



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:01 AM UTC

PDB ID : 3R7W / pdb_00003r7w
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

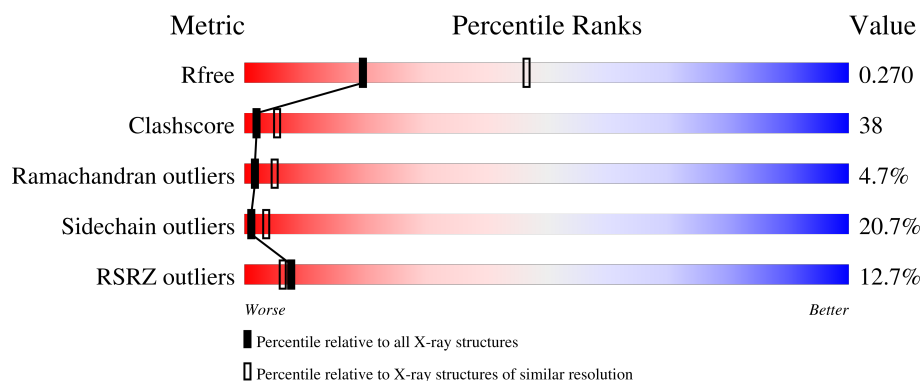
1 Overall quality at a glance

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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 38% 41% 14% 6%
1	C	307	4% 41% 42% 10% 6%
2	B	331	14% 31% 39% 17% 11%
2	D	331	18% 24% 35% 9% 31%

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			

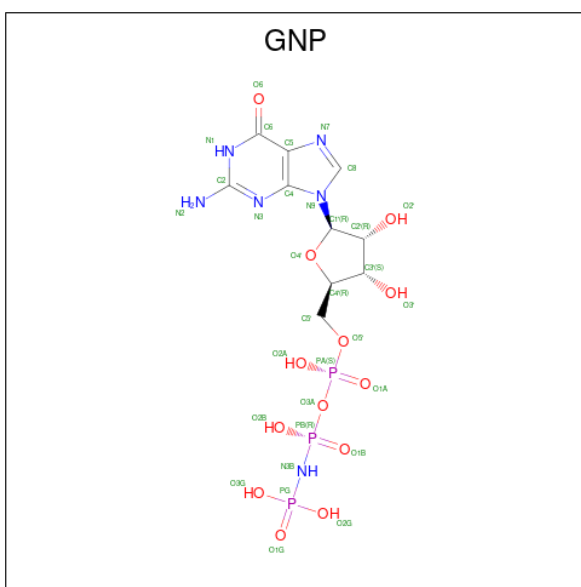
There are 8 discrepancies between the modelled and reference sequences:

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 (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

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

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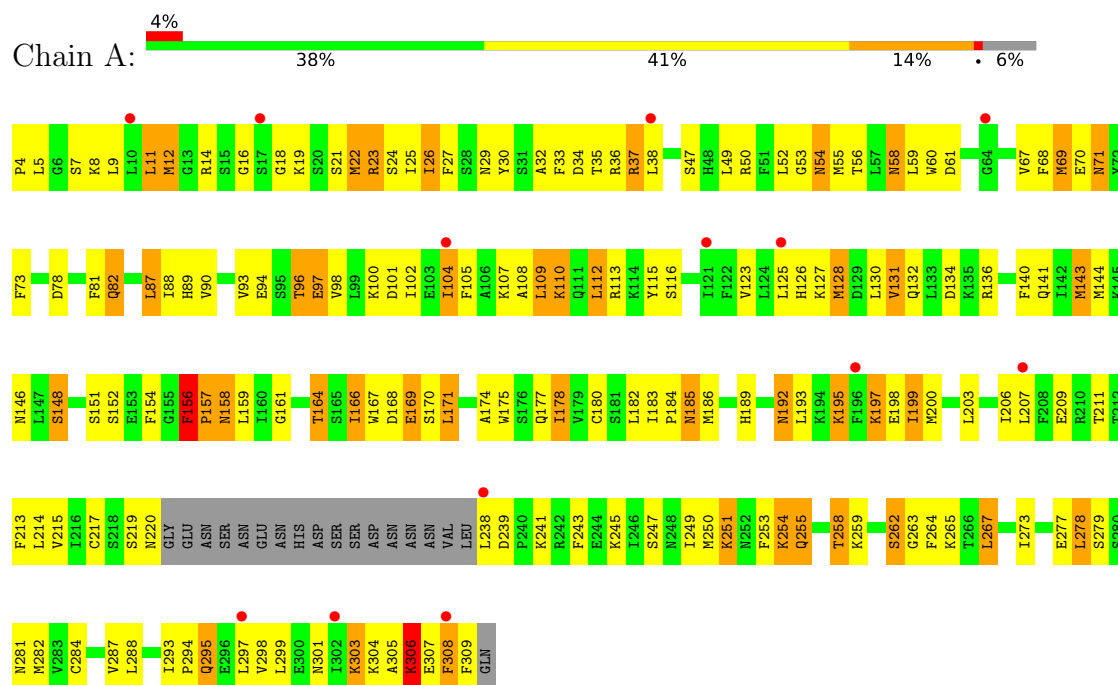
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		

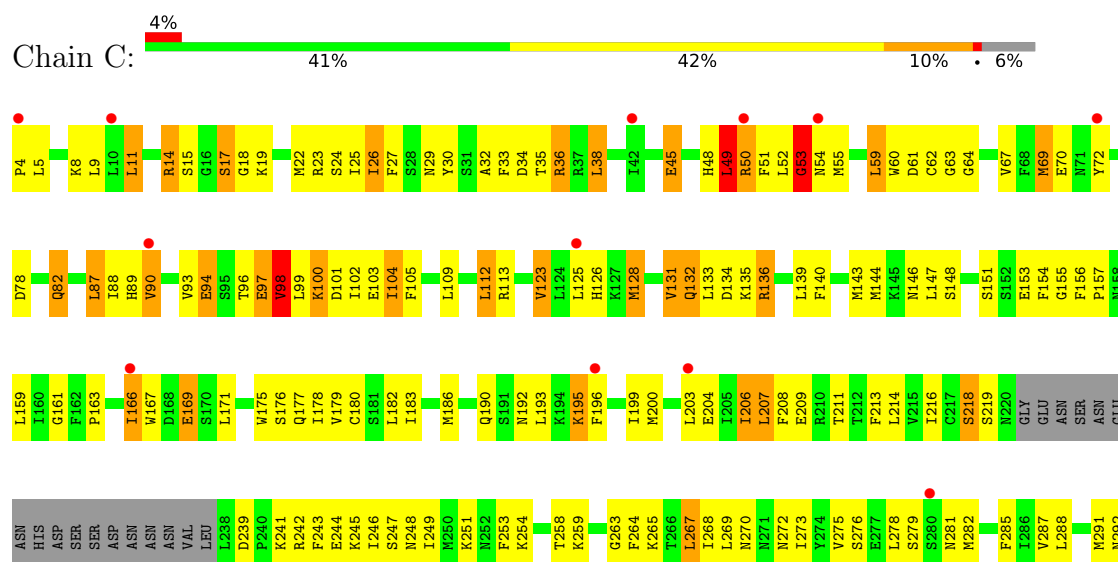
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: GTP-binding protein GTR1

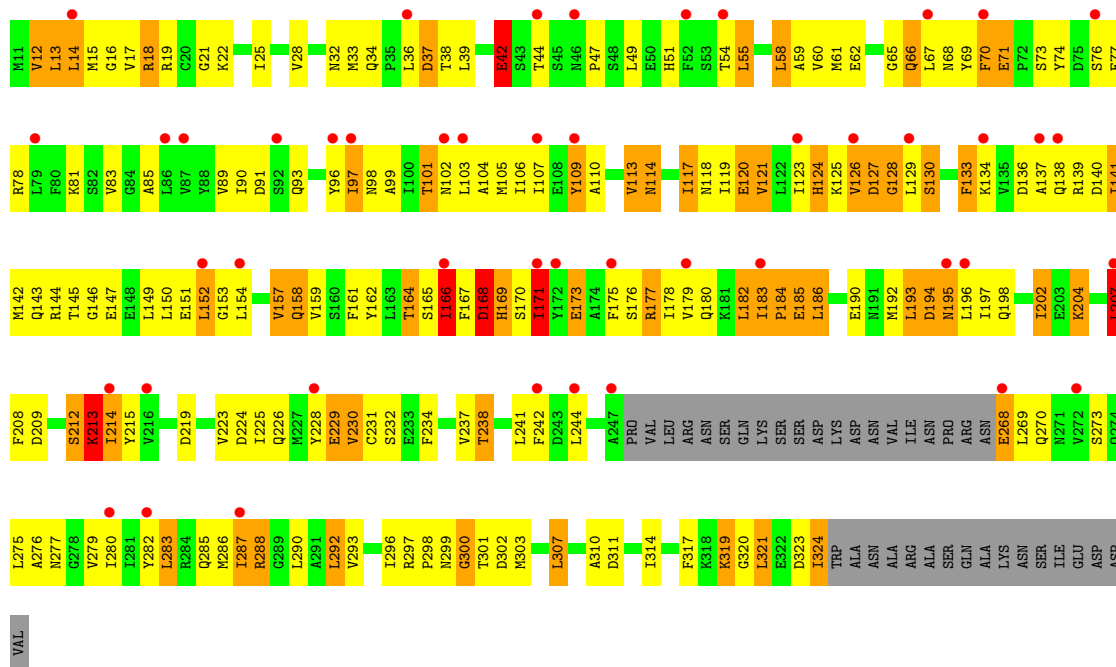


• Molecule 1: GTP-binding protein GTR1

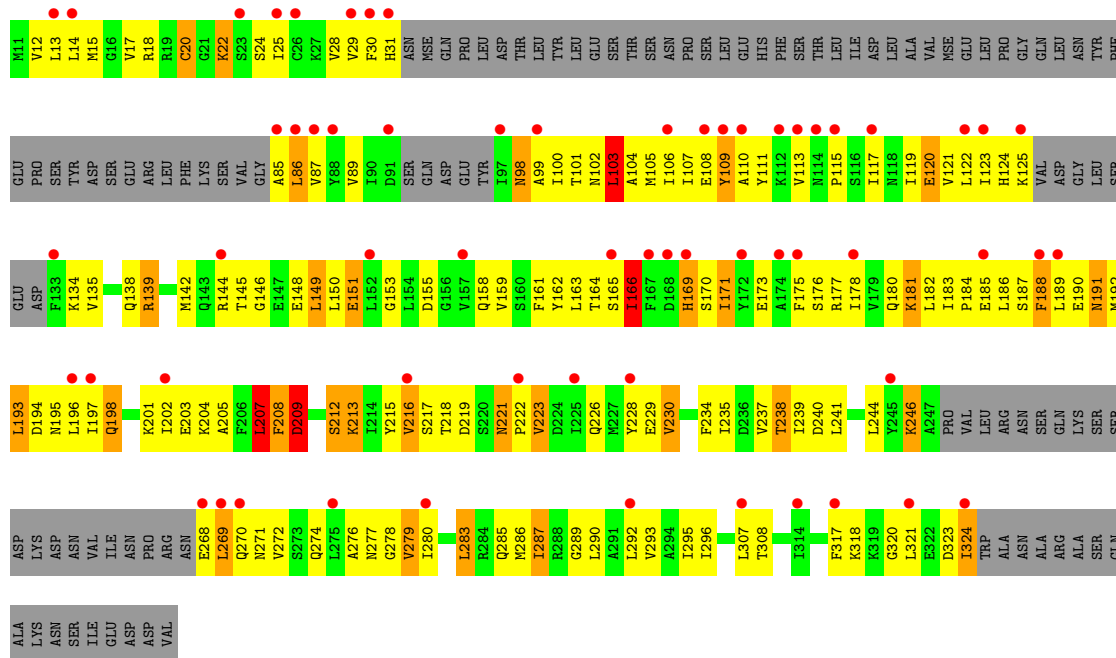
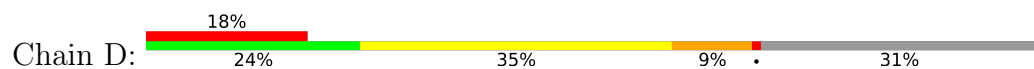




