



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:00 AM UTC

PDB ID : 1D2E / pdb_00001d2e
Title : CRYSTAL STRUCTURE OF MITOCHONDRIAL EF-TU IN COMPLEX WITH GDP
Authors : Andersen, G.R.; Thirup, S.; Spemulli, L.L.; Nyborg, J.
Deposited on : 1999-09-23
Resolution : 1.94 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

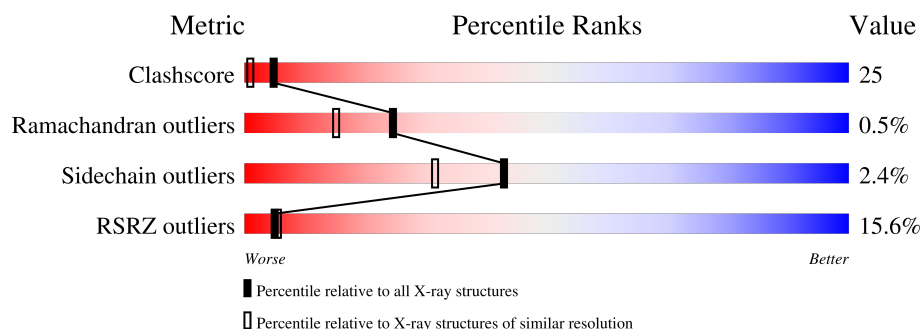
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	397	5% 68% 29% .
1	B	397	13% 56% 43% .
1	C	397	12% 62% 36% .
1	D	397	32% 50% 45% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13597 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 ELONGATION FACTOR TU (EF-TU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			
1	B	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			
1	C	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			
1	D	397	Total	C	N	O	S	0	0	0
			3070	1938	539	577	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

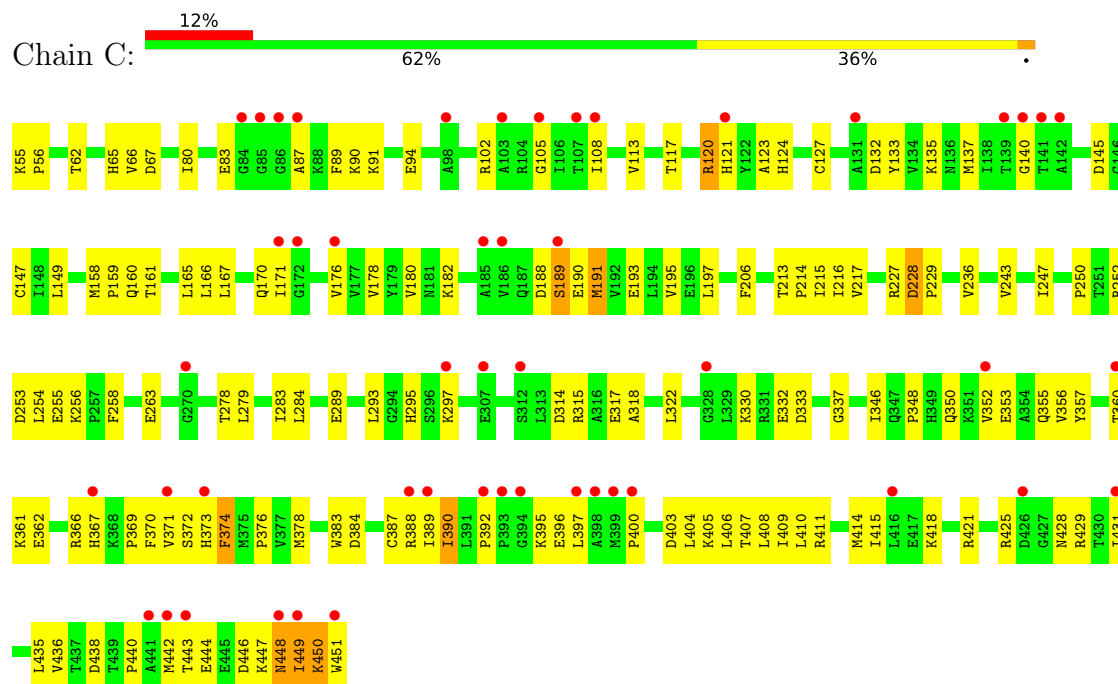


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

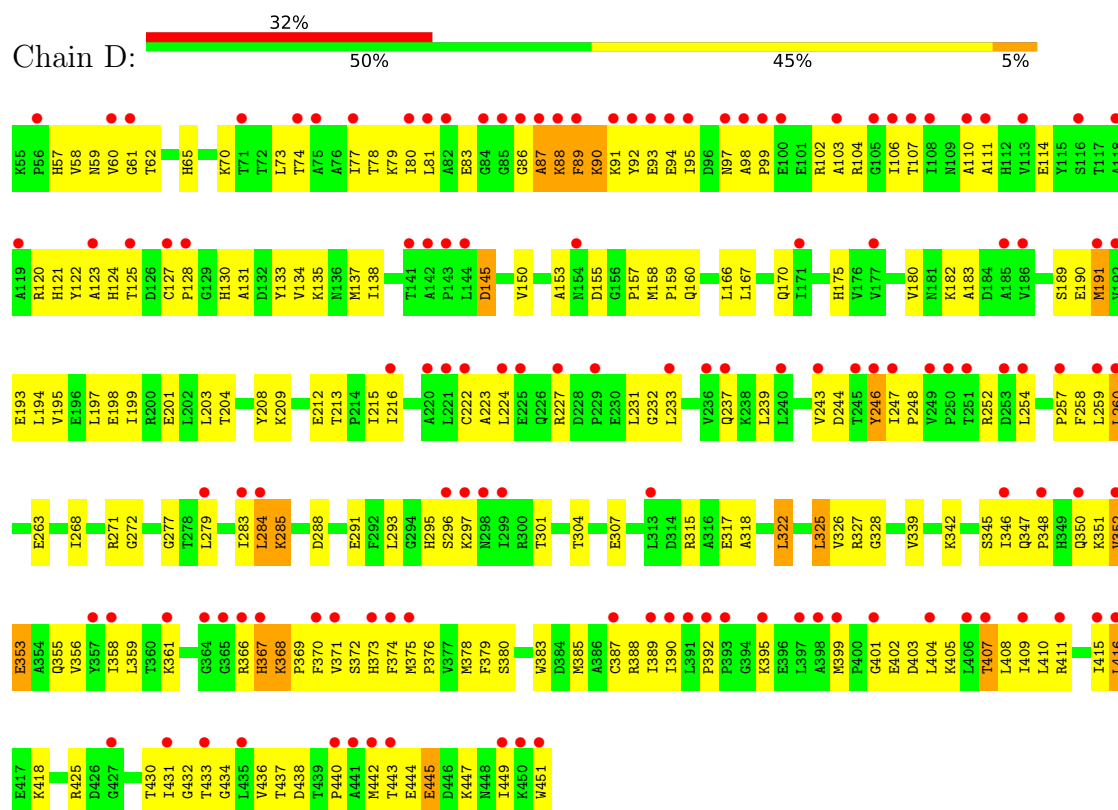
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	387	Total O 387 387	0	0
4	B	274	Total O 274 274	0	0
4	C	295	Total O 295 295	0	0
4	D	245	Total O 245 245	0	0

• Molecule 1: ELONGATION FACTOR TU (EF-TU)



• Molecule 1: ELONGATION FACTOR TU (EF-TU)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.09Å 119.78Å 128.89Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	34.70 – 1.94 34.70 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.70-1.94) 98.2 (34.70-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.94Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.237 , 0.257 0.254 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13597	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	0.47	0/3127	1.04	13/4232 (0.3%)
1	B	0.37	0/3127	0.95	6/4232 (0.1%)
1	C	0.40	0/3127	0.98	10/4232 (0.2%)
1	D	0.38	0/3127	0.98	11/4232 (0.3%)
All	All	0.41	0/12508	0.99	40/16928 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	GLU	N-CA-C	-7.87	97.44	109.95
1	A	117	THR	N-CA-C	-7.40	99.51	110.46
1	D	268	ILE	N-CA-C	-7.25	100.97	108.15
1	C	189	SER	N-CA-C	-7.06	104.40	112.87
1	C	123	ALA	N-CA-C	-6.90	97.27	108.52
1	C	117	THR	N-CA-C	-6.69	99.49	109.86
1	A	355	GLN	N-CA-C	-6.47	98.68	108.96
1	D	322	LEU	N-CA-C	6.45	117.95	108.86
1	D	87	ALA	N-CA-C	-6.43	106.15	112.97
1	C	228	ASP	CA-C-N	6.38	126.86	119.47
1	C	228	ASP	C-N-CA	6.38	126.86	119.47
1	D	444	GLU	N-CA-C	-6.18	104.84	112.38
1	B	189	SER	N-CA-C	-5.91	105.91	113.01
1	C	87	ALA	N-CA-C	5.77	118.36	109.07
1	B	355	GLN	N-CA-C	-5.71	99.88	108.96
1	A	327	ARG	N-CA-C	5.58	118.41	110.10
1	A	322	LEU	N-CA-C	5.53	116.66	108.86
1	B	374	PHE	N-CA-C	-5.53	102.22	110.23
1	A	245	THR	N-CA-C	5.50	120.09	112.45
1	B	190	GLU	N-CA-C	-5.48	105.46	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	VAL	N-CA-C	-5.47	100.60	108.53
1	D	145	ASP	N-CA-C	-5.46	106.78	113.50
1	A	367	HIS	N-CA-C	-5.39	106.83	113.41
1	B	123	ALA	N-CA-C	-5.38	98.48	107.99
1	D	246	TYR	N-CA-C	5.33	117.17	111.36
1	A	161	THR	N-CA-C	-5.23	105.48	111.07
1	C	161	THR	N-CA-C	-5.20	105.51	111.07
1	A	375	MET	N-CA-C	5.18	118.58	108.21
1	D	90	LYS	N-CA-C	-5.18	100.46	108.90
1	A	120	ARG	N-CA-C	5.17	116.85	109.14
1	D	272	GLY	N-CA-C	5.17	117.58	111.63
1	D	434	GLY	N-CA-C	5.13	118.77	111.12
1	C	355	GLN	N-CA-C	-5.13	100.37	108.73
1	C	120	ARG	N-CA-C	5.10	116.74	109.14
1	D	407	THR	N-CA-C	-5.07	101.43	109.59
1	C	374	PHE	N-CA-C	-5.06	103.36	110.50
1	D	353	GLU	N-CA-C	-5.06	101.91	109.95
1	A	123	ALA	N-CA-C	-5.05	99.05	107.99
1	A	119	ALA	N-CA-C	5.02	117.86	111.69
1	B	321	ASN	N-CA-C	-5.02	100.33	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3070	0	3122	117	0
1	B	3070	0	3122	173	0
1	C	3070	0	3122	135	0
1	D	3070	0	3123	213	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	1	0
3	C	28	0	12	1	0
3	D	28	0	12	1	0
4	A	387	0	0	7	0
4	B	274	0	0	8	0
4	C	295	0	0	13	0
4	D	245	0	0	16	0
All	All	13597	0	12537	634	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 25.

