



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:50 PM UTC

PDB ID : 2V55 / pdb_00002v55
Title : Mechanism of multi-site phosphorylation from a ROCK-I:RhoE complex structure
Authors : Komander, D.; Garg, R.; Wan, P.T.C.; Ridley, A.J.; Barford, D.
Deposited on : 2008-10-01
Resolution : 3.71 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

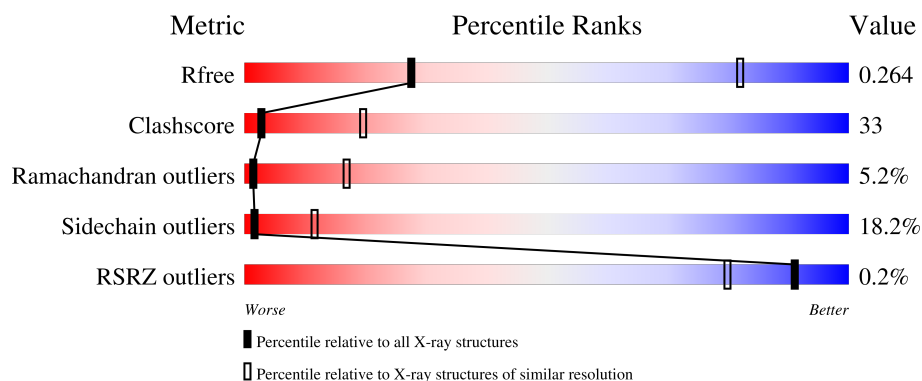
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

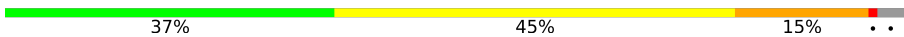
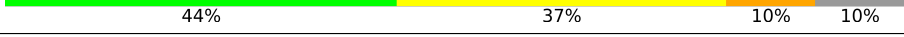
The reported resolution of this entry is 3.71 Å.

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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	406	
1	C	406	
2	B	200	
2	D	200	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9188 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.

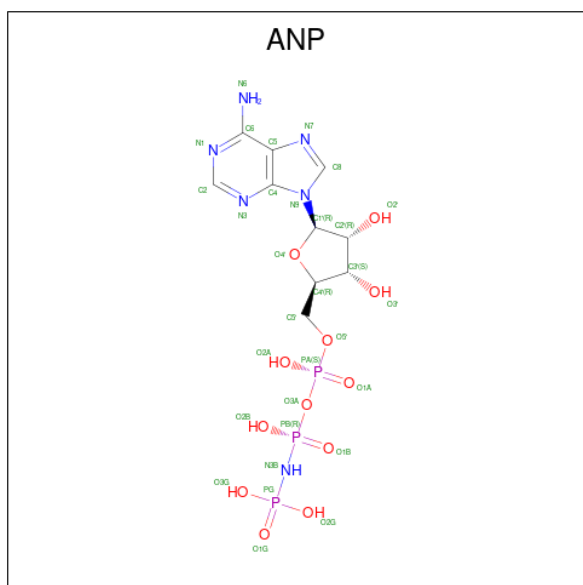
- Molecule 1 is a protein called RHO-ASSOCIATED PROTEIN KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3133	1999	519	594	21			
1	C	396	Total	C	N	O	S	0	0	0
			3152	2015	522	594	21			

- Molecule 2 is a protein called RHO-RELATED GTP-BINDING PROTEIN RHOE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1383	873	227	273	10			
2	D	182	Total	C	N	O	S	0	0	0
			1385	874	227	274	10			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

