LEU:HD23	2.37	0.54
1:C:168:GLU:HG2	1:C:201:ALA:CB	2.38	0.54
1:A:353:VAL:CG2	3:E:20:PHE:CD2	2.91	0.54
1:A:3:GLU:HB2	1:A:129:CYS:SG	2.47	0.54
1:A:60:LYS:NZ	1:A:85:GLN:O	2.27	0.54
2:B:166:MET:HE2	2:B:166:MET:HA	1.89	0.54
1:C:402:ARG:O	1:C:403:ALA:C	2.45	0.54
1:A:72:PRO:HD3	1:A:96:LYS:HA	1.89	0.54
2:B:135:PHE:HB2	2:B:166:MET:CE	2.38	0.54
2:B:38:GLY:O	2:B:40:SER:N	2.37	0.54
2:D:111:GLY:HA2	2:D:149:MET:CE	2.38	0.54
2:D:336:GLN:NE2	2:D:351:VAL:HG11	2.22	0.54
1:A:174:ALA:HB1	1:A:207:GLU:HB2	1.90	0.54
2:D:267:PHE:N	2:D:267:PHE:CD1	2.76	0.54
2:D:343:PHE:O	2:D:344:VAL:C	2.46	0.54
2:B:241:CYS:HB2	7:B:700:POD:H203	1.89	0.54
1:A:154:MET:HE1	1:A:166:LYS:HD2	1.90	0.54
1:A:51:THR:CB	1:A:243:ARG:HA	2.37	0.54
2:D:177:VAL:O	2:D:177:VAL:HG12	2.08	0.54
1:A:179:THR:HG22	1:A:180:ALA:N	2.23	0.54
1:A:265:ILE:O	1:A:266:HIS:O	2.26	0.54
1:A:395:PHE:C	1:A:395:PHE:CD2	2.80	0.54
1:C:198:SER:HB2	1:C:265:ILE:HD12	1.89	0.54
3:E:27:PRO:HG2	3:E:29:PHE:CB	2.38	0.54
2:D:151:THR:HG22	2:D:193:GLN:HB3	1.90	0.54
3:E:114:ALA:O	3:E:116:LEU:N	2.41	0.54
1:A:119:LEU:CD1	1:A:156:ARG:HB3	2.38	0.53
1:C:256:GLN:C	1:C:258:ASN:N	2.61	0.53
1:C:66:VAL:HG11	1:C:122:ILE:HG22	1.90	0.53
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.42	0.53
2:B:298:ALA:HB1	2:B:306:ASP:HB3	1.89	0.53
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.90	0.53
2:B:207:GLU:HB2	2:B:304:ALA:HB2	1.89	0.53
2:D:254:LYS:O	2:D:258:ASN:HB2	2.08	0.53
2:D:371:LEU:HD13	2:D:371:LEU:H	1.73	0.53
3:E:139:LEU:HG	3:E:140:LYS:N	2.24	0.53
1:A:135:PHE:CD1	1:A:135:PHE:N	2.76	0.53
1:A:234:ILE:HG22	1:A:235:VAL:N	2.24	0.53
1:C:139:HIS:CG	1:C:150:THR:HG21	2.43	0.53
1:A:180:ALA:HB2	2:B:258:ASN:HD21	1.74	0.53
2:B:405:LEU:C	2:B:407:TRP:N	2.57	0.53
1:C:240:ALA:HA	1:C:243:ARG:HD3	1.91	0.53
1:C:253:THR:O	1:C:257:THR:HB	2.09	0.53
2:D:227:LEU:O	2:D:230:LEU:HB2	2.09	0.53
2:D:255:LEU:HD22	2:D:255:LEU:O	2.08	0.53
2:D:312:TYR:HB2	2:D:343:PHE:CD2	2.44	0.53
1:A:35:GLN:O	1:A:37:PRO:HD3	2.09	0.53
1:C:102:ASN:OD1	1:C:105:ARG:HB2	2.09	0.53
2:D:403:ALA:O	2:D:405:LEU:N	2.41	0.53
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.91	0.53
1:C:224:TYR:O	1:C:228:ASN:ND2	2.36	0.53
2:B:251:ASP:OD1	2:B:254:LYS:HG3	2.09	0.53
1:C:219:ILE:C	1:C:221:ARG:H	2.12	0.53
1:C:90:GLU:O	1:C:121:ARG:HD2	2.08	0.53
3:E:94:ILE:O	3:E:98:LYS:CB	2.56	0.53
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.43	0.53
2:B:371:LEU:H	2:B:371:LEU:HD13	1.73	0.53
2:B:66:ILE:HD11	2:B:121:VAL:HG12	1.91	0.53
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.73	0.53
2:B:38:GLY:C	2:B:40:SER:H	2.11	0.53
1:C:239:THR:O	1:C:241:SER:N	2.37	0.53
2:D:165:ILE:CD1	2:D:252:LEU:HD23	2.39	0.53
2:D:312:TYR:HD1	2:D:343:PHE:CE2	2.27	0.53
2:D:66:ILE:HD11	2:D:121:VAL:HG12	1.89	0.53
1:C:256:GLN:O	1:C:258:ASN:N	2.41	0.52
1:C:333:ALA:O	1:C:336:LYS:HB2	2.10	0.52
1:C:35:GLN:O	1:C:37:PRO:HD3	2.09	0.52
2:D:209:LEU:HD21	2:D:231:VAL:CG2	2.39	0.52
2:D:87:PHE:CD2	2:D:87:PHE:N	2.77	0.52
1:A:98:ASP:HB2	1:A:110:ILE:HD13	1.91	0.52
2:D:174:SER:OG	2:D:176:LYS:O	2.20	0.52
2:D:180:THR:CG2	2:D:182:VAL:HG22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:CYS:O	1:A:348:PRO:C	2.44	0.52
1:A:415:GLU:O	1:A:418:PHE:HB2	2.09	0.52
1:C:105:ARG:NH2	2:D:2:ARG:NH2	2.57	0.52
2:D:274:PRO:HB3	2:D:286:LEU:HD21	1.90	0.52
2:D:62:VAL:HG22	2:D:62:VAL:O	2.09	0.52
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.91	0.52
2:B:325:MET:HG2	2:B:355:VAL:HG11	1.92	0.52
2:D:255:LEU:HD22	2:D:259:MET:HG3	1.91	0.52
2:D:259:MET:HE2	2:D:378:ILE:CG2	2.39	0.52
1:A:211:ASP:O	1:A:214:ARG:HB2	2.10	0.52
2:B:12:CYS:HG	2:B:171:VAL:HG21	1.74	0.52
1:C:133:GLN:HE21	1:C:252:LEU:HG	1.75	0.52
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.75	0.52
2:D:255:LEU:CD2	2:D:259:MET:CG	2.88	0.52
2:D:87:PHE:HD2	2:D:87:PHE:H	1.55	0.52
2:B:177:VAL:CG1	2:B:177:VAL:O	2.57	0.52
1:C:9:VAL:HG11	1:C:150:THR:OG1	2.10	0.52
2:D:284:ARG:O	2:D:286:LEU:HD12	2.09	0.52
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.44	0.52
2:D:296:PHE:CE2	2:D:377:PHE:HE1	2.27	0.52
1:A:278:ALA:O	1:A:279:GLU:CB	2.58	0.52
2:B:135:PHE:CD1	2:B:135:PHE:N	2.77	0.52
3:E:119:MET:HA	3:E:122:ARG:HH21	1.75	0.52
1:A:395:PHE:CD2	1:A:396:ASP:N	2.78	0.52
2:B:111:GLY:HA2	2:B:149:MET:CE	2.39	0.52
2:B:154:ILE:O	2:B:156:LYS:N	2.43	0.52
2:B:198:THR:OG1	2:B:265:LEU:HD22	2.10	0.52
2:B:180:THR:HG23	1:C:258:ASN:ND2	2.25	0.52
1:C:102:ASN:HB2	1:C:408:TYR:CE2	2.45	0.52
2:D:142:GLY:HA3	2:D:173:PRO:HG3	1.92	0.52
1:A:432:TYR:O	1:A:433:GLU:C	2.47	0.51
1:A:53:PHE:CD1	1:A:53:PHE:N	2.78	0.51
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.91	0.51
2:B:195:VAL:CG1	2:B:196:GLU:HG2	2.40	0.51
2:D:244:PHE:CB	2:D:245:PRO:CD	2.85	0.51
1:A:137:VAL:O	1:A:137:VAL:HG12	2.11	0.51
2:B:406:HIS:HE1	2:B:407:TRP:CD1	2.28	0.51
2:B:195:VAL:HG21	2:B:428:LEU:HD13	1.93	0.51
2:B:205:ASP:OD1	2:B:207:GLU:HB2	2.11	0.51
2:B:284:ARG:O	2:B:286:LEU:N	2.44	0.51
2:D:255:LEU:CD2	2:D:259:MET:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:GLY:C	2:D:40:SER:H	2.13	0.51
1:C:180:ALA:N	1:C:183:GLU:OE1	2.44	0.51
1:C:191:THR:CG2	1:C:425:MET:HE3	2.40	0.51
2:D:251:ASP:C	2:D:253:ARG:N	2.62	0.51
1:A:11:GLN:HB3	5:A:600:GTP:O2A	2.11	0.51
2:B:388:PHE:CD2	2:B:425:MET:CE	2.91	0.51
1:C:346:TRP:CE3	1:C:347:CYS:HB2	2.46	0.51
2:D:205:ASP:OD1	2:D:207:GLU:CB	2.56	0.51
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.93	0.51
1:A:313:MET:O	1:A:314:ALA:HB2	2.10	0.51
1:C:101:ASN:H	1:C:144:GLY:HA3	1.74	0.51
2:D:264:ARG:O	2:D:266:HIS:CD2	2.64	0.51
2:D:337:ASN:C	2:D:339:ASN:H	2.14	0.51
1:A:402:ARG:O	1:A:403:ALA:C	2.49	0.51
1:C:313:MET:O	1:C:314:ALA:HB2	2.10	0.51
2:D:264:ARG:O	2:D:266:HIS:N	2.27	0.51
1:A:404:PHE:O	1:A:405:VAL:C	2.49	0.50
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.94	0.50
2:D:315:VAL:HG22	2:D:379:GLY:HA2	1.92	0.50
2:B:343:PHE:O	2:B:344:VAL:C	2.49	0.50
2:D:48:ARG:O	2:D:49:ILE:C	2.48	0.50
3:E:61:ARG:O	3:E:62:LYS:C	2.49	0.50
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.46	0.50
1:A:249:ASN:HA	1:A:254:GLU:CD	2.31	0.50
2:D:263:PRO:C	2:D:265:LEU:H	2.14	0.50
1:A:368:LEU:CD1	1:A:368:LEU:H	2.11	0.50
2:B:177:VAL:HG12	2:B:177:VAL:O	2.10	0.50
2:B:3:GLU:O	2:B:133:GLN:N	2.43	0.50
1:C:227:LEU:O	1:C:231:ILE:HG12	2.11	0.50
1:A:100:ALA:CB	1:A:105:ARG:HG2	2.41	0.50
1:A:278:ALA:C	1:A:280:LYS:H	2.14	0.50
1:C:395:PHE:C	1:C:395:PHE:CD2	2.85	0.50
1:C:406:HIS:HA	1:C:409:VAL:HG23	1.93	0.50
3:E:70:LYS:C	3:E:72:LEU:H	2.15	0.50
1:A:106:GLY:O	1:A:108:TYR:N	2.43	0.50
1:A:236:SER:HA	1:A:243:ARG:NH2	2.27	0.50
1:A:325:PRO:HB3	3:E:20:PHE:HE1	1.76	0.50
2:B:139:HIS:HE1	2:B:170:SER:OG	1.94	0.50
2:B:259:MET:HE2	2:B:378:ILE:CG2	2.40	0.50
2:D:114:LEU:O	2:D:115:VAL:C	2.49	0.50
1:A:270:ALA:HB3	1:A:302:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLY:O	2:B:147:SER:HB3	2.11	0.50
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.94	0.50
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.94	0.50
1:A:210:TYR:C	1:A:210:TYR:CD1	2.85	0.50
1:A:207:GLU:O	1:A:211:ASP:HB2	2.11	0.50
2:B:107:HIS:CE1	2:B:193:GLN:HE22	2.29	0.50
1:A:181:VAL:HG23	2:B:258:ASN:OD1	2.12	0.50
2:B:287:THR:O	2:B:288:VAL:CB	2.58	0.50
7:B:700:POD:O6	7:B:700:POD:C21	2.59	0.50
2:D:158:ARG:O	2:D:159:GLU:CB	2.51	0.50
2:D:38:GLY:O	2:D:40:SER:N	2.43	0.50
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.46	0.49
1:C:3:GLU:HB2	1:C:129:CYS:SG	2.51	0.49
1:C:185:TYR:O	1:C:189:LEU:HB2	2.11	0.49
1:A:348:PRO:CG	3:E:27:PRO:HD3	2.27	0.49
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.93	0.49
2:B:291:LEU:CD2	2:B:375:ALA:HB3	2.40	0.49
1:C:115:ILE:O	1:C:119:LEU:HB2	2.11	0.49
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.94	0.49
2:D:255:LEU:HD22	2:D:259:MET:HG2	1.94	0.49
1:A:112:LYS:HD2	3:E:58:GLU:OE1	2.12	0.49
1:A:255:PHE:O	1:A:259:LEU:HB2	2.13	0.49
1:A:287:SER:C	1:A:289:ALA:N	2.63	0.49
1:A:398:MET:CE	2:B:348:PRO:HD2	2.41	0.49
2:B:191:VAL:CG1	2:B:425:MET:HE3	2.16	0.49
1:A:387:ALA:HA	1:A:390:ARG:HD3	1.93	0.49
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.95	0.49
2:B:385:GLN:HG3	2:B:429:VAL:HG13	1.94	0.49
1:A:191:THR:HA	1:A:194:THR:CG2	2.40	0.49
1:A:133:GLN:CD	1:A:251:ASP:HA	2.32	0.49
2:B:140:SER:O	2:B:147:SER:HB2	2.13	0.49
2:B:199:ASP:N	2:B:199:ASP:OD1	2.46	0.49
2:B:408:TYR:O	2:B:409:THR:C	2.50	0.49
2:D:199:ASP:N	2:D:199:ASP:OD1	2.46	0.49
2:D:284:ARG:O	2:D:286:LEU:N	2.45	0.49
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.47	0.49
2:B:69:ASP:OD1	2:B:71:GLU:HG2	2.11	0.49
2:D:36:TYR:HD1	2:D:37:HIS:H	1.60	0.49
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.77	0.49
1:C:111:GLY:O	1:C:113:GLU:N	2.46	0.49
2:B:336:GLN:NE2	2:B:351:VAL:HG11	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:O	2:B:51:VAL:HG23	2.13	0.49
1:C:161:TYR:HB3	1:C:164:LYS:HG3	1.94	0.49
2:D:152:LEU:O	2:D:153:LEU:C	2.51	0.49
2:B:395:PHE:O	2:B:398:MET:N	2.45	0.49
1:C:287:SER:C	1:C:289:ALA:N	2.66	0.49
2:D:31:ASP:HB3	2:D:32:PRO:HD2	1.94	0.49
1:A:240:ALA:HB2	1:A:243:ARG:CZ	2.42	0.48
2:D:198:THR:OG1	2:D:265:LEU:HD22	2.13	0.48
2:D:337:ASN:HA	2:D:340:SER:HB3	1.94	0.48
1:A:102:ASN:N	1:A:102:ASN:OD1	2.46	0.48
2:B:256:ALA:O	2:B:258:ASN:N	2.41	0.48
2:B:68:VAL:HG13	2:B:118:VAL:CG2	2.36	0.48
1:C:240:ALA:HB2	1:C:243:ARG:CZ	2.30	0.48
1:A:101:ASN:ND2	2:B:254:LYS:HE2	2.28	0.48
2:B:256:ALA:C	2:B:258:ASN:H	2.15	0.48
2:B:36:TYR:HD1	2:B:37:HIS:N	2.09	0.48
1:A:295:CYS:HB3	1:A:296:PHE:HD1	1.78	0.48
2:D:140:SER:O	2:D:147:SER:HB2	2.14	0.48
2:D:188:THR:HG23	2:D:391:ILE:CD1	2.44	0.48
1:A:164:LYS:HG2	1:A:164:LYS:H	1.46	0.48
1:A:360:PRO:HD2	1:A:371:VAL:O	2.14	0.48
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.94	0.48
2:D:408:TYR:O	2:D:409:THR:C	2.52	0.48
1:A:180:ALA:N	1:A:183:GLU:OE1	2.45	0.48
2:B:11:GLN:HG2	2:B:11:GLN:O	2.12	0.48
1:C:198:SER:CB	1:C:265:ILE:CD1	2.92	0.48
1:C:98:ASP:HB2	1:C:110:ILE:HD13	1.96	0.48
2:D:102:ASN:O	2:D:105:LYS:N	2.46	0.48
1:A:174:ALA:HB2	1:A:207:GLU:H	1.78	0.48
1:C:360:PRO:HD2	1:C:371:VAL:O	2.13	0.48
1:C:415:GLU:O	1:C:418:PHE:HB2	2.13	0.48