All (634) 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:368:LYS:HD3	1:A:368:LYS:H	1.08	1.08
1:A:352:VAL:HG11	1:A:416:LEU:HD12	1.30	1.06
1:C:137:MET:HE3	1:C:167:LEU:HD23	1.38	1.02
1:A:352:VAL:HG11	1:A:416:LEU:CD1	1.92	0.99
1:B:388:ARG:HH12	1:B:450:LYS:HE2	1.30	0.97
1:D:405:LYS:NZ	1:D:437:THR:HG21	1.80	0.96
1:A:449:ILE:HD13	1:A:449:ILE:H	1.35	0.91
1:A:368:LYS:HD3	1:A:368:LYS:N	1.86	0.88
1:B:352:VAL:CG2	1:B:436:VAL:HG13	2.02	0.88
1:A:446:ASP:O	1:A:449:ILE:HG23	1.74	0.87
1:D:416:LEU:HD22	1:D:436:VAL:HG21	1.58	0.86
1:D:443:THR:HG22	1:D:445:GLU:H	1.42	0.84
1:A:332:GLU:HB3	1:C:229:PRO:HG3	1.60	0.84
1:D:81:LEU:HB2	4:D:1380:HOH:O	1.78	0.84
1:C:145:ASP:CG	1:C:250:PRO:HG3	2.02	0.84
1:D:405:LYS:HZ1	1:D:437:THR:HG21	1.42	0.84
1:A:446:ASP:O	1:A:449:ILE:HD12	1.78	0.83
1:D:91:LYS:HD3	1:D:92:TYR:H	1.42	0.82
1:A:449:ILE:HG12	1:A:451:TRP:HE1	1.41	0.82
1:B:352:VAL:HG21	1:B:436:VAL:HG13	1.59	0.82
1:B:409:ILE:HG23	1:B:442:MET:HE1	1.61	0.82
1:C:108:ILE:HD11	1:C:135:LYS:HB2	1.59	0.82
1:C:392:PRO:HG3	1:C:405:LYS:O	1.78	0.82
1:D:368:LYS:HD3	1:D:368:LYS:N	1.95	0.81
1:A:392:PRO:HG3	1:A:405:LYS:O	1.81	0.80
1:B:416:LEU:HD22	1:B:436:VAL:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:MET:HE3	1:B:313:LEU:HD12	1.63	0.80
1:C:189:SER:O	1:C:193:GLU:HG3	1.82	0.80
1:B:145:ASP:CG	1:B:250:PRO:HG3	2.07	0.79
1:D:78:THR:HB	1:D:89:PHE:HA	1.63	0.79
1:C:361:LYS:HE2	1:C:367:HIS:O	1.82	0.79
1:A:108:ILE:HD11	1:A:110:ALA:HB2	1.66	0.78
1:D:73:LEU:O	1:D:77:ILE:HG13	1.83	0.78
1:A:416:LEU:CD1	1:A:436:VAL:HG21	2.13	0.78
1:D:304:THR:OG1	1:D:325:LEU:HD22	1.83	0.78
1:D:368:LYS:HD3	1:D:368:LYS:H	1.48	0.77
1:C:352:VAL:CG2	1:C:436:VAL:HG13	2.13	0.77
1:B:308:MET:HE3	1:B:313:LEU:CD1	2.15	0.76
1:B:90:LYS:NZ	1:B:94:GLU:HG2	2.01	0.76
1:A:374:PHE:CE2	1:A:376:PRO:HG3	2.20	0.76
1:D:97:ASN:HB3	4:D:1533:HOH:O	1.86	0.76
1:A:193:GLU:O	1:A:197:LEU:HG	1.86	0.76
1:A:449:ILE:CG1	1:A:451:TRP:HE1	1.96	0.75
1:D:90:LYS:HG2	1:D:94:GLU:HG2	1.68	0.75
1:A:449:ILE:HG12	1:A:451:TRP:NE1	2.00	0.75
1:D:98:ALA:HB2	1:D:111:ALA:HB2	1.65	0.75
1:B:353:GLU:HG3	1:B:440:PRO:HG2	1.67	0.75
1:B:98:ALA:HB2	1:B:111:ALA:HB2	1.66	0.75
1:A:209:LYS:HB3	1:A:212:GLU:OE2	1.87	0.74
1:B:90:LYS:HZ1	1:B:94:GLU:HG2	1.51	0.74
1:D:79:LYS:O	1:D:83:GLU:HG2	1.87	0.74
1:D:153:ALA:HB2	1:D:180:VAL:HG12	1.70	0.74
1:A:266:TYR:HA	1:A:331:ARG:HE	1.52	0.73
1:D:418:LYS:HE2	1:D:438:ASP:HA	1.70	0.73
1:B:228:ASP:HB3	1:B:230:GLU:OE2	1.89	0.72
1:B:58:VAL:HG21	1:B:120:ARG:HH21	1.55	0.72
1:C:243:VAL:HG13	1:C:247:ILE:HD12	1.72	0.71
1:A:409:ILE:CG2	1:A:442:MET:HE1	2.20	0.71
1:B:332:GLU:H	1:B:332:GLU:CD	1.99	0.70
1:D:392:PRO:HD2	1:D:395:LYS:HD2	1.73	0.70
1:D:375:MET:CE	1:D:388:ARG:HD3	2.21	0.70
1:D:405:LYS:NZ	1:D:437:THR:CG2	2.55	0.70
1:A:145:ASP:CG	1:A:250:PRO:HG3	2.16	0.70
1:B:58:VAL:HG21	1:B:120:ARG:NH2	2.06	0.70
1:D:353:GLU:HG3	1:D:440:PRO:HG2	1.73	0.70
1:C:387:CYS:HB3	1:C:410:LEU:HD23	1.72	0.69
1:A:93:GLU:CD	1:A:93:GLU:H	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:HD11	1:A:436:VAL:HG21	1.75	0.69
1:B:388:ARG:NH1	1:B:450:LYS:HE2	2.07	0.69
1:C:443:THR:HG22	1:C:446:ASP:OD2	1.93	0.68
1:C:352:VAL:HG21	1:C:436:VAL:HG13	1.73	0.68
1:D:252:ARG:HH21	1:D:254:LEU:HD11	1.57	0.68
1:D:301:THR:OG1	1:D:327:ARG:HG2	1.93	0.68
1:D:375:MET:HE3	1:D:388:ARG:HD3	1.75	0.68
1:B:389:ILE:HG12	1:B:408:LEU:CD2	2.23	0.68
1:A:352:VAL:CG1	1:A:416:LEU:HD12	2.15	0.67
1:B:66:VAL:HG13	1:B:160:GLN:OE1	1.95	0.67
1:B:387:CYS:HB3	1:B:410:LEU:HD23	1.76	0.67
1:B:450:LYS:HD3	1:B:450:LYS:H	1.59	0.67
1:B:268:ILE:HG23	1:B:271:ARG:HB2	1.75	0.67
1:D:104:ARG:HG2	1:D:104:ARG:HH11	1.60	0.67
1:C:166:LEU:O	1:C:170:GLN:HG3	1.94	0.66
1:C:389:ILE:C	1:C:390:ILE:HD12	2.20	0.66
1:D:209:LYS:O	1:D:213:THR:HG23	1.94	0.66
1:D:447:LYS:HB3	4:D:1522:HOH:O	1.95	0.66
1:B:291:GLU:OE2	1:B:293:LEU:HD21	1.95	0.66
1:B:451:TRP:HB3	4:B:1451:HOH:O	1.96	0.66
1:D:65:HIS:HD2	1:D:160:GLN:H	1.44	0.66
1:A:368:LYS:H	1:A:368:LYS:CD	1.97	0.66
1:C:371:VAL:HG12	1:C:397:LEU:HD23	1.78	0.66
1:C:145:ASP:OD1	1:C:250:PRO:HG3	1.95	0.65
1:C:371:VAL:HG12	1:C:397:LEU:CD2	2.27	0.65
1:A:416:LEU:HD13	1:A:436:VAL:HG21	1.78	0.65
1:D:322:LEU:C	1:D:322:LEU:HD12	2.22	0.65
1:A:372:SER:O	1:A:373:HIS:HB2	1.97	0.65
1:C:443:THR:HG22	1:C:446:ASP:CG	2.22	0.65
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.61	0.65
1:C:102:ARG:HE	1:C:105:GLY:HA2	1.61	0.65
1:A:298:ASN:HB2	4:A:1664:HOH:O	1.97	0.64
1:A:449:ILE:H	1:A:449:ILE:CD1	2.08	0.64
1:A:416:LEU:HD11	1:A:436:VAL:CG2	2.27	0.64
1:A:344:GLY:O	1:D:418:LYS:NZ	2.31	0.63
1:B:352:VAL:HG23	1:B:438:ASP:O	1.98	0.63
1:C:102:ARG:HB2	4:C:1543:HOH:O	1.99	0.63
1:C:279:LEU:HD23	1:C:317:GLU:C	2.23	0.63
1:D:231:LEU:HD23	4:D:1351:HOH:O	1.98	0.63
1:D:252:ARG:NH2	1:D:254:LEU:HD21	2.14	0.63
1:A:229:PRO:O	1:A:234:LYS:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLY:HA3	1:C:421:ARG:NE	2.13	0.63
1:C:449:ILE:C	1:C:449:ILE:HD12	2.23	0.63
1:B:390:ILE:HB	1:B:407:THR:HB	1.81	0.62
1:B:268:ILE:HD13	1:B:271:ARG:HD3	1.81	0.62
1:B:65:HIS:HD2	1:B:160:GLN:H	1.46	0.62
1:D:89:PHE:CD1	1:D:89:PHE:C	2.78	0.62
1:D:246:TYR:O	1:D:248:PRO:HD3	2.00	0.62
1:B:137:MET:HE3	1:B:167:LEU:HD13	1.82	0.62
1:B:268:ILE:CG2	1:B:271:ARG:HB2	2.29	0.62
1:D:60:VAL:HG12	1:D:61:GLY:N	2.15	0.61
1:D:366:ARG:NH1	1:D:368:LYS:O	2.33	0.61
1:D:239:LEU:O	1:D:243:VAL:HG23	2.01	0.60
1:D:80:ILE:HD13	1:D:233:LEU:HD12	1.82	0.60
1:A:409:ILE:HG23	1:A:442:MET:HE1	1.82	0.60
1:B:216:ILE:HD12	1:B:216:ILE:N	2.16	0.60
1:C:108:ILE:HD12	1:C:132:ASP:HA	1.83	0.60
1:D:431:ILE:HD12	1:D:432:GLY:N	2.16	0.60
1:B:93:GLU:CD	1:B:93:GLU:H	2.08	0.60
1:D:353:GLU:HG3	1:D:440:PRO:CG	2.31	0.60
1:D:131:ALA:O	1:D:135:LYS:HG3	2.01	0.60
1:D:352:VAL:HG22	1:D:436:VAL:HG13	1.83	0.60
1:D:350:GLN:HG3	1:D:410:LEU:O	2.02	0.59
1:C:65:HIS:HE1	4:C:1571:HOH:O	1.85	0.59
1:D:194:LEU:HD23	4:D:1541:HOH:O	2.01	0.59
1:D:431:ILE:HD12	1:D:431:ILE:C	2.27	0.59
1:C:425:ARG:HD3	4:C:1546:HOH:O	2.01	0.59
1:A:330:LYS:HG2	1:A:333:ASP:OD1	2.03	0.59
1:D:405:LYS:HZ2	1:D:437:THR:CB	2.15	0.59
1:C:293:LEU:HB3	1:C:348:PRO:HG3	1.83	0.59
1:B:83:GLU:C	1:B:85:GLY:H	2.09	0.59
1:C:171:ILE:HG22	1:C:435:LEU:HD22	1.83	0.59
1:B:265:VAL:HB	1:B:331:ARG:HH12	1.68	0.59
1:B:438:ASP:C	1:B:440:PRO:HD3	2.28	0.59
1:A:368:LYS:N	1:A:368:LYS:CD	2.63	0.59
1:B:192:VAL:O	1:B:195:VAL:HG12	2.02	0.58
1:C:322:LEU:HD12	1:C:322:LEU:C	2.28	0.58
1:D:433:THR:HG22	4:D:1362:HOH:O	2.03	0.58
1:A:65:HIS:HD2	1:A:160:GLN:H	1.51	0.58
1:C:390:ILE:HD12	1:C:390:ILE:N	2.17	0.58
1:D:374:PHE:CD2	1:D:376:PRO:HG3	2.39	0.58
1:B:373:HIS:HA	1:B:388:ARG:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:MET:SD	1:D:411:ARG:HG3	2.44	0.58
1:C:360:THR:HG22	1:C:362:GLU:H	1.67	0.58
1:B:352:VAL:HG23	1:B:436:VAL:HG13	1.82	0.58
1:B:146:GLY:HA3	1:B:247:ILE:HD12	1.85	0.57
1:C:278:THR:HG23	4:C:1367:HOH:O	2.04	0.57
1:D:361:LYS:HD3	1:D:367:HIS:CD2	2.38	0.57
1:A:307:GLU:HG2	4:A:1352:HOH:O	2.02	0.57
1:D:166:LEU:O	1:D:170:GLN:HG3	2.05	0.57
1:D:315:ARG:HG2	4:D:1394:HOH:O	2.05	0.57
1:D:385:MET:SD	1:D:411:ARG:CG	2.92	0.57
1:C:428:ASN:HA	4:C:1546:HOH:O	2.04	0.57
1:A:442:MET:HE3	1:A:446:ASP:HB3	1.86	0.57
1:D:368:LYS:N	1:D:368:LYS:CD	2.66	0.57
1:A:197:LEU:O	1:A:201:GLU:HG3	2.04	0.57
1:C:372:SER:O	1:C:373:HIS:HB2	2.04	0.57
1:A:449:ILE:CG1	1:A:451:TRP:NE1	2.61	0.57
1:C:145:ASP:OD2	1:C:250:PRO:HG3	2.04	0.57
1:B:119:ALA:C	1:B:120:ARG:HG3	2.30	0.57
1:A:260:LEU:HD13	1:A:260:LEU:C	2.30	0.56
1:B:395:LYS:HE2	1:B:404:LEU:HD13	1.86	0.56
1:C:133:TYR:HB3	1:C:137:MET:HE2	1.87	0.56
1:A:449:ILE:HD13	1:A:449:ILE:N	2.15	0.56
1:B:135:LYS:HE2	1:B:357:TYR:CZ	2.40	0.56
1:B:395:LYS:HE2	1:B:404:LEU:CD1	2.36	0.56
1:D:366:ARG:HD3	1:D:370:PHE:HD2	1.71	0.56
1:A:120:ARG:NH1	1:A:247:ILE:O	2.37	0.56
1:B:127:CYS:HB2	1:B:133:TYR:CE1	2.40	0.56
1:B:133:TYR:HB3	1:B:137:MET:HE2	1.86	0.56
1:C:62:THR:HG23	1:C:124:HIS:CE1	2.40	0.56
1:D:197:LEU:O	1:D:201:GLU:HG2	2.05	0.56
1:D:295:HIS:O	1:D:297:LYS:HG3	2.05	0.56
1:D:258:PHE:HB2	1:D:279:LEU:HD11	1.88	0.56
1:C:188:ASP:HB2	1:C:190:GLU:OE1	2.06	0.56
1:A:191:MET:HE3	1:A:191:MET:HA	1.87	0.55
1:B:57:HIS:HB2	4:B:1431:HOH:O	2.05	0.55
1:B:335:ARG:NH2	4:B:1309:HOH:O	2.39	0.55
1:C:429:ARG:HH11	1:C:429:ARG:HB2	1.71	0.55
1:B:392:PRO:HG3	1:B:405:LYS:O	2.07	0.55
1:D:98:ALA:HB1	1:D:110:ALA:C	2.31	0.55
1:D:222:CYS:HB3	1:D:227:ARG:O	2.07	0.55
1:A:216:ILE:N	1:A:216:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:CD2	1:B:160:GLN:HB2	2.42	0.55
1:D:390:ILE:HB	1:D:407:THR:HB	1.86	0.55
1:B:433:THR:HG22	4:B:1357:HOH:O	2.06	0.55
1:A:322:LEU:HD12	1:A:322:LEU:C	2.31	0.55
1:D:399:MET:HB2	1:D:402:GLU:CD	2.32	0.55
1:B:330:LYS:HB3	1:B:332:GLU:OE2	2.07	0.55
1:C:121:HIS:HB2	4:C:1471:HOH:O	2.07	0.55
1:C:65:HIS:HD2	1:C:160:GLN:H	1.53	0.55
1:D:57:HIS:CE1	1:D:123:ALA:HB2	2.41	0.55
1:C:102:ARG:NE	1:C:105:GLY:HA2	2.22	0.55
1:D:79:LYS:HD2	1:D:91:LYS:NZ	2.22	0.55
1:C:295:HIS:CE1	1:C:414:MET:HE1	2.42	0.54
1:D:191:MET:O	1:D:195:VAL:HG23	2.07	0.54
1:D:58:VAL:HB	1:D:122:TYR:CE1	2.41	0.54
1:D:263:GLU:HG3	4:D:1384:HOH:O	2.06	0.54
1:A:390:ILE:N	1:A:390:ILE:HD12	2.22	0.54
1:D:223:ALA:HB2	1:D:232:GLY:C	2.33	0.54
1:D:351:LYS:HB2	1:D:442:MET:SD	2.47	0.54
1:A:209:LYS:O	1:A:213:THR:HG23	2.08	0.54
1:A:404:LEU:HD23	1:A:404:LEU:N	2.22	0.54
1:B:312:SER:O	1:B:313:LEU:HD23	2.08	0.54
1:B:353:GLU:HG3	1:B:440:PRO:CG	2.37	0.54
1:C:378:MET:CE	1:C:408:LEU:HD22	2.38	0.54
