



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:52 AM UTC

PDB ID : 4M0L / pdb_00004m0l
Title : Gamma subunit of the translation initiation factor 2 from *Sulfolobus solfataricus* complexed with GDP
Authors : Nikonov, O.S.; Stolboushkina, E.A.; Arkhipova, V.I.; Gabdulkhakov, A.G.; Nikulin, A.D.; Lazopulo, A.M.; Lazopulo, S.M.; Garber, M.B.; Nikonov, S.V.
Deposited on : 2013-08-01
Resolution : 2.60 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

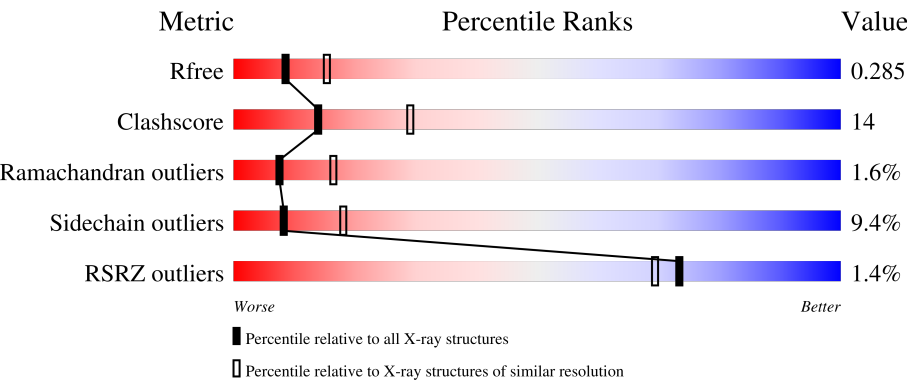
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	415	% 66%29%..
1	B	415	66%27%.5%
1	C	415	2%68%26%...
1	D	415	%61%30%6%.

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Mol	Chain	Length	Quality of chain
1	E	415	2% 67% 25% 6%
1	F	415	2% 60% 33% 7%

2 Entry composition [i](#)

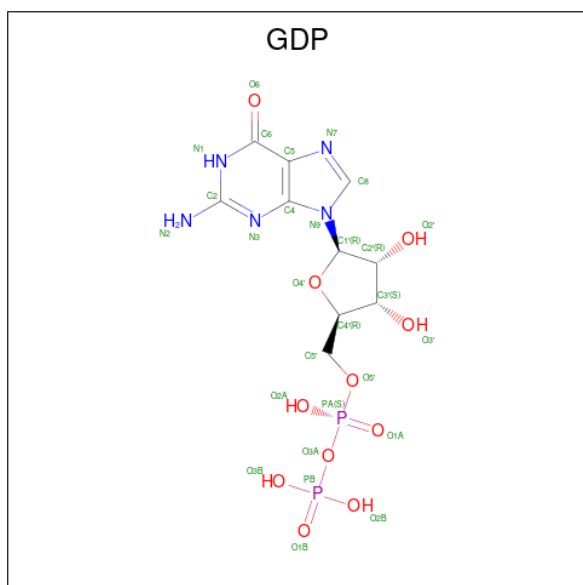
There are 5 unique types of molecules in this entry. The entry contains 19444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3197	2050	543	592	12			
1	B	396	Total	C	N	O	S	0	0	0
			3068	1970	521	565	12			
1	C	406	Total	C	N	O	S	0	0	0
			3148	2020	536	581	11			
1	D	405	Total	C	N	O	S	0	0	0
			3138	2014	533	580	11			
1	E	405	Total	C	N	O	S	0	0	0
			3138	2014	533	580	11			
1	F	414	Total	C	N	O	S	0	0	0
			3212	2058	548	594	12			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

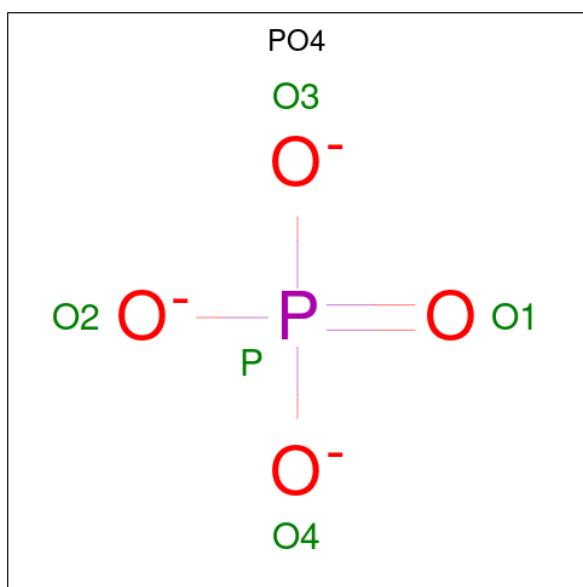


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		

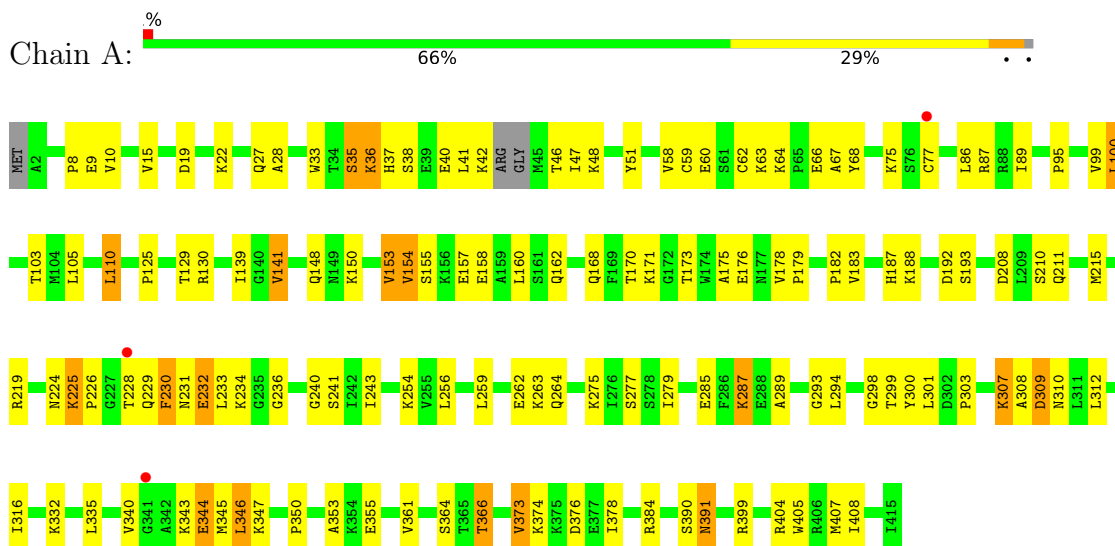
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	73	Total	O	0	0
			73	73		
5	C	77	Total	O	0	0
			77	77		
5	D	65	Total	O	0	0
			65	65		
5	E	51	Total	O	0	0
			51	51		
5	F	27	Total	O	0	0
			27	27		

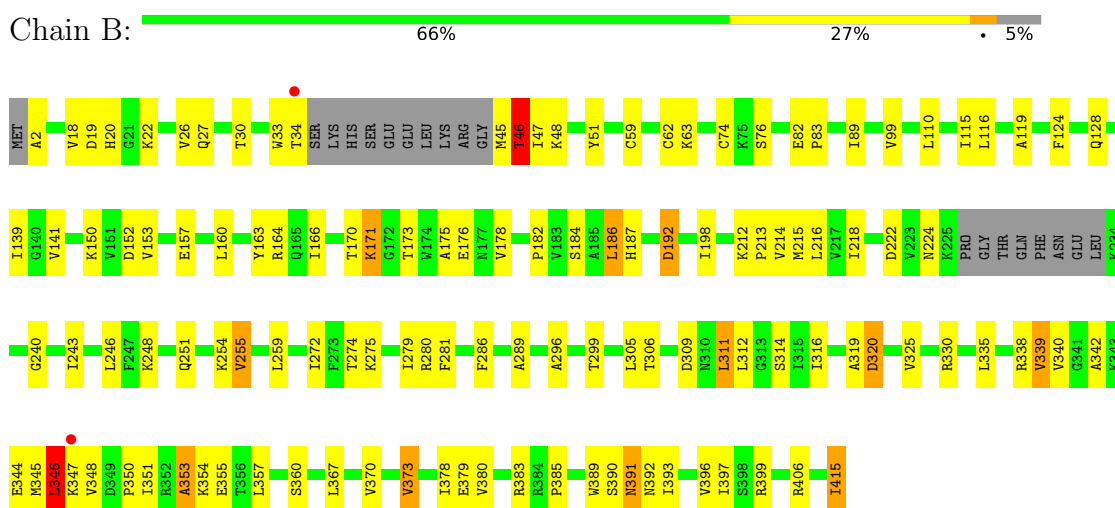
3 Residue-property plots [i](#)