• Molecule 2: GTP-binding protein GTR2



• 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, α , β , γ	68.91Å 148.44Å 98.51Å 90.00° 100.61° 90.00°	Depositor
Resolution (Å)	44.06 – 2.77 44.06 – 2.77	Depositor EDS
% Data completeness (in resolution range)	95.0 (44.06-2.77) 95.1 (44.06-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.236 , 0.283 0.227 , 0.270	Depositor DCC
R_{free} test set	2290 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9011	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.75	0/2375	1.07	6/3165 (0.2%)
1	C	0.73	0/2384	1.06	3/3177 (0.1%)
2	B	0.60	0/2378	0.97	9/3205 (0.3%)
2	D	0.58	0/1847	1.00	6/2480 (0.2%)
All	All	0.67	0/8984	1.03	24/12027 (0.2%)

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 (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	ILE	N-CA-C	7.96	118.66	111.81
2	D	207	LEU	N-CA-C	-7.17	101.30	110.19
2	B	207	LEU	N-CA-C	-6.20	101.34	110.52
1	A	156	PHE	CA-C-N	6.17	127.56	119.84
1	A	156	PHE	C-N-CA	6.17	127.56	119.84
1	C	179	VAL	N-CA-C	6.00	116.74	110.62
2	B	124	HIS	N-CA-C	5.91	117.95	110.33
2	D	241	LEU	N-CA-C	-5.87	104.97	111.36
1	A	209	GLU	N-CA-C	-5.63	102.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	209	ASP	N-CA-C	5.52	117.18	108.96
2	B	76	SER	N-CA-C	-5.41	107.33	114.04
2	B	93	GLN	N-CA-C	-5.41	106.52	113.23
1	A	115	TYR	N-CA-C	5.40	117.99	111.40
1	C	49	LEU	N-CA-C	5.34	116.52	108.46
2	D	235	ILE	N-CA-C	-5.33	105.18	110.62
2	B	171	ILE	CB-CA-C	-5.30	104.98	112.14
2	B	183	ILE	CA-C-N	5.29	126.46	119.84
2	B	183	ILE	C-N-CA	5.29	126.46	119.84
2	B	121	VAL	N-CA-C	5.27	115.54	108.17
2	D	221	ASN	CA-C-N	5.26	124.71	119.24
2	D	221	ASN	C-N-CA	5.26	124.71	119.24
1	A	199	ILE	CB-CA-C	-5.26	105.24	111.97
1	C	219	SER	N-CA-C	5.24	117.90	111.82
1	A	69	MSE	N-CA-C	5.01	116.74	111.28

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	177	0
1	C	2353	0	2404	151	0
2	B	2348	0	2348	185	0
2	D	1830	0	1866	197	0
3	A	32	0	13	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	692	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 38.

