



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:49 am BST

PDB ID : 1U0L
Title : Crystal structure of YjeQ from *Thermotoga maritima*
Authors : Shin, D.H.; Lou, Y.; Jaru, J.; Kim, R.; Yokota, H.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2004-07-13
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

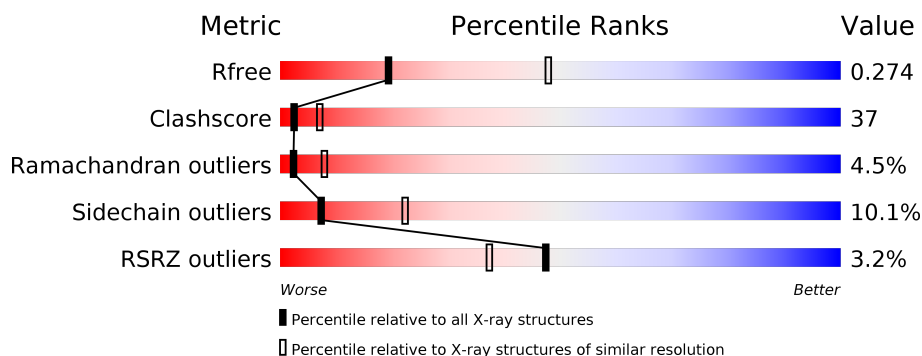
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 ≥ 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	301	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>43%</div> <div>8%</div> <div>8%</div> </div> </div>
1	B	301	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>39%</div> <div>5%</div> <div>8%</div> </div> </div>
1	C	301	<div> <div>3%</div> <div> <div></div> <div>43%</div> <div>39%</div> <div>9%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6806 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 Probable GTPase engC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2221	1410	371	429	11			
1	B	278	Total	C	N	O	S	0	0	0
			2221	1410	371	429	11			
1	C	278	Total	C	N	O	S	0	0	0
			2221	1410	371	429	11			

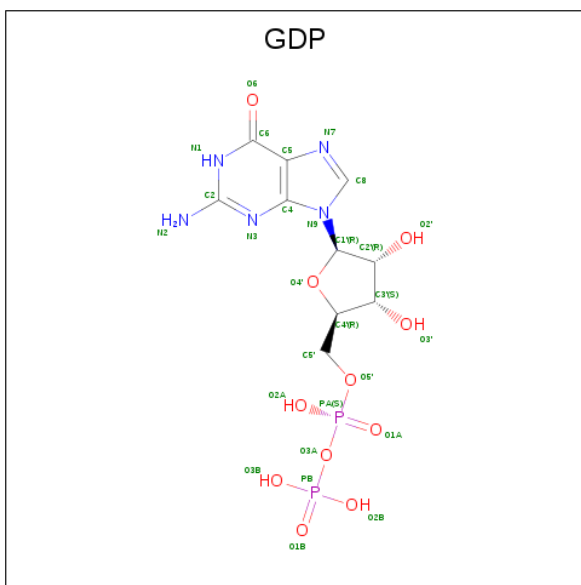
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP Q9X242
A	-4	GLY	-	CLONING ARTIFACT	UNP Q9X242
A	-3	GLY	-	CLONING ARTIFACT	UNP Q9X242
A	-2	GLY	-	CLONING ARTIFACT	UNP Q9X242
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9X242
A	0	GLY	-	CLONING ARTIFACT	UNP Q9X242
B	-5	GLY	-	CLONING ARTIFACT	UNP Q9X242
B	-4	GLY	-	CLONING ARTIFACT	UNP Q9X242
B	-3	GLY	-	CLONING ARTIFACT	UNP Q9X242
B	-2	GLY	-	CLONING ARTIFACT	UNP Q9X242
B	-1	GLY	-	CLONING ARTIFACT	UNP Q9X242
B	0	GLY	-	CLONING ARTIFACT	UNP Q9X242
C	-5	GLY	-	CLONING ARTIFACT	UNP Q9X242
C	-4	GLY	-	CLONING ARTIFACT	UNP Q9X242
C	-3	GLY	-	CLONING ARTIFACT	UNP Q9X242
C	-2	GLY	-	CLONING ARTIFACT	UNP Q9X242
C	-1	GLY	-	CLONING ARTIFACT	UNP Q9X242
C	0	GLY	-	CLONING ARTIFACT	UNP Q9X242

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

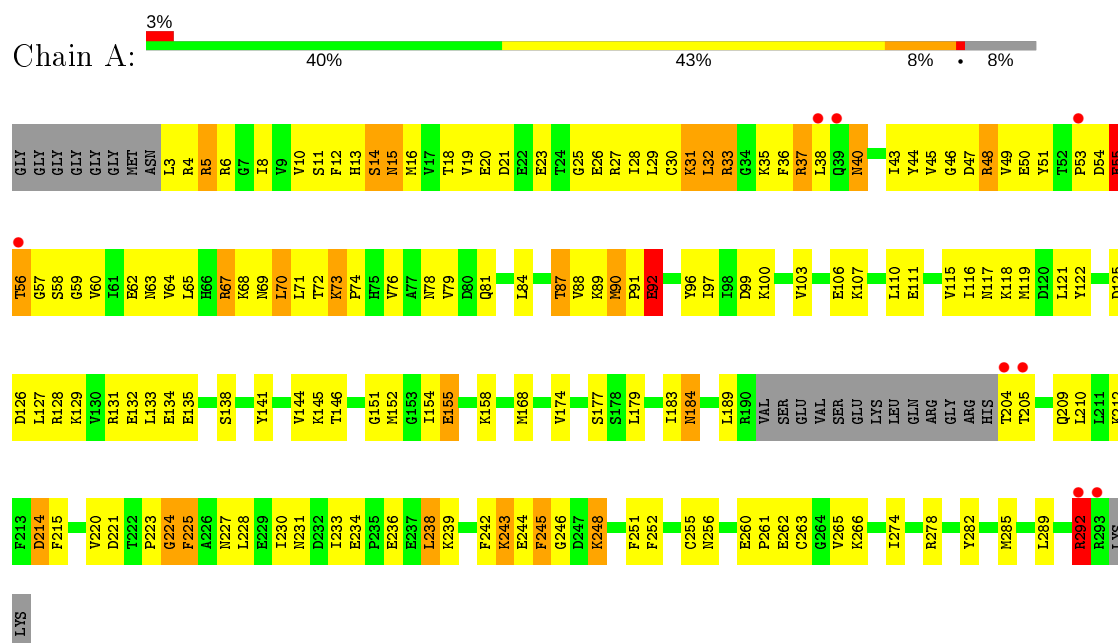
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	16	Total	O	0	0
			16	16		
4	C	18	Total	O	0	0
			18	18		