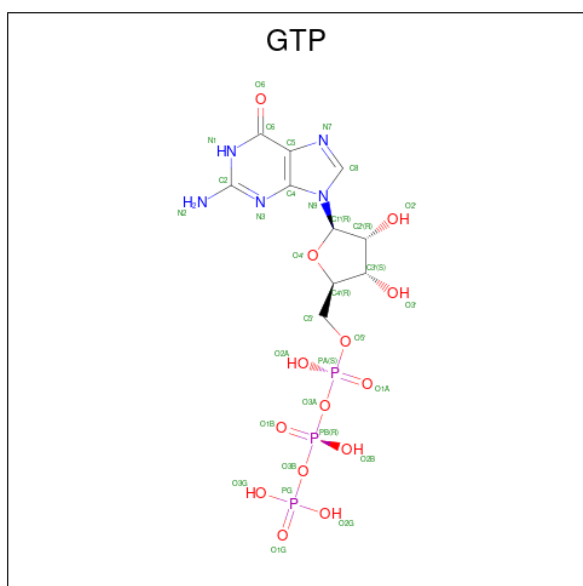


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

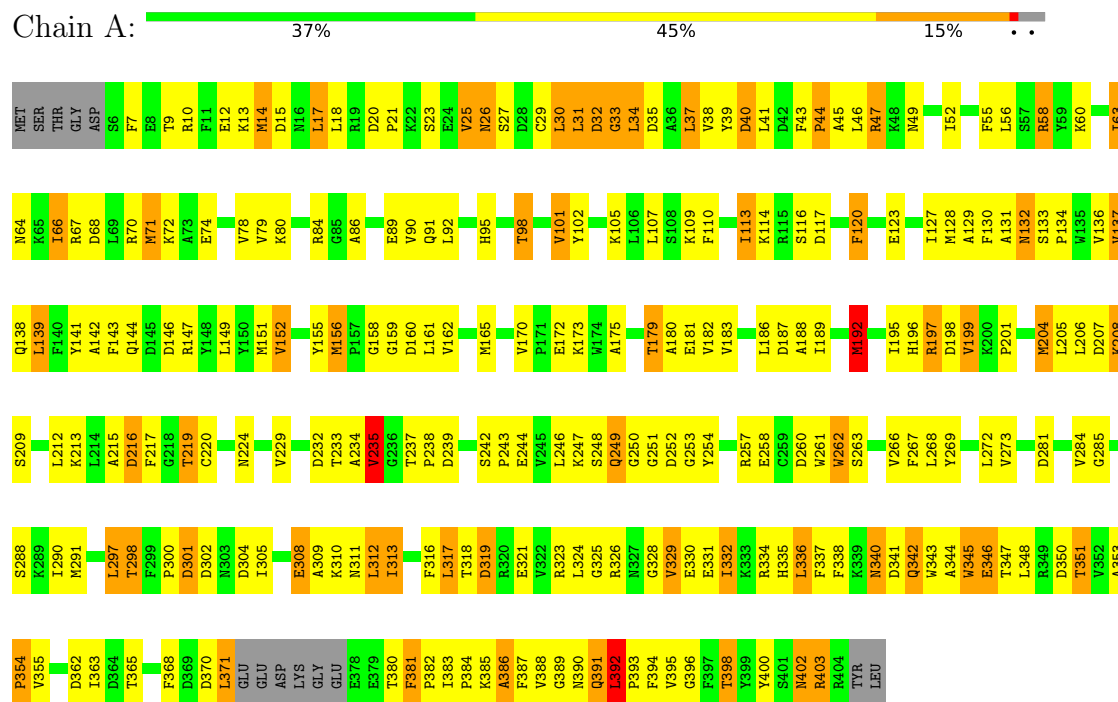


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

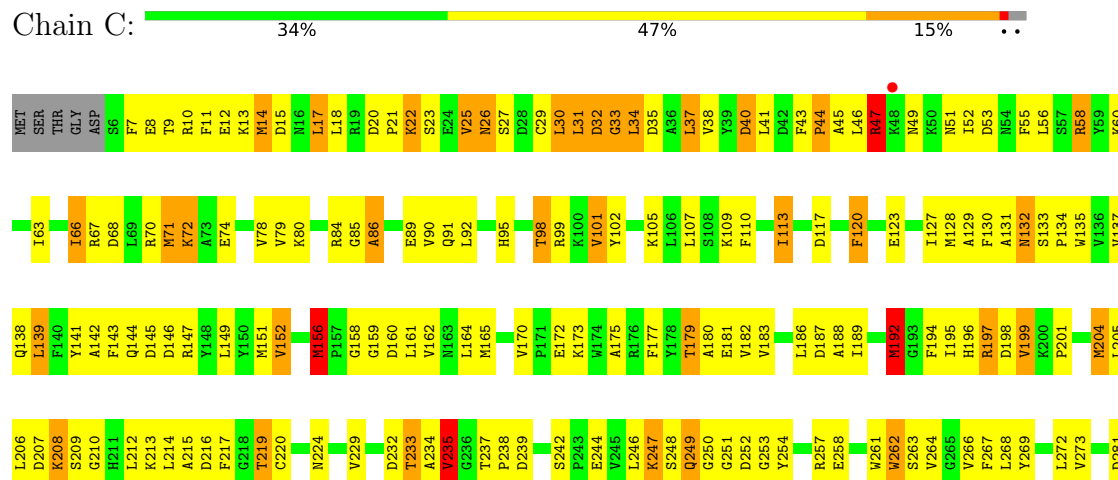
3 Residue-property plots

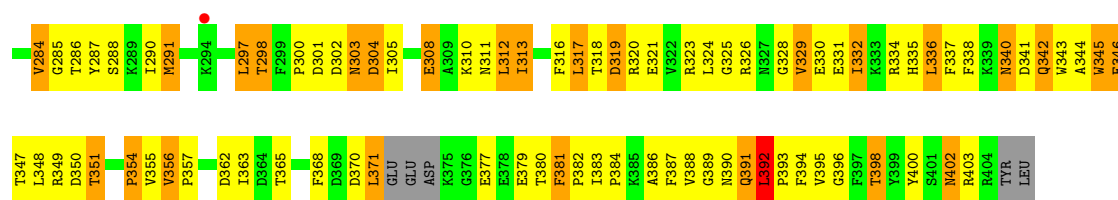
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: RHO-ASSOCIATED PROTEIN KINASE 1



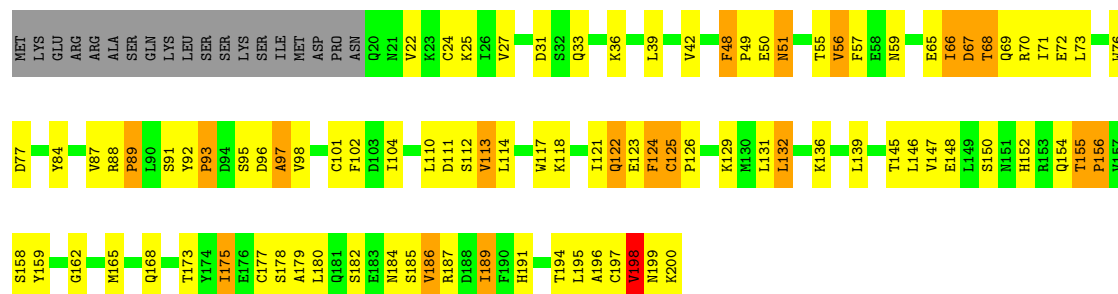
• Molecule 1: RHO-ASSOCIATED PROTEIN KINASE 1