All (692) 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
1:A:54:ASN:H	1:A:54:ASN:HD22	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:A:125:LEU:HD11	1:A:143:MSE:HG3	1.56	0.87
1:C:131:VAL:CG1	1:C:132:GLN:H	1.86	0.87
2:D:171:ILE:HD12	2:D:171:ILE:H	1.36	0.87
2:D:209:ASP:HB2	2:D:212:SER:C	2.00	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:LYS:HE3	1:A:60:TRP:CZ2	2.13	0.83
1:A:54:ASN:HD22	1:A:54:ASN:N	1.76	0.83
1:A:195:LYS:O	1:A:199:ILE:HG13	1.79	0.83
1:A:101:ASP:O	1:A:104:ILE:HD13	1.77	0.82
2:D:215:TYR:C	2:D:217:SER:H	1.87	0.81
2:D:142:MSE:HE2	2:D:161:PHE:HB2	1.61	0.81
2:D:234:PHE:O	2:D:238:THR:HG22	1.81	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
1:A:304:LYS:HA	1:A:305:ALA:C	2.06	0.80
2:B:149:LEU:HD13	2:B:157:VAL:HG21	1.63	0.80
2:D:120:GLU:HG2	2:D:178:ILE:HG12	1.61	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
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:50:ARG:HG3	1:C:50:ARG:HH11	1.48	0.78
1:C:94:GLU:O	1:C:94:GLU:HG2	1.83	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
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:254:LYS:NZ	1:A:254:LYS:HB3	2.01	0.75
2:B:323:ASP:O	2:B:324:ILE:HG13	1.87	0.75
1:C:23:ARG:HG3	1:C:59:LEU:HD12	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:HD21	1:C:22:MSE:HE1	1.69	0.74
2:B:234:PHE:O	2:B:238:THR:HG22	1.86	0.74
2:D:238:THR:HB	2:D:271:ASN:ND2	1.96	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:H	1:A:54:ASN:ND2	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:15:MSE:HA	2:B:22:LYS:HZ3	1.53	0.71
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
1:A:109:LEU:CD2	1:A:156:PHE:HD2	2.03	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
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:124:HIS:HA	2:D:164:THR:HB	1.74	0.70
2:D:189:LEU:HD13	2:D:189:LEU:O	1.92	0.70
1:A:207:LEU:HD13	1:A:282:MSE:HE1	1.74	0.69
2:B:283:LEU:HB2	2:B:293:VAL:HG22	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
1:A:12:MSE:CE	1:A:87:LEU:HD21	2.24	0.68
2:B:193:LEU:HB2	2:B:317:PHE:CE1	2.26	0.68
2:B:226:GLN:O	2:B:230:VAL:HG23	1.92	0.68
1:A:305:ALA:H	1:A:309:PHE:HD1	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:MSE:HE2	2:D:292:LEU:HB2	1.76	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
2:D:209:ASP:HB2	2:D:213:LYS:H	1.58	0.68
1:A:186:MSE:CE	1:A:217:CYS:HB3	2.23	0.68
2:D:146:GLY:O	2:D:150:LEU:HB2	1.94	0.68
2:D:212:SER:CA	2:D:213:LYS:HB2	2.19	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
1:A:267:LEU:C	1:A:267:LEU:HD12	2.20	0.67
2:B:215:TYR:CD1	2:B:215:TYR:O	2.47	0.67
2:D:286:MSE:HE3	2:D:317:PHE:CE2	2.30	0.67
2:B:70:PHE:CA	2:B:71:GLU:CB	2.73	0.67
1:C:203:LEU:HD12	1:C:203:LEU:O	1.95	0.67
2:D:193:LEU:HD23	2:D:193:LEU:N	2.10	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
1:A:23:ARG:HG2	1:A:23:ARG:NH2	2.10	0.66
1:A:259:LYS:HE3	2:B:229:GLU:OE1	1.96	0.65
2:B:198:GLN:HA	2:B:198:GLN:HE21	1.59	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
1:C:259:LYS:HE2	2:D:229:GLU:CD	2.22	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
1:C:207:LEU:HG	1:C:282:MSE:HE1	1.77	0.65
2:D:176:SER:HB3	2:D:215:TYR:CG	2.32	0.65
2:B:298:PRO:C	2:B:300:GLY:H	2.05	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:50:ARG:HG3	1:C:50:ARG:NH1	2.12	0.64
1:C:207:LEU:HG	1:C:282:MSE:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:O	1:A:245:LYS:HG3	1.97	0.64
2:D:100:ILE:HG13	2:D:145:THR:HG23	1.79	0.64
1:A:200:MSE:HE1	1:A:301:ASN:HB2	1.78	0.64
2:B:85:ALA:HB2	2:B:182:LEU:HD11	1.79	0.64
1:C:293:ILE:HG13	1:C:294:PRO:HD2	1.80	0.64
2:D:171:ILE:H	2:D:171:ILE:CD1	2.05	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:C:169:GLU:CD	1:C:169:GLU:H	2.05	0.64
1:A:265:LYS:HD3	2:B:276:ALA:HA	1.79	0.63
1:C:140:PHE:CZ	1:C:144:MSE:HE3	2.33	0.63
2:D:181:LYS:CA	2:D:186:LEU:HD21	2.26	0.63
1:C:128:MSE:HG3	1:C:128:MSE:O	1.97	0.63
2:D:24:SER:O	2:D:28:VAL:HG23	1.99	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
1:A:192:ASN:N	1:A:192:ASN:HD22	1.96	0.63
2:D:101:THR:HG22	2:D:148:GLU:HG3	1.79	0.63
1:C:166:ILE:HD13	3:C:500:GNP:N7	2.14	0.63
2:D:12:VAL:HG22	2:D:85:ALA:HB3	1.80	0.63
1:A:25:ILE:HD12	1:A:166:ILE:HD11	1.81	0.62
2:B:119:ILE:H	2:B:158:GLN:HG2	1.64	0.62
2:D:125:LYS:HE3	3:D:500:GNP:N3	2.14	0.62
2:B:74:TYR:CE1	1:C:308:PHE:HE1	2.17	0.62
2:D:197:ILE:HG22	2:D:197:ILE:O	1.98	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: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:O	2:D:283:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:85:ALA:HA	2:D:117:ILE:HG23	1.84	0.60
1:C:93:VAL:HG11	1:C:128:MSE:HE1	1.83	0.60
1:C:101:ASP:O	1:C:104:ILE:HD13	2.01	0.60
2:B:165:SER:C	2:B:167:PHE:H	2.10	0.59
2:D:215:TYR:C	2:D:217:SER:N	2.55	0.59
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:126:VAL:HG12	2:B:126:VAL:O	2.02	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
2:D:277:ASN:HB3	2:D:279:VAL:H	1.67	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
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:B:223:VAL:O	2:B:224:ASP:HB3	2.02	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:B:234:PHE:O	2:B:238:THR:CG2	2.51	0.58
2:D:86:LEU:O	2:D:120:GLU:HB2	2.03	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
1:A:151:SER:C	1:A:157:PRO:HD2	2.29	0.58
2:D:145:THR:O	2:D:149:LEU:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:125:LYS:HD3	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
1:C:22:MSE:CE	1:C:175:TRP:HZ2	2.16	0.57
2:D:166:ILE:H	2:D:171:ILE:CG1	2.18	0.57
1:A:174:ALA:O	1:A:178:ILE:HG13	2.05	0.57
1:C:193:LEU:HD13	1:C:207:LEU:HD21	1.84	0.57
2:D:103:LEU:HD12	2:D:145:THR:HG22	1.85	0.57
2:B:140:ASP:O	2:B:143:GLN:HB2	2.04	0.57
2:D:25:ILE:O	2:D:29:VAL:HG23	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:A:169:GLU:HG2	1:A:245:LYS:HG2	1.87	0.56
1:C:14:ARG:O	1:C:17:SER:OG	2.23	0.56
1:C:200:MSE:HE3	1:C:200:MSE:HA	1.85	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
1:A:157:PRO:HA	1:A:158:ASN:C	2.31	0.56
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
1:A:254:LYS:HB3	1:A:254:LYS:HZ2	1.68	0.55
2:B:159:VAL:HB	2:B:161:PHE:CE2	2.41	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
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:A:12:MSE:HE3	1:A:87:LEU:HD21	1.87	0.55
1:C:26:ILE:CD1	1:C:175:TRP:CG	2.90	0.55
1:C:18:GLY:HA2	3:C:500:GNP:PA	2.47	0.55
1:C:50:ARG:HB3	1:C:54:ASN:OD1	2.06	0.55
1:A:37:ARG:H	1:A:37:ARG:HD3	1.71	0.55
2:D:166:ILE:HA	2:D:171:ILE:HG12	1.89	0.55
1:A:125:LEU:CD1	1:A:143:MSE:HG3	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLU:O	2:B:81:LYS:HG3	2.07	0.54
2:D:138:GLN:HE22	2:D:163:LEU:HD11	1.72	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:28:VAL:HG11	2:B:166:ILE:CG1	2.37	0.54
2:B:124:HIS:CG	2:B:125:LYS:N	2.75	0.54
1:A:253:PHE:HB2	2:B:237:VAL:HG21	1.90	0.54
1:A:23:ARG:HH21	1:A:23:ARG:CG	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
2:D:283:LEU:HD12	2:D:283:LEU:C	2.32	0.53
1:C:25:ILE:HD12	1:C:166:ILE:HG13	1.90	0.53
1:C:36:ARG:NH1	1:C:36:ARG:HB3	2.23	0.53
2:D:104:ALA:CB	2:D:148:GLU:HB3	2.38	0.53
2:B:90:ILE:HG22	2:B:90:ILE:O	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:N	2:D:193:LEU:CD2	2.71	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:D:28:VAL:HG12	2:D:28:VAL:O	2.08	0.53
2:B:25:ILE:HA	2:B:28:VAL:CG1	2.37	0.53
1:A:131:VAL:HG22	1:A:136:ARG:CG	2.39	0.52
2:B:118:ASN:HA	2:B:158:GLN:HG2	1.91	0.52
2:D:181:LYS:HB3	2:D:186:LEU:HD21	1.91	0.52
2:B:109:TYR:O	2:B:113:VAL:HG23	2.10	0.52
2:D:221:ASN:HB3	2:D:222:PRO:HD2	1.90	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
1:A:239:ASP:C	1:A:239:ASP:OD1	2.50	0.52
1:C:169:GLU:HG2	1:C:245:LYS:HG2	1.90	0.52
2:D:142:MSE:HG2	2:D:161:PHE:CE2	2.45	0.52
2:D:234:PHE:O	2:D:238:THR:CG2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HG	1:A:140:PHE:HD1	1.75	0.52
1:C:94:GLU:O	1:C:94:GLU:CG	2.57	0.52
2:D:166:ILE:HG21	3:D:500:GNP:O6	2.10	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
1:A:61:ASP:OD1	1:A:61:ASP:C	2.53	0.51
2:B:120:GLU:HG2	2:B:178:ILE:CG1	2.27	0.51
1:A:52:LEU:HD12	1:A:55:MSE:HE3	1.91	0.51
2:D:89:VAL:HG23	2:D:124:HIS:CB	2.40	0.51
1:A:192:ASN:HD22	1:A:192:ASN:H	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:B:77:GLU:OE1	2:B:113:VAL:HG21	2.10	0.51
1:C:61:ASP:C	1:C:61:ASP:OD1	2.52	0.51
2:D:286:MSE:HE3	2:D:317:PHE:CD2	2.46	0.51
2:B:168:ASP:HB3	2:B:170:SER:H	1.75	0.51
2:D:188:PHE:O	2:D:192:MSE:HG3	2.11	0.51
2:B:123:ILE:O	2:B:126:VAL:HG23	2.10	0.51
2:D:207:LEU:HD22	2:D:290:LEU:CD2	2.40	0.51
1:A:26:ILE:HG13	1:A:27:PHE:CD2	2.46	0.51
1:A:151:SER:OG	1:A:157:PRO:HD3	2.11	0.51
1:A:299:LEU:HD12	1:A:299:LEU:H	1.75	0.51
2:D:29:VAL:HG12	2:D:30:PHE:CD1	2.46	0.51
2:D:164:THR:HG22	2:D:165:SER:N	2.22	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
1:A:29:ASN:ND2	1:A:255:GLN:NE2	2.55	0.50
1:A:55:MSE:HE1	1:A:183:ILE:HA	1.93	0.50
2:B:19:ARG:HA	3:B:500:GNP:H5'2	1.94	0.50
2:B:242:PHE:CD1	2:B:242:PHE:C	2.89	0.50
2:D:86:LEU:HD22	2:D:87:VAL:N	2.26	0.50
2:D:106:ILE:HA	2:D:109:TYR:OH	2.12	0.50
2:D:197:ILE:HG21	2:D:202:ILE:HD12	1.93	0.50
2:D:269:LEU:HD12	2:D:285:GLN:HB2	1.93	0.50
2:B:197:ILE:O	2:B:198:GLN:CD	2.55	0.50
1:C:279:SER:C	1:C:281:ASN:H	2.18	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:D:186:LEU:HD12	2:D:186:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:OE1	1:A:130:LEU:HD13	2.12	0.50
1:A:131:VAL:HG22	1:A:136:ARG:HG2	1.93	0.50
2:B:69:TYR:HE1	2:B:101:THR:OG1	1.93	0.50
2:D:190:GLU:O	2:D:190:GLU:HG2	2.10	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:A:278:LEU:N	1:A:278:LEU:HD23	2.26	0.49
1:C:123:VAL:O	1:C:161:GLY:HA2	2.12	0.49
2:B:151:GLU:O	2:B:153:GLY:N	2.44	0.49
2:D:22:LYS:HB2	3:D:500:GNP:O1B	2.12	0.49
2:B:123:ILE:O	2:B:126:VAL:CG2	2.59	0.49
1:C:89:HIS:HE1	1:C:104:ILE:HD11	1.77	0.49
2:D:14:LEU:C	2:D:15:MSE:HG3	2.38	0.49
2:D:87:VAL:HG22	2:D:120:GLU:HB3	1.93	0.49
2:D:209:ASP:CB	2:D:213:LYS:N	2.68	0.49
1:A:88:ILE:HG12	1:A:178:ILE:HD13	1.94	0.49
1:A:109:LEU:HD22	1:A:154:PHE:HB2	1.94	0.49
1:A:277:GLU:C	1:A:278:LEU:HD23	2.37	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
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
1:C:275:VAL:HG22	1:C:285:PHE:CD1	2.47	0.49
1:A:219:SER:OG	1:A:220:ASN:ND2	2.45	0.49
1:A:299:LEU:HD12	1:A:299:LEU:N	2.28	0.49
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:A:16:GLY:O	1:A:127:LYS:NZ	2.40	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
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:TYR:CD1	2:B:105:MSE:SE	3.17	0.48
2:B:73:SER:CB	1:C:192:ASN:HD21	2.27	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:B:32:ASN:C	2:B:32:ASN:HD22	2.22	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:104:ILE:HG12	1:A:105:PHE:N	2.19	0.48
1:A:125:LEU:O	1:A:128:MSE:HE3	2.14	0.48
1:A:168:ASP:OD2	1:A:170:SER:OG	2.26	0.48
1:C:11:LEU:HD13	1:C:19:LYS:HB3	1.94	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
2:B:33:MSE:HG2	2:B:34:GLN:N	2.28	0.47
2:D:86:LEU:HD13	2:D:86:LEU:C	2.38	0.47
1:A:8:LYS:HE3	1:A:60:TRP:CE2	2.49	0.47
1:A:180:CYS:C	1:A:182:LEU:N	2.72	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
2:D:138:GLN:CG	2:D:142:MSE:HE3	2.45	0.47
