



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:24 PM GMT

PDB ID : 3R7W  
Title : Crystal Structure of Gtr1p-Gtr2p complex  
Authors : Gong, R.; Li, L.; Liu, Y.; Wang, P.; Yang, H.; Wang, L.; Cheng, J.; Guan, K.L.; Xu, Y.  
Deposited on : 2011-03-23  
Resolution : 2.77 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

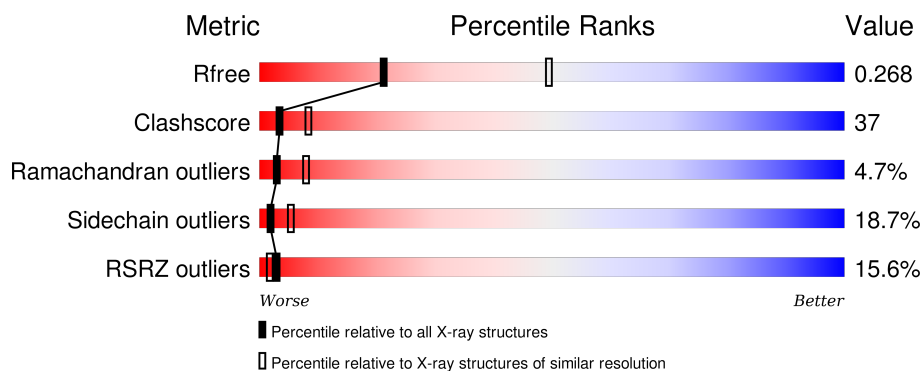
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	<div> <div>4%</div> <div>40%</div> <div>42%</div> <div>12%</div> <div>6%</div> </div>
1	C	307	<div> <div>7%</div> <div>44%</div> <div>40%</div> <div>9%</div> <div>6%</div> </div>
2	B	331	<div> <div>21%</div> <div>34%</div> <div>40%</div> <div>14%</div> <div>11%</div> </div>
2	D	331	<div> <div>19%</div> <div>24%</div> <div>35%</div> <div>9%</div> <div>31%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	600	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9011 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 GTP-binding protein GTR1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	Se	0	0	0
			2344	1513	388	425	5	13			
1	C	290	Total	C	N	O	S	Se	0	0	0
			2353	1518	390	427	5	13			

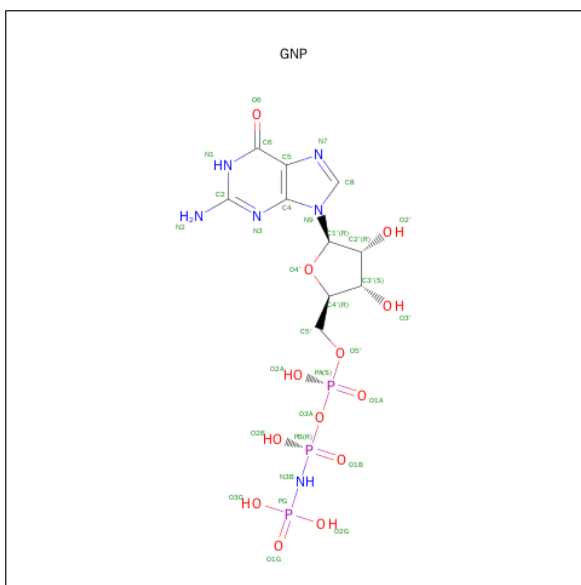
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	PRO	-	EXPRESSION TAG	UNP Q00582
A	5	LEU	-	EXPRESSION TAG	UNP Q00582
A	6	GLY	-	EXPRESSION TAG	UNP Q00582
A	7	SER	-	EXPRESSION TAG	UNP Q00582
C	4	PRO	-	EXPRESSION TAG	UNP Q00582
C	5	LEU	-	EXPRESSION TAG	UNP Q00582
C	6	GLY	-	EXPRESSION TAG	UNP Q00582
C	7	SER	-	EXPRESSION TAG	UNP Q00582

- Molecule 2 is a protein called GTP-binding protein GTR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	Se	0	0	0
			2348	1508	371	455	4	10			
2	D	229	Total	C	N	O	S	Se	0	0	0
			1830	1182	294	342	4	8			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0

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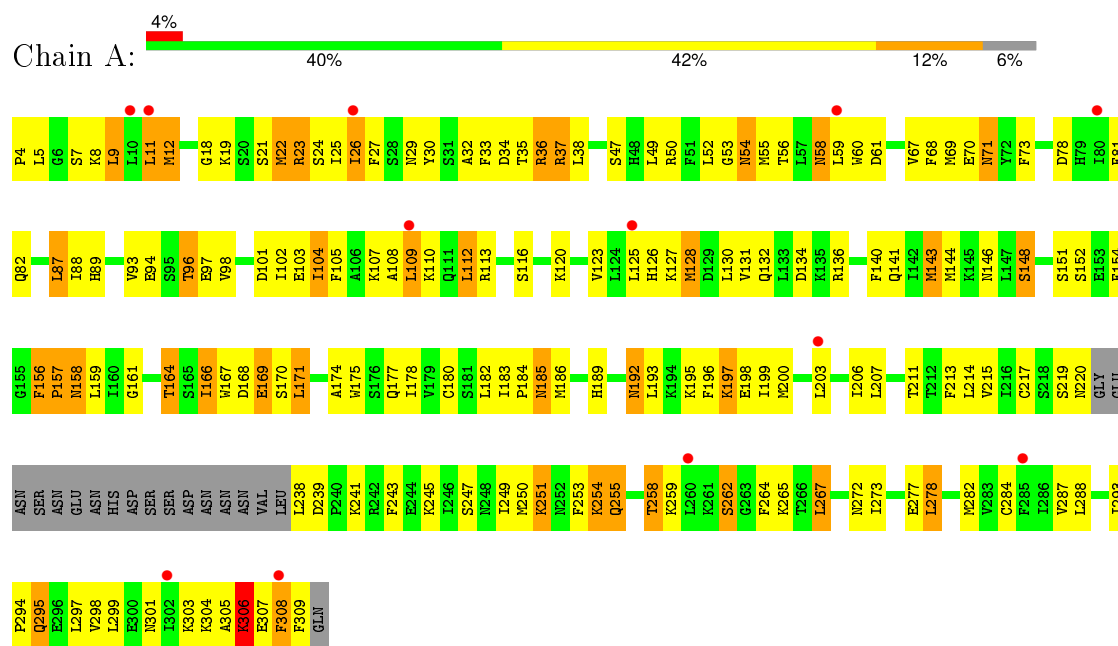
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		

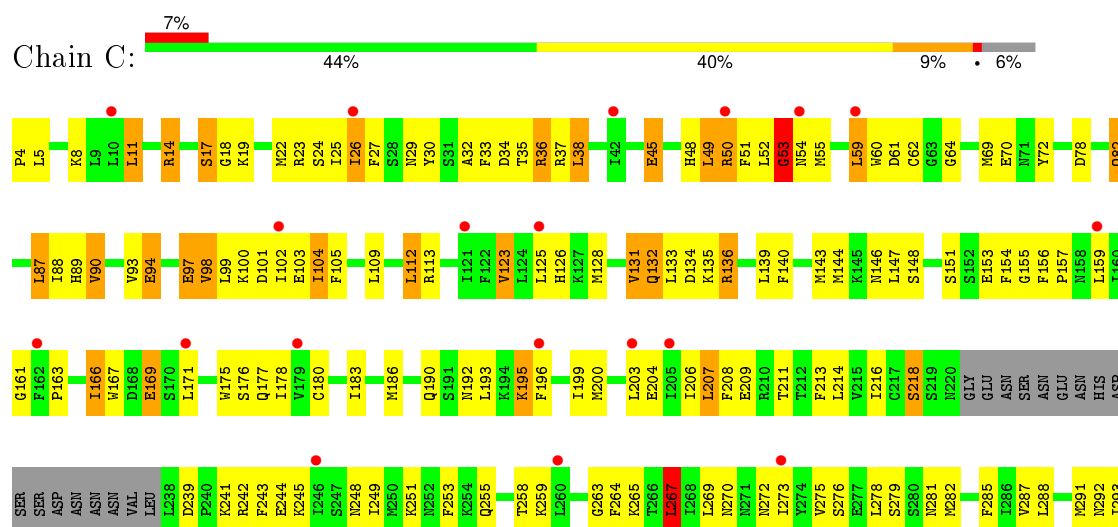
### 3 Residue-property plots [i](#)

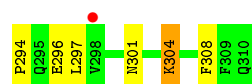
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: GTP-binding protein GTR1