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

- Molecule 1: Translation initiation factor 2 subunit gamma

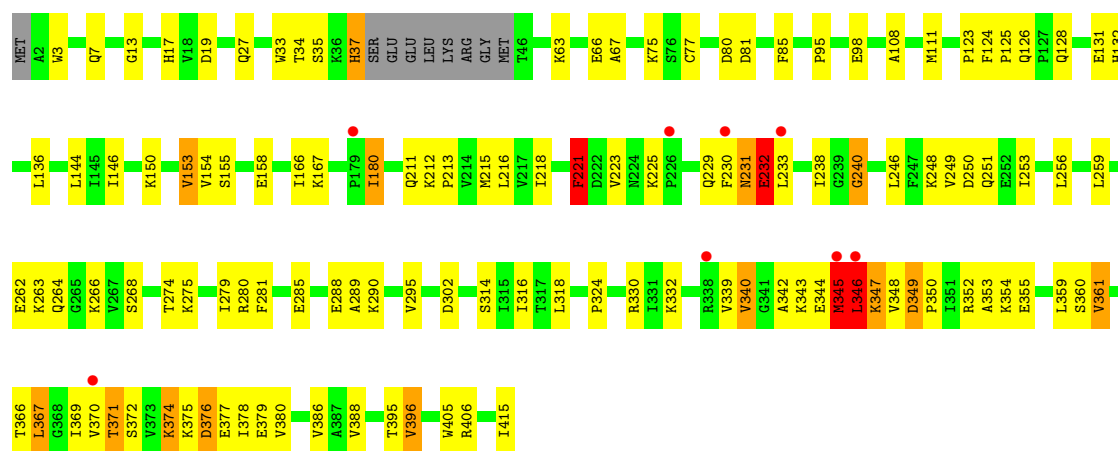


- Molecule 1: Translation initiation factor 2 subunit gamma

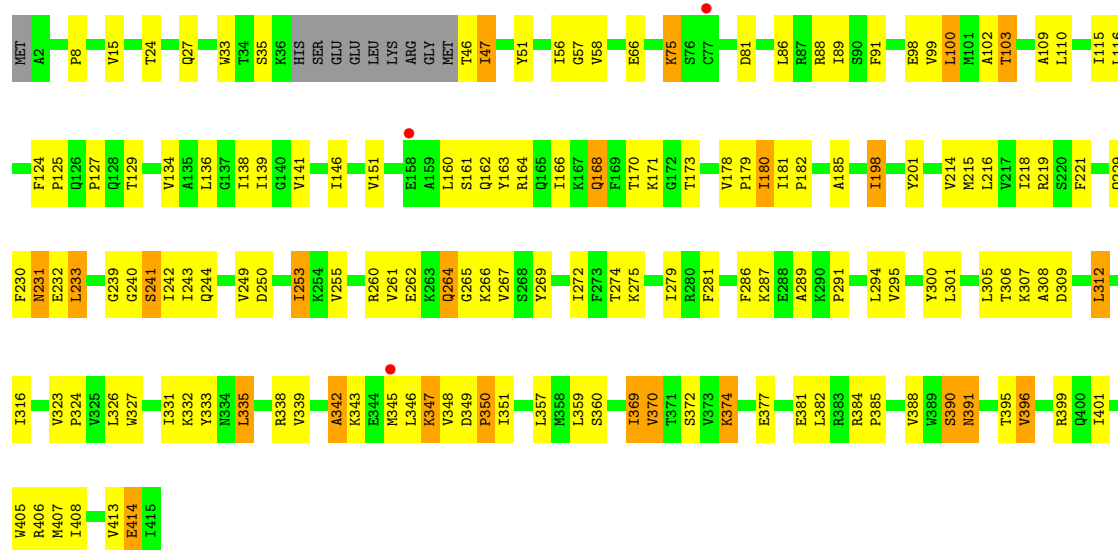


- Molecule 1: Translation initiation factor 2 subunit gamma

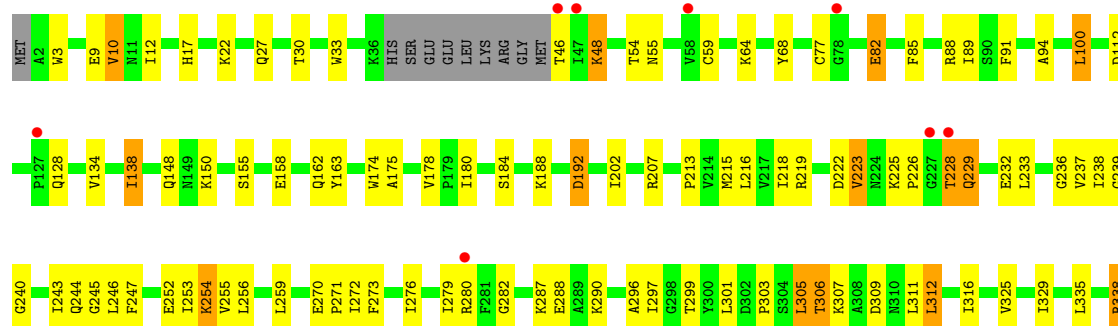


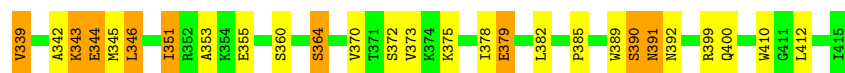


• Molecule 1: Translation initiation factor 2 subunit gamma

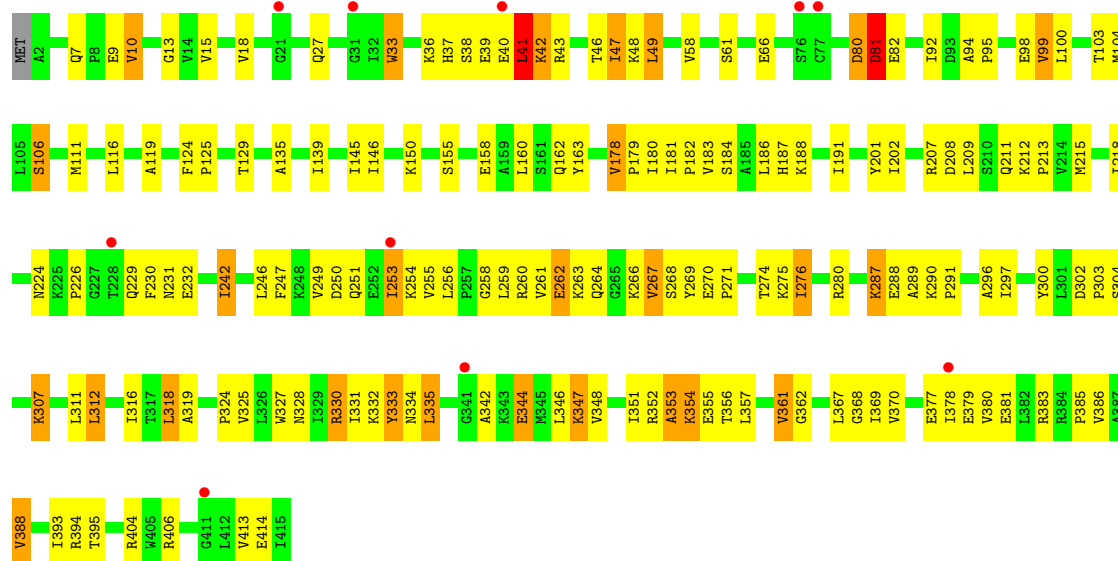


• Molecule 1: Translation initiation factor 2 subunit gamma





- Molecule 1: Translation initiation factor 2 subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.05Å 106.55Å 156.30Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	19.81 – 2.60 19.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.81-2.60) 96.6 (19.81-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.234 , 0.286 0.234 , 0.285	Depositor DCC
R_{free} test set	4213 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19444	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, PO4, 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	0.37	0/3255	0.81	4/4408 (0.1%)
1	B	0.36	1/3122 (0.0%)	0.77	1/4228 (0.0%)
1	C	0.36	1/3206 (0.0%)	0.82	6/4344 (0.1%)
1	D	0.35	0/3195	0.83	5/4329 (0.1%)
1	E	0.32	0/3195	0.77	0/4329
1	F	0.40	0/3271	0.85	3/4430 (0.1%)
All	All	0.36	2/19244 (0.0%)	0.81	19/26068 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	350	PRO	N-CD	5.47	1.55	1.47
1	B	182	PRO	N-CD	5.06	1.54	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	181	ILE	N-CA-C	7.27	115.78	109.02
1	C	346	LEU	N-CA-C	6.68	118.56	111.28
1	B	346	LEU	N-CA-C	6.13	116.69	108.23
1	F	178	VAL	CA-C-N	6.12	126.57	119.47
1	F	178	VAL	C-N-CA	6.12	126.57	119.47
1	C	240	GLY	N-CA-C	5.84	119.03	110.80
1	D	374	LYS	CB-CA-C	-5.57	109.04	117.07
1	A	232	GLU	N-CA-C	-5.57	106.37	112.72
1	C	231	ASN	N-CA-C	5.49	117.34	111.36
1	A	309	ASP	N-CA-C	-5.47	104.36	111.74
1	D	342	ALA	N-CA-C	5.45	116.90	111.07
1	F	229	GLN	N-CA-C	5.31	118.14	110.28
1	C	232	GLU	N-CA-C	5.30	117.14	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	PHE	N-CA-C	5.21	115.41	108.38
1	A	230	PHE	N-CA-C	5.13	116.92	110.91
1	D	350	PRO	CA-N-CD	-5.11	104.84	112.00
1	C	345	MET	N-CA-C	5.08	116.89	111.36
1	D	374	LYS	CA-C-O	5.05	120.87	117.94
1	A	240	GLY	N-CA-C	5.03	118.48	111.19

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	3197	0	3314	94	0
1	B	3068	0	3190	77	0
1	C	3148	0	3264	88	0
1	D	3138	0	3257	108	0
1	E	3138	0	3258	82	0
1	F	3212	0	3331	120	0
2	A	28	0	12	3	0
2	B	28	0	12	2	0
2	C	28	0	12	1	0
2	D	28	0	12	0	0
2	E	28	0	12	2	0
2	F	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	E	5	0	0	0	0
5	A	70	0	0	0	0
5	B	73	0	0	1	0
5	C	77	0	0	0	0
5	D	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	51	0	0	2	0
5	F	27	0	0	1	0
All	All	19444	0	19686	558	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 14.