1:A:243:VAL:HG13	1:A:247:ILE:HD12	1.88	0.54
1:D:233:LEU:O	1:D:237:GLN:HG3	2.08	0.54
1:C:135:LYS:HE2	1:C:357:TYR:CZ	2.42	0.54
1:B:416:LEU:HD22	1:B:436:VAL:CG2	2.35	0.53
1:D:60:VAL:CG1	1:D:61:GLY:N	2.71	0.53
1:B:139:THR:O	1:B:139:THR:HG22	2.08	0.53
1:B:106:ILE:HG23	1:B:363:GLU:OE2	2.08	0.53
1:B:190:GLU:H	1:B:190:GLU:CD	2.17	0.53
1:B:227:ARG:O	1:B:228:ASP:C	2.51	0.53
1:C:353:GLU:OE2	1:C:440:PRO:HG2	2.08	0.53
1:D:366:ARG:C	1:D:368:LYS:H	2.16	0.53
1:A:352:VAL:HG11	1:A:416:LEU:HD11	1.87	0.53
1:C:252:ARG:HH21	1:C:254:LEU:HD11	1.73	0.53
1:B:62:THR:HG23	1:B:124:HIS:CE1	2.44	0.53
1:B:140:GLY:HA3	1:B:421:ARG:NE	2.24	0.53
1:D:104:ARG:HG2	1:D:104:ARG:NH1	2.23	0.53
1:C:360:THR:CG2	1:C:362:GLU:HG2	2.38	0.53
1:C:360:THR:HG22	1:C:361:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PRO:HD2	1:A:395:LYS:CB	2.39	0.53
1:B:450:LYS:HD2	4:B:1457:HOH:O	2.09	0.53
1:C:366:ARG:NH1	1:C:370:PHE:HB3	2.23	0.52
1:B:120:ARG:HH11	1:B:244:ASP:HA	1.73	0.52
1:D:378:MET:CE	1:D:408:LEU:HD13	2.39	0.52
1:D:443:THR:CG2	1:D:445:GLU:HB3	2.38	0.52
1:D:443:THR:C	1:D:445:GLU:N	2.66	0.52
1:A:65:HIS:CD2	1:A:160:GLN:HB2	2.44	0.52
1:B:65:HIS:CE1	1:B:66:VAL:HG22	2.45	0.52
1:A:82:ALA:HA	1:A:87:ALA:O	2.09	0.52
1:B:178:VAL:HB	1:B:215:ILE:HG12	1.91	0.52
1:C:411:ARG:HA	1:C:451:TRP:CZ2	2.45	0.52
1:D:257:PRO:CB	1:D:345:SER:HB2	2.39	0.52
1:D:387:CYS:HB3	1:D:410:LEU:HD23	1.91	0.52
1:A:89:PHE:CE2	1:A:91:LYS:HG2	2.45	0.52
1:A:158:MET:HB3	1:A:159:PRO:CD	2.39	0.52
1:A:279:LEU:HD23	1:A:317:GLU:C	2.35	0.52
1:B:89:PHE:CD1	1:B:89:PHE:C	2.88	0.52
1:C:448:ASN:ND2	1:C:448:ASN:O	2.43	0.52
1:D:375:MET:HA	1:D:387:CYS:O	2.09	0.52
1:D:62:THR:O	1:D:133:TYR:CE2	2.63	0.52
1:D:243:VAL:HG13	1:D:247:ILE:HD12	1.90	0.52
1:D:404:LEU:N	1:D:404:LEU:HD23	2.25	0.52
1:B:58:VAL:CG2	1:B:120:ARG:HH21	2.22	0.51
1:B:316:ALA:CB	1:B:322:LEU:HD22	2.41	0.51
1:D:352:VAL:CG2	1:D:436:VAL:HG13	2.40	0.51
1:B:118:ALA:HB3	4:B:1561:HOH:O	2.09	0.51
1:B:187:GLN:HA	4:B:1458:HOH:O	2.11	0.51
1:D:213:THR:HG22	4:D:1500:HOH:O	2.11	0.51
1:D:346:ILE:CD1	1:D:415:ILE:HG23	2.41	0.51
1:B:378:MET:HE2	1:B:408:LEU:HD13	1.92	0.51
1:B:389:ILE:HG12	1:B:408:LEU:HD21	1.91	0.51
1:A:374:PHE:CD2	1:A:376:PRO:HG3	2.45	0.51
1:B:57:HIS:CE1	1:B:123:ALA:HB2	2.45	0.51
1:B:260:LEU:C	1:B:260:LEU:HD13	2.36	0.51
1:B:449:ILE:HG12	1:B:450:LYS:N	2.26	0.51
1:B:188:ASP:HB3	1:B:190:GLU:OE1	2.11	0.51
1:B:349:HIS:ND1	1:B:439:THR:HG21	2.25	0.51
1:D:191:MET:HE3	1:D:191:MET:HA	1.93	0.51
1:D:271:ARG:HG2	1:D:325:LEU:HD11	1.92	0.51
1:B:443:THR:CG2	1:B:445:GLU:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:MET:O	1:B:402:GLU:HB3	2.11	0.51
1:D:65:HIS:HA	1:D:160:GLN:HB2	1.92	0.51
1:B:350:GLN:HG2	1:B:442:MET:CE	2.41	0.51
1:B:352:VAL:HG22	1:B:353:GLU:N	2.26	0.51
1:D:284:LEU:HD23	1:D:285:LYS:N	2.26	0.51
1:C:55:LYS:HB2	1:C:56:PRO:CD	2.40	0.50
1:A:332:GLU:CB	1:C:229:PRO:HG3	2.39	0.50
1:C:147:CYS:O	1:C:176:VAL:HG13	2.11	0.50
1:C:369:PRO:HG3	1:C:400:PRO:CG	2.42	0.50
1:D:106:ILE:HD11	1:D:433:THR:OG1	2.11	0.50
1:D:405:LYS:NZ	1:D:437:THR:OG1	2.43	0.50
1:B:167:LEU:O	1:B:171:ILE:HG23	2.11	0.50
1:D:104:ARG:NH2	1:D:430:THR:OG1	2.44	0.50
1:B:234:LYS:O	1:B:238:LYS:HG3	2.11	0.50
1:D:74:THR:HG22	1:D:95:ILE:HD13	1.92	0.50
1:A:252:ARG:HD3	4:A:1418:HOH:O	2.12	0.50
1:B:283:ILE:HD13	1:B:315:ARG:NH2	2.27	0.50
1:D:93:GLU:CD	1:D:93:GLU:H	2.20	0.50
1:C:451:TRP:HB2	4:C:1523:HOH:O	2.12	0.50
1:D:98:ALA:CB	1:D:111:ALA:HB2	2.36	0.50
1:D:137:MET:HE3	1:D:167:LEU:HD13	1.94	0.50
1:B:378:MET:CE	1:B:408:LEU:HD13	2.42	0.50
1:C:443:THR:HG23	1:C:446:ASP:H	1.77	0.50
1:D:283:ILE:HD12	1:D:315:ARG:NH2	2.27	0.50
1:D:389:ILE:HG12	1:D:408:LEU:CD2	2.42	0.50
1:B:58:VAL:HG21	1:B:120:ARG:CZ	2.42	0.50
1:B:265:VAL:HB	1:B:331:ARG:NH1	2.26	0.50
1:C:91:LYS:HD3	1:C:94:GLU:OE2	2.12	0.50
1:D:259:LEU:HD11	1:D:339:VAL:HG11	1.93	0.50
1:D:285:LYS:N	1:D:288:ASP:OD2	2.44	0.49
1:B:443:THR:HG22	1:B:445:GLU:H	1.76	0.49
1:C:188:ASP:C	1:C:190:GLU:N	2.69	0.49
1:D:216:ILE:N	1:D:216:ILE:HD12	2.26	0.49
1:A:57:HIS:CE1	1:A:123:ALA:HB2	2.47	0.49
1:B:369:PRO:CG	1:B:399:MET:SD	3.00	0.49
1:D:79:LYS:HD2	1:D:91:LYS:HZ3	1.77	0.49
1:B:446:ASP:O	1:B:449:ILE:HG22	2.13	0.49
1:D:291:GLU:CD	1:D:293:LEU:HD21	2.37	0.49
1:A:86:GLY:O	1:A:87:ALA:HB2	2.12	0.49
1:B:418:LYS:HA	1:B:436:VAL:HG12	1.95	0.49
1:C:450:LYS:HD3	1:C:450:LYS:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:C	1:A:431:ILE:HD12	2.38	0.49
1:D:285:LYS:HB2	1:D:285:LYS:NZ	2.28	0.49
1:D:418:LYS:HA	1:D:436:VAL:HG12	1.95	0.49
1:C:89:PHE:CZ	1:C:91:LYS:HE3	2.48	0.49
1:D:62:THR:HG23	1:D:124:HIS:NE2	2.28	0.49
1:D:158:MET:HB3	1:D:159:PRO:CD	2.43	0.49
1:C:188:ASP:OD2	1:C:191:MET:HB2	2.13	0.49
1:B:186:VAL:HG12	1:B:188:ASP:H	1.78	0.49
1:D:120:ARG:HD2	1:D:122:TYR:OH	2.12	0.49
1:C:127:CYS:HB2	1:C:133:TYR:CE1	2.48	0.49
1:C:216:ILE:N	1:C:216:ILE:HD12	2.28	0.49
1:A:192:VAL:HG12	1:A:196:GLU:OE2	2.12	0.48
1:A:204:THR:HA	1:A:208:TYR:O	2.12	0.48
1:B:149:LEU:HD11	1:B:161:THR:HG23	1.94	0.48
1:B:350:GLN:HB2	1:B:413:PRO:HG3	1.95	0.48
1:C:65:HIS:HA	1:C:160:GLN:HB2	1.95	0.48
1:D:346:ILE:HD11	1:D:415:ILE:HG23	1.95	0.48
1:D:355:GLN:OE1	1:D:405:LYS:HE2	2.14	0.48
1:C:418:LYS:HA	1:C:436:VAL:HG12	1.94	0.48
1:C:373:HIS:CD2	1:C:388:ARG:NE	2.81	0.48
1:A:369:PRO:CG	1:A:399:MET:SD	3.01	0.48
1:B:380:SER:HB3	1:B:383:TRP:CZ2	2.49	0.48
1:B:443:THR:HB	1:B:446:ASP:OD2	2.12	0.48
1:C:279:LEU:HD23	1:C:317:GLU:CA	2.42	0.48
1:D:371:VAL:HG23	1:D:373:HIS:H	1.78	0.48
1:B:88:LYS:HD3	1:B:89:PHE:N	2.28	0.48
1:B:431:ILE:C	1:B:431:ILE:HD12	2.39	0.48
1:D:87:ALA:O	1:D:88:LYS:C	2.56	0.48
1:B:350:GLN:HG2	1:B:442:MET:HE3	1.95	0.48
1:B:404:LEU:HD11	1:B:406:LEU:HD21	1.95	0.48
1:C:295:HIS:O	1:C:297:LYS:HG3	2.13	0.48
1:A:188:ASP:OD2	1:A:190:GLU:HG2	2.14	0.48
1:B:67:ASP:OD1	1:B:67:ASP:O	2.31	0.48
1:B:373:HIS:HA	1:B:388:ARG:HG2	1.94	0.48
1:A:389:ILE:C	1:A:390:ILE:HD12	2.39	0.48
1:B:225:GLU:HB2	1:B:227:ARG:HD3	1.96	0.48
1:A:142:ALA:HB2	4:A:1496:HOH:O	2.14	0.48
1:A:295:HIS:CE1	1:A:414:MET:HE1	2.49	0.48
1:B:409:ILE:HG23	1:B:442:MET:CE	2.40	0.48
1:B:204:THR:HA	1:B:208:TYR:O	2.14	0.47
1:B:418:LYS:HE2	1:B:439:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HE	1:C:105:GLY:CA	2.26	0.47
1:C:350:GLN:HG3	1:C:410:LEU:O	2.14	0.47
1:B:73:LEU:O	1:B:77:ILE:HG13	2.14	0.47
1:B:308:MET:CE	1:B:313:LEU:HD12	2.41	0.47
1:B:409:ILE:CG2	1:B:442:MET:HE1	2.40	0.47
1:D:283:ILE:HD12	1:D:315:ARG:CZ	2.44	0.47
1:A:62:THR:HG23	1:A:124:HIS:CE1	2.50	0.47
1:D:79:LYS:HD3	1:D:224:LEU:HD12	1.96	0.47
1:D:342:LYS:HE3	4:D:1451:HOH:O	2.13	0.47
1:D:358:ILE:O	1:D:401:GLY:N	2.38	0.47
1:C:252:ARG:NH2	1:C:317:GLU:OE2	2.48	0.47
1:B:190:GLU:O	1:B:194:LEU:HG	2.15	0.47
1:B:225:GLU:O	1:B:227:ARG:HG3	2.14	0.47
1:C:374:PHE:HE2	1:C:431:ILE:CD1	2.27	0.47
1:B:190:GLU:CD	1:B:190:GLU:N	2.73	0.47
1:B:371:VAL:HG12	1:B:397:LEU:HD23	1.97	0.47
1:C:409:ILE:CG2	1:C:442:MET:HE1	2.45	0.47
1:B:58:VAL:HG21	1:B:120:ARG:NE	2.30	0.47
1:C:451:TRP:CD1	1:C:451:TRP:N	2.83	0.47
1:D:130:HIS:ND1	1:D:160:GLN:HG2	2.30	0.47
1:D:260:LEU:HD13	1:D:260:LEU:C	2.39	0.47
1:C:158:MET:HB3	1:C:159:PRO:CD	2.45	0.46
1:C:346:ILE:HD12	1:C:415:ILE:HD12	1.97	0.46
1:D:215:ILE:C	1:D:216:ILE:HD12	2.39	0.46
1:A:79:LYS:HB2	1:A:89:PHE:CE1	2.51	0.46
1:A:80:ILE:HD12	1:A:236:VAL:HG11	1.96	0.46
1:C:438:ASP:C	1:C:440:PRO:HD3	2.41	0.46
1:D:252:ARG:NH2	1:D:317:GLU:OE2	2.35	0.46
1:D:385:MET:SD	1:D:411:ARG:NE	2.80	0.46
1:D:405:LYS:HB3	4:D:1478:HOH:O	2.15	0.46
1:B:82:ALA:HA	4:B:1330:HOH:O	2.15	0.46
1:C:332:GLU:CD	1:C:332:GLU:N	2.72	0.46
1:C:421:ARG:HG2	1:C:421:ARG:HH11	1.79	0.46
1:A:114:GLU:OE1	1:A:121:HIS:NE2	2.46	0.46
1:B:404:LEU:N	1:B:404:LEU:HD23	2.30	0.46
1:C:90:LYS:HD2	1:C:113:VAL:HG12	1.96	0.46
1:D:366:ARG:HG3	1:D:368:LYS:O	2.16	0.46
1:B:263:GLU:HG2	1:B:277:GLY:HA2	1.97	0.46
1:D:57:HIS:HE1	1:D:123:ALA:HB2	1.81	0.46
1:D:283:ILE:HG22	4:D:1450:HOH:O	2.16	0.46
1:B:331:ARG:HG3	1:B:331:ARG:NH1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG22	1:B:445:GLU:HG2	1.98	0.46
1:C:253:ASP:HB3	1:C:256:LYS:HD2	1.97	0.46
1:D:158:MET:HE3	1:D:159:PRO:HD3	1.97	0.46
1:D:195:VAL:O	1:D:199:ILE:HG13	2.15	0.46
1:D:252:ARG:NH2	1:D:254:LEU:HD11	2.27	0.46
1:D:260:LEU:HD11	1:D:277:GLY:HA3	1.98	0.46
1:B:215:ILE:C	1:B:216:ILE:HD12	2.41	0.46
1:B:225:GLU:OE1	1:B:227:ARG:NH1	2.46	0.46
1:C:376:PRO:HG3	1:C:389:ILE:HD11	1.97	0.46
1:D:91:LYS:HD3	1:D:92:TYR:N	2.20	0.46
1:D:190:GLU:O	1:D:194:LEU:HG	2.16	0.46
1:D:366:ARG:HD3	1:D:370:PHE:CD2	2.49	0.46
1:D:373:HIS:HB3	1:D:388:ARG:NH2	2.30	0.46
1:B:145:ASP:OD1	1:B:250:PRO:HG3	2.13	0.46
1:C:227:ARG:O	1:C:228:ASP:C	2.58	0.46
1:D:134:VAL:O	1:D:138:ILE:HG13	2.16	0.46
1:B:124:HIS:C	1:B:124:HIS:CD2	2.94	0.46
1:B:442:MET:SD	1:B:446:ASP:HB3	2.56	0.46
1:C:254:LEU:HD22	1:C:317:GLU:HB2	1.98	0.46
1:A:392:PRO:HD2	1:A:395:LYS:HB2	1.98	0.45
1:B:292:PHE:HZ	1:B:326:VAL:HG11	1.81	0.45
1:B:297:LYS:HE2	1:B:297:LYS:HB3	1.77	0.45
1:A:222:CYS:HB3	1:A:227:ARG:O	2.17	0.45
1:B:158:MET:HB3	1:B:159:PRO:CD	2.46	0.45
1:D:366:ARG:O	1:D:368:LYS:N	2.49	0.45
1:D:392:PRO:HG2	1:D:405:LYS:O	2.16	0.45
1:D:409:ILE:O	1:D:451:TRP:HH2	1.99	0.45
1:A:108:ILE:CD1	1:A:110:ALA:HB2	2.40	0.45
1:A:188:ASP:OD2	1:A:190:GLU:HB2	2.17	0.45
1:B:356:VAL:O	1:B:403:ASP:HA	2.17	0.45
1:D:157:PRO:HD2	1:D:198:GLU:OE2	2.16	0.45
1:B:418:LYS:HE2	1:B:438:ASP:HA	1.98	0.45
1:C:182:LYS:HG2	3:C:1303:GDP:C6	2.52	0.45