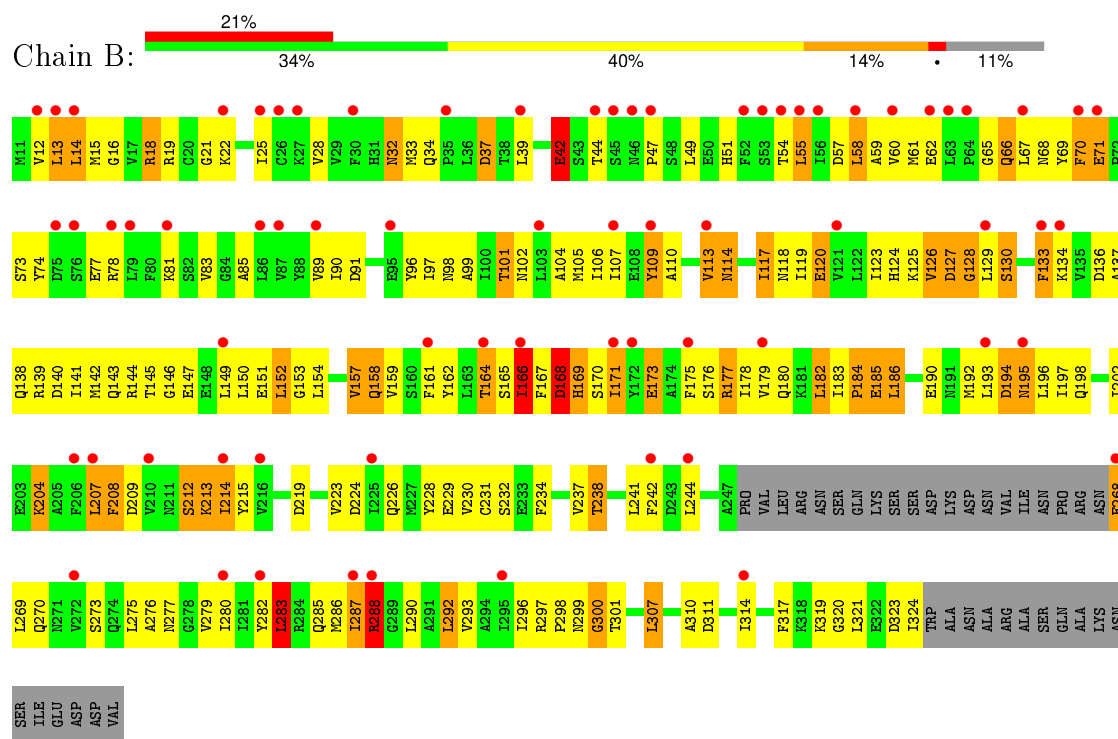


#### • Molecule 1: GTP-binding protein GTR1

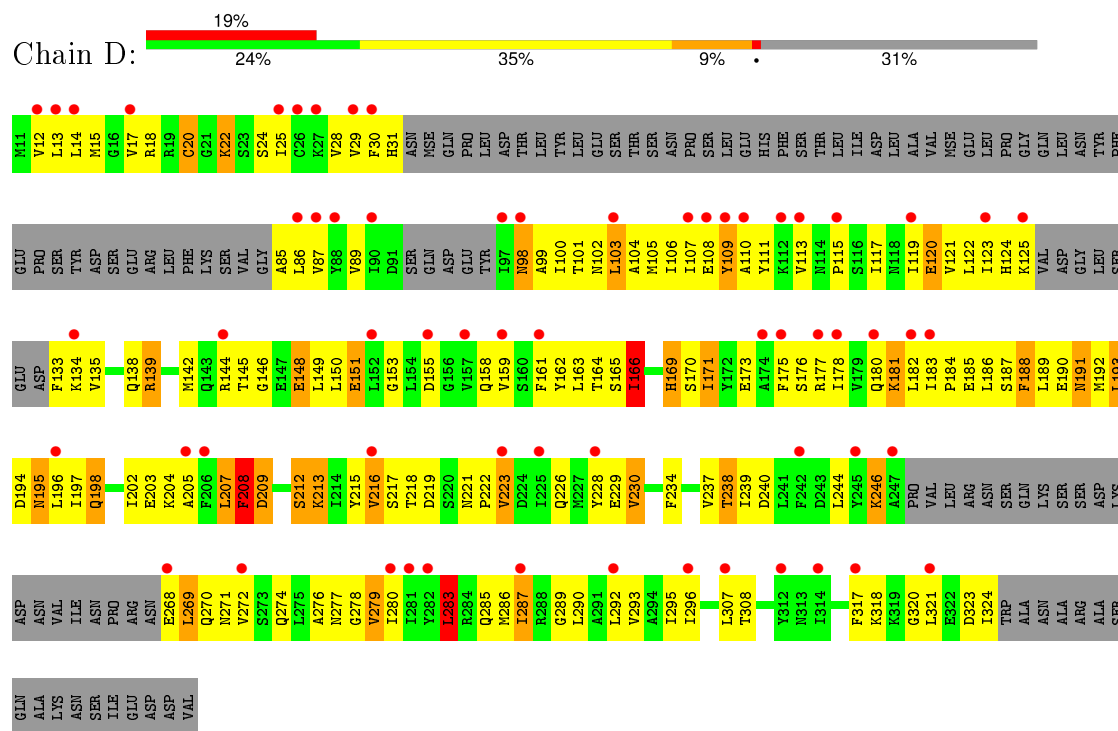




• Molecule 2: GTP-binding protein GTR2



• Molecule 2: GTP-binding protein GTR2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.91Å 148.44Å 98.51Å 90.00° 100.61° 90.00°	Depositor
Resolution (Å)	44.06 – 2.77 74.22 – 2.77	Depositor EDS
% Data completeness (in resolution range)	95.0 (44.06-2.77) 95.2 (74.22-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.236 , 0.283 0.224 , 0.268	Depositor DCC
$R_{free}$ test set	2286 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 46935 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2042e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GNP, MG

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	0.62	0/2375	0.77	1/3165 (0.0%)
1	C	0.59	0/2384	0.76	1/3177 (0.0%)
2	B	0.46	0/2378	0.64	1/3205 (0.0%)
2	D	0.45	0/1847	0.68	1/2480 (0.0%)
All	All	0.54	0/8984	0.71	4/12027 (0.0%)

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	C	0	1
2	B	0	1
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	283	LEU	CA-CB-CG	6.88	131.13	115.30
2	B	283	LEU	CA-CB-CG	6.74	130.79	115.30
1	C	267	LEU	CA-CB-CG	5.91	128.88	115.30
1	A	9	LEU	CA-CB-CG	5.37	127.66	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	268	GLU	Peptide
1	C	53	GLY	Peptide
2	D	208	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2344	0	2396	169	0
1	C	2353	0	2404	146	0
2	B	2348	0	2348	172	0
2	D	1830	0	1866	193	0
3	A	32	0	13	1	0
3	B	32	0	13	7	0
3	C	32	0	13	5	0
3	D	32	0	13	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
All	All	9011	0	9066	662	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 37.