All (558) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:HG12	1:C:342:ALA:HB2	1.14	1.14
1:F:263:LYS:HE3	1:F:264:GLN:HG2	1.29	1.09
1:F:94:ALA:HB2	1:F:100:LEU:HD13	1.30	1.08
1:B:373:VAL:HG23	1:B:378:ILE:HG22	1.38	0.99
1:A:35:SER:CB	1:A:36:LYS:HA	1.94	0.97
1:E:344:GLU:N	1:E:344:GLU:OE2	2.00	0.94
1:F:262:GLU:HG3	1:F:267:VAL:HB	1.53	0.90
1:F:94:ALA:CB	1:F:100:LEU:HD13	2.02	0.89
1:F:263:LYS:CE	1:F:264:GLN:HG2	2.04	0.88
1:E:338:ARG:HD2	1:E:345:MET:HA	1.53	0.88
1:D:115:ILE:HD11	1:D:198:ILE:HD11	1.57	0.86
1:C:352:ARG:HG2	1:C:355:GLU:OE1	1.76	0.85
1:C:339:VAL:HG12	1:C:342:ALA:CB	2.02	0.85
1:D:179:PRO:O	1:D:180:ILE:HG22	1.76	0.85
1:C:339:VAL:CG1	1:C:342:ALA:HB2	2.04	0.84
1:B:216:LEU:HG	1:B:243:ILE:HD11	1.59	0.84
1:E:232:GLU:O	1:E:233:LEU:HG	1.77	0.84
1:F:15:VAL:HG12	1:F:100:LEU:HD21	1.59	0.84
1:A:225:LYS:HG3	1:A:226:PRO:HD2	1.61	0.82
1:F:37:HIS:CD2	1:F:38:SER:H	1.97	0.82
1:B:338:ARG:HE	1:B:345:MET:HG3	1.45	0.81
1:A:219:ARG:HH21	1:A:294:LEU:HD11	1.46	0.81
1:A:35:SER:HB3	1:A:36:LYS:HG2	1.63	0.80
1:A:41:LEU:HD11	1:D:35:SER:HB3	1.62	0.80
1:D:338:ARG:HB3	1:D:345:MET:O	1.80	0.80
1:F:262:GLU:HA	1:F:266:LYS:O	1.82	0.80
1:C:374:LYS:HB2	1:C:377:GLU:O	1.82	0.79
1:D:347:LYS:HZ2	1:D:348:VAL:H	1.30	0.78
1:F:249:VAL:HA	1:F:276:ILE:HD11	1.66	0.77
1:A:225:LYS:HG3	1:A:226:PRO:CD	2.15	0.77
1:D:347:LYS:NZ	1:D:348:VAL:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:HB2	1:A:233:LEU:HD23	1.67	0.75
1:D:229:GLN:HB3	1:D:231:ASN:HD21	1.50	0.75
1:A:87:ARG:HE	1:A:89:ILE:HD11	1.52	0.75
1:E:192:ASP:OD1	1:E:192:ASP:N	2.19	0.74
1:B:218:ILE:HG12	1:B:240:GLY:HA2	1.69	0.74
1:A:35:SER:HB3	1:A:36:LYS:HA	1.69	0.74
1:B:110:LEU:HD11	1:B:243:ILE:HD13	1.68	0.74
1:A:332:LYS:NZ	1:A:376:ASP:OD2	2.21	0.73
1:F:7:GLN:NE2	1:F:290:LYS:O	2.22	0.73
1:C:75:LYS:NZ	1:C:80:ASP:OD1	2.20	0.73
1:F:81:ASP:OD1	1:F:81:ASP:N	2.22	0.71
1:F:230:PHE:HD1	1:F:231:ASN:H	1.37	0.71
1:D:218:ILE:HG22	1:D:219:ARG:HG3	1.71	0.71
1:E:252:GLU:HG2	5:E:639:HOH:O	1.89	0.71
1:E:351:ILE:N	1:E:351:ILE:HD12	2.06	0.71
1:F:325:VAL:HG12	1:F:385:PRO:HB2	1.72	0.70
1:F:49:LEU:HD21	1:F:103:THR:HG21	1.74	0.70
1:A:15:VAL:HG12	1:A:100:LEU:HD11	1.74	0.70
1:D:229:GLN:HB3	1:D:231:ASN:ND2	2.07	0.70
2:E:501:GDP:H8	2:E:501:GDP:H5"	1.56	0.69
1:B:346:LEU:HD22	1:F:209:LEU:HD22	1.74	0.69
1:E:392:ASN:HB3	1:E:412:LEU:HB3	1.75	0.69
1:D:260:ARG:HB2	1:D:269:TYR:CZ	2.27	0.69
1:D:347:LYS:HA	1:D:347:LYS:HZ3	1.58	0.69
1:F:318:LEU:HD12	1:F:318:LEU:H	1.56	0.69
1:A:215:MET:HB3	1:A:316:ILE:HB	1.74	0.69
1:D:179:PRO:O	1:D:180:ILE:CG2	2.41	0.68
1:E:351:ILE:HD12	1:E:351:ILE:H	1.58	0.68
1:D:168:GLN:OE1	1:D:171:LYS:NZ	2.26	0.68
1:D:24:THR:HG22	1:D:185:ALA:HB1	1.76	0.68
1:A:229:GLN:HB2	1:A:233:LEU:CD2	2.23	0.68
1:E:148:GLN:OE1	1:E:162:GLN:NE2	2.27	0.68
1:F:208:ASP:HB3	1:F:211:GLN:HE22	1.58	0.68
1:D:390:SER:OG	1:D:391:ASN:N	2.24	0.67
1:E:55:ASN:OD1	1:E:88:ARG:NH1	2.27	0.67
1:D:342:ALA:O	1:D:343:LYS:CB	2.43	0.67
1:D:342:ALA:O	1:D:343:LYS:HB3	1.96	0.66
1:F:353:ALA:O	1:F:355:GLU:N	2.26	0.66
1:E:391:ASN:OD1	1:E:392:ASN:N	2.27	0.66
1:D:216:LEU:HD23	1:D:243:ILE:HD11	1.79	0.65
1:E:232:GLU:C	1:E:233:LEU:HG	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:GLN:CG	1:C:232:GLU:HB3	2.28	0.64
1:C:330:ARG:HG2	1:C:379:GLU:HG2	1.80	0.64
1:F:47:ILE:HD13	1:F:218:ILE:HG22	1.79	0.64
1:B:222:ASP:OD2	1:B:224:ASN:ND2	2.31	0.64
1:D:338:ARG:CB	1:D:345:MET:O	2.44	0.64
1:A:63:LYS:HE3	1:C:264:GLN:HA	1.80	0.64
1:B:339:VAL:HG13	1:B:342:ALA:HB2	1.80	0.64
1:D:360:SER:HB2	1:D:396:VAL:HG13	1.78	0.64
1:E:10:VAL:HG23	1:E:112:ASP:HB2	1.80	0.64
1:B:340:VAL:O	1:B:406:ARG:NH1	2.30	0.63
1:C:263:LYS:HD2	1:C:266:LYS:HE3	1.79	0.63
1:C:123:PRO:O	1:C:126:GLN:NE2	2.32	0.63
1:A:58:VAL:HG23	1:A:86:LEU:HD11	1.81	0.63
1:F:48:LYS:HB3	1:F:95:PRO:HG3	1.80	0.63
1:C:7:GLN:NE2	1:C:290:LYS:O	2.30	0.62
1:F:213:PRO:HG2	1:F:318:LEU:HD11	1.80	0.62
1:F:262:GLU:CG	1:F:267:VAL:HB	2.27	0.62
1:C:361:VAL:HG13	1:C:395:THR:HB	1.82	0.62
1:E:373:VAL:HG22	1:E:378:ILE:HG22	1.82	0.62
1:F:287:LYS:H	1:F:287:LYS:HD3	1.65	0.61
1:C:360:SER:HB2	1:C:396:VAL:HG13	1.82	0.61
1:D:229:GLN:OE1	1:D:229:GLN:HA	2.00	0.61
1:C:146:ILE:O	1:C:180:ILE:HA	2.00	0.61
1:A:346:LEU:HD12	1:A:346:LEU:H	1.65	0.61
1:F:342:ALA:HB1	1:F:344:GLU:HG2	1.82	0.61
1:D:260:ARG:HB2	1:D:269:TYR:CE2	2.36	0.61
1:B:390:SER:OG	1:B:391:ASN:N	2.33	0.61
1:E:219:ARG:HE	1:E:239:GLY:HA3	1.66	0.61
1:F:40:GLU:O	1:F:41:LEU:HB2	2.01	0.60
1:F:324:PRO:HG2	1:F:388:VAL:HG13	1.83	0.60
1:D:146:ILE:CG2	1:D:180:ILE:HD13	2.31	0.60
1:C:324:PRO:HG2	1:C:388:VAL:HG23	1.83	0.60
1:C:352:ARG:HG3	1:C:355:GLU:HB2	1.82	0.60
1:A:27:GLN:HG3	1:A:33:TRP:CE2	2.37	0.60
1:C:230:PHE:O	1:C:233:LEU:HD23	2.01	0.60
1:A:309:ASP:O	1:A:312:LEU:HB2	2.02	0.60
1:B:171:LYS:HD3	1:C:250:ASP:OD1	2.01	0.60
1:B:248:LYS:HE3	1:B:251:GLN:NE2	2.17	0.60
1:F:254:LYS:HD3	1:F:256:LEU:HD21	1.84	0.60
1:C:229:GLN:O	1:C:229:GLN:HG3	2.02	0.60
1:F:116:LEU:HD11	1:F:129:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ILE:HD13	1:D:399:ARG:NH2	2.16	0.59
1:B:115:ILE:HD11	1:B:198:ILE:HD11	1.83	0.59
1:E:351:ILE:H	1:E:351:ILE:CD1	2.16	0.59
1:F:230:PHE:CD1	1:F:231:ASN:N	2.71	0.59
1:C:332:LYS:NZ	1:C:376:ASP:OD2	2.36	0.59
1:E:372:SER:OG	1:E:379:GLU:OE1	2.21	0.59
1:A:345:MET:O	1:A:347:LYS:N	2.35	0.59
1:F:95:PRO:HG2	1:F:99:VAL:HG11	1.83	0.58
1:A:139:ILE:HG13	1:A:141:VAL:HG13	1.85	0.58
1:A:225:LYS:CG	1:A:226:PRO:HD2	2.32	0.58
1:F:356:THR:HA	1:F:368:GLY:O	2.03	0.58
1:D:146:ILE:O	1:D:180:ILE:HA	2.03	0.58
1:F:262:GLU:HG3	1:F:267:VAL:CB	2.31	0.58
1:A:308:ALA:O	1:A:309:ASP:HB2	2.03	0.58
1:D:24:THR:HG22	1:D:185:ALA:CB	2.34	0.57
1:E:82:GLU:N	1:E:82:GLU:OE1	2.37	0.57
1:E:238:ILE:HG21	1:E:316:ILE:HD11	1.84	0.57
2:E:501:GDP:H5"	2:E:501:GDP:C8	2.39	0.57
1:A:335:LEU:HD11	1:A:350:PRO:HA	1.85	0.57
1:B:320:ASP:OD1	1:B:320:ASP:N	2.32	0.57
1:C:154:VAL:HG13	1:C:158:GLU:HB2	1.86	0.57
1:B:367:LEU:HB2	1:B:383:ARG:HD3	1.85	0.57
1:C:229:GLN:HG3	1:C:232:GLU:HB3	1.87	0.57
1:F:370:VAL:HG22	1:F:380:VAL:HG22	1.87	0.57
1:C:229:GLN:HE21	1:C:232:GLU:HB2	1.69	0.57
1:D:103:THR:HB	1:D:109:ALA:HB2	1.86	0.57
1:D:399:ARG:HD2	1:D:408:ILE:HD13	1.87	0.57
1:A:59:CYS:HB3	1:A:62:CYS:SG	2.45	0.56
1:A:399:ARG:HG2	1:A:408:ILE:HG21	1.87	0.56
1:E:246:LEU:HD11	1:E:288:GLU:HB2	1.86	0.56
1:A:229:GLN:HB3	1:A:232:GLU:HB3	1.87	0.56
1:B:255:VAL:HG13	1:B:272:ILE:HG13	1.88	0.56
1:B:370:VAL:HG22	1:B:380:VAL:HG22	1.88	0.56
1:B:355:GLU:OE2	1:B:399:ARG:NE	2.36	0.56
1:E:223:VAL:HG13	1:E:237:VAL:HG11	1.86	0.56
1:F:94:ALA:HB2	1:F:100:LEU:CD1	2.21	0.56
1:B:360:SER:HB2	1:B:396:VAL:HG12	1.88	0.56
1:C:361:VAL:HG21	1:C:386:VAL:HG11	1.87	0.56
1:E:343:LYS:HE2	1:E:344:GLU:HG3	1.88	0.56
1:F:104:MET:O	1:F:139:ILE:HG21	2.06	0.56
1:C:274:THR:OG1	1:C:275:LYS:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PRO:HG2	1:A:293:GLY:HA3	1.88	0.56
1:C:352:ARG:CG	1:C:355:GLU:HB2	2.36	0.56
1:E:389:TRP:CE3	1:E:390:SER:HB3	2.41	0.56
1:C:230:PHE:HA	1:C:233:LEU:HD23	1.89	0.55
1:D:347:LYS:HZ2	1:D:348:VAL:N	2.01	0.55
1:C:229:GLN:HG2	1:C:232:GLU:HB3	1.87	0.55
1:D:127:PRO:HB3	1:D:338:ARG:HH22	1.71	0.55
1:A:171:LYS:HA	1:A:176:GLU:HG3	1.88	0.55
1:B:164:ARG:NH1	1:C:302:ASP:OD1	2.39	0.55
1:A:154:VAL:HG13	1:A:158:GLU:HB2	1.88	0.55
1:D:345:MET:SD	1:D:345:MET:N	2.80	0.55
1:E:30:THR:HG22	1:E:54:THR:HB	1.88	0.55
1:A:35:SER:HB3	1:A:36:LYS:CA	2.37	0.55
1:C:67:ALA:HA	1:C:77:CYS:SG	2.46	0.55
1:C:280:ARG:NH1	1:C:285:GLU:OE1	2.40	0.55
1:B:45:MET:HG2	1:B:46:THR:HG22	1.88	0.55
1:F:261:VAL:HG23	1:F:261:VAL:O	2.06	0.55
1:F:328:ASN:HD21	1:F:381:GLU:CD	2.14	0.55
1:E:225:LYS:HB3	1:E:226:PRO:HD2	1.89	0.55
1:F:212:LYS:HE2	1:F:318:LEU:HD13	1.87	0.55
1:A:22:LYS:N	2:A:501:GDP:O1B	2.34	0.55
1:C:352:ARG:NH1	1:C:354:LYS:O	2.40	0.55
1:F:287:LYS:HG2	1:F:288:GLU:HG2	1.88	0.55
1:A:355:GLU:OE1	1:A:399:ARG:NE	2.36	0.54
1:D:306:THR:O	1:D:308:ALA:N	2.40	0.54
1:F:215:MET:HB2	1:F:242:ILE:HG22	1.89	0.54
1:B:192:ASP:OD1	1:B:192:ASP:N	2.40	0.54
1:E:255:VAL:HG11	1:E:311:LEU:HD12	1.87	0.54
1:C:150:LYS:HG2	2:C:501:GDP:C6	2.43	0.54
1:F:357:LEU:O	1:F:368:GLY:N	2.35	0.54
1:A:259:LEU:HD21	1:D:75:LYS:HB3	1.90	0.54
1:B:344:GLU:OE1	1:B:344:GLU:N	2.40	0.54
1:E:48:LYS:NZ	1:E:309:ASP:OD2	2.41	0.54
1:C:370:VAL:HG11	1:C:378:ILE:HD11	1.90	0.54
1:F:215:MET:HA	1:F:242:ILE:HA	1.89	0.54
1:E:243:ILE:HG21	1:E:389:TRP:CH2	2.42	0.54
1:D:214:VAL:HG12	1:D:244:GLN:HG2	1.90	0.54
1:D:351:ILE:CD1	1:D:399:ARG:NH2	2.71	0.54
1:F:7:GLN:HE22	1:F:290:LYS:H	1.56	0.54
1:A:263:LYS:O	1:A:264:GLN:HG2	2.08	0.53
1:D:146:ILE:HG22	1:D:180:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:PRO:C	1:D:180:ILE:HG22	2.33	0.53
1:C:229:GLN:CG	1:C:232:GLU:CB	2.85	0.53
1:F:37:HIS:CG	1:F:38:SER:N	2.77	0.53
1:F:39:GLU:CD	1:F:40:GLU:H	2.16	0.53
1:D:274:THR:OG1	1:D:275:LYS:N	2.42	0.53
1:F:290:LYS:HG2	1:F:291:PRO:HD2	1.91	0.53
1:B:248:LYS:H	1:B:251:GLN:CD	2.15	0.53
1:C:230:PHE:O	1:C:233:LEU:CD2	2.57	0.53
1:C:370:VAL:HG22	1:C:380:VAL:HG22	1.91	0.53
1:D:347:LYS:HE3	1:D:349:ASP:OD2	2.09	0.53
1:A:307:LYS:HG3	1:A:308:ALA:N	2.23	0.53
1:E:329:ILE:HD13	1:E:382:LEU:HD11	1.91	0.53
1:F:361:VAL:HG13	1:F:395:THR:HB	1.91	0.52
1:A:35:SER:OG	1:A:36:LYS:HA	2.09	0.52
1:E:134:VAL:O	1:E:138:ILE:HG22	2.08	0.52
1:B:391:ASN:O	1:B:393:ILE:N	2.42	0.52
1:C:218:ILE:HG12	1:C:240:GLY:HA2	1.91	0.52
1:F:27:GLN:OE1	1:F:33:TRP:CE2	2.63	0.52
1:A:150:LYS:HG2	2:A:501:GDP:C6	2.44	0.52
1:B:338:ARG:NE	1:B:345:MET:HG3	2.20	0.52
1:B:373:VAL:CG2	1:B:378:ILE:HG22	2.26	0.52
1:A:219:ARG:HH21	1:A:294:LEU:CD1	2.18	0.52
1:B:344:GLU:HG2	1:B:346:LEU:HG	1.91	0.52
1:E:325:VAL:HG12	1:E:385:PRO:HB2	1.91	0.52
1:C:279:ILE:HG21	1:C:289:ALA:HB2	1.90	0.52
1:E:253:ILE:HD12	1:E:316:ILE:HG21	1.91	0.52
1:A:224:ASN:HD21	1:A:234:LYS:N	2.08	0.52
1:D:348:VAL:HG12	1:D:348:VAL:O	2.09	0.52
1:F:275:LYS:HB3	1:F:300:TYR:CD1	2.45	0.51
1:C:13:GLY:HA3	1:C:111:MET:SD	2.51	0.51
1:C:346:LEU:N	1:C:346:LEU:CD2	2.73	0.51
1:D:116:LEU:HD11	1:D:129:THR:HG23	1.93	0.51
1:E:351:ILE:N	1:E:351:ILE:CD1	2.73	0.51
1:F:37:HIS:CG	1:F:38:SER:H	2.26	0.51
1:B:139:ILE:HG13	1:B:141:VAL:HG23	1.92	0.51
1:D:102:ALA:HA	1:D:407:MET:HE3	1.92	0.51
1:E:225:LYS:O	1:E:228:THR:HG22	2.10	0.51
1:E:390:SER:OG	1:E:391:ASN:N	2.42	0.51
1:C:347:LYS:N	1:C:347:LYS:CD	2.73	0.51
1:D:161:SER:O	1:D:164:ARG:HG2	2.10	0.51
1:E:229:GLN:OE1	1:E:229:GLN:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:TYR:CE1	1:F:385:PRO:HD2	2.46	0.51
1:B:274:THR:HG21	1:B:299:THR:HB	1.92	0.51
1:D:231:ASN:ND2	1:D:232:GLU:HG2	2.26	0.51
1:E:309:ASP:HB3	1:E:312:LEU:HD23	1.93	0.51
1:B:171:LYS:HA	1:B:176:GLU:HG3	1.92	0.51
1:D:27:GLN:HG3	1:D:33:TRP:CE2	2.46	0.51
1:E:3:TRP:CD1	1:E:85:PHE:HB2	2.46	0.51
1:F:393:ILE:HG23	1:F:413:VAL:HB	1.92	0.50
1:F:250:ASP:H	1:F:276:ILE:HG13	1.76	0.50
1:C:256:LEU:O	1:C:314:SER:HB2	2.11	0.50
1:B:243:ILE:HG21	1:B:389:TRP:CH2	2.47	0.50
1:E:17:HIS:ND1	1:E:128:GLN:HB2	2.26	0.50
1:A:287:LYS:HE2	1:E:353:ALA:HB3	1.92	0.50
1:B:279:ILE:HG21	1:B:289:ALA:HB2	1.92	0.50
1:D:401:ILE:HD13	1:D:406:ARG:HB2	1.93	0.50
1:D:327:TRP:CE2	1:D:385:PRO:HG3	2.46	0.50
1:B:18:VAL:HG23	1:B:128:GLN:OE1	2.11	0.50
1:F:9:GLU:HG3	1:F:10:VAL:HG12	1.93	0.50
1:F:106:SER:OG	1:F:362:GLY:O	2.26	0.50
1:A:361:VAL:O	1:A:364:SER:OG	2.24	0.50
1:B:254:LYS:NZ	1:B:319:ALA:O	2.42	0.50
1:C:131:GLU:OE2	1:C:340:VAL:HA	2.12	0.50
1:D:146:ILE:HG13	1:D:178:VAL:HG11	1.94	0.50
1:A:59:CYS:CB	1:A:62:CYS:SG	3.00	0.50
1:E:64:LYS:HE3	1:E:68:TYR:HE2	1.77	0.50
1:E:213:PRO:HB2	1:E:247:PHE:CE2	2.46	0.50
1:F:247:PHE:CE1	1:F:253:ILE:HD11	2.47	0.50
1:B:46:THR:O	1:B:48:LYS:HG3	2.11	0.49
1:D:160:LEU:O	1:D:163:TYR:HB3	2.12	0.49
1:F:255:VAL:HG11	1:F:311:LEU:HD23	1.94	0.49
1:C:17:HIS:ND1	1:C:128:GLN:HB2	2.28	0.49
1:D:351:ILE:CD1	1:D:399:ARG:CZ	2.90	0.49
1:F:13:GLY:HA2	1:F:92:ILE:HG12	1.94	0.49
1:F:47:ILE:O	1:F:47:ILE:HD12	2.12	0.49
1:D:249:VAL:HG23	1:D:287:LYS:O	2.13	0.49
1:D:396:VAL:CG2	1:D:407:MET:HG2	2.43	0.49
1:C:246:LEU:HD11	1:C:288:GLU:HB2	1.94	0.49
1:F:9:GLU:O	1:F:207:ARG:NH1	2.43	0.49
1:F:268:SER:HA	1:F:327:TRP:CZ2	2.47	0.49
1:B:26:VAL:O	1:B:30:THR:OG1	2.26	0.49
1:F:160:LEU:O	1:F:163:TYR:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASP:O	1:A:150:LYS:NZ	2.37	0.49
1:A:58:VAL:CG2	1:A:86:LEU:HD11	2.42	0.49
1:A:187:HIS:CE1	1:C:367:LEU:HD13	2.48	0.49
1:D:264:GLN:OE1	1:D:264:GLN:HA	2.12	0.49
1:F:330:ARG:HD3	1:F:379:GLU:CG	2.43	0.49
1:B:152:ASP:OD1	1:B:184:SER:OG	2.25	0.49