1:C:366:ARG:HH11	1:C:370:PHE:HB3	1.80	0.45
1:D:60:VAL:O	1:D:124:HIS:HA	2.16	0.45
1:D:65:HIS:CD2	1:D:160:GLN:HB2	2.51	0.45
1:D:90:LYS:HE2	1:D:94:GLU:HG2	1.98	0.45
1:D:120:ARG:NH1	1:D:247:ILE:O	2.44	0.45
1:D:449:ILE:HG22	4:D:1508:HOH:O	2.15	0.45
1:C:252:ARG:NH2	1:C:254:LEU:HD11	2.30	0.45
1:D:271:ARG:NH2	4:D:1448:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:CD	1:A:93:GLU:N	2.71	0.45
1:A:404:LEU:HD11	1:A:406:LEU:HD21	1.99	0.45
1:B:83:GLU:C	1:B:85:GLY:N	2.75	0.45
1:C:404:LEU:HD11	1:C:406:LEU:HD21	1.99	0.45
1:B:195:VAL:O	1:B:199:ILE:HG13	2.17	0.45
1:D:91:LYS:HG3	1:D:93:GLU:OE1	2.15	0.45
1:A:106:ILE:HD13	1:A:433:THR:HG21	1.98	0.45
1:B:55:LYS:NZ	1:B:117:THR:O	2.48	0.45
1:B:388:ARG:NH2	1:B:449:ILE:HG13	2.32	0.45
1:D:356:VAL:O	1:D:403:ASP:HA	2.17	0.45
1:C:149:LEU:HD22	1:C:165:LEU:HD21	1.98	0.45
1:D:353:GLU:HB2	1:D:438:ASP:HB2	1.98	0.45
1:B:103:ALA:O	1:B:104:ARG:HB2	2.16	0.45
1:D:158:MET:HB3	1:D:159:PRO:HD2	1.99	0.45
1:A:409:ILE:HG21	1:A:442:MET:HE1	1.97	0.44
1:B:108:ILE:HD11	1:B:135:LYS:HB3	1.98	0.44
1:B:259:LEU:HD23	1:B:259:LEU:C	2.42	0.44
1:D:62:THR:O	1:D:133:TYR:HE2	1.99	0.44
1:D:366:ARG:H	1:D:431:ILE:HG22	1.82	0.44
1:A:189:SER:O	1:A:190:GLU:C	2.60	0.44
1:A:190:GLU:O	1:A:194:LEU:HG	2.17	0.44
1:A:362:GLU:OE1	1:A:362:GLU:N	2.41	0.44
1:A:416:LEU:HD13	1:A:416:LEU:C	2.43	0.44
1:A:449:ILE:HG13	1:A:451:TRP:HE1	1.80	0.44
1:C:283:ILE:HD13	1:C:315:ARG:NH2	2.32	0.44
1:D:367:HIS:HA	4:D:1336:HOH:O	2.16	0.44
1:A:188:ASP:HA	4:A:1477:HOH:O	2.17	0.44
1:A:260:LEU:C	1:A:260:LEU:CD1	2.90	0.44
1:B:182:LYS:HG2	3:B:1302:GDP:C6	2.52	0.44
1:D:252:ARG:HH22	1:D:317:GLU:CD	2.21	0.44
1:A:57:HIS:HE1	1:A:123:ALA:HB2	1.83	0.44
1:A:298:ASN:CG	1:A:298:ASN:O	2.60	0.44
1:C:378:MET:O	1:C:384:ASP:HA	2.17	0.44
1:C:102:ARG:HD3	4:C:1508:HOH:O	2.17	0.44
1:C:337:GLY:CA	1:C:383:TRP:HB3	2.48	0.44
1:C:443:THR:CG2	1:C:446:ASP:H	2.30	0.44
1:D:78:THR:C	4:D:1380:HOH:O	2.60	0.44
1:D:209:LYS:CB	1:D:212:GLU:HG2	2.46	0.44
1:A:212:GLU:OE2	1:A:212:GLU:N	2.49	0.44
1:D:62:THR:HG23	1:D:124:HIS:CE1	2.52	0.44
1:A:390:ILE:HB	1:A:407:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LYS:NZ	1:D:437:THR:CB	2.81	0.44
1:A:366:ARG:NH2	1:A:368:LYS:HG2	2.33	0.44
1:B:140:GLY:HA3	1:B:421:ARG:CZ	2.48	0.44
1:C:180:VAL:HB	1:C:217:VAL:HG22	2.00	0.44
1:D:102:ARG:NH1	1:D:102:ARG:HG3	2.32	0.44
1:D:103:ALA:O	1:D:104:ARG:HB3	2.18	0.44
1:D:291:GLU:HG2	1:D:293:LEU:HD21	2.00	0.44
1:A:353:GLU:HG3	1:A:440:PRO:HG2	1.99	0.44
1:C:263:GLU:HG3	4:C:1514:HOH:O	2.18	0.44
1:D:98:ALA:HA	1:D:99:PRO:HD3	1.80	0.44
1:D:380:SER:HB3	1:D:383:TRP:CZ2	2.53	0.44
1:D:130:HIS:O	1:D:134:VAL:HG23	2.18	0.43
1:D:252:ARG:CZ	1:D:254:LEU:HD21	2.47	0.43
1:A:378:MET:CE	1:A:408:LEU:HD22	2.48	0.43
1:B:349:HIS:CE1	1:B:439:THR:HG21	2.53	0.43
1:B:111:ALA:O	1:B:125:THR:HA	2.18	0.43
1:B:373:HIS:O	1:B:375:MET:HG3	2.19	0.43
1:B:388:ARG:HH12	1:B:450:LYS:CE	2.15	0.43
1:D:86:GLY:C	1:D:88:LYS:H	2.25	0.43
1:D:153:ALA:HB2	1:D:180:VAL:CG1	2.42	0.43
1:D:203:LEU:HD13	1:D:213:THR:OG1	2.18	0.43
1:D:347:GLN:HA	1:D:348:PRO:HD3	1.82	0.43
1:D:411:ARG:HA	1:D:451:TRP:CZ2	2.54	0.43
1:B:157:PRO:HD2	1:B:198:GLU:OE1	2.18	0.43
1:B:188:ASP:O	1:B:191:MET:HB3	2.19	0.43
1:C:171:ILE:HA	1:C:435:LEU:HD21	1.99	0.43
1:D:322:LEU:C	1:D:322:LEU:CD1	2.90	0.43
1:D:70:LYS:HA	1:D:150:VAL:HG21	2.00	0.43
1:A:233:LEU:O	1:A:237:GLN:HG3	2.19	0.43
1:B:171:ILE:HG22	1:B:435:LEU:HD22	2.00	0.43
1:B:290:CYS:SG	1:B:301:THR:HG23	2.59	0.43
1:C:188:ASP:C	1:C:190:GLU:H	2.26	0.43
1:C:361:LYS:NZ	4:C:1560:HOH:O	2.50	0.43
1:C:374:PHE:HE2	1:C:431:ILE:HD11	1.83	0.43
1:D:307:GLU:C	1:D:307:GLU:CD	2.86	0.43
1:C:55:LYS:HB2	1:C:56:PRO:HD2	1.99	0.43
1:D:371:VAL:C	1:D:373:HIS:H	2.25	0.43
1:A:130:HIS:ND1	1:A:160:GLN:HG2	2.34	0.43
1:C:356:VAL:O	1:C:403:ASP:HA	2.19	0.43
1:D:114:GLU:HB3	1:D:121:HIS:HE1	1.83	0.43
1:D:285:LYS:HB2	1:D:285:LYS:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:THR:C	1:D:445:GLU:H	2.27	0.43
1:A:106:ILE:CD1	1:A:433:THR:HG21	2.49	0.43
1:C:330:LYS:HB3	1:C:333:ASP:OD1	2.18	0.43
1:C:444:GLU:HA	1:C:447:LYS:HD3	2.01	0.43
1:D:158:MET:HE3	1:D:159:PRO:CD	2.49	0.43
1:D:405:LYS:HZ2	1:D:437:THR:CG2	2.32	0.43
1:A:438:ASP:C	1:A:440:PRO:HD3	2.43	0.42
1:B:181:ASN:CG	1:B:182:LYS:N	2.77	0.42
1:B:216:ILE:N	1:B:216:ILE:CD1	2.81	0.42
1:B:353:GLU:CG	1:B:440:PRO:HG2	2.44	0.42
1:C:373:HIS:HD2	1:C:388:ARG:NE	2.17	0.42
1:C:396:GLU:O	1:C:397:LEU:HD23	2.18	0.42
1:B:395:LYS:HE3	1:B:395:LYS:HB3	1.88	0.42
1:C:360:THR:HG21	1:C:362:GLU:HG2	2.01	0.42
1:D:79:LYS:CD	1:D:224:LEU:HD12	2.49	0.42
1:D:183:ALA:HB3	1:D:231:LEU:HD22	2.01	0.42
1:D:366:ARG:HH12	1:D:369:PRO:C	2.27	0.42
1:B:181:ASN:CG	1:B:182:LYS:H	2.28	0.42
1:C:176:VAL:O	1:C:213:THR:HG23	2.19	0.42
1:C:258:PHE:HB2	1:C:279:LEU:HD11	2.02	0.42
1:D:372:SER:O	1:D:389:ILE:O	2.38	0.42
1:A:69:GLY:HA3	1:A:181:ASN:ND2	2.35	0.42
1:B:335:ARG:HG3	1:B:336:ARG:N	2.34	0.42
1:D:107:THR:O	1:D:135:LYS:NZ	2.45	0.42
1:D:189:SER:O	1:D:193:GLU:HG3	2.20	0.42
1:A:266:TYR:HB2	1:A:331:ARG:HH21	1.84	0.42
1:A:399:MET:O	1:A:402:GLU:HB3	2.20	0.42
1:B:58:VAL:HG21	1:B:120:ARG:HE	1.83	0.42
1:C:392:PRO:HD2	1:C:395:LYS:HB2	2.02	0.42
1:D:209:LYS:HB2	1:D:212:GLU:HG2	2.00	0.42
1:D:379:PHE:CE1	1:D:425:ARG:HD3	2.54	0.42
1:B:169:ARG:HA	1:B:169:ARG:HD2	1.91	0.42
1:C:390:ILE:HB	1:C:407:THR:HB	2.01	0.42
1:C:425:ARG:CD	4:C:1546:HOH:O	2.65	0.42
1:D:127:CYS:HB2	1:D:133:TYR:CE1	2.55	0.42
1:D:285:LYS:HB2	1:D:288:ASP:OD2	2.20	0.42
1:A:372:SER:O	1:A:373:HIS:CB	2.67	0.42
1:B:204:THR:HG23	1:C:255:GLU:HB3	2.01	0.42
1:B:379:PHE:CE1	1:B:425:ARG:HD2	2.54	0.42
1:C:56:PRO:HB2	1:C:120:ARG:HG2	2.02	0.42
1:C:197:LEU:HD23	4:C:1405:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:ASP:C	1:D:440:PRO:HD3	2.45	0.42
1:A:71:THR:HG23	1:A:95:ILE:HG22	2.02	0.42
1:A:79:LYS:HE3	1:A:89:PHE:CD1	2.55	0.42
1:B:80:ILE:HD13	1:B:233:LEU:HD12	2.02	0.42
1:C:191:MET:O	1:C:195:VAL:HG23	2.20	0.42
1:D:90:LYS:CG	1:D:94:GLU:HG2	2.45	0.42
1:D:405:LYS:HD3	1:D:405:LYS:HA	1.85	0.42
1:C:91:LYS:N	1:C:91:LYS:HD2	2.35	0.42
1:C:404:LEU:N	1:C:404:LEU:HD23	2.35	0.42
1:A:400:PRO:HD2	4:A:1631:HOH:O	2.20	0.41
1:A:447:LYS:O	1:A:449:ILE:HD13	2.20	0.41
1:A:55:LYS:HE2	1:A:118:ALA:O	2.19	0.41
1:A:127:CYS:HA	1:A:128:PRO:HD3	1.89	0.41
1:A:404:LEU:HD23	1:A:404:LEU:H	1.85	0.41
1:B:145:ASP:OD2	1:B:250:PRO:HG3	2.21	0.41
1:B:176:VAL:O	1:B:213:THR:HG23	2.21	0.41
1:C:80:ILE:HD12	1:C:236:VAL:HG11	2.02	0.41
1:C:135:LYS:HE2	1:C:357:TYR:CE1	2.55	0.41
1:A:408:LEU:HD12	1:A:408:LEU:N	2.34	0.41
1:B:339:VAL:HB	1:B:415:ILE:HG13	2.02	0.41
1:C:411:ARG:HG2	1:C:411:ARG:HH11	1.85	0.41
1:D:204:THR:HA	1:D:208:TYR:O	2.21	0.41
1:D:252:ARG:NH1	1:D:318:ALA:O	2.53	0.41
1:B:308:MET:SD	1:B:320:ASP:HB3	2.60	0.41
1:D:258:PHE:CD1	1:D:258:PHE:C	2.98	0.41
1:A:158:MET:HB3	1:A:159:PRO:HD2	2.02	0.41
1:C:158:MET:HB3	1:C:159:PRO:HD2	2.03	0.41
1:D:352:VAL:HG22	1:D:438:ASP:O	2.20	0.41
1:D:366:ARG:NH1	1:D:369:PRO:C	2.79	0.41
1:B:135:LYS:HE2	1:B:357:TYR:OH	2.20	0.41
1:B:350:GLN:CG	1:B:442:MET:HE3	2.51	0.41
1:C:166:LEU:HB2	1:C:206:PHE:CE2	2.56	0.41
1:C:258:PHE:CD1	1:C:258:PHE:C	2.98	0.41
1:D:325:LEU:HD23	1:D:326:VAL:N	2.35	0.41
1:A:186:VAL:CG1	1:A:191:MET:HB3	2.51	0.41
1:B:291:GLU:OE1	1:B:300:ARG:HD3	2.21	0.41
1:B:332:GLU:CD	1:B:332:GLU:N	2.75	0.41
1:B:352:VAL:CG2	1:B:353:GLU:N	2.84	0.41
1:D:104:ARG:CZ	1:D:430:THR:OG1	2.68	0.41
1:D:122:TYR:OH	1:D:244:ASP:HA	2.20	0.41
1:D:180:VAL:N	1:D:216:ILE:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LYS:HG2	3:D:1304:GDP:C6	2.55	0.41
1:A:275:VAL:CG1	1:A:334:LEU:HD13	2.51	0.41
1:C:55:LYS:N	4:C:1510:HOH:O	2.54	0.41
1:B:389:ILE:HD11	1:B:424:LEU:HD13	2.03	0.41
1:B:443:THR:HG22	1:B:444:GLU:N	2.35	0.41
1:C:66:VAL:O	1:C:67:ASP:HB2	2.21	0.41
1:C:374:PHE:CD2	1:C:376:PRO:HD3	2.56	0.41
1:D:74:THR:O	1:D:77:ILE:HB	2.20	0.41
1:D:359:LEU:N	1:D:359:LEU:HD12	2.35	0.41
1:D:361:LYS:HD3	1:D:367:HIS:NE2	2.35	0.41
1:D:416:LEU:HD22	1:D:436:VAL:CG2	2.38	0.41
1:A:149:LEU:HD22	1:A:165:LEU:HD21	2.01	0.41
1:B:80:ILE:HD12	1:B:236:VAL:HG11	2.03	0.41
1:C:213:THR:HA	1:C:214:PRO:HD3	1.95	0.41
1:C:421:ARG:HG2	1:C:421:ARG:NH1	2.36	0.41
1:D:279:LEU:HD23	1:D:317:GLU:C	2.46	0.41
1:B:268:ILE:HG23	1:B:268:ILE:O	2.21	0.40
1:B:301:THR:OG1	1:B:302:VAL:N	2.48	0.40
1:C:228:ASP:N	1:C:229:PRO:HD3	2.35	0.40
1:C:317:GLU:O	1:C:318:ALA:C	2.64	0.40
1:A:260:LEU:HD21	1:A:277:GLY:C	2.46	0.40
1:D:104:ARG:C	1:D:106:ILE:H	2.29	0.40
1:A:271:ARG:HD2	4:A:1684:HOH:O	2.21	0.40
1:C:178:VAL:HB	1:C:215:ILE:HG12	2.02	0.40
1:C:188:ASP:O	1:C:191:MET:HB3	2.20	0.40
1:D:175:HIS:CD2	1:D:248:PRO:HD2	2.56	0.40
1:D:260:LEU:HD21	1:D:277:GLY:C	2.46	0.40
1:D:366:ARG:C	1:D:368:LYS:N	2.79	0.40
1:D:371:VAL:C	1:D:373:HIS:N	2.78	0.40
1:B:130:HIS:HB2	1:B:160:GLN:OE1	2.21	0.40
1:B:197:LEU:O	1:B:201:GLU:HG3	2.22	0.40
1:D:59:ASN:N	1:D:145:ASP:OD2	2.41	0.40
1:D:89:PHE:CE1	1:D:91:LYS:HE2	2.57	0.40
1:D:293:LEU:CD1	1:D:346:ILE:HG23	2.51	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	395/397 (100%)	381 (96%)	14 (4%)	0	100	100
1	B	395/397 (100%)	376 (95%)	18 (5%)	1 (0%)	36	30
1	C	395/397 (100%)	381 (96%)	12 (3%)	2 (0%)	24	15
1	D	395/397 (100%)	361 (91%)	29 (7%)	5 (1%)	9	3
All	All	1580/1588 (100%)	1499 (95%)	73 (5%)	8 (0%)	24	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	83	GLU
1	D	88	LYS
1	D	367	HIS
1	C	448	ASN
1	D	128	PRO
1	D	328	GLY
1	B	92	TYR
1	D	296	SER

