



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GJX  
Title : Crystal Structure of the Nuclear Export Complex CRM1-Snurportin1-RanGTP  
Authors : Monecke, T.; Guettler, T.; Neumann, P.; Dickmanns, A.; Goerlich, D.; Ficner, R.  
Deposited on : 2009-03-09  
Resolution : 2.50 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

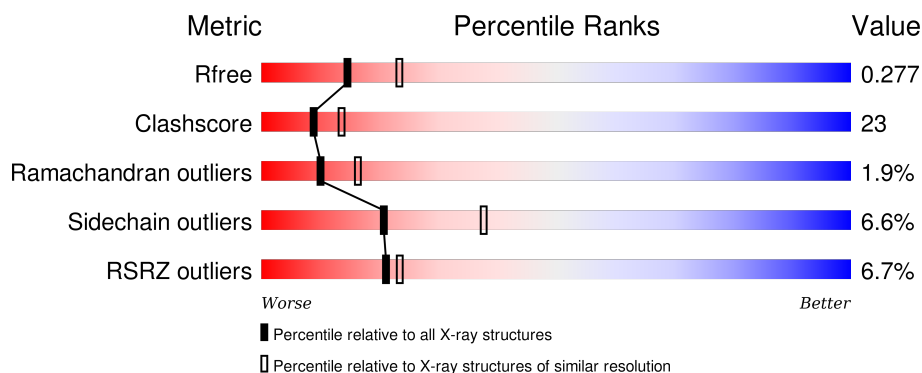
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	B	365	<div> <div>2%</div> <div>44% 26% 5% • 25%</div> </div>
1	E	365	<div> <div>3%</div> <div>43% 30% • 24%</div> </div>
2	C	216	<div> <div>%</div> <div>47% 28% • 21%</div> </div>
2	F	216	<div> <div></div> <div>53% 23% • 21%</div> </div>
3	A	1073	<div> <div>7%</div> <div>56% 36% 5% •</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1073	<div><div></div><div>9%</div><div>55%</div><div>37%</div><div></div><div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25280 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 Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	274	Total	C	N	O	S	0	2	0
			2222	1413	379	415	15			
1	E	279	Total	C	N	O	S	0	8	0
			2303	1466	394	427	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP O95149
B	-3	PRO	-	EXPRESSION TAG	UNP O95149
B	-2	LEU	-	EXPRESSION TAG	UNP O95149
B	-1	GLY	-	EXPRESSION TAG	UNP O95149
B	0	SER	-	EXPRESSION TAG	UNP O95149
E	-4	GLY	-	EXPRESSION TAG	UNP O95149
E	-3	PRO	-	EXPRESSION TAG	UNP O95149
E	-2	LEU	-	EXPRESSION TAG	UNP O95149
E	-1	GLY	-	EXPRESSION TAG	UNP O95149
E	0	SER	-	EXPRESSION TAG	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	1	0
			1399	910	246	238	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	ENGINEERED	UNP P62826
F	69	LEU	GLN	ENGINEERED	UNP P62826

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	5	0
			8456	5424	1421	1557	54			
3	D	1041	Total	C	N	O	S	0	8	0
			8483	5438	1427	1564	54			

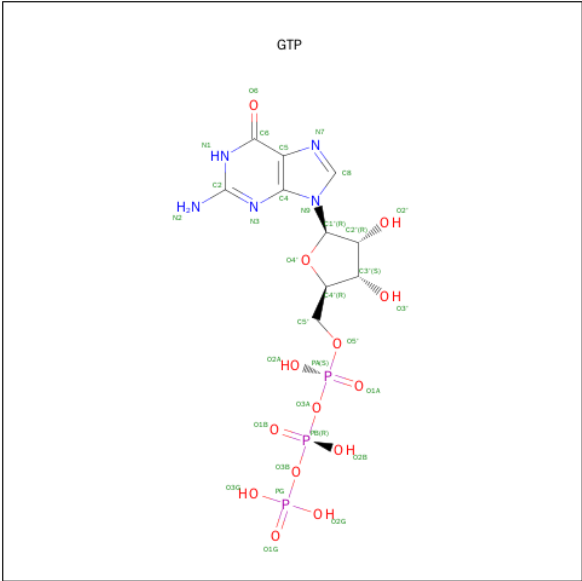
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q6P5F9
A	0	SER	-	EXPRESSION TAG	UNP Q6P5F9
D	-1	GLY	-	EXPRESSION TAG	UNP Q6P5F9
D	0	SER	-	EXPRESSION TAG	UNP Q6P5F9

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 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
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Cl	0	0
			1	1		

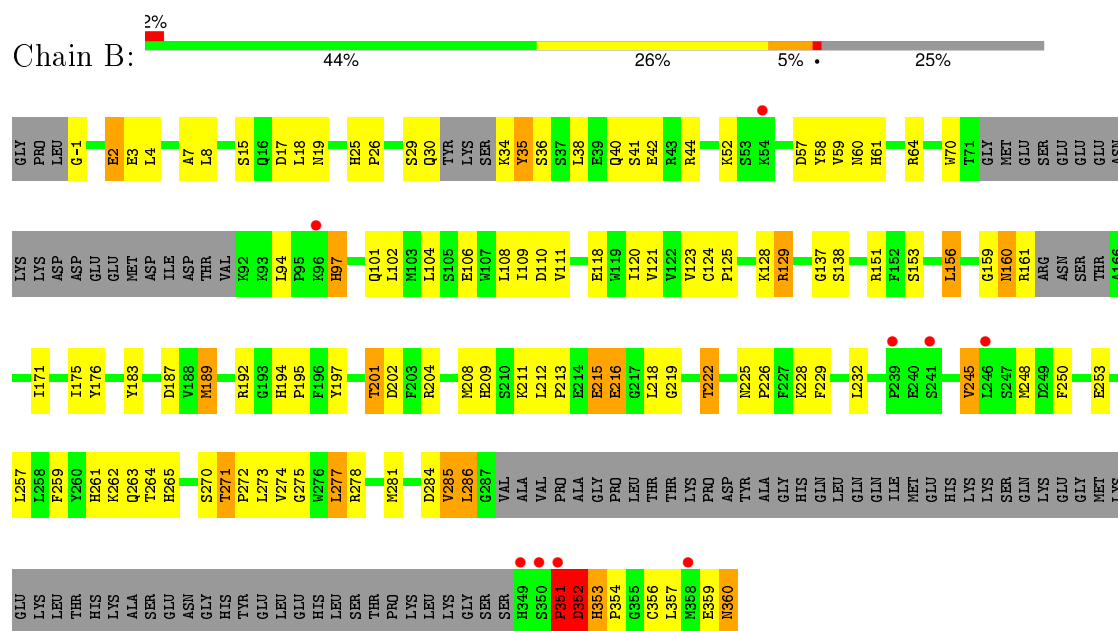
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	134	Total	O	0	0
			134	134		
8	C	58	Total	O	0	0
			58	58		
8	A	258	Total	O	0	0
			258	258		
8	E	130	Total	O	0	0
			130	130		
8	F	46	Total	O	0	0
			46	46		
8	D	333	Total	O	0	0
			333	333		

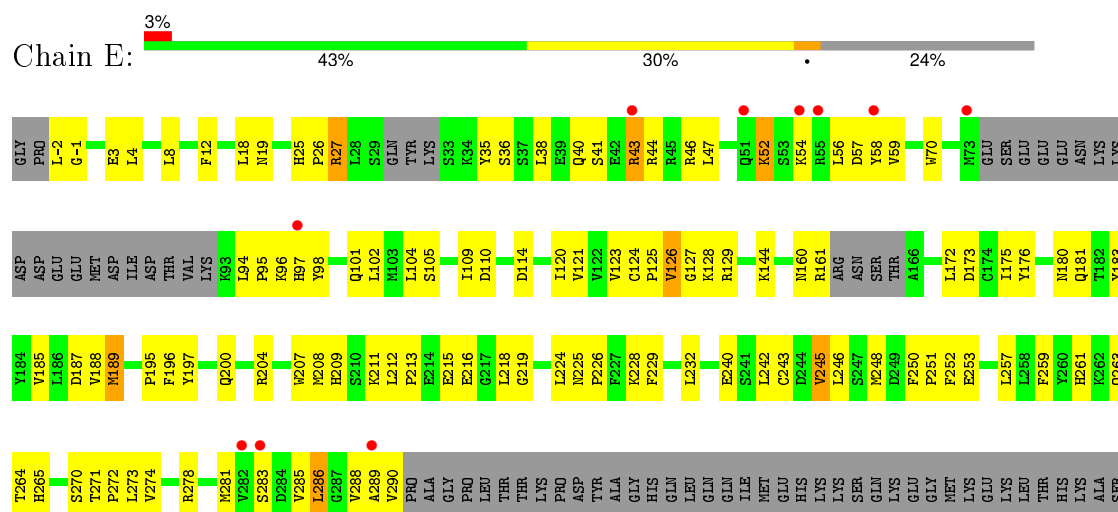
### 3 Residue-property plots

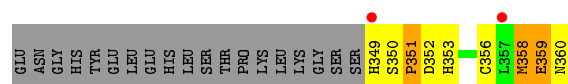
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Snurportin-1

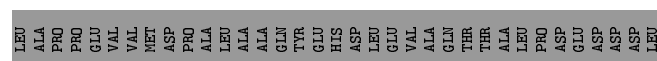
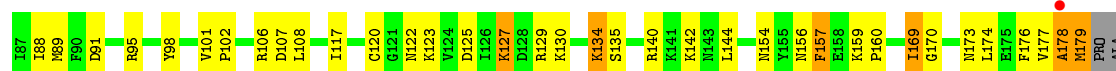


#### • Molecule 1: Snurportin-1

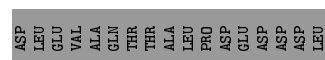
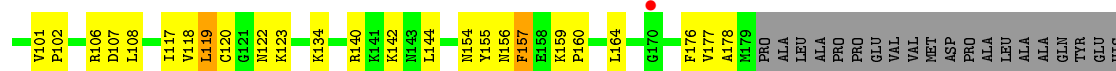




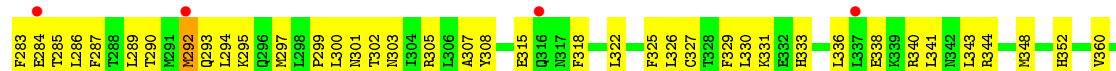
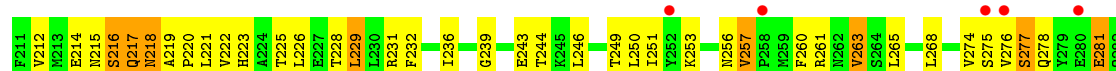
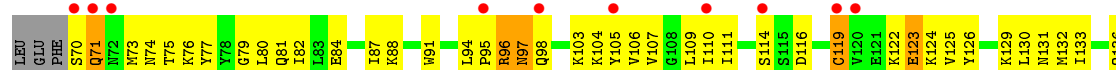
• Molecule 2: GTP-binding nuclear protein Ran



• Molecule 2: GTP-binding nuclear protein Ran



• Molecule 3: Exportin-1









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.17Å 225.74Å 163.45Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	38.84 – 2.50 47.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.84-2.50) 86.9 (47.81-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.244 , 0.281 0.240 , 0.277	Depositor DCC
$R_{free}$ test set	8604 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 172100 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	25280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: GTP, NA, MG, CL

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	B	0.42	0/2283	0.74	3/3090 (0.1%)
1	E	0.40	0/2364	0.64	0/3202
2	C	0.34	0/1434	0.52	0/1936
2	F	0.33	0/1423	0.56	2/1921 (0.1%)
3	A	0.36	0/8628	0.51	0/11687
3	D	0.36	0/8656	0.51	0/11724
All	All	0.37	0/24788	0.55	5/33560 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PRO	CA-N-CD	-10.95	96.18	111.50
1	B	352	ASP	N-CA-C	6.65	128.97	111.00
2	F	13	LEU	CA-CB-CG	5.79	128.61	115.30
1	B	215	GLU	N-CA-C	-5.18	97.00	111.00
2	F	13	LEU	CB-CG-CD1	5.02	119.54	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2222	0	2151	107	0
1	E	2303	0	2223	105	0
2	C	1399	0	1425	60	0
2	F	1389	0	1419	52	0
3	A	8456	0	8516	419	0
3	D	8483	0	8530	417	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	C	32	0	12	2	0
5	F	32	0	12	2	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	E	1	0	0	1	0
8	A	258	0	0	15	0
8	B	134	0	0	8	0
8	C	58	0	0	3	0
8	D	333	0	0	9	0
8	E	130	0	0	7	0
8	F	46	0	0	2	0
All	All	25280	0	24288	1137	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 23.