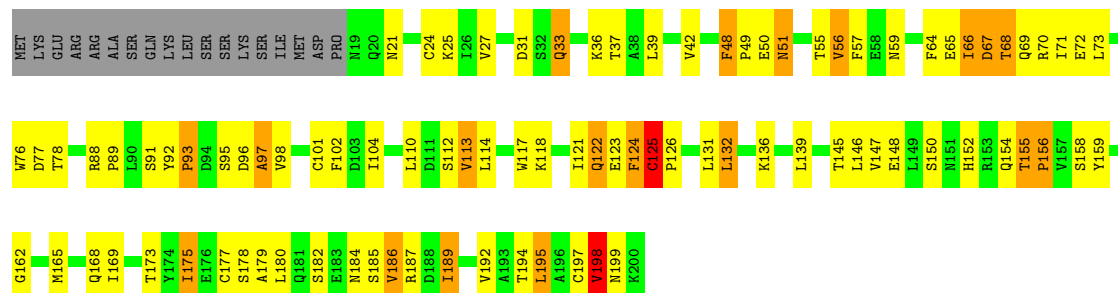
• Molecule 2: RHO-RELATED GTP-BINDING PROTEIN RHOE

Chain B: 44% 37% 10% 10%



• Molecule 2: RHO-RELATED GTP-BINDING PROTEIN RHOE

Chain D: 45% 36% 10% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.48Å 152.48Å 531.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.29 – 3.71 49.29 – 3.71	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.29-3.71) 98.2 (49.29-3.71)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.269 0.229 , 0.264	Depositor DCC
R_{free} test set	809 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: GTP, MG, ANP, SO4

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	0.55	0/3208	1.00	18/4349 (0.4%)
1	C	0.54	0/3228	1.00	21/4374 (0.5%)
2	B	0.56	0/1410	1.02	8/1921 (0.4%)
2	D	0.53	0/1413	1.00	10/1929 (0.5%)
All	All	0.55	0/9259	1.00	57/12573 (0.5%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	TRP	N-CA-C	7.79	120.90	111.40
2	B	198	VAL	N-CA-C	7.78	117.85	110.53
1	A	345	TRP	N-CA-C	7.01	120.31	111.69
1	C	170	VAL	CA-C-N	6.93	128.34	120.85
1	C	170	VAL	C-N-CA	6.93	128.34	120.85
1	C	381	PHE	CA-C-N	6.93	128.50	119.84
1	C	381	PHE	C-N-CA	6.93	128.50	119.84
1	A	47	ARG	NE-CZ-NH1	-6.86	114.64	121.50
1	A	170	VAL	CA-C-N	6.86	128.14	120.66
1	A	170	VAL	C-N-CA	6.86	128.14	120.66
2	D	155	THR	CA-C-N	6.59	128.07	119.84
2	D	155	THR	C-N-CA	6.59	128.07	119.84
1	A	381	PHE	CA-C-N	6.54	128.01	119.84
1	A	381	PHE	C-N-CA	6.54	128.01	119.84
1	A	47	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	C	304	ASP	N-CA-C	-6.48	105.76	113.21
1	C	235	VAL	N-CA-C	6.42	116.83	108.35
1	C	44	PRO	N-CA-C	-6.19	105.10	113.40
2	B	155	THR	CA-C-N	6.14	127.51	119.84
2	B	155	THR	C-N-CA	6.14	127.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	PHE	CA-C-N	6.02	126.33	119.83
2	B	48	PHE	C-N-CA	6.02	126.33	119.83
1	C	17	LEU	N-CA-C	-5.92	105.41	114.16
1	C	396	GLY	N-CA-C	-5.90	106.95	115.27
1	A	44	PRO	N-CA-C	-5.86	105.55	113.40
1	A	192	MET	N-CA-C	-5.85	105.90	113.16
1	A	260	ASP	N-CA-C	-5.82	105.28	112.90
1	C	47	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	A	17	LEU	N-CA-C	-5.79	105.59	114.16
1	A	396	GLY	N-CA-C	-5.79	107.11	115.27
1	A	120	PHE	N-CA-C	-5.77	105.15	114.09
1	C	343	TRP	N-CA-C	5.72	116.95	107.73
1	A	284	VAL	CB-CA-C	-5.71	100.61	110.94
1	A	343	TRP	N-CA-C	5.70	116.91	107.73
2	D	48	PHE	CA-C-N	5.69	126.58	119.98
2	D	48	PHE	C-N-CA	5.69	126.58	119.98
2	B	131	LEU	N-CA-C	5.58	116.68	107.20
2	D	198	VAL	N-CA-C	5.56	116.34	110.72
2	D	131	LEU	N-CA-C	5.56	116.65	107.20
1	A	235	VAL	N-CA-C	5.55	115.68	108.35
2	B	111	ASP	N-CA-C	-5.54	106.60	113.19
1	C	120	PHE	N-CA-C	-5.49	105.58	114.09
2	D	125	CYS	CA-C-N	5.47	124.81	118.85
2	D	125	CYS	C-N-CA	5.47	124.81	118.85
1	A	18	LEU	N-CA-C	-5.39	106.71	113.72
1	C	377	GLU	N-CA-C	5.32	117.94	109.96
2	D	78	THR	N-CA-C	5.29	115.27	108.34
1	C	18	LEU	N-CA-C	-5.26	106.88	113.72
1	C	192	MET	N-CA-C	-5.24	106.66	113.16
1	C	310	LYS	N-CA-C	-5.18	105.75	111.71
1	C	156	MET	CA-C-N	5.08	125.76	120.12
1	C	156	MET	C-N-CA	5.08	125.76	120.12
2	B	101	CYS	N-CA-C	5.07	118.00	110.14
1	C	356	VAL	CA-C-N	5.07	125.36	119.93
1	C	356	VAL	C-N-CA	5.07	125.36	119.93
1	A	310	LYS	N-CA-C	-5.05	105.90	111.71
2	D	101	CYS	N-CA-C	5.02	117.79	109.85