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	332/332 (100%)	324 (98%)	8 (2%)	43	31
1	B	332/332 (100%)	327 (98%)	5 (2%)	57	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	332/332 (100%)	325 (98%)	7 (2%)	47	37
1	D	332/332 (100%)	320 (96%)	12 (4%)	31	17
All	All	1328/1328 (100%)	1296 (98%)	32 (2%)	43	31

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	A	108	ILE
1	A	191	MET
1	A	260	LEU
1	A	284	LEU
1	A	368	LYS
1	A	405	LYS
1	A	449	ILE
1	B	125	THR
1	B	141	THR
1	B	284	LEU
1	B	307	GLU
1	B	332	GLU
1	C	191	MET
1	C	284	LEU
1	C	289	GLU
1	C	314	ASP
1	C	390	ILE
1	C	449	ILE
1	C	450	LYS
1	D	89	PHE
1	D	125	THR
1	D	155	ASP
1	D	191	MET
1	D	260	LEU
1	D	284	LEU
1	D	285	LYS
1	D	325	LEU
1	D	352	VAL
1	D	368	LYS
1	D	416	LEU
1	D	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	175	HIS
1	A	295	HIS
1	A	367	HIS
1	A	412	GLN
1	B	57	HIS
1	B	59	ASN
1	B	65	HIS
1	B	97	ASN
1	B	109	ASN
1	B	355	GLN
1	C	65	HIS
1	C	97	ASN
1	C	109	ASN
1	C	136	ASN
1	C	347	GLN
1	C	349	HIS
1	C	373	HIS
1	C	428	ASN
1	C	448	ASN
1	D	65	HIS
1	D	170	GLN
1	D	175	HIS
1	D	295	HIS
1	D	347	GLN
1	D	367	HIS
1	D	448	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	GDP	C	1303	2	29,30,30	1.04	2 (6%)	45,47,47	0.78	1 (2%)
3	GDP	B	1302	2	29,30,30	1.08	2 (6%)	45,47,47	0.79	1 (2%)
3	GDP	A	1301	2	29,30,30	0.99	2 (6%)	45,47,47	0.79	1 (2%)
3	GDP	D	1304	2	29,30,30	1.18	2 (6%)	45,47,47	0.82	1 (2%)