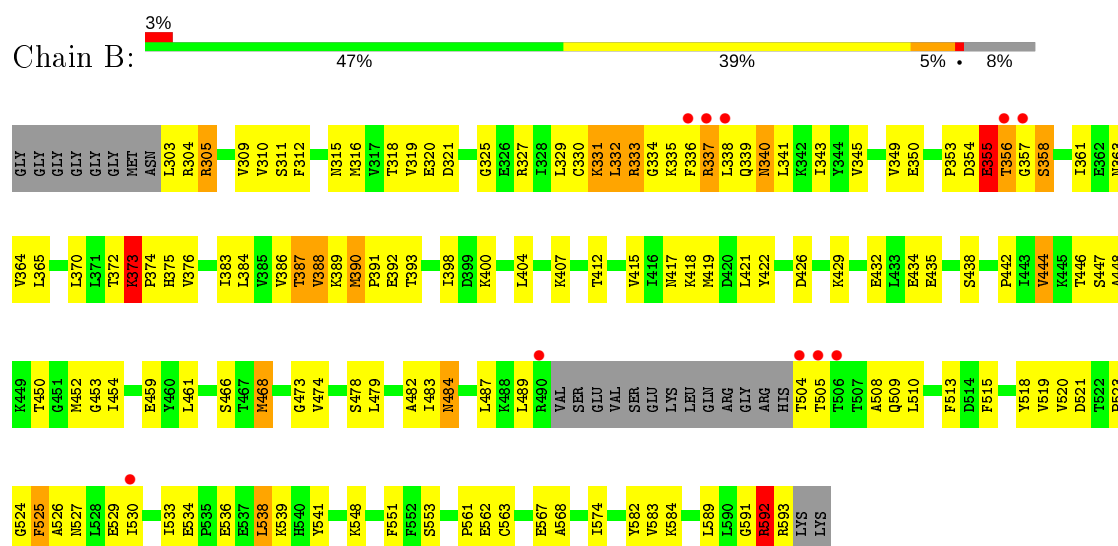
3 Residue-property plots

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

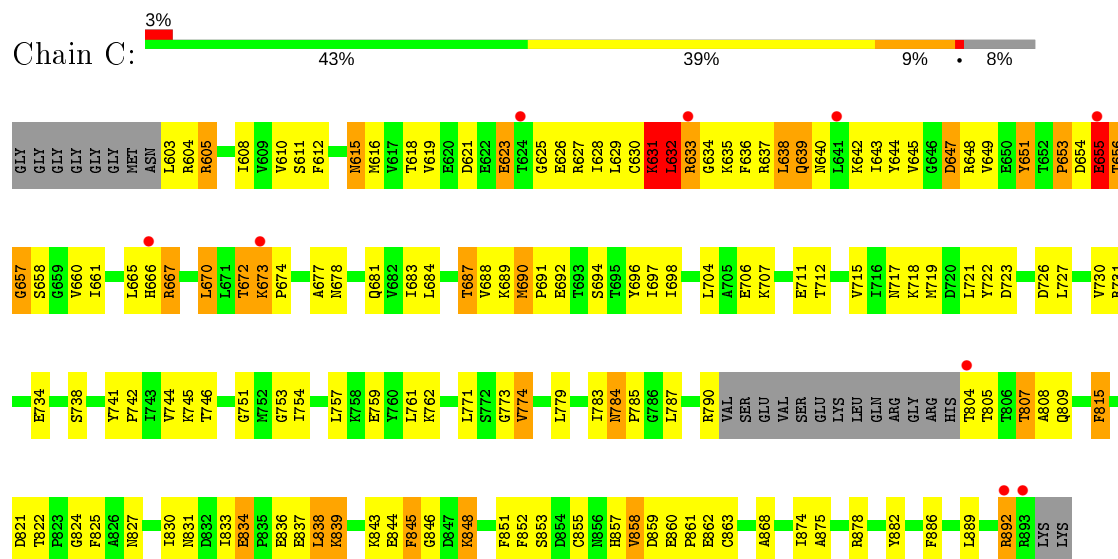
• Molecule 1: Probable GTPase engC



• Molecule 1: Probable GTPase engC



• Molecule 1: Probable GTPase engC



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.82Å 114.80Å 77.09Å 90.00° 105.72° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 45.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (20.00-2.80) 94.7 (45.40-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.284 0.210 , 0.274	Depositor DCC
R_{free} test set	3295 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.6	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	0.92	EDS
Total number of atoms	6806	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GDP, ZN

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	0.42	0/2255	0.71	0/3036
1	B	0.39	0/2255	0.68	1/3036 (0.0%)
1	C	0.36	0/2255	0.66	0/3036
All	All	0.39	0/6765	0.68	1/9108 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	LYS	C-N-CD	5.29	139.51	128.40

There are no chirality outliers.

There are no planarity outliers.