1:A:33:PHE:O	1:A:35:THR:N	2.47	0.47
1:A:180:CYS:C	1:A:182:LEU:H	2.23	0.47
2:B:42:GLU:CD	2:B:42:GLU:H	2.21	0.47
2:B:119:ILE:N	2:B:119:ILE:HD12	2.30	0.47
2:B:207:LEU:CD2	2:B:290:LEU:HD13	2.44	0.47
1:C:102:ILE:HD13	1:C:146:ASN:ND2	2.30	0.47
2:D:177:ARG:NH1	2:D:180:GLN:HE22	2.13	0.47
1:A:125:LEU:HD11	1:A:143:MSE:CG	2.37	0.47
2:B:22:LYS:HB3	2:B:89:VAL:HG11	1.97	0.47
2:B:66:GLN:HB3	2:B:67:LEU:H	1.50	0.47
2:B:138:GLN:O	2:B:140:ASP:N	2.48	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: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
2:B:58:LEU:HD13	2:B:58:LEU:O	2.14	0.47
2:B:126:VAL:HG12	2:B:134:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:PRO:C	2:B:300:GLY:N	2.71	0.47
1:C:11:LEU:HD21	1:C:22:MSE:CE	2.42	0.47
2:D:135:VAL:HG13	2:D:139:ARG:HH21	1.80	0.47
2:D:283:LEU:C	2:D:283:LEU:CD1	2.88	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
1:C:206:ILE:HB	1:C:208:PHE:HE1	1.80	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
2:D:124:HIS:CG	2:D:125:LYS:H	2.30	0.46
1:C:88:ILE:HG12	1:C:178:ILE:HD13	1.96	0.46
1:A:22:MSE:HE2	1:A:22:MSE:HB2	1.76	0.46
1:A:151:SER:HB3	1:A:157:PRO:CG	2.45	0.46
1:A:297:LEU:C	1:A:297:LEU:HD13	2.41	0.46
2:B:77:GLU:OE1	2:B:77:GLU:HA	2.15	0.46
1:C:253:PHE:HB2	2:D:237:VAL:HG21	1.96	0.46
2:D:103:LEU:HD13	2:D:104:ALA:N	2.31	0.46
2:D:180:GLN:O	2:D:183:ILE:HG22	2.14	0.46
1:A:73:PHE:HE1	1:A:108:ALA:HA	1.79	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:78:ASP:O	1:C:82:GLN:HG3	2.15	0.46
1:C:206:ILE:HB	1:C:208:PHE:CE1	2.51	0.46
1:C:133:LEU:C	1:C:135:LYS:H	2.24	0.46
1:A:215:VAL:HG21	1:A:243:PHE:HB3	1.97	0.46
1:C:136:ARG:H	1:C:136:ARG:HG2	1.52	0.46
2:D:103:LEU:HD12	2:D:145:THR:CG2	2.45	0.46
1:A:7:SER:CB	1:A:182:LEU:HD13	2.46	0.46
1:A:267:LEU:HB2	2:B:273:SER:HB2	1.97	0.46
1:A:304:LYS:HA	1:A:305:ALA:O	2.14	0.46
2:B:146:GLY:O	2:B:150:LEU:HG	2.14	0.46
1:C:125:LEU:O	1:C:128:MSE:HE3	2.15	0.46
2:D:202:ILE:HG22	2:D:203:GLU:N	2.31	0.46
2:B:128:GLY:C	2:B:129:LEU:HD12	2.40	0.46
2:D:12:VAL:C	2:D:13:LEU:HD23	2.40	0.46
2:B:98:ASN:O	2:B:102:ASN:OD1	2.33	0.45
2:B:197:ILE:O	2:B:197:ILE:HG22	2.15	0.45
1:C:183:ILE:CG2	1:C:186:MSE:HE2	2.45	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:207:LEU:HD22	2:D:208:PHE:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:ASP:O	2:D:244:LEU:HD23	2.16	0.45
1:A:128:MSE:O	1:A:128:MSE:HG3	2.15	0.45
2:D:25:ILE:HD11	2:D:124:HIS:CD2	2.52	0.45
2:D:122:LEU:O	2:D:124:HIS:N	2.45	0.45
1:A:303:LYS:O	1:A:306:LYS:HB2	2.16	0.45
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.56	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
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.77	0.45
1:C:128:MSE:HE3	1:C:128:MSE:HB2	1.87	0.45
1:C:263:GLY:O	1:C:264:PHE:C	2.59	0.45
1:A:25:ILE:HD11	1:A:166:ILE:HG13	1.99	0.45
1:C:82:GLN:HE21	1:C:82:GLN:HB3	1.67	0.45
1:C:155:GLY:O	1:C:157:PRO:HD3	2.17	0.45
2:D:269:LEU:C	2:D:269:LEU:HD22	2.42	0.45
2:D:274:GLN:NE2	2:D:278:GLY:HA2	2.32	0.45
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.66	0.45
2:B:179:VAL:O	2:B:179:VAL:CG1	2.65	0.45
1:C:175:TRP:O	1:C:176:SER:C	2.60	0.45
1:C:239:ASP:C	1:C:239:ASP:OD1	2.57	0.45
2:D:119:ILE:HD13	2:D:158:GLN:H	1.82	0.45
2:D:221:ASN:HB3	2:D:222:PRO:CD	2.46	0.45
1:C:25:ILE:HD11	1:C:166:ILE:HG13	1.98	0.45
2:D:119:ILE:N	2:D:119:ILE:HD12	2.32	0.45
2:B:192:MSE:C	2:B:196:LEU:HB2	2.42	0.45
1:C:239:ASP:O	1:C:242:ARG:HB3	2.16	0.45
2:D:171:ILE:HG22	2:D:175:PHE:CE2	2.52	0.45
2:D:181:LYS:CB	2:D:186:LEU:HD21	2.47	0.45
2:D:197:ILE:CG2	2:D:202:ILE:HD12	2.47	0.45
2:D:212:SER:CA	2:D:213:LYS:CB	2.88	0.45
1:A:193:LEU:HD13	1:A:207:LEU:HG	1.98	0.44
2:B:22:LYS:HZ1	2:B:65:GLY:CA	2.30	0.44
2:B:142:MSE:HG2	2:B:161:PHE:CD1	2.52	0.44
1:C:4:PRO:HG2	1:C:5:LEU:H	1.81	0.44
1:C:4:PRO:CG	1:C:5:LEU:H	2.29	0.44
2:D:85:ALA:CA	2:D:117:ILE:HG23	2.45	0.44
1:A:47:SER:O	1:A:58:ASN:HA	2.17	0.44
2:B:119:ILE:HB	2:B:158:GLN:O	2.16	0.44
2:D:113:VAL:HG12	2:D:113:VAL:O	2.17	0.44
2:D:169:HIS:CG	2:D:229:GLU:HG2	2.52	0.44
2:D:197:ILE:O	2:D:198:GLN:OE1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:ASP:O	2:D:289:GLY:O	2.35	0.44
1:A:47:SER:HB3	1:A:49:LEU:HD21	1.98	0.44
1:A:263:GLY:O	1:A:264:PHE:C	2.60	0.44
2:B:55:LEU:HD11	2:B:288:ARG:HD2	2.00	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
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
1:A:107:LYS:O	1:A:110:LYS:HB3	2.18	0.44
2:D:170:SER:HA	2:D:173:GLU:HB3	2.00	0.44
1:A:151:SER:C	1:A:157:PRO:CD	2.91	0.44
2:B:99:ALA:HA	2:B:102:ASN:CG	2.43	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
1:C:97:GLU:O	1:C:98:VAL:C	2.57	0.44
2:D:171:ILE:HG22	2:D:175:PHE:HE2	1.83	0.44
2:D:286:MSE:SE	2:D:318:LYS:HB2	2.68	0.44
1:A:88:ILE:HD13	1:A:175:TRP:CH2	2.53	0.44
2:B:120:GLU:HG3	2:B:162:TYR:CE2	2.53	0.44
2:B:124:HIS:CG	2:B:125:LYS:H	2.36	0.44
2:D:246:LYS:HE2	2:D:246:LYS:HB2	1.74	0.44
2:B:13:LEU:HD13	2:B:15:MSE:HE1	1.99	0.44
2:B:114:ASN:HB3	2:B:117:ILE:HG13	2.00	0.44
1:C:249:ILE:CD1	2:D:240:ASP:HB3	2.47	0.44
2:D:14:LEU:HD23	2:D:15:MSE:N	2.33	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:HD23	1:C:59:LEU:HA	1.72	0.43
1:C:246:ILE:O	1:C:247:SER:C	2.60	0.43
2:D:99:ALA:O	2:D:103:LEU:HB2	2.18	0.43
1:A:206:ILE:H	1:A:206:ILE:HD12	1.83	0.43
2:D:22:LYS:HG3	3:D:500:GNP:O3G	2.18	0.43
1:A:157:PRO:HB3	1:A:159:LEU:H	1.83	0.43
1:A:197:LYS:HG3	1:A:198:GLU:N	2.32	0.43
1:C:62:CYS:HB3	1:C:72:TYR:CE1	2.53	0.43
1:C:259:LYS:HE2	2:D:229:GLU:OE2	2.18	0.43
1:A:55:MSE:HE2	1:A:184:PRO:HD3	2.01	0.43
1:A:68:PHE:O	1:A:71:ASN:HB2	2.19	0.43
1:A:126:HIS:O	1:A:127:LYS:HB2	2.18	0.43
2:B:16:GLY:H	2:B:22:LYS:NZ	2.16	0.43
2:B:74:TYR:O	2:B:78:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASP:O	1:C:104:ILE:CD1	2.67	0.43
1:A:307:GLU:O	1:A:308:PHE:O	2.37	0.43
2:B:14:LEU:HD13	2:B:22:LYS:O	2.18	0.43
2:D:119:ILE:HD13	2:D:158:GLN:N	2.34	0.43
2:B:277:ASN:OD1	2:B:277:ASN:C	2.61	0.43
1:C:125:LEU:HD23	1:C:140:PHE:HA	2.00	0.43
1:C:207:LEU:CG	1:C:282:MSE:CE	2.97	0.43
2:D:151:GLU:O	2:D:153:GLY:O	2.36	0.43
2:B:33:MSE:HE2	2:B:37:ASP:CB	2.48	0.43
2:B:231:CYS:CB	2:B:293:VAL:HG11	2.49	0.43
2:B:104:ALA:O	2:B:107:ILE:HG12	2.19	0.43
1:C:14:ARG:O	1:C:15:SER:C	2.61	0.43
1:C:52:LEU:O	1:C:53:GLY:C	2.61	0.43
1:C:193:LEU:HD22	1:C:207:LEU:HD23	2.01	0.43
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
2:D:119:ILE:HG22	2:D:159:VAL:HG13	2.01	0.42
1:A:207:LEU:HB3	1:A:282:MSE:HE2	2.00	0.42
1:A:267:LEU:C	1:A:267:LEU:CD1	2.90	0.42
1:A:298:VAL:HG12	1:A:299:LEU:N	2.33	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:253:PHE:O	1:C:254:LYS:C	2.62	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:A:185:ASN:O	1:A:186:MSE:C	2.63	0.42
2:B:102:ASN:O	2:B:106:ILE:HG13	2.19	0.42
2:B:119:ILE:N	2:B:158:GLN:HG2	2.31	0.42
2:B:195:ASN:O	2:B:198:GLN:N	2.43	0.42
1:C:55:MSE:HE2	1:C:55:MSE:HB3	1.72	0.42
1:C:131:VAL:HG21	1:C:139:LEU:HD23	2.01	0.42
1:A:14:ARG:HH22	1:A:97:GLU:CD	2.27	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:279:SER:C	1:A:281:ASN:H	2.28	0.42
2:D:171:ILE:HD12	2:D:171:ILE:N	2.18	0.42
1:A:33:PHE:CD1	1:A:36:ARG:NH1	2.87	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
2:B:283:LEU:HA	2:B:292:LEU:O	2.19	0.42
2:B:176:SER:OG	2:B:215:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:VAL:HG12	2:B:224:ASP:O	2.19	0.42
1:C:33:PHE:O	1:C:35:THR:N	2.53	0.42
2:D:213:LYS:CA	2:D:213:LYS:HE3	2.49	0.42
1:A:19:LYS:NZ	3:A:500:GNP:O3G	2.51	0.42
1:A:245:LYS:O	1:A:249:ILE:HG13	2.19	0.42
1:A:251:LYS:HD2	1:A:255:GLN:HE22	1.85	0.42
2:D:188:PHE:CD1	2:D:191:ASN:HB3	2.54	0.42
2:B:215:TYR:HD2	2:B:228:TYR:CD1	2.38	0.42
2:B:297:ARG:CZ	2:B:297:ARG:HB2	2.50	0.42
1:C:22:MSE:HG2	1:C:171:LEU:HD21	2.02	0.42
1:C:52:LEU:HD11	1:C:216:ILE:HD12	2.01	0.42
1:C:125:LEU:CD2	1:C:140:PHE:HA	2.50	0.42
1:C:183:ILE:HG21	1:C:186:MSE:HE2	2.00	0.42
2:D:98:ASN:HD21	2:D:102:ASN:ND2	2.17	0.42
1:A:200:MSE:HE1	1:A:301:ASN:CB	2.49	0.42
2:B:17:VAL:O	2:B:18:ARG:C	2.63	0.42
2:B:319:LYS:HA	2:B:319:LYS:HD2	1.66	0.42
1:C:62:CYS:O	1:C:63:GLY:C	2.63	0.42
1:C:249:ILE:HD13	2:D:240:ASP:HB3	2.02	0.42
2:D:222:PRO:O	2:D:223:VAL:CB	2.68	0.42
2:D:272:VAL:HG11	2:D:307:LEU:HD11	2.01	0.42
2:B:107:ILE:HA	2:B:110:ALA:HB3	2.01	0.41
2:B:282:TYR:O	2:B:293:VAL:HA	2.19	0.41
2:D:119:ILE:HD12	2:D:119:ILE:H	1.84	0.41
1:A:50:ARG:NH1	1:A:53:GLY:O	2.51	0.41
2:B:97:ILE:HD13	2:B:144:ARG:HH12	1.85	0.41
2:B:204:LYS:HE2	2:B:204:LYS:HB2	1.71	0.41
2:B:207:LEU:CD2	2:B:290:LEU:HB3	2.51	0.41
2:B:319:LYS:C	2:B:321:LEU:H	2.28	0.41
2:D:15:MSE:O	2:D:89:VAL:HG12	2.20	0.41
2:D:100:ILE:HG12	2:D:144:ARG:CB	2.50	0.41
1:A:192:ASN:N	1:A:192:ASN:ND2	2.67	0.41
2:B:180:GLN:HA	2:B:183:ILE:HD12	2.02	0.41
1:C:45:GLU:O	1:C:45:GLU:HG2	2.20	0.41
2:D:100:ILE:HG12	2:D:144:ARG:HB2	2.03	0.41
2:D:209:ASP:OD1	2:D:213:LYS:NZ	2.43	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:A:25:ILE:CD1	1:A:166:ILE:HG13	2.50	0.41
1:A:166:ILE:HD12	1:A:166:ILE:HA	1.47	0.41
2:B:209:ASP:HB3	2:B:212:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:VAL:HG22	2:D:18:ARG:N	2.28	0.41
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.87	0.41
1:C:112:LEU:HB3	1:C:156:PHE:CZ	2.55	0.41
2:D:25:ILE:HD11	2:D:124:HIS:CG	2.55	0.41
2:D:125:LYS:HG3	3:D:500:GNP:C2	2.51	0.41
2:B:103:LEU:HD13	2:B:103:LEU:C	2.46	0.41
1:A:262:SER:HB3	2:B:275:LEU:HB3	2.03	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:C:304:LYS:HE3	1:C:304:LYS:O	2.21	0.41
2:D:14:LEU:C	2:D:14:LEU:HD23	2.46	0.41
1:A:18:GLY:HA2	3:A:500:GNP:O1A	2.19	0.41
2:D:122:LEU:C	2:D:124:HIS:N	2.79	0.41
1:A:125:LEU:HB3	1:A:128:MSE:HE1	2.03	0.41
1:A:206:ILE:HD12	1:A:206:ILE:N	2.35	0.41
1:A:305:ALA:HA	1:A:309:PHE:HD1	1.85	0.41
1:A:308:PHE:HB2	1:A:309:PHE:H	1.65	0.41
2:B:103:LEU:O	2:B:104:ALA:C	2.63	0.41
2:B:125:LYS:HG2	3:B:500:GNP:N1	2.35	0.41
2:B:165:SER:C	2:B:167:PHE:N	2.78	0.41
2:B:169:HIS:HB2	2:B:229:GLU:OE2	2.21	0.41
2:B:286:MSE:HE2	2:B:292:LEU:CB	2.43	0.41
1:C:24:SER:HB3	1:C:30:TYR:HB2	2.03	0.41
1:C:177:GLN:HE21	1:C:177:GLN:HB3	1.66	0.41
2:D:24:SER:O	2:D:166:ILE:HD11	2.21	0.41
1:A:305:ALA:CA	1:A:309:PHE:HD1	2.34	0.41
2:D:189:LEU:O	2:D:193:LEU:HD21	2.21	0.41
2:B:36:LEU:C	2:B:38:THR:H	2.28	0.40
2:B:127:ASP:O	2:B:129:LEU:N	2.53	0.40
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
1:A:141:GLN:O	1:A:141:GLN:NE2	2.54	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:A:128:MSE:HE3	1:A:128:MSE:HB2	1.80	0.40
1:A:131:VAL:HG22	1:A:136:ARG:HG3	2.02	0.40
2:B:283:LEU:HD12	2:B:283:LEU:C	2.46	0.40
2:D:101:THR:O	2:D:105:MSE:HB2	2.21	0.40
2:D:103:LEU:O	2:D:104:ALA:C	2.64	0.40
1:A:11:LEU:HD11	1:A:22:MSE:CE	2.51	0.40
2:B:13:LEU:HD13	2:B:15:MSE:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:HIS:HE2	3:B:500:GNP:C5	2.33	0.40
2:B:287:ILE:H	2:B:287:ILE:HG12	1.63	0.40
2:B:302:ASP:OD1	2:B:302:ASP:C	2.64	0.40
1:C:52:LEU:HB3	1:C:53:GLY:H	1.71	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:B:283:LEU:C	2:B:283:LEU:CD1	2.94	0.40
2:D:215:TYR:O	2:D:216:VAL:HB	2.22	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%)	5	17
1	C	286/307 (93%)	245 (86%)	35 (12%)	6 (2%)	5	17
2	B	290/331 (88%)	225 (78%)	38 (13%)	27 (9%)	0	1
2	D	219/331 (66%)	170 (78%)	37 (17%)	12 (6%)	1	4
All	All	1080/1276 (85%)	887 (82%)	142 (13%)	51 (5%)	2	5