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	C	1303	2	-	2/16/32/32	0/3/3/3
3	GDP	B	1302	2	-	2/16/32/32	0/3/3/3
3	GDP	A	1301	2	-	2/16/32/32	0/3/3/3
3	GDP	D	1304	2	-	2/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1304	GDP	PA-O3A	4.15	1.64	1.59
3	B	1302	GDP	PA-O3A	3.33	1.63	1.59
3	C	1303	GDP	PA-O3A	2.62	1.62	1.59
3	C	1303	GDP	PB-O2B	-2.36	1.46	1.54
3	B	1302	GDP	PB-O2B	-2.31	1.46	1.54
3	A	1301	GDP	PB-O3B	-2.17	1.46	1.54
3	D	1304	GDP	PB-O2B	-2.10	1.47	1.54
3	A	1301	GDP	PB-O2B	-2.02	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1303	GDP	O3'-C3'-C4'	-2.39	104.22	111.08
3	D	1304	GDP	O3'-C3'-C4'	-2.34	104.36	111.08
3	B	1302	GDP	O3'-C3'-C4'	-2.30	104.48	111.08
3	A	1301	GDP	O3'-C3'-C4'	-2.24	104.64	111.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

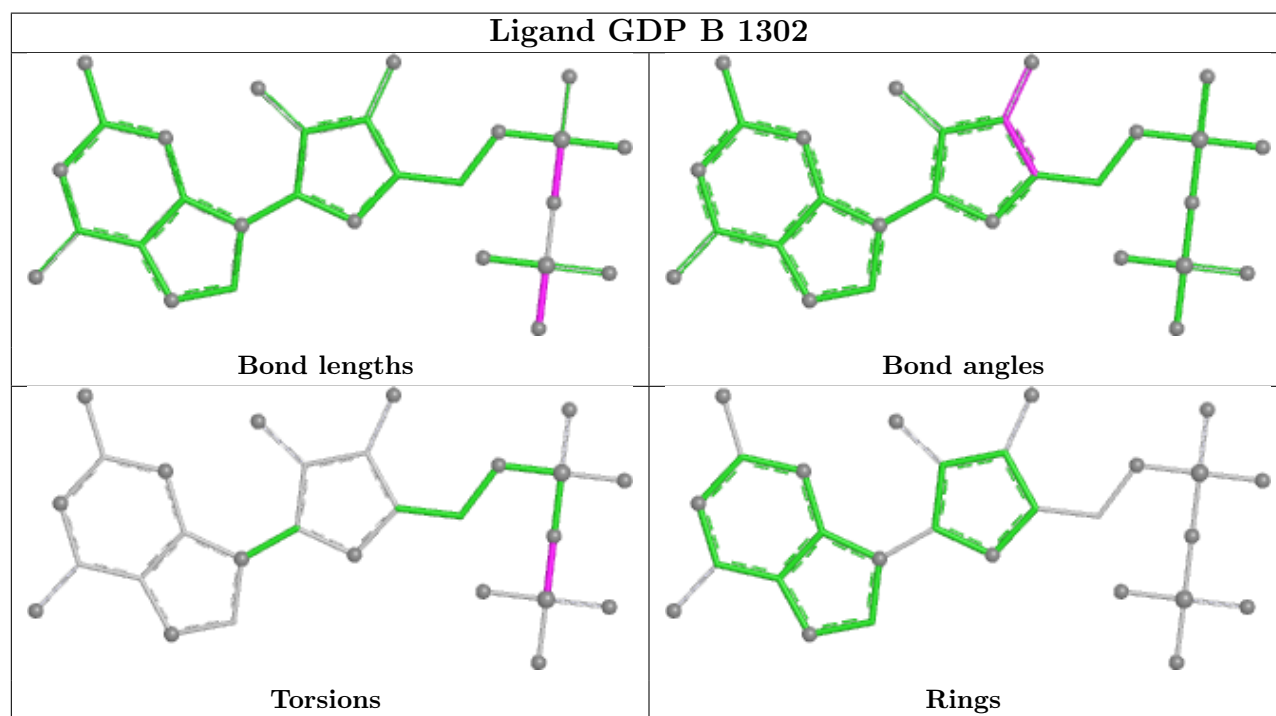
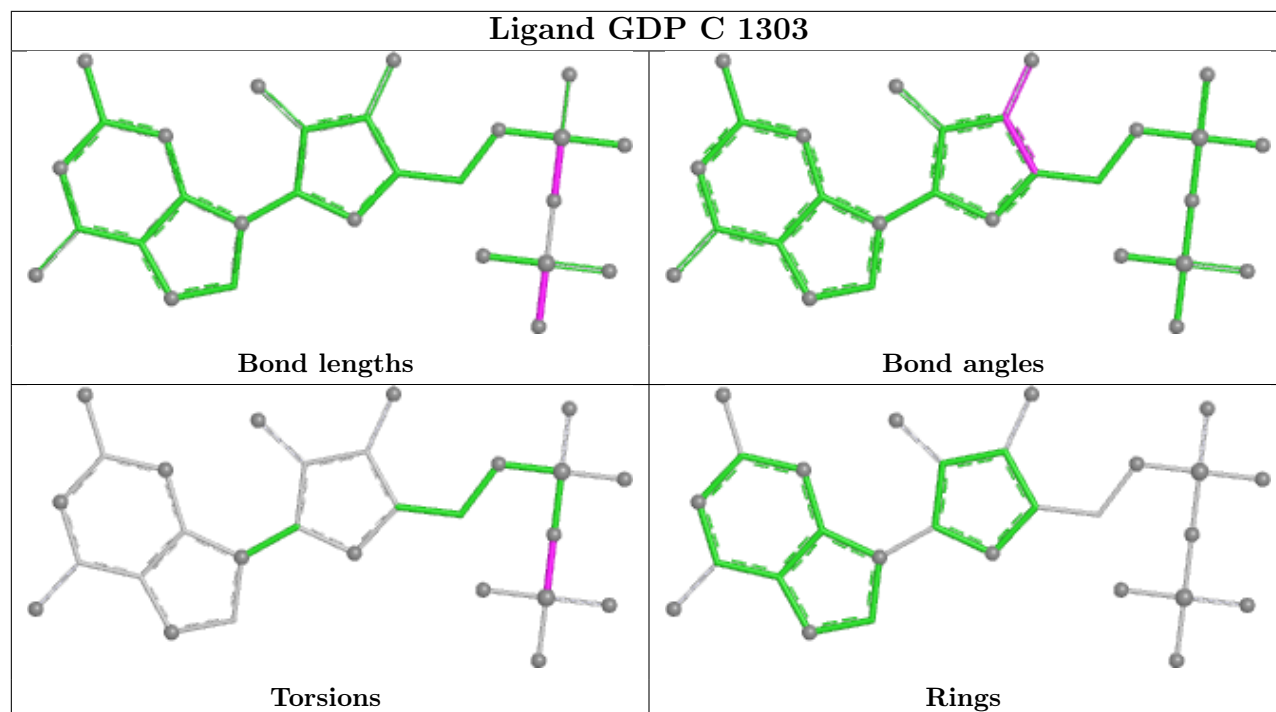
Mol	Chain	Res	Type	Atoms
3	A	1301	GDP	PA-O3A-PB-O2B
3	B	1302	GDP	PA-O3A-PB-O2B
3	C	1303	GDP	PA-O3A-PB-O2B
3	D	1304	GDP	PA-O3A-PB-O2B
3	D	1304	GDP	PA-O3A-PB-O1B
3	A	1301	GDP	PA-O3A-PB-O1B
3	C	1303	GDP	PA-O3A-PB-O1B
3	B	1302	GDP	PA-O3A-PB-O1B