All (1137) 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:A:476:MET:HE3	3:A:501:ILE:HG12	1.18	1.13
2:F:54:THR:HG22	2:F:176:PHE:HB3	1.19	1.11
3:D:33:ASN:HB2	3:D:44:ARG:HG3	1.33	1.09
3:A:1008:ILE:HG23	3:A:1009:PRO:HD3	1.35	1.07
1:E:350:SER:HB3	1:E:351:PRO:HD2	1.37	1.05
1:E:351:PRO:HB3	7:E:362:CL:CL	1.97	1.01
3:A:256:ASN:HB3	3:A:293:GLN:HE21	1.22	1.00
3:D:426:LYS:HD2	3:D:426:LYS:H	1.25	0.99
3:D:131:ASN:HD21	3:D:166:ASN:HD21	1.07	0.98
3:D:960:THR:HG23	3:D:968:VAL:HG11	1.41	0.98
3:D:1008:ILE:HG23	3:D:1009:PRO:HD3	1.42	0.97
3:A:33:ASN:HB2	3:A:44:ARG:HG3	1.47	0.97
3:A:426:LYS:H	3:A:426:LYS:HD2	1.28	0.96
3:A:962:LEU:HD23	3:A:968:VAL:HG21	1.44	0.95
3:D:434:GLU:HG3	3:D:440:VAL:HG12	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:ARG:HB3	2:F:157:PHE:HZ	1.31	0.95
3:A:131:ASN:HD21	3:A:166:ASN:HD21	1.09	0.94
3:A:1016:ARG:HH11	3:A:1016:ARG:HG2	1.30	0.94
3:D:46:ALA:O	3:D:50:LEU:HB2	1.66	0.94
3:D:62:ARG:HB3	3:D:66:ILE:HD11	1.51	0.93
2:C:29:ARG:HB3	2:C:157:PHE:HZ	1.34	0.92
3:A:807:ILE:HD11	3:A:815:ILE:HD12	1.50	0.92
2:C:21:THR:HG23	2:C:89:MET:HG2	1.48	0.92
3:A:144:LYS:HG3	3:A:145:HIS:CD2	2.05	0.91
1:B:159:GLY:O	1:B:160:ASN:HB2	1.69	0.91
3:D:53:LEU:HD12	3:D:54:LYS:H	1.35	0.91
3:D:340:ARG:HG2	3:D:342:ASN:OD1	1.71	0.91
3:A:141:GLU:HA	3:A:144:LYS:HE2	1.54	0.90
1:E:43:ARG:HD2	1:E:46:ARG:HH12	1.35	0.89
3:A:46:ALA:O	3:A:50:LEU:HB2	1.72	0.88
3:D:770:GLN:HB3	8:D:1380:HOH:O	1.72	0.88
3:D:79:GLY:O	3:D:82:ILE:HG22	1.74	0.88
1:E:52[A]:LYS:HE3	1:E:265:HIS:H	1.39	0.87
2:C:134:LYS:HE3	2:C:135:SER:OG	1.75	0.86
3:D:63:VAL:HA	3:D:76:LYS:HG2	1.54	0.86
3:A:62:ARG:HH11	3:A:79:GLY:HA2	1.41	0.86
3:A:740:THR:HA	3:A:745[B]:ILE:HD13	1.58	0.86
2:F:29:ARG:HB3	2:F:157:PHE:CZ	2.11	0.85
3:A:53:LEU:HD12	3:A:54:LYS:H	1.41	0.85
3:A:393:LEU:HD22	3:A:398:GLN:HA	1.55	0.85
3:A:990:GLN:H	3:A:993:GLN:HE21	1.24	0.85
2:C:29:ARG:HB3	2:C:157:PHE:CZ	2.12	0.84
3:A:62:ARG:NH1	3:A:79:GLY:HA2	1.93	0.84
3:D:476:MET:HE3	3:D:501:ILE:HA	1.59	0.84
1:B:52:LYS:HE3	1:B:264:THR:HA	1.57	0.84
1:E:43:ARG:HD2	1:E:46:ARG:NH1	1.92	0.83
3:A:451:ILE:HG12	8:A:1203:HOH:O	1.78	0.82
3:D:393:LEU:HD12	3:D:395:SER:H	1.44	0.82
3:D:990:GLN:H	3:D:993:GLN:HE21	1.27	0.82
1:B:285:VAL:HG12	1:B:286:LEU:HD12	1.62	0.82
1:E:200:GLN:HG2	8:E:497:HOH:O	1.80	0.80
1:B:38:LEU:HG	1:B:40:GLN:H	1.46	0.80
3:A:1048:GLU:HG3	3:A:1052:LEU:HG	1.63	0.80
3:A:30:ASN:ND2	3:A:47:GLN:HE22	1.80	0.79
1:B:156:LEU:HD13	1:B:218:LEU:HD11	1.65	0.79
3:A:94:LEU:HD23	3:A:95:PRO:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:426:LYS:CD	3:D:426:LYS:H	1.94	0.79
3:D:476:MET:CE	3:D:501:ILE:HG12	2.12	0.79
3:A:276:VAL:HG21	3:A:336:LEU:HD22	1.64	0.79
1:B:264:THR:HG22	1:B:265:HIS:O	1.84	0.78
3:D:276:VAL:HG21	3:D:336:LEU:HD22	1.65	0.78
3:D:23:LEU:HD23	3:D:26:ASN:HB2	1.66	0.78
1:B:108:LEU:HB3	1:B:277:LEU:HD13	1.66	0.78
3:A:962:LEU:HB2	3:A:973:PHE:CD2	2.19	0.77
3:A:214:GLU:HG3	3:A:215:ASN:ND2	2.00	0.77
3:A:509[B]:HIS:HD2	3:A:511:GLU:H	1.33	0.77
3:D:214:GLU:HG3	3:D:215:ASN:ND2	2.00	0.77
3:A:107:VAL:O	3:A:111:ILE:HG12	1.85	0.77
3:D:781:LEU:HD11	3:D:821:GLN:HG3	1.67	0.77
3:D:962:LEU:HB2	3:D:973:PHE:CD2	2.20	0.76
1:E:38:LEU:HG	1:E:40:GLN:H	1.48	0.76
3:A:32:VAL:HG22	3:A:71:GLN:HG2	1.66	0.76
3:A:990:GLN:HG3	3:A:993:GLN:HG3	1.68	0.76
3:A:289:LEU:O	3:A:292:MET:HG3	1.84	0.76
1:B:102:LEU:HD13	1:B:129:ARG:HH11	1.51	0.76
3:A:476:MET:HE3	3:A:501:ILE:CG1	2.09	0.76
3:A:426:LYS:CD	3:A:426:LYS:H	1.98	0.76
3:D:990:GLN:HG3	3:D:993:GLN:HG3	1.68	0.75
1:B:359:GLU:HG2	8:B:494:HOH:O	1.84	0.75
3:D:392:PRO:HA	3:D:399:HIS:NE2	2.02	0.75
3:A:704:HIS:CD2	3:A:767[B]:ASN:H	2.05	0.74
1:B:102:LEU:HB3	1:B:129:ARG:NH1	2.02	0.74
3:A:55:GLU:HG2	3:A:56:HIS:H	1.52	0.74
2:F:54:THR:CG2	2:F:176:PHE:HB3	2.10	0.74
3:A:476:MET:HE2	3:A:516:PHE:HZ	1.52	0.73
3:D:53:LEU:HD12	3:D:54:LYS:N	2.02	0.73
3:A:476:MET:HE2	3:A:516:PHE:CZ	2.24	0.73
3:D:56:HIS:CG	3:D:56:HIS:O	2.41	0.73
3:D:1033:LEU:HD12	3:D:1035:LEU:HD11	1.71	0.73
3:A:56:HIS:CG	3:A:56:HIS:O	2.42	0.72
3:A:116:ASP:O	3:A:119:CYS:HB3	1.90	0.72
3:A:888:ASN:ND2	3:A:889:VAL:H	1.88	0.72
2:C:95:ARG:HD2	2:C:130:LYS:HB3	1.71	0.72
3:D:798:PRO:HG3	3:D:844:HIS:CE1	2.24	0.72
3:D:341:LEU:HD23	3:D:344:ARG:HD2	1.70	0.72
3:A:97:ASN:ND2	3:A:97:ASN:H	1.87	0.72
3:D:678:ILE:HD12	3:D:679:LEU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:509[B]:HIS:CD2	3:A:511:GLU:HB3	2.24	0.71
3:A:665:TRP:O	3:A:669:ILE:HG12	1.88	0.71
3:A:509[B]:HIS:CD2	3:A:511:GLU:H	2.07	0.71
3:A:704:HIS:CD2	3:A:767[A]:ASN:H	2.09	0.71
3:D:738:MET:HG3	8:D:1269:HOH:O	1.90	0.71
3:D:32:VAL:O	3:D:36:TYR:HD2	1.72	0.71
3:A:739:VAL:O	3:A:745[B]:ILE:HG21	1.90	0.71
3:D:434:GLU:HG3	3:D:440:VAL:CG1	2.19	0.71
3:A:20:SER:HB2	3:A:22:LYS:HG3	1.72	0.71
3:D:144:LYS:HG3	3:D:145[A]:HIS:CD2	2.26	0.71
3:A:32:VAL:O	3:A:36:TYR:HD2	1.73	0.70
3:D:888:ASN:ND2	3:D:889:VAL:H	1.89	0.70
3:A:1043:ARG:NH1	3:A:1046:GLN:HG2	2.06	0.70
3:D:476:MET:HE3	3:D:501:ILE:HG12	1.71	0.70
3:D:672:ALA:HA	3:D:678:ILE:HD11	1.72	0.70
3:A:249:THR:O	3:A:253:LYS:HB2	1.90	0.70
2:C:21:THR:HG22	2:C:23:LYS:HG3	1.72	0.70
3:D:312:LYS:HA	3:D:312:LYS:HE3	1.73	0.70
3:D:28:LEU:HD11	3:D:66:ILE:HG23	1.73	0.70
3:A:179:PHE:CE1	3:A:195:LYS:HG2	2.25	0.70
3:D:131:ASN:ND2	3:D:166:ASN:HD21	1.85	0.70
3:A:672:ALA:HA	3:A:678:ILE:HD11	1.72	0.70
3:D:665:TRP:O	3:D:669:ILE:HG12	1.90	0.69
3:D:249:THR:O	3:D:253:LYS:HB2	1.90	0.69
3:D:179:PHE:HE1	3:D:195:LYS:HE2	1.58	0.69
3:A:71:GLN:HA	3:A:74:ASN:OD1	1.92	0.69
3:A:226:LEU:HD23	3:A:263:VAL:HB	1.75	0.69
3:D:58:ASP:OD1	3:D:61:THR:HB	1.92	0.69
1:E:70:TRP:CE3	1:E:96:LYS:O	2.45	0.69
3:D:957:LYS:NZ	3:D:961:PRO:HB3	2.07	0.69
3:A:803:THR:O	3:A:807:ILE:HG23	1.92	0.69
1:B:159:GLY:O	1:B:160:ASN:CB	2.40	0.69
3:A:53:LEU:HD12	3:A:54:LYS:N	2.06	0.69
3:D:141:GLU:HA	3:D:144:LYS:HE2	1.75	0.69
2:C:70:GLU:O	2:C:76:ARG:NH2	2.26	0.69
3:D:704:HIS:CD2	3:D:767:ASN:H	2.11	0.69
2:C:169:ILE:HG22	2:C:170:GLY:H	1.58	0.68
3:D:424:MET:HA	3:D:457:MET:HE2	1.76	0.68
3:A:957:LYS:NZ	3:A:961:PRO:HB3	2.07	0.68
3:D:962:LEU:C	3:D:964:PRO:HD3	2.13	0.68
3:A:179:PHE:HE1	3:A:195:LYS:HE2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:300:LEU:O	3:A:352:HIS:HE1	1.76	0.68
3:A:1016:ARG:NH1	3:A:1016:ARG:HG2	1.98	0.68
3:D:737[A]:GLU:O	3:D:740:THR:HB	1.93	0.68
3:D:759:ILE:HD13	3:D:780:LEU:HD21	1.76	0.68
3:A:205:ILE:HD11	3:A:232:PHE:CZ	2.28	0.68
3:D:97:ASN:H	3:D:97:ASN:ND2	1.89	0.68
3:A:399:HIS:HD2	3:A:401:ASP:HB2	1.58	0.68
3:A:737:GLU:O	3:A:740:THR:HB	1.94	0.68
3:A:704:HIS:HD2	3:A:767[B]:ASN:H	1.38	0.68
1:E:105:SER:HA	1:E:274:VAL:HG13	1.76	0.68
3:A:887:ARG:HD3	3:A:937:ALA:HB3	1.76	0.68
1:B:261:HIS:HD2	1:B:263:GLN:H	1.40	0.68
3:A:28:LEU:O	3:A:32:VAL:HG23	1.94	0.68
3:D:300:LEU:O	3:D:352:HIS:HE1	1.77	0.67
3:A:815:ILE:HG12	3:A:818:GLU:HG2	1.76	0.67
1:E:43:ARG:CD	1:E:46:ARG:HH12	2.07	0.67
1:E:123:VAL:HG21	1:E:250:PHE:CZ	2.29	0.67
2:C:38:LYS:HG2	3:A:842:PRO:HG3	1.76	0.67
3:D:251:ILE:HG21	3:D:289:LEU:HB3	1.76	0.67
3:A:962:LEU:HD13	3:A:973:PHE:HE2	1.60	0.67
3:D:226:LEU:HD23	3:D:263:VAL:HB	1.76	0.67
3:D:1043:ARG:NH1	3:D:1046:GLN:HG2	2.09	0.67
3:D:815:ILE:HG12	3:D:818:GLU:HG2	1.77	0.67
3:A:759:ILE:HD13	3:A:780:LEU:HD21	1.77	0.67
2:F:106:ARG:HD3	3:D:181:PHE:CE2	2.30	0.67
1:B:222:THR:HG22	1:B:225:ASN:H	1.59	0.67
3:A:131:ASN:ND2	3:A:166:ASN:HD21	1.87	0.67
2:C:21:THR:CG2	2:C:89:MET:HG2	2.24	0.67
1:E:52[A]:LYS:CE	1:E:265:HIS:H	2.08	0.66
3:D:678:ILE:HD12	3:D:679:LEU:N	2.09	0.66
3:D:179:PHE:CE1	3:D:195:LYS:HG2	2.29	0.66
1:B:176:TYR:HB2	1:B:183:TYR:CE1	2.29	0.66
3:D:737[B]:GLU:O	3:D:740:THR:HB	1.94	0.66
3:D:482:ASN:HB3	3:D:488:GLU:HB2	1.76	0.66
3:A:63:VAL:HA	3:A:76:LYS:HG2	1.76	0.66
1:E:176:TYR:HB2	1:E:183:TYR:CE1	2.29	0.66
2:C:37:LYS:HE3	8:A:1199:HOH:O	1.96	0.66
1:E:207:TRP:HB3	8:E:492:HOH:O	1.95	0.66
3:D:435:ASN:ND2	3:D:439:GLU:HB2	2.09	0.66
1:E:160:ASN:O	1:E:161:ARG:HG2	1.96	0.66
3:D:887:ARG:HD3	3:D:937:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:482:ASN:HB3	3:A:488:GLU:HB2	1.77	0.66
3:D:434:GLU:CG	3:D:440:VAL:HG12	2.25	0.66
3:A:388:THR:HG22	3:A:399:HIS:HE2	1.61	0.66
1:B:160:ASN:CG	1:B:161:ARG:H	1.99	0.66
3:D:206:PHE:CE1	3:D:240:TYR:HB3	2.31	0.66
3:D:926:ILE:HG21	3:D:946:LEU:HD11	1.77	0.66
3:D:548:VAL:HG13	3:D:555:LEU:HD21	1.78	0.66
3:A:962:LEU:HD22	3:A:968:VAL:HG11	1.77	0.65
3:D:202:PHE:O	3:D:205:ILE:HG12	1.96	0.65
1:B:4:LEU:HD11	3:A:521:ILE:HG13	1.78	0.65
3:A:887:ARG:HH21	3:A:891:ASP:HB3	1.61	0.65
3:D:28:LEU:O	3:D:32:VAL:HG23	1.96	0.65
3:A:729:SER:OG	3:A:792:VAL:HG22	1.97	0.65
3:D:33:ASN:HB2	3:D:44:ARG:CG	2.18	0.65
3:A:424:MET:HA	3:A:457:MET:HE2	1.79	0.65
1:E:127:GLY:HA2	8:E:549:HOH:O	1.97	0.65
2:C:55:ASN:OD1	2:C:174:LEU:HD12	1.97	0.65
1:E:95:PRO:HB2	1:E:101:GLN:NE2	2.12	0.65
3:A:171:LEU:HD13	3:A:205:ILE:HD12	1.79	0.65
2:C:106:ARG:HD3	3:A:181:PHE:CE2	2.32	0.64
3:D:489:TRP:O	3:D:490:SER:HB3	1.97	0.64
3:A:704:HIS:HD2	3:A:767[A]:ASN:H	1.42	0.64
3:A:62:ARG:HH12	3:A:82:ILE:HG13	1.63	0.64
1:B:18:LEU:HA	1:B:36:SER:O	1.97	0.64
3:D:52:HIS:ND1	3:D:82:ILE:HD12	2.12	0.64
1:E:261:HIS:HD2	1:E:263:GLN:H	1.44	0.64
3:D:201:GLU:O	3:D:204:GLN:HG3	1.97	0.64
3:A:437:GLN:HG2	3:A:746:ARG:HG2	1.79	0.64
1:E:4:LEU:HD11	3:D:521:ILE:HG13	1.78	0.64
3:A:678:ILE:HD12	3:A:679:LEU:N	2.12	0.64
3:D:210:GLN:O	3:D:214:GLU:HG2	1.97	0.64
1:B:123:VAL:HG21	1:B:250:PHE:CZ	2.33	0.64
3:D:887:ARG:HH21	3:D:891:ASP:HB3	1.63	0.63
3:A:146:TRP:CE3	3:A:149:PHE:HB2	2.33	0.63
3:A:677:ASP:O	3:A:680:LYS:HB3	1.98	0.63
3:A:548:VAL:HG13	3:A:555:LEU:HD21	1.80	0.63
3:D:677:ASP:O	3:D:680:LYS:HB3	1.98	0.63
3:A:30:ASN:HD22	3:A:47:GLN:HE22	1.45	0.63
3:D:257:VAL:HG21	3:D:260:PHE:HD2	1.63	0.63
3:A:489:TRP:O	3:A:490:SER:HB3	1.98	0.63
3:A:678:ILE:HD12	3:A:679:LEU:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:257:VAL:HG21	3:A:260:PHE:HD2	1.64	0.63
3:A:926:ILE:HG21	3:A:946:LEU:HD11	1.80	0.63
3:D:704:HIS:HD2	3:D:767:ASN:H	1.45	0.63
3:A:788:TYR:CE1	3:A:796:ARG:HB3	2.34	0.63
3:D:22:LYS:HG2	3:D:58:ASP:CG	2.19	0.63
3:D:276:VAL:HA	3:D:283:PHE:CE2	2.34	0.63
3:D:678:ILE:C	3:D:680:LYS:H	2.02	0.63
3:D:146:TRP:CE3	3:D:149:PHE:HB2	2.34	0.63
3:A:678:ILE:C	3:A:680:LYS:H	2.02	0.63
1:B:102:LEU:HB3	1:B:129:ARG:HH12	1.64	0.62
3:A:961:PRO:HD3	3:A:970:ASN:HD21	1.62	0.62
3:A:888:ASN:HD22	3:A:889:VAL:H	1.46	0.62
1:E:18:LEU:HA	1:E:36:SER:O	1.99	0.62
3:A:388:THR:HG23	3:A:401:ASP:HB3	1.81	0.62
3:A:229:LEU:HD11	3:A:246:LEU:HD11	1.80	0.62
3:D:45:MET:O	3:D:49:VAL:HG12	1.98	0.62
3:A:187:THR:HG22	3:A:190:LYS:HB2	1.81	0.62
2:C:42:THR:HG23	8:C:826:HOH:O	1.98	0.62
3:A:276:VAL:HA	3:A:283:PHE:CE2	2.35	0.62
3:A:681:ASP:OD2	3:A:684:THR:HG23	2.00	0.62
3:A:583:MET:HG2	8:A:1255:HOH:O	1.98	0.62
3:A:810:LYS:HD3	3:A:810:LYS:O	1.99	0.62
3:D:437:GLN:HG2	3:D:746:ARG:HG2	1.81	0.62
3:D:476:MET:CE	3:D:516:PHE:HZ	2.13	0.62
3:A:1046:GLN:O	3:A:1049:LYS:HB2	1.99	0.62
1:E:278:ARG:HG2	1:E:281:MET:HE3	1.82	0.62
3:D:429:GLU:HG3	3:D:445:MET:HG3	1.82	0.62
3:D:485:ASN:C	3:D:487:THR:H	2.04	0.62
3:D:90:ARG:O	3:D:94:LEU:HG	1.99	0.62
3:D:476:MET:HE2	3:D:501:ILE:HG12	1.80	0.61
3:D:229:LEU:HD11	3:D:246:LEU:HD11	1.81	0.61
3:A:476:MET:CE	3:A:501:ILE:HG12	2.12	0.61
3:A:216:SER:O	3:A:217:GLN:HG2	1.98	0.61
1:B:-1:GLY:O	1:B:3:GLU:HG2	1.99	0.61
3:D:32:VAL:HG22	3:D:71:GLN:HB2	1.82	0.61
3:A:187:THR:HG22	3:A:190:LYS:HE3	1.81	0.61
1:B:285:VAL:HG12	1:B:286:LEU:CD1	2.29	0.61
3:A:210:GLN:O	3:A:214:GLU:HG2	1.99	0.61
3:A:33:ASN:CB	3:A:44:ARG:HG3	2.28	0.61
3:D:141:GLU:HG2	3:D:145[A]:HIS:HD2	1.63	0.61
3:A:110:ILE:CD1	3:A:130:LEU:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1003:SER:HA	3:A:1046:GLN:NE2	2.15	0.61
2:C:50:LEU:HD12	2:C:63:VAL:HG21	1.82	0.61
3:A:30:ASN:HA	3:A:44:ARG:HD2	1.82	0.61
3:D:888:ASN:HD22	3:D:889:VAL:H	1.46	0.61
1:B:261:HIS:CD2	1:B:263:GLN:H	2.19	0.61
3:D:28:LEU:CD1	3:D:66:ILE:HG23	2.29	0.61
3:D:544:ILE:HG22	3:D:545:MET:HE1	1.83	0.61
2:F:54:THR:HA	2:F:176:PHE:HA	1.83	0.61
1:B:160:ASN:CG	1:B:161:ARG:N	2.54	0.61
1:E:52[A]:LYS:HE3	1:E:265:HIS:N	2.12	0.61
3:A:62:ARG:NH1	3:A:82:ILE:HG13	2.15	0.60
3:D:402:ILE:HD13	3:D:407:GLN:NE2	2.16	0.60
3:D:1050:HIS:O	3:D:1054:MET:HG2	2.01	0.60
3:A:485:ASN:C	3:A:487:THR:H	2.05	0.60
1:B:211:LYS:N	1:B:211:LYS:HD2	2.16	0.60
3:A:131:ASN:HD21	3:A:166:ASN:ND2	1.91	0.60
1:B:218:LEU:HG	1:B:229:PHE:HB2	1.83	0.60
3:A:962:LEU:C	3:A:964:PRO:HD3	2.22	0.60
3:D:218:ASN:HD22	3:D:220:PRO:HD2	1.67	0.60
3:A:962:LEU:O	3:A:963:ASN:HB2	2.01	0.60
3:A:45:MET:O	3:A:49:VAL:HG12	2.00	0.60
2:F:117:ILE:HB	2:F:144:LEU:HD22	1.84	0.60
3:A:33:ASN:HB2	3:A:44:ARG:CG	2.26	0.60