All (662) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:HG12	1:C:132:GLN:H	1.05	1.13
2:D:238:THR:HB	2:D:271:ASN:HD22	1.11	1.08
2:D:212:SER:HA	2:D:213:LYS:HB2	1.36	1.07
2:B:70:PHE:HA	2:B:71:GLU:HB3	1.40	1.01
2:B:164:THR:HG22	2:B:171:ILE:HA	1.39	1.01
2:D:192:MSE:HE1	2:D:320:GLY:HA3	1.42	1.01
1:A:126:HIS:ND1	1:A:164:THR:HG22	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HD22	1:A:54:ASN:H	0.99	0.99
1:A:250:MSE:HE1	2:B:241:LEU:HD11	1.46	0.98
2:B:120:GLU:HG2	2:B:178:ILE:HG12	1.41	0.98
2:B:139:ARG:HA	2:B:142:MSE:HE2	1.45	0.98
2:B:70:PHE:HA	2:B:71:GLU:CB	1.94	0.96
2:D:193:LEU:HD22	2:D:317:PHE:HE1	1.29	0.96
2:D:287:ILE:HD11	2:D:321:LEU:HB3	1.45	0.96
1:C:131:VAL:HG12	1:C:132:GLN:N	1.81	0.93
1:A:186:MSE:HE1	1:A:217:CYS:HB3	1.50	0.92
2:B:166:ILE:HA	2:B:171:ILE:HG12	1.52	0.90
2:D:181:LYS:HA	2:D:186:LEU:HD21	1.54	0.88
2:B:165:SER:HB2	2:B:168:ASP:HB2	1.54	0.88
1:C:131:VAL:CG1	1:C:132:GLN:H	1.86	0.87
2:D:171:ILE:H	2:D:171:ILE:HD12	1.36	0.87
1:A:125:LEU:HD11	1:A:143:MSE:HG3	1.56	0.87
2:D:215:TYR:OH	2:D:223:VAL:HG11	1.74	0.86
2:D:198:GLN:OE1	2:D:198:GLN:HA	1.74	0.85
2:D:188:PHE:HA	2:D:191:ASN:HB2	1.58	0.85
2:D:209:ASP:HB2	2:D:212:SER:O	1.77	0.85
1:A:11:LEU:HD21	1:A:22:MSE:HE1	1.59	0.84
1:A:255:GLN:O	1:A:258:THR:HB	1.76	0.84
1:C:193:LEU:HD13	1:C:207:LEU:CD2	2.06	0.84
1:A:126:HIS:ND1	1:A:164:THR:CG2	2.40	0.84
1:A:109:LEU:HD23	1:A:156:PHE:CD2	2.13	0.83
2:B:193:LEU:HB2	2:B:317:PHE:HE1	1.41	0.83
1:A:54:ASN:N	1:A:54:ASN:HD22	1.76	0.83
1:A:195:LYS:O	1:A:199:ILE:HG13	1.79	0.83
1:A:8:LYS:HE3	1:A:60:TRP:CZ2	2.13	0.83
1:A:101:ASP:O	1:A:104:ILE:HD13	1.77	0.82
2:D:209:ASP:HB2	2:D:212:SER:C	2.00	0.81
2:D:234:PHE:O	2:D:238:THR:HG22	1.81	0.81
2:D:142:MSE:HE2	2:D:161:PHE:HB2	1.61	0.81
2:D:164:THR:HG22	2:D:165:SER:H	1.46	0.81
1:A:29:ASN:HD22	1:A:255:GLN:NE2	1.78	0.80
2:D:120:GLU:HG2	2:D:178:ILE:HG12	1.61	0.80
2:B:149:LEU:HD13	2:B:157:VAL:HG21	1.63	0.80
2:B:25:ILE:HA	2:B:28:VAL:HG12	1.63	0.80
2:B:286:MSE:HE2	2:B:292:LEU:HB2	1.64	0.80
2:B:107:ILE:HD11	2:B:149:LEU:HD21	1.61	0.80
1:A:23:ARG:HG2	1:A:23:ARG:HH21	1.44	0.80
1:A:109:LEU:HD23	1:A:156:PHE:HD2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HD11	1:A:27:PHE:CZ	2.18	0.79
2:D:193:LEU:HD23	2:D:193:LEU:H	1.47	0.79
1:C:242:ARG:HB2	2:D:244:LEU:HD12	1.65	0.79
1:A:93:VAL:HG11	1:A:128:MSE:HE1	1.64	0.79
1:C:113:ARG:HD3	1:C:154:PHE:O	1.83	0.79
1:C:94:GLU:HG2	1:C:94:GLU:O	1.83	0.78
1:C:50:ARG:HH11	1:C:50:ARG:HG3	1.48	0.78
2:D:134:LYS:HD3	2:D:163:LEU:HD13	1.65	0.78
2:D:87:VAL:HA	2:D:120:GLU:O	1.84	0.78
2:D:277:ASN:HD22	2:D:279:VAL:CG2	1.98	0.77
2:D:215:TYR:C	2:D:217:SER:H	1.87	0.76
1:A:295:GLN:HG3	1:A:299:LEU:HD11	1.66	0.76
2:D:209:ASP:HB2	2:D:213:LYS:N	1.99	0.76
1:C:123:VAL:HG11	1:C:159:LEU:HD21	1.66	0.76
1:A:293:ILE:HD11	1:A:297:LEU:HD12	1.68	0.76
1:A:304:LYS:HA	1:A:305:ALA:C	2.06	0.76
1:A:254:LYS:HB3	1:A:254:LYS:NZ	2.01	0.75
1:C:23:ARG:HG3	1:C:59:LEU:HD12	1.69	0.75
2:B:323:ASP:O	2:B:324:ILE:HG13	1.87	0.75
1:A:156:PHE:O	1:A:157:PRO:O	2.04	0.75
2:B:277:ASN:OD1	2:B:279:VAL:HG23	1.87	0.75
1:C:11:LEU:HD21	1:C:22:MSE:HE1	1.69	0.74
2:D:238:THR:HB	2:D:271:ASN:ND2	1.96	0.74
2:B:234:PHE:O	2:B:238:THR:HG22	1.86	0.74
2:D:212:SER:HA	2:D:213:LYS:CB	2.15	0.74
2:D:193:LEU:HD22	2:D:317:PHE:CE1	2.20	0.74
2:D:205:ALA:HB1	2:D:292:LEU:HD11	1.70	0.74
1:C:29:ASN:ND2	1:C:251:LYS:HE3	2.03	0.74
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.69	0.74
1:A:54:ASN:ND2	1:A:54:ASN:H	1.80	0.73
1:A:250:MSE:CE	2:B:241:LEU:HD11	2.18	0.73
2:B:13:LEU:HD12	2:B:83:VAL:HG21	1.71	0.73
1:A:180:CYS:HA	1:A:183:ILE:HD12	1.70	0.73
2:B:25:ILE:HG22	2:B:166:ILE:HG13	1.71	0.73
2:D:119:ILE:HB	2:D:159:VAL:HA	1.71	0.72
1:C:23:ARG:HG3	1:C:59:LEU:CD1	2.19	0.72
2:B:198:GLN:HA	2:B:198:GLN:NE2	2.03	0.72
1:C:104:ILE:HD13	1:C:105:PHE:H	1.55	0.72
1:C:104:ILE:HD13	1:C:105:PHE:N	2.04	0.72
2:B:18:ARG:HG2	2:B:19:ARG:HG2	1.71	0.71
1:A:26:ILE:HD11	1:A:27:PHE:CE2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:CD2	1:A:156:PHE:HD2	2.03	0.71
2:B:15:MSE:HA	2:B:22:LYS:HZ3	1.54	0.71
1:C:140:PHE:CE1	1:C:144:MSE:HE3	2.26	0.70
2:B:298:PRO:O	2:B:300:GLY:N	2.21	0.70
1:C:200:MSE:HE1	1:C:301:ASN:HD22	1.55	0.70
2:D:209:ASP:CB	2:D:213:LYS:H	2.04	0.70
2:D:124:HIS:HA	2:D:164:THR:HB	1.74	0.70
1:C:25:ILE:CD1	1:C:166:ILE:HG13	2.21	0.70
2:D:17:VAL:HG22	2:D:18:ARG:H	1.55	0.70
2:D:189:LEU:HD13	2:D:189:LEU:O	1.92	0.70
2:B:283:LEU:HB2	2:B:293:VAL:HG22	1.74	0.69
1:A:207:LEU:HD13	1:A:282:MSE:HE1	1.74	0.69
1:C:193:LEU:HD13	1:C:207:LEU:HD22	1.74	0.69
2:D:102:ASN:O	2:D:106:ILE:HG13	1.92	0.69
2:D:119:ILE:HG21	2:D:159:VAL:HG22	1.75	0.69
2:D:124:HIS:CG	2:D:125:LYS:N	2.61	0.68
1:A:305:ALA:N	1:A:309:PHE:HD1	1.91	0.68
2:B:193:LEU:HB2	2:B:317:PHE:CE1	2.26	0.68
1:A:12:MSE:CE	1:A:87:LEU:HD21	2.24	0.68
2:B:226:GLN:O	2:B:230:VAL:HG23	1.92	0.68
2:D:286:MSE:HE2	2:D:292:LEU:HB2	1.76	0.68
1:A:305:ALA:H	1:A:309:PHE:HD1	1.41	0.68
2:D:209:ASP:HB2	2:D:213:LYS:H	1.58	0.68
1:A:78:ASP:HB2	1:A:82:GLN:OE1	1.92	0.68
1:C:209:GLU:HB2	1:C:216:ILE:HD11	1.76	0.68
1:A:186:MSE:CE	1:A:217:CYS:HB3	2.23	0.68
2:D:212:SER:CA	2:D:213:LYS:HB2	2.19	0.68
2:D:146:GLY:O	2:D:150:LEU:HB2	1.94	0.68
2:B:13:LEU:HD21	2:B:61:MSE:HE3	1.76	0.67
1:C:125:LEU:HD22	1:C:140:PHE:CD1	2.30	0.67
2:B:180:GLN:O	2:B:186:LEU:HG	1.95	0.67
2:D:286:MSE:HE3	2:D:317:PHE:CE2	2.30	0.67
2:B:215:TYR:O	2:B:215:TYR:CD1	2.47	0.67
2:B:70:PHE:CA	2:B:71:GLU:CB	2.73	0.67
2:D:193:LEU:HD23	2:D:193:LEU:N	2.10	0.67
1:C:203:LEU:HD12	1:C:203:LEU:O	1.95	0.67
1:A:93:VAL:HG11	1:A:128:MSE:CE	2.24	0.66
2:B:130:SER:HB2	2:B:133:PHE:HB2	1.77	0.66
1:A:152:SER:N	1:A:157:PRO:HG2	2.10	0.66
1:C:126:HIS:HE1	3:C:500:GNP:N7	1.93	0.66
1:A:156:PHE:HB2	1:A:157:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HG2	1:A:23:ARG:NH2	2.10	0.66
2:B:198:GLN:HE21	2:B:198:GLN:HA	1.59	0.65
1:A:259:LYS:HE3	2:B:229:GLU:OE1	1.96	0.65
1:C:200:MSE:CE	1:C:301:ASN:HD22	2.08	0.65
2:D:277:ASN:HD22	2:D:279:VAL:HG21	1.60	0.65
1:C:265:LYS:HD3	2:D:276:ALA:HA	1.79	0.65
1:C:17:SER:HB2	1:C:90:VAL:HG22	1.78	0.65
2:B:39:LEU:HA	3:B:500:GNP:O2'	1.96	0.65
1:A:295:GLN:HG3	1:A:299:LEU:CD1	2.26	0.65
2:B:165:SER:O	2:B:167:PHE:N	2.27	0.65
2:D:176:SER:HB3	2:D:215:TYR:CG	2.32	0.65
1:C:207:LEU:HG	1:C:282:MSE:HE1	1.77	0.65
2:D:100:ILE:HG21	2:D:144:ARG:HB3	1.79	0.64
1:C:22:MSE:HE3	1:C:175:TRP:HZ2	1.61	0.64
1:C:32:ALA:HB1	1:C:166:ILE:HG23	1.79	0.64
2:B:49:LEU:HD11	2:B:59:ALA:HB1	1.79	0.64
1:C:207:LEU:HG	1:C:282:MSE:CE	2.28	0.64
1:C:50:ARG:HG3	1:C:50:ARG:NH1	2.12	0.64
2:D:100:ILE:HG13	2:D:145:THR:HG23	1.79	0.64
1:A:241:LYS:O	1:A:245:LYS:HG3	1.97	0.64
2:D:171:ILE:H	2:D:171:ILE:CD1	2.05	0.64
1:A:200:MSE:HE1	1:A:301:ASN:HB2	1.78	0.64
1:C:293:ILE:HG13	1:C:294:PRO:HD2	1.80	0.64
2:B:85:ALA:HB2	2:B:182:LEU:HD11	1.79	0.64
2:B:197:ILE:HG21	2:B:202:ILE:HD12	1.80	0.64
2:B:190:GLU:O	2:B:194:ASP:HB2	1.96	0.64
2:B:287:ILE:HD11	2:B:321:LEU:HB3	1.80	0.64
1:A:265:LYS:HD3	2:B:276:ALA:HA	1.79	0.63
2:D:181:LYS:CA	2:D:186:LEU:HD21	2.26	0.63
1:C:140:PHE:CZ	1:C:144:MSE:HE3	2.33	0.63
2:D:24:SER:O	2:D:28:VAL:HG23	1.99	0.63
1:C:128:MSE:O	1:C:128:MSE:HG3	1.97	0.63
1:A:203:LEU:HD12	1:A:203:LEU:O	1.98	0.63
2:B:33:MSE:HE2	2:B:37:ASP:HB2	1.81	0.63
2:B:73:SER:HB2	1:C:192:ASN:HD21	1.64	0.63
1:C:109:LEU:CD1	1:C:151:SER:HA	2.28	0.63
2:D:101:THR:HG22	2:D:148:GLU:HG3	1.79	0.63
1:A:192:ASN:N	1:A:192:ASN:HD22	1.96	0.63
2:D:12:VAL:HG22	2:D:85:ALA:HB3	1.80	0.63
1:C:166:ILE:HD13	3:C:500:GNP:N7	2.14	0.63
2:D:125:LYS:HE3	3:D:500:GNP:N3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ILE:H	2:B:158:GLN:HG2	1.64	0.62
1:A:25:ILE:HD12	1:A:166:ILE:HD11	1.81	0.62
2:D:197:ILE:HG22	2:D:197:ILE:O	1.98	0.62
2:B:74:TYR:CE1	1:C:308:PHE:HE1	2.17	0.62
2:D:25:ILE:HD11	2:D:124:HIS:CE1	2.35	0.62
2:D:277:ASN:HB3	2:D:279:VAL:HG23	1.80	0.62
2:B:65:GLY:O	2:B:66:GLN:HG3	1.99	0.62
1:A:267:LEU:C	1:A:267:LEU:HD12	2.20	0.62
1:A:25:ILE:HD12	1:A:166:ILE:CD1	2.29	0.62
1:A:166:ILE:HG22	1:A:167:TRP:CD1	2.35	0.62
1:A:156:PHE:CB	1:A:157:PRO:HD3	2.30	0.62
2:D:25:ILE:HG23	2:D:171:ILE:HG21	1.82	0.61
2:D:283:LEU:HD12	2:D:283:LEU:O	2.00	0.61
1:A:278:LEU:HD21	1:A:284:CYS:SG	2.39	0.61
2:D:270:GLN:HA	2:D:283:LEU:O	2.00	0.61
2:B:212:SER:HB2	2:B:214:ILE:HD13	1.83	0.61
1:A:98:VAL:O	1:A:102:ILE:HG13	2.01	0.61
2:D:145:THR:O	2:D:149:LEU:HD12	2.00	0.61
2:B:22:LYS:HG2	3:B:500:GNP:O1B	2.01	0.61
2:D:185:GLU:HA	2:D:185:GLU:OE2	2.02	0.60
2:D:207:LEU:HD22	2:D:290:LEU:HD23	1.82	0.60
1:C:29:ASN:HD21	1:C:251:LYS:HE3	1.66	0.60
1:C:259:LYS:HE2	2:D:229:GLU:CD	2.22	0.60
2:B:70:PHE:HA	2:B:71:GLU:HB2	1.84	0.60
1:A:207:LEU:HD13	1:A:282:MSE:CE	2.31	0.60
2:B:137:ALA:O	2:B:141:ILE:HB	2.01	0.60
2:B:173:GLU:O	2:B:177:ARG:HG3	2.00	0.60
2:B:298:PRO:C	2:B:300:GLY:H	2.05	0.60
2:D:85:ALA:HA	2:D:117:ILE:HG23	1.84	0.60
1:C:101:ASP:O	1:C:104:ILE:HD13	2.01	0.60
1:C:93:VAL:HG11	1:C:128:MSE:HE1	1.83	0.60
2:B:192:MSE:O	2:B:196:LEU:HB2	2.03	0.59
1:A:109:LEU:CD2	1:A:156:PHE:CD2	2.83	0.59
2:B:223:VAL:O	2:B:224:ASP:HB3	2.02	0.59
2:D:277:ASN:HB3	2:D:279:VAL:H	1.67	0.59
2:B:133:PHE:O	2:B:136:ASP:HB2	2.02	0.59
2:D:107:ILE:HG21	2:D:149:LEU:HD21	1.84	0.59
1:C:169:GLU:H	1:C:169:GLU:CD	2.05	0.59
2:B:126:VAL:HG12	2:B:126:VAL:O	2.02	0.59
1:A:4:PRO:HG2	1:A:5:LEU:H	1.67	0.59
2:B:143:GLN:O	2:B:147:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:HE1	1:A:104:ILE:HD11	1.67	0.59
1:A:207:LEU:HB3	1:A:282:MSE:CE	2.32	0.59
2:D:222:PRO:O	2:D:223:VAL:HB	2.03	0.59
2:D:223:VAL:HG12	2:D:223:VAL:O	2.02	0.58
2:D:277:ASN:HD22	2:D:279:VAL:HG23	1.67	0.58
2:B:124:HIS:CD2	2:B:125:LYS:N	2.71	0.58
1:C:18:GLY:HA2	3:C:500:GNP:O1A	2.02	0.58
1:C:180:CYS:HA	1:C:183:ILE:HD12	1.85	0.58