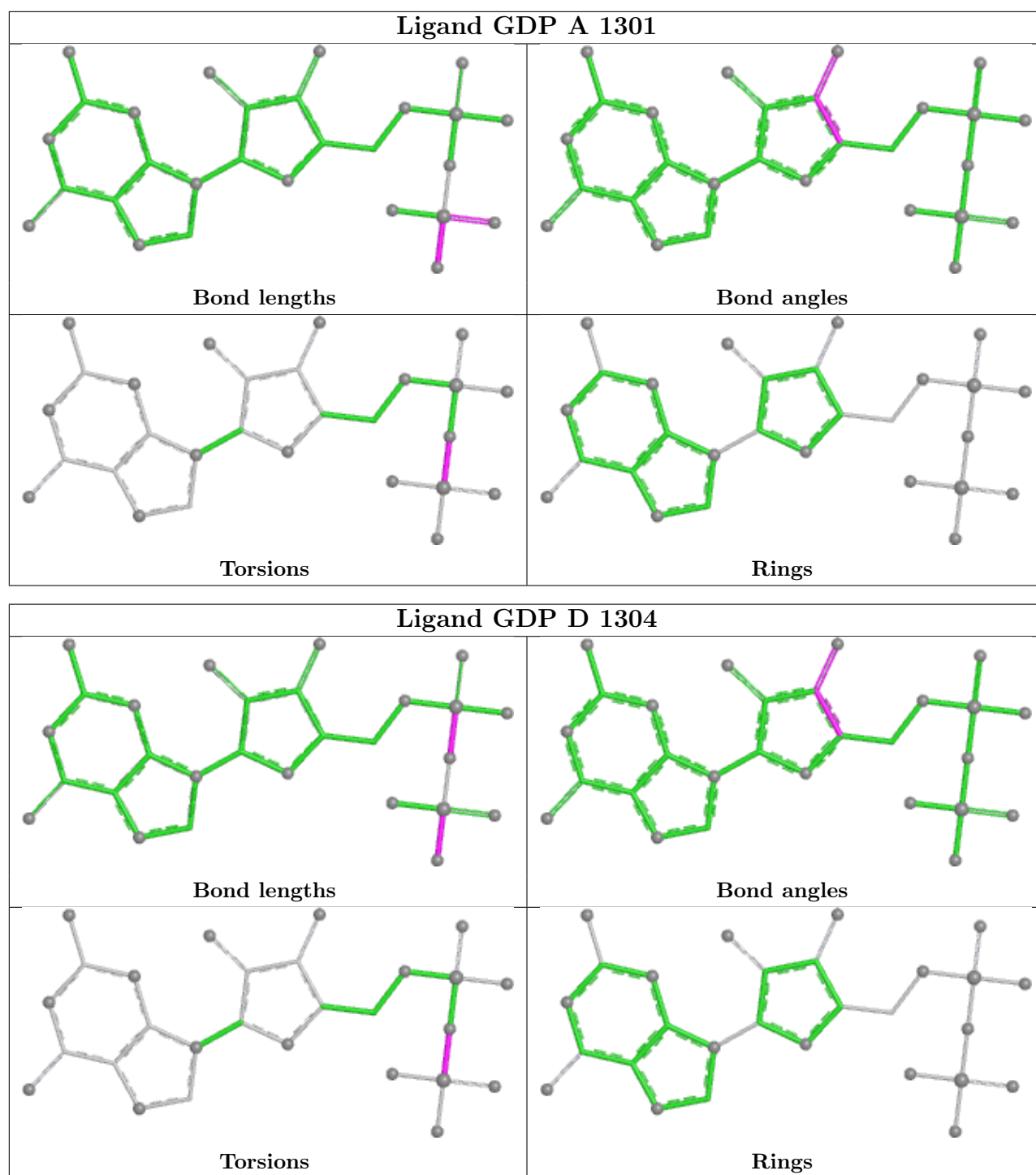
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1303	GDP	1	0
3	B	1302	GDP	1	0
3	D	1304	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	397/397 (100%)	0.54	19 (4%) 35 40	19, 35, 58, 69	0
1	B	397/397 (100%)	1.10	51 (12%) 7 8	33, 47, 66, 71	0
1	C	397/397 (100%)	0.93	49 (12%) 8 9	28, 44, 63, 71	0
1	D	397/397 (100%)	1.56	128 (32%) 1 0	27, 53, 67, 71	0
All	All	1588/1588 (100%)	1.03	247 (15%) 5 5	19, 45, 65, 71	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	5.4
1	C	85	GLY	5.4
1	B	141	THR	4.8
1	D	370	PHE	4.6
1	B	143	PRO	4.6
1	B	87	ALA	4.5
1	D	374	PHE	4.5
1	C	393	PRO	4.4
1	B	86	GLY	4.4
1	D	389	ILE	4.3
1	C	86	GLY	4.3
1	C	87	ALA	4.2
1	B	89	PHE	4.0
1	D	186	VAL	4.0
1	B	188	ASP	3.9
1	D	449	ILE	3.9
1	A	187	GLN	3.8
1	D	89	PHE	3.7
1	C	84	GLY	3.7
1	D	233	LEU	3.6
1	C	108	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	449	ILE	3.6
1	D	373	HIS	3.6
1	D	87	ALA	3.5
1	D	392	PRO	3.5
1	D	144	LEU	3.5
1	D	393	PRO	3.5
1	D	416	LEU	3.5
1	B	451	TRP	3.4
1	B	144	LEU	3.4
1	D	240	LEU	3.4
1	D	99	PRO	3.4
1	D	192	VAL	3.4
1	D	390	ILE	3.3
1	D	398	ALA	3.3
1	C	142	ALA	3.3
1	C	394	GLY	3.3
1	D	251	THR	3.2
1	D	84	GLY	3.2
1	D	387	CYS	3.2
1	D	250	PRO	3.2
1	B	231	LEU	3.2
1	D	95	ILE	3.2
1	C	312	SER	3.2
1	B	442	MET	3.1
1	B	119	ALA	3.1
1	D	118	ALA	3.1
1	C	392	PRO	3.1
1	D	229	PRO	3.1
1	A	451	TRP	3.1
1	D	397	LEU	3.1
1	D	123	ALA	3.1
1	D	221	LEU	3.0
1	D	97	ASN	3.0
1	D	105	GLY	3.0
1	D	80	ILE	3.0
1	C	451	TRP	3.0
1	D	297	LYS	2.9
1	B	121	HIS	2.9
1	D	451	TRP	2.9
1	C	388	ARG	2.9
1	D	81	LEU	2.9
1	D	391	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	222	CYS	2.9
1	B	268	ILE	2.9
1	D	61	GLY	2.9
1	B	92	TYR	2.8
1	B	67	ASP	2.8
1	D	404	LEU	2.8
1	A	186	VAL	2.8
1	D	352	VAL	2.8
1	B	84	GLY	2.8
1	D	406	LEU	2.8
1	B	98	ALA	2.8
1	B	154	ASN	2.8
1	C	140	GLY	2.8
1	A	87	ALA	2.7
1	D	119	ALA	2.7
1	D	128	PRO	2.7
1	D	249	VAL	2.7
1	B	91	LYS	2.7
1	C	297	LYS	2.7
1	D	56	PRO	2.7
1	C	389	ILE	2.7
1	D	346	ILE	2.7
1	B	118	ALA	2.7
1	D	110	ALA	2.7
1	D	441	ALA	2.7
1	C	399	MET	2.7
1	B	443	THR	2.7
1	D	224	LEU	2.7
1	D	91	LYS	2.7
1	D	371	VAL	2.7
1	D	227	ARG	2.6
1	D	443	THR	2.6
1	C	352	VAL	2.6
1	A	119	ALA	2.6
1	A	188	ASP	2.6
1	B	418	LYS	2.6
1	D	107	THR	2.6
1	D	77	ILE	2.6
1	B	103	ALA	2.6
1	D	82	ALA	2.6
1	D	191	MET	2.6
1	D	350	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	358	ILE	2.6
1	D	113	VAL	2.6
1	D	142	ALA	2.6
1	D	143	PRO	2.5
1	D	253	ASP	2.5
1	A	449	ILE	2.5
1	D	411	ARG	2.5
1	C	416	LEU	2.5
1	D	86	GLY	2.5
1	B	95	ILE	2.5
1	D	216	ILE	2.5
1	B	111	ALA	2.5
1	D	177	VAL	2.5
1	D	243	VAL	2.5
1	C	270	GLY	2.5
1	D	366	ARG	2.5
1	D	367	HIS	2.5
1	B	185	ALA	2.5
1	D	220	ALA	2.5
1	D	442	MET	2.5
1	D	125	THR	2.5
1	A	197	LEU	2.4
1	D	93	GLU	2.4
1	D	399	MET	2.4
1	C	171	ILE	2.4
1	C	431	ILE	2.4
1	A	213	THR	2.4
1	D	401	GLY	2.4
1	D	313	LEU	2.4
1	B	251	THR	2.4
1	C	141	THR	2.4
1	D	98	ALA	2.4
1	D	257	PRO	2.4
1	A	195	VAL	2.4
1	C	448	ASN	2.4
1	A	191	MET	2.4
1	D	296	SER	2.4
1	D	245	THR	2.4
1	D	103	ALA	2.4
1	C	121	HIS	2.4
1	C	107	THR	2.3
1	D	94	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	100	GLU	2.3
1	B	82	ALA	2.3
1	B	110	ALA	2.3
1	B	449	ILE	2.3
1	D	108	ILE	2.3
1	A	143	PRO	2.3
1	C	371	VAL	2.3
1	C	397	LEU	2.3
1	D	357	TYR	2.3
1	C	400	PRO	2.3
1	B	140	GLY	2.3
1	B	66	VAL	2.3
1	B	186	VAL	2.3
1	B	352	VAL	2.3
1	B	371	VAL	2.3
1	C	426	ASP	2.3
1	D	279	LEU	2.3
1	D	435	LEU	2.3
1	C	185	ALA	2.3
1	A	427	GLY	2.3
1	D	106	ILE	2.3
1	D	299	ILE	2.3
1	D	427	GLY	2.3
1	B	139	THR	2.3
1	B	328	GLY	2.2
1	D	75	ALA	2.2
1	C	176	VAL	2.2
1	C	186	VAL	2.2
1	B	57	HIS	2.2
1	C	373	HIS	2.2
1	D	375	MET	2.2
1	D	141	THR	2.2
1	D	364	GLY	2.2
1	D	365	GLY	2.2
1	C	103	ALA	2.2
1	C	139	THR	2.2
1	A	144	LEU	2.2
1	D	259	LEU	2.2
1	C	105	GLY	2.2
1	A	118	ALA	2.2
1	D	246	TYR	2.2
1	D	298	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	443	THR	2.2
1	B	107	THR	2.2
1	C	360	THR	2.2
1	A	85	GLY	2.2
1	B	221	LEU	2.2
1	D	85	GLY	2.2
1	D	284	LEU	2.2
1	D	111	ALA	2.2
1	D	171	ILE	2.1
1	D	283	ILE	2.1
1	D	237	GLN	2.1
1	B	228	ASP	2.1
1	D	71	THR	2.1
1	C	189	SER	2.1
1	C	328	GLY	2.1
1	D	348	PRO	2.1
1	B	373	HIS	2.1
1	C	367	HIS	2.1
1	A	428	ASN	2.1
1	B	309	PHE	2.1
1	B	104	ARG	2.1
1	C	172	GLY	2.1
1	A	212	GLU	2.1
1	D	440	PRO	2.1
1	D	185	ALA	2.1
1	B	390	ILE	2.1
1	D	92	TYR	2.1
1	D	409	ILE	2.1
1	D	415	ILE	2.1
1	D	431	ILE	2.1
1	C	307	GLU	2.1
1	D	225	GLU	2.1
1	D	154	ASN	2.1
1	D	127	CYS	2.1
1	D	254	LEU	2.1
1	D	260	LEU	2.1
1	C	131	ALA	2.1
1	C	441	ALA	2.1
1	B	106	ILE	2.0
1	D	88	LYS	2.0
1	D	247	ILE	2.0
1	D	395	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	442	MET	2.0
1	D	407	THR	2.0
1	D	433	THR	2.0
1	B	187	GLN	2.0
1	D	60	VAL	2.0
1	B	81	LEU	2.0
1	B	404	LEU	2.0
1	C	98	ALA	2.0
1	C	398	ALA	2.0
1	D	361	LYS	2.0
1	D	450	LYS	2.0
1	D	116	SER	2.0
1	C	443	THR	2.0
1	D	74	THR	2.0
1	B	448	ASN	2.0
1	D	236	VAL	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 oligosaccharides 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(Å ²)	Q<0.9
3	GDP	D	1304	28/28	0.86	0.11	50,54,58,58	0
2	MG	D	504	1/1	0.91	0.10	52,52,52,52	0
3	GDP	B	1302	28/28	0.94	0.08	44,51,53,55	0
3	GDP	C	1303	28/28	0.95	0.07	31,34,37,39	0
3	GDP	A	1301	28/28	0.97	0.07	18,29,31,32	0
2	MG	B	502	1/1	0.98	0.04	49,49,49,49	0
2	MG	C	503	1/1	0.99	0.03	35,35,35,35	0