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	3133	0	2963	210	0
1	C	3152	0	2984	228	0
2	B	1383	0	1334	84	0
2	D	1385	0	1319	84	0
3	A	31	0	13	1	0
3	C	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	32	0	12	7	0
5	D	32	0	12	6	0
6	D	5	0	0	0	0
All	All	9188	0	8650	586	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 33.

All (586) 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:31:LEU:HD13	1:C:70:ARG:HD2	1.31	1.10
1:C:285:GLY:HA2	2:D:173:THR:HB	1.33	1.07
1:A:31:LEU:HD13	1:A:70:ARG:HD2	1.37	1.06
2:D:175:ILE:HD11	2:D:189:ILE:HG12	1.37	1.05
1:A:340:ASN:HB2	1:A:342:GLN:HG2	1.40	1.03
1:C:340:ASN:HB2	1:C:342:GLN:HG2	1.41	1.03
1:C:131:ALA:HB2	1:C:192:MET:SD	2.00	1.02
2:B:175:ILE:HD11	2:B:189:ILE:HG12	1.43	1.00
1:A:131:ALA:HB2	1:A:192:MET:SD	2.03	0.99
2:D:25:LYS:HD3	2:D:95:SER:HA	1.50	0.91
2:B:25:LYS:HD3	2:B:95:SER:HA	1.51	0.90
1:A:105:LYS:HD3	1:A:151:MET:HE2	1.55	0.89
1:C:105:LYS:HD3	1:C:151:MET:HE2	1.58	0.85
1:C:109:LYS:HB2	1:C:147:ARG:O	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:LEU:HA	2:D:113:VAL:HG13	1.60	0.84
1:C:187:ASP:OD1	1:C:329:VAL:HG11	1.78	0.83
1:A:109:LYS:HE3	1:A:394:PHE:CD2	2.15	0.82
1:C:25:VAL:HB	1:C:30:LEU:HD21	1.58	0.82
1:C:308:GLU:HB3	1:C:336:LEU:HD13	1.62	0.81
2:B:110:LEU:HA	2:B:113:VAL:HG13	1.62	0.81
2:B:136:LYS:HB3	2:B:139:LEU:HD13	1.60	0.81
1:A:109:LYS:HB2	1:A:147:ARG:O	1.80	0.80
1:C:158:GLY:HA3	1:C:206:LEU:HB2	1.64	0.80
2:D:136:LYS:HB3	2:D:139:LEU:HD13	1.63	0.79
1:A:187:ASP:OD1	1:A:329:VAL:HG11	1.82	0.79
1:A:158:GLY:HA3	1:A:206:LEU:HB2	1.65	0.79
1:A:25:VAL:HB	1:A:30:LEU:HD21	1.65	0.78
1:C:147:ARG:HH22	1:C:380:THR:HB	1.49	0.78
2:B:66:ILE:HD12	2:B:71:ILE:HD11	1.65	0.77
1:A:308:GLU:HB3	1:A:336:LEU:HD13	1.66	0.77
1:C:47:ARG:HD2	1:C:53:ASP:OD1	1.85	0.77
1:C:285:GLY:HA2	2:D:173:THR:CB	2.13	0.76
1:C:31:LEU:HD13	1:C:70:ARG:CD	2.13	0.76
1:C:107:LEU:HB2	1:C:149:LEU:HB2	1.68	0.75
1:A:313:ILE:HG23	1:A:317:LEU:HD23	1.66	0.75
1:C:113:ILE:HD11	1:C:381:PHE:CZ	2.22	0.75
1:C:250:GLY:HA3	2:D:65:GLU:O	1.88	0.74
1:A:113:ILE:HD11	1:A:381:PHE:CZ	2.23	0.74
1:C:47:ARG:HD3	1:C:53:ASP:HA	1.69	0.74
2:D:98:VAL:HG11	2:D:121:ILE:CD1	2.18	0.73
1:C:109:LYS:HE3	1:C:394:PHE:CD2	2.24	0.73
1:C:22:LYS:HG3	1:C:130:PHE:HE1	1.54	0.73
1:C:389:GLY:O	1:C:392:LEU:HB2	1.90	0.72
1:C:302:ASP:O	1:C:304:ASP:N	2.19	0.72
1:A:147:ARG:HH22	1:A:380:THR:HB	1.54	0.71
1:C:313:ILE:HG23	1:C:317:LEU:HD23	1.72	0.71
2:D:66:ILE:HD12	2:D:71:ILE:HD11	1.71	0.71
1:A:113:ILE:HD11	1:A:381:PHE:HZ	1.54	0.71
1:A:389:GLY:O	1:A:392:LEU:HB2	1.91	0.71
1:A:189:ILE:HD11	1:A:217:PHE:HE1	1.55	0.71
2:B:154:GLN:O	2:B:155:THR:HG23	1.90	0.71
2:B:179:ALA:HB3	5:B:1201:GTP:O6	1.91	0.71
1:C:285:GLY:CA	2:D:173:THR:HB	2.17	0.71
2:D:179:ALA:HB3	5:D:1201:GTP:O6	1.91	0.71