2:D:154:ILE:C	2:D:156:LYS:H	2.17	0.48
3:E:114:ALA:C	3:E:116:LEU:N	2.66	0.48
3:E:140:LYS:O	3:E:141:GLU:C	2.52	0.48
2:B:335:VAL:C	2:B:337:ASN:H	2.17	0.48
1:A:327:ASP:O	1:A:328:VAL:C	2.51	0.48
1:C:306:ASP:HA	1:C:307:PRO:HD3	1.69	0.48
2:D:135:PHE:HB2	2:D:166:MET:CE	2.42	0.48
2:D:102:ASN:O	2:D:103:TRP:C	2.52	0.47
2:D:225:GLY:O	2:D:228:ASN:N	2.47	0.47
2:B:132:LEU:HD23	2:B:164:ARG:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:O	1:A:74:VAL:N	2.48	0.47
1:A:81:GLY:O	1:A:82:THR:C	2.51	0.47
2:B:382:THR:HA	2:B:432:TYR:CD2	2.49	0.47
1:C:250:VAL:O	1:C:251:ASP:HB3	2.14	0.47
2:B:401:ARG:NH2	1:C:434:GLU:O	2.43	0.47
2:D:324:SER:C	2:D:326:LYS:N	2.68	0.47
2:D:42:LEU:O	2:D:44:LEU:N	2.47	0.47
1:C:119:LEU:HD22	1:C:156:ARG:HE	1.78	0.47
2:D:195:VAL:HA	2:D:265:LEU:CD2	2.44	0.47
3:E:116:LEU:C	3:E:118:ALA:H	2.16	0.47
1:A:100:ALA:O	1:A:101:ASN:HB2	2.13	0.47
2:B:251:ASP:OD1	2:B:254:LYS:HE3	2.13	0.47
1:C:191:THR:O	1:C:195:LEU:HB3	2.14	0.47
2:B:157:ILE:O	2:B:158:ARG:C	2.51	0.47
2:B:306:ASP:O	2:B:307:PRO:C	2.53	0.47
2:B:381:SER:C	2:B:383:ALA:H	2.18	0.47
2:B:97:SER:OG	2:B:98:GLY:O	2.32	0.47
1:C:430:LYS:O	1:C:434:GLU:HB2	2.15	0.47
2:D:248:LEU:O	2:D:249:ASN:HB2	2.13	0.47
1:A:231:ILE:HG12	1:A:231:ILE:H	1.36	0.47
2:B:381:SER:C	2:B:383:ALA:N	2.67	0.47
1:C:72:PRO:HD3	1:C:96:LYS:HA	1.96	0.47
3:E:90:ASN:C	3:E:92:ASN:N	2.68	0.47
1:A:416:GLY:O	1:A:420:GLU:HB3	2.15	0.47
1:A:98:ASP:O	1:A:99:ALA:C	2.52	0.47
2:B:313:LEU:HB2	2:B:380:ASN:O	2.14	0.47
1:C:273:ALA:HB2	1:C:375:VAL:H	1.78	0.47
1:C:404:PHE:O	1:C:405:VAL:C	2.52	0.47
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.62	0.47
2:D:96:GLN:HA	2:D:96:GLN:OE1	2.15	0.47
3:E:127:ASP:C	3:E:129:HIS:H	2.18	0.47
1:C:198:SER:CB	1:C:265:ILE:HD11	2.44	0.47
1:C:281:ALA:HB2	1:C:369:ALA:CB	2.45	0.47
3:E:33:PRO:CB	3:E:35:PHE:CE1	2.97	0.47
1:A:350:GLY:O	1:A:351:PHE:CG	2.67	0.47
2:B:251:ASP:O	2:B:253:ARG:HB2	2.15	0.47
1:A:219:ILE:C	1:A:221:ARG:N	2.69	0.47
1:A:302:MET:HA	1:A:302:MET:HE2	1.96	0.47
2:B:159:GLU:HG3	3:E:72:LEU:HD23	1.97	0.47
1:A:176:GLN:HG2	1:A:177:VAL:N	2.30	0.46
2:B:6:HIS:HD2	2:B:136:GLN:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:CB	1:C:243:ARG:HA	2.45	0.46
2:B:248:LEU:O	2:B:249:ASN:HB2	2.15	0.46
2:B:47:GLU:HG2	2:B:47:GLU:H	1.60	0.46
1:C:102:ASN:O	1:C:105:ARG:N	2.46	0.46
1:A:66:VAL:HG11	1:A:122:ILE:HG22	1.97	0.46
1:A:95:GLY:C	1:A:97:GLU:H	2.17	0.46
1:C:355:ILE:H	1:C:355:ILE:HG13	1.54	0.46
1:C:390:ARG:H	1:C:390:ARG:HG2	1.54	0.46
2:D:132:LEU:HD23	2:D:164:ARG:HG3	1.97	0.46
2:D:48:ARG:C	2:D:50:ASN:N	2.68	0.46
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.80	0.46
1:A:224:TYR:CE2	5:A:600:GTP:C5	3.03	0.46
2:B:106:GLY:O	2:B:149:MET:HA	2.15	0.46
2:B:202:TYR:CE2	2:B:238:VAL:HG11	2.51	0.46
2:B:269:MET:CE	2:B:307:PRO:HG3	2.46	0.46
2:B:337:ASN:C	2:B:339:ASN:N	2.68	0.46
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.50	0.46
2:B:86:ILE:HG22	2:B:87:PHE:N	2.30	0.46
1:C:132:LEU:CG	1:C:133:GLN:N	2.76	0.46
7:D:701:POD:C20	7:D:701:POD:H213	2.45	0.46
1:A:171:ILE:HG23	1:A:206:ASN:HD21	1.80	0.46
1:A:223:THR:CG2	1:A:225:THR:HG23	2.46	0.46
1:A:367:ASP:H	1:A:368:LEU:HD12	1.81	0.46
1:A:406:HIS:CE1	2:B:263:PRO:HD3	2.50	0.46
1:C:143:GLY:O	1:C:147:SER:HB3	2.15	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.15	0.46
1:A:221:ARG:N	1:A:222:PRO:HD2	2.31	0.46
1:C:278:ALA:C	1:C:280:LYS:H	2.19	0.46
1:C:105:ARG:NH1	1:C:411:GLU:OE1	2.37	0.46
1:C:416:GLY:O	1:C:420:GLU:HB3	2.15	0.46
2:D:111:GLY:HA2	2:D:149:MET:HE1	1.98	0.46
2:D:132:LEU:HD23	2:D:164:ARG:CD	2.46	0.46
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.50	0.46
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.46	0.46
2:B:100:GLY:O	2:B:101:ASN:HB2	2.15	0.46
2:B:296:PHE:CE2	2:B:377:PHE:CE1	3.04	0.46
1:C:27:GLU:CD	1:C:320:ARG:HH22	2.19	0.46
2:D:308:ARG:CA	2:D:308:ARG:HH11	2.29	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HB2	2.51	0.46
1:A:316:CYS:O	1:A:377:MET:HA	2.15	0.46
1:A:311:LYS:H	1:A:382:THR:HG23	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASP:C	2:B:307:PRO:O	2.50	0.46
2:B:424:ASN:O	2:B:427:ASP:HB2	2.15	0.46
2:D:325:MET:HG2	2:D:355:VAL:HG11	1.98	0.46
1:A:163:LYS:H	1:A:163:LYS:HE3	1.80	0.46
2:B:132:LEU:HD23	2:B:164:ARG:CD	2.46	0.46
2:B:83:PHE:HD2	2:B:83:PHE:HA	1.71	0.46
2:D:238:VAL:HG13	2:D:378:ILE:CD1	2.44	0.46
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.81	0.46
1:A:151:SER:OG	1:A:193:THR:HB	2.16	0.46
1:A:221:ARG:N	1:A:222:PRO:CD	2.79	0.46
1:A:288:VAL:HA	1:A:291:ILE:CD1	2.45	0.46
2:B:255:LEU:HD22	2:B:255:LEU:O	2.15	0.46
2:B:60:LYS:O	2:B:61:TYR:HD2	1.99	0.46
1:C:256:GLN:HB3	1:C:257:THR:H	1.58	0.46
2:D:277:SER:O	2:D:278:ARG:CG	2.52	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.26	0.46
1:A:240:ALA:CA	1:A:243:ARG:CG	2.75	0.45
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.98	0.45
2:B:165:ILE:HG21	2:B:253:ARG:HD3	1.98	0.45
1:C:174:ALA:O	1:C:176:GLN:N	2.49	0.45
2:D:2:ARG:HB2	2:D:133:GLN:HG3	1.97	0.45
2:D:48:ARG:O	2:D:50:ASN:N	2.50	0.45
2:B:320:ARG:NH1	2:B:360:PRO:HG3	2.30	0.45
2:D:195:VAL:HG12	2:D:196:GLU:HG2	1.99	0.45
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.81	0.45
2:B:253:ARG:HG3	2:B:253:ARG:HH11	1.81	0.45
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.84	0.45
2:D:12:CYS:HG	2:D:171:VAL:HG21	1.81	0.45
2:B:312:TYR:HB2	2:B:343:PHE:CD2	2.51	0.45
2:D:119:LEU:CD1	2:D:156:LYS:HB3	2.46	0.45
3:E:33:PRO:O	3:E:34:GLU:CB	2.65	0.45
1:A:100:ALA:HB2	1:A:105:ARG:HG2	1.98	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:CB	2.83	0.45
1:A:287:SER:O	1:A:289:ALA:N	2.50	0.45
1:A:287:SER:O	1:A:290:GLU:N	2.49	0.45
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.32	0.45
2:B:180:THR:HG22	2:B:182:VAL:H	1.81	0.45
2:B:347:ILE:O	2:B:348:PRO:C	2.55	0.45
2:B:86:ILE:HG22	2:B:87:PHE:CD2	2.51	0.45
1:C:62:VAL:CG2	1:C:91:GLN:HE22	2.30	0.45
2:B:191:VAL:CG1	2:B:425:MET:CE	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLN:O	1:C:236:SER:HB3	2.17	0.45
1:A:185:TYR:CD1	1:A:418:PHE:HE2	2.34	0.45
2:B:393:GLU:O	2:B:393:GLU:HG3	2.15	0.45
2:B:185:TYR:HD1	2:B:408:TYR:CE1	2.35	0.45
1:C:108:TYR:CD2	3:E:108:ASN:ND2	2.85	0.45
1:C:107:HIS:CD2	1:C:108:TYR:CE1	2.99	0.45
1:C:11:GLN:HB3	5:C:601:GTP:O2A	2.17	0.45
1:C:406:HIS:HA	1:C:409:VAL:CG2	2.47	0.45
1:C:7:ILE:HG12	1:C:66:VAL:HG23	1.99	0.45
2:D:104:ALA:HB2	2:D:408:TYR:HD2	1.82	0.45
2:D:93:VAL:HG21	2:D:118:VAL:HG22	1.99	0.45
2:B:133:GLN:HE21	2:B:252:LEU:CB	2.24	0.45
2:B:96:GLN:O	2:B:97:SER:O	2.35	0.45
3:E:136:ASN:ND2	3:E:139:LEU:HD23	2.32	0.45
1:A:90:GLU:O	1:A:121:ARG:HD2	2.17	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.45
1:C:168:GLU:CG	1:C:201:ALA:HB1	2.47	0.45
1:C:386:GLU:O	1:C:390:ARG:HG2	2.16	0.45
1:C:398:MET:CE	2:D:348:PRO:HD2	2.46	0.45
1:C:53:PHE:CD1	1:C:53:PHE:N	2.84	0.45
2:D:255:LEU:CD2	2:D:259:MET:HG2	2.47	0.45
2:D:359:PRO:HB3	2:D:371:LEU:O	2.17	0.45
2:D:259:MET:CE	2:D:378:ILE:CG2	2.94	0.45
3:E:27:PRO:O	3:E:28:SER:CB	2.64	0.45
1:A:198:SER:OG	1:A:265:ILE:HD12	2.16	0.44
1:A:208:ALA:O	1:A:212:ILE:HD12	2.16	0.44
1:A:234:ILE:HG13	1:A:272:TYR:HB2	1.98	0.44
2:B:316:ALA:HB1	7:B:700:POD:C22	2.47	0.44
1:C:68:VAL:CG1	1:C:118:VAL:HG21	2.46	0.44
1:C:405:VAL:CG1	1:C:406:HIS:H	2.28	0.44
1:C:432:TYR:O	1:C:433:GLU:C	2.55	0.44
3:E:90:ASN:O	3:E:91:ASN:C	2.54	0.44
1:A:392:ASP:O	1:A:395:PHE:HB3	2.17	0.44
2:B:260:VAL:HG12	2:B:266:HIS:HB2	1.98	0.44
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.82	0.44
2:D:112:ALA:CB	3:E:134:ARG:HH22	2.30	0.44
2:D:245:PRO:HB2	2:D:246:GLY:H	1.58	0.44
2:B:158:ARG:HD2	2:B:197:ASN:CB	2.47	0.44
2:B:227:LEU:O	2:B:230:LEU:HB2	2.18	0.44
2:B:335:VAL:O	2:B:339:ASN:HB2	2.17	0.44
1:C:392:ASP:O	1:C:395:PHE:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:N	1:C:70:LEU:CD1	2.79	0.44
3:E:136:ASN:OD1	3:E:139:LEU:CD2	2.65	0.44
2:B:153:LEU:O	2:B:157:ILE:HG12	2.16	0.44
2:B:263:PRO:O	2:B:265:LEU:N	2.35	0.44
1:C:120:ASP:O	1:C:122:ILE:N	2.51	0.44
2:D:306:ASP:OD2	2:D:306:ASP:N	2.50	0.44
2:D:402:LYS:O	2:D:403:ALA:O	2.34	0.44
2:D:406:HIS:CE1	2:D:407:TRP:CD1	3.05	0.44
1:A:88:HIS:O	1:A:91:GLN:HG3	2.17	0.44
2:B:262:PHE:O	2:B:263:PRO:C	2.56	0.44
2:B:32:PRO:HA	2:B:83:PHE:CD2	2.53	0.44
1:C:176:GLN:HG2	1:C:177:VAL:N	2.33	0.44
1:C:16:ILE:HG22	1:C:17:GLY:N	2.32	0.44
1:C:350:GLY:O	1:C:351:PHE:CG	2.70	0.44
2:D:195:VAL:CG1	2:D:196:GLU:HG2	2.48	0.44
2:B:347:ILE:CG2	2:B:347:ILE:O	2.63	0.44
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.95	0.44
2:B:427:ASP:O	2:B:430:SER:N	2.51	0.44
1:C:284:GLU:O	1:C:285:GLN:CB	2.65	0.44
1:C:405:VAL:O	1:C:407:TRP:N	2.51	0.44
2:D:135:PHE:CD1	2:D:135:PHE:N	2.86	0.44
2:D:236:SER:OG	2:D:237:GLY:N	2.51	0.44
2:D:6:HIS:HD2	2:D:136:GLN:HG3	1.83	0.44
1:A:258:ASN:OD1	1:A:352:LYS:HG3	2.18	0.44
2:B:194:LEU:HD22	2:B:194:LEU:HA	1.89	0.44
2:B:324:SER:C	2:B:326:LYS:N	2.71	0.44
2:B:375:ALA:C	2:B:376:THR:HG22	2.37	0.44
1:C:154:MET:HE1	1:C:166:LYS:HD2	1.99	0.44
2:D:287:THR:O	2:D:288:VAL:CB	2.66	0.44
2:D:335:VAL:O	2:D:339:ASN:HB2	2.18	0.44
1:A:107:HIS:CD2	1:A:108:TYR:CE1	2.99	0.43
2:D:134:GLY:HA3	2:D:165:ILE:O	2.18	0.43
2:D:36:TYR:CE1	2:D:38:GLY:O	2.71	0.43
3:E:6:MET:O	3:E:7:GLU:O	2.34	0.43
2:B:315:VAL:O	2:B:351:VAL:HA	2.19	0.43
2:B:402:LYS:O	2:B:403:ALA:O	2.36	0.43
1:C:142:GLY:HA3	1:C:183:GLU:HG3	2.00	0.43
1:C:346:TRP:CZ3	1:C:347:CYS:HB2	2.52	0.43
2:D:204:ILE:N	2:D:204:ILE:HD12	2.34	0.43
1:A:353:VAL:HG23	3:E:20:PHE:CD2	2.54	0.43
2:B:102:ASN:O	2:B:103:TRP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:C	2:B:156:LYS:N	2.71	0.43
2:B:217:LEU:O	2:B:219:LEU:N	2.50	0.43
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.53	0.43
2:B:195:VAL:HA	2:B:265:LEU:HD23	2.00	0.43
2:B:93:VAL:HG21	2:B:118:VAL:HG22	2.00	0.43
1:C:304:LYS:O	1:C:305:CYS:HB3	2.19	0.43
2:D:206:ASN:HA	2:D:209:LEU:HB2	2.00	0.43
2:D:242:LEU:HA	2:D:249:ASN:O	2.18	0.43
2:D:20:PHE:CZ	2:D:24:ILE:HG21	2.52	0.43
3:E:70:LYS:O	3:E:74:GLU:HB2	2.18	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.43
1:A:25:CYS:O	1:A:26:LEU:C	2.56	0.43