1:D:242:ILE:HB	1:D:291:PRO:HA	1.93	0.49
1:D:309:ASP:O	1:D:312:LEU:HB2	2.13	0.49
1:E:338:ARG:HB3	1:E:345:MET:O	2.13	0.49
1:F:351:ILE:HG12	1:F:357:LEU:HD11	1.95	0.48
1:F:357:LEU:N	1:F:368:GLY:O	2.39	0.48
1:A:225:LYS:HG3	1:A:226:PRO:HD3	1.94	0.48
1:C:372:SER:O	1:C:378:ILE:HG13	2.13	0.48
1:D:275:LYS:HD2	1:D:300:TYR:HE2	1.79	0.48
1:E:389:TRP:H	1:E:389:TRP:CD1	2.31	0.48
1:E:391:ASN:CG	1:E:392:ASN:H	2.11	0.48
1:F:13:GLY:HA3	1:F:111:MET:HE3	1.94	0.48
1:F:302:ASP:OD1	1:F:303:PRO:HD2	2.13	0.48
1:A:28:ALA:HA	1:A:188:LYS:HE3	1.95	0.48
1:B:274:THR:CG2	1:B:275:LYS:N	2.77	0.48
1:D:47:ILE:HD11	1:D:218:ILE:HG23	1.95	0.48
1:C:215:MET:HB3	1:C:316:ILE:HB	1.95	0.48
1:D:231:ASN:N	1:D:231:ASN:HD22	2.11	0.48
1:D:281:PHE:HB2	1:D:286:PHE:CE2	2.48	0.48
1:F:344:GLU:HG3	1:F:347:LYS:HZ1	1.78	0.48
1:B:2:ALA:HA	1:B:82:GLU:OE2	2.14	0.48
1:E:213:PRO:HA	1:E:244:GLN:O	2.13	0.48
1:B:325:VAL:HG12	1:B:385:PRO:HB2	1.94	0.48
1:B:338:ARG:HH21	1:B:345:MET:HG3	1.79	0.48
1:D:301:LEU:HB3	1:D:305:LEU:HD11	1.95	0.48
1:D:374:LYS:HD2	1:D:377:GLU:HB3	1.94	0.48
1:D:338:ARG:HD3	1:D:345:MET:HA	1.95	0.48
1:F:119:ALA:O	1:F:162:GLN:NE2	2.42	0.48
1:A:229:GLN:CB	1:A:233:LEU:HD23	2.40	0.47
1:D:15:VAL:HG12	1:D:100:LEU:HD11	1.96	0.47
1:F:145:ILE:HD11	1:F:201:TYR:HB2	1.96	0.47
1:F:258:GLY:HA3	1:F:271:PRO:HA	1.96	0.47
1:C:249:VAL:HG12	1:C:250:ASP:OD1	2.15	0.47
1:F:208:ASP:HB3	1:F:211:GLN:NE2	2.27	0.47
1:A:303:PRO:O	1:A:307:LYS:HB3	2.14	0.47
1:B:170:THR:HB	1:B:175:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:SER:OG	1:C:158:GLU:HG3	2.13	0.47
1:A:41:LEU:HD23	1:A:42:LYS:HG2	1.95	0.47
1:A:236:GLY:O	1:A:299:THR:OG1	2.28	0.47
1:A:340:VAL:HG11	1:A:407:MET:HE3	1.96	0.47
1:D:351:ILE:HD13	1:D:399:ARG:CZ	2.45	0.47
1:E:27:GLN:HG3	1:E:33:TRP:CD1	2.50	0.47
1:E:184:SER:O	1:E:188:LYS:N	2.48	0.47
1:A:110:LEU:HD21	1:A:243:ILE:HG12	1.96	0.47
1:A:157:GLU:O	1:A:160:LEU:HB3	2.15	0.47
1:D:57:GLY:HA2	1:D:86:LEU:HD13	1.96	0.47
1:E:213:PRO:HB2	1:E:247:PHE:CZ	2.50	0.47
1:E:246:LEU:HD13	1:E:290:LYS:HG3	1.97	0.47
1:A:64:LYS:NZ	1:A:68:TYR:OH	2.47	0.47
1:B:274:THR:CG2	1:B:275:LYS:H	2.28	0.47
1:C:229:GLN:HG3	1:C:232:GLU:CB	2.44	0.47
1:C:238:ILE:HD12	1:C:316:ILE:HD11	1.97	0.47
1:D:102:ALA:N	1:D:407:MET:HE1	2.30	0.47
1:D:124:PHE:CE2	1:D:166:ILE:HA	2.50	0.47
1:A:155:SER:OG	1:A:158:GLU:HG3	2.15	0.47
1:C:153:VAL:HG23	1:D:405:TRP:CD1	2.50	0.46
1:D:231:ASN:ND2	1:D:231:ASN:N	2.61	0.46
1:D:331:ILE:HG12	1:D:413:VAL:HG22	1.96	0.46
1:F:135:ALA:O	1:F:139:ILE:HG13	2.15	0.46
1:A:48:LYS:HB3	1:A:95:PRO:HG2	1.98	0.46
1:B:330:ARG:HG3	1:B:379:GLU:HG2	1.96	0.46
1:D:170:THR:O	1:D:173:THR:OG1	2.21	0.46
1:E:27:GLN:HG3	1:E:33:TRP:CG	2.51	0.46
1:F:242:ILE:HD11	1:F:291:PRO:N	2.30	0.46
1:A:9:GLU:HG3	1:A:10:VAL:HG23	1.96	0.46
1:B:335:LEU:HD11	1:B:350:PRO:HA	1.96	0.46
1:A:59:CYS:O	1:A:67:ALA:HB1	2.15	0.46
1:B:150:LYS:HG2	2:B:501:GDP:C6	2.50	0.46
1:E:218:ILE:HG12	1:E:240:GLY:HA2	1.98	0.46
1:F:230:PHE:CD2	1:F:232:GLU:OE2	2.69	0.46
1:F:255:VAL:HG22	1:F:316:ILE:HD11	1.98	0.46
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.58	0.46
1:A:58:VAL:HG22	1:A:68:TYR:CE1	2.51	0.46
1:C:7:GLN:HE22	1:C:290:LYS:C	2.22	0.46
1:E:138:ILE:HG13	1:E:410:TRP:CZ2	2.51	0.46
1:F:260:ARG:HH22	1:F:383:ARG:NH2	2.14	0.46
1:B:274:THR:HG22	1:B:275:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:SER:HA	1:C:37:HIS:CE1	2.50	0.46
1:D:388:VAL:HG12	1:D:390:SER:O	2.16	0.46
1:D:396:VAL:HG21	1:D:407:MET:HG2	1.97	0.46
1:E:355:GLU:OE1	1:E:399:ARG:NE	2.46	0.46
1:B:212:LYS:HA	1:B:213:PRO:HD3	1.78	0.46
1:E:213:PRO:HA	1:E:245:GLY:HA3	1.97	0.46
1:E:254:LYS:HD2	1:E:256:LEU:HD11	1.97	0.46
1:F:46:THR:C	1:F:47:ILE:HG13	2.41	0.46
1:C:340:VAL:O	1:C:406:ARG:NH2	2.49	0.46
1:D:230:PHE:HA	1:D:233:LEU:CD2	2.46	0.46
1:E:12:ILE:HD12	1:E:202:ILE:HG21	1.97	0.46
1:E:94:ALA:HB3	1:E:100:LEU:HG	1.98	0.46
1:A:36:LYS:O	1:A:37:HIS:C	2.59	0.46
1:A:340:VAL:HG13	1:A:340:VAL:O	2.16	0.46
1:B:351:ILE:O	1:B:373:VAL:HG21	2.16	0.46
1:D:58:VAL:HG12	1:D:86:LEU:HD11	1.97	0.46
1:F:40:GLU:O	1:F:48:LYS:NZ	2.44	0.46
1:A:182:PRO:C	1:A:183:VAL:HG13	2.41	0.45
1:B:309:ASP:HB3	1:B:312:LEU:HD13	1.98	0.45
1:D:253:ILE:HD11	1:D:316:ILE:HG21	1.97	0.45
1:D:333:TYR:HE2	1:D:335:LEU:HD13	1.80	0.45
1:A:37:HIS:O	1:A:38:SER:C	2.59	0.45
1:D:384:ARG:HA	1:D:385:PRO:HD3	1.85	0.45
1:A:366:THR:HB	1:A:384:ARG:HB3	1.97	0.45
1:B:415:ILE:HD12	1:B:415:ILE:HA	1.78	0.45
1:B:216:LEU:O	1:B:240:GLY:HA3	2.15	0.45
1:C:374:LYS:HD3	1:C:377:GLU:HG3	1.99	0.45
1:F:261:VAL:HG22	1:F:268:SER:O	2.17	0.45
1:F:331:ILE:O	1:F:377:GLU:HA	2.16	0.45
1:F:333:TYR:HE2	1:F:351:ILE:HD13	1.82	0.45
1:E:155:SER:OG	1:E:158:GLU:HG3	2.17	0.45
1:E:338:ARG:CD	1:E:345:MET:HA	2.37	0.45
1:A:51:TYR:CD2	1:A:294:LEU:HB2	2.52	0.45
1:E:222:ASP:CG	1:E:303:PRO:HB3	2.42	0.45
1:F:80:ASP:OD1	1:F:80:ASP:N	2.49	0.45
1:C:371:THR:N	1:C:379:GLU:O	2.42	0.45
1:A:148:GLN:HB3	1:A:182:PRO:HA	1.98	0.45
1:A:277:SER:N	1:A:298:GLY:O	2.49	0.45
1:A:404:ARG:HD3	1:A:405:TRP:N	2.31	0.45
1:B:20:HIS:HD1	1:B:119:ALA:H	1.65	0.45
1:F:254:LYS:HG2	1:F:319:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:ASP:OD2	1:F:304:SER:OG	2.24	0.45
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.75	0.44
1:D:332:LYS:HB2	1:D:414:GLU:OE1	2.17	0.44
1:F:42:LYS:HE2	1:F:95:PRO:HB2	1.99	0.44
1:E:9:GLU:O	1:E:207:ARG:NH2	2.50	0.44
1:F:262:GLU:HG3	1:F:267:VAL:HA	1.99	0.44
1:B:27:GLN:HG3	1:B:33:TRP:CE2	2.52	0.44
1:B:59:CYS:SG	1:B:83:PRO:HB3	2.57	0.44
1:D:347:LYS:NZ	1:D:348:VAL:N	2.60	0.44
1:B:215:MET:HE3	1:B:316:ILE:HB	1.99	0.44
1:C:345:MET:H	1:C:345:MET:HG2	1.51	0.44
1:D:215:MET:HE3	1:D:240:GLY:HA3	1.99	0.44
1:A:225:LYS:CG	1:A:226:PRO:CD	2.92	0.44
1:C:124:PHE:CE2	1:C:166:ILE:HA	2.53	0.44
1:F:344:GLU:HG3	1:F:347:LYS:NZ	2.32	0.44
1:B:63:LYS:HB2	5:B:663:HOH:O	2.18	0.44
1:A:373:VAL:HB	1:A:378:ILE:HG22	2.00	0.44
1:D:180:ILE:O	1:D:180:ILE:HG13	2.17	0.44
1:E:10:VAL:HG13	1:E:89:ILE:HG22	2.00	0.44
1:C:352:ARG:HG2	1:C:355:GLU:CD	2.42	0.44
1:C:132:HIS:O	1:C:136:LEU:HB2	2.18	0.44
1:C:281:PHE:CE1	1:C:295:VAL:HB	2.52	0.44
1:F:36:LYS:HE3	1:F:36:LYS:HB2	1.62	0.44
1:B:215:MET:HE3	1:B:316:ILE:HD12	2.00	0.43
1:B:373:VAL:HG23	1:B:378:ILE:CG2	2.29	0.43
1:C:229:GLN:HG2	1:C:232:GLU:CB	2.47	0.43
1:A:170:THR:O	1:A:173:THR:OG1	2.25	0.43
1:B:274:THR:CG2	1:B:299:THR:HB	2.48	0.43
1:D:339:VAL:HB	1:D:342:ALA:HB2	2.00	0.43
1:B:309:ASP:O	1:B:312:LEU:HB2	2.19	0.43
1:E:22:LYS:HE2	5:E:637:HOH:O	2.19	0.43
1:B:124:PHE:CE1	1:B:166:ILE:HA	2.54	0.43
1:B:152:ASP:O	1:E:400:GLN:NE2	2.52	0.43
1:B:353:ALA:O	1:B:370:VAL:HB	2.19	0.43
1:D:81:ASP:N	1:D:81:ASP:OD1	2.51	0.43
1:D:239:GLY:HA2	1:D:295:VAL:O	2.19	0.43
1:E:163:TYR:CE2	1:E:180:ILE:HB	2.54	0.43
1:F:146:ILE:HG13	1:F:178:VAL:HG11	2.00	0.43
1:D:264:GLN:HB3	1:D:265:GLY:H	1.61	0.43
1:E:236:GLY:HA3	1:E:306:THR:HG21	2.01	0.43
1:E:339:VAL:HB	1:E:342:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:TRP:CZ3	1:E:390:SER:HB3	2.53	0.43
1:F:377:GLU:C	1:F:378:ILE:HD12	2.43	0.43
1:A:192:ASP:OD1	1:A:193:SER:N	2.52	0.43
1:A:275:LYS:HB3	1:A:300:TYR:CD1	2.53	0.43
1:C:3:TRP:CD1	1:C:85:PHE:HB2	2.54	0.43
1:C:359:LEU:HD11	1:C:380:VAL:HG11	2.00	0.43
1:D:110:LEU:HD21	1:D:241:SER:HB3	2.01	0.43
1:E:303:PRO:HA	1:E:306:THR:HG22	2.01	0.43
1:F:124:PHE:HA	1:F:125:PRO:HA	1.77	0.43
1:A:287:LYS:HD3	1:A:287:LYS:N	2.34	0.43
1:B:214:VAL:O	1:B:243:ILE:N	2.51	0.43
1:B:280:ARG:HB2	1:B:296:ALA:HB3	1.99	0.43
1:C:66:GLU:HG3	1:D:262:GLU:O	2.18	0.43
1:C:136:LEU:HD21	1:C:144:LEU:HD13	2.01	0.43
1:F:81:ASP:HB2	1:F:82:GLU:H	1.51	0.43
1:F:262:GLU:HG3	1:F:267:VAL:CA	2.49	0.43
1:F:335:LEU:HD12	1:F:335:LEU:HA	1.73	0.43
1:F:178:VAL:HG13	1:F:179:PRO:HD2	2.01	0.43
1:A:404:ARG:HD3	1:A:405:TRP:H	1.84	0.42
1:F:247:PHE:HB2	1:F:289:ALA:HB3	2.01	0.42
1:C:27:GLN:HG3	1:C:33:TRP:CE2	2.53	0.42
1:D:51:TYR:HA	1:D:91:PHE:O	2.19	0.42
1:D:279:ILE:HG21	1:D:289:ALA:HB2	2.01	0.42
1:D:324:PRO:HB2	1:D:326:LEU:CD1	2.49	0.42
1:A:343:LYS:O	1:A:344:GLU:HB3	2.19	0.42
1:A:345:MET:HB3	1:A:346:LEU:HD12	2.02	0.42
1:B:357:LEU:HD13	1:B:397:ILE:HG23	2.00	0.42
1:B:360:SER:HB2	1:B:396:VAL:CG1	2.49	0.42
1:E:270:GLU:HA	1:E:271:PRO:HD3	1.87	0.42
1:E:346:LEU:HA	1:E:346:LEU:HD22	1.73	0.42
1:A:390:SER:OG	1:A:391:ASN:N	2.52	0.42
1:C:37:HIS:NE2	1:C:95:PRO:HB3	2.34	0.42
1:C:124:PHE:HA	1:C:125:PRO:HA	1.74	0.42
1:C:221:PHE:N	1:C:221:PHE:CD1	2.86	0.42
1:E:280:ARG:HG2	1:E:296:ALA:HB3	2.01	0.42
1:F:139:ILE:HG22	1:F:394:ARG:CZ	2.49	0.42
1:A:19:ASP:HA	2:A:501:GDP:H5'	2.00	0.42
1:A:153:VAL:HG13	1:C:405:TRP:CD1	2.55	0.42
1:C:221:PHE:N	1:C:221:PHE:HD1	2.18	0.42
1:C:229:GLN:NE2	1:C:232:GLU:HB2	2.34	0.42
1:F:332:LYS:NZ	1:F:414:GLU:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:ILE:HG22	1:D:381:GLU:HB3	2.01	0.42
1:F:215:MET:SD	1:F:297:ILE:HD13	2.59	0.42
1:D:253:ILE:HD11	1:D:316:ILE:CG2	2.49	0.42
1:B:22:LYS:NZ	2:B:501:GDP:O1B	2.36	0.42
1:B:186:LEU:HD12	1:B:187:HIS:CE1	2.55	0.42
1:D:261:VAL:O	1:D:267:VAL:HG13	2.20	0.42
1:E:12:ILE:HB	1:E:91:PHE:CD1	2.55	0.42
1:A:125:PRO:HG2	1:A:130:ARG:CZ	2.50	0.42
1:C:318:LEU:HD23	1:C:318:LEU:HA	1.86	0.42
1:D:56:ILE:HG13	1:D:89:ILE:HD12	2.00	0.42
1:E:27:GLN:HG3	1:E:33:TRP:CD2	2.55	0.42
1:E:236:GLY:O	1:E:299:THR:OG1	2.29	0.42
1:F:186:LEU:HD23	1:F:187:HIS:CD2	2.55	0.42
1:F:304:SER:HA	1:F:307:LYS:HZ3	1.85	0.42
1:C:248:LYS:O	1:C:251:GLN:HB2	2.20	0.41
1:C:374:LYS:HD3	1:C:377:GLU:OE2	2.20	0.41
1:E:174:TRP:CZ3	1:E:175:ALA:HB2	2.54	0.41
1:E:254:LYS:HE3	1:E:273:PHE:CE1	2.55	0.41
1:F:280:ARG:HB3	1:F:296:ALA:HB3	2.01	0.41
1:F:330:ARG:HD3	1:F:379:GLU:HG2	2.02	0.41
1:A:254:LYS:HE3	1:A:256:LEU:HD21	2.01	0.41
1:A:262:GLU:HG2	1:D:66:GLU:HG2	2.02	0.41
1:D:8:PRO:HA	1:D:88:ARG:HB3	2.01	0.41
1:D:164:ARG:HB2	1:D:168:GLN:HE22	1.86	0.41
1:D:255:VAL:HB	1:D:272:ILE:HB	2.01	0.41
1:F:13:GLY:HA2	1:F:92:ILE:CG1	2.50	0.41
1:A:99:VAL:O	1:A:103:THR:HG23	2.19	0.41
1:A:345:MET:HB3	1:A:346:LEU:H	1.59	0.41
1:B:338:ARG:HH21	1:B:345:MET:CG	2.34	0.41
1:F:361:VAL:HG21	1:F:386:VAL:HG11	2.02	0.41
1:F:146:ILE:N	5:F:622:HOH:O	2.52	0.41
1:A:373:VAL:O	1:A:373:VAL:HG22	2.21	0.41
1:D:231:ASN:ND2	1:D:231:ASN:H	2.18	0.41
1:E:301:LEU:HD22	1:E:305:LEU:HD11	2.03	0.41
1:F:404:ARG:HA	1:F:404:ARG:HD2	1.85	0.41
1:B:89:ILE:HD12	1:B:89:ILE:C	2.45	0.41
1:F:155:SER:OG	1:F:158:GLU:HG3	2.21	0.41
1:C:154:VAL:CG1	1:C:158:GLU:HB2	2.49	0.41
1:C:212:LYS:HA	1:C:213:PRO:HD3	1.92	0.41
1:D:134:VAL:O	1:D:138:ILE:HG13	2.21	0.41
1:E:360:SER:HA	1:E:364:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LEU:O	1:F:269:TYR:HA	2.21	0.41
1:C:27:GLN:HG3	1:C:33:TRP:CD1	2.56	0.41
1:C:81:ASP:OD1	1:C:81:ASP:N	2.54	0.41
1:C:263:LYS:HD2	1:C:266:LYS:CE	2.49	0.41
1:D:139:ILE:HG13	1:D:141:VAL:HG23	2.02	0.41
1:D:162:GLN:O	1:D:166:ILE:HG13	2.21	0.41
1:E:253:ILE:HD13	1:E:276:ILE:HG12	2.03	0.41
1:F:37:HIS:CE1	1:F:39:GLU:H	2.39	0.41
1:F:333:TYR:CE2	1:F:351:ILE:HD13	2.56	0.41
1:F:344:GLU:HG2	1:F:344:GLU:H	1.60	0.41
1:A:175:ALA:O	1:A:178:VAL:HG22	2.20	0.41
1:B:163:TYR:CD1	1:B:163:TYR:C	2.98	0.41
1:B:281:PHE:HB2	1:B:286:PHE:CE1	2.56	0.41
1:C:108:ALA:HA	1:C:216:LEU:HD21	2.03	0.41
1:A:279:ILE:HG21	1:A:289:ALA:HB2	2.03	0.40
1:D:168:GLN:HA	1:D:171:LYS:HD2	2.01	0.40
1:A:224:ASN:ND2	1:A:233:LEU:HD22	2.36	0.40
1:B:353:ALA:O	1:B:355:GLU:N	2.45	0.40
1:D:179:PRO:HG3	1:D:201:TYR:CE1	2.56	0.40
1:E:279:ILE:HG12	1:E:297:ILE:HD13	2.03	0.40
1:F:92:ILE:O	1:F:92:ILE:HG13	2.21	0.40
1:F:270:GLU:HA	1:F:271:PRO:HD3	1.95	0.40
1:B:305:LEU:O	1:B:311:LEU:HD13	2.22	0.40
1:C:253:ILE:HD12	1:C:316:ILE:HG21	2.03	0.40
1:D:124:PHE:HA	1:D:125:PRO:HA	1.72	0.40
1:D:178:VAL:HA	1:D:179:PRO:HD3	1.81	0.40
1:D:347:LYS:HZ3	1:D:347:LYS:CA	2.31	0.40
1:F:47:ILE:HG12	1:F:312:LEU:HD11	2.03	0.40
1:C:348:VAL:HG22	1:C:349:ASP:N	2.37	0.40
1:F:184:SER:O	1:F:188:LYS:N	2.54	0.40
1:F:209:LEU:HD11	1:F:246:LEU:HB2	2.04	0.40
1:A:208:ASP:OD2	1:A:211:GLN:HG3	2.21	0.40
1:A:230:PHE:O	1:A:231:ASN:CB	2.70	0.40
1:F:181:ILE:HA	1:F:182:PRO:HD3	1.96	0.40
1:F:183:VAL:HB	1:F:191:ILE:HD13	2.02	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	408/415 (98%)	378 (93%)	24 (6%)	6 (2%)	8	18
1	B	390/415 (94%)	355 (91%)	27 (7%)	8 (2%)	5	11
1	C	402/415 (97%)	383 (95%)	16 (4%)	3 (1%)	18	38
1	D	401/415 (97%)	371 (92%)	25 (6%)	5 (1%)	10	23
1	E	401/415 (97%)	367 (92%)	29 (7%)	5 (1%)	10	23
1	F	412/415 (99%)	371 (90%)	29 (7%)	12 (3%)	3	6
All	All	2414/2490 (97%)	2225 (92%)	150 (6%)	39 (2%)	7	16