1:A:185:ASN:HB2	1:A:189:HIS:CD2	2.38	0.58
2:D:280:ILE:HB	2:D:296:ILE:HB	1.86	0.58
2:B:67:LEU:HB3	2:B:71:GLU:OE2	2.03	0.58
2:D:86:LEU:O	2:D:120:GLU:HB2	2.03	0.58
2:B:234:PHE:O	2:B:238:THR:CG2	2.51	0.58
2:B:98:ASN:O	2:B:101:THR:HG23	2.04	0.58
2:B:125:LYS:HE2	3:B:500:GNP:N2	2.18	0.58
2:D:218:THR:HG23	2:D:219:ASP:O	2.03	0.58
1:A:55:MSE:HE1	1:A:183:ILE:CG1	2.34	0.58
2:D:145:THR:O	2:D:149:LEU:HB2	2.04	0.58
1:A:96:THR:HG22	1:A:97:GLU:HG2	1.86	0.57
1:A:156:PHE:CB	1:A:157:PRO:CD	2.82	0.57
1:C:100:LYS:O	1:C:103:GLU:HB3	2.04	0.57
2:B:125:LYS:HD3	2:B:125:LYS:O	2.04	0.57
1:C:93:VAL:HG11	1:C:128:MSE:CE	2.34	0.57
2:D:13:LEU:HB3	2:D:15:MSE:HE3	1.87	0.57
2:D:166:ILE:H	2:D:171:ILE:CG1	2.18	0.57
1:C:22:MSE:CE	1:C:175:TRP:HZ2	2.16	0.57
1:C:193:LEU:HD13	1:C:207:LEU:HD21	1.84	0.57
1:A:104:ILE:HG12	1:A:105:PHE:N	2.19	0.57
2:D:103:LEU:HD12	2:D:145:THR:HG22	1.85	0.57
1:A:174:ALA:O	1:A:178:ILE:HG13	2.05	0.57
2:D:25:ILE:O	2:D:29:VAL:HG23	2.04	0.57
2:B:140:ASP:O	2:B:143:GLN:HB2	2.04	0.57
1:C:125:LEU:HB3	1:C:128:MSE:HE1	1.86	0.56
1:A:123:VAL:O	1:A:161:GLY:HA2	2.05	0.56
1:C:200:MSE:HA	1:C:200:MSE:HE3	1.85	0.56
1:A:169:GLU:HG2	1:A:245:LYS:HG2	1.87	0.56
1:C:126:HIS:CE1	3:C:500:GNP:N7	2.73	0.56
2:B:125:LYS:HG2	3:B:500:GNP:C2	2.35	0.56
2:D:283:LEU:HB2	2:D:293:VAL:HG22	1.87	0.56
2:B:287:ILE:CD1	2:B:321:LEU:HB3	2.34	0.56
2:B:270:GLN:HA	2:B:283:LEU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:ILE:HA	2:D:109:TYR:CZ	2.41	0.56
1:A:24:SER:HB3	1:A:30:TYR:CG	2.41	0.55
2:B:159:VAL:HB	2:B:161:PHE:CE2	2.41	0.55
1:A:254:LYS:HB3	1:A:254:LYS:HZ2	1.68	0.55
1:C:22:MSE:HE3	1:C:175:TRP:CZ2	2.39	0.55
1:A:55:MSE:HE1	1:A:183:ILE:HG12	1.88	0.55
2:B:280:ILE:HB	2:B:296:ILE:HB	1.87	0.55
2:D:215:TYR:C	2:D:217:SER:N	2.55	0.55
1:A:305:ALA:HA	1:A:309:PHE:CD1	2.42	0.55
2:D:20:CYS:SG	2:D:89:VAL:HG13	2.47	0.55
2:D:109:TYR:O	2:D:113:VAL:HG23	2.06	0.55
1:C:26:ILE:CD1	1:C:175:TRP:CG	2.90	0.55
1:A:12:MSE:HE3	1:A:87:LEU:HD21	1.87	0.55
2:B:165:SER:C	2:B:167:PHE:H	2.10	0.55
1:C:50:ARG:HB3	1:C:54:ASN:OD1	2.06	0.55
1:C:18:GLY:HA2	3:C:500:GNP:PA	2.47	0.55
2:D:166:ILE:HA	2:D:171:ILE:HG12	1.89	0.55
1:A:37:ARG:H	1:A:37:ARG:HD3	1.71	0.55
1:A:125:LEU:CD1	1:A:143:MSE:HG3	2.34	0.55
2:D:138:GLN:HE22	2:D:163:LEU:HD11	1.72	0.54
2:B:77:GLU:O	2:B:81:LYS:HG3	2.07	0.54
1:C:14:ARG:O	1:C:17:SER:OG	2.23	0.54
2:B:213:LYS:HD3	2:B:232:SER:OG	2.07	0.54
1:A:293:ILE:CG1	1:A:294:PRO:HD2	2.36	0.54
2:B:124:HIS:CG	2:B:125:LYS:N	2.75	0.54
2:B:28:VAL:HG11	2:B:166:ILE:CG1	2.37	0.54
1:A:253:PHE:HB2	2:B:237:VAL:HG21	1.90	0.54
1:A:23:ARG:CG	1:A:23:ARG:HH21	2.19	0.54
2:D:142:MSE:HG2	2:D:161:PHE:CD2	2.43	0.54
2:B:12:VAL:HB	2:B:60:VAL:HG22	1.90	0.54
1:C:8:LYS:HE3	1:C:60:TRP:CE2	2.43	0.54
2:B:286:MSE:HE3	2:B:317:PHE:CE2	2.43	0.54
2:D:25:ILE:HA	2:D:166:ILE:HD11	1.90	0.54
2:D:169:HIS:HD2	2:D:228:TYR:CE2	2.26	0.54
1:C:25:ILE:HD12	1:C:166:ILE:HG13	1.90	0.53
2:D:104:ALA:CB	2:D:148:GLU:HB3	2.38	0.53
1:C:36:ARG:NH1	1:C:36:ARG:HB3	2.23	0.53
2:B:90:ILE:O	2:B:90:ILE:HG22	2.09	0.53
1:C:166:ILE:HG22	1:C:167:TRP:CD1	2.42	0.53
2:D:188:PHE:O	2:D:192:MSE:N	2.31	0.53
2:D:193:LEU:CD2	2:D:193:LEU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:VAL:O	2:D:28:VAL:HG12	2.08	0.53
1:A:151:SER:C	1:A:157:PRO:HD2	2.29	0.53
2:B:179:VAL:HG12	2:B:179:VAL:O	2.08	0.53
2:B:231:CYS:HB3	2:B:293:VAL:HG11	1.90	0.53
1:C:48:HIS:O	1:C:49:LEU:HB3	2.09	0.53
2:B:25:ILE:HA	2:B:28:VAL:CG1	2.37	0.53
2:B:118:ASN:HA	2:B:158:GLN:HG2	1.91	0.52
1:A:131:VAL:HG22	1:A:136:ARG:CG	2.39	0.52
2:D:181:LYS:HB3	2:D:186:LEU:HD21	1.91	0.52
2:D:221:ASN:HB3	2:D:222:PRO:HD2	1.90	0.52
2:B:109:TYR:O	2:B:113:VAL:HG23	2.10	0.52
1:A:156:PHE:HB2	1:A:157:PRO:CD	2.39	0.52
2:B:55:LEU:HD13	2:B:288:ARG:NE	2.25	0.52
2:D:234:PHE:O	2:D:238:THR:CG2	2.54	0.52
2:D:142:MSE:HG2	2:D:161:PHE:CE2	2.45	0.52
1:C:169:GLU:HG2	1:C:245:LYS:HG2	1.90	0.52
2:D:323:ASP:O	2:D:324:ILE:HD12	2.09	0.52
1:C:87:LEU:HB2	1:C:112:LEU:HD21	1.91	0.52
1:C:123:VAL:CG1	1:C:159:LEU:HD21	2.38	0.52
2:D:166:ILE:HG21	3:D:500:GNP:O6	2.10	0.52
1:A:125:LEU:HG	1:A:140:PHE:HD1	1.75	0.52
1:C:94:GLU:CG	1:C:94:GLU:O	2.57	0.52
2:B:166:ILE:CA	2:B:171:ILE:HG12	2.32	0.52
1:C:35:THR:O	1:C:38:LEU:HB2	2.10	0.52
2:B:120:GLU:HG2	2:B:178:ILE:CG1	2.27	0.51
2:D:89:VAL:HG23	2:D:124:HIS:CB	2.40	0.51
1:A:52:LEU:HD12	1:A:55:MSE:HE3	1.91	0.51
1:A:192:ASN:H	1:A:192:ASN:HD22	1.58	0.51
2:B:307:LEU:O	2:B:311:ASP:HB2	2.11	0.51
2:D:89:VAL:HG23	2:D:124:HIS:HB3	1.92	0.51
2:D:274:GLN:HE21	2:D:278:GLY:HA2	1.75	0.51
2:D:286:MSE:HE3	2:D:317:PHE:CD2	2.46	0.51
1:A:157:PRO:HA	1:A:158:ASN:C	2.31	0.51
2:B:77:GLU:OE1	2:B:113:VAL:HG21	2.10	0.51
2:D:188:PHE:O	2:D:192:MSE:HG3	2.11	0.51
2:B:168:ASP:HB3	2:B:170:SER:H	1.75	0.51
2:D:207:LEU:HD22	2:D:290:LEU:CD2	2.40	0.51
2:B:123:ILE:O	2:B:126:VAL:HG23	2.10	0.51
2:D:164:THR:HG22	2:D:165:SER:N	2.22	0.51
2:D:29:VAL:HG12	2:D:30:PHE:CD1	2.46	0.51
1:A:151:SER:OG	1:A:157:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HG13	1:A:27:PHE:CD2	2.46	0.51
1:A:299:LEU:H	1:A:299:LEU:HD12	1.75	0.51
2:D:190:GLU:O	2:D:194:ASP:CB	2.59	0.51
2:D:238:THR:CB	2:D:271:ASN:HD22	2.02	0.50
2:B:169:HIS:ND1	2:B:229:GLU:CG	2.75	0.50
2:B:19:ARG:HA	3:B:500:GNP:H5'2	1.94	0.50
2:D:197:ILE:HG21	2:D:202:ILE:HD12	1.93	0.50
1:A:29:ASN:ND2	1:A:255:GLN:NE2	2.55	0.50
2:D:86:LEU:HD22	2:D:87:VAL:N	2.26	0.50
1:A:55:MSE:HE1	1:A:183:ILE:HA	1.93	0.50
2:D:106:ILE:HA	2:D:109:TYR:OH	2.12	0.50
2:D:269:LEU:HD12	2:D:285:GLN:HB2	1.93	0.50
2:D:186:LEU:HD12	2:D:186:LEU:H	1.76	0.50
1:A:144:MSE:O	1:A:148:SER:HB2	2.12	0.50
1:C:64:GLY:HA2	1:C:69:MSE:HE2	1.94	0.50
2:B:69:TYR:HE1	2:B:101:THR:OG1	1.93	0.50
1:A:131:VAL:HG22	1:A:136:ARG:HG2	1.93	0.50
2:D:190:GLU:O	2:D:190:GLU:HG2	2.10	0.50
1:A:94:GLU:OE1	1:A:130:LEU:HD13	2.12	0.50
2:B:70:PHE:CA	2:B:71:GLU:HB3	2.28	0.50
1:C:207:LEU:HD12	1:C:282:MSE:HE2	1.94	0.50
1:C:264:PHE:HE2	1:C:267:LEU:HB3	1.77	0.50
1:C:123:VAL:O	1:C:161:GLY:HA2	2.12	0.49
1:A:278:LEU:HD23	1:A:278:LEU:N	2.26	0.49
2:D:22:LYS:HB2	3:D:500:GNP:O1B	2.12	0.49
2:B:151:GLU:O	2:B:153:GLY:N	2.44	0.49
2:D:209:ASP:CB	2:D:213:LYS:N	2.68	0.49
2:D:87:VAL:HG22	2:D:120:GLU:HB3	1.93	0.49
1:C:89:HIS:HE1	1:C:104:ILE:HD11	1.77	0.49
2:B:123:ILE:O	2:B:126:VAL:CG2	2.59	0.49
1:A:109:LEU:HD22	1:A:154:PHE:HB2	1.94	0.49
1:C:26:ILE:HD12	1:C:175:TRP:CG	2.47	0.49
1:C:293:ILE:HG13	1:C:294:PRO:CD	2.42	0.49
1:A:88:ILE:HG12	1:A:178:ILE:HD13	1.94	0.49
2:D:269:LEU:HD13	2:D:269:LEU:O	2.11	0.49
1:C:35:THR:HA	1:C:38:LEU:HD22	1.94	0.49
2:B:33:MSE:HG2	2:B:34:GLN:H	1.77	0.49
2:D:283:LEU:HD12	2:D:283:LEU:C	2.32	0.49
1:C:275:VAL:HG22	1:C:285:PHE:CD1	2.47	0.49
1:A:299:LEU:N	1:A:299:LEU:HD12	2.28	0.49
1:A:219:SER:OG	1:A:220:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ALA:HB1	1:A:166:ILE:HG23	1.93	0.49
2:B:126:VAL:O	2:B:127:ASP:O	2.31	0.49
2:D:177:ARG:HD3	2:D:180:GLN:NE2	2.27	0.49
2:D:286:MSE:HE2	2:D:292:LEU:CB	2.43	0.48
1:A:47:SER:HB3	1:A:49:LEU:CD2	2.43	0.48
2:B:28:VAL:HG11	2:B:166:ILE:HG12	1.94	0.48
2:B:207:LEU:HD23	2:B:208:PHE:H	1.78	0.48
2:B:310:ALA:O	2:B:314:ILE:HG13	2.14	0.48
1:A:152:SER:HA	1:A:157:PRO:HD2	1.96	0.48
2:D:195:ASN:HB3	2:D:196:LEU:HD22	1.94	0.48
1:C:144:MSE:O	1:C:148:SER:HB2	2.13	0.48
1:A:55:MSE:HE2	1:A:184:PRO:CD	2.43	0.48
2:B:73:SER:CB	1:C:192:ASN:HD21	2.27	0.48
2:B:69:TYR:CD1	2:B:105:MSE:SE	3.17	0.48
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.60	0.48
1:C:24:SER:HB3	1:C:30:TYR:CG	2.49	0.48
1:A:151:SER:O	1:A:157:PRO:HD2	2.14	0.48
2:D:120:GLU:HG3	2:D:162:TYR:CE2	2.49	0.48
2:B:169:HIS:ND1	2:B:229:GLU:HG2	2.28	0.48
1:A:125:LEU:O	1:A:128:MSE:HE3	2.14	0.48
1:C:11:LEU:HD13	1:C:19:LYS:HB3	1.94	0.48
1:A:168:ASP:OD2	1:A:170:SER:OG	2.26	0.48
1:A:55:MSE:CE	1:A:183:ILE:HA	2.44	0.47
2:B:197:ILE:CG2	2:B:202:ILE:HD12	2.44	0.47
2:B:207:LEU:HD11	2:B:321:LEU:HD11	1.96	0.47
2:D:190:GLU:O	2:D:194:ASP:HB2	2.14	0.47
1:A:19:LYS:HA	1:A:22:MSE:HE2	1.96	0.47
2:B:99:ALA:HA	2:B:102:ASN:ND2	2.30	0.47
1:A:239:ASP:C	1:A:239:ASP:OD1	2.50	0.47
2:B:22:LYS:HZ1	2:B:65:GLY:CA	2.28	0.47
2:B:33:MSE:HG2	2:B:34:GLN:N	2.28	0.47
1:C:131:VAL:CG1	1:C:132:GLN:N	2.54	0.47
2:D:14:LEU:O	2:D:15:MSE:HG3	2.15	0.47
1:A:8:LYS:HE3	1:A:60:TRP:CE2	2.49	0.47
2:D:138:GLN:CG	2:D:142:MSE:HE3	2.45	0.47
2:B:207:LEU:CD2	2:B:290:LEU:HD13	2.44	0.47
2:B:119:ILE:N	2:B:119:ILE:HD12	2.30	0.47
2:D:177:ARG:NH1	2:D:180:GLN:HE22	2.13	0.47
1:A:33:PHE:O	1:A:35:THR:N	2.47	0.47
1:C:102:ILE:HD13	1:C:146:ASN:ND2	2.30	0.47
2:B:22:LYS:HB3	2:B:89:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLN:HB3	2:B:67:LEU:H	1.50	0.47
1:A:125:LEU:HD11	1:A:143:MSE:CG	2.37	0.47
2:B:138:GLN:O	2:B:140:ASP:N	2.48	0.47
1:C:23:ARG:O	1:C:27:PHE:HB2	2.15	0.47
1:C:203:LEU:O	1:C:204:GLU:HB3	2.15	0.47
1:A:4:PRO:CG	1:A:5:LEU:H	2.27	0.47
2:B:184:PRO:O	2:B:185:GLU:HB2	2.15	0.47
1:C:11:LEU:HD21	1:C:22:MSE:CE	2.42	0.47
2:B:126:VAL:HG12	2:B:134:LYS:HE2	1.97	0.47
2:D:135:VAL:HG13	2:D:139:ARG:HH21	1.80	0.47
2:B:58:LEU:O	2:B:58:LEU:HD13	2.14	0.47
2:B:69:TYR:HD1	2:B:105:MSE:SE	2.48	0.46
1:C:8:LYS:HE3	1:C:60:TRP:CZ2	2.50	0.46
2:D:124:HIS:CG	2:D:125:LYS:H	2.30	0.46
2:D:86:LEU:HD22	2:D:87:VAL:H	1.80	0.46
2:D:107:ILE:O	2:D:110:ALA:HB3	2.15	0.46
1:C:61:ASP:C	1:C:61:ASP:OD1	2.52	0.46
1:C:206:ILE:HB	1:C:208:PHE:HE1	1.80	0.46
1:C:88:ILE:HG12	1:C:178:ILE:HD13	1.96	0.46
1:A:22:MSE:HB2	1:A:22:MSE:HE2	1.76	0.46
1:A:151:SER:HB3	1:A:157:PRO:CG	2.45	0.46
1:A:304:LYS:HA	1:A:305:ALA:O	2.14	0.46
2:D:103:LEU:HD13	2:D:104:ALA:N	2.31	0.46
2:B:77:GLU:OE1	2:B:77:GLU:HA	2.15	0.46
2:D:180:GLN:O	2:D:183:ILE:HG22	2.14	0.46
1:C:253:PHE:HB2	2:D:237:VAL:HG21	1.96	0.46
2:B:286:MSE:HE3	2:B:317:PHE:CD2	2.50	0.46
1:C:17:SER:HB2	1:C:90:VAL:CG2	2.43	0.46