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	206 (76%)	64 (24%)	1	2
1	C	271/274 (99%)	218 (80%)	53 (20%)	1	4
2	B	269/292 (92%)	212 (79%)	57 (21%)	1	3
2	D	208/292 (71%)	171 (82%)	37 (18%)	2	5
All	All	1018/1132 (90%)	807 (79%)	211 (21%)	1	3

All (211) 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	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	82	GLN
1	A	87	LEU

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Mol	Chain	Res	Type
1	A	90	VAL
1	A	96	THR
1	A	97	GLU
1	A	100	LYS
1	A	104	ILE
1	A	109	LEU
1	A	110	LYS
1	A	112	LEU
1	A	113	ARG
1	A	116	SER
1	A	128	MSE
1	A	131	VAL
1	A	132	GLN
1	A	134	ASP
1	A	143	MSE
1	A	146	ASN
1	A	148	SER
1	A	158	ASN
1	A	164	THR
1	A	166	ILE
1	A	169	GLU
1	A	171	LEU
1	A	177	GLN
1	A	178	ILE
1	A	192	ASN
1	A	195	LYS
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	267	LEU
1	A	273	ILE
1	A	278	LEU
1	A	287	VAL
1	A	288	LEU

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Mol	Chain	Res	Type
1	A	295	GLN
1	A	303	LYS
1	A	306	LYS
2	B	12	VAL
2	B	13	LEU
2	B	14	LEU
2	B	42	GLU
2	B	44	THR
2	B	51	HIS
2	B	54	THR
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
2	B	117	ILE
2	B	120	GLU
2	B	121	VAL
2	B	133	PHE
2	B	141	ILE
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	193	LEU
2	B	195	ASN
2	B	202	ILE
2	B	204	LYS
2	B	207	LEU

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Mol	Chain	Res	Type
2	B	213	LYS
2	B	214	ILE
2	B	219	ASP
2	B	225	ILE
2	B	229	GLU
2	B	230	VAL
2	B	238	THR
2	B	244	LEU
2	B	268	GLU
2	B	283	LEU
2	B	287	ILE
2	B	292	LEU
2	B	301	THR
2	B	303	MSE
2	B	307	LEU
2	B	319	LYS
2	B	321	LEU
2	B	324	ILE
1	C	9	LEU
1	C	11	LEU
1	C	14	ARG
1	C	17	SER
1	C	26	ILE
1	C	36	ARG
1	C	38	LEU
1	C	45	GLU
1	C	49	LEU
1	C	50	ARG
1	C	59	LEU
1	C	67	VAL
1	C	69	MSE
1	C	70	GLU
1	C	82	GLN
1	C	87	LEU
1	C	90	VAL
1	C	94	GLU
1	C	96	THR
1	C	97	GLU
1	C	98	VAL
1	C	99	LEU
1	C	100	LYS
1	C	104	ILE

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Mol	Chain	Res	Type
1	C	112	LEU
1	C	123	VAL
1	C	128	MSE
1	C	132	GLN
1	C	136	ARG
1	C	153	GLU
1	C	166	ILE
1	C	169	GLU
1	C	182	LEU
1	C	190	GLN
1	C	195	LYS
1	C	206	ILE
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	258	THR
1	C	267	LEU
1	C	268	ILE
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	86	LEU
2	D	98	ASN
2	D	103	LEU
2	D	108	GLU
2	D	109	TYR
2	D	111	TYR
2	D	120	GLU
2	D	121	VAL
2	D	139	ARG
2	D	149	LEU
2	D	166	ILE

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Mol	Chain	Res	Type
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	198	GLN
2	D	201	LYS
2	D	204	LYS
2	D	207	LEU
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
2	D	324	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	58	ASN
1	A	65	GLN
1	A	89	HIS
1	A	132	GLN
1	A	141	GLN
1	A	192	ASN
1	A	220	ASN
1	A	248	ASN
1	A	255	GLN
1	A	272	ASN
1	A	281	ASN
2	B	32	ASN
2	B	98	ASN

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Mol	Chain	Res	Type
2	B	158	GLN
2	B	191	ASN
2	B	195	ASN
2	B	198	GLN
2	B	199	HIS
2	B	274	GLN
2	B	285	GLN
2	B	313	ASN
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	114	ASN
2	D	138	GLN
2	D	169	HIS
2	D	180	GLN
2	D	221	ASN
2	D	274	GLN
2	D	277	ASN
2	D	313	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	500	4	34,34,34	1.52	5 (14%)	47,54,54	1.15	5 (10%)
3	GNP	A	500	4	34,34,34	1.35	6 (17%)	47,54,54	1.42	5 (10%)
3	GNP	D	500	4	34,34,34	1.61	5 (14%)	47,54,54	1.12	3 (6%)
3	GNP	C	500	4	34,34,34	1.37	6 (17%)	47,54,54	1.13	6 (12%)