3:A:295:LYS:HG2	3:A:300:LEU:HD11	1.83	0.60
3:D:429:GLU:HB3	3:D:445:MET:HB2	1.84	0.60
3:A:225:THR:O	3:A:228:THR:HG22	2.02	0.60
1:E:264:THR:HB	1:E:273:LEU:HD13	1.84	0.60
3:D:225:THR:O	3:D:228:THR:HG22	2.01	0.60
2:F:10:GLN:HG2	2:F:60:LYS:HD3	1.83	0.60
2:F:54:THR:HG22	2:F:176:PHE:CB	2.13	0.59
3:D:22:LYS:HG2	3:D:58:ASP:OD1	2.02	0.59
3:D:300:LEU:HD12	3:D:300:LEU:H	1.66	0.59
1:E:261:HIS:CD2	1:E:263:GLN:H	2.20	0.59
3:A:32:VAL:HG22	3:A:71:GLN:CG	2.32	0.59
2:F:50:LEU:HD12	2:F:63:VAL:HG21	1.84	0.59
1:E:211:LYS:N	1:E:211:LYS:HD2	2.18	0.59
3:A:216:SER:HB2	3:A:222:VAL:CG2	2.33	0.59
3:A:206:PHE:HE2	3:A:244:THR:HG21	1.66	0.59
1:E:128:LYS:O	1:E:175:ILE:HA	2.03	0.59
3:A:33:ASN:ND2	3:A:44:ARG:HE	1.99	0.59
3:D:295:LYS:HG2	3:D:300:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:218:ASN:ND2	3:D:220:PRO:HD2	2.18	0.59
3:A:483:GLN:HE22	3:A:489:TRP:HA	1.68	0.59
1:B:52:LYS:CE	1:B:265:HIS:H	2.15	0.59
1:B:52:LYS:HD3	1:B:265:HIS:CG	2.37	0.59
3:A:728:ILE:HD13	3:A:749:ARG:HD2	1.85	0.59
3:A:476:MET:CE	3:A:516:PHE:HZ	2.15	0.58
1:B:201:THR:HG22	1:B:264:THR:O	2.03	0.58
3:D:681:ASP:OD2	3:D:684:THR:HG23	2.03	0.58
3:A:429:GLU:HG3	3:A:445:MET:HG3	1.85	0.58
3:D:476:MET:HE1	3:D:516:PHE:CZ	2.38	0.58
3:A:300:LEU:HD12	3:A:300:LEU:H	1.67	0.58
3:A:218:ASN:HD22	3:A:220:PRO:HD2	1.68	0.58
3:D:788:TYR:CE1	3:D:796:ARG:HB3	2.38	0.58
3:A:838:PHE:HA	3:A:845:ARG:NH2	2.18	0.58
2:C:177:VAL:O	2:C:178:ALA:HB3	2.04	0.58
3:A:30:ASN:ND2	3:A:47:GLN:NE2	2.49	0.58
3:D:216:SER:HB2	3:D:222:VAL:CG2	2.34	0.58
1:E:209:HIS:CE1	1:E:232:LEU:O	2.57	0.58
3:D:926:ILE:HG21	3:D:946:LEU:CD1	2.34	0.58
3:D:483:GLN:HE22	3:D:489:TRP:HA	1.69	0.58
3:D:293:GLN:O	3:D:297:MET:HG3	2.02	0.58
3:D:963:ASN:N	3:D:964:PRO:HD3	2.18	0.58
1:E:52[B]:LYS:NZ	1:E:263:GLN:O	2.34	0.58
3:A:265:LEU:HD21	3:A:322:LEU:HA	1.84	0.58
3:A:745[A]:ILE:HD13	3:A:748:MET:CE	2.33	0.58
1:E:185:VAL:HG12	1:E:208:MET:SD	2.44	0.58
2:C:117:ILE:HB	2:C:144:LEU:HD22	1.86	0.58
3:D:146:TRP:N	3:D:147:PRO:HD3	2.18	0.58
3:D:62:ARG:O	3:D:66:ILE:HG13	2.04	0.58
2:F:52:PHE:HB2	2:F:59:ILE:HG22	1.86	0.58
3:D:340:ARG:HB3	3:D:343:LEU:HD12	1.85	0.57
3:D:545:MET:HG3	3:D:583:MET:SD	2.43	0.57
1:E:259:PHE:O	1:E:274:VAL:HA	2.03	0.57
1:B:128:LYS:HE3	1:B:176:TYR:HD2	1.69	0.57
3:D:150:ILE:HD11	3:D:205:ILE:HG23	1.85	0.57
3:D:360:VAL:HG11	3:D:365:ILE:HD12	1.85	0.57
3:D:597:ARG:HE	3:D:601:GLN:NE2	2.02	0.57
1:E:173:ASP:HB2	1:E:189:MET:HE1	1.85	0.57
3:A:218:ASN:ND2	3:A:220:PRO:HD2	2.20	0.57
3:D:150:ILE:HG21	3:D:201:GLU:CD	2.24	0.57
3:D:92:LYS:HD2	3:D:1030:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:962:LEU:O	3:A:964:PRO:HD3	2.03	0.57
3:A:399:HIS:CD2	3:A:401:ASP:HB2	2.40	0.57
3:A:705:PRO:O	3:A:708:ILE:HG22	2.04	0.57
3:D:485:ASN:O	3:D:487:THR:N	2.38	0.57
3:A:146:TRP:N	3:A:147:PRO:HD3	2.18	0.57
3:A:799:GLU:HG2	8:A:1286:HOH:O	2.04	0.57
3:D:1005:ASN:OD1	3:D:1049:LYS:HE3	2.05	0.57
2:C:52:PHE:HB2	2:C:59:ILE:HG22	1.86	0.57
3:A:303:ASN:HD21	3:A:305:ARG:NH2	2.03	0.57
3:D:728:ILE:HD13	3:D:749:ARG:HD2	1.87	0.57
3:D:107:VAL:O	3:D:111:ILE:HG12	2.05	0.57
3:A:160:SER:HB3	3:A:163:LEU:HD12	1.87	0.57
1:B:259:PHE:O	1:B:274:VAL:HA	2.05	0.57
3:A:341:LEU:HD23	3:A:341:LEU:O	2.05	0.57
3:D:21:GLN:HG2	3:D:22:LYS:N	2.20	0.57
3:A:388:THR:HG23	3:A:401:ASP:CB	2.35	0.57
1:E:26:PRO:HG2	1:E:109:ILE:HD11	1.87	0.57
3:D:1038:ARG:HH21	3:D:1042:LEU:HD21	1.69	0.57
3:D:265:LEU:HD21	3:D:322:LEU:HA	1.86	0.57
2:F:123:LYS:HE2	5:F:217:GTP:C4	2.40	0.56
3:D:810:LYS:O	3:D:810:LYS:HD3	2.05	0.56
3:A:681:ASP:O	3:A:685:VAL:HG13	2.05	0.56
3:D:91:TRP:HA	3:D:94:LEU:HD12	1.88	0.56
3:A:441:VAL:HB	3:A:628:GLN:OE1	2.05	0.56
1:B:278:ARG:HG2	1:B:281:MET:HE3	1.87	0.56
2:F:9:VAL:HG22	2:F:9:VAL:O	2.04	0.56
3:A:961:PRO:HD3	3:A:970:ASN:ND2	2.21	0.56
2:C:31:LEU:HD12	2:C:32:THR:CG2	2.36	0.56
3:A:344:ARG:NH1	3:A:408:LEU:HD21	2.21	0.56
3:D:851:LEU:O	3:D:855:VAL:HG23	2.06	0.56
1:E:52[A]:LYS:HZ2	1:E:265:HIS:HB2	1.70	0.56
3:A:481:GLN:OE1	3:A:481:GLN:HA	2.04	0.56
2:C:31:LEU:HD12	2:C:32:THR:HG23	1.88	0.56
1:B:52:LYS:HE3	1:B:265:HIS:H	1.71	0.56
3:D:142:TRP:HH2	3:D:198:MET:HA	1.71	0.56
3:A:150:ILE:HD11	3:A:205:ILE:HG22	1.86	0.56
3:A:926:ILE:HG21	3:A:946:LEU:CD1	2.36	0.56
1:B:351:PRO:HB3	1:B:352:ASP:OD2	2.06	0.56
3:D:426:LYS:N	3:D:426:LYS:HD2	2.08	0.56
3:D:888:ASN:N	3:D:888:ASN:HD22	2.01	0.56
3:D:431:LEU:HD22	3:D:445:MET:CE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:HIS:CE1	1:B:232:LEU:O	2.58	0.56
3:D:84:GLU:O	3:D:88:LYS:HG3	2.05	0.56
3:A:360:VAL:HG11	3:A:365:ILE:HD12	1.86	0.56
3:D:709:GLN:O	3:D:712:ARG:HB3	2.06	0.56
3:A:256:ASN:HB3	3:A:293:GLN:NE2	2.07	0.56
3:A:962:LEU:HB2	3:A:973:PHE:HD2	1.68	0.56
3:D:21:GLN:HG2	3:D:22:LYS:H	1.71	0.56
3:A:340:ARG:HB2	3:A:343:LEU:HD12	1.86	0.56
3:A:142:TRP:HH2	3:A:198:MET:HA	1.71	0.56
3:A:841:TYR:O	3:A:845:ARG:HG3	2.05	0.56
3:A:957:LYS:HZ1	3:A:961:PRO:HB3	1.71	0.56
1:E:19:ASN:HD21	1:E:38:LEU:H	1.53	0.56
3:D:312:LYS:HG3	3:D:313:ASP:H	1.70	0.56
3:A:485:ASN:O	3:A:487:THR:N	2.39	0.56
1:B:212:LEU:HB2	1:B:213:PRO:HD3	1.88	0.56
3:D:93:ILE:HG22	3:D:1027:GLY:HA3	1.88	0.56
2:C:10:GLN:HG2	2:C:60:LYS:HE2	1.87	0.55
3:D:962:LEU:HB2	3:D:973:PHE:HD2	1.68	0.55
3:D:66:ILE:HG22	3:D:72:ASN:HB3	1.87	0.55
1:E:52[A]:LYS:HE3	1:E:264:THR:HA	1.88	0.55
3:D:1003:SER:HA	3:D:1046:GLN:NE2	2.21	0.55
3:D:187:THR:HG23	3:D:190:LYS:H	1.72	0.55
1:B:61:HIS:HE1	1:B:101:GLN:HE22	1.53	0.55
3:A:388:THR:HG22	3:A:389:SER:N	2.21	0.55
3:D:399:HIS:C	3:D:401:ASP:H	2.09	0.55
3:A:150:ILE:HG21	3:A:201:GLU:CD	2.26	0.55
3:D:132:MET:O	3:D:136:GLN:HG2	2.06	0.55
1:B:137:GLY:O	1:B:160:ASN:HB2	2.07	0.55
3:A:218:ASN:HB3	3:A:221:LEU:HB3	1.87	0.55
3:A:23:LEU:HD12	3:A:23:LEU:H	1.71	0.55
2:F:71:LYS:HG3	8:F:915:HOH:O	2.05	0.55
3:A:1016:ARG:HH11	3:A:1016:ARG:CG	2.13	0.55
3:A:709:GLN:O	3:A:712:ARG:HB3	2.06	0.55
3:A:293:GLN:O	3:A:297:MET:HG3	2.06	0.55
3:D:960:THR:HG23	3:D:968:VAL:CG1	2.28	0.55
3:D:957:LYS:HZ1	3:D:961:PRO:HB3	1.71	0.55
1:B:201:THR:HG22	1:B:204:ARG:NH1	2.21	0.55
3:D:681:ASP:O	3:D:685:VAL:HG13	2.06	0.55
3:A:514:LYS:NZ	8:A:1321:HOH:O	2.39	0.55
1:B:26:PRO:HG2	1:B:109:ILE:HD11	1.89	0.55
1:B:360:ASN:HB2	8:B:494:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:N	8:B:363:HOH:O	2.39	0.55
1:E:349:HIS:CE1	3:D:708[A]:ILE:HD12	2.42	0.55
3:D:66:ILE:HG21	3:D:75:THR:HB	1.89	0.55
1:B:19:ASN:HD21	1:B:38:LEU:H	1.54	0.55
2:F:155:TYR:HB2	3:D:445:MET:HE1	1.88	0.55
1:E:218:LEU:HG	1:E:229:PHE:HB2	1.89	0.55
1:B:264:THR:OG1	1:B:273:LEU:HD13	2.07	0.54
3:A:888:ASN:ND2	3:A:889:VAL:N	2.55	0.54
3:A:132:MET:O	3:A:136:GLN:HG2	2.06	0.54
3:A:239:GLY:HA2	3:A:243:GLU:HG3	1.88	0.54
3:D:402:ILE:HG21	3:D:407:GLN:HE21	1.72	0.54
3:D:888:ASN:ND2	3:D:889:VAL:N	2.55	0.54
3:D:939:LEU:CD2	3:D:1016:ARG:HH11	2.20	0.54
3:D:66:ILE:HD13	3:D:75:THR:HG22	1.90	0.54
3:D:344:ARG:NH1	3:D:408:LEU:HD21	2.23	0.54
3:A:483:GLN:NE2	3:A:489:TRP:HA	2.23	0.54
3:D:284:GLU:HG3	3:D:343:LEU:HD21	1.89	0.54
3:A:73:MET:HG3	3:A:126:TYR:HB2	1.88	0.54
1:B:61:HIS:CE1	1:B:101:GLN:HE22	2.25	0.54
3:D:894:LEU:HD13	3:D:941:MET:HB2	1.90	0.54
3:A:251:ILE:HG21	3:A:289:LEU:HB3	1.89	0.54
3:D:218:ASN:HB3	3:D:221:LEU:HB3	1.89	0.54
3:D:73:MET:HG3	3:D:126:TYR:HB2	1.89	0.54
3:A:888:ASN:HD22	3:A:888:ASN:N	2.04	0.54
3:A:887:ARG:HD3	3:A:937:ALA:CB	2.37	0.54
3:A:429:GLU:CG	3:A:445:MET:HG3	2.38	0.54
1:B:171:ILE:O	1:B:189:MET:HG2	2.08	0.54
3:A:187:THR:HG23	3:A:190:LYS:H	1.73	0.54
3:A:274:VAL:HG12	3:A:275:SER:N	2.23	0.54
2:C:89:MET:HE2	2:C:120:CYS:HB2	1.90	0.54
1:E:70:TRP:CD2	1:E:96:LYS:O	2.61	0.54
3:A:187:THR:H	3:A:190:LYS:HZ2	1.55	0.54
2:C:123:LYS:HE2	5:C:217:GTP:C4	2.43	0.54
3:A:864:LEU:HD11	3:A:907:GLU:OE1	2.08	0.54
3:D:22:LYS:HE2	3:D:58:ASP:HB2	1.88	0.53
3:A:672:ALA:CA	3:A:678:ILE:HD11	2.38	0.53
3:A:437:GLN:HB3	8:A:1267:HOH:O	2.07	0.53
3:D:390:ALA:HB3	8:D:1367:HOH:O	2.09	0.53
3:D:511:GLU:HB2	8:D:1128:HOH:O	2.07	0.53
3:D:274:VAL:HG12	3:D:275:SER:N	2.24	0.53
2:F:176:PHE:O	2:F:176:PHE:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:705:PRO:O	3:D:708[A]:ILE:HG22	2.08	0.53
3:D:153:ILE:HD11	3:D:171:LEU:HD21	1.89	0.53
3:D:160:SER:HB3	3:D:163:LEU:HD12	1.90	0.53
3:A:87:ILE:O	3:A:91:TRP:HB2	2.08	0.53
3:A:30:ASN:HA	3:A:33:ASN:HD22	1.73	0.53
1:B:138:SER:HA	1:B:159:GLY:O	2.09	0.53
3:A:393:LEU:HB3	3:A:399:HIS:ND1	2.23	0.53
3:D:256:ASN:HB3	3:D:293:GLN:NE2	2.22	0.53
3:D:284:GLU:CD	3:D:343:LEU:HD11	2.29	0.53
1:B:352:ASP:HB3	3:A:711:GLY:O	2.08	0.53
1:B:171:ILE:HG22	1:B:189:MET:HG3	1.90	0.53
2:F:28:LYS:HG2	8:F:745:HOH:O	2.08	0.53
3:D:716:ASP:O	3:D:720:VAL:HG13	2.09	0.53
3:A:187:THR:H	3:A:190:LYS:NZ	2.07	0.53
3:A:739:VAL:HG12	3:A:745[A]:ILE:HG13	1.89	0.53
3:A:32:VAL:HG22	3:A:71:GLN:CB	2.38	0.53
3:A:299:PRO:HB2	3:A:302:THR:HG23	1.89	0.53
3:D:299:PRO:HB2	3:D:302:THR:HG23	1.89	0.53
3:D:1033:LEU:HB2	3:D:1035:LEU:HG	1.91	0.53
3:A:153:ILE:HD11	3:A:171:LEU:HD21	1.90	0.53
3:D:87:ILE:O	3:D:91:TRP:HB2	2.08	0.53
3:A:142:TRP:HB3	3:A:143:PRO:HD3	1.90	0.53
3:A:84:GLU:O	3:A:88:LYS:HG3	2.08	0.53
3:D:912:GLN:O	3:D:916[B]:GLN:HG3	2.09	0.53
3:D:887:ARG:HD3	3:D:937:ALA:CB	2.39	0.52
3:D:393:LEU:HD21	3:D:397:SER:HB3	1.90	0.52
3:A:962:LEU:HD13	3:A:973:PHE:CE2	2.43	0.52
3:A:990:GLN:HG2	3:A:993:GLN:HE21	1.74	0.52
1:B:187:ASP:OD1	1:B:204:ARG:HD2	2.10	0.52
3:A:437:GLN:HG2	3:A:746:ARG:CG	2.39	0.52
3:A:142:TRP:CZ3	3:A:197:SER:HB3	2.44	0.52
1:E:104:LEU:O	1:E:270:SER:HA	2.09	0.52
3:D:1029:ASP:OD1	3:D:1029:ASP:N	2.42	0.52
3:A:142:TRP:O	3:A:146:TRP:HB3	2.09	0.52
2:F:89:MET:HE2	2:F:120:CYS:HB2	1.91	0.52
3:A:960:THR:HG22	3:A:963:ASN:H	1.74	0.52
3:A:285:THR:O	3:A:289:LEU:HD13	2.08	0.52
3:D:672:ALA:CA	3:D:678:ILE:HD11	2.39	0.52
3:D:142:TRP:HB3	3:D:143:PRO:HD3	1.90	0.52
3:D:212:VAL:O	3:D:216:SER:HB3	2.09	0.52
3:A:724:LEU:HD12	3:A:751:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:ARG:CB	2:F:157:PHE:HZ	2.14	0.52
3:A:735:ASN:HB2	3:A:739:VAL:CG2	2.40	0.52
3:D:142:TRP:CZ3	3:D:197:SER:HB3	2.44	0.52
3:A:284:GLU:CD	3:A:343:LEU:HD11	2.30	0.52
3:D:735:ASN:HB2	3:D:739:VAL:CG2	2.40	0.52
1:E:352:ASP:HB2	3:D:711:GLY:O	2.09	0.52
3:D:957:LYS:HZ3	3:D:961:PRO:HB3	1.74	0.52
3:D:290:THR:HG21	3:D:325:PHE:CE2	2.45	0.52
3:D:141:GLU:HG2	3:D:145[A]:HIS:CD2	2.43	0.52
1:E:358:MET:O	1:E:359:GLU:HB2	2.10	0.52
3:D:960:THR:HG22	3:D:963:ASN:H	1.75	0.52
3:D:990:GLN:HG2	3:D:993:GLN:HE21	1.74	0.52
1:E:172:LEU:HD22	1:E:188[B]:VAL:HG12	1.92	0.52
3:D:105:TYR:O	3:D:109:LEU:HG	2.10	0.52
3:D:963:ASN:N	3:D:964:PRO:CD	2.73	0.51
3:D:961:PRO:HD3	3:D:970:ASN:OD1	2.11	0.51
3:D:476:MET:CE	3:D:516:PHE:CZ	2.93	0.51
3:D:821:GLN:OE1	3:D:821:GLN:HA	2.10	0.51
3:D:127:ILE:N	3:D:127:ILE:HD12	2.25	0.51
3:A:566:VAL:HG11	3:A:610:PHE:HE2	1.74	0.51
3:D:437:GLN:HG2	3:D:746:ARG:CG	2.39	0.51
3:A:333:HIS:HB3	3:A:336:LEU:HD23	1.92	0.51
1:B:128:LYS:O	1:B:175:ILE:HA	2.11	0.51
2:F:59:ILE:HD13	2:F:60:LYS:N	2.25	0.51
3:A:912:GLN:NE2	3:A:958:ILE:HG23	2.25	0.51
3:D:131:ASN:HD21	3:D:166:ASN:ND2	1.90	0.51
1:B:59:VAL:HA	1:B:195:PRO:HG2	1.91	0.51
3:A:212:VAL:O	3:A:216:SER:HB3	2.10	0.51
3:D:788:TYR:CD2	3:D:826:VAL:HG12	2.45	0.51
1:E:188[A]:VAL:HG13	1:E:188[A]:VAL:O	2.10	0.51
3:D:434:GLU:HA	3:D:439:GLU:O	2.10	0.51
3:D:436:ASP:O	3:D:437:GLN:HG3	2.11	0.51
3:A:509[B]:HIS:HD2	3:A:511:GLU:HB3	1.71	0.51
3:A:219:ALA:HB3	3:A:220:PRO:HD3	1.91	0.51
3:D:912:GLN:NE2	3:D:958:ILE:HG23	2.25	0.51
1:E:44:ARG:NH2	1:E:272:PRO:HG3	2.26	0.51
3:A:491:TRP:CH2	3:A:535:ASP:HB3	2.46	0.51
3:D:305:ARG:HG3	8:D:1384:HOH:O	2.11	0.51
3:D:518:VAL:O	3:D:522:LYS:HB2	2.10	0.51
3:A:110:ILE:HD13	3:A:130:LEU:HD13	1.93	0.51
3:A:664:VAL:CG1	3:A:691:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:755:THR:O	3:A:759:ILE:HG13	2.11	0.51
3:D:429:GLU:OE1	3:D:429:GLU:HA	2.10	0.51
3:D:104:LYS:HA	3:D:107:VAL:HG22	1.92	0.51
1:B:353:HIS:N	1:B:353:HIS:CD2	2.79	0.51
3:A:261:ARG:HD2	3:A:318:PHE:CG	2.46	0.51
3:A:851:LEU:O	3:A:855:VAL:HG23	2.11	0.51
3:D:19:PHE:O	3:D:19:PHE:CD1	2.64	0.51
1:E:356:CYS:HB3	3:D:673:THR:OG1	2.11	0.51
3:D:962:LEU:O	3:D:963:ASN:CB	2.59	0.50
3:D:58:ASP:CG	3:D:62:ARG:HE	2.14	0.50
2:C:98:TYR:O	2:C:101:VAL:HG23	2.11	0.50
3:A:1048:GLU:O	3:A:1052:LEU:N	2.45	0.50
3:A:887:ARG:NH2	3:A:891:ASP:HB3	2.25	0.50
3:D:219:ALA:HB3	3:D:220:PRO:HD3	1.92	0.50
1:E:187:ASP:HB3	1:E:189:MET:HE1	1.93	0.50
3:D:887:ARG:NH2	3:D:891:ASP:HB3	2.25	0.50
1:B:57:ASP:OD1	1:B:59:VAL:HB	2.10	0.50
3:D:881:ALA:O	3:D:884:HIS:HB2	2.11	0.50
3:A:129:LYS:O	3:A:133:ILE:HG13	2.11	0.50
3:A:105:TYR:O	3:A:109:LEU:HG	2.11	0.50
2:F:176:PHE:O	2:F:176:PHE:CD2	2.64	0.50
2:C:32:THR:OG1	2:C:34:GLU:HG2	2.11	0.50