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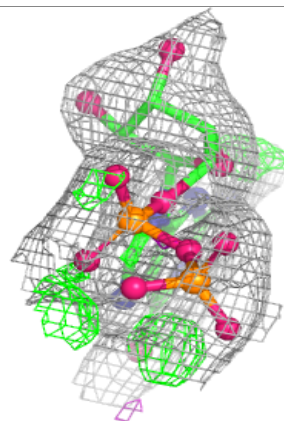
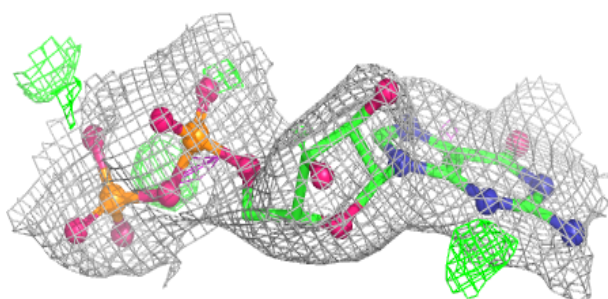
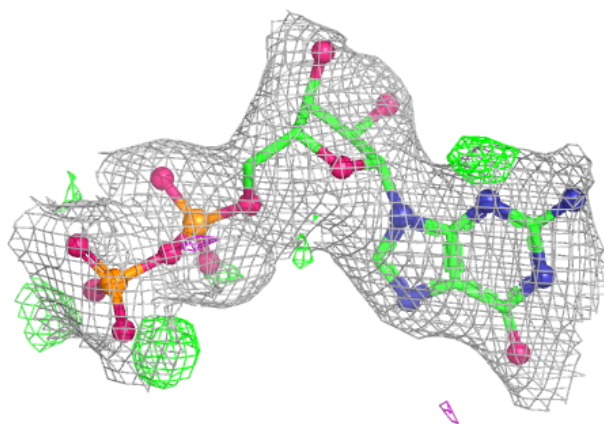
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	501	1/1	0.99	0.03	26,26,26,26	0

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.

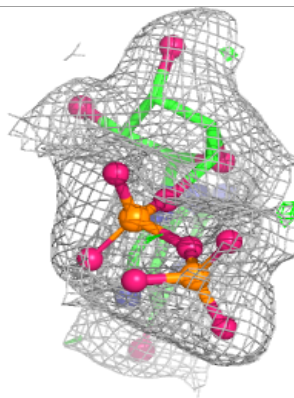
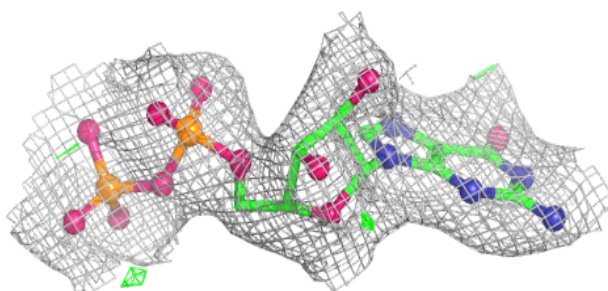
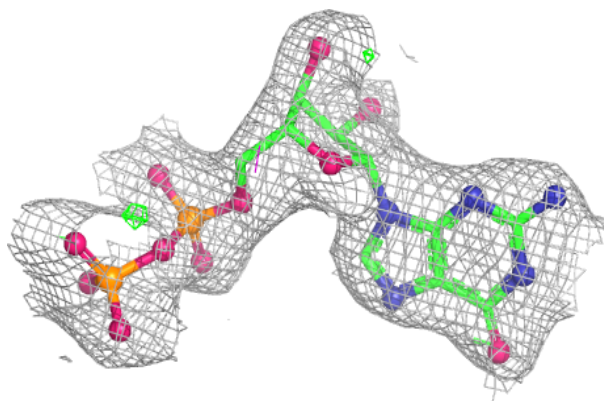
Electron density around GDP D 1304:

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

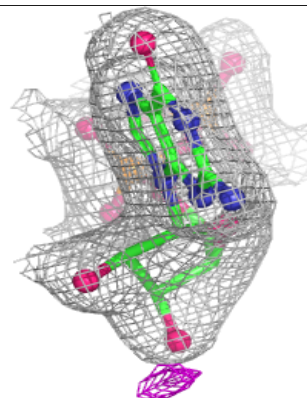
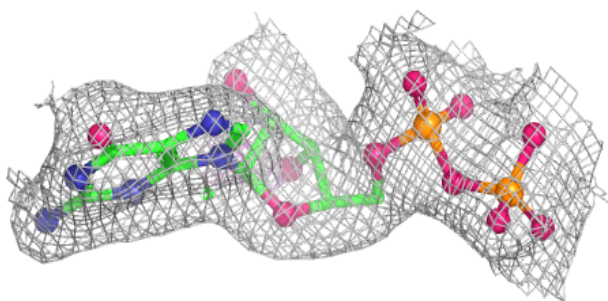
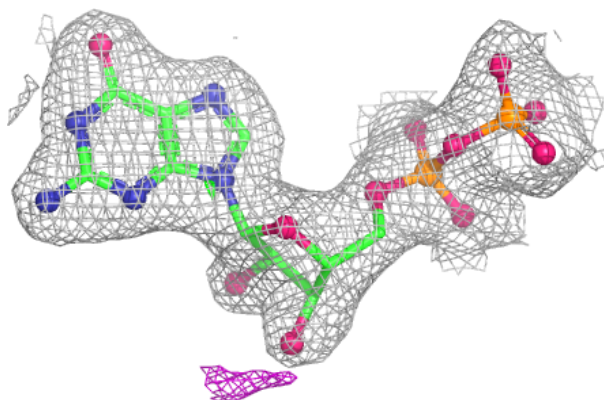


Electron density around GDP B 1302:

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

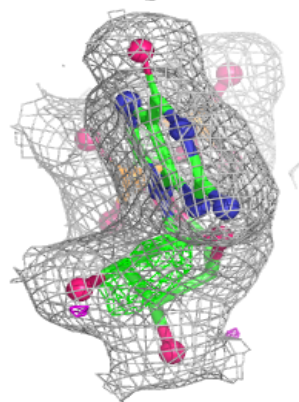
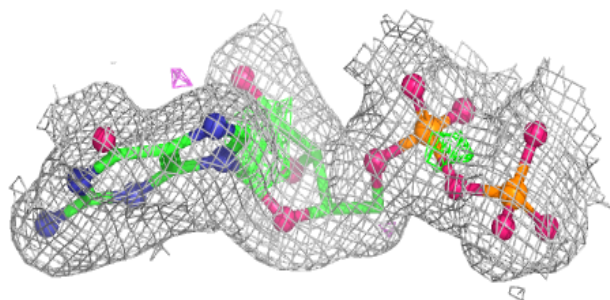
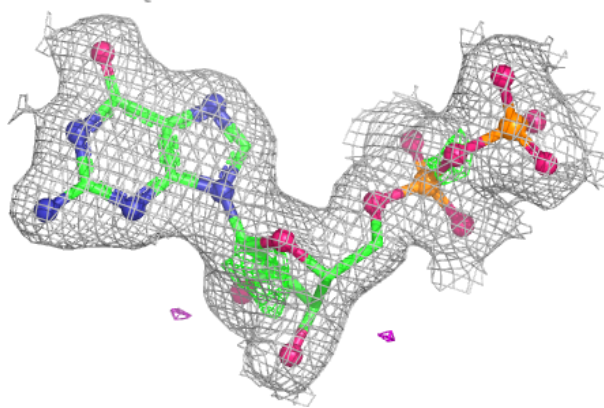
**Electron density around GDP C 1303:**

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



Electron density around GDP A 1301:

$2mF_o-DF_c$ (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.