1:A:189:ILE:CD1	1:A:217:PHE:HE1	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ILE:HD11	1:C:381:PHE:HZ	1.55	0.71
1:C:302:ASP:C	1:C:304:ASP:H	1.99	0.70
1:C:159:GLY:HA2	1:C:368:PHE:CE1	2.26	0.70
1:A:159:GLY:HA2	1:A:368:PHE:CE1	2.27	0.70
2:B:129:LYS:HD2	2:B:196:ALA:O	1.92	0.70
1:A:90:VAL:HG22	1:A:105:LYS:HA	1.72	0.70
1:A:80:LYS:HE2	1:A:370:ASP:OD1	1.93	0.69
1:C:234:ALA:HB2	1:C:249:GLN:HB2	1.75	0.69
1:A:107:LEU:HB2	1:A:149:LEU:HB2	1.74	0.69
1:A:31:LEU:HD13	1:A:70:ARG:CD	2.17	0.69
2:B:98:VAL:HG11	2:B:121:ILE:CD1	2.23	0.69
1:C:90:VAL:HG22	1:C:105:LYS:HA	1.73	0.68
1:C:308:GLU:HB3	1:C:336:LEU:CD1	2.23	0.68
2:D:98:VAL:HG11	2:D:121:ILE:HD12	1.76	0.68
1:A:234:ALA:HB2	1:A:249:GLN:HB2	1.76	0.68
1:C:284:VAL:HG23	2:D:192:VAL:HG13	1.75	0.68
1:C:189:ILE:CD1	1:C:217:PHE:HE1	2.07	0.67
1:C:92:LEU:HD21	1:C:363:ILE:HB	1.76	0.67
1:A:37:LEU:HD23	1:A:38:VAL:N	2.09	0.67
1:C:20:ASP:O	1:C:23:SER:HB3	1.95	0.67
1:A:162:VAL:HG13	1:A:201:PRO:HB2	1.77	0.67
1:C:37:LEU:HD23	1:C:38:VAL:N	2.09	0.67
1:C:80:LYS:HE2	1:C:370:ASP:OD1	1.96	0.66
2:B:48:PHE:HE2	2:B:180:LEU:HB2	1.61	0.65
1:A:269:TYR:HB2	1:A:313:ILE:HD13	1.78	0.65
1:C:392:LEU:C	1:C:394:PHE:H	2.05	0.65
1:A:72:LYS:HE2	1:A:74:GLU:OE2	1.97	0.64
1:A:144:GLN:HE22	1:A:394:PHE:HB3	1.62	0.64
1:A:92:LEU:HD21	1:A:363:ILE:HB	1.80	0.64
1:C:72:LYS:HE2	1:C:74:GLU:OE2	1.97	0.64
1:C:22:LYS:HG3	1:C:130:PHE:CE1	2.33	0.63
1:C:313:ILE:CG2	1:C:317:LEU:HD23	2.28	0.63
1:A:392:LEU:C	1:A:394:PHE:H	2.06	0.63
1:C:189:ILE:HD11	1:C:217:PHE:HE1	1.62	0.63
2:D:110:LEU:C	2:D:112:SER:H	2.06	0.63
1:C:162:VAL:HG13	1:C:201:PRO:HB2	1.81	0.62
1:A:308:GLU:HB3	1:A:336:LEU:CD1	2.29	0.62
1:A:313:ILE:CG2	1:A:317:LEU:HD23	2.28	0.62
2:D:168:GLN:O	2:D:168:GLN:HG2	1.97	0.62
2:D:48:PHE:HE2	2:D:180:LEU:HB2	1.63	0.62
5:D:1201:GTP:O2G	5:D:1201:GTP:O2B	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:C	2:B:112:SER:H	2.07	0.62
1:C:102:TYR:HB2	1:C:152:VAL:HG12	1.82	0.62
1:C:14:MET:O	1:C:17:LEU:HB3	2.00	0.61
2:B:118:LYS:O	2:B:122:GLN:HB2	2.00	0.61
1:A:20:ASP:O	1:A:23:SER:HB3	2.01	0.61
1:A:249:GLN:HG3	2:B:67:ASP:OD1	2.00	0.61
1:A:262:TRP:CD1	1:A:262:TRP:C	2.78	0.61
1:A:250:GLY:HA3	2:B:65:GLU:O	2.01	0.60
1:A:14:MET:O	1:A:17:LEU:HB3	2.01	0.60
2:D:88:ARG:N	2:D:89:PRO:HD2	2.16	0.60
1:A:313:ILE:HG23	1:A:317:LEU:CD2	2.29	0.60
2:D:71:ILE:N	2:D:71:ILE:HD12	2.15	0.60
2:B:139:LEU:HD11	5:B:1201:GTP:N2	2.17	0.60
1:A:266:VAL:CG2	1:A:317:LEU:HD11	2.32	0.60
2:B:88:ARG:N	2:B:89:PRO:HD2	2.17	0.60
1:C:101:VAL:HG11	1:C:363:ILE:HG22	1.83	0.60
1:A:344:ALA:O	1:A:347:THR:HG22	2.02	0.60
1:C:269:TYR:HB2	1:C:313:ILE:HD13	1.84	0.60
1:A:12:GLU:O	1:A:14:MET:N	2.34	0.60
1:C:144:GLN:HE22	1:C:394:PHE:HB3	1.67	0.60
1:A:392:LEU:HB3	1:A:393:PRO:HD3	1.84	0.59
1:C:266:VAL:HG23	1:C:317:LEU:HD11	1.84	0.59
1:C:392:LEU:HB3	1:C:393:PRO:HD3	1.83	0.59