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	2221	0	2235	180	0
1	B	2221	0	2235	166	0
1	C	2221	0	2235	185	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	4	0
3	C	28	0	12	5	0
4	A	22	0	0	3	0
4	B	16	0	0	2	0
4	C	18	0	0	0	0
All	All	6806	0	6741	503	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 (503) 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:A:21:ASP:HB3	1:A:25:GLY:HA3	1.30	1.12
1:C:673:LYS:HB3	1:C:674:PRO:HD3	1.28	1.10
1:A:72:THR:HG23	1:A:73:LYS:H	1.15	1.06
1:B:373:LYS:HB3	1:B:374:PRO:HD3	1.34	1.04
1:A:209:GLN:H	1:A:221:ASP:HB2	1.17	1.03
1:C:673:LYS:HB3	1:C:674:PRO:CD	1.93	0.99
1:B:391:PRO:HG2	1:B:474:VAL:HA	1.45	0.97
1:B:329:LEU:O	1:B:358:SER:HB2	1.65	0.96
1:A:73:LYS:HB3	1:A:74:PRO:HD3	1.47	0.96
1:B:321:ASP:HB3	1:B:325:GLY:HA3	1.44	0.95
1:B:311:SER:HB2	1:B:509:GLN:HG2	1.49	0.94
1:A:263:CYS:H	1:C:615:ASN:HD21	1.05	0.93
1:A:90:MET:HB3	1:A:91:PRO:HD3	1.49	0.92
1:C:635:LYS:HA	1:C:638:LEU:HD23	1.51	0.92
1:B:373:LYS:HB3	1:B:374:PRO:CD	1.97	0.91
1:A:6:ARG:NH2	1:A:65:LEU:HD21	1.88	0.88
1:B:335:LYS:HA	1:B:338:LEU:HD23	1.56	0.88
1:A:209:GLN:N	1:A:221:ASP:HB2	1.91	0.85
1:B:305:ARG:HH11	1:B:305:ARG:HB3	1.39	0.85
1:C:746:THR:HG22	1:C:753:GLY:HA3	1.58	0.84
1:A:230:ILE:HG22	1:A:289:LEU:HD21	1.60	0.83
1:C:683:ILE:HD11	1:C:761:LEU:HD21	1.59	0.83
1:C:621:ASP:HB3	1:C:625:GLY:HA3	1.58	0.83
1:A:29:LEU:HD23	1:A:30:CYS:N	1.95	0.81
1:A:72:THR:HG23	1:A:73:LYS:N	1.93	0.81
1:C:605:ARG:HB3	1:C:605:ARG:HH11	1.46	0.81
1:A:87:THR:HB	1:A:174:VAL:HG23	1.63	0.80
1:C:616:MET:SD	1:C:629:LEU:HD21	2.21	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:ARG:HB3	1:C:667:ARG:NH1	1.96	0.80
1:B:461:LEU:HD22	1:B:513:PHE:HE1	1.46	0.80
1:B:387:THR:HG21	1:B:391:PRO:HD2	1.64	0.80
1:C:830:ILE:HG22	1:C:889:LEU:HD21	1.64	0.79
1:B:461:LEU:HD22	1:B:513:PHE:CE1	2.17	0.79
1:C:771:LEU:O	1:C:774:VAL:HB	1.83	0.79
1:A:292:ARG:HD3	1:A:292:ARG:O	1.82	0.79
1:B:318:THR:HG22	1:B:327:ARG:HG2	1.65	0.78
1:B:434:GLU:O	1:B:438:SER:HB2	1.84	0.78
1:A:21:ASP:HB3	1:A:25:GLY:CA	2.11	0.77
1:A:21:ASP:CB	1:A:25:GLY:HA3	2.14	0.76
1:A:263:CYS:H	1:C:615:ASN:ND2	1.82	0.76
1:C:610:VAL:HG21	1:C:627:ARG:NH1	2.00	0.76
1:C:691:PRO:HG2	1:C:774:VAL:HA	1.68	0.76
1:C:667:ARG:HB3	1:C:667:ARG:HH11	1.51	0.75
1:B:383:ILE:HD11	1:B:461:LEU:HD21	1.68	0.75
1:A:90:MET:HB3	1:A:91:PRO:CD	2.18	0.74
1:B:533:ILE:HD12	1:B:533:ILE:H	1.52	0.73
1:A:31:LYS:HA	1:A:31:LYS:HE3	1.70	0.73
1:C:621:ASP:HB3	1:C:625:GLY:CA	2.18	0.73
1:A:29:LEU:O	1:A:58:SER:HB2	1.88	0.72
1:B:391:PRO:HD3	1:B:418:LYS:HE3	1.71	0.72
1:C:809:GLN:HB2	1:C:821:ASP:HB2	1.72	0.72
1:A:73:LYS:HB3	1:A:74:PRO:CD	2.18	0.72
1:A:115:VAL:HG22	1:A:144:VAL:HG22	1.72	0.71
1:A:37:ARG:HG2	1:B:551:PHE:O	1.91	0.71
1:A:261:PRO:CG	1:C:643:ILE:HG22	2.22	0.70
1:A:10:VAL:HG21	1:A:27:ARG:HH11	1.56	0.70
1:C:603:LEU:HG	1:C:604:ARG:H	1.56	0.70
1:A:48:ARG:HB3	1:A:65:LEU:HD22	1.74	0.69
1:B:338:LEU:H	1:B:338:LEU:HD22	1.56	0.69
1:A:209:GLN:H	1:A:221:ASP:CB	2.01	0.69
1:C:629:LEU:O	1:C:658:SER:HB2	1.92	0.69
1:A:43:ILE:HG22	1:B:561:PRO:HG2	1.75	0.69
1:A:47:ASP:CG	1:A:67:ARG:HH12	1.96	0.69
1:C:683:ILE:CD1	1:C:761:LEU:HD21	2.22	0.68
1:B:312:PHE:CE1	1:B:345:VAL:HG23	2.28	0.68
1:C:719:MET:HA	1:C:722:TYR:CD2	2.29	0.68
1:A:100:LYS:HE2	1:A:230:ILE:HD12	1.76	0.68
1:A:261:PRO:HG2	1:C:643:ILE:HG22	1.76	0.68
1:B:489:LEU:HD13	1:B:523:PRO:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HB2	4:A:315:HOH:O	1.94	0.67
1:A:238:LEU:HD11	1:A:285:MET:HB3	1.76	0.67
1:A:292:ARG:NH2	1:B:593:ARG:HG3	2.09	0.67
1:C:681:GLN:HG2	1:C:711:GLU:HB2	1.76	0.67
1:C:790:ARG:HB2	1:C:822:THR:HG22	1.76	0.67
1:A:31:LYS:HE3	1:A:32:LEU:H	1.59	0.67
1:B:303:LEU:HG	1:B:304:ARG:H	1.59	0.67
1:B:318:THR:CG2	1:B:327:ARG:HG2	2.25	0.66
1:C:687:THR:HG21	1:C:691:PRO:HD2	1.77	0.66
1:C:688:VAL:HG22	1:C:722:TYR:CE1	2.30	0.66
1:B:335:LYS:O	1:B:339:GLN:CD	2.34	0.66
1:B:339:GLN:O	1:B:341:LEU:N	2.27	0.66
1:A:47:ASP:OD1	1:A:67:ARG:NH1	2.29	0.65
1:C:670:LEU:HD23	1:C:677:ALA:HB2	1.79	0.65
1:B:309:VAL:HG12	1:B:345:VAL:HA	1.78	0.65
1:B:568:ALA:CB	1:B:574:ILE:HD13	2.27	0.65
1:A:5:ARG:HB3	1:A:5:ARG:HH11	1.61	0.65
1:A:15:ASN:ND2	1:B:562:GLU:HA	2.12	0.65
1:B:337:ARG:NE	1:C:853:SER:HB2	2.11	0.65
1:C:683:ILE:HD11	1:C:761:LEU:CD2	2.27	0.65
1:A:35:LYS:HA	1:A:38:LEU:HD23	1.80	0.64
1:B:479:LEU:O	1:B:483:ILE:HG13	1.97	0.64
1:C:633:ARG:HB2	1:C:633:ARG:HH11	1.61	0.64
1:A:10:VAL:HG21	1:A:27:ARG:NH1	2.12	0.64
1:C:690:MET:CB	1:C:691:PRO:HD3	2.28	0.64
1:C:721:LEU:HD11	3:C:899:GDP:HN21	1.61	0.64
1:A:72:THR:O	1:A:73:LYS:C	2.33	0.63
1:B:530:ILE:O	1:B:530:ILE:HG22	1.98	0.63
1:C:721:LEU:HD11	3:C:899:GDP:N2	2.13	0.63
1:A:43:ILE:HG22	1:B:561:PRO:CG	2.27	0.63
1:A:158:LYS:HG2	1:A:215:PHE:CE2	2.33	0.63
1:B:446:THR:HG22	1:B:453:GLY:HA3	1.80	0.63
1:C:667:ARG:CB	1:C:667:ARG:HH11	2.11	0.63
1:A:134:GLU:O	1:A:138:SER:HB2	1.98	0.63
1:A:90:MET:CB	1:A:91:PRO:CD	2.77	0.63
1:B:333:ARG:HB2	1:B:333:ARG:HH11	1.64	0.62
1:B:400:LYS:HD3	1:B:530:ILE:HD13	1.81	0.62
1:C:629:LEU:C	1:C:629:LEU:HD23	2.20	0.62
1:B:533:ILE:HD12	1:B:533:ILE:N	2.15	0.62
1:B:504:THR:HG22	1:B:505:THR:H	1.64	0.62
1:C:696:TYR:HD2	1:C:697:ILE:HD12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:MET:CB	1:B:391:PRO:HD3	2.29	0.62
1:C:673:LYS:CB	1:C:674:PRO:HD3	2.18	0.62
1:A:33:ARG:HB2	1:A:33:ARG:HH11	1.65	0.61
1:B:387:THR:HG22	1:B:392:GLU:H	1.64	0.61
1:B:389:LYS:HD2	1:B:426:ASP:OD2	2.00	0.61
1:C:687:THR:HB	1:C:774:VAL:HG22	1.81	0.61
1:C:610:VAL:HG21	1:C:627:ARG:HH11	1.66	0.61
1:C:857:HIS:HA	1:C:863:CYS:SG	2.41	0.61
1:B:447:SER:HB3	1:B:450:THR:HB	1.82	0.61
1:C:631:LYS:HE3	1:C:631:LYS:C	2.21	0.61
1:B:316:MET:SD	1:B:329:LEU:HD21	2.41	0.61
1:B:524:GLY:O	1:B:526:ALA:N	2.30	0.61
1:C:626:GLU:O	1:C:628:ILE:HD12	2.01	0.61
1:A:184:ASN:HD21	1:A:214:ASP:HB2	1.65	0.60
1:B:331:LYS:HE2	1:B:332:LEU:HD12	1.83	0.60
1:B:373:LYS:O	1:B:375:HIS:N	2.34	0.60
1:B:404:LEU:HD13	1:B:525:PHE:HB3	1.82	0.60
1:C:612:PHE:HE1	1:C:645:VAL:HG23	1.66	0.60
1:C:612:PHE:CE1	1:C:645:VAL:HG23	2.37	0.59
1:A:54:ASP:OD1	1:A:59:GLY:HA2	2.02	0.59
1:B:332:LEU:HD12	1:B:332:LEU:O	2.01	0.59
1:C:779:LEU:O	1:C:783:ILE:HG13	2.02	0.59
1:C:651:TYR:HD2	1:C:651:TYR:H	1.49	0.59
1:A:33:ARG:HG2	1:A:60:VAL:CG1	2.33	0.59
1:B:412:THR:O	1:B:442:PRO:HD2	2.02	0.59
1:A:99:ASP:O	1:A:103:VAL:HG23	2.03	0.59
1:C:623:GLU:O	1:C:625:GLY:N	2.36	0.59
1:C:621:ASP:CB	1:C:625:GLY:HA3	2.31	0.59
1:A:117:ASN:ND2	1:A:118:LYS:H	2.00	0.58
1:B:330:CYS:HB3	1:B:361:ILE:HG13	1.86	0.58
1:B:321:ASP:HB3	1:B:325:GLY:CA	2.27	0.58
1:C:631:LYS:CE	1:C:632:LEU:HD12	2.34	0.58
1:C:809:GLN:H	1:C:821:ASP:HB3	1.68	0.58
1:A:263:CYS:SG	1:A:265:VAL:HB	2.43	0.58
1:B:316:MET:HB3	1:B:329:LEU:HD21	1.85	0.58
1:A:121:LEU:HD13	3:A:299:GDP:N2	2.19	0.58
1:A:31:LYS:HA	1:A:31:LYS:CE	2.32	0.58
1:A:248:LYS:HE3	1:A:274:ILE:HD11	1.85	0.58
1:B:530:ILE:HG22	1:B:589:LEU:HD21	1.86	0.57
1:C:773:GLY:HA2	3:C:899:GDP:H5'	1.85	0.57
1:A:263:CYS:HB3	1:A:266:LYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:C	1:A:57:GLY:H	2.07	0.57
1:B:303:LEU:O	1:B:305:ARG:HG3	2.05	0.57
1:B:386:VAL:HG13	1:B:393:THR:HB	1.86	0.57
1:A:26:GLU:O	1:A:28:ILE:HD12	2.05	0.57
1:A:4:ARG:NH1	1:A:62:GLU:HG3	2.19	0.57
1:A:68:LYS:HG2	1:A:78:ASN:HA	1.87	0.57
1:C:631:LYS:HE3	1:C:632:LEU:HD12	1.87	0.57
1:C:672:THR:O	1:C:673:LYS:C	2.42	0.57
1:A:43:ILE:HD11	1:A:49:VAL:HG11	1.86	0.57
1:B:338:LEU:HD22	1:B:338:LEU:N	2.19	0.57
1:A:115:VAL:HG22	1:A:144:VAL:CG2	2.33	0.57
1:A:28:ILE:HD12	1:A:28:ILE:N	2.20	0.57