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	B	500	4	-	3/18/38/38	0/3/3/3
3	GNP	A	500	4	-	9/18/38/38	0/3/3/3
3	GNP	D	500	4	-	6/18/38/38	0/3/3/3
3	GNP	C	500	4	-	5/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	GNP	PA-O3A	-5.49	1.53	1.59
3	B	500	GNP	PA-O3A	-4.58	1.54	1.59
3	D	500	GNP	PB-O3A	-4.11	1.54	1.59
3	C	500	GNP	PA-O3A	-3.92	1.55	1.59
3	B	500	GNP	PG-O1G	3.88	1.52	1.46
3	D	500	GNP	PG-O1G	3.71	1.51	1.46
3	A	500	GNP	PG-O1G	3.70	1.51	1.46
3	B	500	GNP	PB-O3A	-3.50	1.54	1.59
3	A	500	GNP	PA-O3A	-3.41	1.55	1.59
3	C	500	GNP	PG-O1G	3.18	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	GNP	PB-O2B	-3.00	1.48	1.56
3	B	500	GNP	PB-O2B	-2.99	1.48	1.56
3	D	500	GNP	PB-O2B	-2.85	1.49	1.56
3	C	500	GNP	PB-O3A	-2.76	1.55	1.59
3	A	500	GNP	PB-O2B	-2.51	1.50	1.56
3	A	500	GNP	PG-O2G	-2.43	1.50	1.56
3	A	500	GNP	PB-O3A	-2.25	1.56	1.59
3	C	500	GNP	PG-O3G	-2.16	1.51	1.56
3	A	500	GNP	PG-O3G	-2.14	1.51	1.56
3	C	500	GNP	PG-O2G	-2.07	1.51	1.56
3	D	500	GNP	PG-O3G	-2.02	1.51	1.56
3	B	500	GNP	PG-O2G	-2.02	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	GNP	O1G-PG-N3B	-5.21	104.10	111.77
3	D	500	GNP	O2B-PB-O1B	3.96	118.36	109.87
3	B	500	GNP	O2B-PB-O1B	3.93	118.29	109.87
3	D	500	GNP	O3G-PG-O1G	-3.67	104.25	113.45
3	A	500	GNP	O3A-PB-N3B	3.66	116.73	106.59
3	B	500	GNP	O3G-PG-O1G	-3.42	104.87	113.45
3	C	500	GNP	O2G-PG-O3G	3.28	116.42	107.59
3	A	500	GNP	O3'-C3'-C4'	-3.15	102.04	111.08
3	D	500	GNP	O2G-PG-O3G	3.08	115.87	107.59
3	A	500	GNP	O2B-PB-O1B	3.02	116.34	109.87
3	B	500	GNP	O2G-PG-O3G	2.88	115.32	107.59
3	C	500	GNP	O5'-PA-O1A	-2.82	97.76	108.94
3	A	500	GNP	O1B-PB-N3B	-2.73	107.75	111.77
3	C	500	GNP	O3G-PG-O1G	-2.54	107.08	113.45
3	B	500	GNP	O1B-PB-N3B	-2.49	108.10	111.77
3	C	500	GNP	O1G-PG-N3B	-2.47	108.14	111.77
3	C	500	GNP	O2B-PB-O1B	2.24	114.66	109.87
3	C	500	GNP	C2'-C1'-N9	2.23	119.46	113.25
3	B	500	GNP	O1G-PG-N3B	-2.16	108.59	111.77

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	GNP	PB-N3B-PG-O1G
3	A	500	GNP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	A	500	GNP	PG-N3B-PB-O3A
3	A	500	GNP	C5'-O5'-PA-O3A
3	A	500	GNP	C5'-O5'-PA-O1A
3	B	500	GNP	PG-N3B-PB-O1B
3	B	500	GNP	PA-O3A-PB-O2B
3	C	500	GNP	PB-N3B-PG-O1G
3	C	500	GNP	PG-N3B-PB-O1B
3	C	500	GNP	PG-N3B-PB-O3A
3	D	500	GNP	PB-N3B-PG-O1G
3	D	500	GNP	PG-N3B-PB-O1B
3	D	500	GNP	PG-N3B-PB-O3A
3	D	500	GNP	O4'-C4'-C5'-O5'
3	D	500	GNP	C3'-C4'-C5'-O5'
3	A	500	GNP	O4'-C4'-C5'-O5'
3	A	500	GNP	C3'-C4'-C5'-O5'
3	B	500	GNP	PG-N3B-PB-O3A
3	D	500	GNP	C5'-O5'-PA-O3A
3	C	500	GNP	PA-O3A-PB-O2B
3	A	500	GNP	PB-O3A-PA-O1A
3	A	500	GNP	PA-O3A-PB-O1B
3	C	500	GNP	PA-O3A-PB-O1B

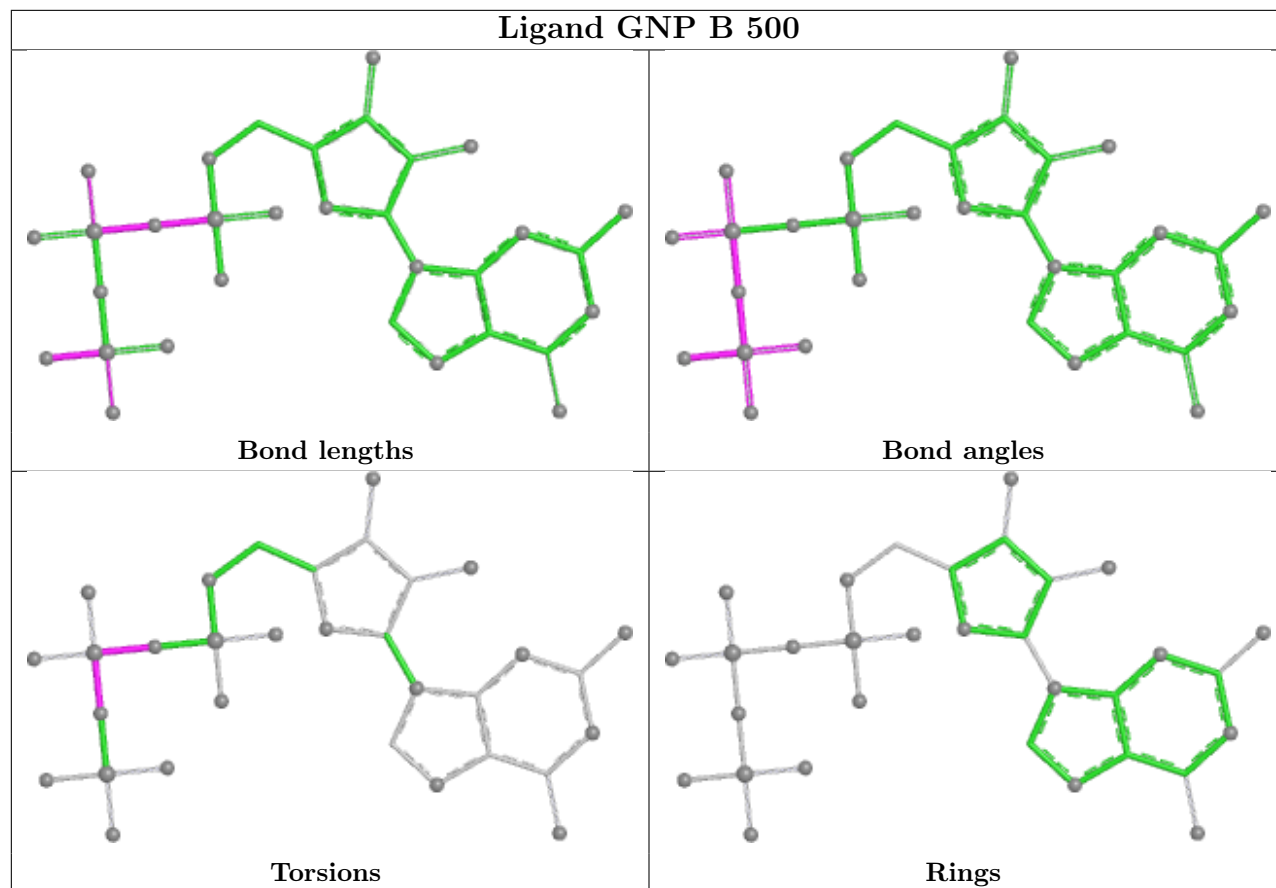
There are no ring outliers.