2:D:139:LEU:HD11	5:D:1201:GTP:N2	2.16	0.59
1:A:102:TYR:HB2	1:A:152:VAL:HG12	1.83	0.59
1:A:370:ASP:C	1:A:371:LEU:HG	2.27	0.59
1:C:370:ASP:C	1:C:371:LEU:HG	2.27	0.59
1:A:101:VAL:HG11	1:A:363:ILE:HG22	1.84	0.59
2:B:98:VAL:HG11	2:B:121:ILE:HD12	1.83	0.59
1:C:313:ILE:HG23	1:C:317:LEU:CD2	2.32	0.59
1:A:105:LYS:HD3	1:A:151:MET:CE	2.30	0.59
1:A:127:ILE:HG21	1:A:217:PHE:CE1	2.38	0.58
1:A:204:MET:HE1	1:A:267:PHE:CE2	2.37	0.58
1:A:266:VAL:HG23	1:A:317:LEU:HD11	1.85	0.58
1:C:266:VAL:CG2	1:C:317:LEU:HD11	2.34	0.58
1:C:46:LEU:O	1:C:52:ILE:HD12	2.03	0.58
1:C:141:TYR:O	1:C:152:VAL:HG23	2.03	0.58
1:A:79:VAL:HG11	1:A:363:ILE:HD12	1.86	0.58
1:A:340:ASN:N	1:A:340:ASN:HD22	2.01	0.58
1:C:127:ILE:HG21	1:C:217:PHE:CE1	2.39	0.58
1:C:233:THR:HG22	2:D:67:ASP:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ILE:CD1	2:B:71:ILE:HD11	2.34	0.58
1:C:262:TRP:CD1	1:C:262:TRP:C	2.81	0.58
1:A:70:ARG:O	1:A:71:MET:C	2.47	0.57
1:A:46:LEU:O	1:A:52:ILE:HD12	2.03	0.57
1:C:70:ARG:HG2	1:C:400:TYR:OH	2.04	0.57
2:D:57:PHE:CE1	2:D:91:SER:HB3	2.40	0.57
1:C:204:MET:HE1	1:C:267:PHE:CE2	2.39	0.57
1:A:312:LEU:HG	1:A:335:HIS:CD2	2.39	0.57
1:C:44:PRO:HD2	1:C:45:ALA:H	1.70	0.57
2:B:168:GLN:O	2:B:168:GLN:HG2	2.05	0.57
1:C:127:ILE:HG21	1:C:217:PHE:CD1	2.40	0.57
1:C:248:SER:HB2	1:C:253:GLY:HA3	1.86	0.57
1:C:70:ARG:O	1:C:71:MET:C	2.48	0.56
1:C:302:ASP:C	1:C:304:ASP:N	2.63	0.56
1:A:189:ILE:HD11	1:A:217:PHE:CE1	2.38	0.56
2:B:71:ILE:N	2:B:71:ILE:HD12	2.20	0.56
1:C:312:LEU:HG	1:C:335:HIS:CD2	2.40	0.56
1:C:344:ALA:O	1:C:347:THR:HG22	2.05	0.56
2:D:118:LYS:O	2:D:122:GLN:HB2	2.05	0.56
1:A:141:TYR:O	1:A:152:VAL:HG23	2.06	0.56
1:A:248:SER:HB2	1:A:253:GLY:HA3	1.87	0.56
1:C:105:LYS:HD3	1:C:151:MET:CE	2.33	0.56
1:A:95:HIS:ND1	1:A:98:THR:HG23	2.21	0.56
5:B:1201:GTP:O2B	5:B:1201:GTP:O2G	2.24	0.55
1:C:12:GLU:C	1:C:14:MET:N	2.64	0.55
1:C:303:ASN:C	1:C:305:ILE:H	2.13	0.55
2:D:113:VAL:O	2:D:113:VAL:HG23	2.05	0.55
1:C:142:ALA:O	1:C:398:THR:HA	2.07	0.55
1:A:40:ASP:OD1	1:A:391:GLN:HB2	2.07	0.55
1:A:251:GLY:O	1:A:253:GLY:N	2.40	0.55
1:C:388:VAL:HG23	1:C:389:GLY:H	1.72	0.55
2:D:55:THR:HG21	2:D:77:ASP:OD2	2.07	0.55
1:C:129:ALA:C	1:C:130:PHE:HD2	2.15	0.55
1:C:196:HIS:O	1:C:197:ARG:HB2	2.07	0.55
1:A:207:ASP:C	1:A:209:SER:H	2.15	0.55
1:C:340:ASN:N	1:C:340:ASN:HD22	2.05	0.55
1:A:127:ILE:HG21	1:A:217:PHE:CD1	2.41	0.54
1:A:44:PRO:HD2	1:A:45:ALA:H	1.73	0.54
2:D:71:ILE:HD12	2:D:71:ILE:H	1.72	0.54
1:A:402:ASN:O	1:C:402:ASN:O	2.25	0.54
1:A:180:ALA:HB2	1:A:338:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HA	2:B:117:TRP:HD1	1.73	0.54
1:C:40:ASP:OD1	1:C:391:GLN:HB2	2.07	0.54
1:A:70:ARG:HG2	1:A:400:TYR:OH	2.07	0.53
1:C:346:GLU:CD	1:C:346:GLU:H	2.15	0.53
2:B:55:THR:HG21	2:B:77:ASP:OD2	2.08	0.53
1:C:251:GLY:O	1:C:253:GLY:N	2.41	0.53