1:A:73:LYS:CB	1:A:74:PRO:HD3	2.29	0.56
1:A:87:THR:HG23	1:A:89:LYS:O	2.05	0.56
1:C:834:GLU:O	1:C:837:GLU:HB3	2.05	0.56
1:C:654:ASP:O	1:C:656:THR:N	2.38	0.56
1:A:18:THR:HG22	1:A:27:ARG:HG2	1.87	0.56
1:C:805:THR:C	1:C:807:THR:H	2.08	0.56
1:C:845:PHE:N	1:C:845:PHE:HD1	2.03	0.56
1:B:343:ILE:CG2	1:C:861:PRO:HG2	2.35	0.56
1:C:618:THR:CG2	1:C:627:ARG:HG2	2.35	0.56
1:B:332:LEU:HD13	1:C:851:PHE:CZ	2.41	0.56
1:C:696:TYR:CD2	1:C:697:ILE:HD12	2.40	0.56
1:B:444:VAL:HG23	1:B:446:THR:HG23	1.87	0.56
1:A:239:LYS:HE2	1:A:256:ASN:HA	1.87	0.55
1:A:37:ARG:HH21	1:B:553:SER:HB2	1.71	0.55
1:A:51:TYR:HB2	1:A:60:VAL:O	2.06	0.55
1:B:387:THR:CG2	1:B:392:GLU:H	2.19	0.55
1:B:568:ALA:HB1	1:B:574:ILE:HD13	1.87	0.55
1:C:690:MET:HB3	1:C:691:PRO:HD3	1.87	0.55
1:A:252:PHE:CE2	1:C:642:LYS:HD3	2.41	0.55
1:A:154:ILE:HD12	1:A:154:ILE:N	2.21	0.55
1:C:825:PHE:N	1:C:825:PHE:CD1	2.74	0.55
1:C:875:ALA:HB3	1:C:878:ARG:HG2	1.88	0.55
1:A:29:LEU:HD23	1:A:30:CYS:H	1.70	0.55
1:B:391:PRO:HG2	1:B:474:VAL:CA	2.30	0.55
1:C:875:ALA:HB3	1:C:878:ARG:CG	2.37	0.55
1:A:28:ILE:HD12	1:A:28:ILE:H	1.71	0.55
1:B:484:ASN:HB2	1:B:487:LEU:HD12	1.88	0.55
1:C:665:LEU:N	1:C:665:LEU:HD12	2.22	0.55
1:B:387:THR:HG21	1:B:391:PRO:CD	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:CB	1:A:29:LEU:HD21	2.37	0.54
1:A:245:PHE:N	1:A:245:PHE:CD1	2.73	0.54
1:C:762:LYS:HG2	1:C:815:PHE:CD1	2.42	0.54
1:C:831:ASN:C	1:C:833:ILE:H	2.10	0.54
1:A:49:VAL:HG12	1:A:64:VAL:HA	1.89	0.54
1:B:417:ASN:ND2	1:B:418:LYS:H	2.05	0.54
1:A:18:THR:CG2	1:A:27:ARG:HG2	2.38	0.54
1:A:16:MET:HB3	1:A:29:LEU:HD21	1.89	0.54
1:C:845:PHE:N	1:C:845:PHE:CD1	2.73	0.54
1:C:616:MET:HE2	1:C:631:LYS:HB2	1.88	0.54
1:C:647:ASP:CG	1:C:667:ARG:HH12	2.11	0.54
1:A:72:THR:CG2	1:A:73:LYS:H	2.01	0.54
1:B:568:ALA:HB3	1:B:574:ILE:HD13	1.90	0.54
1:A:292:ARG:HH21	1:B:593:ARG:HG3	1.71	0.54
1:C:651:TYR:CD2	1:C:651:TYR:N	2.74	0.54
1:A:71:LEU:HD12	1:A:79:VAL:HG21	1.89	0.54
1:B:504:THR:HG22	1:B:505:THR:N	2.22	0.54
1:C:628:ILE:HD12	1:C:628:ILE:N	2.23	0.54
1:C:616:MET:CE	1:C:629:LEU:HD21	2.38	0.54
1:C:673:LYS:HG2	1:C:827:ASN:ND2	2.22	0.54
1:C:721:LEU:CD1	3:C:899:GDP:HN21	2.22	0.53
1:B:339:GLN:C	1:B:341:LEU:H	2.12	0.53
1:B:536:GLU:CD	1:B:536:GLU:H	2.10	0.53
1:C:632:LEU:HA	1:C:661:ILE:HB	1.90	0.53
1:C:687:THR:HG21	1:C:691:PRO:CD	2.38	0.53
1:B:529:GLU:C	1:B:530:ILE:HD12	2.29	0.53
1:B:388:VAL:HG22	1:B:422:TYR:CE1	2.44	0.53
1:C:644:TYR:O	1:C:647:ASP:HB2	2.08	0.53
1:A:8:ILE:HD12	1:A:8:ILE:N	2.24	0.53
1:A:33:ARG:HG2	1:A:60:VAL:HG12	1.91	0.53
1:C:634:GLY:C	1:C:636:PHE:H	2.11	0.53
1:C:804:THR:HG22	1:C:805:THR:N	2.24	0.53
1:B:390:MET:CB	1:B:391:PRO:CD	2.87	0.53
1:A:32:LEU:HD13	1:B:551:PHE:CZ	2.44	0.53
1:A:87:THR:CB	1:A:174:VAL:HG23	2.36	0.53
1:C:629:LEU:HD23	1:C:630:CYS:N	2.24	0.53
1:A:131:ARG:O	1:A:135:GLU:HB2	2.09	0.52
1:C:655:GLU:C	1:C:657:GLY:H	2.12	0.52
1:C:846:GLY:C	1:C:848:LYS:H	2.11	0.52
1:B:305:ARG:HD2	1:B:353:PRO:HG2	1.90	0.52
1:A:11:SER:CB	1:A:209:GLN:HG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:VAL:HG22	1:C:744:VAL:HG22	1.92	0.52
1:B:338:LEU:CD2	1:B:338:LEU:H	2.22	0.52
1:B:383:ILE:CD1	1:B:461:LEU:HD21	2.37	0.52
1:B:421:LEU:HD13	3:B:599:GDP:HN21	1.75	0.52
1:A:31:LYS:HE3	1:A:31:LYS:CA	2.38	0.51
1:C:704:LEU:HD21	1:C:830:ILE:HD13	1.92	0.51
1:C:690:MET:CB	1:C:691:PRO:CD	2.88	0.51
1:A:155:GLU:OE2	1:A:158:LYS:HD2	2.10	0.51
1:A:204:THR:HG22	1:A:205:THR:N	2.25	0.51
1:C:712:THR:O	1:C:742:PRO:HD2	2.09	0.51
1:A:245:PHE:HD1	1:A:245:PHE:N	2.08	0.51
1:A:31:LYS:HE3	1:A:32:LEU:N	2.26	0.51
1:B:329:LEU:HD23	1:B:330:CYS:N	2.25	0.51
1:B:407:LYS:HA	1:B:541:TYR:CE2	2.46	0.51
1:C:734:GLU:O	1:C:738:SER:HB2	2.10	0.51
1:B:390:MET:HB3	1:B:391:PRO:HD3	1.92	0.51
1:A:146:THR:HA	1:A:152:MET:O	2.11	0.51
1:A:89:LYS:O	1:A:90:MET:C	2.49	0.51
1:B:337:ARG:HE	1:C:853:SER:HB2	1.76	0.50
1:B:419:MET:HA	1:B:422:TYR:CD2	2.45	0.50
1:C:651:TYR:CE1	1:C:653:PRO:HG3	2.47	0.50
1:A:242:PHE:O	1:A:243:LYS:C	2.50	0.50
1:A:35:LYS:C	1:A:37:ARG:N	2.62	0.50
1:A:38:LEU:N	1:A:38:LEU:HD22	2.27	0.50
1:A:69:ASN:HB2	4:A:306:HOH:O	2.12	0.50
1:C:719:MET:CE	1:C:745:LYS:HD3	2.41	0.50
1:A:204:THR:HG22	1:A:205:THR:H	1.77	0.50
1:C:734:GLU:O	1:C:738:SER:CB	2.60	0.49
1:C:704:LEU:HG	1:C:830:ILE:HD11	1.94	0.49
1:A:236:GLU:CD	1:A:236:GLU:H	2.14	0.49
1:A:87:THR:CG2	1:A:89:LYS:O	2.60	0.49
1:B:432:GLU:O	1:B:435:GLU:HB3	2.12	0.49
1:B:331:LYS:NZ	1:C:862:GLU:OE1	2.35	0.49
1:C:605:ARG:CB	1:C:605:ARG:HH11	2.22	0.49
1:B:350:GLU:OE2	1:B:363:ASN:HB3	2.13	0.49
1:A:151:GLY:C	1:A:154:ILE:HD13	2.32	0.49
1:B:563:CYS:O	1:B:567:GLU:HB2	2.12	0.49
1:C:707:LYS:HD2	1:C:833:ILE:HD11	1.95	0.49
1:C:830:ILE:O	1:C:830:ILE:HG22	2.12	0.49
1:C:836:GLU:CD	1:C:836:GLU:H	2.15	0.49
1:A:262:GLU:OE1	1:C:631:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PHE:HZ	1:A:63:ASN:HA	1.77	0.49
1:B:311:SER:CB	1:B:509:GLN:HG2	2.32	0.49
1:A:15:ASN:HD21	1:B:562:GLU:HA	1.77	0.49
1:C:610:VAL:HG22	1:C:618:THR:O	2.11	0.49
1:B:536:GLU:O	1:B:539:LYS:HE3	2.13	0.49
1:C:633:ARG:HG2	1:C:660:VAL:CG1	2.42	0.49
1:A:11:SER:HB2	1:A:209:GLN:HG2	1.94	0.49
1:A:6:ARG:HH22	1:A:65:LEU:HD21	1.74	0.49
1:C:731:ARG:HA	1:C:734:GLU:OE1	2.12	0.49
1:B:330:CYS:CB	1:B:361:ILE:HG13	2.42	0.49
1:C:809:GLN:H	1:C:821:ASP:CB	2.25	0.49
1:A:231:ASN:C	1:A:233:ILE:H	2.16	0.49
1:B:312:PHE:CD1	1:B:345:VAL:HG23	2.47	0.49
1:A:38:LEU:H	1:A:38:LEU:HD22	1.78	0.48
1:A:96:TYR:HD2	1:A:97:ILE:HD12	1.78	0.48
1:A:261:PRO:HA	1:C:612:PHE:CD2	2.49	0.48
1:A:20:GLU:OE2	1:A:212:LYS:HE3	2.12	0.48
1:A:79:VAL:O	1:A:110:LEU:HD22	2.13	0.48
1:B:383:ILE:HB	1:B:468:MET:HE3	1.95	0.48
1:A:71:LEU:CD1	1:A:79:VAL:HG21	2.43	0.48
1:A:38:LEU:H	1:A:38:LEU:CD2	2.26	0.48
1:B:530:ILE:HD12	1:B:530:ILE:N	2.28	0.48
1:B:390:MET:HB2	1:B:391:PRO:HD3	1.94	0.48
1:A:35:LYS:HB3	1:A:38:LEU:HB2	1.95	0.48
1:C:636:PHE:O	1:C:639:GLN:O	2.32	0.48
1:A:26:GLU:N	1:A:26:GLU:OE2	2.47	0.48
1:A:179:LEU:O	1:A:183:ILE:HG13	2.14	0.47
1:B:305:ARG:CB	1:B:305:ARG:HH11	2.18	0.47
1:C:704:LEU:HB3	1:C:825:PHE:CE2	2.49	0.47
1:B:312:PHE:CE2	1:C:861:PRO:HG3	2.49	0.47
1:C:632:LEU:O	1:C:632:LEU:CD1	2.62	0.47
1:A:72:THR:CG2	1:A:73:LYS:N	2.66	0.47
1:C:608:ILE:HD11	1:C:648:ARG:CZ	2.44	0.47
1:C:868:ALA:HB3	1:C:874:ILE:HD12	1.96	0.47
1:B:504:THR:CG2	1:B:505:THR:H	2.26	0.47
1:A:223:PRO:O	1:A:224:GLY:O	2.33	0.47
1:A:230:ILE:O	1:A:230:ILE:HG22	2.14	0.47
1:A:70:LEU:HD22	1:A:71:LEU:O	2.15	0.47
1:B:374:PRO:O	1:B:376:VAL:HG23	2.14	0.47
1:B:393:THR:HG22	1:B:398:ILE:HG13	1.95	0.47
1:B:533:ILE:H	1:B:533:ILE:CD1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ASP:O	1:C:730:VAL:HG23	2.14	0.47
1:A:116:ILE:CD1	1:A:133:LEU:HD13	2.45	0.47
1:A:107:LYS:HD2	1:A:233:ILE:HD11	1.97	0.47
1:C:851:PHE:HB2	1:C:862:GLU:HB3	1.95	0.47
1:B:305:ARG:O	1:B:350:GLU:HA	2.15	0.47
1:B:484:ASN:HB2	1:B:487:LEU:CD1	2.44	0.47
1:C:673:LYS:CB	1:C:674:PRO:CD	2.80	0.47
1:A:125:ASP:O	1:A:129:LYS:HD3	2.15	0.46
1:A:73:LYS:CB	1:A:74:PRO:CD	2.90	0.46
1:B:509:GLN:HB2	1:B:521:ASP:HB2	1.97	0.46
1:B:373:LYS:HG2	1:B:527:ASN:ND2	2.29	0.46
1:B:373:LYS:HG2	1:B:527:ASN:HD22	1.81	0.46
1:C:846:GLY:C	1:C:848:LYS:N	2.68	0.46
1:B:332:LEU:HD13	1:C:851:PHE:CE2	2.50	0.46
1:C:892:ARG:HH11	1:C:892:ARG:HG2	1.80	0.46
1:A:119:MET:HG3	1:A:152:MET:CE	2.45	0.46
1:A:225:PHE:HB3	4:A:308:HOH:O	2.16	0.46
1:A:71:LEU:HD21	1:A:110:LEU:HD11	1.97	0.46
1:A:87:THR:HG22	1:A:92:GLU:N	2.30	0.46
1:A:46:GLY:HA2	1:A:210:LEU:HD11	1.97	0.46
1:A:87:THR:HG21	1:A:91:PRO:HB2	1.96	0.46
1:B:303:LEU:HG	1:B:304:ARG:N	2.27	0.46