1:A:21:TRP:CH2	1:A:63:PRO:CB	3.02	0.43
2:B:104:ALA:HB2	2:B:408:TYR:HD2	1.82	0.43
2:B:232:SER:OG	2:B:233:ALA:N	2.50	0.43
2:B:406:HIS:C	2:B:406:HIS:ND1	2.72	0.43
1:C:163:LYS:O	1:C:164:LYS:C	2.57	0.43
1:C:206:ASN:H	1:C:206:ASN:HD22	1.65	0.43
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.80	0.43
1:C:270:ALA:O	1:C:302:MET:HB2	2.19	0.43
1:C:72:PRO:O	1:C:74:VAL:N	2.51	0.43
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.46	0.43
1:C:252:LEU:O	1:C:253:THR:C	2.57	0.43
3:E:33:PRO:HB2	3:E:34:GLU:H	1.63	0.43
1:A:70:LEU:HB2	1:A:145:THR:HG21	2.01	0.43
2:D:312:TYR:CD1	2:D:343:PHE:CE2	3.06	0.43
2:D:86:ILE:HG22	2:D:87:PHE:CD2	2.53	0.43
1:A:191:THR:O	1:A:195:LEU:HB3	2.19	0.43
1:A:168:GLU:HG2	1:A:201:ALA:CB	2.49	0.43
1:A:206:ASN:C	1:A:208:ALA:N	2.72	0.43
1:A:38:SER:O	1:A:39:ASP:C	2.56	0.43
2:B:185:TYR:HD1	2:B:408:TYR:HE1	1.67	0.43
1:C:106:GLY:O	1:C:108:TYR:N	2.51	0.43
1:C:375:VAL:HG12	1:C:376:CYS:N	2.30	0.43
1:C:377:MET:O	1:C:377:MET:CG	2.66	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.43
2:B:88:ARG:HG2	2:B:89:PRO:HD2	2.00	0.43
1:C:177:VAL:O	1:C:177:VAL:HG12	2.19	0.43
1:C:262:TYR:O	1:C:263:PRO:C	2.55	0.43
1:C:288:VAL:HA	1:C:291:ILE:CD1	2.47	0.43
1:C:302:MET:HE2	1:C:302:MET:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:HIS:CE1	2:D:263:PRO:HD3	2.54	0.43
2:D:325:MET:HA	2:D:328:VAL:HB	2.01	0.43
2:D:273:ALA:CB	2:D:375:ALA:H	2.31	0.43
3:E:90:ASN:C	3:E:92:ASN:H	2.21	0.43
1:A:226:ASN:HD22	1:A:226:ASN:HA	1.66	0.43
2:B:205:ASP:HB3	2:B:303:ALA:HA	2.01	0.43
2:B:407:TRP:HH2	1:C:256:GLN:HB3	1.84	0.43
2:D:139:HIS:HD2	2:D:146:GLY:O	2.00	0.43
2:D:96:GLN:HB3	2:D:97:SER:H	1.66	0.43
1:A:139:HIS:CG	1:A:150:THR:HG21	2.54	0.43
1:A:266:HIS:O	1:A:268:PRO:HD3	2.19	0.43
1:A:387:ALA:HA	1:A:390:ARG:HH11	1.84	0.43
2:B:109:THR:HB	2:B:110:GLU:H	1.72	0.43
2:B:306:ASP:OD2	2:B:306:ASP:N	2.51	0.43
1:C:103:TYR:CD1	1:C:148:GLY:HA2	2.53	0.43
1:C:281:ALA:HB2	1:C:369:ALA:HB3	2.01	0.43
1:C:387:ALA:HA	1:C:390:ARG:HH11	1.84	0.43
2:D:158:ARG:HD2	2:D:197:ASN:CB	2.46	0.43
3:E:109:LYS:O	3:E:113:GLU:HB2	2.19	0.43
2:B:174:SER:CB	2:B:207:GLU:HG2	2.49	0.42
2:D:269:MET:CE	2:D:307:PRO:HG3	2.49	0.42
2:D:273:ALA:HB2	2:D:375:ALA:H	1.84	0.42
2:D:315:VAL:O	2:D:351:VAL:HA	2.18	0.42
2:D:67:LEU:HD12	2:D:92:PHE:HD2	1.82	0.42
2:B:273:ALA:CB	2:B:375:ALA:H	2.32	0.42
2:D:151:THR:CG2	2:D:193:GLN:HB3	2.49	0.42
2:B:165:ILE:HD11	2:B:252:LEU:HD23	2.00	0.42
2:B:339:ASN:HD22	2:B:339:ASN:HA	1.68	0.42
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.67	0.42
1:C:287:SER:O	1:C:290:GLU:N	2.53	0.42
1:C:88:HIS:CD2	1:C:89:PRO:HD2	2.54	0.42
2:D:164:ARG:HG2	2:D:164:ARG:H	1.51	0.42
2:D:112:ALA:HB2	3:E:134:ARG:HH22	1.83	0.42
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.42
2:B:152:LEU:HD12	2:B:152:LEU:O	2.19	0.42
2:B:315:VAL:HG22	2:B:379:GLY:HA2	2.02	0.42
2:B:317:ALA:O	2:B:353:THR:HA	2.19	0.42
2:B:67:LEU:HD12	2:B:92:PHE:HD2	1.82	0.42
1:C:22:GLU:HB2	1:C:83:TYR:CE1	2.53	0.42
2:D:253:ARG:HH11	2:D:253:ARG:HG3	1.85	0.42
2:D:332:MET:CG	2:D:353:THR:HG21	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:O	1:A:176:GLN:N	2.52	0.42
2:D:347:ILE:CG2	2:D:347:ILE:O	2.65	0.42
1:A:287:SER:C	1:A:289:ALA:H	2.21	0.42
2:B:391:ILE:HD11	2:B:425:MET:CE	2.50	0.42
1:C:168:GLU:HG3	1:C:201:ALA:HB1	2.02	0.42
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.85	0.42
1:C:327:ASP:O	1:C:328:VAL:C	2.57	0.42
2:D:273:ALA:HB2	2:D:375:ALA:O	2.20	0.42
2:D:54:ASN:O	2:D:62:VAL:O	2.38	0.42
1:A:154:MET:HE2	1:A:154:MET:HB3	1.97	0.42
2:B:183:GLU:O	2:B:184:PRO:C	2.58	0.42
2:B:408:TYR:C	2:B:410:GLY:N	2.69	0.42
1:C:205:ASP:OD1	1:C:207:GLU:N	2.52	0.42
1:C:236:SER:O	1:C:243:ARG:NH1	2.52	0.42
2:D:385:GLN:HG3	2:D:429:VAL:HG13	2.01	0.42
2:D:7:ILE:HA	2:D:66:ILE:HG22	2.02	0.42
3:E:63:TYR:O	3:E:66:ALA:N	2.53	0.42
1:A:190:THR:HG22	1:A:191:THR:N	2.34	0.42
1:A:347:CYS:C	1:A:348:PRO:O	2.53	0.42
2:B:225:GLY:O	2:B:228:ASN:N	2.52	0.42
2:B:312:TYR:CD1	2:B:343:PHE:CE2	3.07	0.42
1:C:428:LEU:O	1:C:431:ASP:HB2	2.20	0.42
2:D:274:PRO:HB3	2:D:286:LEU:CD2	2.50	0.42
1:A:117:LEU:O	1:A:120:ASP:HB3	2.19	0.42
1:A:132:LEU:CG	1:A:133:GLN:N	2.78	0.42
1:A:17:GLY:O	1:A:19:ALA:N	2.53	0.42
2:B:151:THR:CG2	2:B:193:GLN:HB3	2.49	0.42
2:B:21:TRP:O	2:B:25:SER:HB2	2.20	0.42
2:B:254:LYS:O	2:B:258:ASN:HB2	2.19	0.42
1:C:105:ARG:HD2	1:C:411:GLU:OE1	2.19	0.42
2:D:132:LEU:HD23	2:D:164:ARG:CG	2.50	0.42
2:D:377:PHE:C	2:D:377:PHE:CD2	2.93	0.42
2:D:47:GLU:HG2	2:D:47:GLU:H	1.56	0.42
1:A:428:LEU:O	1:A:431:ASP:HB2	2.20	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.58	0.42
2:B:119:LEU:HD11	2:B:156:LYS:HB3	2.02	0.42
1:C:135:PHE:CD1	1:C:135:PHE:N	2.87	0.42
1:C:138:PHE:N	1:C:138:PHE:CD1	2.88	0.42
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.75	0.42
1:C:210:TYR:C	1:C:210:TYR:CD1	2.92	0.42
1:C:219:ILE:C	1:C:221:ARG:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.02	0.42
2:D:272:PHE:CD2	2:D:273:ALA:N	2.88	0.42
2:D:287:THR:CB	2:D:290:GLU:HG3	2.46	0.42
2:D:380:ASN:HA	2:D:380:ASN:HD22	1.55	0.42
2:B:20:PHE:CZ	2:B:24:ILE:HG21	2.55	0.41
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.54	0.41
2:D:256:ALA:C	2:D:258:ASN:N	2.73	0.41
3:E:94:ILE:HG22	3:E:95:LYS:N	2.35	0.41
1:A:138:PHE:N	1:A:138:PHE:CD1	2.89	0.41
1:A:381:THR:HG23	1:A:381:THR:O	2.19	0.41
1:A:88:HIS:H	1:A:91:GLN:NE2	2.18	0.41
2:B:31:ASP:HB2	2:B:34:GLY:HA3	2.00	0.41
2:B:145:THR:HG23	6:B:602:GDP:O3B	2.20	0.41
1:C:396:ASP:OD1	1:C:422:ARG:NE	2.46	0.41
2:D:119:LEU:O	2:D:122:VAL:HG22	2.20	0.41
2:D:274:PRO:HG3	2:D:286:LEU:HD22	2.02	0.41
2:D:403:ALA:C	2:D:405:LEU:H	2.23	0.41
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.78	0.41
1:C:273:ALA:CB	1:C:375:VAL:N	2.76	0.41
1:C:395:PHE:HD2	1:C:396:ASP:N	2.18	0.41
2:D:111:GLY:O	2:D:149:MET:HE1	2.19	0.41
2:D:16:ILE:CG2	2:D:17:GLY:N	2.83	0.41
2:D:298:ALA:C	2:D:300:ASN:H	2.23	0.41
2:D:298:ALA:CB	2:D:306:ASP:HB3	2.50	0.41
3:E:58:GLU:HB2	3:E:61:ARG:NH2	2.34	0.41
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.03	0.41
1:A:210:TYR:C	1:A:210:TYR:HD1	2.23	0.41
1:A:398:MET:HE3	2:B:348:PRO:HD2	2.01	0.41
1:C:9:VAL:CG1	1:C:150:THR:OG1	2.69	0.41
1:C:21:TRP:HZ3	1:C:53:PHE:CZ	2.38	0.41
1:C:256:GLN:O	1:C:257:THR:C	2.59	0.41
1:C:311:LYS:H	1:C:382:THR:HG23	1.86	0.41
1:C:69:ASP:C	1:C:70:LEU:HD12	2.40	0.41
2:D:269:MET:HE1	2:D:307:PRO:HG3	2.02	0.41
2:D:224:TYR:OH	6:D:603:GDP:H2'	2.19	0.41
1:A:182:VAL:HG23	1:A:186:ASN:ND2	2.35	0.41
1:A:270:ALA:HB3	1:A:302:MET:CG	2.49	0.41
1:A:346:TRP:CZ3	1:A:347:CYS:HB2	2.55	0.41
1:A:62:VAL:CG2	1:A:91:GLN:HE22	2.34	0.41
2:B:318:VAL:HG11	7:B:700:POD:H211	2.02	0.41
1:C:242:LEU:HA	1:C:250:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:CYS:O	2:D:131:CYS:SG	2.79	0.41
2:D:2:ARG:HD3	2:D:133:GLN:HG3	2.02	0.41
1:A:284:GLU:O	1:A:285:GLN:CB	2.69	0.41
2:B:118:VAL:O	2:B:120:ASP:N	2.54	0.41
2:B:165:ILE:HG21	2:B:253:ARG:CD	2.51	0.41
1:C:287:SER:HB2	1:C:290:GLU:H	1.85	0.41
1:C:277:SER:HA	1:C:367:ASP:O	2.21	0.41
2:D:13:GLY:HA3	2:D:139:HIS:HA	2.02	0.41
2:D:204:ILE:H	2:D:204:ILE:HD12	1.85	0.41
2:D:82:PRO:HB2	2:D:83:PHE:H	1.49	0.41
1:A:111:GLY:O	1:A:113:GLU:N	2.54	0.41
1:A:141:PHE:CE2	1:A:191:THR:HB	2.56	0.41
1:A:262:TYR:O	1:A:263:PRO:C	2.58	0.41
1:A:377:MET:HE3	1:A:377:MET:HA	2.03	0.41
1:A:385:ALA:O	1:A:386:GLU:C	2.58	0.41
2:B:308:ARG:NH1	2:B:308:ARG:HA	2.19	0.41
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.38	0.41
1:C:345:ASP:HB3	1:C:346:TRP:CD1	2.55	0.41
2:B:41:ASP:O	2:B:42:LEU:C	2.59	0.41
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.54	0.41
1:A:355:ILE:HG13	1:A:355:ILE:H	1.45	0.41
1:A:91:GLN:O	1:A:92:LEU:HD23	2.21	0.41
2:B:146:GLY:HA2	2:B:150:GLY:H	1.85	0.41
2:B:164:ARG:H	2:B:164:ARG:HG2	1.70	0.41
2:B:245:PRO:HB2	2:B:246:GLY:H	1.65	0.41
1:C:240:ALA:HB2	1:C:243:ARG:HD3	2.03	0.41
1:C:278:ALA:O	1:C:279:GLU:CB	2.69	0.41
2:D:135:PHE:HB2	2:D:166:MET:HE1	2.03	0.41
2:D:10:GLY:O	2:D:13:GLY:N	2.53	0.41
1:C:105:ARG:HH12	2:D:253:ARG:HH22	1.69	0.41
1:A:345:ASP:HB3	1:A:346:TRP:CD1	2.56	0.41
2:B:188:THR:HG23	2:B:391:ILE:CD1	2.51	0.41
1:C:108:TYR:O	1:C:112:LYS:HB2	2.21	0.41
2:B:264:ARG:C	2:B:266:HIS:CD2	2.95	0.41
1:C:266:HIS:CB	1:C:380:ASN:OD1	2.67	0.41
1:C:26:LEU:HD21	1:C:364:PRO:HD3	2.03	0.41
1:C:98:ASP:O	1:C:99:ALA:C	2.59	0.41
2:D:3:GLU:HA	2:D:51:VAL:HG13	2.03	0.41
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.85	0.40
2:B:139:HIS:CE1	2:B:170:SER:OG	2.74	0.40
2:B:224:TYR:O	2:B:228:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:MET:HA	2:B:328:VAL:HB	2.02	0.40
2:B:325:MET:CG	2:B:355:VAL:HG11	2.51	0.40
2:B:75:MET:HG2	2:B:75:MET:H	1.69	0.40
1:C:2:ARG:HB2	1:C:131:GLY:O	2.21	0.40
1:C:180:ALA:O	1:C:181:VAL:C	2.57	0.40
2:B:141:LEU:O	2:B:187:ALA:HA	2.22	0.40
2:B:210:TYR:O	2:B:213:CYS:HB2	2.21	0.40
2:D:313:LEU:HB2	2:D:380:ASN:O	2.22	0.40
3:E:8:VAL:HA	3:E:21:GLU:O	2.21	0.40
1:A:118:VAL:HG12	1:A:119:LEU:N	2.35	0.40
1:A:230:LEU:O	1:A:230:LEU:HD12	2.21	0.40
1:A:265:ILE:O	1:A:266:HIS:C	2.59	0.40
2:B:165:ILE:CD1	2:B:252:LEU:HD23	2.51	0.40
2:B:392:SER:O	2:B:396:THR:N	2.44	0.40
2:D:109:THR:HB	2:D:110:GLU:H	1.73	0.40
1:A:177:VAL:O	1:A:177:VAL:HG12	2.22	0.40
1:A:319:TYR:HB2	1:A:355:ILE:HA	2.02	0.40
2:B:209:LEU:HD21	2:B:231:VAL:CG2	2.49	0.40
2:B:391:ILE:HD11	2:B:425:MET:SD	2.61	0.40
1:C:256:GLN:O	1:C:259:LEU:N	2.41	0.40
1:C:291:ILE:HB	1:C:375:VAL:HG23	2.03	0.40
2:D:187:ALA:O	2:D:191:VAL:HB	2.22	0.40
2:D:165:ILE:HG21	2:D:253:ARG:HD3	2.03	0.40
2:D:106:GLY:O	2:D:149:MET:HA	2.22	0.40
1:C:180:ALA:HB1	2:D:258:ASN:HD21	1.84	0.40
2:D:50:ASN:HB3	2:D:51:VAL:H	1.73	0.40
2:D:63:PRO:CD	2:D:86:ILE:HG23	2.51	0.40
3:E:81:GLU:HA	3:E:84:GLN:HB3	2.04	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	429/451 (95%)	288 (67%)	88 (20%)	53 (12%)	0	5
1	C	426/451 (94%)	289 (68%)	90 (21%)	47 (11%)	0	8
2	B	418/445 (94%)	274 (66%)	87 (21%)	57 (14%)	0	4
2	D	424/445 (95%)	276 (65%)	87 (20%)	61 (14%)	0	4
3	E	130/142 (92%)	81 (62%)	29 (22%)	20 (15%)	0	3
All	All	1827/1934 (94%)	1208 (66%)	381 (21%)	238 (13%)	0	5