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLU
1	A	346	LEU
1	B	46	THR
1	B	353	ALA
1	C	353	ALA
1	D	307	LYS
1	D	391	ASN
1	F	81	ASP
1	F	307	LYS
1	F	354	LYS
1	A	353	ALA
1	A	391	ASN
1	B	392	ASN
1	D	370	VAL
1	E	375	LYS
1	F	41	LEU
1	F	180	ILE
1	F	347	LYS
1	F	353	ALA
1	A	374	LYS

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Mol	Chain	Res	Type
1	B	354	LYS
1	B	391	ASN
1	E	391	ASN
1	F	80	ASP
1	F	348	VAL
1	A	40	GLU
1	C	180	ILE
1	E	306	THR
1	F	346	LEU
1	B	51	TYR
1	C	340	VAL
1	D	182	PRO
1	E	307	LYS
1	B	347	LYS
1	F	47	ILE
1	E	282	GLY
1	F	226	PRO
1	B	47	ILE
1	D	350	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	355/357 (99%)	327 (92%)	28 (8%)	11	26
1	B	340/357 (95%)	312 (92%)	28 (8%)	10	24
1	C	349/357 (98%)	317 (91%)	32 (9%)	8	19
1	D	348/357 (98%)	312 (90%)	36 (10%)	7	15
1	E	348/357 (98%)	315 (90%)	33 (10%)	8	18
1	F	356/357 (100%)	317 (89%)	39 (11%)	6	13
All	All	2096/2142 (98%)	1900 (91%)	196 (9%)	8	18

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	36	LYS
1	A	46	THR
1	A	47	ILE
1	A	60	GLU
1	A	66	GLU
1	A	75	LYS
1	A	77	CYS
1	A	100	LEU
1	A	105	LEU
1	A	110	LEU
1	A	129	THR
1	A	141	VAL
1	A	153	VAL
1	A	154	VAL
1	A	162	GLN
1	A	168	GLN
1	A	210	SER
1	A	225	LYS
1	A	228	THR
1	A	241	SER
1	A	285	GLU
1	A	287	LYS
1	A	301	LEU
1	A	307	LYS
1	A	310	ASN
1	A	366	THR
1	A	373	VAL
1	B	19	ASP
1	B	34	THR
1	B	46	THR
1	B	62	CYS
1	B	74	CYS
1	B	76	SER
1	B	99	VAL
1	B	116	LEU
1	B	153	VAL
1	B	157	GLU
1	B	160	LEU
1	B	171	LYS
1	B	173	THR
1	B	178	VAL
1	B	186	LEU

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Mol	Chain	Res	Type
1	B	192	ASP
1	B	246	LEU
1	B	255	VAL
1	B	259	LEU
1	B	306	THR
1	B	311	LEU
1	B	314	SER
1	B	320	ASP
1	B	339	VAL
1	B	346	LEU
1	B	348	VAL
1	B	373	VAL
1	B	415	ILE
1	C	19	ASP
1	C	34	THR
1	C	37	HIS
1	C	63	LYS
1	C	98	GLU
1	C	153	VAL
1	C	167	LYS
1	C	211	GLN
1	C	221	PHE
1	C	223	VAL
1	C	225	LYS
1	C	231	ASN
1	C	232	GLU
1	C	259	LEU
1	C	262	GLU
1	C	268	SER
1	C	343	LYS
1	C	344	GLU
1	C	345	MET
1	C	346	LEU
1	C	347	LYS
1	C	349	ASP
1	C	361	VAL
1	C	366	THR
1	C	367	LEU
1	C	369	ILE
1	C	371	THR
1	C	374	LYS
1	C	375	LYS