3:A:276:VAL:HB	3:A:333:HIS:ND1	2.25	0.50
3:A:284:GLU:HG3	3:A:343:LEU:HD21	1.93	0.50
1:B:106[B]:GLU:O	1:B:275:GLY:HA2	2.12	0.50
3:D:996:LEU:O	3:D:999:THR:HG22	2.11	0.50
3:D:333:HIS:HB3	3:D:336:LEU:HD23	1.93	0.50
3:D:491:TRP:CH2	3:D:535:ASP:HB3	2.46	0.50
1:E:59:VAL:HA	1:E:195:PRO:HG2	1.92	0.50
2:C:129:ARG:NH1	3:A:447:ASP:O	2.45	0.50
3:D:66:ILE:CD1	3:D:75:THR:HG22	2.42	0.50
3:D:1050:HIS:HA	3:D:1053:GLN:HG2	1.92	0.50
1:E:225:ASN:N	1:E:226:PRO:HD3	2.27	0.50
3:D:566:VAL:HG11	3:D:610:PHE:HE2	1.75	0.50
3:D:755:THR:O	3:D:759:ILE:HG13	2.12	0.50
3:A:123:GLU:OE1	3:A:123:GLU:HA	2.11	0.50
2:F:38:LYS:HG2	3:D:842:PRO:HG3	1.94	0.50
3:D:1008:ILE:CG2	3:D:1009:PRO:HD3	2.30	0.50
3:A:1038:ARG:HH21	3:A:1042:LEU:HD21	1.76	0.50
1:B:202:ASP:HB3	1:B:262:LYS:HG2	1.94	0.50
2:C:29:ARG:CB	2:C:157:PHE:HZ	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:483:GLN:NE2	3:D:489:TRP:HA	2.26	0.50
2:C:52:PHE:HE1	2:C:61:PHE:HD2	1.60	0.50
3:D:729:SER:OG	3:D:792:VAL:HG22	2.12	0.50
3:A:968:VAL:HG12	3:A:973:PHE:HB2	1.93	0.49
3:A:181:PHE:O	3:A:185:GLN:HG2	2.12	0.49
2:C:59:ILE:HD13	2:C:60:LYS:N	2.26	0.49
3:A:559:TRP:CD2	3:A:603:GLN:HG3	2.46	0.49
3:A:957:LYS:HZ3	3:A:961:PRO:HB3	1.75	0.49
3:A:393:LEU:HD22	3:A:398:GLN:CA	2.35	0.49
3:D:326:LEU:O	3:D:330:LEU:HG	2.12	0.49
1:B:215:GLU:O	1:B:216:GLU:C	2.50	0.49
2:F:29:ARG:HG2	2:F:34:GLU:O	2.12	0.49
3:D:476:MET:HE2	3:D:516:PHE:HZ	1.77	0.49
3:D:788:TYR:O	3:D:796:ARG:HG2	2.12	0.49
1:E:25:HIS:HE1	1:E:27:ARG:HD3	1.78	0.49
1:E:57:ASP:OD1	1:E:59:VAL:HB	2.11	0.49
3:D:175[B]:SER:OG	3:D:232:PHE:HE1	1.95	0.49
3:A:894:LEU:HD13	3:A:941:MET:HB2	1.95	0.49
3:D:435:ASN:CG	3:D:439:GLU:HB2	2.32	0.49
1:E:358:MET:O	1:E:359:GLU:CB	2.60	0.49
3:D:261:ARG:HD2	3:D:318:PHE:CG	2.48	0.49
3:D:129:LYS:O	3:D:133:ILE:HG13	2.12	0.49
1:B:8:LEU:HD22	3:A:564:THR:HG22	1.93	0.49
3:D:30:ASN:HB3	3:D:44:ARG:HD2	1.94	0.49
3:D:344:ARG:O	3:D:348:MET:HG2	2.12	0.49
3:D:103:LYS:HE3	3:D:146:TRP:CD1	2.47	0.49
1:B:222:THR:HG22	1:B:225:ASN:N	2.26	0.49
3:D:882:PHE:C	3:D:882:PHE:CD1	2.86	0.49
3:A:875:LEU:O	3:A:879:ILE:HG12	2.13	0.49
1:B:70:TRP:CD1	1:B:97:HIS:CE1	3.00	0.49
3:D:56:HIS:CD2	3:D:56:HIS:O	2.66	0.49
3:D:797:GLU:OE2	3:D:798:PRO:HD2	2.13	0.49
3:A:26:ASN:HB3	8:A:1204:HOH:O	2.12	0.49
3:A:996:LEU:O	3:A:999:THR:HG22	2.12	0.49
3:D:875:LEU:O	3:D:879:ILE:HG12	2.13	0.49
3:A:967:PRO:HG2	3:A:968:VAL:HG23	1.95	0.49
3:D:142:TRP:O	3:D:146:TRP:HB3	2.12	0.49
3:A:76:LYS:HB3	3:A:126:TYR:CE1	2.47	0.49
3:A:187:THR:CG2	3:A:190:LYS:HB2	2.43	0.49
2:F:86:ALA:HB3	2:F:108:LEU:HD21	1.94	0.49
3:A:990:GLN:H	3:A:993:GLN:NE2	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ALA:HB3	2:C:108:LEU:HD21	1.93	0.49
3:D:28:LEU:HD12	3:D:75:THR:OG1	2.13	0.49
3:D:54:LYS:O	3:D:55:GLU:HG2	2.13	0.49
3:D:276:VAL:HB	3:D:333:HIS:ND1	2.27	0.49
3:A:882:PHE:CD1	3:A:882:PHE:C	2.86	0.49
1:E:114:ASP:HB3	8:E:876:HOH:O	2.13	0.49
2:C:47:VAL:HG13	2:C:47:VAL:O	2.12	0.49
3:D:1033:LEU:CD1	3:D:1035:LEU:HD21	2.43	0.49
1:E:219:GLY:O	1:E:228:LYS:HD2	2.13	0.49
1:E:350:SER:CB	1:E:351:PRO:HD2	2.17	0.48
3:A:435:ASN:C	3:A:437:GLN:H	2.16	0.48
3:A:429:GLU:HA	3:A:429:GLU:OE1	2.12	0.48
3:D:988:HIS:H	3:D:988:HIS:CD2	2.31	0.48
3:D:406:ARG:HD3	8:D:1182:HOH:O	2.13	0.48
3:A:545:MET:SD	3:A:569:LEU:HD11	2.52	0.48
3:D:208:LEU:HD23	3:D:208:LEU:C	2.33	0.48
3:A:56:HIS:O	3:A:56:HIS:CD2	2.66	0.48
3:A:290:THR:HG21	3:A:325:PHE:CE2	2.48	0.48
3:A:23:LEU:H	3:A:23:LEU:CD1	2.26	0.48
3:D:429:GLU:CG	3:D:445:MET:HG3	2.42	0.48
3:D:841:TYR:O	3:D:845:ARG:HG3	2.13	0.48
3:D:357:VAL:HG13	3:D:369:CYS:SG	2.53	0.48
2:C:29:ARG:HG2	2:C:34:GLU:O	2.14	0.48
3:D:517:LEU:HD11	3:D:551:TYR:CD1	2.47	0.48
3:A:962:LEU:CD2	3:A:968:VAL:HG11	2.40	0.48
3:D:486:GLY:O	3:D:487:THR:C	2.51	0.48
2:F:52:PHE:HE1	2:F:61:PHE:HD2	1.61	0.48
3:A:344:ARG:O	3:A:348:MET:HG2	2.13	0.48
1:E:283:SER:O	1:E:288:VAL:HG13	2.14	0.48
3:A:27:LEU:O	3:A:31:VAL:HG23	2.14	0.48
1:B:44:ARG:NH2	1:B:272:PRO:HG3	2.29	0.48
2:F:81:ILE:O	2:F:82:GLN:HB2	2.13	0.48
2:F:156:ASN:ND2	2:F:159:LYS:HZ1	2.11	0.48
3:D:145[A]:HIS:C	3:D:147:PRO:HD3	2.33	0.48
3:A:881:ALA:O	3:A:884:HIS:HB2	2.13	0.48
2:C:125:ASP:O	2:C:127:LYS:HE3	2.13	0.48
3:A:518:VAL:O	3:A:522:LYS:HB2	2.12	0.48
1:E:289:ALA:O	1:E:290:VAL:HB	2.13	0.48
3:D:268:LEU:HD22	3:D:286:LEU:HD11	1.95	0.48
3:A:76:LYS:HB3	3:A:126:TYR:HE1	1.78	0.48
2:C:178:ALA:O	2:C:179:MET:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:838:PHE:HA	3:D:845:ARG:NH2	2.29	0.48
3:A:953:VAL:CG2	3:A:974:ILE:HD12	2.43	0.48
1:B:104:LEU:O	1:B:270:SER:HA	2.13	0.48
3:D:354:MET:HB3	3:D:373:TRP:CZ2	2.49	0.48
3:D:52:HIS:CE1	3:D:82:ILE:HD12	2.49	0.48
3:A:62:ARG:HH11	3:A:79:GLY:CA	2.17	0.48
3:A:993:GLN:HG2	3:A:1033:LEU:HD22	1.96	0.48
3:D:185:GLN:HG3	3:D:186:ILE:HG13	1.95	0.48
3:A:23:LEU:HD13	3:A:26:ASN:HB2	1.96	0.48
3:D:27:LEU:O	3:D:31:VAL:HG23	2.14	0.48
3:D:120:VAL:HG23	3:D:121:GLU:N	2.28	0.48
1:B:60:ASN:O	1:B:64:ARG:HG3	2.14	0.48
3:A:104:LYS:HA	3:A:107:VAL:HG22	1.95	0.48
3:D:181:PHE:O	3:D:185:GLN:HG2	2.13	0.48
3:A:136:GLN:OE1	3:A:136:GLN:HA	2.14	0.48
3:D:175[B]:SER:OG	3:D:232:PHE:CE1	2.66	0.48
2:C:31:LEU:CD1	2:C:32:THR:HG23	2.44	0.47
3:A:1030:THR:HG23	3:A:1032:ASP:OD1	2.14	0.47
3:A:578:ASP:HA	8:A:1148:HOH:O	2.13	0.47
1:E:204:ARG:HA	8:E:492:HOH:O	2.13	0.47
3:D:739:VAL:HG12	3:D:745:ILE:HG13	1.95	0.47
1:E:358:MET:HB3	1:E:359:GLU:H	1.39	0.47
2:C:86:ALA:CB	2:C:108:LEU:HD21	2.44	0.47
1:B:245:VAL:HA	1:B:248:MET:SD	2.54	0.47
3:A:486:GLY:O	3:A:487:THR:C	2.52	0.47
3:D:575:GLU:HG2	3:D:580:VAL:HG11	1.97	0.47
2:C:15:LEU:HD22	2:C:23:LYS:HD2	1.96	0.47
1:E:43:ARG:HB3	1:E:43:ARG:HE	1.41	0.47
3:D:511:GLU:HG2	3:D:515:ARG:NH1	2.29	0.47
3:D:607:VAL:HG23	3:D:608:MET:HG2	1.96	0.47
3:A:28:LEU:HD12	3:A:75:THR:OG1	2.14	0.47
2:C:52:PHE:CE1	2:C:61:PHE:HD2	2.32	0.47
3:A:716:ASP:O	3:A:720:VAL:HG13	2.15	0.47
3:A:960:THR:HA	3:A:961:PRO:HD3	1.74	0.47
3:A:962:LEU:O	3:A:963:ASN:CB	2.61	0.47
3:D:399:HIS:C	3:D:401:ASP:N	2.68	0.47
3:D:344:ARG:CZ	3:D:408:LEU:HD11	2.44	0.47
3:A:688:LEU:O	3:A:692:LEU:HG	2.14	0.47
3:A:424:MET:HA	3:A:457:MET:CE	2.44	0.47
3:D:257:VAL:HG21	3:D:260:PHE:CD2	2.48	0.47
1:B:171:ILE:HG22	1:B:189:MET:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:122:LYS:O	3:A:123:GLU:O	2.33	0.47
3:A:953:VAL:HG21	3:A:974:ILE:HD12	1.97	0.47
3:D:664:VAL:CG1	3:D:691:ILE:HD11	2.45	0.47
2:F:101:VAL:HB	2:F:102:PRO:HD3	1.96	0.47
3:D:996:LEU:HD22	3:D:1035:LEU:HD23	1.97	0.47
1:B:128:LYS:HG3	1:B:176:TYR:HB3	1.96	0.47
3:A:257:VAL:HG21	3:A:260:PHE:CD2	2.49	0.47
2:F:88:ILE:HG21	2:F:101:VAL:HG13	1.96	0.47
3:A:326:LEU:O	3:A:330:LEU:HG	2.15	0.47
1:E:126:VAL:HG13	1:E:253:GLU:HB2	1.95	0.47
1:B:42:GLU:HB3	8:B:948:HOH:O	2.14	0.47
3:D:688:LEU:O	3:D:692:LEU:HG	2.14	0.47
3:A:185:GLN:HG3	3:A:186:ILE:HG13	1.96	0.47
3:D:135:VAL:HG12	3:D:139:LYS:HE2	1.96	0.47
3:D:436:ASP:C	3:D:437:GLN:HG3	2.34	0.47
3:D:453:LEU:O	3:D:457:MET:HG3	2.15	0.47
3:D:136:GLN:OE1	3:D:136:GLN:HA	2.15	0.47
3:A:988:HIS:H	3:A:988:HIS:CD2	2.32	0.47
1:B:219:GLY:O	1:B:228:LYS:HD2	2.15	0.47
3:A:73:MET:CG	3:A:126:TYR:HB2	2.45	0.46
3:A:453:LEU:O	3:A:457:MET:HG3	2.15	0.46
3:A:837:ASP:O	3:A:845:ARG:NH2	2.46	0.46
2:C:88:ILE:HG21	2:C:101:VAL:HG13	1.96	0.46
3:D:953:VAL:CG2	3:D:974:ILE:HD12	2.45	0.46
3:D:35:LEU:HD12	3:D:71:GLN:OE1	2.14	0.46
3:A:788:TYR:O	3:A:796:ARG:HG2	2.15	0.46
1:E:25:HIS:CE1	1:E:27:ARG:HD3	2.50	0.46
3:D:327:CYS:HB2	3:D:354:MET:CE	2.45	0.46
1:B:29:SER:O	1:B:30:GLN:C	2.52	0.46
3:A:962:LEU:HB2	3:A:973:PHE:CE2	2.50	0.46
3:D:73:MET:CG	3:D:126:TYR:HB2	2.45	0.46
1:E:176:TYR:HB2	1:E:183:TYR:CD1	2.50	0.46
3:D:202:PHE:CZ	3:D:236:ILE:HG21	2.51	0.46
3:A:139:LYS:HD3	3:A:186:ILE:HD11	1.97	0.46
3:A:146:TRP:CD2	3:A:149:PHE:HB2	2.50	0.46
2:C:91:ASP:OD1	2:C:123:LYS:HD2	2.15	0.46
3:D:760:SER:HB3	3:D:803:THR:HG23	1.98	0.46
1:B:106[A]:GLU:HG3	1:B:271:THR:O	2.15	0.46
2:C:81:ILE:O	2:C:82:GLN:HB2	2.15	0.46
3:A:476:MET:CE	3:A:516:PHE:CZ	2.94	0.46
3:D:435:ASN:HD21	3:D:439:GLU:HB2	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:96:ARG:NH2	3:A:145:HIS:CG	2.83	0.46
1:E:265:HIS:CE1	8:E:497:HOH:O	2.68	0.46
3:A:788:TYR:CD2	3:A:826:VAL:HG12	2.50	0.46
3:A:517:LEU:HD11	3:A:551:TYR:CD1	2.50	0.46
3:A:721:TYR:CD2	3:A:721:TYR:C	2.88	0.46
3:D:24:ASP:OD2	3:D:62:ARG:HA	2.16	0.46
1:E:52[A]:LYS:HD3	1:E:265:HIS:CG	2.50	0.46
3:A:239:GLY:O	3:A:243:GLU:HB2	2.15	0.46
3:D:716:ASP:O	3:D:720:VAL:CG1	2.64	0.46
3:D:739:VAL:O	3:D:742:GLN:HG2	2.16	0.46
2:F:36:GLU:OE2	2:F:38:LYS:HE3	2.16	0.46
3:A:525:LEU:CD1	3:A:544:ILE:HD13	2.46	0.46
3:D:721:TYR:C	3:D:721:TYR:CD2	2.89	0.46
1:B:285:VAL:O	1:B:286:LEU:HD12	2.16	0.46
2:F:122:ASN:O	2:F:123:LYS:HB2	2.15	0.46
3:A:797:GLU:OE2	3:A:798:PRO:HD2	2.16	0.46
3:A:668:ILE:HG12	8:A:1279:HOH:O	2.15	0.46
3:A:124:LYS:H	3:A:124:LYS:HD2	1.81	0.46
2:F:53:HIS:O	2:F:176:PHE:HB2	2.15	0.46
3:A:509[B]:HIS:HD2	3:A:511:GLU:N	2.09	0.46
2:C:178:ALA:O	2:C:179:MET:CB	2.63	0.46
1:E:349:HIS:NE2	3:D:708[A]:ILE:HD12	2.31	0.46
3:A:575:GLU:HG2	3:A:580:VAL:HG11	1.98	0.46
3:A:393:LEU:CD2	3:A:398:GLN:HA	2.39	0.46
3:A:678:ILE:C	3:A:680:LYS:N	2.69	0.46
3:D:815:ILE:HA	3:D:818:GLU:OE1	2.16	0.46
3:A:106:VAL:O	3:A:110:ILE:HG12	2.15	0.46
1:E:212:LEU:N	1:E:213:PRO:CD	2.79	0.46
3:D:119:CYS:SG	3:D:127:ILE:HG12	2.56	0.46
3:A:268:LEU:HD22	3:A:286:LEU:HD11	1.97	0.46
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.97	0.46
3:D:217:GLN:HB2	3:D:217:GLN:HE21	1.54	0.46
3:A:307:ALA:O	3:A:315:GLU:OE2	2.34	0.46
3:D:485:ASN:C	3:D:487:THR:N	2.68	0.46
3:D:982:LEU:HD13	3:D:1018:PHE:CZ	2.51	0.46
3:D:124:LYS:HD2	3:D:124:LYS:H	1.81	0.46
1:B:52:LYS:HD3	1:B:265:HIS:ND1	2.30	0.45
3:D:678:ILE:C	3:D:680:LYS:N	2.69	0.45
2:F:52:PHE:CE1	2:F:61:PHE:HD2	2.33	0.45
1:B:208:MET:HG2	1:B:212:LEU:CD1	2.46	0.45
1:B:209:HIS:O	1:B:213:PRO:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:GLU:HB3	3:D:722:LYS:HD3	1.98	0.45
3:D:829:CYS:O	3:D:833:MET:HG3	2.16	0.45
3:A:815:ILE:HA	3:A:818:GLU:OE1	2.16	0.45
1:E:189:MET:O	1:E:196:PHE:N	2.43	0.45
2:F:159:LYS:HB2	2:F:160:PRO:HD3	1.97	0.45
3:D:953:VAL:HG21	3:D:974:ILE:HD12	1.98	0.45
1:E:360:ASN:CG	1:E:360:ASN:O	2.54	0.45
3:A:440:VAL:O	3:A:440:VAL:HG23	2.16	0.45
3:D:600:VAL:HG13	3:D:644:GLN:NE2	2.30	0.45
3:D:424:MET:HA	3:D:457:MET:CE	2.45	0.45
3:D:544:ILE:HG22	3:D:545:MET:CE	2.46	0.45
3:D:402:ILE:HG21	3:D:407:GLN:NE2	2.31	0.45
3:D:654:ILE:HB	3:D:708[B]:ILE:HD11	1.99	0.45
3:A:611:ILE:HG13	3:A:615[B]:LEU:HD22	1.99	0.45
3:D:497:LEU:HD12	3:D:497:LEU:O	2.16	0.45
3:A:186:ILE:HG22	3:A:187:THR:O	2.17	0.45
3:D:290:THR:HG21	3:D:325:PHE:CZ	2.51	0.45
2:F:81:ILE:HD11	3:D:77:TYR:CD2	2.51	0.45
2:F:77:ASP:OD1	2:F:77:ASP:N	2.50	0.45
3:A:829:CYS:O	3:A:833:MET:HG3	2.17	0.45
3:A:739:VAL:O	3:A:742:GLN:HG2	2.17	0.45
3:D:665:TRP:CZ3	3:D:692:LEU:HD21	2.50	0.45
3:A:223:HIS:CE1	3:A:263:VAL:HG21	2.51	0.45
1:B:225:ASN:N	1:B:226:PRO:HD3	2.32	0.45
2:F:98:TYR:O	2:F:101:VAL:HG23	2.17	0.45
3:D:593:GLN:HB3	8:D:1328:HOH:O	2.16	0.45
1:B:160:ASN:O	1:B:161:ARG:HB2	2.17	0.45
3:A:70:SER:O	3:A:71:GLN:HB2	2.16	0.45
1:E:173:ASP:HB2	1:E:189:MET:CE	2.46	0.45
1:E:129:ARG:HG2	1:E:144:LYS:HE3	1.98	0.45
3:D:146:TRP:CD2	3:D:149:PHE:HB2	2.52	0.45
3:A:485:ASN:C	3:A:487:THR:N	2.69	0.45
1:E:209:HIS:HE1	1:E:232:LEU:O	1.99	0.45
2:C:123:LYS:HG2	5:C:217:GTP:C6	2.51	0.45
3:D:480:LEU:O	3:D:483:GLN:HB2	2.16	0.45
1:B:209:HIS:NE2	1:B:232:LEU:O	2.50	0.45
1:B:212:LEU:N	1:B:213:PRO:CD	2.79	0.45
3:D:837:ASP:O	3:D:845:ARG:NH2	2.47	0.45
3:A:19:PHE:O	3:A:19:PHE:CG	2.70	0.45
3:A:940:THR:O	3:A:944:SER:HB2	2.17	0.45
1:B:264:THR:OG1	1:B:273:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:ARG:NH1	2:C:130:LYS:HE2	2.32	0.45
3:A:534:LYS:HE2	3:A:577:HIS:HB2	1.99	0.45
3:D:989:LEU:HD11	3:D:1022:ILE:HG22	1.99	0.45
1:E:41:SER:HB2	1:E:110:ASP:HB3	1.97	0.45
3:D:962:LEU:O	3:D:963:ASN:HB2	2.17	0.45
3:A:95:PRO:HG2	3:A:98:GLN:HB2	1.99	0.45
3:A:110:ILE:HD11	3:A:130:LEU:HB3	1.96	0.45
3:D:127:ILE:N	3:D:127:ILE:CD1	2.80	0.45
2:F:86:ALA:CB	2:F:108:LEU:HD21	2.47	0.45
2:C:156:ASN:ND2	2:C:159:LYS:HZ1	2.15	0.45
3:D:772:VAL:HG12	3:D:811:LEU:HD11	1.98	0.45
3:A:989:LEU:HD11	3:A:1022:ILE:HG22	1.99	0.45
1:B:7:ALA:HA	8:B:410:HOH:O	2.16	0.45
3:A:458:ARG:HG3	3:A:503:SER:HB2	1.99	0.45
1:B:285:VAL:O	1:B:286:LEU:HB2	2.17	0.44
3:A:274:VAL:HG12	3:A:275:SER:H	1.82	0.44
1:B:57:ASP:HB3	8:B:903:HOH:O	2.16	0.44
1:E:8:LEU:HD22	3:D:564:THR:HG22	1.99	0.44
3:A:55:GLU:HG2	3:A:56:HIS:N	2.28	0.44
1:E:187:ASP:OD1	1:E:204:ARG:HD2	2.17	0.44
1:B:208:MET:HG2	1:B:212:LEU:HD11	1.98	0.44
2:C:101:VAL:HB	2:C:102:PRO:HD3	1.98	0.44