1:C:206:ILE:HB	1:C:208:PHE:CE1	2.51	0.46
1:A:73:PHE:HE1	1:A:108:ALA:HA	1.79	0.46
1:C:78:ASP:O	1:C:82:GLN:HG3	2.15	0.46
2:D:103:LEU:HD12	2:D:145:THR:CG2	2.45	0.46
1:C:136:ARG:HG2	1:C:136:ARG:H	1.52	0.46
1:A:61:ASP:C	1:A:61:ASP:OD1	2.53	0.46
1:A:215:VAL:HG21	1:A:243:PHE:HB3	1.97	0.46
2:D:202:ILE:HG22	2:D:203:GLU:N	2.31	0.46
1:A:7:SER:CB	1:A:182:LEU:HD13	2.46	0.46
1:C:125:LEU:O	1:C:128:MSE:HE3	2.15	0.46
1:A:267:LEU:HB2	2:B:273:SER:HB2	1.97	0.46
1:C:279:SER:C	1:C:281:ASN:H	2.18	0.46
2:B:146:GLY:O	2:B:150:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PHE:C	2:B:242:PHE:CD1	2.89	0.46
2:B:197:ILE:HG22	2:B:197:ILE:O	2.15	0.45
2:B:197:ILE:O	2:B:198:GLN:CD	2.55	0.45
1:C:183:ILE:CG2	1:C:186:MSE:HE2	2.45	0.45
2:B:98:ASN:O	2:B:102:ASN:OD1	2.33	0.45
1:C:269:LEU:HB3	1:C:273:ILE:HB	1.98	0.45
1:A:109:LEU:HD23	1:A:156:PHE:CE2	2.50	0.45
2:D:240:ASP:O	2:D:244:LEU:HD23	2.16	0.45
2:D:207:LEU:HD22	2:D:208:PHE:H	1.80	0.45
2:D:122:LEU:O	2:D:124:HIS:N	2.45	0.45
2:D:25:ILE:HD11	2:D:124:HIS:CD2	2.52	0.45
1:A:128:MSE:O	1:A:128:MSE:HG3	2.15	0.45
2:D:124:HIS:CD2	2:D:125:LYS:HB2	2.51	0.45
2:D:138:GLN:HE21	2:D:163:LEU:HD21	1.80	0.45
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.56	0.45
1:A:303:LYS:O	1:A:306:LYS:HB2	2.16	0.45
1:C:128:MSE:HB2	1:C:128:MSE:HE3	1.87	0.45
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.77	0.45
1:A:25:ILE:HD11	1:A:166:ILE:HG13	1.99	0.45
1:A:277:GLU:C	1:A:278:LEU:HD23	2.37	0.45
2:D:274:GLN:NE2	2:D:278:GLY:HA2	2.32	0.45
1:C:82:GLN:HB3	1:C:82:GLN:HE21	1.67	0.45
1:C:155:GLY:O	1:C:157:PRO:HD3	2.17	0.45
2:D:221:ASN:HB3	2:D:222:PRO:CD	2.46	0.45
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.66	0.45
2:D:119:ILE:HD13	2:D:158:GLN:H	1.82	0.45
2:B:179:VAL:O	2:B:179:VAL:CG1	2.65	0.45
2:D:14:LEU:C	2:D:15:MSE:HG3	2.38	0.45
2:D:119:ILE:HD12	2:D:119:ILE:N	2.32	0.45
1:C:25:ILE:HD11	1:C:166:ILE:HG13	1.98	0.45
2:D:212:SER:CA	2:D:213:LYS:CB	2.88	0.45
2:D:181:LYS:CB	2:D:186:LEU:HD21	2.47	0.45
2:D:171:ILE:HG22	2:D:175:PHE:CE2	2.52	0.45
2:D:197:ILE:CG2	2:D:202:ILE:HD12	2.47	0.45
1:C:239:ASP:O	1:C:242:ARG:HB3	2.16	0.45
2:B:142:MSE:HG2	2:B:161:PHE:CD1	2.52	0.44
2:D:85:ALA:CA	2:D:117:ILE:HG23	2.45	0.44
1:A:193:LEU:HD13	1:A:207:LEU:HG	1.98	0.44
1:C:4:PRO:CG	1:C:5:LEU:H	2.29	0.44
1:C:4:PRO:HG2	1:C:5:LEU:H	1.81	0.44
2:D:209:ASP:O	2:D:289:GLY:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:ILE:O	2:D:198:GLN:OE1	2.34	0.44
2:D:113:VAL:O	2:D:113:VAL:HG12	2.17	0.44
2:B:119:ILE:HB	2:B:158:GLN:O	2.16	0.44
2:D:169:HIS:CG	2:D:229:GLU:HG2	2.52	0.44
1:A:47:SER:O	1:A:58:ASN:HA	2.17	0.44
2:D:209:ASP:HB3	2:D:213:LYS:H	1.80	0.44
2:D:215:TYR:HB3	2:D:217:SER:N	2.33	0.44
2:B:55:LEU:HD11	2:B:288:ARG:HD2	2.00	0.44
1:A:47:SER:HB3	1:A:49:LEU:HD21	1.98	0.44
1:C:4:PRO:O	1:C:5:LEU:HD23	2.18	0.44
1:C:218:SER:HG	1:C:243:PHE:HZ	1.60	0.44
2:D:170:SER:HA	2:D:173:GLU:HB3	2.00	0.44
1:A:107:LYS:O	1:A:110:LYS:HB3	2.18	0.44
2:B:269:LEU:HB3	2:B:285:GLN:HB2	1.99	0.44
1:C:272:ASN:HB3	1:C:291:MSE:HG2	2.00	0.44
2:D:286:MSE:SE	2:D:318:LYS:HB2	2.68	0.44
2:D:171:ILE:HG22	2:D:175:PHE:HE2	1.83	0.44
2:B:124:HIS:CG	2:B:125:LYS:H	2.36	0.44
2:B:120:GLU:HG3	2:B:162:TYR:CE2	2.53	0.44
1:A:88:ILE:HD13	1:A:175:TRP:CH2	2.53	0.44
2:D:246:LYS:HB2	2:D:246:LYS:HE2	1.74	0.44
2:B:13:LEU:HD13	2:B:15:MSE:HE1	1.99	0.44
2:D:14:LEU:HD23	2:D:15:MSE:N	2.33	0.44
1:C:249:ILE:CD1	2:D:240:ASP:HB3	2.47	0.44
2:B:114:ASN:HB3	2:B:117:ILE:HG13	2.00	0.44
1:A:81:PHE:HD1	1:A:112:LEU:HD13	1.82	0.43
1:C:196:PHE:O	1:C:196:PHE:CD2	2.71	0.43
1:C:59:LEU:HA	1:C:59:LEU:HD23	1.72	0.43
2:D:99:ALA:O	2:D:103:LEU:HB2	2.18	0.43
2:D:22:LYS:HG3	3:D:500:GNP:O3G	2.18	0.43
1:A:206:ILE:HD12	1:A:206:ILE:H	1.83	0.43
1:A:157:PRO:HB3	1:A:159:LEU:H	1.83	0.43
1:C:239:ASP:OD1	1:C:239:ASP:C	2.57	0.43
1:C:259:LYS:HE2	2:D:229:GLU:OE2	2.18	0.43
1:A:197:LYS:HG3	1:A:198:GLU:N	2.32	0.43
2:B:32:ASN:C	2:B:32:ASN:HD22	2.22	0.43
1:C:62:CYS:HB3	1:C:72:TYR:CE1	2.53	0.43
2:B:16:GLY:H	2:B:22:LYS:NZ	2.16	0.43
1:A:126:HIS:O	1:A:127:LYS:HB2	2.18	0.43
1:A:55:MSE:HE2	1:A:184:PRO:HD3	2.01	0.43
1:C:101:ASP:O	1:C:104:ILE:CD1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:TYR:O	2:B:78:ARG:HB2	2.19	0.43
1:A:68:PHE:O	1:A:71:ASN:HB2	2.19	0.43
2:B:14:LEU:HD13	2:B:22:LYS:O	2.18	0.43
1:A:307:GLU:O	1:A:308:PHE:O	2.37	0.43
1:A:180:CYS:C	1:A:182:LEU:N	2.72	0.43
2:D:119:ILE:HD13	2:D:158:GLN:N	2.34	0.43
1:C:207:LEU:CG	1:C:282:MSE:CE	2.97	0.43
1:C:125:LEU:HD23	1:C:140:PHE:HA	2.00	0.43
2:D:151:GLU:O	2:D:153:GLY:O	2.36	0.43
2:B:42:GLU:CD	2:B:42:GLU:H	2.21	0.43
2:B:231:CYS:CB	2:B:293:VAL:HG11	2.49	0.43
2:D:86:LEU:HD13	2:D:86:LEU:C	2.38	0.43
2:B:33:MSE:HE2	2:B:37:ASP:CB	2.48	0.43
1:C:193:LEU:HD22	1:C:207:LEU:HD23	2.01	0.43
2:B:104:ALA:O	2:B:107:ILE:HG12	2.19	0.43
2:D:119:ILE:HG22	2:D:159:VAL:HG13	2.01	0.42
1:A:207:LEU:CD1	1:A:282:MSE:HE1	2.44	0.42
1:C:269:LEU:O	1:C:270:ASN:HB2	2.19	0.42
1:A:298:VAL:HG12	1:A:299:LEU:N	2.33	0.42
1:A:207:LEU:HB3	1:A:282:MSE:HE2	2.00	0.42
1:C:143:MSE:HE2	1:C:147:LEU:HD21	2.01	0.42
1:C:195:LYS:O	1:C:199:ILE:HG13	2.19	0.42
1:C:97:GLU:O	1:C:98:VAL:C	2.57	0.42
1:A:78:ASP:O	1:A:82:GLN:HB2	2.19	0.42
2:D:183:ILE:HG13	2:D:184:PRO:HD2	2.01	0.42
1:C:131:VAL:HG21	1:C:139:LEU:HD23	2.01	0.42
2:B:195:ASN:O	2:B:198:GLN:N	2.43	0.42
2:B:119:ILE:N	2:B:158:GLN:HG2	2.31	0.42
2:B:102:ASN:O	2:B:106:ILE:HG13	2.19	0.42
1:C:55:MSE:HB3	1:C:55:MSE:HE2	1.72	0.42
2:D:171:ILE:N	2:D:171:ILE:HD12	2.18	0.42
1:A:148:SER:O	1:A:152:SER:HB2	2.18	0.42
1:A:157:PRO:HG3	1:A:159:LEU:HB2	2.02	0.42
1:A:180:CYS:C	1:A:182:LEU:H	2.23	0.42
2:B:283:LEU:HA	2:B:292:LEU:O	2.19	0.42
1:A:55:MSE:HE2	1:A:184:PRO:HD2	2.01	0.42
2:B:215:TYR:O	2:B:215:TYR:HD1	1.98	0.42
1:A:33:PHE:CD1	1:A:36:ARG:NH1	2.87	0.42
2:D:213:LYS:CA	2:D:213:LYS:HE3	2.49	0.42
2:B:176:SER:OG	2:B:215:TYR:N	2.52	0.42
2:B:223:VAL:HG12	2:B:224:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:PHE:O	1:C:35:THR:N	2.53	0.42
2:D:188:PHE:CD1	2:D:191:ASN:HB3	2.54	0.42
1:A:251:LYS:HD2	1:A:255:GLN:HE22	1.85	0.42
1:A:245:LYS:O	1:A:249:ILE:HG13	2.19	0.42
1:C:22:MSE:HG2	1:C:171:LEU:HD21	2.02	0.42
1:C:125:LEU:CD2	1:C:140:PHE:HA	2.50	0.42
2:D:98:ASN:HD21	2:D:102:ASN:ND2	2.17	0.42
1:C:52:LEU:HD11	1:C:216:ILE:HD12	2.01	0.42
2:B:215:TYR:HD2	2:B:228:TYR:CD1	2.38	0.42
2:D:283:LEU:CD1	2:D:283:LEU:C	2.88	0.42
1:C:183:ILE:HG21	1:C:186:MSE:HE2	2.00	0.42
2:B:297:ARG:CZ	2:B:297:ARG:HB2	2.50	0.42
2:D:209:ASP:OD1	2:D:213:LYS:NZ	2.43	0.42
2:D:12:VAL:C	2:D:13:LEU:HD23	2.40	0.42
2:D:222:PRO:O	2:D:223:VAL:CB	2.68	0.42
1:C:249:ILE:HD13	2:D:240:ASP:HB3	2.02	0.42
1:A:200:MSE:HE1	1:A:301:ASN:CB	2.49	0.42
2:B:319:LYS:HA	2:B:319:LYS:HD2	1.66	0.42
2:D:272:VAL:HG11	2:D:307:LEU:HD11	2.01	0.42
2:B:282:TYR:O	2:B:293:VAL:HA	2.19	0.41
2:B:107:ILE:HA	2:B:110:ALA:HB3	2.01	0.41
2:D:119:ILE:H	2:D:119:ILE:HD12	1.84	0.41
2:D:15:MSE:O	2:D:89:VAL:HG12	2.20	0.41
1:A:297:LEU:C	1:A:297:LEU:HD13	2.41	0.41
2:D:100:ILE:HG12	2:D:144:ARG:CB	2.50	0.41
2:B:207:LEU:CD2	2:B:290:LEU:HB3	2.51	0.41
1:A:50:ARG:NH1	1:A:53:GLY:O	2.51	0.41
2:B:204:LYS:HB2	2:B:204:LYS:HE2	1.71	0.41
2:B:97:ILE:HD13	2:B:144:ARG:HH12	1.85	0.41
2:B:180:GLN:HA	2:B:183:ILE:HD12	2.02	0.41
2:D:100:ILE:HG12	2:D:144:ARG:HB2	2.03	0.41
1:A:192:ASN:N	1:A:192:ASN:ND2	2.67	0.41
2:D:218:THR:HG23	2:D:219:ASP:N	2.36	0.41
2:D:226:GLN:O	2:D:230:VAL:HG23	2.20	0.41
1:C:45:GLU:HG2	1:C:45:GLU:O	2.20	0.41
2:D:17:VAL:HG22	2:D:18:ARG:N	2.28	0.41
1:A:166:ILE:HD12	1:A:166:ILE:HA	1.47	0.41
1:A:25:ILE:CD1	1:A:166:ILE:HG13	2.50	0.41
2:B:209:ASP:HB3	2:B:212:SER:OG	2.20	0.41
2:D:125:LYS:HG3	3:D:500:GNP:C2	2.51	0.41
2:D:25:ILE:HD11	2:D:124:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LEU:HB3	1:C:156:PHE:CZ	2.55	0.41
1:A:112:LEU:HA	1:A:112:LEU:HD12	1.87	0.41
1:C:133:LEU:C	1:C:135:LYS:H	2.24	0.41
2:B:195:ASN:ND2	2:B:196:LEU:HD22	2.36	0.41
1:C:51:PHE:O	1:C:55:MSE:HB2	2.21	0.41
1:A:262:SER:HB3	2:B:275:LEU:HB3	2.03	0.41
1:C:304:LYS:O	1:C:304:LYS:HE3	2.21	0.41
2:B:128:GLY:C	2:B:129:LEU:HD12	2.40	0.41
1:A:18:GLY:HA2	3:A:500:GNP:O1A	2.19	0.41
2:B:125:LYS:HG2	3:B:500:GNP:N1	2.35	0.41
2:D:24:SER:O	2:D:166:ILE:HD11	2.21	0.41
1:A:125:LEU:HB3	1:A:128:MSE:HE1	2.03	0.41
2:B:286:MSE:HE2	2:B:292:LEU:CB	2.43	0.41
1:A:308:PHE:HB2	1:A:309:PHE:H	1.65	0.41
1:A:305:ALA:HA	1:A:309:PHE:HD1	1.85	0.41
2:B:169:HIS:HB2	2:B:229:GLU:OE2	2.21	0.41
1:C:24:SER:HB3	1:C:30:TYR:HB2	2.03	0.41
1:A:206:ILE:HD12	1:A:206:ILE:N	2.35	0.41
1:C:177:GLN:HB3	1:C:177:GLN:HE21	1.66	0.41
2:D:189:LEU:O	2:D:193:LEU:HD21	2.21	0.41
1:A:305:ALA:CA	1:A:309:PHE:HD1	2.34	0.41
1:C:19:LYS:HG2	1:C:90:VAL:CG1	2.50	0.40
1:C:125:LEU:N	1:C:125:LEU:CD1	2.84	0.40
2:B:127:ASP:O	2:B:129:LEU:N	2.53	0.40
1:A:259:LYS:HB3	2:B:226:GLN:HG3	2.03	0.40
1:C:36:ARG:HB3	1:C:36:ARG:CZ	2.51	0.40
1:C:263:GLY:O	1:C:264:PHE:C	2.59	0.40
1:A:141:GLN:NE2	1:A:141:GLN:O	2.54	0.40
1:A:128:MSE:HE3	1:A:128:MSE:HB2	1.80	0.40
2:D:101:THR:O	2:D:105:MSE:HB2	2.21	0.40
1:A:131:VAL:HG22	1:A:136:ARG:HG3	2.02	0.40
2:B:124:HIS:HE2	3:B:500:GNP:C5	2.33	0.40
2:B:13:LEU:HD13	2:B:15:MSE:CE	2.52	0.40
1:A:11:LEU:HD11	1:A:22:MSE:CE	2.51	0.40
1:C:52:LEU:HB3	1:C:53:GLY:H	1.71	0.40
2:B:287:ILE:H	2:B:287:ILE:HG12	1.63	0.40
1:C:241:LYS:O	1:C:245:LYS:HG3	2.20	0.40
1:C:241:LYS:O	1:C:244:GLU:HG2	2.21	0.40
2:D:215:TYR:O	2:D:216:VAL:HB	2.22	0.40
1:C:175:TRP:O	1:C:176:SER:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	285/307 (93%)	247 (87%)	32 (11%)	6 (2%)	9	27
1	C	286/307 (93%)	245 (86%)	35 (12%)	6 (2%)	9	27
2	B	290/331 (88%)	225 (78%)	38 (13%)	27 (9%)	1	1
2	D	219/331 (66%)	170 (78%)	37 (17%)	12 (6%)	2	6
All	All	1080/1276 (85%)	887 (82%)	142 (13%)	51 (5%)	3	8