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Mol	Chain	Res	Type
1	C	376	ASP
1	C	396	VAL
1	C	415	ILE
1	D	46	THR
1	D	47	ILE
1	D	75	LYS
1	D	98	GLU
1	D	99	VAL
1	D	100	LEU
1	D	103	THR
1	D	136	LEU
1	D	151	VAL
1	D	168	GLN
1	D	180	ILE
1	D	198	ILE
1	D	221	PHE
1	D	231	ASN
1	D	233	LEU
1	D	241	SER
1	D	250	ASP
1	D	253	ILE
1	D	264	GLN
1	D	266	LYS
1	D	294	LEU
1	D	312	LEU
1	D	323	VAL
1	D	335	LEU
1	D	346	LEU
1	D	347	LYS
1	D	357	LEU
1	D	359	LEU
1	D	369	ILE
1	D	370	VAL
1	D	372	SER
1	D	382	LEU
1	D	390	SER
1	D	395	THR
1	D	396	VAL
1	D	414	GLU
1	E	10	VAL
1	E	46	THR
1	E	48	LYS

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Mol	Chain	Res	Type
1	E	59	CYS
1	E	77	CYS
1	E	82	GLU
1	E	100	LEU
1	E	138	ILE
1	E	150	LYS
1	E	178	VAL
1	E	192	ASP
1	E	215	MET
1	E	216	LEU
1	E	223	VAL
1	E	228	THR
1	E	229	GLN
1	E	254	LYS
1	E	259	LEU
1	E	272	ILE
1	E	287	LYS
1	E	305	LEU
1	E	312	LEU
1	E	335	LEU
1	E	338	ARG
1	E	339	VAL
1	E	343	LYS
1	E	344	GLU
1	E	346	LEU
1	E	351	ILE
1	E	364	SER
1	E	370	VAL
1	E	379	GLU
1	E	390	SER
1	F	10	VAL
1	F	18	VAL
1	F	33	TRP
1	F	41	LEU
1	F	42	LYS
1	F	43	ARG
1	F	49	LEU
1	F	58	VAL
1	F	61	SER
1	F	66	GLU
1	F	81	ASP
1	F	98	GLU

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Mol	Chain	Res	Type
1	F	99	VAL
1	F	106	SER
1	F	150	LYS
1	F	202	ILE
1	F	224	ASN
1	F	242	ILE
1	F	251	GLN
1	F	253	ILE
1	F	262	GLU
1	F	267	VAL
1	F	274	THR
1	F	276	ILE
1	F	287	LYS
1	F	312	LEU
1	F	318	LEU
1	F	330	ARG
1	F	333	TYR
1	F	334	ASN
1	F	335	LEU
1	F	344	GLU
1	F	352	ARG
1	F	354	LYS
1	F	361	VAL
1	F	367	LEU
1	F	369	ILE
1	F	388	VAL
1	F	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	A	310	ASN
1	B	55	ASN
1	B	187	HIS
1	B	334	ASN
1	B	391	ASN
1	B	392	ASN
1	C	128	GLN
1	C	229	GLN
1	C	400	GLN
1	D	231	ASN

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Mol	Chain	Res	Type
1	E	143	ASN
1	E	148	GLN
1	E	162	GLN
1	E	400	GLN
1	F	7	GLN
1	F	224	ASN
1	F	244	GLN
1	F	264	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\# Z > 2$
2	GDP	A	501	3	29,30,30	1.18	3 (10%)	45,47,47	1.81	7 (15%)
2	GDP	F	501	3	29,30,30	1.17	3 (10%)	45,47,47	1.79	6 (13%)
4	PO4	E	503	-	4,4,4	1.01	0	6,6,6	0.51	0
2	GDP	D	501	3	29,30,30	1.20	4 (13%)	45,47,47	1.73	6 (13%)
2	GDP	E	501	3	29,30,30	1.16	3 (10%)	45,47,47	1.76	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	C	501	3	29,30,30	1.18	3 (10%)	45,47,47	1.77	6 (13%)
2	GDP	B	501	3	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)

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
2	GDP	A	501	3	-	3/16/32/32	0/3/3/3
2	GDP	F	501	3	-	0/16/32/32	0/3/3/3
2	GDP	D	501	3	-	3/16/32/32	0/3/3/3
2	GDP	E	501	3	-	6/16/32/32	0/3/3/3
2	GDP	C	501	3	-	4/16/32/32	0/3/3/3
2	GDP	B	501	3	-	1/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	GDP	C5-C4	3.03	1.47	1.38
2	A	501	GDP	C5-C4	3.01	1.47	1.38
2	F	501	GDP	C5-C4	2.98	1.46	1.38
2	B	501	GDP	C5-C4	2.94	1.46	1.38
2	E	501	GDP	C5-C4	2.93	1.46	1.38
2	D	501	GDP	C5-C4	2.86	1.46	1.38
2	D	501	GDP	C6-N1	-2.73	1.33	1.38
2	A	501	GDP	C6-N1	-2.70	1.33	1.38
2	F	501	GDP	C6-N1	-2.69	1.33	1.38
2	C	501	GDP	C6-N1	-2.69	1.33	1.38
2	B	501	GDP	C6-N1	-2.65	1.33	1.38
2	E	501	GDP	C6-N1	-2.58	1.34	1.38
2	A	501	GDP	C5-N7	-2.44	1.34	1.39
2	D	501	GDP	C5-N7	-2.33	1.34	1.39
2	B	501	GDP	C5-N7	-2.32	1.34	1.39
2	F	501	GDP	C5-N7	-2.27	1.34	1.39
2	E	501	GDP	C5-N7	-2.21	1.34	1.39
2	C	501	GDP	C5-N7	-2.20	1.34	1.39
2	D	501	GDP	C4-N9	-2.12	1.32	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	GDP	C5-C4-N3	-6.27	118.42	128.39
2	A	501	GDP	C5-C4-N3	-6.24	118.45	128.39
2	C	501	GDP	C5-C4-N3	-6.10	118.69	128.39
2	B	501	GDP	C5-C4-N3	-5.93	118.96	128.39
2	E	501	GDP	C5-C4-N3	-5.90	119.00	128.39
2	D	501	GDP	C5-C4-N3	-5.76	119.22	128.39
2	F	501	GDP	C2-N3-C4	5.03	120.97	112.30
2	C	501	GDP	C2-N3-C4	4.97	120.86	112.30
2	E	501	GDP	C2-N3-C4	4.94	120.81	112.30
2	A	501	GDP	C2-N3-C4	4.93	120.79	112.30
2	B	501	GDP	C2-N3-C4	4.86	120.67	112.30
2	D	501	GDP	C2-N3-C4	4.86	120.66	112.30
2	F	501	GDP	N9-C4-N3	4.72	135.38	125.95
2	A	501	GDP	N9-C4-N3	4.68	135.30	125.95
2	C	501	GDP	N9-C4-N3	4.49	134.93	125.95
2	B	501	GDP	N9-C4-N3	4.40	134.76	125.95
2	D	501	GDP	N9-C4-N3	4.19	134.34	125.95
2	E	501	GDP	N9-C4-N3	4.13	134.22	125.95
2	E	501	GDP	C6-C5-N7	3.51	136.68	130.29
2	D	501	GDP	C6-C5-N7	3.46	136.58	130.29
2	C	501	GDP	C6-C5-N7	3.41	136.49	130.29
2	B	501	GDP	C6-C5-N7	3.34	136.36	130.29
2	F	501	GDP	C6-C5-N7	3.16	136.04	130.29
2	A	501	GDP	C6-C5-N7	3.01	135.76	130.29
2	E	501	GDP	C4-C5-N7	-2.80	106.23	110.67
2	C	501	GDP	C4-C5-N7	-2.71	106.38	110.67
2	D	501	GDP	C4-C5-N7	-2.58	106.57	110.67
2	B	501	GDP	C4-C5-N7	-2.57	106.59	110.67
2	F	501	GDP	C4-C5-N7	-2.56	106.61	110.67
2	A	501	GDP	C4-C5-N7	-2.47	106.75	110.67
2	A	501	GDP	O6-C6-C5	-2.18	120.78	126.53
2	A	501	GDP	C3'-C2'-C1'	2.16	105.56	101.46
2	B	501	GDP	O6-C6-C5	-2.14	120.89	126.53
2	F	501	GDP	O6-C6-C5	-2.09	121.01	126.53
2	D	501	GDP	O6-C6-C5	-2.08	121.04	126.53
2	C	501	GDP	O6-C6-C5	-2.04	121.14	126.53

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GDP	PA-O3A-PB-O3B
2	E	501	GDP	C5'-O5'-PA-O3A

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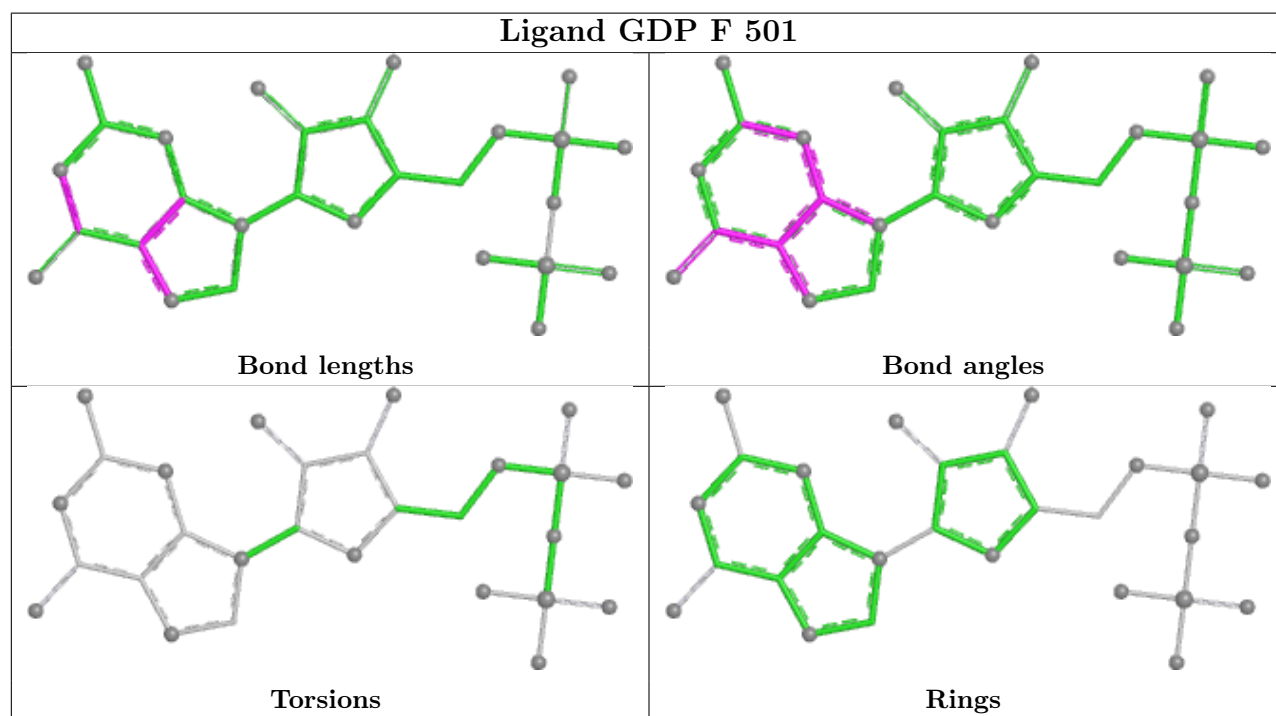
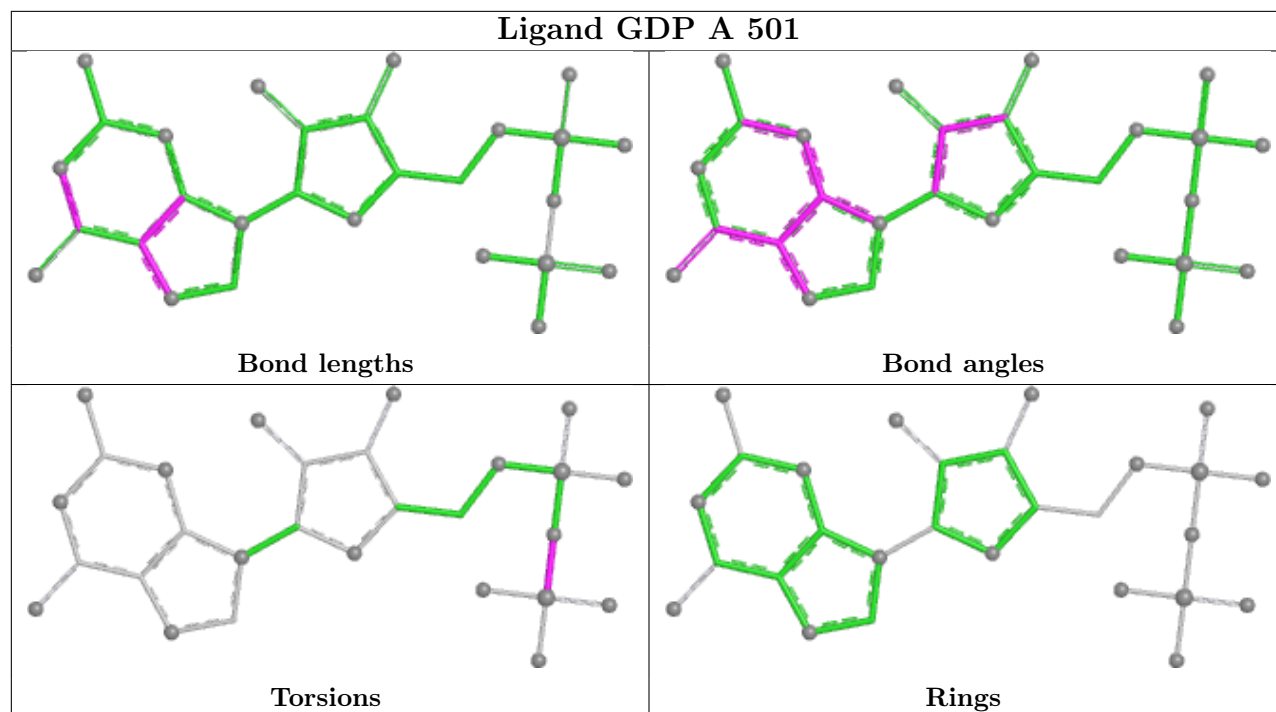
Mol	Chain	Res	Type	Atoms
2	E	501	GDP	C5'-O5'-PA-O1A
2	E	501	GDP	C5'-O5'-PA-O2A
2	E	501	GDP	C3'-C4'-C5'-O5'
2	E	501	GDP	O4'-C4'-C5'-O5'
2	C	501	GDP	C3'-C4'-C5'-O5'
2	B	501	GDP	PA-O3A-PB-O1B
2	C	501	GDP	PB-O3A-PA-O2A
2	D	501	GDP	PB-O3A-PA-O2A
2	C	501	GDP	O4'-C4'-C5'-O5'
2	A	501	GDP	PA-O3A-PB-O2B
2	D	501	GDP	O4'-C4'-C5'-O5'
2	C	501	GDP	PB-O3A-PA-O1A
2	D	501	GDP	PB-O3A-PA-O1A
2	E	501	GDP	PB-O3A-PA-O1A
2	A	501	GDP	PA-O3A-PB-O1B