All (238) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	47	ASP
1	A	62	VAL
1	A	73	THR
1	A	96	LYS
1	A	99	ALA
1	A	100	ALA
1	A	112	LYS
1	A	129	CYS
1	A	247	ALA
1	A	273	ALA
1	A	284	GLU
1	A	345	ASP
1	A	348	PRO
1	A	403	ALA
1	A	437	VAL
2	B	34	GLY
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	50	ASN
2	B	60	LYS
2	B	62	VAL
2	B	72	PRO
2	B	73	GLY
2	B	82	PRO
2	B	97	SER
2	B	115	VAL
2	B	145	THR
2	B	217	LEU
2	B	226	ASP

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Mol	Chain	Res	Type
2	B	240	THR
2	B	244	PHE
2	B	265	LEU
2	B	266	HIS
2	B	273	ALA
2	B	285	ALA
2	B	288	VAL
2	B	308	ARG
2	B	343	PHE
2	B	350	ASN
2	B	360	PRO
2	B	369	ARG
2	B	371	LEU
2	B	400	ARG
2	B	403	ALA
2	B	404	PHE
2	B	406	HIS
1	C	62	VAL
1	C	73	THR
1	C	96	LYS
1	C	99	ALA
1	C	100	ALA
1	C	112	LYS
1	C	129	CYS
1	C	256	GLN
1	C	257	THR
1	C	265	ILE
1	C	273	ALA
1	C	284	GLU
1	C	345	ASP
1	C	351	PHE
1	C	403	ALA
1	C	437	VAL
2	D	34	GLY
2	D	42	LEU
2	D	43	GLN
2	D	50	ASN
2	D	60	LYS
2	D	62	VAL
2	D	72	PRO
2	D	73	GLY
2	D	82	PRO