1:C:744:VAL:HG23	1:C:744:VAL:O	2.15	0.46
1:C:751:GLY:C	1:C:754:ILE:HD13	2.36	0.46
1:B:376:VAL:HG21	1:B:520:VAL:HG11	1.97	0.46
1:C:858:VAL:HG21	1:C:886:PHE:CD2	2.51	0.46
1:A:53:PRO:O	1:A:55:GLU:N	2.45	0.46
1:C:860:GLU:HA	1:C:861:PRO:HD3	1.65	0.46
1:C:616:MET:HE1	1:C:629:LEU:HD21	1.97	0.46
1:C:831:ASN:C	1:C:833:ILE:N	2.69	0.46
1:B:391:PRO:CD	1:B:418:LYS:HE3	2.44	0.46
1:C:615:ASN:HD22	1:C:615:ASN:HA	1.54	0.46
1:A:119:MET:CE	1:A:145:LYS:HD3	2.46	0.45
1:A:3:LEU:HG	1:A:4:ARG:N	2.31	0.45
1:B:589:LEU:HD23	1:B:589:LEU:HA	1.77	0.45
1:C:719:MET:HA	1:C:722:TYR:CE2	2.51	0.45
1:A:134:GLU:OE2	1:A:145:LYS:HE3	2.16	0.45
1:A:251:PHE:HB2	1:A:262:GLU:HB3	1.97	0.45
1:C:690:MET:HB2	1:C:691:PRO:HD3	1.97	0.45
1:C:722:TYR:HB3	1:C:726:ASP:HB2	1.98	0.45
1:C:757:LEU:HD23	1:C:783:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLY:O	1:A:154:ILE:HD13	2.16	0.45
1:A:242:PHE:CZ	1:A:282:TYR:HB2	2.51	0.45
1:B:448:ALA:HB1	1:B:478:SER:HB3	1.98	0.45
1:C:628:ILE:H	1:C:628:ILE:HD12	1.80	0.45
1:C:631:LYS:O	1:C:632:LEU:C	2.55	0.45
1:A:128:ARG:O	1:A:132:GLU:HG3	2.16	0.45
1:B:355:GLU:C	1:B:357:GLY:H	2.20	0.45
1:B:383:ILE:HD11	1:B:461:LEU:CD2	2.41	0.45
1:B:466:SER:O	1:B:519:VAL:HA	2.16	0.45
1:A:43:ILE:HG22	1:B:561:PRO:HG3	1.99	0.45
1:B:331:LYS:HA	1:B:331:LYS:HE3	1.98	0.45
1:A:227:ASN:O	1:A:228:LEU:C	2.54	0.45
1:C:852:PHE:CE1	1:C:861:PRO:HD2	2.52	0.45
1:C:633:ARG:HB3	1:C:660:VAL:CG1	2.47	0.45
1:A:141:TYR:CE1	1:A:243:LYS:HE2	2.53	0.44
1:C:649:VAL:HA	1:C:665:LEU:HD13	1.98	0.44
1:C:635:LYS:HB3	1:C:638:LEU:HB2	1.98	0.44
1:A:87:THR:HG21	1:A:91:PRO:N	2.32	0.44
1:B:310:VAL:HG22	1:B:318:THR:O	2.17	0.44
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.32	0.44
1:C:673:LYS:HA	1:C:673:LYS:HD2	1.80	0.44
1:B:336:PHE:O	1:B:339:GLN:O	2.36	0.44
1:A:40:ASN:HD22	1:A:40:ASN:HA	1.54	0.44
1:A:33:ARG:HG2	1:A:60:VAL:HG11	1.98	0.44
1:B:387:THR:HB	1:B:474:VAL:HG23	2.00	0.44
1:B:454:ILE:HG21	1:B:482:ALA:O	2.18	0.44
1:C:647:ASP:HA	1:C:678:ASN:ND2	2.33	0.44
1:C:855:CYS:SG	1:C:860:GLU:CB	3.06	0.44
1:B:415:VAL:HG12	1:B:415:VAL:O	2.18	0.44
1:B:419:MET:HA	1:B:422:TYR:CE2	2.53	0.44
1:B:574:ILE:HA	4:B:45:HOH:O	2.17	0.44
1:B:592:ARG:HH11	1:B:592:ARG:HG2	1.83	0.44
1:B:355:GLU:O	1:B:357:GLY:N	2.45	0.44
1:C:633:ARG:O	1:C:633:ARG:HG3	2.18	0.44
1:C:634:GLY:HA3	1:C:636:PHE:CD2	2.53	0.44
1:B:331:LYS:HE3	1:B:331:LYS:CA	2.48	0.43
1:B:386:VAL:HG13	1:B:393:THR:CB	2.48	0.43
1:B:415:VAL:HG22	1:B:444:VAL:HG22	2.00	0.43
1:B:421:LEU:CD1	3:B:599:GDP:HN21	2.31	0.43
1:C:704:LEU:HB3	1:C:825:PHE:CD2	2.53	0.43
1:B:473:GLY:HA2	3:B:599:GDP:O3A	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ARG:CG	1:C:633:ARG:O	2.66	0.43
1:B:345:VAL:HG13	1:B:510:LEU:HG	2.00	0.43
1:B:429:LYS:HE3	4:B:52:HOH:O	2.18	0.43
1:C:689:LYS:O	1:C:690:MET:C	2.56	0.43
1:B:319:VAL:CG1	1:B:361:ILE:HD11	2.49	0.43
1:C:838:LEU:HB3	1:C:882:TYR:HE1	1.83	0.43
1:A:5:ARG:O	1:A:50:GLU:HA	2.18	0.43
1:B:365:LEU:CD1	1:B:365:LEU:N	2.82	0.43
1:B:387:THR:HG23	1:B:389:LYS:H	1.83	0.43
1:C:717:ASN:CG	1:C:718:LYS:H	2.22	0.43
1:B:407:LYS:HD2	1:B:533:ILE:HG13	2.00	0.43
1:C:631:LYS:HE2	1:C:632:LEU:HD12	2.01	0.43
1:C:848:LYS:HE3	1:C:874:ILE:HD11	2.00	0.43
1:C:741:TYR:CE1	1:C:843:LYS:HE2	2.54	0.43
1:A:122:TYR:HB3	1:A:126:ASP:HB2	1.99	0.43
1:A:45:VAL:HG12	1:A:210:LEU:HG	2.00	0.43
1:A:54:ASP:O	1:A:56:THR:N	2.51	0.43
1:A:87:THR:CG2	1:A:92:GLU:H	2.32	0.43
1:C:633:ARG:HG2	1:C:660:VAL:HG11	2.01	0.43
1:A:31:LYS:HE2	1:B:562:GLU:OE1	2.18	0.42
1:A:100:LYS:HG3	1:A:230:ILE:CD1	2.49	0.42
1:A:260:GLU:HA	1:A:261:PRO:HD3	1.63	0.42
1:B:419:MET:HB3	1:B:452:MET:HE1	2.01	0.42
1:C:645:VAL:HG21	1:C:808:ALA:O	2.20	0.42
1:A:88:VAL:HG22	1:A:122:TYR:CZ	2.55	0.42
1:B:365:LEU:N	1:B:365:LEU:HD12	2.33	0.42
1:B:417:ASN:CG	1:B:418:LYS:H	2.21	0.42
1:A:245:PHE:HE2	1:A:282:TYR:CD2	2.38	0.42
1:A:88:VAL:CG2	1:A:89:LYS:N	2.82	0.42
1:B:509:GLN:H	1:B:521:ASP:HB3	1.84	0.42
1:B:592:ARG:HD3	1:B:592:ARG:O	2.20	0.42
1:C:855:CYS:SG	1:C:860:GLU:CG	3.08	0.42
1:B:354:ASP:CG	1:B:354:ASP:O	2.58	0.42
1:B:390:MET:O	1:B:391:PRO:C	2.56	0.42
1:C:687:THR:HB	1:C:774:VAL:CG2	2.46	0.42
1:A:177:SER:HB2	1:A:189:LEU:HD12	2.00	0.42
1:A:32:LEU:HD13	1:B:551:PHE:CE2	2.55	0.42
1:A:68:LYS:HG3	1:A:69:ASN:ND2	2.34	0.42
1:B:335:LYS:CA	1:B:338:LEU:HD23	2.37	0.42
1:B:309:VAL:CG1	1:B:345:VAL:HA	2.47	0.42
1:C:855:CYS:SG	1:C:860:GLU:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:857:HIS:N	1:C:860:GLU:OE1	2.52	0.42
1:A:12:PHE:CE1	1:A:45:VAL:HG22	2.55	0.42
1:B:320:GLU:OE2	1:B:518:TYR:OH	2.38	0.42
1:C:655:GLU:C	1:C:657:GLY:N	2.72	0.42
1:C:694:SER:O	1:C:698:ILE:HG13	2.19	0.42
1:C:673:LYS:HB2	1:C:827:ASN:HD21	1.85	0.42
1:A:89:LYS:HG2	1:A:90:MET:H	1.85	0.42
1:B:333:ARG:HD3	1:B:334:GLY:N	2.35	0.42
1:B:373:LYS:HA	1:B:373:LYS:HD2	1.90	0.42
1:C:651:TYR:N	1:C:651:TYR:HD2	2.13	0.42
1:C:844:GLU:OE2	1:C:878:ARG:NE	2.42	0.42
1:A:70:LEU:HD23	1:A:76:VAL:O	2.20	0.42
1:B:373:LYS:O	1:B:374:PRO:C	2.52	0.42
1:B:345:VAL:CG1	1:B:510:LEU:HG	2.50	0.42
1:C:719:MET:HE2	1:C:745:LYS:HD3	2.02	0.42
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.87	0.42
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.85	0.42
1:B:337:ARG:HE	1:B:337:ARG:C	2.23	0.42
1:A:255:CYS:SG	1:A:260:GLU:HB2	2.60	0.41
1:B:349:VAL:HG12	1:B:364:VAL:HA	2.02	0.41
1:A:244:GLU:OE2	1:A:278:ARG:NE	2.50	0.41
1:C:621:ASP:HB3	1:C:625:GLY:HA2	2.01	0.41
1:C:673:LYS:CG	1:C:827:ASN:ND2	2.83	0.41
1:A:81:GLN:HG2	1:A:111:GLU:HB2	2.02	0.41
1:C:762:LYS:HE3	1:C:815:PHE:HB2	2.02	0.41
1:C:721:LEU:CD1	3:C:899:GDP:N2	2.82	0.41
1:A:15:ASN:HD21	1:B:563:CYS:N	2.18	0.41
1:A:36:PHE:CZ	1:A:63:ASN:HA	2.54	0.41
1:C:719:MET:HE1	1:C:745:LYS:HD3	2.00	0.41
1:C:784:ASN:HB2	1:C:787:LEU:HD12	2.01	0.41
1:A:90:MET:O	1:A:91:PRO:C	2.58	0.41
1:B:354:ASP:O	1:B:356:THR:N	2.53	0.41
1:C:751:GLY:O	1:C:754:ILE:HD13	2.20	0.41
1:C:603:LEU:HG	1:C:604:ARG:N	2.29	0.41
1:A:44:TYR:O	1:A:47:ASP:HB2	2.21	0.41
1:B:421:LEU:CD1	3:B:599:GDP:N2	2.84	0.41
1:B:583:VAL:O	1:B:584:LYS:C	2.59	0.41
1:B:375:HIS:CD2	1:C:859:ASP:OD2	2.74	0.41
1:C:633:ARG:HH11	1:C:633:ARG:CB	2.30	0.41
1:C:635:LYS:O	1:C:638:LEU:HB2	2.21	0.41
1:C:717:ASN:CG	1:C:718:LYS:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:C	1:A:57:GLY:N	2.73	0.41
1:A:87:THR:HG21	1:A:91:PRO:CB	2.51	0.41
1:A:87:THR:HG22	1:A:87:THR:O	2.21	0.41
1:A:87:THR:HG21	1:A:91:PRO:CD	2.50	0.41
1:B:310:VAL:HG21	1:B:327:ARG:HH11	1.86	0.41
1:C:665:LEU:CD1	1:C:665:LEU:N	2.84	0.41
1:A:6:ARG:NH1	1:A:6:ARG:HG2	2.36	0.41
1:C:687:THR:HG21	1:C:691:PRO:HB2	2.02	0.41
1:C:611:SER:HB3	1:C:809:GLN:HG2	2.03	0.41
1:C:838:LEU:O	1:C:839:LYS:C	2.59	0.41
1:B:533:ILE:HG21	1:B:538:LEU:HD23	2.03	0.40
1:C:621:ASP:HB2	1:C:651:TYR:OH	2.21	0.40
1:C:707:LYS:HD2	1:C:833:ILE:CG1	2.50	0.40
1:C:784:ASN:O	1:C:785:PRO:C	2.57	0.40
1:A:13:HIS:ND1	1:A:14:SER:OG	2.44	0.40
1:A:76:VAL:HG21	1:A:220:VAL:HG11	2.04	0.40
1:B:327:ARG:HG3	1:B:327:ARG:HH11	1.86	0.40
1:C:723:ASP:O	1:C:727:LEU:HG	2.22	0.40
1:A:251:PHE:HD2	1:A:252:PHE:CD1	2.39	0.40
1:B:434:GLU:O	1:B:438:SER:CB	2.61	0.40
1:B:539:LYS:HA	1:B:582:TYR:CE1	2.56	0.40
1:C:673:LYS:HG2	1:C:827:ASN:HD22	1.87	0.40
1:C:616:MET:CE	1:C:631:LYS:HB2	2.50	0.40
1:C:616:MET:HE2	1:C:630:CYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/301 (91%)	233 (85%)	31 (11%)	10 (4%)	3 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	274/301 (91%)	225 (82%)	37 (14%)	12 (4%)	2	8
1	C	274/301 (91%)	218 (80%)	41 (15%)	15 (6%)	2	5
All	All	822/903 (91%)	676 (82%)	109 (13%)	37 (4%)	2	8