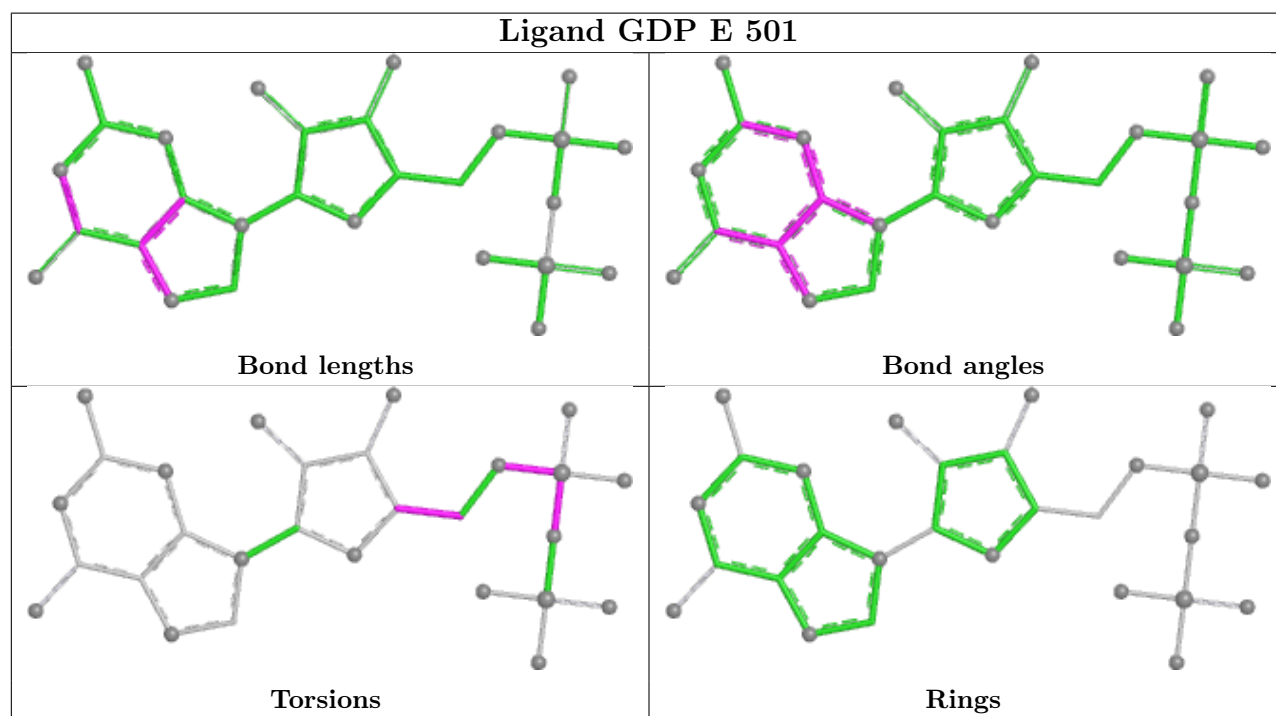
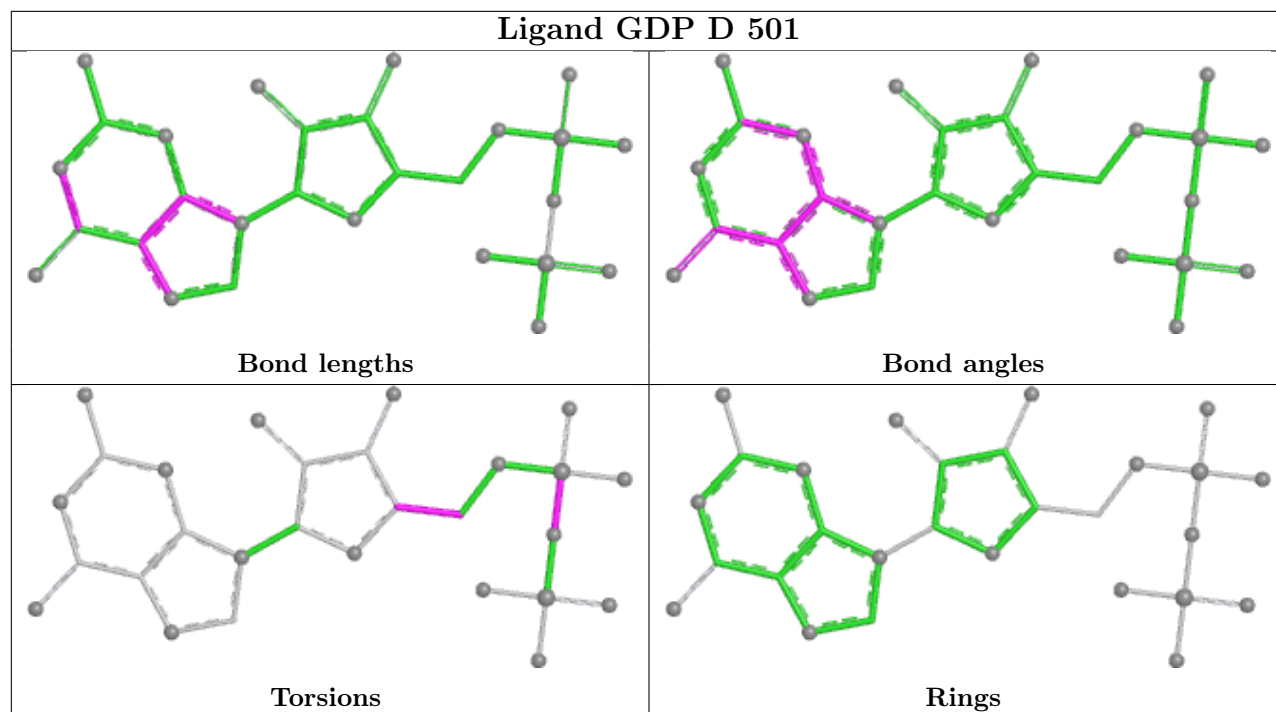
There are no ring outliers.

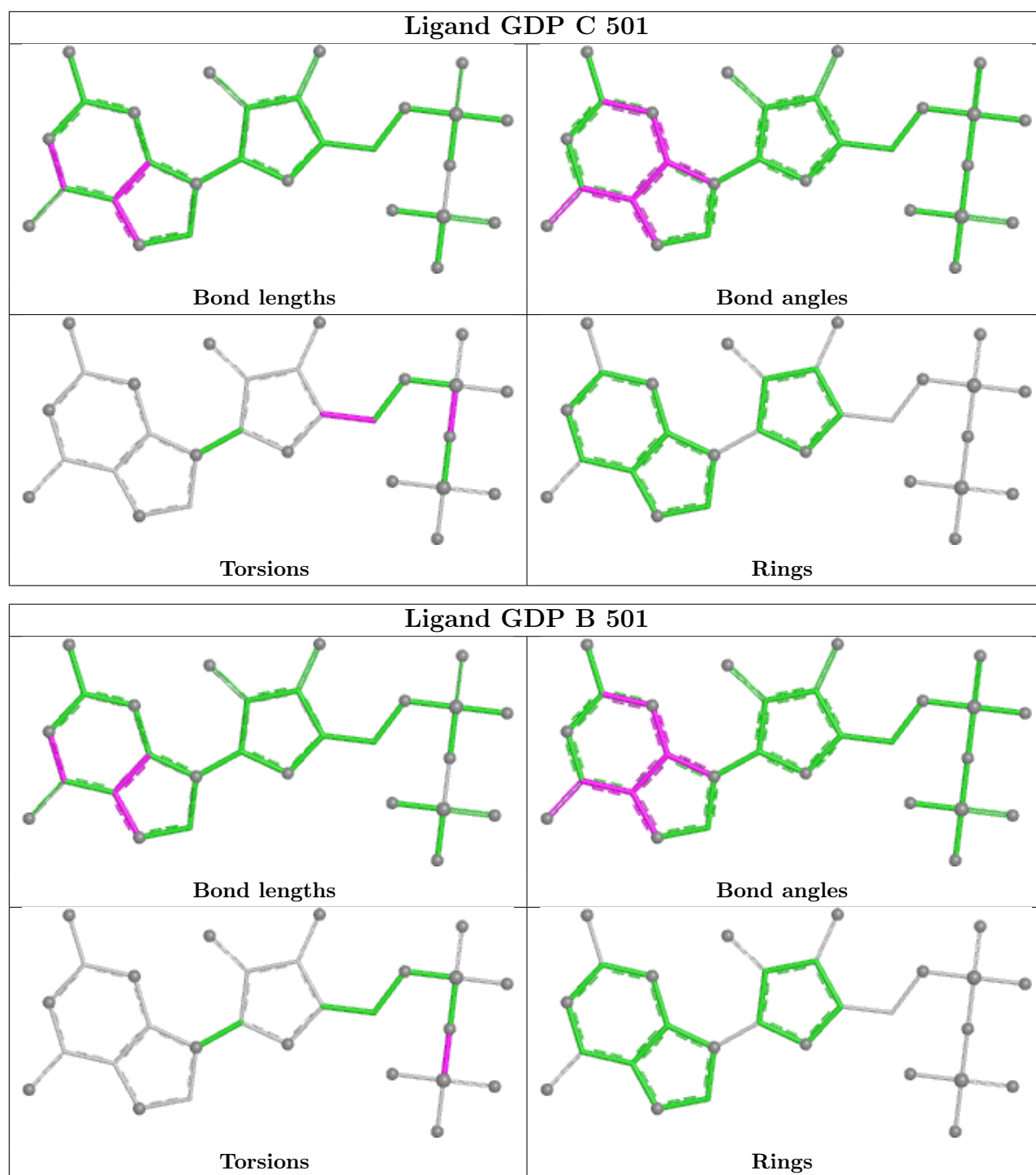
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GDP	3	0
2	E	501	GDP	2	0
2	C	501	GDP	1	0
2	B	501	GDP	2	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	412/415 (99%)	-0.12	3 (0%) 84 82	18, 34, 53, 90	366 (88%)
1	B	396/415 (95%)	-0.10	2 (0%) 87 85	19, 37, 55, 81	323 (81%)
1	C	406/415 (97%)	-0.04	8 (1%) 65 60	15, 32, 73, 122	332 (81%)
1	D	405/415 (97%)	0.07	3 (0%) 84 82	15, 37, 64, 133	341 (84%)
1	E	405/415 (97%)	0.11	8 (1%) 65 60	20, 48, 72, 119	298 (73%)
1	F	414/415 (99%)	0.37	10 (2%) 59 54	28, 55, 83, 151	291 (70%)
All	All	2438/2490 (97%)	0.05	34 (1%) 73 69	15, 41, 73, 151	1951 (80%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	411	GLY	3.8
1	A	77	CYS	3.4
1	E	47	ILE	3.4
1	E	78	GLY	3.3
1	F	228	THR	3.2
1	A	228	THR	3.2
1	E	58	VAL	3.2
1	C	230	PHE	3.1
1	D	77	CYS	3.0
1	C	370	VAL	2.9
1	F	341	GLY	2.8
1	B	34	THR	2.8
1	E	46	THR	2.7
1	D	158	GLU	2.6
1	E	228	THR	2.6
1	C	346	LEU	2.4
1	A	341	GLY	2.4
1	F	21	GLY	2.3
1	B	347	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	179	PRO	2.3
1	E	227	GLY	2.3
1	D	345	MET	2.2
1	F	40	GLU	2.2
1	F	77	CYS	2.2
1	E	127	PRO	2.2
1	F	31	GLY	2.2
1	F	76	SER	2.2
1	C	345	MET	2.1
1	C	338	ARG	2.0
1	E	280	ARG	2.0
1	C	226	PRO	2.0
1	C	233	LEU	2.0
1	F	378	ILE	2.0
1	F	253	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