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Mol	Chain	Res	Type
2	D	97	SER
2	D	115	VAL
2	D	145	THR
2	D	217	LEU
2	D	226	ASP
2	D	227	LEU
2	D	240	THR
2	D	244	PHE
2	D	265	LEU
2	D	266	HIS
2	D	273	ALA
2	D	277	SER
2	D	280	SER
2	D	285	ALA
2	D	288	VAL
2	D	308	ARG
2	D	343	PHE
2	D	344	VAL
2	D	350	ASN
2	D	360	PRO
2	D	371	LEU
2	D	400	ARG
2	D	403	ALA
2	D	406	HIS
3	E	7	GLU
3	E	28	SER
3	E	34	GLU
3	E	63	TYR
3	E	64	GLN
3	E	68	LEU
1	A	32	PRO
1	A	72	PRO
1	A	101	ASN
1	A	144	GLY
1	A	222	PRO
1	A	239	THR
1	A	245	ASP
1	A	249	ASN
1	A	251	ASP
1	A	264	ARG
1	A	265	ILE
1	A	285	GLN

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Mol	Chain	Res	Type
1	A	351	PHE
1	A	377	MET
1	A	386	GLU
1	A	405	VAL
2	B	99	ALA
2	B	103	TRP
2	B	109	THR
2	B	144	GLY
2	B	155	SER
2	B	157	ILE
2	B	159	GLU
2	B	227	LEU
2	B	245	PRO
2	B	264	ARG
2	B	344	VAL
2	B	370	GLY
1	C	72	PRO
1	C	107	HIS
1	C	120	ASP
1	C	144	GLY
1	C	175	PRO
1	C	222	PRO
1	C	239	THR
1	C	285	GLN
1	C	357	TYR
1	C	386	GLU
2	D	11	GLN
2	D	39	ASP
2	D	103	TRP
2	D	159	GLU
2	D	245	PRO
2	D	257	VAL
2	D	264	ARG
2	D	276	THR
2	D	370	GLY
2	D	402	LYS
2	D	404	PHE
3	E	9	ILE
3	E	32	VAL
3	E	33	PRO
3	E	91	ASN
3	E	115	HIS

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Mol	Chain	Res	Type
1	A	46	ASP
1	A	107	HIS
1	A	120	ASP
1	A	207	GLU
1	A	248	LEU
1	A	314	ALA
1	A	326	LYS
1	A	396	ASP
2	B	11	GLN
2	B	218	LYS
2	B	257	VAL
2	B	299	LYS
2	B	305	CYS
2	B	402	LYS
1	C	32	PRO
1	C	33	ASP
1	C	98	ASP
1	C	101	ASN
1	C	251	ASP
1	C	253	THR
1	C	264	ARG
1	C	305	CYS
1	C	314	ALA
1	C	377	MET
1	C	405	VAL
2	D	109	THR
2	D	144	GLY
2	D	218	LYS
2	D	278	ARG
2	D	299	LYS
2	D	305	CYS
2	D	336	GLN
3	E	21	GLU
3	E	36	ASN
3	E	71	HIS
1	A	83	TYR
1	A	175	PRO
1	A	305	CYS
1	A	432	TYR
2	B	223	THR
2	B	248	LEU
2	B	336	GLN

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Mol	Chain	Res	Type
1	C	59	GLY
1	C	83	TYR
1	C	163	LYS
1	C	200	CYS
1	C	248	LEU
2	D	59	ASN
2	D	99	ALA
2	D	251	ASP
2	D	325	MET
2	D	369	ARG
3	E	20	PHE
3	E	90	ASN
3	E	123	LEU
3	E	138	GLU
1	A	266	HIS
1	A	357	TYR
1	A	370	LYS
2	B	59	ASN
2	B	252	LEU
1	C	121	ARG
1	C	124	LYS
1	C	146	GLY
2	D	248	LEU
2	D	338	LYS
3	E	50	ILE
1	A	146	GLY
1	A	274	PRO
2	B	96	GLN
1	C	106	GLY
1	A	328	VAL
2	B	13	GLY
1	A	250	VAL
3	E	31	GLY
1	A	59	GLY
1	C	274	PRO
2	D	13	GLY
2	D	157	ILE
1	A	221	ARG
2	D	307	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/378 (90%)	217 (64%)	125 (36%)	0	1
1	C	340/378 (90%)	219 (64%)	121 (36%)	0	1
2	B	343/381 (90%)	216 (63%)	127 (37%)	0	0
2	D	348/381 (91%)	214 (62%)	134 (38%)	0	0
3	E	65/126 (52%)	45 (69%)	20 (31%)	0	2
All	All	1438/1644 (88%)	911 (63%)	527 (37%)	0	1

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	15	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	53	PHE
1	A	60	LYS
1	A	66	VAL
1	A	68	VAL
1	A	71	GLU
1	A	73	THR
1	A	74	VAL
1	A	77	GLU
1	A	82	THR
1	A	84	ARG
1	A	88	HIS
1	A	91	GLN
1	A	94	THR
1	A	96	LYS
1	A	105	ARG
1	A	110	ILE

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Mol	Chain	Res	Type
1	A	112	LYS
1	A	113	GLU
1	A	115	ILE
1	A	125	LEU
1	A	127	ASP
1	A	128	GLN
1	A	129	CYS
1	A	132	LEU
1	A	135	PHE
1	A	138	PHE
1	A	140	SER
1	A	141	PHE
1	A	147	SER
1	A	151	SER
1	A	153	LEU
1	A	154	MET
1	A	155	GLU
1	A	156	ARG
1	A	157	LEU
1	A	163	LYS
1	A	166	LYS
1	A	172	TYR
1	A	178	SER
1	A	183	GLU
1	A	187	SER
1	A	190	THR
1	A	192	HIS
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	200	CYS
1	A	203	MET
1	A	205	ASP
1	A	206	ASN
1	A	210	TYR
1	A	211	ASP
1	A	212	ILE
1	A	215	ARG
1	A	219	ILE
1	A	224	TYR
1	A	225	THR

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Mol	Chain	Res	Type
1	A	226	ASN
1	A	227	LEU
1	A	229	ARG
1	A	230	LEU
1	A	231	ILE
1	A	234	ILE
1	A	238	ILE
1	A	242	LEU
1	A	243	ARG
1	A	249	ASN
1	A	258	ASN
1	A	260	VAL
1	A	271	THR
1	A	275	VAL
1	A	277	SER
1	A	280	LYS
1	A	284	GLU
1	A	287	SER
1	A	290	GLU
1	A	292	THR
1	A	295	CYS
1	A	302	MET
1	A	313	MET
1	A	315	CYS
1	A	316	CYS
1	A	318	LEU
1	A	329	ASN
1	A	341	ILE
1	A	343	PHE
1	A	349	THR
1	A	351	PHE
1	A	353	VAL
1	A	355	ILE
1	A	356	ASN
1	A	362	VAL
1	A	363	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	376	CYS
1	A	377	MET
1	A	379	SER

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Mol	Chain	Res	Type
1	A	380	ASN
1	A	381	THR
1	A	382	THR
1	A	384	ILE
1	A	390	ARG
1	A	394	LYS
1	A	396	ASP
1	A	397	LEU
1	A	401	LYS
1	A	413	MET
1	A	414	GLU
1	A	419	SER
1	A	423	GLU
1	A	430	LYS
1	A	432	TYR
1	A	433	GLU
1	A	434	GLU
1	A	438	ASP
2	B	4	ILE
2	B	15	GLN
2	B	16	ILE
2	B	23	VAL
2	B	24	ILE
2	B	25	SER
2	B	26	ASP
2	B	27	GLU
2	B	33	THR
2	B	36	TYR
2	B	41	ASP
2	B	42	LEU
2	B	44	LEU
2	B	47	GLU
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	66	ILE
2	B	74	THR
2	B	75	MET
2	B	76	ASP
2	B	80	SER
2	B	83	PHE

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Mol	Chain	Res	Type
2	B	86	ILE
2	B	87	PHE
2	B	88	ARG
2	B	90	ASP
2	B	94	PHE
2	B	97	SER
2	B	101	ASN
2	B	105	LYS
2	B	109	THR
2	B	110	GLU
2	B	120	ASP
2	B	122	VAL
2	B	128	SER
2	B	129	CYS
2	B	131	CYS
2	B	135	PHE
2	B	137	LEU
2	B	140	SER
2	B	145	THR
2	B	149	MET
2	B	151	THR
2	B	153	LEU
2	B	155	SER
2	B	156	LYS
2	B	159	GLU
2	B	163	ASP
2	B	164	ARG
2	B	166	MET
2	B	170	SER
2	B	171	VAL
2	B	178	SER
2	B	183	GLU
2	B	188	THR
2	B	191	VAL
2	B	192	HIS
2	B	193	GLN
2	B	194	LEU
2	B	195	VAL
2	B	197	ASN
2	B	199	ASP
2	B	201	THR
2	B	203	CYS