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	73	LYS
1	A	90	MET
1	A	224	GLY
1	B	340	ASN
1	B	372	THR
1	B	373	LYS
1	B	525	PHE
1	C	655	GLU
1	C	672	THR
1	C	673	LYS
1	C	690	MET
1	A	55	GLU
1	A	92	GLU
1	B	355	GLU
1	B	592	ARG
1	C	638	LEU
1	C	824	GLY
1	B	356	THR
1	B	390	MET
1	C	623	GLU
1	C	632	LEU
1	A	243	LYS
1	A	292	ARG
1	B	358	SER
1	B	508	ALA
1	B	515	PHE
1	C	631	LYS
1	C	656	THR
1	A	56	THR
1	C	657	GLY
1	C	815	PHE
1	C	839	LYS
1	A	246	GLY

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Mol	Chain	Res	Type
1	C	858	VAL
1	B	591	GLY
1	C	653	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	248/264 (94%)	221 (89%)	27 (11%)	6	19
1	B	248/264 (94%)	228 (92%)	20 (8%)	11	33
1	C	248/264 (94%)	220 (89%)	28 (11%)	6	18
All	All	744/792 (94%)	669 (90%)	75 (10%)	7	22

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	14	SER
1	A	15	ASN
1	A	19	VAL
1	A	31	LYS
1	A	32	LEU
1	A	33	ARG
1	A	37	ARG
1	A	40	ASN
1	A	48	ARG
1	A	55	GLU
1	A	67	ARG
1	A	70	LEU
1	A	84	LEU
1	A	87	THR
1	A	92	GLU
1	A	106	GLU
1	A	155	GLU
1	A	168	MET

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	214	ASP
1	A	225	PHE
1	A	234	GLU
1	A	238	LEU
1	A	245	PHE
1	A	248	LYS
1	A	292	ARG
1	B	305	ARG
1	B	315	ASN
1	B	331	LYS
1	B	332	LEU
1	B	333	ARG
1	B	337	ARG
1	B	340	ASN
1	B	355	GLU
1	B	370	LEU
1	B	384	LEU
1	B	387	THR
1	B	388	VAL
1	B	444	VAL
1	B	459	GLU
1	B	468	MET
1	B	484	ASN
1	B	534	GLU
1	B	538	LEU
1	B	548	LYS
1	B	592	ARG
1	C	605	ARG
1	C	615	ASN
1	C	619	VAL
1	C	631	LYS
1	C	632	LEU
1	C	633	ARG
1	C	637	ARG
1	C	639	GLN
1	C	640	ASN
1	C	647	ASP
1	C	651	TYR
1	C	655	GLU
1	C	666	HIS
1	C	667	ARG