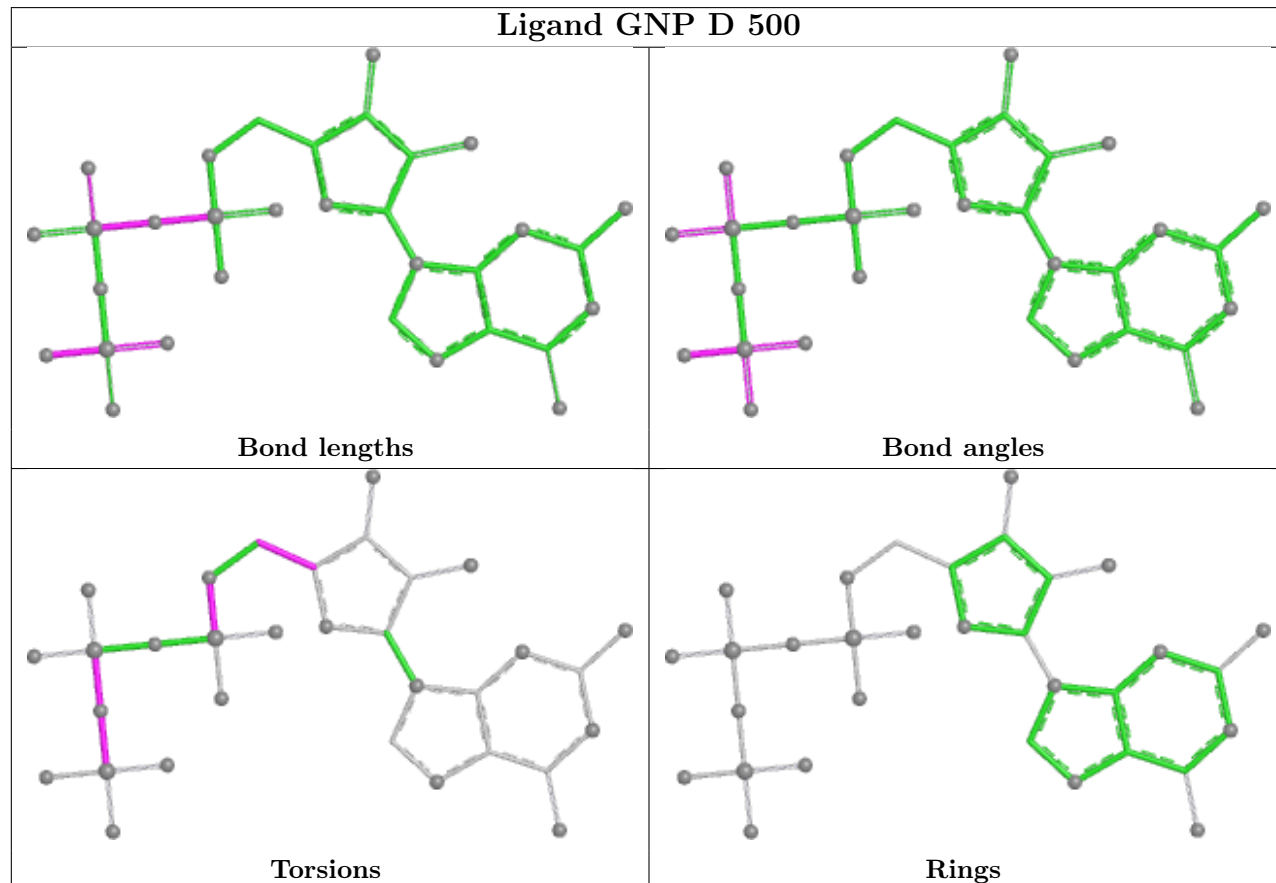
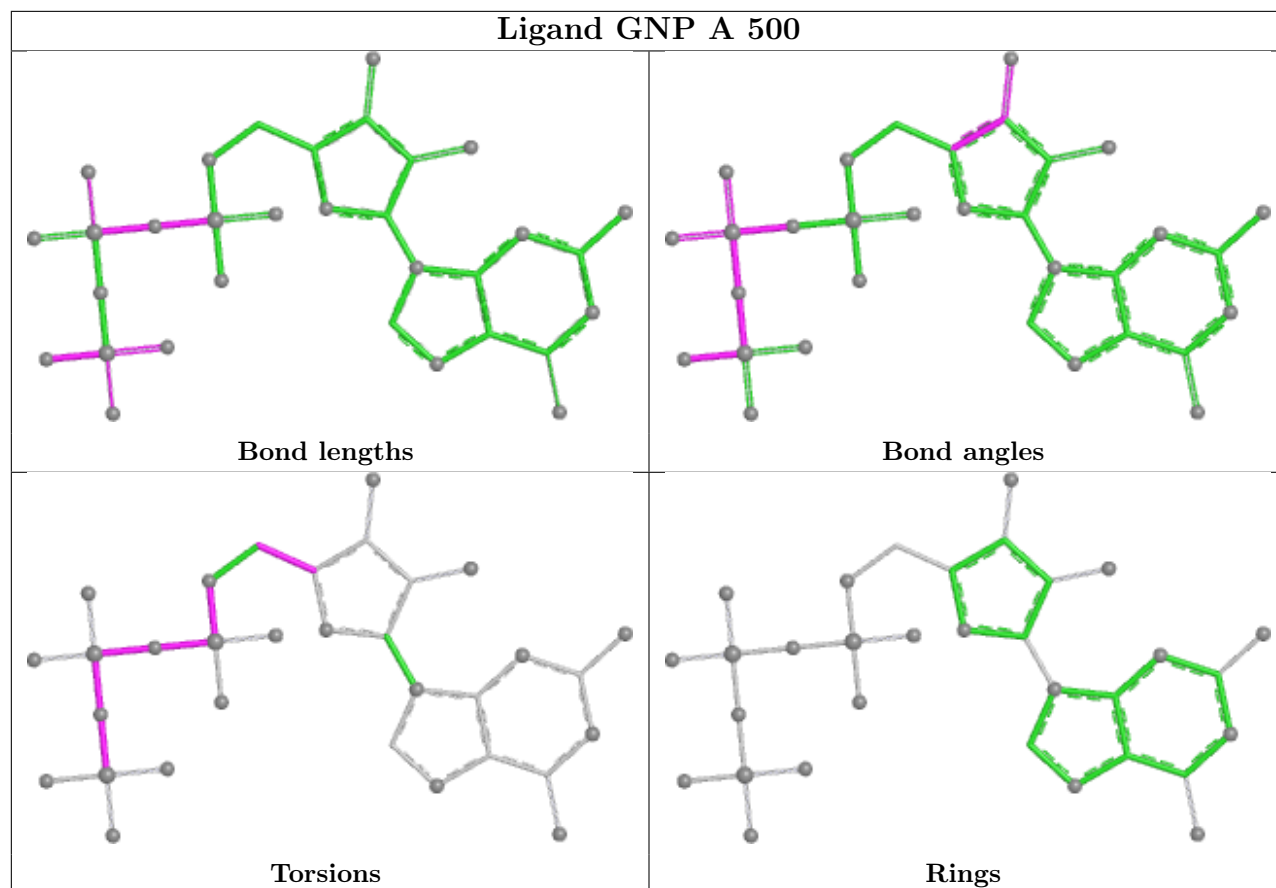
4 monomers are involved in 19 short contacts:

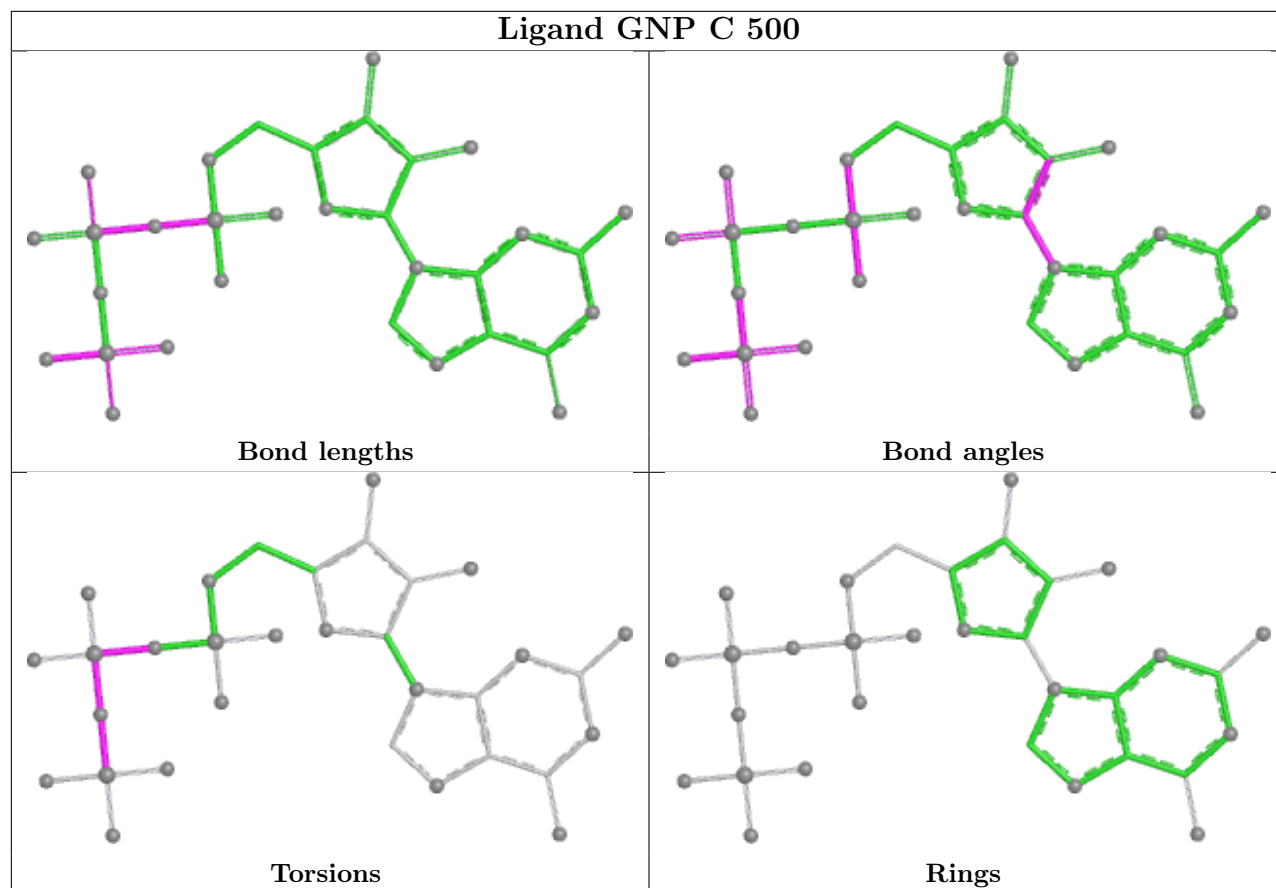
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	GNP	7	0
3	A	500	GNP	2	0
3	D	500	GNP	5	0
3	C	500	GNP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/307 (89%)	0.56	13 (4%) 36 31	56, 72, 112, 132	0
1	C	277/307 (90%)	0.51	13 (4%) 36 31	55, 71, 98, 122	0
2	B	284/331 (85%)	1.12	47 (16%) 4 3	65, 120, 156, 164	0
2	D	221/331 (66%)	1.39	61 (27%) 1 1	62, 120, 181, 188	0
All	All	1058/1276 (82%)	0.87	134 (12%) 8 6	55, 85, 160, 188	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	152	LEU	5.7
2	D	174	ALA	5.6
2	D	175	PHE	5.2
2	D	216	VAL	5.0
2	D	123	ILE	4.8
2	D	268	GLU	4.5
2	D	14	LEU	4.4
2	D	125	LYS	4.4
2	D	321	LEU	4.3
2	D	110	ALA	4.1
2	D	13	LEU	4.0
2	B	247	ALA	3.9
2	B	67	LEU	3.9
2	D	30	PHE	3.8
2	B	152	LEU	3.8
2	B	36	LEU	3.7
2	B	166	ILE	3.7
2	D	97	ILE	3.7
2	D	87	VAL	3.6
1	C	42	ILE	3.6
2	B	14	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	70	PHE	3.5
2	D	85	ALA	3.5
2	D	165	SER	3.4
2	B	171	ILE	3.3
2	B	196	LEU	3.3
1	C	125	LEU	3.3
1	A	17	SER	3.3
2	D	86	LEU	3.2
2	D	113	VAL	3.2
2	B	107	ILE	3.2
1	A	302	ILE	3.2
2	B	216	VAL	3.1
2	D	25	ILE	3.1
2	B	287	ILE	3.1
2	D	91	ASP	3.0
2	B	87	VAL	3.0
1	C	54	ASN	3.0
2	D	324	ILE	3.0
2	B	46	ASN	2.9
2	D	112	LYS	2.9
2	B	86	LEU	2.9
2	D	115	PRO	2.8
1	C	166	ILE	2.8
2	B	79	LEU	2.8
2	B	175	PHE	2.8
2	B	109	TYR	2.8
2	D	169	HIS	2.8
2	D	108	GLU	2.8
2	D	196	LEU	2.8
2	B	54	THR	2.8
2	B	242	PHE	2.8
2	B	97	ILE	2.7
2	B	179	VAL	2.7
2	D	117	ILE	2.7
2	B	137	ALA	2.7
2	D	157	VAL	2.7
2	B	123	ILE	2.7
2	B	183	ILE	2.7
2	B	207	LEU	2.7
2	B	134	LYS	2.7
2	D	314	ILE	2.7
2	B	76	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	228	TYR	2.6
2	D	189	LEU	2.6
2	D	185	GLU	2.6
1	C	203	LEU	2.6
1	C	280	SER	2.6
2	D	225	ILE	2.6
2	B	103	LEU	2.6
2	D	144	ARG	2.6
2	D	245	TYR	2.6
2	B	195	ASN	2.6
2	B	272	VAL	2.5
1	C	196	PHE	2.5
1	C	50	ARG	2.5
2	D	168	ASP	2.5
1	A	104	ILE	2.5
1	A	297	LEU	2.5
1	C	4	PRO	2.5
1	C	293	ILE	2.4
2	D	26	CYS	2.4
2	D	109	TYR	2.4
2	D	114	ASN	2.4
2	B	172	TYR	2.4
2	D	133	PHE	2.4
1	A	121	ILE	2.4
2	B	44	THR	2.4
2	D	307	LEU	2.4
2	B	96	TYR	2.4
1	A	207	LEU	2.4
2	B	244	LEU	2.3
2	B	280	ILE	2.3
2	D	222	PRO	2.3
2	B	126	VAL	2.3
2	D	317	PHE	2.3
2	B	138	GLN	2.3
2	D	172	TYR	2.3
2	D	23	SER	2.3
2	D	270	GLN	2.3
1	A	38	LEU	2.3
2	B	52	PHE	2.3
2	D	197	ILE	2.2
1	A	125	LEU	2.2
1	A	238	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	31	HIS	2.2
2	B	268	GLU	2.2
2	B	228	TYR	2.2
2	B	129	LEU	2.2
2	D	122	LEU	2.2
2	D	269	LEU	2.2
2	B	214	ILE	2.2
2	D	106	ILE	2.2
2	B	92	SER	2.2
2	D	178	ILE	2.2
1	A	308	PHE	2.2
2	B	282	TYR	2.1
1	C	10	LEU	2.1
2	B	154	LEU	2.1
2	D	99	ALA	2.1
2	D	88	TYR	2.1
2	D	29	VAL	2.1
1	A	196	PHE	2.1
2	D	292	LEU	2.1
1	A	64	GLY	2.1
1	C	90	VAL	2.1
2	D	280	ILE	2.1
2	D	167	PHE	2.1
2	D	188	PHE	2.1
1	A	10	LEU	2.1
2	D	275	LEU	2.1
2	D	202	ILE	2.0
2	B	102	ASN	2.0
1	C	72	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