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Mol	Chain	Res	Type
2	B	205	ASP
2	B	212	ILE
2	B	216	THR
2	B	220	THR
2	B	223	THR
2	B	224	TYR
2	B	229	HIS
2	B	231	VAL
2	B	232	SER
2	B	236	SER
2	B	240	THR
2	B	242	LEU
2	B	248	LEU
2	B	251	ASP
2	B	252	LEU
2	B	253	ARG
2	B	255	LEU
2	B	258	ASN
2	B	265	LEU
2	B	267	PHE
2	B	269	MET
2	B	275	LEU
2	B	282	GLN
2	B	286	LEU
2	B	287	THR
2	B	291	LEU
2	B	292	THR
2	B	302	MET
2	B	305	CYS
2	B	306	ASP
2	B	308	ARG
2	B	313	LEU
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	336	GLN
2	B	342	TYR
2	B	343	PHE
2	B	350	ASN
2	B	353	THR
2	B	357	ASP
2	B	371	LEU

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Mol	Chain	Res	Type
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	378	ILE
2	B	380	ASN
2	B	382	THR
2	B	384	ILE
2	B	385	GLN
2	B	386	GLU
2	B	401	ARG
2	B	402	LYS
2	B	405	LEU
2	B	406	HIS
2	B	409	THR
2	B	414	ASP
2	B	416	MET
2	B	419	THR
2	B	425	MET
2	B	430	SER
1	C	2	ARG
1	C	4	CYS
1	C	16	ILE
1	C	22	GLU
1	C	23	LEU
1	C	26	LEU
1	C	53	PHE
1	C	66	VAL
1	C	68	VAL
1	C	74	VAL
1	C	77	GLU
1	C	82	THR
1	C	84	ARG
1	C	88	HIS
1	C	91	GLN
1	C	92	LEU
1	C	94	THR
1	C	96	LYS
1	C	98	ASP
1	C	105	ARG
1	C	110	ILE
1	C	112	LYS
1	C	113	GLU

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Mol	Chain	Res	Type
1	C	114	ILE
1	C	115	ILE
1	C	125	LEU
1	C	127	ASP
1	C	128	GLN
1	C	129	CYS
1	C	132	LEU
1	C	135	PHE
1	C	140	SER
1	C	141	PHE
1	C	147	SER
1	C	151	SER
1	C	153	LEU
1	C	154	MET
1	C	155	GLU
1	C	156	ARG
1	C	157	LEU
1	C	163	LYS
1	C	166	LYS
1	C	172	TYR
1	C	178	SER
1	C	183	GLU
1	C	187	SER
1	C	190	THR
1	C	192	HIS
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	198	SER
1	C	199	ASP
1	C	200	CYS
1	C	203	MET
1	C	205	ASP
1	C	206	ASN
1	C	210	TYR
1	C	211	ASP
1	C	212	ILE
1	C	219	ILE
1	C	224	TYR
1	C	225	THR
1	C	226	ASN

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Mol	Chain	Res	Type
1	C	227	LEU
1	C	229	ARG
1	C	231	ILE
1	C	234	ILE
1	C	242	LEU
1	C	243	ARG
1	C	249	ASN
1	C	250	VAL
1	C	251	ASP
1	C	252	LEU
1	C	256	GLN
1	C	257	THR
1	C	258	ASN
1	C	275	VAL
1	C	280	LYS
1	C	284	GLU
1	C	287	SER
1	C	290	GLU
1	C	292	THR
1	C	295	CYS
1	C	302	MET
1	C	305	CYS
1	C	313	MET
1	C	316	CYS
1	C	318	LEU
1	C	341	ILE
1	C	343	PHE
1	C	344	VAL
1	C	349	THR
1	C	353	VAL
1	C	355	ILE
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	382	THR
1	C	384	ILE

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Mol	Chain	Res	Type
1	C	390	ARG
1	C	394	LYS
1	C	396	ASP
1	C	397	LEU
1	C	401	LYS
1	C	413	MET
1	C	414	GLU
1	C	419	SER
1	C	423	GLU
1	C	430	LYS
1	C	432	TYR
1	C	433	GLU
1	C	434	GLU
1	C	438	ASP
2	D	4	ILE
2	D	12	CYS
2	D	15	GLN
2	D	16	ILE
2	D	23	VAL
2	D	24	ILE
2	D	25	SER
2	D	26	ASP
2	D	27	GLU
2	D	33	THR
2	D	36	TYR
2	D	41	ASP
2	D	42	LEU
2	D	44	LEU
2	D	47	GLU
2	D	51	VAL
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	66	ILE
2	D	75	MET
2	D	76	ASP
2	D	80	SER
2	D	83	PHE
2	D	86	ILE
2	D	87	PHE
2	D	88	ARG
2	D	90	ASP

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Mol	Chain	Res	Type
2	D	94	PHE
2	D	97	SER
2	D	101	ASN
2	D	105	LYS
2	D	109	THR
2	D	110	GLU
2	D	120	ASP
2	D	122	VAL
2	D	128	SER
2	D	129	CYS
2	D	131	CYS
2	D	135	PHE
2	D	137	LEU
2	D	140	SER
2	D	145	THR
2	D	149	MET
2	D	151	THR
2	D	153	LEU
2	D	155	SER
2	D	156	LYS
2	D	163	ASP
2	D	164	ARG
2	D	166	MET
2	D	170	SER
2	D	171	VAL
2	D	177	VAL
2	D	178	SER
2	D	181	VAL
2	D	183	GLU
2	D	188	THR
2	D	191	VAL
2	D	192	HIS
2	D	193	GLN
2	D	194	LEU
2	D	195	VAL
2	D	197	ASN
2	D	199	ASP
2	D	201	THR
2	D	203	CYS
2	D	205	ASP
2	D	216	THR
2	D	220	THR

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Mol	Chain	Res	Type
2	D	223	THR
2	D	224	TYR
2	D	229	HIS
2	D	232	SER
2	D	236	SER
2	D	240	THR
2	D	242	LEU
2	D	248	LEU
2	D	251	ASP
2	D	252	LEU
2	D	253	ARG
2	D	255	LEU
2	D	258	ASN
2	D	265	LEU
2	D	267	PHE
2	D	268	PHE
2	D	269	MET
2	D	275	LEU
2	D	278	ARG
2	D	280	SER
2	D	281	GLN
2	D	286	LEU
2	D	287	THR
2	D	291	LEU
2	D	292	THR
2	D	302	MET
2	D	306	ASP
2	D	308	ARG
2	D	313	LEU
2	D	320	ARG
2	D	322	ARG
2	D	323	MET
2	D	325	MET
2	D	331	GLN
2	D	336	GLN
2	D	338	LYS
2	D	342	TYR
2	D	343	PHE
2	D	345	GLU
2	D	350	ASN
2	D	353	THR
2	D	357	ASP

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Mol	Chain	Res	Type
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	382	THR
2	D	384	ILE
2	D	385	GLN
2	D	386	GLU
2	D	390	ARG
2	D	392	SER
2	D	401	ARG
2	D	402	LYS
2	D	405	LEU
2	D	406	HIS
2	D	414	ASP
2	D	416	MET
2	D	419	THR
2	D	425	MET
2	D	430	SER
3	E	6	MET
3	E	10	GLU
3	E	35	PHE
3	E	55	GLU
3	E	58	GLU
3	E	69	LEU
3	E	78	HIS
3	E	93	PHE
3	E	94	ILE
3	E	101	LEU
3	E	105	MET
3	E	109	LYS
3	E	112	ARG
3	E	113	GLU
3	E	116	LEU
3	E	122	ARG
3	E	124	GLN
3	E	126	LYS
3	E	134	ARG
3	E	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	88	HIS
1	A	91	GLN
1	A	101	ASN
1	A	107	HIS
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	ASN
1	A	301	GLN
1	A	329	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	107	HIS
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	206	ASN
2	B	266	HIS
2	B	294	GLN
2	B	300	ASN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	406	HIS
1	C	8	HIS
1	C	11	GLN
1	C	88	HIS
1	C	91	GLN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	216	ASN
1	C	258	ASN
1	C	301	GLN
2	D	6	HIS
2	D	8	GLN

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Mol	Chain	Res	Type
2	D	14	ASN
2	D	43	GLN
2	D	107	HIS
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	193	GLN
2	D	206	ASN
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	300	ASN
2	D	309	HIS
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
3	E	78	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 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
7	POD	D	701	-	34,34,34	3.27	12 (35%)	51,51,51	4.08	21 (41%)
6	GDP	D	603	-	24,30,30	0.98	1 (4%)	31,47,47	2.09	8 (25%)
5	GTP	C	601	4	26,34,34	1.22	3 (11%)	33,54,54	2.08	11 (33%)
7	POD	B	700	-	34,34,34	3.27	11 (32%)	51,51,51	4.32	25 (49%)
5	GTP	A	600	4	26,34,34	1.09	1 (3%)	33,54,54	2.18	8 (24%)
6	GDP	B	602	-	24,30,30	1.17	2 (8%)	31,47,47	2.34	10 (32%)