3:A:534:LYS:HB3	3:A:577:HIS:CD2	2.51	0.44
3:D:216:SER:HB2	3:D:222:VAL:HG22	1.99	0.44
2:F:38:LYS:HE3	2:F:38:LYS:HB2	1.77	0.44
1:E:180:ASN:O	1:E:181:GLN:C	2.53	0.44
3:D:693:LYS:O	3:D:697:ARG:HG2	2.17	0.44
3:A:287:PHE:HB2	3:A:329:PHE:CZ	2.51	0.44
3:A:30:ASN:CA	3:A:44:ARG:HD2	2.48	0.44
3:D:53:LEU:CD1	3:D:54:LYS:H	2.19	0.44
1:E:97[A]:HIS:CD2	1:E:98:TYR:N	2.85	0.44
3:D:939:LEU:HD21	3:D:1016:ARG:HH11	1.82	0.44
3:D:966:ASN:N	3:D:967:PRO:HD2	2.33	0.44
3:A:594:LYS:HE2	3:A:594:LYS:HA	2.00	0.44
3:D:218:ASN:O	3:D:222:VAL:HG23	2.18	0.44
3:D:716:ASP:HA	8:D:1253:HOH:O	2.16	0.44
3:A:1046:GLN:OE1	3:A:1049:LYS:HD3	2.17	0.44
3:D:257:VAL:HG22	3:D:260:PHE:HB2	2.00	0.44
3:D:402:ILE:HG23	3:D:402:ILE:O	2.17	0.44
3:A:600:VAL:HG13	3:A:644:GLN:NE2	2.32	0.44
3:D:458:ARG:HG3	3:D:503:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:VAL:O	2:F:47:VAL:HG23	2.18	0.44
3:A:693:LYS:O	3:A:697:ARG:HG2	2.18	0.44
3:D:685:VAL:HA	3:D:688:LEU:HD12	2.00	0.44
3:A:437:GLN:C	3:A:439:GLU:H	2.21	0.44
1:E:12:PHE:HE2	3:D:545:MET:HE3	1.83	0.44
3:D:849:PHE:CZ	3:D:881:ALA:HB2	2.52	0.44
3:A:607:VAL:HG23	3:A:608:MET:HG2	1.99	0.44
1:B:58:TYR:HB3	1:B:197:TYR:HD1	1.83	0.44
3:A:388:THR:HG22	3:A:389:SER:H	1.81	0.44
1:B:176:TYR:HB2	1:B:183:TYR:CD1	2.52	0.44
3:D:887:ARG:HA	3:D:887:ARG:HD2	1.58	0.44
3:A:216:SER:HB2	3:A:222:VAL:HG22	2.00	0.44
3:D:1038:ARG:O	3:D:1042:LEU:HG	2.18	0.44
2:F:123:LYS:HG2	5:F:217:GTP:C6	2.53	0.44
1:E:-1:GLY:O	1:E:3[A]:GLU:HG2	2.17	0.44
3:A:277:SER:HB3	3:A:278:GLN:OE1	2.18	0.44
3:A:414:SER:OG	3:A:471:ASP:OD2	2.32	0.44
3:D:17:LEU:HD12	3:D:17:LEU:HA	1.76	0.44
1:E:240:GLU:CD	1:E:240:GLU:H	2.20	0.44
3:D:223:HIS:CE1	3:D:263:VAL:HG21	2.52	0.44
3:A:186:ILE:HG23	3:A:190:LYS:HD2	1.99	0.44
3:A:216:SER:HB2	3:A:222:VAL:HG21	2.00	0.44
1:E:208:MET:HG2	1:E:212:LEU:CD1	2.48	0.44
3:D:731:ALA:HB1	3:D:739:VAL:HG11	1.99	0.44
3:A:286:LEU:O	3:A:286:LEU:HD12	2.18	0.44
3:D:22:LYS:HB2	3:D:61:THR:HG21	1.98	0.43
3:D:66:ILE:HD13	3:D:75:THR:CG2	2.48	0.43
2:F:91:ASP:OD1	2:F:123:LYS:HD2	2.18	0.43
2:C:91:ASP:CG	2:C:123:LYS:HD2	2.38	0.43
1:E:102:LEU:CD1	1:E:129:ARG:HG3	2.48	0.43
2:F:40:VAL:HG13	3:D:839:GLU:OE1	2.18	0.43
3:D:393:LEU:HD12	3:D:395:SER:N	2.23	0.43
3:D:397:SER:O	3:D:398:GLN:HB2	2.18	0.43
3:A:94:LEU:HD22	3:A:98:GLN:HG2	1.99	0.43
3:A:223:HIS:CE1	3:A:263:VAL:CG2	3.01	0.43
3:D:274:VAL:HG12	3:D:275:SER:H	1.83	0.43
1:B:253:GLU:H	1:B:253:GLU:HG3	1.66	0.43
1:E:351:PRO:O	1:E:352:ASP:OD1	2.37	0.43
3:A:738:MET:C	3:A:740:THR:H	2.21	0.43
3:A:993:GLN:HG2	3:A:1033:LEU:CD2	2.48	0.43
3:D:186:ILE:HG22	3:D:187:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:294:LEU:HD21	3:A:322:LEU:HD11	1.99	0.43
1:E:212:LEU:HB2	1:E:213:PRO:HD3	2.01	0.43
3:A:344:ARG:CZ	3:A:408:LEU:HD11	2.48	0.43
3:A:545:MET:SD	3:A:569:LEU:CD1	3.06	0.43
2:C:81:ILE:HD11	3:A:77:TYR:CD2	2.53	0.43
3:D:435:ASN:C	3:D:437:GLN:H	2.21	0.43
3:A:24:ASP:O	3:A:28:LEU:HB2	2.17	0.43
1:E:209:HIS:O	1:E:213:PRO:HG2	2.19	0.43
3:A:778:PRO:HB2	3:A:779:PRO:HD3	2.01	0.43
1:E:215:GLU:O	1:E:216:GLU:C	2.57	0.43
3:D:303:ASN:HD21	3:D:305:ARG:NH2	2.15	0.43
3:D:666:ASP:O	3:D:670:GLN:HG3	2.19	0.43
2:C:45:VAL:HG22	2:C:46:GLU:N	2.33	0.43
3:D:534:LYS:HE2	3:D:577:HIS:HB2	2.00	0.43
3:D:961:PRO:HD2	3:D:962:LEU:H	1.83	0.43
3:A:223:HIS:NE2	3:A:263:VAL:HG21	2.34	0.43
1:E:173:ASP:CB	1:E:189:MET:HE1	2.49	0.43
3:A:218:ASN:O	3:A:222:VAL:HG23	2.19	0.43
3:D:294:LEU:HD21	3:D:322:LEU:HD11	1.99	0.43
3:A:907:GLU:N	3:A:907:GLU:OE2	2.52	0.43
3:A:689:GLY:O	3:A:693:LYS:HG3	2.18	0.43
3:D:753:ARG:NH1	8:D:1310:HOH:O	2.51	0.43
3:D:778:PRO:HB2	3:D:779:PRO:HD3	2.01	0.43
3:A:898:PHE:CE1	3:A:902:GLN:NE2	2.87	0.43
3:A:820:PRO:HB2	8:A:1212:HOH:O	2.18	0.43
3:D:54:LYS:O	3:D:55:GLU:CG	2.66	0.43
3:A:388:THR:CG2	3:A:399:HIS:HE2	2.29	0.43
2:C:169:ILE:HG22	2:C:170:GLY:N	2.31	0.43
2:F:142:LYS:HB2	2:F:144:LEU:HG	2.01	0.43
3:A:206:PHE:CE2	3:A:244:THR:HG21	2.50	0.43
1:B:25:HIS:ND1	1:B:26:PRO:HD2	2.34	0.43
2:C:142:LYS:HB2	2:C:144:LEU:HG	2.01	0.43
1:B:192:ARG:O	1:B:194:HIS:CD2	2.72	0.43
3:A:19:PHE:C	3:A:21:GLN:H	2.20	0.43
3:D:363:THR:O	3:D:367:LYS:HG3	2.19	0.43
1:B:2:GLU:OE2	1:B:2:GLU:C	2.56	0.43
3:D:426:LYS:N	3:D:426:LYS:CD	2.72	0.43
3:A:888:ASN:HD22	3:A:889:VAL:N	2.15	0.43
3:D:223:HIS:NE2	3:D:263:VAL:HG21	2.34	0.43
3:D:92:LYS:HD2	3:D:1030:THR:CG2	2.49	0.43
3:A:1038:ARG:O	3:A:1042:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:716:ASP:O	3:A:720:VAL:CG1	2.67	0.43
3:A:720:VAL:HG22	8:A:1183:HOH:O	2.18	0.43
2:C:80:TYR:O	2:C:81:ILE:C	2.57	0.43
3:D:689:GLY:O	3:D:693:LYS:HG3	2.18	0.43
1:B:356:CYS:O	3:A:719:ASN:ND2	2.52	0.43
3:D:287:PHE:HB2	3:D:329:PHE:CZ	2.53	0.43
3:D:777:VAL:O	3:D:780:LEU:HB2	2.19	0.42
3:D:294:LEU:HD21	3:D:322:LEU:CD1	2.49	0.42
3:A:978:VAL:O	3:A:981:LEU:HB3	2.19	0.42
3:A:511:GLU:HG2	3:A:515:ARG:NH1	2.34	0.42
1:E:70:TRP:CZ2	1:E:97[A]:HIS:HA	2.54	0.42
1:B:128:LYS:HE3	1:B:176:TYR:CD2	2.51	0.42
3:D:202:PHE:HD1	3:D:205:ILE:HD11	1.83	0.42
3:A:840:GLU:O	3:A:845:ARG:HD2	2.18	0.42
1:B:194:HIS:HA	1:B:195:PRO:HD3	1.92	0.42
3:A:1036:GLU:OE1	3:A:1037:GLU:HG3	2.18	0.42
2:F:13:LEU:HB2	2:F:85:CYS:SG	2.59	0.42
2:C:9:VAL:HG13	2:C:9:VAL:O	2.19	0.42
3:A:704:HIS:HB3	3:A:705:PRO:HD3	2.02	0.42
3:D:888:ASN:HD22	3:D:889:VAL:N	2.16	0.42
3:D:87:ILE:HD13	3:D:137:ILE:HG13	2.00	0.42
3:A:290:THR:O	3:A:294:LEU:HB2	2.19	0.42
3:D:978:VAL:O	3:D:981:LEU:HB3	2.19	0.42
3:D:960:THR:CG2	3:D:968:VAL:HG11	2.29	0.42
3:A:961:PRO:HD2	3:A:962:LEU:H	1.85	0.42
3:A:257:VAL:HG22	3:A:260:PHE:HB2	2.02	0.42
1:B:353:HIS:HA	1:B:354:PRO:HD3	1.63	0.42
3:A:607:VAL:HA	8:A:1224:HOH:O	2.18	0.42
3:A:409:TYR:O	3:A:410:LEU:C	2.57	0.42
1:E:251:PRO:HG2	1:E:252:PHE:CD1	2.54	0.42
2:C:36:GLU:HA	8:C:673:HOH:O	2.19	0.42
3:A:497:LEU:HD12	3:A:497:LEU:O	2.19	0.42
3:A:202:PHE:CZ	3:A:236:ILE:HG21	2.55	0.42
3:A:731:ALA:HB1	3:A:739:VAL:HG11	2.00	0.42
3:D:393:LEU:O	3:D:395:SER:N	2.52	0.42
1:B:359:GLU:O	1:B:360:ASN:C	2.58	0.42
2:C:106:ARG:NH1	2:C:107:ASP:OD1	2.52	0.42
3:A:218:ASN:C	3:A:218:ASN:HD22	2.22	0.42
3:D:330:LEU:HB3	3:D:372:TYR:CE1	2.54	0.42
3:A:978:VAL:HG12	3:A:998:VAL:HG22	2.02	0.42
2:F:15:LEU:HD22	2:F:23:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:281:GLU:HA	3:A:281:GLU:OE2	2.20	0.42
3:A:971:GLN:NE2	8:A:1078:HOH:O	2.51	0.42
3:D:437:GLN:O	3:D:439:GLU:N	2.53	0.42
3:D:55:GLU:HB3	3:D:56:HIS:H	1.69	0.42
3:A:665:TRP:CZ3	3:A:692:LEU:HD21	2.53	0.42
3:A:1036:GLU:HG2	3:A:1037:GLU:N	2.35	0.42
1:E:58:TYR:HB3	1:E:197:TYR:HD1	1.85	0.42
3:D:724:LEU:CD2	3:D:751:VAL:HG11	2.49	0.42
1:E:95:PRO:HB2	1:E:101:GLN:HE22	1.85	0.42
3:A:294:LEU:HD21	3:A:322:LEU:CD1	2.50	0.42
3:D:916[A]:GLN:HA	3:D:916[A]:GLN:NE2	2.34	0.42
3:A:982:LEU:HD13	3:A:1018:PHE:CZ	2.55	0.42
3:A:930:VAL:HG12	3:A:931:THR:N	2.33	0.42
3:D:481:GLN:OE1	3:D:485:ASN:ND2	2.53	0.42
3:D:482:ASN:HA	3:D:486:GLY:HA3	2.01	0.42
3:A:87:ILE:HD13	3:A:137:ILE:HG13	2.01	0.42
3:A:327:CYS:O	3:A:331:LYS:HB2	2.20	0.42
3:D:106:VAL:O	3:D:110:ILE:HG13	2.20	0.42
1:B:151:ARG:NH1	8:B:384:HOH:O	2.52	0.42
3:D:569:LEU:HD11	3:D:591:ILE:HD12	2.02	0.42
1:E:52[B]:LYS:HD2	1:E:265:HIS:CG	2.55	0.42
2:F:106:ARG:NH1	2:F:107:ASP:OD1	2.52	0.42
3:A:482:ASN:HA	3:A:486:GLY:HA3	2.01	0.42
3:A:882:PHE:HA	3:A:890:ALA:HA	2.01	0.42
1:B:123:VAL:HG22	1:B:257:LEU:CD2	2.50	0.42
1:E:128:LYS:CE	3:D:623:CYS:O	2.68	0.42
3:D:19:PHE:O	3:D:19:PHE:CG	2.72	0.42
3:D:286:LEU:HD12	3:D:286:LEU:O	2.19	0.42
1:B:104:LEU:HB2	1:B:270:SER:HA	2.01	0.42
3:A:920:CYS:O	3:A:923:LEU:HB2	2.20	0.42
1:E:224:LEU:HA	8:E:767:HOH:O	2.19	0.42
3:A:231:ARG:HA	3:A:231:ARG:HD3	1.90	0.42
3:A:685:VAL:HA	3:A:688:LEU:HD12	2.02	0.41
3:D:216:SER:HB2	3:D:222:VAL:HG21	2.02	0.41
1:E:278:ARG:HB2	1:E:281:MET:HG3	2.01	0.41
1:E:208:MET:HG2	1:E:212:LEU:HD11	2.01	0.41
3:D:104:LYS:HD2	3:D:104:LYS:HA	1.76	0.41
3:A:123:GLU:C	3:A:125:VAL:N	2.73	0.41
2:F:88:ILE:HB	2:F:119:LEU:HD23	2.02	0.41
3:D:738:MET:C	3:D:740:THR:H	2.22	0.41
1:B:153:SER:O	1:B:226:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:LEU:O	3:A:250:LEU:HG	2.20	0.41
3:A:23:LEU:HD12	3:A:23:LEU:N	2.35	0.41
3:A:23:LEU:HD13	3:A:26:ASN:CB	2.50	0.41
3:D:403:PRO:HA	3:D:404:PRO:HD3	1.83	0.41
3:D:95:PRO:HG2	3:D:98:GLN:HB2	2.02	0.41
1:E:121:VAL:CG2	1:E:257:LEU:HB3	2.50	0.41
3:A:1054:MET:HA	8:A:1213:HOH:O	2.19	0.41
3:A:251:ILE:HD13	3:A:289:LEU:HB2	2.02	0.41
3:A:114:SER:C	3:A:116:ASP:H	2.23	0.41
3:A:849:PHE:CZ	3:A:881:ALA:HB2	2.54	0.41
3:D:57:PRO:HA	3:D:60:TRP:CZ3	2.55	0.41
3:D:338:GLU:OE2	3:D:409:TYR:HE2	2.03	0.41
3:A:103:LYS:HZ2	3:A:103:LYS:HB2	1.85	0.41
2:C:9:VAL:HG22	2:C:9:VAL:O	2.20	0.41
3:D:920:CYS:O	3:D:923:LEU:HB2	2.21	0.41
3:A:574:HIS:HD2	3:A:624:ASP:CG	2.24	0.41
2:C:39:TYR:HA	8:C:555:HOH:O	2.20	0.41
1:E:43:ARG:CG	1:E:46:ARG:HH12	2.33	0.41
3:A:1003:SER:HA	3:A:1046:GLN:HE21	1.86	0.41
3:A:308:TYR:CE1	3:A:365:ILE:HD11	2.55	0.41
3:D:268:LEU:HD22	3:D:286:LEU:CD1	2.50	0.41
3:D:918:TYR:O	3:D:921:ASP:HB2	2.20	0.41
3:D:930:VAL:HG12	3:D:931:THR:N	2.34	0.41
3:A:403:PRO:HA	3:A:404:PRO:HD3	1.84	0.41
3:D:218:ASN:C	3:D:218:ASN:HD22	2.23	0.41
1:B:121:VAL:CG2	1:B:257:LEU:HB3	2.50	0.41
1:E:25:HIS:ND1	1:E:26:PRO:HD2	2.35	0.41
3:D:398:GLN:O	3:D:399:HIS:O	2.38	0.41
3:A:24:ASP:C	3:A:24:ASP:OD1	2.59	0.41
3:D:888:ASN:N	3:D:888:ASN:ND2	2.68	0.41
3:A:153:ILE:HG13	3:A:154:VAL:N	2.36	0.41
3:A:887:ARG:HA	3:A:887:ARG:HD2	1.59	0.41
3:A:338:GLU:OE2	3:A:409:TYR:HE2	2.03	0.41
1:E:124:CYS:HA	1:E:125:PRO:HD3	1.68	0.41
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.21	0.41
3:D:146:TRP:N	3:D:147:PRO:CD	2.84	0.41
3:D:287:PHE:CE2	3:D:337:LEU:HD13	2.55	0.41
3:D:940:THR:O	3:D:944:SER:HB2	2.21	0.41
2:F:118:VAL:HG23	2:F:164:LEU:HD21	2.03	0.41
3:A:1009:PRO:O	3:A:1013:GLU:HG2	2.20	0.41
3:A:33:ASN:HD22	3:A:44:ARG:HE	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:969:ASN:O	3:A:970:ASN:C	2.60	0.41
3:D:993:GLN:HG2	3:D:1033:LEU:HD13	2.03	0.41
3:D:97:ASN:H	3:D:97:ASN:HD22	1.65	0.41
3:D:223:HIS:CE1	3:D:263:VAL:CG2	3.04	0.41
1:E:187:ASP:HB3	1:E:189:MET:CE	2.51	0.41
3:D:517:LEU:O	3:D:521:ILE:HG12	2.21	0.41
3:A:290:THR:HG21	3:A:325:PHE:CZ	2.55	0.41
2:C:122:ASN:O	2:C:123:LYS:HB2	2.20	0.41
2:F:77:ASP:HA	2:F:80:TYR:CD2	2.56	0.41
2:F:80:TYR:O	2:F:81:ILE:C	2.59	0.41
3:A:417:ARG:NH2	3:A:464:LEU:O	2.47	0.41
3:D:1012:LYS:HB3	3:D:1012:LYS:HE2	1.85	0.41
3:D:24:ASP:O	3:D:28:LEU:HB2	2.20	0.41
3:A:63:VAL:HA	3:A:76:LYS:CG	2.48	0.41
3:D:202:PHE:CE2	3:D:206:PHE:HD1	2.38	0.41
3:A:190:LYS:HB2	3:A:190:LYS:HE3	1.78	0.41
1:B:58:TYR:HB3	1:B:197:TYR:CD1	2.56	0.41
3:A:1034:PHE:C	3:A:1036:GLU:H	2.24	0.41
1:E:242:LEU:O	1:E:246:LEU:HB2	2.21	0.41
3:D:16:LEU:HD12	3:D:16:LEU:C	2.41	0.41
2:C:54:THR:HG22	2:C:176:PHE:HD1	1.86	0.41
3:D:242:PHE:HB3	3:D:282:GLN:HG2	2.03	0.41
3:D:1009:PRO:O	3:D:1013:GLU:HG2	2.21	0.40
3:A:962:LEU:HG	3:A:962:LEU:O	2.20	0.40
2:F:106:ARG:HD3	3:D:181:PHE:CD2	2.54	0.40
3:D:409:TYR:O	3:D:410:LEU:C	2.58	0.40
1:B:15:SER:HB2	8:B:546:HOH:O	2.20	0.40
3:A:467:LEU:N	3:A:467:LEU:HD23	2.36	0.40
3:D:962:LEU:CB	3:D:964:PRO:HD3	2.51	0.40
1:B:201:THR:HG22	1:B:204:ARG:HH12	1.85	0.40
3:D:525:LEU:CD1	3:D:544:ILE:HD13	2.52	0.40
3:D:772:VAL:CG1	3:D:811:LEU:HD11	2.51	0.40
3:D:659:LEU:O	3:D:663:GLN:HG3	2.22	0.40
3:D:975:GLN:HG2	3:D:998:VAL:HG12	2.02	0.40
1:E:245:VAL:HA	1:E:248:MET:HG3	2.03	0.40
3:D:231:ARG:HA	3:D:231:ARG:HD3	1.92	0.40
3:A:738:MET:C	3:A:740:THR:N	2.74	0.40
1:B:187:ASP:OD2	1:B:204:ARG:NH2	2.54	0.40
3:D:179:PHE:HE2	3:D:198:MET:HE3	1.85	0.40
1:B:61:HIS:CG	1:B:94:LEU:HD13	2.55	0.40
1:E:245:VAL:HA	1:E:248:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:419:LEU:HD23	3:A:420:MET:CE	2.52	0.40
3:A:549:GLY:HA3	8:A:1115:HOH:O	2.21	0.40
3:A:422:SER:OG	3:A:479:LYS:HE3	2.21	0.40
3:D:898:PHE:CE1	3:D:902:GLN:NE2	2.89	0.40
1:B:35:TYR:CD2	1:B:35:TYR:O	2.75	0.40
1:B:41:SER:HB2	1:B:110:ASP:HB3	2.02	0.40
1:B:124:CYS:HA	1:B:125:PRO:HD3	1.67	0.40
3:D:222:VAL:O	3:D:226:LEU:HB2	2.21	0.40
3:A:146:TRP:N	3:A:147:PRO:CD	2.84	0.40
3:D:238:LEU:HD22	3:D:242:PHE:HE2	1.86	0.40
3:D:76:LYS:HE2	3:D:126:TYR:CZ	2.56	0.40
3:A:289:LEU:HD12	3:A:289:LEU:N	2.36	0.40
3:A:575:GLU:OE2	3:A:577:HIS:HB2	2.21	0.40
3:A:465:THR:O	3:A:469:TYR:HB3	2.21	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	B	266/365 (73%)	241 (91%)	20 (8%)	5 (2%)	10	16
1	E	277/365 (76%)	253 (91%)	16 (6%)	8 (3%)	6	8
2	C	170/216 (79%)	157 (92%)	11 (6%)	2 (1%)	16	29
2	F	169/216 (78%)	157 (93%)	9 (5%)	3 (2%)	11	18
3	A	1042/1073 (97%)	945 (91%)	79 (8%)	18 (2%)	11	19
3	D	1045/1073 (97%)	952 (91%)	71 (7%)	22 (2%)	9	14
All	All	2969/3308 (90%)	2705 (91%)	206 (7%)	58 (2%)	10	15