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	A	157	PRO
1	A	306	LYS
1	A	308	PHE
2	B	18	ARG
2	B	68	ASN
2	B	71	GLU
2	B	127	ASP
2	B	152	LEU
2	B	166	ILE
2	B	213	LYS
2	B	299	ASN
2	D	115	PRO
2	D	155	ASP
2	D	166	ILE
2	D	182	LEU
2	D	187	SER
2	D	216	VAL
1	A	34	ASP
2	B	55	LEU
2	B	70	PHE
2	B	91	ASP

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Mol	Chain	Res	Type
2	B	128	GLY
1	C	34	ASP
1	C	53	GLY
1	C	98	VAL
2	D	22	LYS
2	D	123	ILE
2	D	151	GLU
2	D	223	VAL
2	B	168	ASP
2	B	194	ASP
2	B	320	GLY
2	D	103	LEU
1	A	185	ASN
2	B	37	ASP
2	B	42	GLU
2	B	66	GLN
2	B	130	SER
2	B	288	ARG
2	B	21	GLY
2	B	185	GLU
2	B	212	SER
1	C	134	ASP
1	C	131	VAL
2	B	126	VAL
2	B	184	PRO
2	B	300	GLY
2	B	47	PRO
2	D	279	VAL
1	C	163	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	270/274 (98%)	209 (77%)	61 (23%)	1	3
1	C	271/274 (99%)	226 (83%)	45 (17%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	269/292 (92%)	221 (82%)	48 (18%)	2	6
2	D	208/292 (71%)	172 (83%)	36 (17%)	2	7
All	All	1018/1132 (90%)	828 (81%)	190 (19%)	2	5