2:D:98:VAL:HG11	2:D:121:ILE:HD11	1.91	0.53
1:A:142:ALA:O	1:A:398:THR:HA	2.07	0.53
2:B:110:LEU:C	2:B:112:SER:N	2.66	0.53
1:C:43:PHE:CE2	1:C:384:PRO:HG2	2.43	0.53
2:D:154:GLN:O	2:D:155:THR:HG23	2.08	0.53
1:A:109:LYS:CE	1:A:394:PHE:CD2	2.90	0.53
1:C:392:LEU:O	1:C:394:PHE:N	2.42	0.53
1:A:346:GLU:H	1:A:346:GLU:CD	2.16	0.53
1:A:43:PHE:CE2	1:A:384:PRO:HG2	2.43	0.53
2:D:113:VAL:HA	2:D:117:TRP:HD1	1.72	0.53
1:A:402:ASN:OD1	1:A:403:ARG:HG2	2.08	0.53
2:D:110:LEU:C	2:D:112:SER:N	2.66	0.53
1:C:207:ASP:C	1:C:209:SER:H	2.16	0.53
1:A:179:THR:O	1:A:183:VAL:HG23	2.08	0.53
1:A:388:VAL:HG23	1:A:389:GLY:H	1.74	0.53
1:A:392:LEU:O	1:A:394:PHE:N	2.42	0.52
2:D:66:ILE:HD13	2:D:66:ILE:O	2.09	0.52
1:A:340:ASN:N	1:A:340:ASN:ND2	2.57	0.52
1:A:12:GLU:C	1:A:14:MET:H	2.16	0.52
1:A:55:PHE:CD2	1:A:56:LEU:N	2.77	0.52
1:A:175:ALA:CB	1:A:272:LEU:HD21	2.39	0.52
1:C:175:ALA:CB	1:C:272:LEU:HD21	2.40	0.52
1:C:183:VAL:HG11	1:C:332:ILE:HG21	1.90	0.52
1:C:390:ASN:C	1:C:392:LEU:H	2.15	0.52
1:A:129:ALA:C	1:A:130:PHE:HD2	2.17	0.52
1:C:288:SER:HB3	2:D:175:ILE:HG22	1.92	0.52
1:A:12:GLU:C	1:A:14:MET:N	2.67	0.52
1:A:335:HIS:C	1:A:337:PHE:H	2.17	0.52
1:C:26:ASN:ND2	1:C:29:CYS:SG	2.83	0.52
1:C:21:PRO:C	1:C:23:SER:H	2.17	0.52
1:C:156:MET:SD	1:C:213:LYS:HD2	2.49	0.52
1:A:288:SER:OG	2:B:173:THR:HG21	2.09	0.52
1:C:66:ILE:HD13	1:C:66:ILE:O	2.09	0.52
1:C:288:SER:HB2	2:D:173:THR:OG1	2.10	0.52
2:B:57:PHE:CE1	2:B:91:SER:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:O	1:C:14:MET:N	2.43	0.52
1:C:55:PHE:CD2	1:C:56:LEU:N	2.77	0.52
1:A:288:SER:HB2	2:B:173:THR:OG1	2.10	0.51
1:C:12:GLU:C	1:C:14:MET:H	2.16	0.51
1:A:55:PHE:CD2	1:A:55:PHE:C	2.89	0.51
1:A:195:ILE:HG22	1:A:197:ARG:HG3	1.92	0.51
1:C:187:ASP:OD2	1:C:329:VAL:HG21	2.10	0.51
2:D:66:ILE:HG23	2:D:71:ILE:CD1	2.40	0.51
1:A:128:MET:HB3	1:A:139:LEU:HB2	1.93	0.51
1:C:80:LYS:HE3	1:C:365:THR:OG1	2.11	0.51
1:C:390:ASN:O	1:C:392:LEU:N	2.38	0.51
1:C:79:VAL:HG11	1:C:363:ILE:HD12	1.93	0.51
1:A:189:ILE:CD1	1:A:217:PHE:CE1	2.90	0.51
1:C:52:ILE:HG22	1:C:56:LEU:HD12	1.93	0.51
1:C:187:ASP:CG	1:C:329:VAL:HG21	2.36	0.51
1:C:189:ILE:HD11	1:C:217:PHE:CE1	2.44	0.51
2:D:112:SER:C	2:D:114:LEU:H	2.17	0.51
2:B:112:SER:C	2:B:114:LEU:H	2.18	0.51
1:C:7:PHE:O	1:C:10:ARG:HB2	2.11	0.51
1:A:66:ILE:HD13	1:A:66:ILE:O	2.12	0.51
1:C:55:PHE:CD2	1:C:55:PHE:C	2.89	0.50
1:A:324:LEU:HD12	1:A:325:GLY:N	2.27	0.50
1:C:15:ASP:C	1:C:17:LEU:H	2.19	0.50
1:C:46:LEU:HB3	1:C:52:ILE:HD13	1.92	0.50
1:C:392:LEU:HB3	1:C:393:PRO:CD	2.41	0.50
2:B:39:LEU:HD11	2:B:189:ILE:HD12	1.93	0.50
1:C:205:LEU:N	1:C:205:LEU:HD22	2.27	0.50
1:A:297:LEU:O	1:A:298:THR:HG23	2.12	0.50
1:C:335:HIS:C	1:C:337:PHE:H	2.19	0.50
1:A:285:GLY:HA2	2:B:173:THR:HB	1.93	0.50
2:B:98:VAL:HG11	2:B:121:ILE:HD11	1.93	0.50