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
7	POD	D	701	-	1/1/5/5	6/10/45/45	0/5/5/5
6	GDP	D	603	-	-	4/12/32/32	0/3/3/3
5	GTP	C	601	4	-	7/18/38/38	0/3/3/3
7	POD	B	700	-	1/1/5/5	6/10/45/45	0/5/5/5
5	GTP	A	600	4	-	8/18/38/38	0/3/3/3
6	GDP	B	602	-	-	4/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	POD	C7-C6	-10.83	1.21	1.39
7	B	700	POD	C7-C6	-9.64	1.23	1.39
7	D	701	POD	C7-C2	-9.57	1.21	1.38
7	B	700	POD	C7-C2	-9.09	1.22	1.38
7	B	700	POD	C10-C13	-6.41	1.42	1.51
7	B	700	POD	C10-C11	-5.79	1.45	1.56
7	D	701	POD	C10-C13	-4.91	1.44	1.51
7	D	701	POD	O4-C13	4.70	1.45	1.35
7	B	700	POD	O1-C3	4.65	1.45	1.38
7	D	701	POD	O1-C3	4.56	1.45	1.38
7	D	701	POD	C10-C11	-4.35	1.48	1.56
7	B	700	POD	O4-C13	3.95	1.43	1.35
7	B	700	POD	C14-C11	-3.95	1.47	1.52
7	D	701	POD	C3-C2	-3.91	1.29	1.39
6	B	602	GDP	C6-N1	3.78	1.39	1.33
7	B	700	POD	O2-C2	3.72	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	POD	C3-C2	-3.59	1.30	1.39
7	D	701	POD	O2-C2	3.14	1.42	1.38
6	D	603	GDP	C6-N1	3.08	1.38	1.33
7	D	701	POD	C14-C11	-3.05	1.48	1.52
5	C	601	GTP	C6-N1	3.00	1.38	1.33
5	A	600	GTP	C6-N1	2.72	1.37	1.33
7	B	700	POD	C10-C9	-2.58	1.49	1.54
6	B	602	GDP	C2-N1	2.50	1.39	1.35
7	B	700	POD	C16-C17	-2.46	1.35	1.41
7	D	701	POD	C16-C17	-2.43	1.35	1.41
5	C	601	GTP	O4'-C4'	-2.42	1.39	1.45
5	C	601	GTP	C2'-C1'	-2.15	1.50	1.53
7	D	701	POD	C18-C17	-2.09	1.36	1.41
7	D	701	POD	C4-C3	-2.06	1.35	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	POD	C2-C7-C6	13.71	149.06	119.42
7	D	701	POD	C2-C7-C6	13.16	147.85	119.42
7	D	701	POD	C7-C6-C5	-12.51	103.81	120.26
7	B	700	POD	C7-C6-C5	-12.19	104.22	120.26
7	B	700	POD	C7-C2-C3	-11.24	107.77	122.02
7	D	701	POD	C7-C2-C3	-9.90	109.47	122.02
7	B	700	POD	C9-C10-C11	9.75	131.61	113.21
7	D	701	POD	C9-C10-C11	9.27	130.69	113.21
7	B	700	POD	O2-C2-C7	8.32	138.97	127.85
7	D	701	POD	O2-C2-C7	8.19	138.81	127.85
6	B	602	GDP	N3-C2-N1	-6.64	118.36	127.22
7	D	701	POD	O4-C13-O5	6.56	128.22	121.42
7	B	700	POD	O4-C13-O5	6.43	128.09	121.42
5	A	600	GTP	N3-C2-N1	-6.27	118.86	127.22
6	D	603	GDP	N3-C2-N1	-6.18	118.98	127.22
7	B	700	POD	C20-O6-C16	5.88	126.40	117.53
5	C	601	GTP	N3-C2-N1	-5.65	119.68	127.22
5	A	600	GTP	C2-N3-C4	5.49	121.63	115.36
7	B	700	POD	C21-O7-C17	5.20	129.02	114.78
7	D	701	POD	C21-O7-C17	4.95	128.34	114.78
6	D	603	GDP	C2-N3-C4	4.86	120.91	115.36
7	B	700	POD	C10-C9-C8	4.82	117.66	109.67
7	B	700	POD	O5-C13-C10	-4.64	123.42	129.38
6	B	602	GDP	C2-N3-C4	4.62	120.63	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	POD	C10-C9-C8	4.52	117.15	109.67
7	D	701	POD	C9-C10-C13	4.33	108.87	103.07
7	B	700	POD	C12-C9-C8	4.27	127.07	117.50
5	C	601	GTP	C2-N3-C4	4.18	120.13	115.36
7	D	701	POD	C14-C11-C10	-4.14	106.73	113.31
7	D	701	POD	C6-C5-C11	4.00	124.96	114.40
7	B	700	POD	C9-C10-C13	3.94	108.34	103.07
5	A	600	GTP	C6-C5-C4	-3.92	117.06	120.80
6	B	602	GDP	C6-N1-C2	3.90	122.12	115.93
7	D	701	POD	C12-C9-C8	3.88	126.20	117.50
7	D	701	POD	C5-C6-C8	3.82	131.08	121.66
7	B	700	POD	C5-C6-C8	3.80	131.01	121.66
7	B	700	POD	C6-C5-C11	3.78	124.38	114.40
7	B	700	POD	C14-C11-C10	-3.77	107.32	113.31
7	B	700	POD	O1-C3-C4	3.67	132.75	127.85
6	B	602	GDP	C5-C6-N1	-3.63	118.47	123.43
7	D	701	POD	C12-O4-C13	3.61	113.57	110.28
7	D	701	POD	O5-C13-C10	-3.56	124.80	129.38
6	D	603	GDP	C5-C6-N1	-3.50	118.65	123.43
5	C	601	GTP	C6-C5-C4	-3.47	117.49	120.80
5	A	600	GTP	C1'-N9-C4	-3.46	120.56	126.64
7	B	700	POD	C12-C9-C10	3.43	106.75	101.79
5	C	601	GTP	PB-O3B-PG	-3.39	121.20	132.83
5	A	600	GTP	PB-O3B-PG	-3.36	121.29	132.83
6	D	603	GDP	C6-N1-C2	3.30	121.18	115.93
6	B	602	GDP	N2-C2-N3	-3.28	112.45	117.79
7	D	701	POD	C12-C9-C10	3.26	106.51	101.79
5	C	601	GTP	C1'-N9-C4	-3.25	120.93	126.64
6	B	602	GDP	PA-O3A-PB	-3.24	121.71	132.83
5	C	601	GTP	N2-C2-N1	3.09	122.06	117.25
7	B	700	POD	O2-C2-C3	3.05	113.26	109.78
6	B	602	GDP	O4'-C1'-C2'	3.03	111.35	106.93
6	D	603	GDP	O3B-PB-O3A	2.99	114.65	104.64
5	C	601	GTP	C2'-C3'-C4'	2.93	108.33	102.64
7	D	701	POD	O1-C3-C4	2.90	131.74	127.85
5	A	600	GTP	N2-C2-N1	2.83	121.65	117.25
5	C	601	GTP	C6-N1-C2	2.77	120.32	115.93
5	A	600	GTP	O3G-PG-O3B	2.71	113.72	104.64
7	D	701	POD	C4-C3-C2	-2.70	118.59	122.02
7	D	701	POD	C7-C6-C8	2.62	125.04	119.37
7	B	700	POD	C12-O4-C13	2.61	112.66	110.28
7	B	700	POD	C19-C14-C11	2.57	125.41	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	603	GDP	C3'-C2'-C1'	2.56	104.83	100.98
6	B	602	GDP	C2'-C3'-C4'	2.52	107.55	102.64
6	B	602	GDP	C1'-N9-C4	-2.52	122.22	126.64
5	A	600	GTP	C2'-C3'-C4'	2.48	107.47	102.64
6	B	602	GDP	C6-C5-C4	-2.48	118.43	120.80
7	B	700	POD	C7-C6-C8	2.48	124.72	119.37
7	D	701	POD	C19-C14-C11	2.45	125.17	120.39
5	C	601	GTP	O3G-PG-O3B	2.36	112.56	104.64
5	C	601	GTP	C5-C6-N1	-2.34	120.23	123.43
6	D	603	GDP	C4-C5-N7	-2.28	107.02	109.40
7	B	700	POD	C6-C8-C9	-2.23	106.05	110.79
7	D	701	POD	O4-C13-C10	-2.13	106.47	109.52
7	B	700	POD	C4-C3-C2	-2.12	119.33	122.02
6	D	603	GDP	O4'-C4'-C3'	2.11	109.29	105.11
5	C	601	GTP	O2G-PG-O3B	2.11	111.72	104.64
7	B	700	POD	O3-C8-C6	2.07	114.58	110.49
7	B	700	POD	C19-C18-C17	2.03	122.52	120.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	701	POD	C10
7	B	700	POD	C10

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	603	GDP	PA-O3A-PB-O2B
6	D	603	GDP	PA-O3A-PB-O3B
6	D	603	GDP	O4'-C4'-C5'-O5'
6	D	603	GDP	C3'-C4'-C5'-O5'
5	C	601	GTP	C3'-C4'-C5'-O5'
5	A	600	GTP	C3'-C4'-C5'-O5'
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	PA-O3A-PB-O3B
6	B	602	GDP	O4'-C4'-C5'-O5'
6	B	602	GDP	C3'-C4'-C5'-O5'
7	B	700	POD	C17-C16-O6-C20
7	D	701	POD	C17-C16-O6-C20
7	D	701	POD	C17-C18-O8-C22
7	B	700	POD	C17-C18-O8-C22
7	D	701	POD	C18-C17-O7-C21

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Mol	Chain	Res	Type	Atoms
5	C	601	GTP	O4'-C4'-C5'-O5'
5	A	600	GTP	O4'-C4'-C5'-O5'
7	D	701	POD	C19-C18-O8-C22
7	B	700	POD	C19-C18-O8-C22
7	D	701	POD	C15-C16-O6-C20
7	B	700	POD	C15-C16-O6-C20
7	B	700	POD	C18-C17-O7-C21
7	D	701	POD	C16-C17-O7-C21
7	B	700	POD	C16-C17-O7-C21
5	C	601	GTP	PB-O3B-PG-O1G
5	A	600	GTP	PB-O3B-PG-O1G
5	C	601	GTP	PB-O3B-PG-O3G
5	A	600	GTP	PB-O3B-PG-O3G
5	A	600	GTP	C5'-O5'-PA-O3A
5	C	601	GTP	C5'-O5'-PA-O2A
5	A	600	GTP	C5'-O5'-PA-O2A
5	C	601	GTP	PB-O3A-PA-O1A
5	A	600	GTP	PB-O3A-PA-O1A
5	C	601	GTP	PA-O3A-PB-O2B
5	A	600	GTP	PA-O3A-PB-O2B

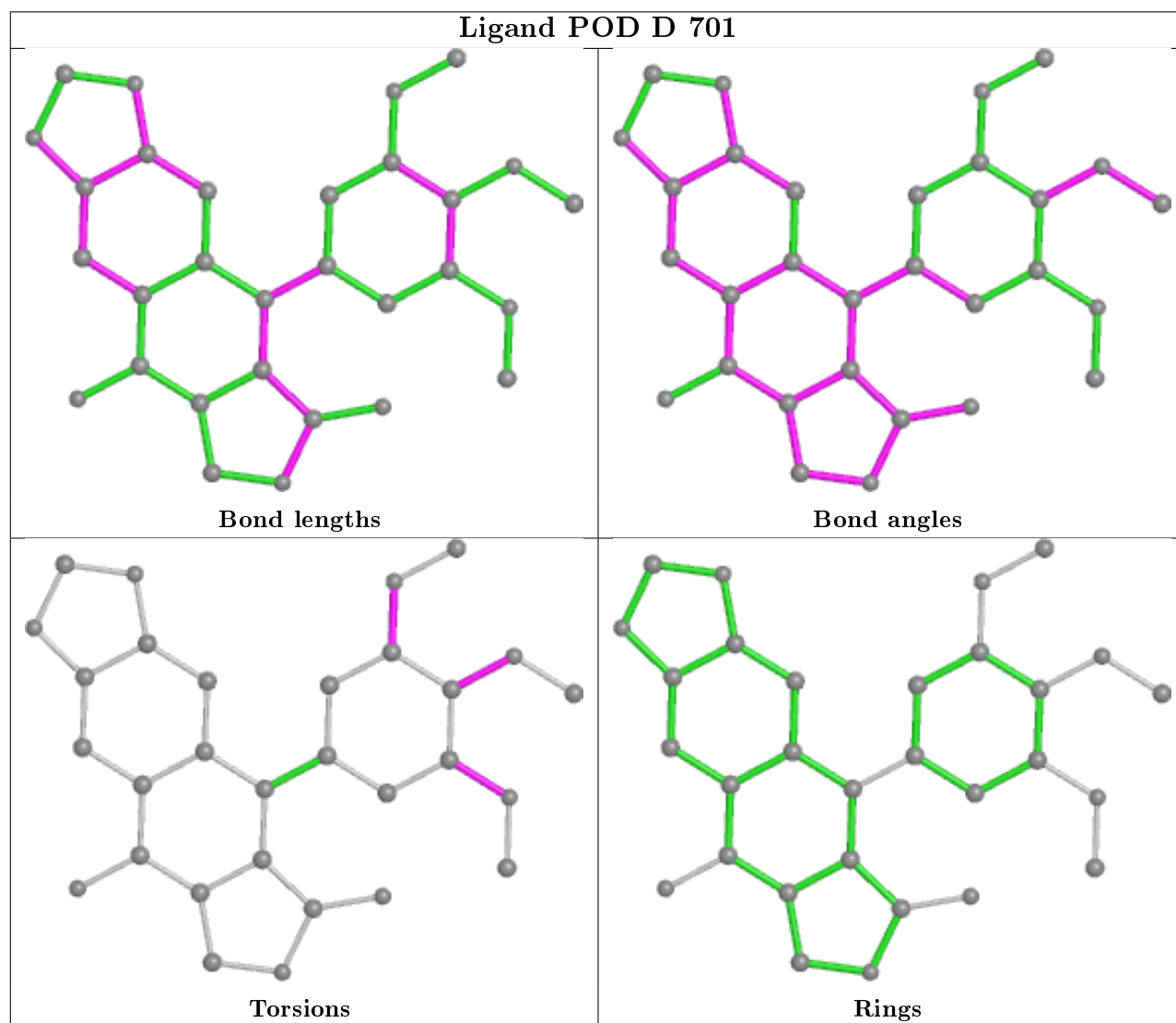
There are no ring outliers.