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	B	216	GLU
1	B	351	PRO
2	C	169	ILE
3	A	123	GLU
3	A	390	ALA
3	A	963	ASN
1	E	94	LEU
1	E	351	PRO
1	E	359	GLU
3	D	399	HIS
3	D	963	ASN
1	B	286	LEU
3	A	54	LYS
3	A	486	GLY
3	A	964	PRO
1	E	286	LEU
2	F	55	ASN
3	D	54	LYS
3	D	216	SER
3	D	486	GLY
3	D	490	SER
3	D	623	CYS
3	A	216	SER
3	A	217	GLN
3	A	490	SER
3	A	623	CYS
3	A	961	PRO
2	F	178	ALA
3	D	217	GLN
3	D	438	GLY
3	D	961	PRO
1	B	97	HIS
2	C	178	ALA
3	A	277	SER
3	A	281	GLU
3	A	743	PRO
1	E	358	MET
3	D	53	LEU
3	D	277	SER
3	D	487	THR
3	D	737[A]	GLU
3	D	737[B]	GLU

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Mol	Chain	Res	Type
3	D	743	PRO
3	A	143	PRO
3	A	487	THR
3	D	143	PRO
3	D	281	GLU
3	D	679	LEU
3	A	55	GLU
3	A	955	GLU
1	E	52[A]	LYS
1	E	52[B]	LYS
1	E	285	VAL
3	D	764	SER
3	D	955	GLU
3	D	111	ILE
2	F	81	ILE