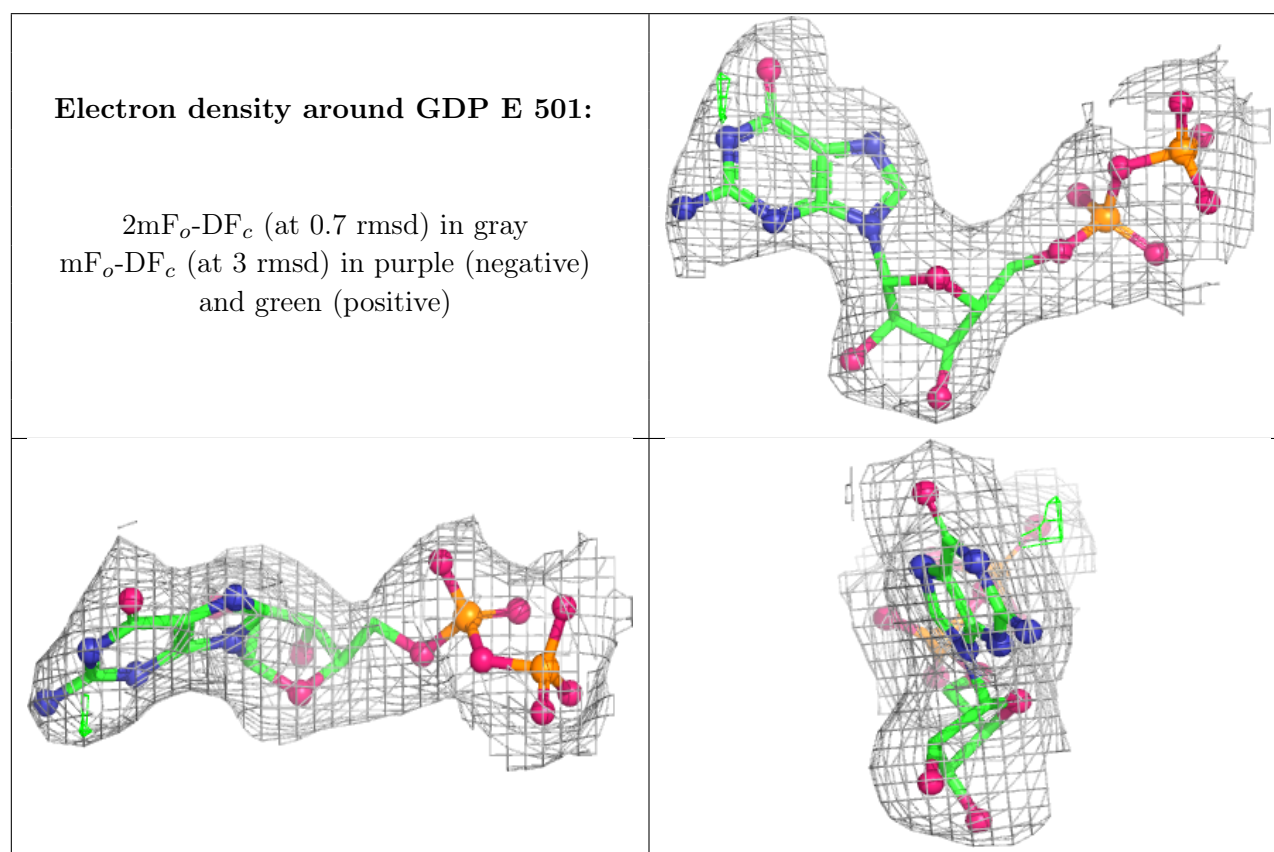
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	C	503	1/1	0.92	0.10	30,30,30,30	0
3	MG	F	502	1/1	0.92	0.09	58,58,58,58	0
2	GDP	E	501	28/28	0.93	0.08	41,55,62,72	28
3	MG	D	502	1/1	0.94	0.07	33,33,33,33	1
3	MG	E	502	1/1	0.94	0.05	46,46,46,46	1
2	GDP	F	501	28/28	0.94	0.08	35,43,48,48	28
3	MG	C	502	1/1	0.96	0.06	25,25,25,25	1
2	GDP	C	501	28/28	0.96	0.08	18,35,39,40	28

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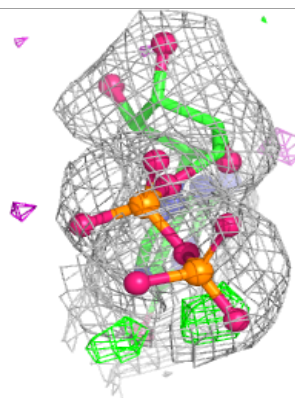
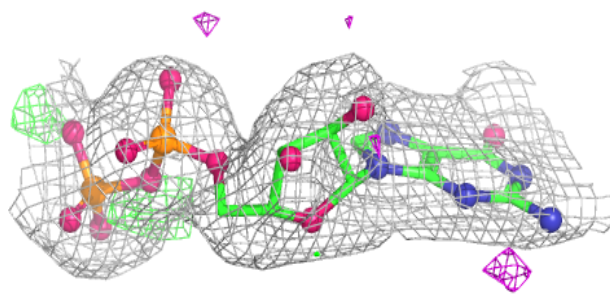
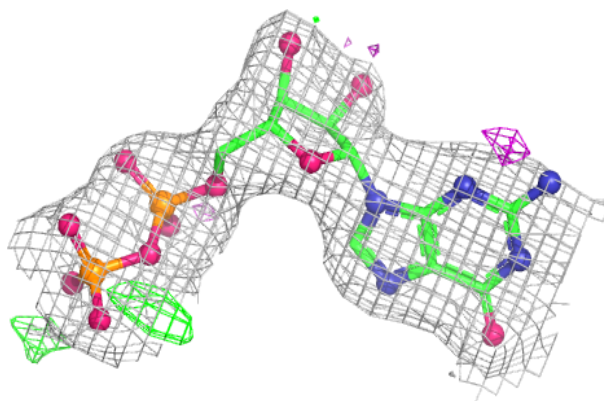
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	D	501	28/28	0.96	0.06	24,30,36,46	28
2	GDP	A	501	28/28	0.96	0.07	26,37,41,44	28
2	GDP	B	501	28/28	0.96	0.07	28,32,38,40	28
4	PO4	E	503	5/5	0.97	0.08	36,42,45,45	5
3	MG	B	502	1/1	0.98	0.05	25,25,25,25	1
3	MG	A	502	1/1	0.99	0.02	24,24,24,24	1

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.

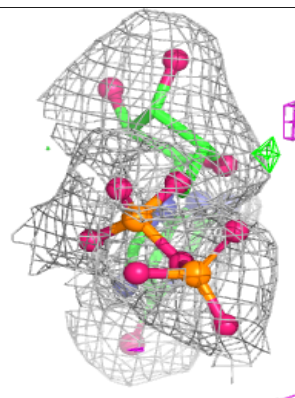
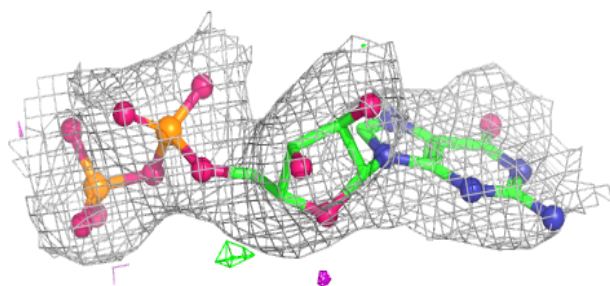
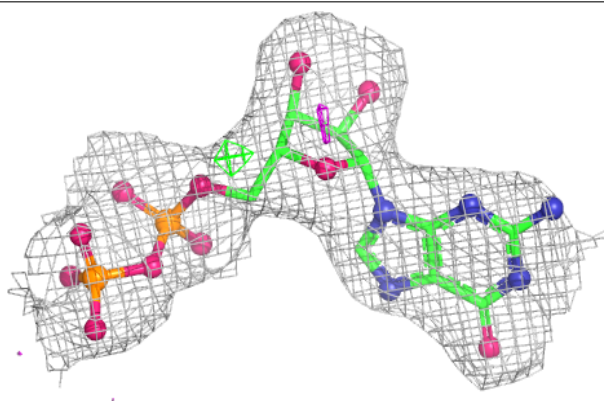


Electron density around GDP F 501:

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

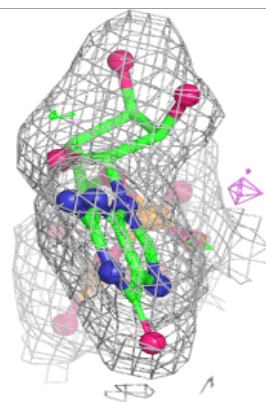
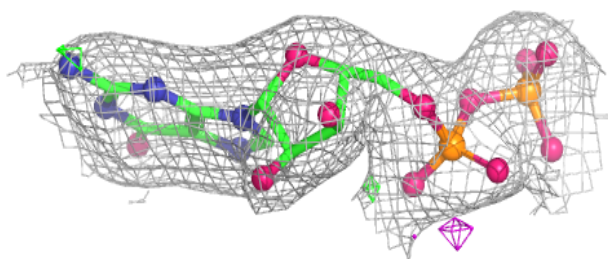
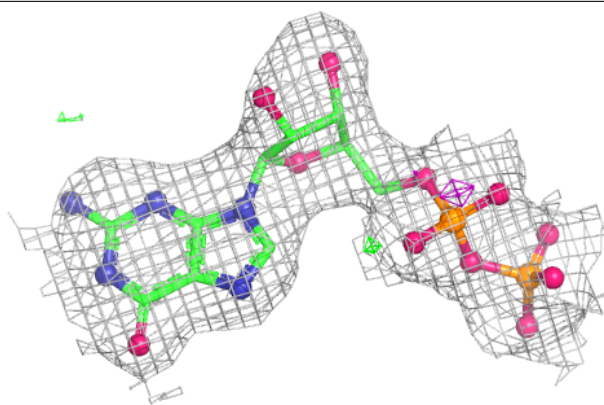
**Electron density around GDP C 501:**

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

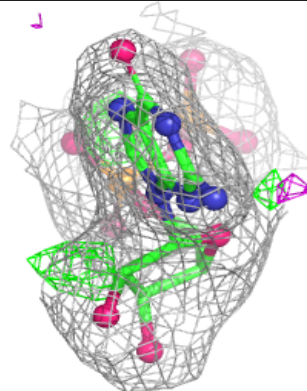
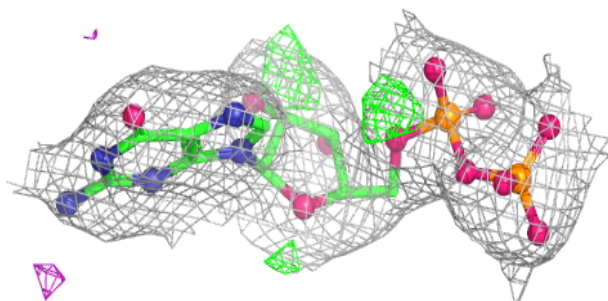
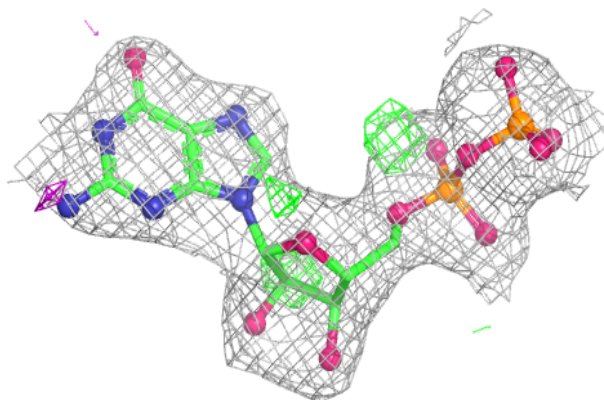


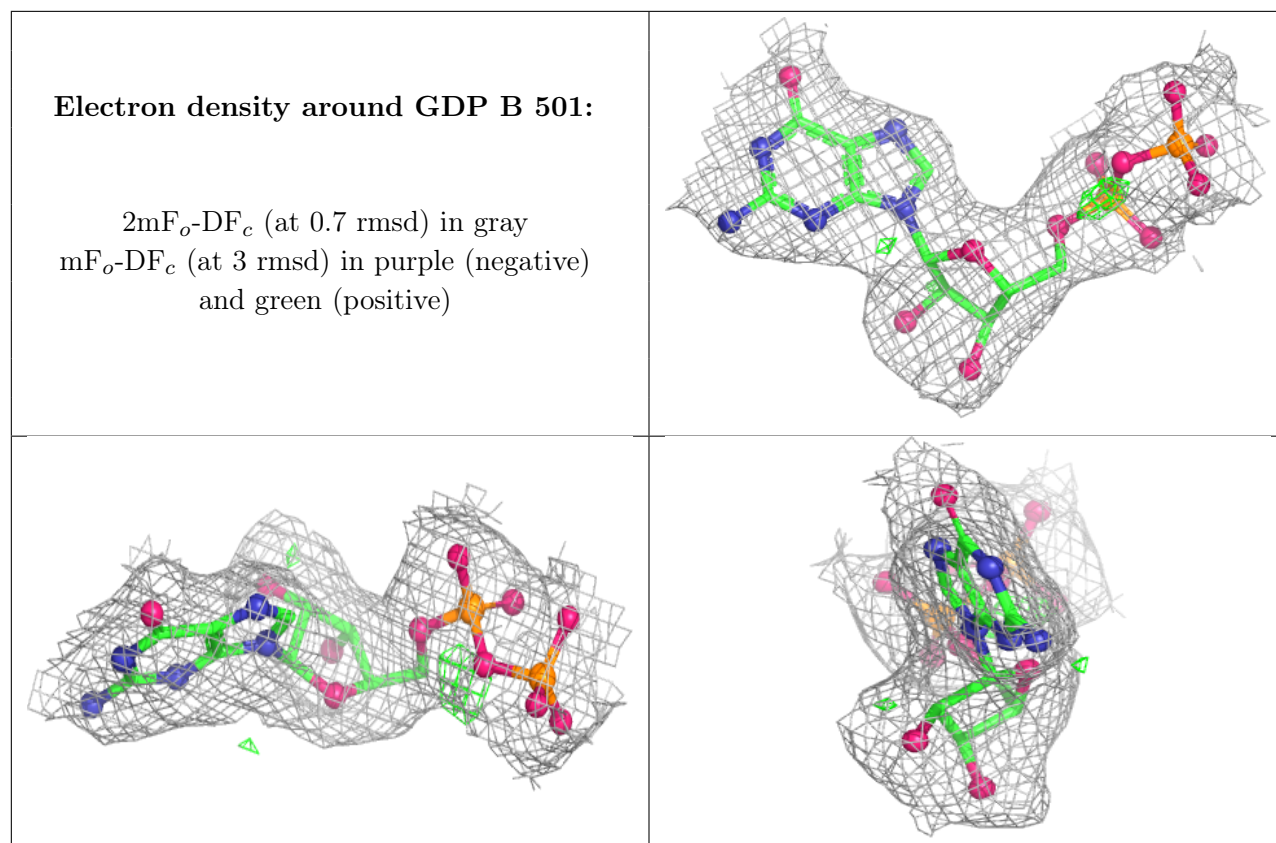
Electron density around GDP D 501:

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

**Electron density around GDP A 501:**

$2mF_o-DF_c$ (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.