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Mol	Chain	Res	Type
1	C	670	LEU
1	C	684	LEU
1	C	687	THR
1	C	692	GLU
1	C	706	GLU
1	C	759	GLU
1	C	774	VAL
1	C	784	ASN
1	C	807	THR
1	C	834	GLU
1	C	838	LEU
1	C	845	PHE
1	C	848	LYS
1	C	892	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	40	ASN
1	A	75	HIS
1	A	117	ASN
1	A	249	GLN
1	A	271	ASN
1	B	315	ASN
1	B	340	ASN
1	B	375	HIS
1	B	417	ASN
1	B	527	ASN
1	B	571	ASN
1	C	615	ASN
1	C	640	ASN
1	C	675	HIS
1	C	681	GLN
1	C	781	ASN
1	C	827	ASN
1	C	840	HIS
1	C	871	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	GDP	B	599	-	24,30,30	1.58	3 (12%)	31,47,47	1.81	3 (9%)
3	GDP	C	899	-	24,30,30	1.37	3 (12%)	31,47,47	1.81	5 (16%)
3	GDP	A	299	-	24,30,30	1.50	4 (16%)	31,47,47	1.83	3 (9%)

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	GDP	B	599	-	-	3/12/32/32	0/3/3/3
3	GDP	C	899	-	-	0/12/32/32	0/3/3/3
3	GDP	A	299	-	-	2/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	599	GDP	C6-N1	5.34	1.42	1.33
3	C	899	GDP	C6-N1	5.02	1.41	1.33
3	A	299	GDP	C6-N1	4.85	1.41	1.33
3	A	299	GDP	O3'-C3'	3.25	1.50	1.43
3	B	599	GDP	O3'-C3'	2.88	1.49	1.43
3	A	299	GDP	C2'-C1'	2.80	1.58	1.53
3	B	599	GDP	C2-N1	2.55	1.39	1.35
3	C	899	GDP	C2-N1	2.47	1.39	1.35
3	C	899	GDP	O3'-C3'	2.20	1.48	1.43
3	A	299	GDP	C2-N1	2.06	1.39	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	599	GDP	C5-C6-N1	-7.34	113.40	123.43
3	C	899	GDP	C5-C6-N1	-7.16	113.63	123.43
3	A	299	GDP	C5-C6-N1	-7.02	113.83	123.43
3	B	599	GDP	C6-N1-C2	4.34	122.83	115.93
3	C	899	GDP	C6-N1-C2	4.25	122.69	115.93
3	A	299	GDP	C6-N1-C2	4.15	122.52	115.93
3	A	299	GDP	N3-C2-N1	-2.97	123.26	127.22
3	B	599	GDP	N3-C2-N1	-2.89	123.36	127.22
3	C	899	GDP	N3-C2-N1	-2.85	123.42	127.22
3	C	899	GDP	O3'-C3'-C4'	-2.10	104.98	111.05
3	C	899	GDP	C2-N3-C4	-2.03	113.04	115.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	599	GDP	PA-O3A-PB-O3B
3	A	299	GDP	PA-O3A-PB-O3B
3	A	299	GDP	PA-O3A-PB-O1B
3	B	599	GDP	PA-O3A-PB-O2B
3	B	599	GDP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 10 short contacts:

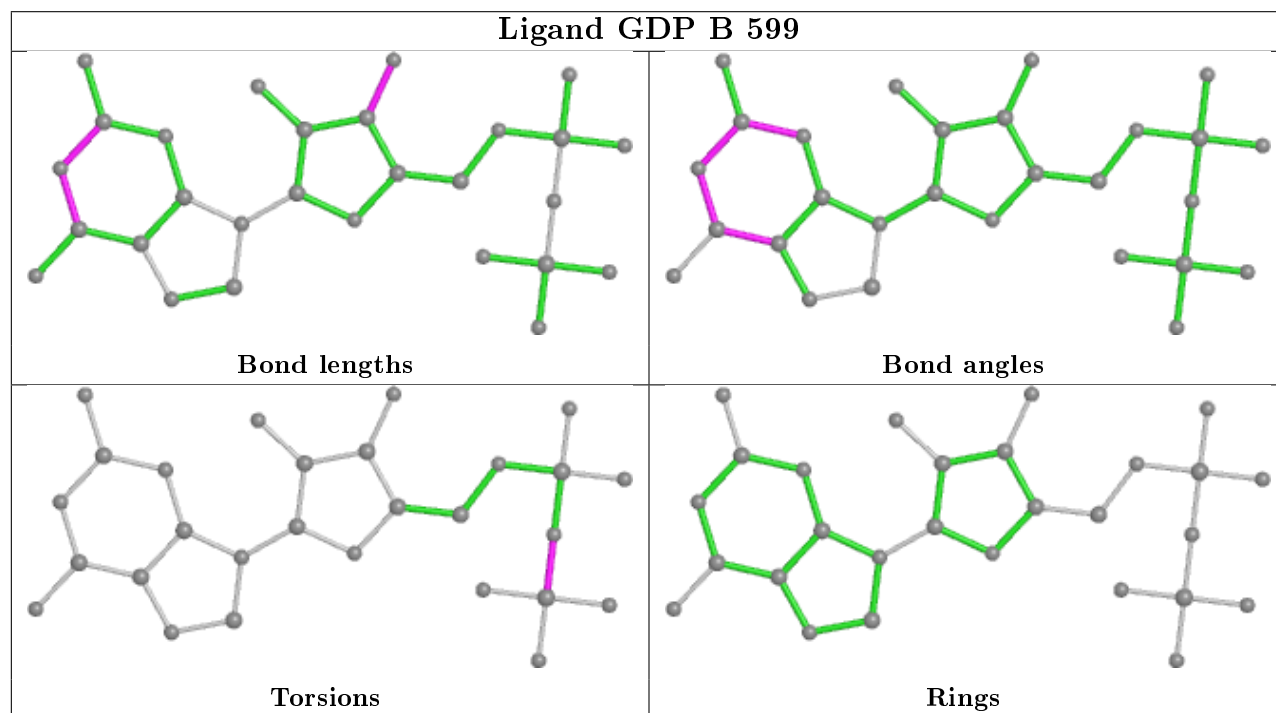
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	599	GDP	4	0
3	C	899	GDP	5	0

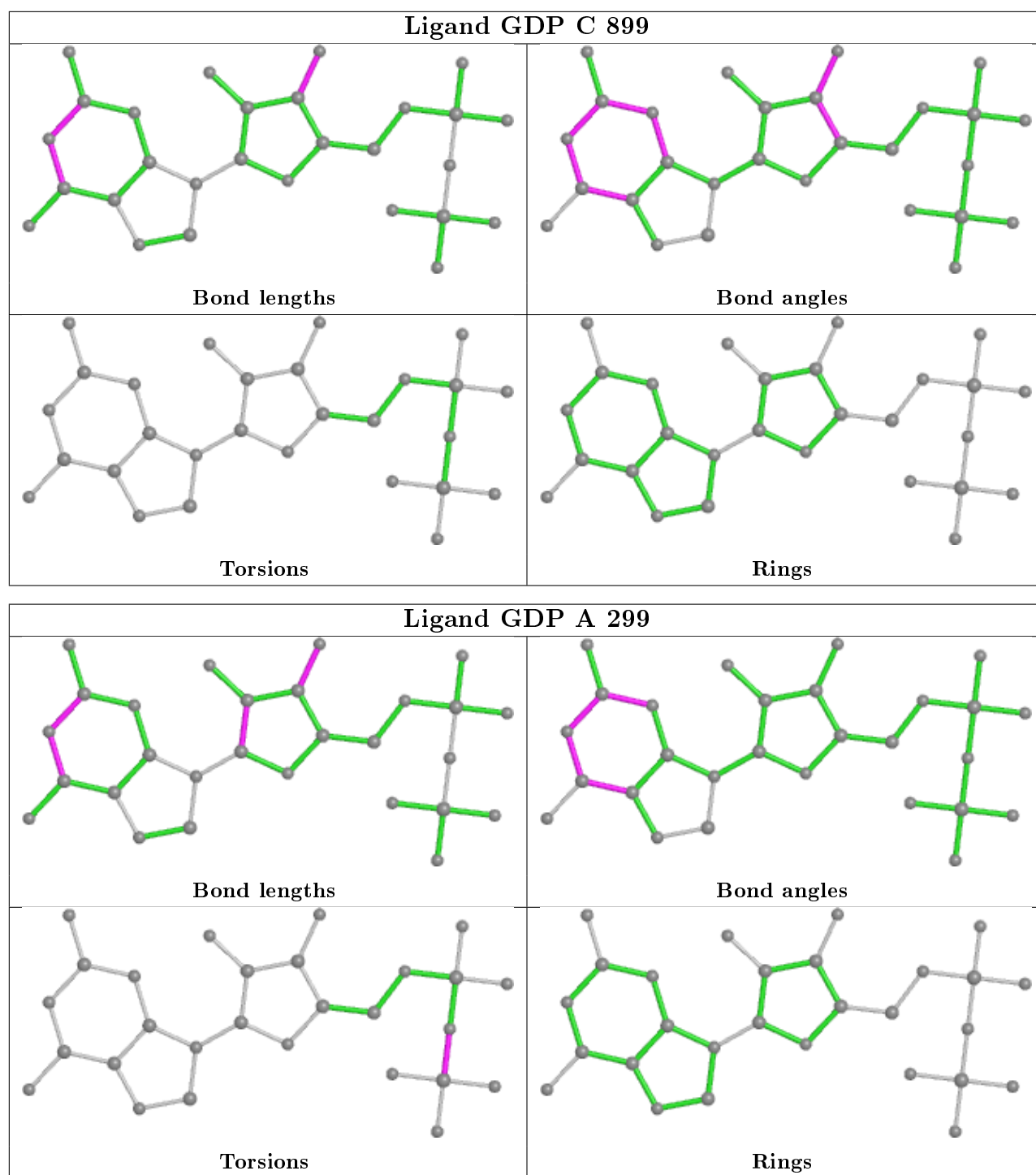
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	299	GDP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	278/301 (92%)	-0.30	8 (2%) 51 41	14, 40, 113, 201	0
1	B	278/301 (92%)	-0.16	10 (3%) 42 32	14, 48, 138, 197	0
1	C	278/301 (92%)	-0.18	9 (3%) 47 37	23, 56, 131, 200	0
All	All	834/903 (92%)	-0.22	27 (3%) 47 37	14, 50, 131, 201	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	LEU	7.8
1	C	893	ARG	6.5
1	B	336	PHE	5.7
1	C	804	THR	5.6
1	B	337	ARG	5.1
1	A	293	ARG	4.5
1	A	38	LEU	4.2
1	C	641	LEU	3.9
1	B	356	THR	3.6
1	C	633	ARG	3.5
1	B	505	THR	3.2
1	A	204	THR	2.9
1	B	504	THR	2.9
1	A	56	THR	2.5
1	C	892	ARG	2.4
1	A	292	ARG	2.4
1	C	666	HIS	2.3
1	B	506	THR	2.3
1	C	655	GLU	2.3
1	A	39	GLN	2.2
1	C	624	THR	2.2
1	A	53	PRO	2.1
1	B	490	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	530	ILE	2.1
1	C	673	LYS	2.1
1	B	357	GLY	2.1
1	A	205	THR	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](#)