### 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	B	249/327 (76%)	229 (92%)	20 (8%)	15	28
1	E	257/327 (79%)	242 (94%)	15 (6%)	25	45
2	C	151/185 (82%)	138 (91%)	13 (9%)	13	24
2	F	150/185 (81%)	139 (93%)	11 (7%)	17	32
3	A	950/973 (98%)	889 (94%)	61 (6%)	22	39
3	D	953/973 (98%)	894 (94%)	59 (6%)	23	41
All	All	2710/2970 (91%)	2531 (93%)	179 (7%)	21	38

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	GLU
1	B	17[A]	ASP
1	B	17[B]	ASP

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Mol	Chain	Res	Type
1	B	35	TYR
1	B	111	VAL
1	B	120	ILE
1	B	129	ARG
1	B	156	LEU
1	B	189	MET
1	B	201	THR
1	B	222	THR
1	B	245	VAL
1	B	271	THR
1	B	277	LEU
1	B	284	ASP
1	B	285	VAL
1	B	352	ASP
1	B	353	HIS
1	B	357	LEU
1	B	360	ASN
2	C	15	LEU
2	C	21	THR
2	C	28	LYS
2	C	40	VAL
2	C	59	ILE
2	C	77	ASP
2	C	127	LYS
2	C	134	LYS
2	C	140	ARG
2	C	154	ASN
2	C	157	PHE
2	C	173	ASN
2	C	179	MET
3	A	18	ASP
3	A	23	LEU
3	A	24	ASP
3	A	25	ILE
3	A	60	TRP
3	A	62	ARG
3	A	71	GLN
3	A	80	LEU
3	A	81	GLN
3	A	96	ARG
3	A	97	ASN
3	A	119	CYS