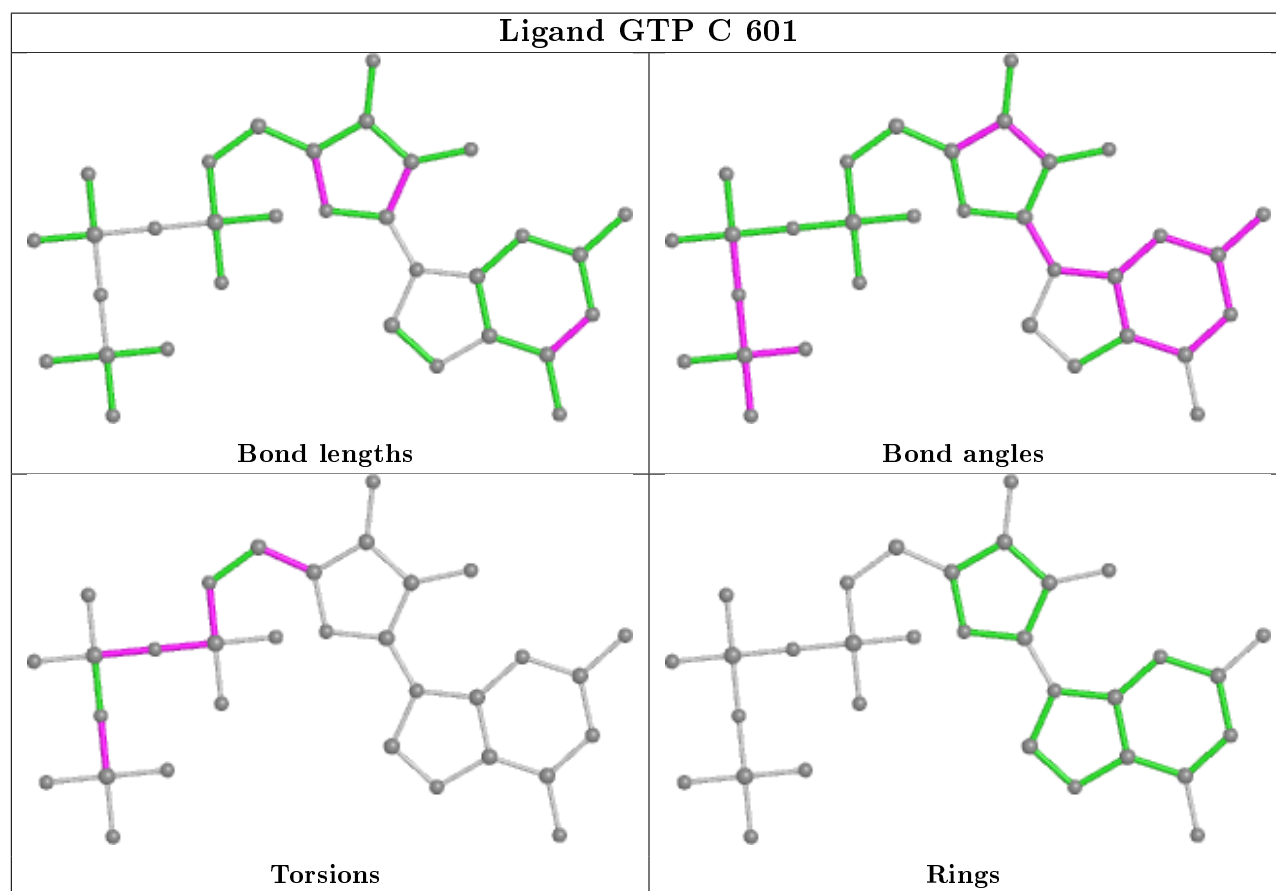
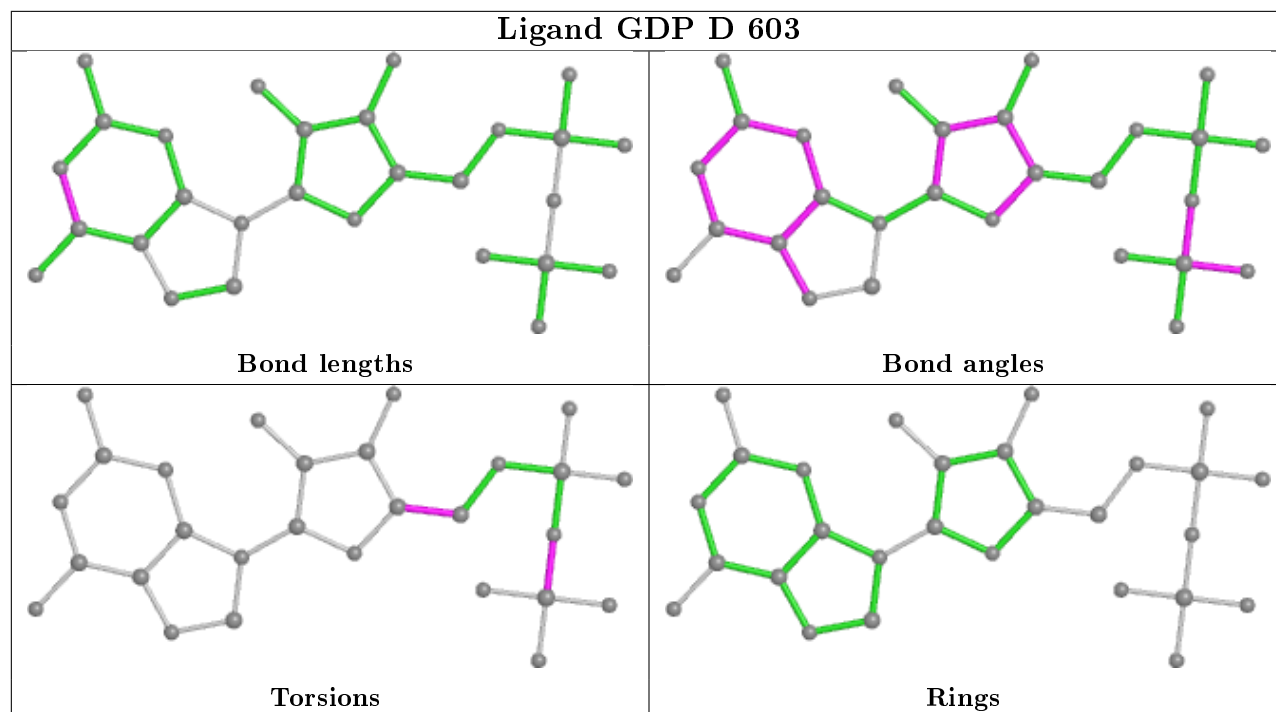
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	701	POD	4	0
6	D	603	GDP	2	0
5	C	601	GTP	2	0
7	B	700	POD	5	0
5	A	600	GTP	3	0
6	B	602	GDP	1	0

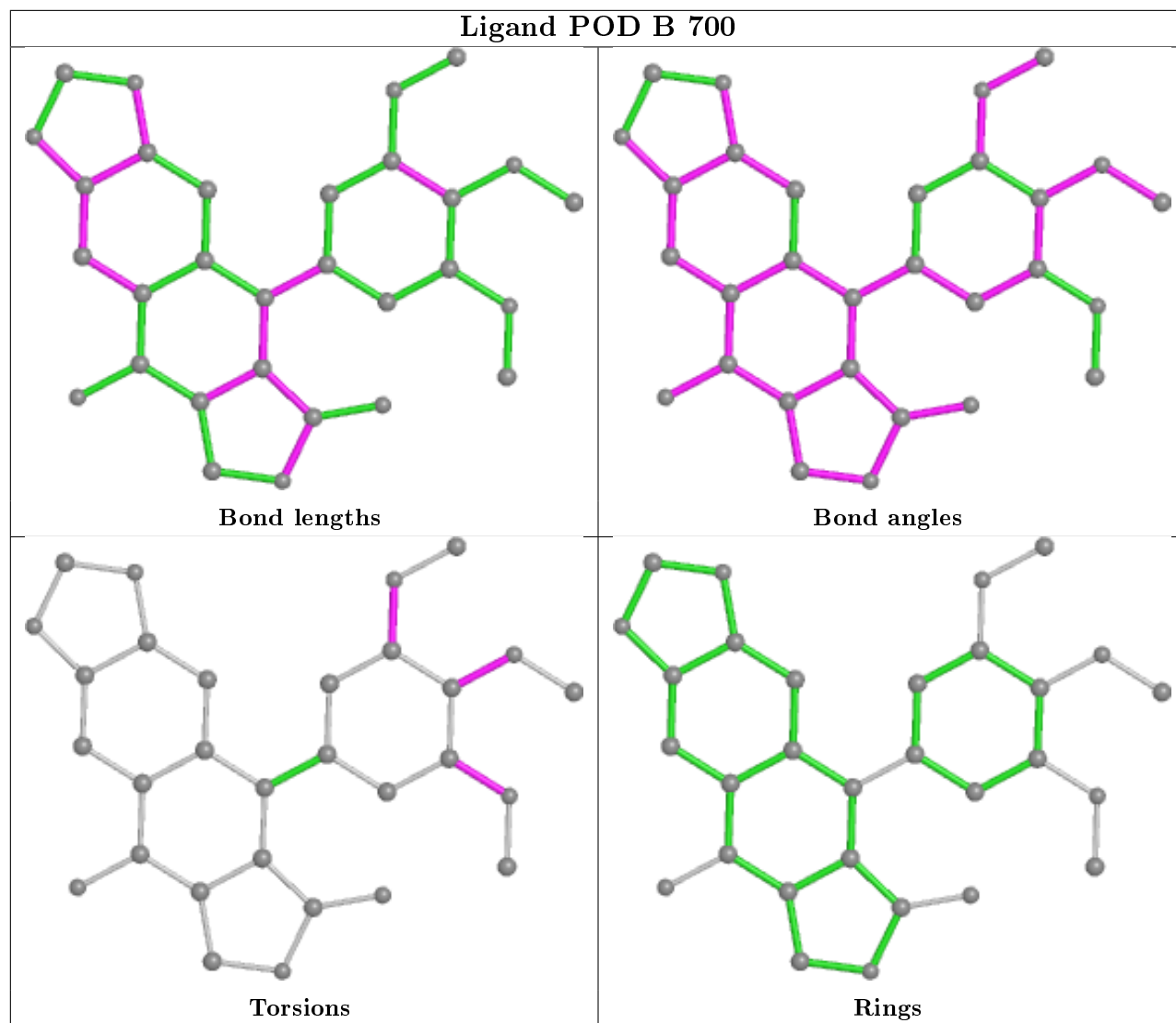
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

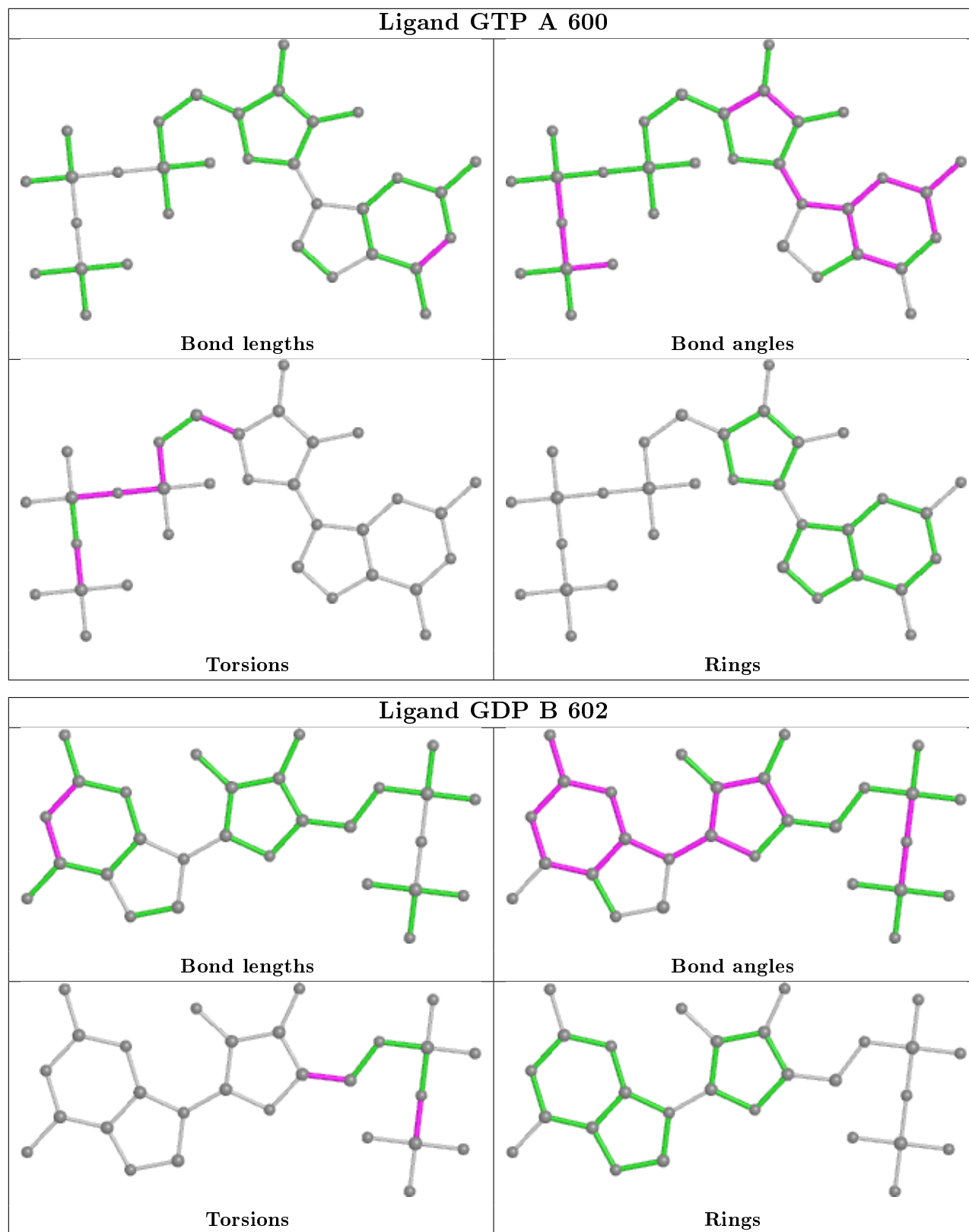
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.