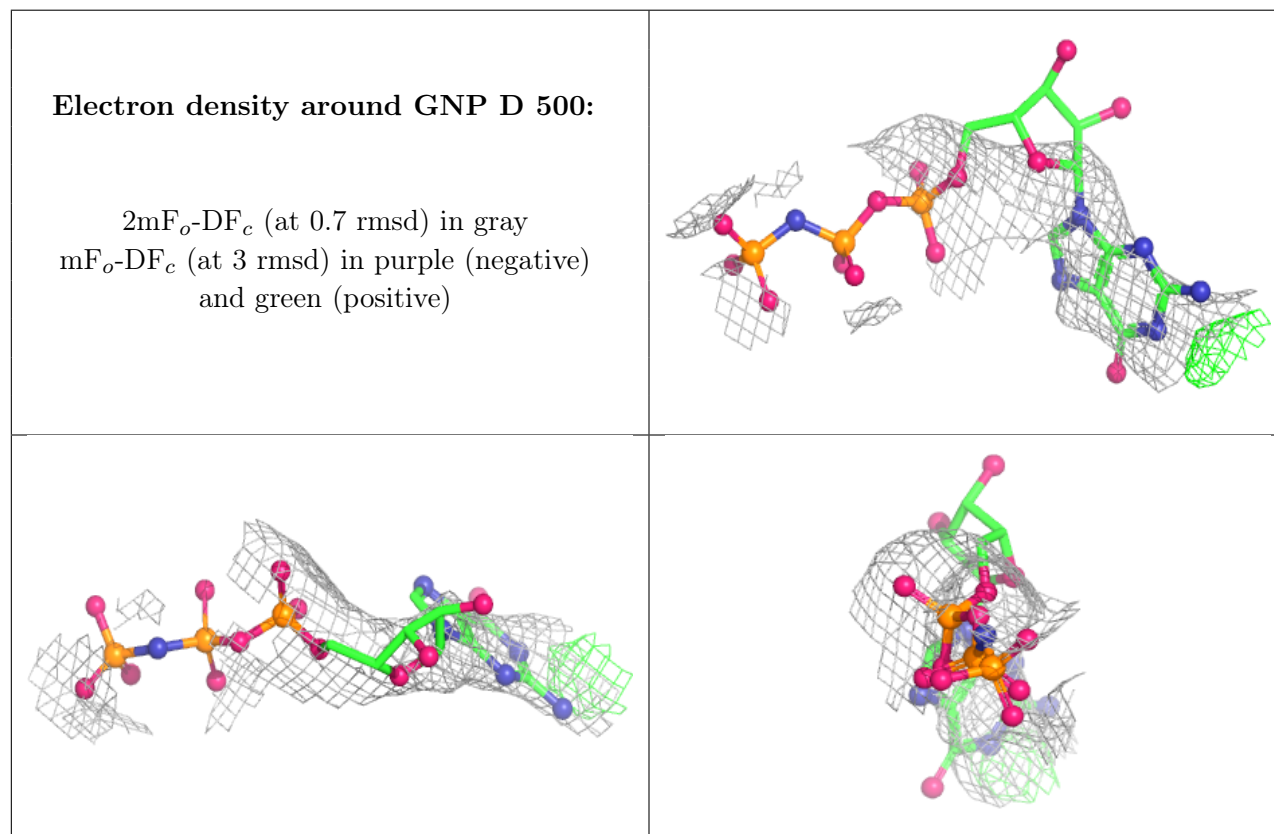
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

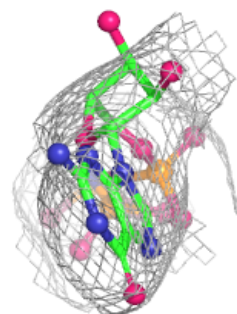
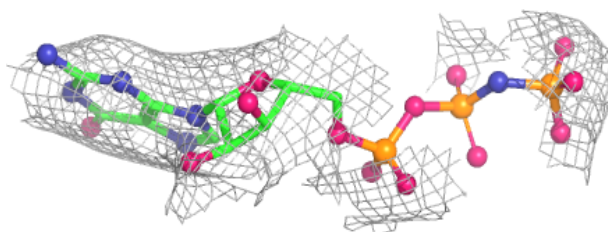
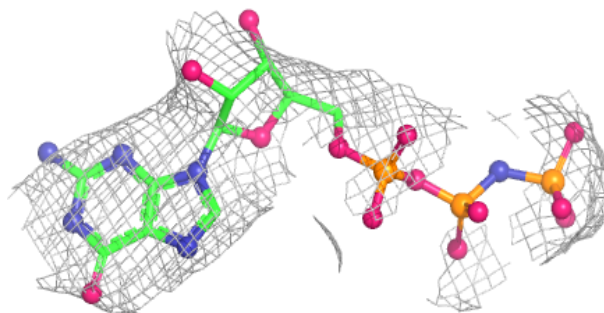
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	600	1/1	0.09	0.18	198,198,198,198	0
3	GNP	D	500	32/32	0.65	0.12	165,189,200,203	0
4	MG	B	600	1/1	0.81	0.09	154,154,154,154	0
3	GNP	B	500	32/32	0.91	0.08	125,142,154,156	0
3	GNP	A	500	32/32	0.95	0.08	59,68,73,74	0
3	GNP	C	500	32/32	0.97	0.08	58,66,74,76	0
4	MG	C	600	1/1	0.99	0.05	63,63,63,63	0
4	MG	A	600	1/1	0.99	0.08	62,62,62,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

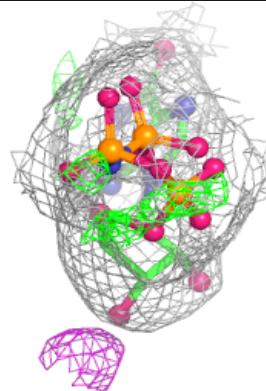
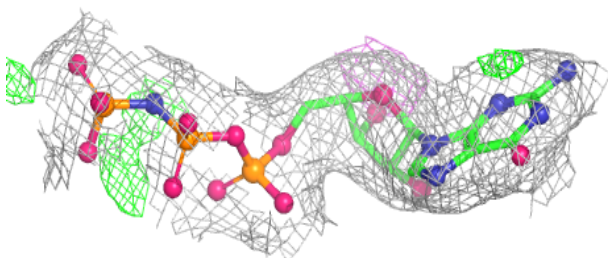
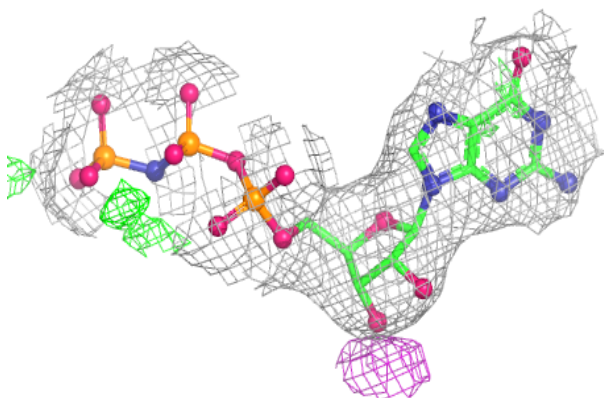


Electron density around GNP B 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

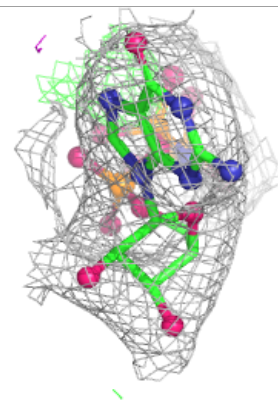
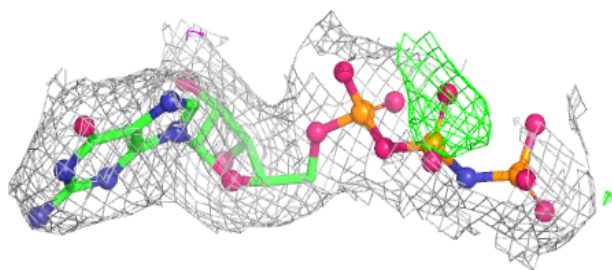
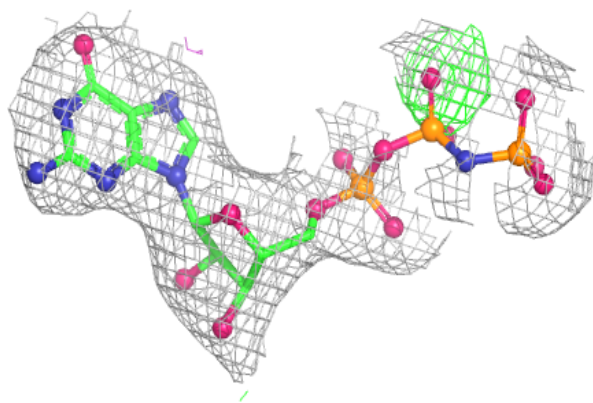
**Electron density around GNP A 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GNP C 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.