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Mol	Chain	Res	Type
3	A	146	TRP
3	A	150	ILE
3	A	165	GLN
3	A	189	VAL
3	A	192	LYS
3	A	194	LEU
3	A	200	ASN
3	A	205	ILE
3	A	208	LEU
3	A	218	ASN
3	A	229	LEU
3	A	257	VAL
3	A	263	VAL
3	A	292	MET
3	A	301	ASN
3	A	387	SER
3	A	393	LEU
3	A	394	LEU
3	A	401	ASP
3	A	426	LYS
3	A	436	ASP
3	A	443	GLU
3	A	481	GLN
3	A	525	LEU
3	A	530	GLN
3	A	535	ASP
3	A	578	ASP
3	A	620	THR
3	A	646	ASP
3	A	653	LEU
3	A	685	VAL
3	A	686	LYS
3	A	710	LEU
3	A	720	VAL
3	A	740	THR
3	A	746	ARG
3	A	749	ARG
3	A	781	LEU
3	A	807	ILE
3	A	875	LEU
3	A	882	PHE
3	A	887	ARG

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Mol	Chain	Res	Type
3	A	888	ASN
3	A	907	GLU
3	A	968	VAL
3	A	999	THR
3	A	1008	ILE
3	A	1016	ARG
3	A	1043	ARG
1	E	-2	LEU
1	E	27	ARG
1	E	35	TYR
1	E	43	ARG
1	E	47	LEU
1	E	54	LYS
1	E	56	LEU
1	E	120	ILE
1	E	126	VAL
1	E	189	MET
1	E	243	CYS
1	E	245	VAL
1	E	271	THR
1	E	286	LEU
1	E	353	HIS
2	F	13	LEU
2	F	15	LEU
2	F	34	GLU
2	F	55	ASN
2	F	59	ILE
2	F	119	LEU
2	F	134	LYS
2	F	140	ARG
2	F	154	ASN
2	F	157	PHE
2	F	177	VAL
3	D	14	ARG
3	D	18	ASP
3	D	25	ILE
3	D	37	HIS
3	D	60	TRP
3	D	80	LEU
3	D	81	GLN
3	D	96	ARG
3	D	97	ASN

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Mol	Chain	Res	Type
3	D	122	LYS
3	D	146	TRP
3	D	150	ILE
3	D	165	GLN
3	D	189	VAL
3	D	192	LYS
3	D	194	LEU
3	D	200	ASN
3	D	204	GLN
3	D	205	ILE
3	D	217	GLN
3	D	218	ASN
3	D	229	LEU
3	D	257	VAL
3	D	263	VAL
3	D	301	ASN
3	D	312	LYS
3	D	341	LEU
3	D	354	MET
3	D	401	ASP
3	D	426	LYS
3	D	436	ASP
3	D	447	ASP
3	D	525	LEU
3	D	535	ASP
3	D	578	ASP
3	D	646	ASP
3	D	653	LEU
3	D	655	GLU
3	D	686	LYS
3	D	710	LEU
3	D	724	LEU
3	D	727	ASN
3	D	740	THR
3	D	749	ARG
3	D	767	ASN
3	D	821	GLN
3	D	875	LEU
3	D	882	PHE
3	D	887	ARG
3	D	888	ASN
3	D	900	LEU

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Mol	Chain	Res	Type
3	D	999	THR
3	D	1008	ILE
3	D	1016	ARG
3	D	1029	ASP
3	D	1030	THR
3	D	1031	SER
3	D	1032	ASP
3	D	1043	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	ASN
1	B	51	GLN
1	B	61	HIS
1	B	101	GLN
1	B	200	GLN
1	B	261	HIS
1	B	353	HIS
2	C	30	HIS
2	C	105	HIS
2	C	145	GLN
2	C	154	ASN
2	C	156	ASN
3	A	30	ASN
3	A	33	ASN
3	A	37	HIS
3	A	56	HIS
3	A	71	GLN
3	A	97	ASN
3	A	145	HIS
3	A	166	ASN
3	A	204	GLN
3	A	210	GLN
3	A	215	ASN
3	A	218	ASN
3	A	293	GLN
3	A	296	GLN
3	A	321	ASN
3	A	352	HIS
3	A	437	GLN
3	A	456	ASN

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Mol	Chain	Res	Type
3	A	483	GLN
3	A	558	HIS
3	A	574	HIS
3	A	577	HIS
3	A	626	GLN
3	A	631	HIS
3	A	704	HIS
3	A	775	ASN
3	A	791	ASN
3	A	821	GLN
3	A	853	GLN
3	A	888	ASN
3	A	924	GLN
3	A	963	ASN
3	A	969	ASN
3	A	970	ASN
3	A	988	HIS
3	A	993	GLN
3	A	1021	GLN
3	A	1046	GLN
3	A	1050	HIS
1	E	19	ASN
1	E	51	GLN
1	E	61	HIS
1	E	101	GLN
1	E	200	GLN
1	E	209	HIS
1	E	261	HIS
1	E	263	GLN
1	E	353	HIS
2	F	30	HIS
2	F	105	HIS
2	F	145	GLN
2	F	154	ASN
2	F	156	ASN
3	D	30	ASN
3	D	43	GLN
3	D	56	HIS
3	D	97	ASN
3	D	166	ASN
3	D	185	GLN
3	D	204	GLN

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Mol	Chain	Res	Type
3	D	210	GLN
3	D	215	ASN
3	D	217	GLN
3	D	218	ASN
3	D	293	GLN
3	D	296	GLN
3	D	321	ASN
3	D	352	HIS
3	D	407	GLN
3	D	437	GLN
3	D	456	ASN
3	D	483	GLN
3	D	558	HIS
3	D	601	GLN
3	D	626	GLN
3	D	704	HIS
3	D	733	GLN
3	D	791	ASN
3	D	853	GLN
3	D	888	ASN
3	D	924	GLN
3	D	988	HIS
3	D	993	GLN
3	D	1021	GLN
3	D	1044	GLN
3	D	1046	GLN

### 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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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$
5	GTP	C	217	-	25,34,34	0.95	1 (4%)	34,54,54	1.86	8 (23%)
5	GTP	F	217	-	25,34,34	0.95	1 (4%)	34,54,54	1.85	7 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	217	-	-	0/18/38/38	0/3/3/3
5	GTP	F	217	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	217	GTP	C6-N1	2.51	1.37	1.33
5	C	217	GTP	C6-N1	2.76	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	217	GTP	N3-C2-N1	-4.63	120.39	127.44
5	F	217	GTP	N3-C2-N1	-4.46	120.65	127.44
5	C	217	GTP	PA-O3A-PB	-4.42	120.32	132.73
5	F	217	GTP	PA-O3A-PB	-4.37	120.46	132.73
5	C	217	GTP	C2'-C1'-N9	-3.84	108.43	114.29
5	F	217	GTP	C2'-C1'-N9	-3.75	108.56	114.29
5	F	217	GTP	C5-C6-N1	-3.37	118.98	123.59
5	C	217	GTP	C5-C6-N1	-3.23	119.17	123.59
5	C	217	GTP	PB-O3B-PG	-3.15	122.09	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	217	GTP	PB-O3B-PG	-2.94	122.80	132.67
5	F	217	GTP	C4-C5-N7	-2.54	107.14	109.48
5	C	217	GTP	C4-C5-N7	-2.19	107.47	109.48
5	C	217	GTP	N2-C2-N1	2.13	120.73	117.20
5	C	217	GTP	C6-N1-C2	2.95	120.03	115.94
5	F	217	GTP	C6-N1-C2	3.23	120.42	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	217	GTP	2	0
5	F	217	GTP	2	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	B	274/365 (75%)	0.29	9 (3%) 50 55	19, 36, 78, 112	3 (1%)
1	E	279/365 (76%)	0.33	12 (4%) 39 44	19, 37, 85, 126	0
2	C	171/216 (79%)	0.28	2 (1%) 81 83	20, 43, 73, 99	0
2	F	171/216 (79%)	0.25	1 (0%) 90 91	20, 42, 77, 99	0
3	A	1041/1073 (97%)	0.50	74 (7%) 19 21	14, 46, 100, 152	1 (0%)
3	D	1041/1073 (97%)	0.60	100 (9%) 10 11	16, 46, 107, 156	5 (0%)
All	All	2977/3308 (89%)	0.47	198 (6%) 21 23	14, 43, 96, 156	9 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1053	GLN	10.3
3	A	1053	GLN	9.3
3	D	967	PRO	8.3
3	D	1055	SER	8.1
3	D	19	PHE	7.9
3	D	966	ASN	7.6
3	D	1054	MET	7.5
3	D	115	SER	7.1
3	D	276	VAL	7.0
3	A	1029	ASP	7.0
3	A	70	SER	6.9
3	A	967	PRO	6.8
3	D	440	VAL	6.5
3	D	53	LEU	6.1
3	D	1052	LEU	5.9
3	D	119	CYS	5.7
3	A	397	SER	5.6
3	D	1025	PHE	5.6
3	D	965	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
3	D	964	PRO	5.5
3	A	1050	HIS	5.3
3	D	154	VAL	5.2
3	A	976	ASP	5.2
3	D	60	TRP	5.1
3	A	392	PRO	4.8
3	D	62	ARG	4.6
3	D	159	THR	4.5
3	A	393	LEU	4.5
3	A	968	VAL	4.4
3	D	70	SER	4.3
3	D	71	GLN	4.3
3	D	441	VAL	4.3
3	A	1030	THR	4.3
3	A	966	ASN	4.2
3	A	1052	LEU	4.2
3	A	1054	MET	4.1
3	D	120	VAL	4.0
3	D	66	ILE	4.0
3	A	394	LEU	4.0
3	D	54	LYS	4.0
3	D	391	SER	4.0
3	D	395	SER	4.0
3	D	22	LYS	4.0
3	D	213	MET	3.9
3	D	436	ASP	3.9
3	D	310	ASN	3.9
3	D	16	LEU	3.9
1	E	73	MET	3.9
3	A	395	SER	3.8
3	A	1027	GLY	3.8
3	D	44	ARG	3.8
3	D	397	SER	3.8
2	C	178	ALA	3.7
3	A	1033	LEU	3.7
3	D	1051	LYS	3.7
3	D	37	HIS	3.7
3	D	1030	THR	3.7
3	A	1026	ALA	3.7
3	A	16	LEU	3.6
3	A	62	ARG	3.6
3	A	337	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	15	GLN	3.6
3	D	52	HIS	3.6
3	D	117	PRO	3.6
1	E	51	GLN	3.6
3	A	120	VAL	3.5
1	E	283	SER	3.5
3	D	123	GLU	3.5
1	E	58	TYR	3.5
3	D	125	VAL	3.5
3	A	114	SER	3.4
3	A	276	VAL	3.3
3	D	336	LEU	3.3
1	E	289	ALA	3.3
3	D	1036	GLU	3.3
3	D	20	SER	3.3
3	A	399	HIS	3.2
3	D	435	ASN	3.2
1	B	350	SER	3.2
3	D	335	GLN	3.2
3	D	64	ASP	3.2
3	D	955	GLU	3.2
3	D	1050	HIS	3.1
3	A	1035	LEU	3.1
3	D	288	THR	3.1
3	D	983	LYS	3.1
3	A	150	ILE	3.0
3	D	399	HIS	3.0
3	A	25	ILE	3.0
3	A	258	PRO	3.0
3	D	996	LEU	3.0
1	B	239	PRO	3.0
3	D	186	ILE	3.0
3	A	1028	GLU	2.9
3	D	337	LEU	2.9
1	B	349	HIS	2.9
1	B	358	MET	2.9
3	A	105	TYR	2.9
3	D	313	ASP	2.9
3	A	939	LEU	2.8
3	D	487	THR	2.8
3	D	98	GLN	2.8
3	D	1027	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	A	71	GLN	2.7
3	D	51	THR	2.7
3	A	63	VAL	2.7
3	D	162	SER	2.7
3	D	434	GLU	2.7
3	A	42	GLN	2.7
3	A	22	LYS	2.7
3	A	955	GLU	2.6
3	A	163	LEU	2.6
3	A	492	LYS	2.6
3	A	284	GLU	2.6
3	D	27	LEU	2.6
3	A	43	GLN	2.6
3	A	316	GLN	2.6
1	B	351	PRO	2.6
3	A	110	ILE	2.6
3	D	939	LEU	2.6
3	A	275	SER	2.6
3	D	230	LEU	2.6
1	E	349	HIS	2.6
3	D	142	TRP	2.5
3	A	37	HIS	2.5
3	A	167	ASN	2.5
3	A	400	PHE	2.5
3	D	604	VAL	2.5
3	A	199	CYS	2.5
3	D	1008	ILE	2.5
3	D	1018	PHE	2.4
3	D	968	VAL	2.4
3	D	396	GLY	2.4
3	D	1004	LEU	2.4
3	D	277	SER	2.4
1	E	97[A]	HIS	2.4
3	A	485	ASN	2.4
1	E	55	ARG	2.4
3	A	119	CYS	2.4
1	B	96	LYS	2.4
3	D	17	LEU	2.4
3	D	271	ILE	2.4
3	A	1055	SER	2.3
3	D	121	GLU	2.3
3	D	446	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	246	LEU	2.3
3	A	208	LEU	2.3
3	D	118	THR	2.3
3	D	346	ALA	2.3
3	A	182	SER	2.3
3	D	1019	LEU	2.3
3	A	280	GLU	2.3
3	D	962	LEU	2.3
3	A	995	LYS	2.3
3	D	989	LEU	2.3
3	A	396	GLY	2.3
3	A	14	ARG	2.3
3	D	1047	GLU	2.2
3	D	206	PHE	2.2
3	D	437	GLN	2.2
2	C	59	ILE	2.2
1	B	54	LYS	2.2
3	D	253	LYS	2.2
3	A	23	LEU	2.2
1	E	282	VAL	2.2
3	A	436	ASP	2.2
3	A	1038	ARG	2.2
3	D	344	ARG	2.2
3	A	98	GLN	2.2
3	D	215	ASN	2.2
3	D	245	LYS	2.1
3	D	134	LEU	2.1
3	D	969	ASN	2.1
3	A	1044	GLN	2.1
3	A	252	TYR	2.1
3	D	65	THR	2.1
3	D	275	SER	2.1
3	A	292	MET	2.1
3	D	36	TYR	2.1
3	D	158	ARG	2.1
3	A	18	ASP	2.1
3	A	72	ASN	2.1
1	B	241	SER	2.1
3	D	1029	ASP	2.1
1	E	43	ARG	2.1
2	F	170	GLY	2.1
3	A	95	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	370	LEU	2.1
3	D	934	SER	2.1
1	E	54	LYS	2.1
3	A	962	LEU	2.1
3	D	109	LEU	2.1
3	A	391	SER	2.1
3	A	158	ARG	2.0
3	D	445	MET	2.0
3	D	972	MET	2.0
1	E	357	LEU	2.0
3	A	974	ILE	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(Å <sup>2</sup> )	Q<0.9
4	NA	B	361	1/1	0.92	0.18	0.84	34,34,34,34	0
4	NA	E	361	1/1	0.83	0.19	0.83	64,64,64,64	0
5	GTP	F	217	32/32	0.98	0.15	-0.14	14,27,40,50	0
6	MG	F	218	1/1	0.95	0.15	-0.36	33,33,33,33	0
6	MG	C	218	1/1	0.77	0.17	-0.50	40,40,40,40	0
5	GTP	C	217	32/32	0.97	0.14	-0.82	13,27,39,52	0
7	CL	E	362	1/1	0.95	0.11	-1.75	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.