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	LEU
1	A	12	MSE
1	A	21	SER
1	A	22	MSE
1	A	23	ARG
1	A	26	ILE
1	A	36	ARG
1	A	37	ARG
1	A	38	LEU
1	A	54	ASN
1	A	56	THR
1	A	58	ASN
1	A	59	LEU
1	A	67	VAL
1	A	69	MSE
1	A	70	GLU
1	A	71	ASN
1	A	87	LEU
1	A	96	THR
1	A	103	GLU
1	A	104	ILE
1	A	109	LEU
1	A	112	LEU
1	A	113	ARG
1	A	116	SER
1	A	120	LYS
1	A	128	MSE
1	A	132	GLN
1	A	134	ASP
1	A	143	MSE
1	A	146	ASN
1	A	148	SER
1	A	158	ASN

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Mol	Chain	Res	Type
1	A	164	THR
1	A	166	ILE
1	A	169	GLU
1	A	171	LEU
1	A	177	GLN
1	A	192	ASN
1	A	196	PHE
1	A	197	LYS
1	A	211	THR
1	A	213	PHE
1	A	214	LEU
1	A	238	LEU
1	A	247	SER
1	A	251	LYS
1	A	254	LYS
1	A	255	GLN
1	A	258	THR
1	A	262	SER
1	A	264	PHE
1	A	267	LEU
1	A	272	ASN
1	A	273	ILE
1	A	278	LEU
1	A	287	VAL
1	A	288	LEU
1	A	295	GLN
1	A	306	LYS
2	B	13	LEU
2	B	14	LEU
2	B	32	ASN
2	B	42	GLU
2	B	44	THR
2	B	51	HIS
2	B	54	THR
2	B	57	ASP
2	B	58	LEU
2	B	62	GLU
2	B	96	TYR
2	B	101	THR
2	B	109	TYR
2	B	113	VAL
2	B	114	ASN

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Mol	Chain	Res	Type
2	B	117	ILE
2	B	120	GLU
2	B	133	PHE
2	B	145	THR
2	B	152	LEU
2	B	154	LEU
2	B	157	VAL
2	B	158	GLN
2	B	164	THR
2	B	166	ILE
2	B	168	ASP
2	B	169	HIS
2	B	171	ILE
2	B	173	GLU
2	B	175	PHE
2	B	177	ARG
2	B	182	LEU
2	B	186	LEU
2	B	195	ASN
2	B	204	LYS
2	B	207	LEU
2	B	208	PHE
2	B	214	ILE
2	B	219	ASP
2	B	238	THR
2	B	244	LEU
2	B	268	GLU
2	B	283	LEU
2	B	287	ILE
2	B	288	ARG
2	B	292	LEU
2	B	301	THR
2	B	307	LEU
1	C	11	LEU
1	C	14	ARG
1	C	17	SER
1	C	26	ILE
1	C	36	ARG
1	C	37	ARG
1	C	38	LEU
1	C	45	GLU
1	C	49	LEU

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Mol	Chain	Res	Type
1	C	50	ARG
1	C	59	LEU
1	C	70	GLU
1	C	82	GLN
1	C	87	LEU
1	C	90	VAL
1	C	94	GLU
1	C	97	GLU
1	C	99	LEU
1	C	104	ILE
1	C	112	LEU
1	C	123	VAL
1	C	132	GLN
1	C	136	ARG
1	C	153	GLU
1	C	166	ILE
1	C	169	GLU
1	C	190	GLN
1	C	195	LYS
1	C	207	LEU
1	C	211	THR
1	C	213	PHE
1	C	214	LEU
1	C	218	SER
1	C	248	ASN
1	C	255	GLN
1	C	258	THR
1	C	267	LEU
1	C	276	SER
1	C	278	LEU
1	C	287	VAL
1	C	288	LEU
1	C	292	ASN
1	C	296	GLU
1	C	297	LEU
1	C	304	LYS
2	D	20	CYS
2	D	31	HIS
2	D	98	ASN
2	D	108	GLU
2	D	109	TYR
2	D	111	TYR

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Mol	Chain	Res	Type
2	D	120	GLU
2	D	121	VAL
2	D	133	PHE
2	D	139	ARG
2	D	148	GLU
2	D	166	ILE
2	D	169	HIS
2	D	171	ILE
2	D	181	LYS
2	D	188	PHE
2	D	191	ASN
2	D	193	LEU
2	D	195	ASN
2	D	198	GLN
2	D	204	LYS
2	D	207	LEU
2	D	208	PHE
2	D	209	ASP
2	D	212	SER
2	D	213	LYS
2	D	230	VAL
2	D	238	THR
2	D	239	ILE
2	D	246	LYS
2	D	268	GLU
2	D	269	LEU
2	D	283	LEU
2	D	287	ILE
2	D	295	ILE
2	D	308	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	89	HIS
1	A	132	GLN
1	A	190	GLN
1	A	192	ASN
1	A	220	ASN
1	A	255	GLN
1	A	272	ASN

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Mol	Chain	Res	Type
1	A	281	ASN
2	B	32	ASN
2	B	158	GLN
2	B	180	GLN
2	B	195	ASN
2	B	198	GLN
2	B	274	GLN
1	C	29	ASN
1	C	82	GLN
1	C	89	HIS
1	C	126	HIS
1	C	146	ASN
1	C	177	GLN
1	C	192	ASN
1	C	248	ASN
1	C	281	ASN
1	C	301	ASN
2	D	98	ASN
2	D	169	HIS
2	D	180	GLN
2	D	195	ASN
2	D	274	GLN
2	D	277	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	GNP	A	500	4	28,34,34	1.70	7 (25%)	33,54,54	2.73	12 (36%)
3	GNP	B	500	4	28,34,34	1.77	6 (21%)	33,54,54	2.44	10 (30%)
3	GNP	C	500	4	28,34,34	1.63	7 (25%)	33,54,54	2.35	11 (33%)
3	GNP	D	500	4	28,34,34	1.77	5 (17%)	33,54,54	2.28	7 (21%)