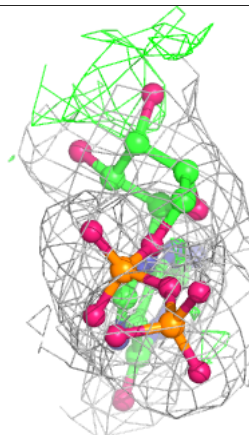
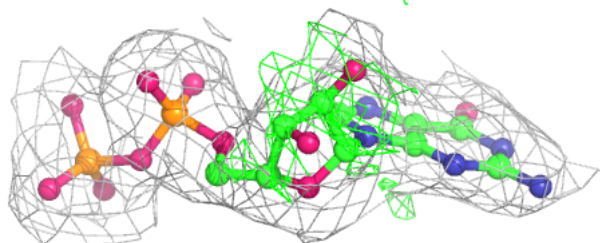
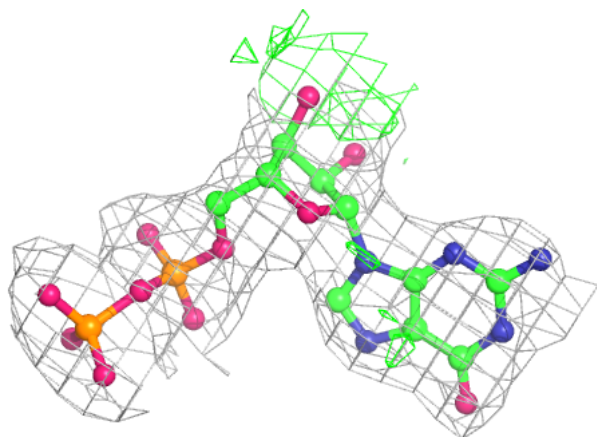
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GDP	B	599	28/28	0.95	0.14	24,39,42,43	0
3	GDP	C	899	28/28	0.96	0.16	38,46,50,51	0
3	GDP	A	299	28/28	0.97	0.17	24,27,31,31	0
2	ZN	C	898	1/1	0.97	0.11	51,51,51,51	0
2	ZN	A	298	1/1	0.97	0.11	62,62,62,62	0
2	ZN	B	598	1/1	0.99	0.12	41,41,41,41	0

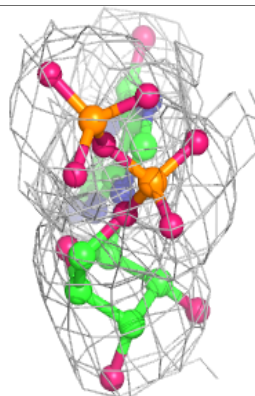
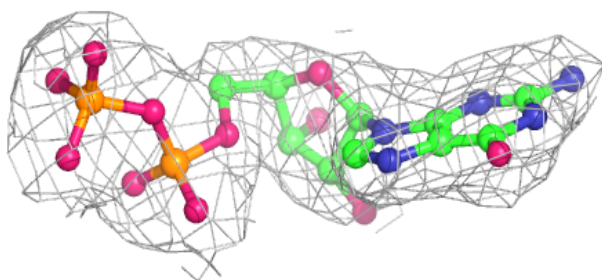
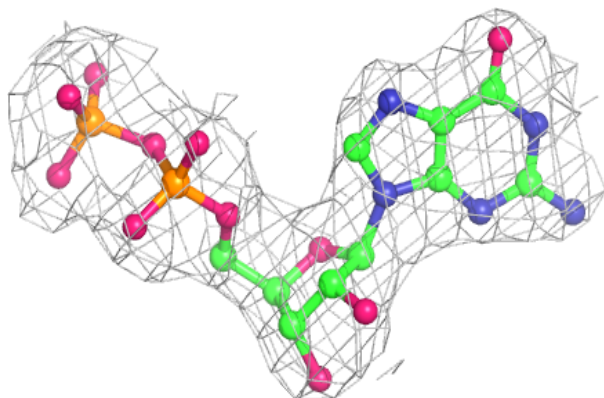
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

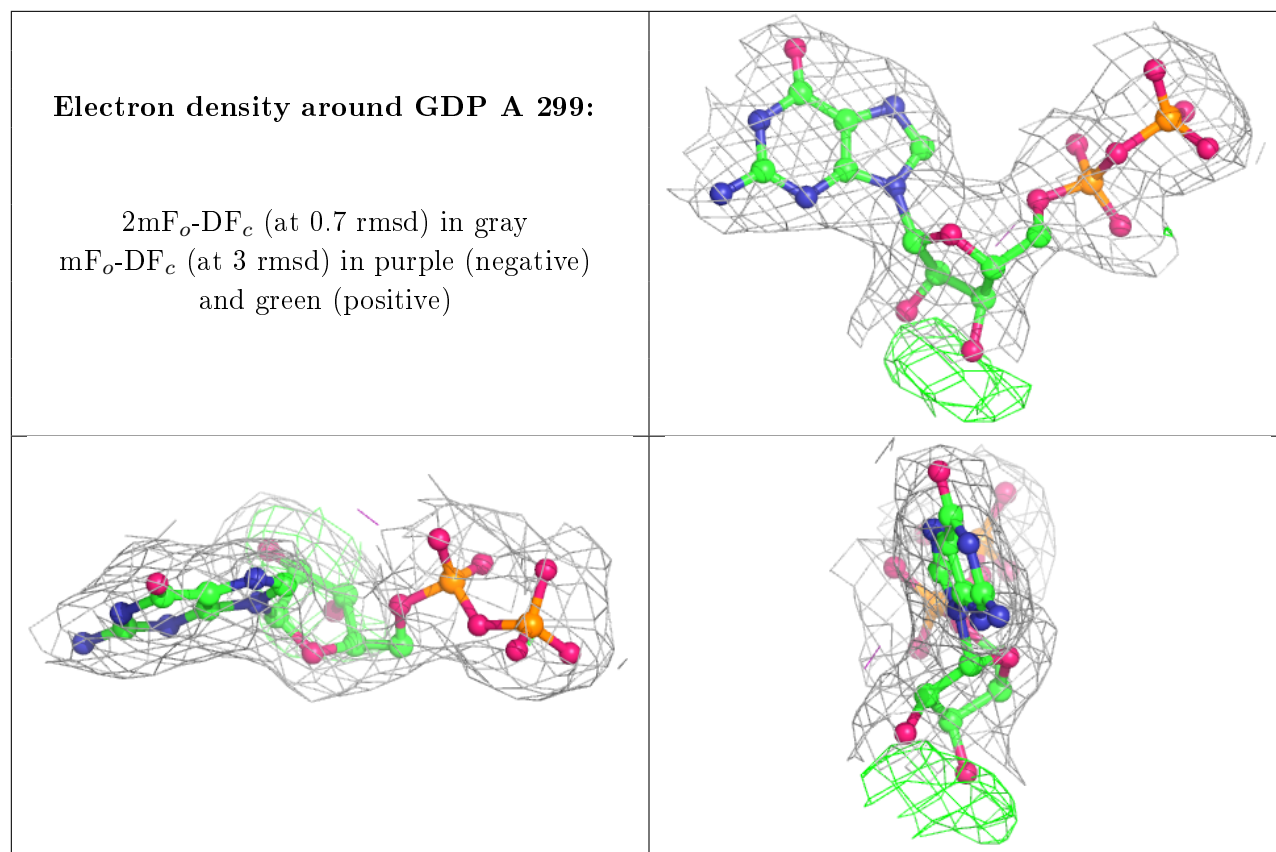
Electron density around GDP B 599:

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

**Electron density around GDP C 899:**

$2mF_o-DF_c$ (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.