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
3	GNP	A	500	4	-	0/12/38/38	0/3/3/3
3	GNP	B	500	4	-	0/12/38/38	0/3/3/3
3	GNP	C	500	4	-	0/12/38/38	0/3/3/3
3	GNP	D	500	4	-	1/12/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	GNP	PB-O3A	-4.10	1.54	1.59
3	B	500	GNP	PB-O3A	-3.49	1.54	1.59
3	C	500	GNP	PB-O2B	-2.82	1.48	1.56
3	B	500	GNP	PB-O2B	-2.81	1.48	1.56
3	C	500	GNP	PB-O3A	-2.75	1.55	1.59
3	D	500	GNP	PB-O2B	-2.68	1.49	1.56
3	A	500	GNP	PB-O2B	-2.35	1.50	1.56
3	A	500	GNP	PG-O2G	-2.27	1.50	1.56
3	A	500	GNP	PB-O3A	-2.25	1.56	1.59
3	B	500	GNP	C8-N7	-2.05	1.30	1.34
3	A	500	GNP	C8-N7	-2.04	1.30	1.34
3	C	500	GNP	PG-O3G	-2.01	1.51	1.56
3	C	500	GNP	PB-O1B	2.04	1.48	1.46
3	D	500	GNP	PB-O1B	2.15	1.48	1.46
3	C	500	GNP	O4'-C1'	2.17	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	GNP	PB-O1B	2.35	1.48	1.46
3	A	500	GNP	PB-O1B	2.41	1.48	1.46
3	C	500	GNP	C6-N1	2.93	1.38	1.33
3	A	500	GNP	C6-N1	3.39	1.39	1.33
3	D	500	GNP	C6-N1	3.57	1.39	1.33
3	B	500	GNP	C6-N1	3.66	1.39	1.33
3	C	500	GNP	PG-O1G	4.27	1.51	1.46
3	A	500	GNP	PG-O1G	4.95	1.51	1.46
3	D	500	GNP	PG-O1G	4.97	1.51	1.46
3	B	500	GNP	PG-O1G	5.19	1.52	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	GNP	C5-C6-N1	-8.39	112.12	123.59
3	A	500	GNP	C5-C6-N1	-8.25	112.31	123.59
3	D	500	GNP	C5-C6-N1	-8.18	112.40	123.59
3	C	500	GNP	C5-C6-N1	-7.31	113.59	123.59
3	A	500	GNP	O1G-PG-N3B	-5.09	104.10	111.90
3	D	500	GNP	O3G-PG-O1G	-3.48	104.25	113.49
3	B	500	GNP	O3G-PG-O1G	-3.24	104.87	113.49
3	C	500	GNP	O5'-PA-O1A	-3.05	97.76	109.62
3	A	500	GNP	PA-O3A-PB	-3.01	122.59	132.67
3	A	500	GNP	O3'-C3'-C4'	-3.00	102.04	111.05
3	C	500	GNP	N3-C2-N1	-2.79	123.19	127.44
3	A	500	GNP	O1B-PB-N3B	-2.70	107.75	111.90
3	A	500	GNP	N3-C2-N1	-2.52	123.60	127.44
3	B	500	GNP	N3-C2-N1	-2.51	123.62	127.44
3	B	500	GNP	O1B-PB-N3B	-2.48	108.10	111.90
3	D	500	GNP	PA-O3A-PB	-2.46	124.43	132.67
3	C	500	GNP	O1G-PG-N3B	-2.45	108.14	111.90
3	C	500	GNP	O3G-PG-O1G	-2.41	107.08	113.49
3	A	500	GNP	C6-C5-C4	-2.39	118.04	120.90
3	B	500	GNP	C6-C5-C4	-2.30	118.15	120.90
3	C	500	GNP	C6-C5-C4	-2.18	118.29	120.90
3	B	500	GNP	O1G-PG-N3B	-2.16	108.59	111.90
3	D	500	GNP	N3-C2-N1	-2.02	124.36	127.44
3	A	500	GNP	N2-C2-N3	2.15	121.92	117.80
3	B	500	GNP	O3A-PA-O5'	2.17	108.69	102.94
3	C	500	GNP	O2B-PB-O1B	2.23	114.66	110.00
3	B	500	GNP	O3G-PG-O2G	2.61	115.32	107.58
3	D	500	GNP	O3G-PG-O2G	2.80	115.87	107.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	500	GNP	O3G-PG-O2G	2.98	116.42	107.58
3	A	500	GNP	O2B-PB-O1B	3.04	116.34	110.00
3	C	500	GNP	C2'-C1'-N9	3.38	119.46	114.29
3	C	500	GNP	O3A-PA-O5'	3.70	112.76	102.94
3	A	500	GNP	O3A-PB-N3B	3.74	116.73	106.44
3	B	500	GNP	O2B-PB-O1B	3.97	118.29	110.00
3	D	500	GNP	O2B-PB-O1B	4.00	118.36	110.00
3	A	500	GNP	O3A-PA-O5'	4.12	113.86	102.94
3	D	500	GNP	C6-N1-C2	5.83	124.03	115.94
3	C	500	GNP	C6-N1-C2	5.86	124.07	115.94
3	B	500	GNP	C6-N1-C2	6.54	125.01	115.94
3	A	500	GNP	C6-N1-C2	6.62	125.13	115.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	500	GNP	O1G-PG-N3B-PB

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GNP	1	0
3	B	500	GNP	7	0
3	C	500	GNP	5	0
3	D	500	GNP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	276/307 (89%)	0.70	12 (4%) 39 31	56, 72, 112, 132	0
1	C	277/307 (90%)	0.72	20 (7%) 18 12	55, 71, 98, 122	0
2	B	284/331 (85%)	1.19	70 (24%) 1 0	65, 120, 156, 164	0
2	D	221/331 (66%)	1.44	63 (28%) 1 0	62, 120, 181, 188	0
All	All	1058/1276 (82%)	0.99	165 (15%) 3 2	55, 85, 160, 188	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	112	LYS	7.5
2	D	157	VAL	6.5
2	B	14	LEU	6.5
2	D	152	LEU	6.5
2	D	268	GLU	6.0
2	D	86	LEU	5.7
2	D	175	PHE	5.7
2	D	14	LEU	5.7
2	B	67	LEU	5.5
2	D	88	TYR	5.5
2	B	56	ILE	5.5
2	D	155	ASP	5.4
2	B	287	ILE	5.4
2	D	13	LEU	5.1
2	B	52	PHE	4.9
2	B	166	ILE	4.9
2	D	115	PRO	4.9
2	D	108	GLU	4.8
2	B	195	ASN	4.6
2	D	321	LEU	4.6
2	B	13	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	109	TYR	4.5
2	B	175	PHE	4.4
1	C	50	ARG	4.3
2	D	216	VAL	4.3
2	B	207	LEU	4.3
2	B	45	SER	4.3
2	B	216	VAL	4.3
2	D	87	VAL	4.2
2	B	54	THR	4.1
2	D	125	LYS	4.1
2	B	86	LEU	4.1
2	B	46	ASN	4.0
2	B	103	LEU	4.0
2	D	174	ALA	4.0
2	B	63	LEU	4.0
2	D	25	ILE	3.9
2	B	109	TYR	3.9
2	B	171	ILE	3.8
2	B	76	SER	3.8
2	B	81	LYS	3.6
2	B	87	VAL	3.5
2	B	55	LEU	3.5
2	D	90	ILE	3.5
2	B	44	THR	3.4
2	D	180	GLN	3.4
2	B	25	ILE	3.4
2	D	123	ILE	3.4
2	D	119	ILE	3.3
2	D	245	TYR	3.3
2	B	26	CYS	3.3
2	D	12	VAL	3.3
2	D	17	VAL	3.3
2	B	214	ILE	3.1
2	D	196	LEU	3.1
2	D	307	LEU	3.1
1	C	125	LEU	3.1
2	B	179	VAL	3.1
2	B	22	LYS	3.1
2	D	317	PHE	3.0
1	A	11	LEU	3.0
1	A	308	PHE	3.0
2	B	39	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	27	LYS	3.0
2	B	70	PHE	3.0
1	C	260	LEU	3.0
2	B	30	PHE	3.0
1	C	26	ILE	3.0
1	C	42	ILE	2.9
2	D	97	ILE	2.9
2	B	113	VAL	2.9
2	B	272	VAL	2.9
2	D	247	ALA	2.9
2	B	107	ILE	2.9
2	D	107	ILE	2.9
1	A	10	LEU	2.9
2	D	223	VAL	2.9
2	D	110	ALA	2.8
2	B	35	PRO	2.8
2	B	133	PHE	2.8
2	B	71	GLU	2.8
1	A	285	PHE	2.8
2	D	26	CYS	2.8
2	B	206	PHE	2.8
2	D	206	PHE	2.8
1	C	196	PHE	2.7
1	C	203	LEU	2.7
2	B	268	GLU	2.7
2	B	53	SER	2.7
1	C	54	ASN	2.6
1	C	273	ILE	2.6
2	B	58	LEU	2.6
1	A	26	ILE	2.6
1	A	302	ILE	2.6
2	B	172	TYR	2.6
2	B	27	LYS	2.6
2	B	280	ILE	2.6
2	D	144	ARG	2.6
2	B	164	THR	2.5
2	B	64	PRO	2.5
1	C	121	ILE	2.5
1	C	205	ILE	2.5
2	B	193	LEU	2.5
2	D	29	VAL	2.5
2	D	205	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	280	ILE	2.5
2	B	288	ARG	2.5
1	C	171	LEU	2.4
2	B	129	LEU	2.4
2	B	161	PHE	2.4
1	A	80	ILE	2.4
2	B	295	ILE	2.4
2	B	314	ILE	2.4
2	D	242	PHE	2.4
2	B	12	VAL	2.4
2	B	244	LEU	2.4
2	B	282	TYR	2.4
2	D	113	VAL	2.4
2	D	281	ILE	2.4
2	B	62	GLU	2.3
2	D	314	ILE	2.3
1	A	125	LEU	2.3
2	D	30	PHE	2.3
2	B	60	VAL	2.3
2	D	183	ILE	2.3
2	B	134	LYS	2.3
2	D	177	ARG	2.3
1	C	59	LEU	2.3
2	D	182	LEU	2.3
1	C	10	LEU	2.3
2	D	103	LEU	2.3
2	D	178	ILE	2.2
2	B	225	ILE	2.2
1	C	298	VAL	2.2
2	D	159	VAL	2.2
2	B	75	ASP	2.2
2	B	47	PRO	2.2
2	B	149	LEU	2.1
2	B	242	PHE	2.1
2	D	272	VAL	2.1
1	C	246	ILE	2.1
2	D	296	ILE	2.1
2	D	98	ASN	2.1
2	D	292	LEU	2.1
2	B	121	VAL	2.1
2	D	134	LYS	2.1
1	A	59	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	159	LEU	2.1
2	B	79	LEU	2.1
2	B	89	VAL	2.1
2	D	225	ILE	2.1
2	D	312	TYR	2.1
2	D	161	PHE	2.0
1	A	109	LEU	2.0
1	C	102	ILE	2.0
1	A	203	LEU	2.0
2	D	282	TYR	2.0
2	B	95	GLU	2.0
2	B	210	VAL	2.0
2	D	287	ILE	2.0
1	A	260	LEU	2.0
2	D	228	TYR	2.0
2	B	78	ARG	2.0
1	C	179	VAL	2.0
1	C	162	PHE	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	MG	A	600	1/1	0.94	0.28	2.84	62,62,62,62	0
3	GNP	C	500	32/32	0.98	0.23	0.65	58,66,74,76	0
3	GNP	A	500	32/32	0.97	0.23	0.34	59,68,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GNP	D	500	32/32	0.74	0.22	-0.60	165,189,200,203	0
3	GNP	B	500	32/32	0.93	0.13	-1.35	125,142,154,156	0
4	MG	D	600	1/1	0.30	0.11	-	198,198,198,198	0
4	MG	B	600	1/1	0.42	0.21	-	154,154,154,154	0
4	MG	C	600	1/1	0.98	0.21	-	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.