2:D:118:LYS:HG2	2:D:122:GLN:NE2	2.27	0.50
1:A:66:ILE:C	1:A:68:ASP:N	2.68	0.50
2:B:48:PHE:CE2	2:B:180:LEU:HB2	2.46	0.50
1:C:95:HIS:ND1	1:C:98:THR:HG23	2.27	0.50
1:A:143:PHE:HA	1:A:398:THR:HG23	1.93	0.49
1:A:187:ASP:CG	1:A:329:VAL:HG21	2.37	0.49
1:A:392:LEU:HB3	1:A:393:PRO:CD	2.42	0.49
1:C:26:ASN:O	1:C:27:SER:C	2.55	0.49
1:C:347:THR:O	1:C:350:ASP:HB2	2.12	0.49
2:D:124:PHE:C	2:D:126:PRO:HD3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ILE:CD1	2:D:71:ILE:HD11	2.40	0.49
1:A:156:MET:SD	1:A:213:LYS:HD2	2.52	0.49
1:A:390:ASN:O	1:A:392:LEU:N	2.42	0.49
2:B:194:THR:O	2:B:198:VAL:HG13	2.13	0.49
1:C:129:ALA:HB2	1:C:139:LEU:HB3	1.95	0.49
1:A:52:ILE:HG22	1:A:56:LEU:HD12	1.95	0.49
1:A:331:GLU:HB3	1:A:334:ARG:NH2	2.27	0.49
2:B:177:CYS:O	2:B:177:CYS:SG	2.71	0.49
2:B:178:SER:C	2:B:180:LEU:H	2.21	0.49
2:B:197:CYS:O	2:B:200:LYS:HD2	2.13	0.49
2:D:139:LEU:HD23	2:D:145:THR:HG21	1.95	0.49
1:A:80:LYS:HE3	1:A:365:THR:OG1	2.13	0.48
1:A:390:ASN:C	1:A:392:LEU:H	2.19	0.48
2:B:113:VAL:HG23	2:B:113:VAL:O	2.12	0.48
1:C:46:LEU:HD21	1:C:386:ALA:O	2.13	0.48
2:D:64:PHE:CG	2:D:65:GLU:N	2.80	0.48
2:D:110:LEU:HA	2:D:113:VAL:CG1	2.38	0.48
1:C:340:ASN:N	1:C:340:ASN:ND2	2.62	0.48
2:B:124:PHE:C	2:B:126:PRO:HD3	2.39	0.48
1:C:402:ASN:OD1	1:C:403:ARG:N	2.46	0.48
1:A:347:THR:O	1:A:350:ASP:HB2	2.13	0.48
1:C:219:THR:HG22	1:C:235:VAL:CG1	2.44	0.48
1:A:129:ALA:HB2	1:A:139:LEU:HB3	1.95	0.48
1:A:335:HIS:CE1	1:A:336:LEU:HD12	2.49	0.48
2:B:150:SER:C	2:B:152:HIS:H	2.22	0.48
1:A:207:ASP:O	1:A:209:SER:N	2.47	0.48
1:A:246:LEU:C	1:A:248:SER:H	2.22	0.48
2:B:162:GLY:O	2:B:165:MET:HB3	2.14	0.48
2:D:194:THR:O	2:D:198:VAL:HG13	2.14	0.48
2:B:124:PHE:N	2:B:124:PHE:CD2	2.81	0.48
1:C:44:PRO:CD	1:C:45:ALA:H	2.26	0.48
2:D:57:PHE:CZ	2:D:91:SER:HB3	2.49	0.48
1:A:38:VAL:HG22	1:A:56:LEU:HD23	1.96	0.48
1:A:247:LYS:O	2:B:187:ARG:NH2	2.47	0.48
2:B:104:ILE:O	2:B:104:ILE:HG22	2.13	0.48
1:A:14:MET:HG3	1:A:15:ASP:N	2.28	0.47
1:A:180:ALA:HB1	1:A:345:TRP:CZ3	2.49	0.47
1:C:14:MET:HG3	1:C:15:ASP:N	2.28	0.47
1:C:179:THR:O	1:C:183:VAL:HG23	2.14	0.47
2:D:92:TYR:O	2:D:93:PRO:C	2.57	0.47
1:A:187:ASP:OD2	1:A:329:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:OG1	1:A:381:PHE:N	2.46	0.47
2:B:96:ASP:O	2:B:97:ALA:HB2	2.13	0.47
2:B:118:LYS:HG2	2:B:122:GLN:NE2	2.28	0.47
1:A:15:ASP:C	1:A:17:LEU:H	2.22	0.47
1:A:205:LEU:N	1:A:205:LEU:HD22	2.30	0.47
1:A:249:GLN:CG	2:B:67:ASP:OD1	2.62	0.47
1:C:66:ILE:C	1:C:68:ASP:N	2.70	0.47
1:C:195:ILE:HG22	1:C:197:ARG:HG3	1.97	0.47
2:D:48:PHE:CE2	2:D:180:LEU:HB2	2.48	0.47
2:D:150:SER:C	2:D:152:HIS:H	2.21	0.47
1:C:215:ALA:HA	1:C:217:PHE:HE2	1.79	0.47
1:A:196:HIS:O	1:A:197:ARG:HB2	2.13	0.47
1:C:247:LYS:O	2:D:187:ARG:NH2	2.48	0.47
1:A:10:ARG:C	1:A:12:GLU:N	2.72	0.47
1:A:46:LEU:HB3	1:A:52:ILE:HD13	1.96	0.47
1:C:37:LEU:O	1:C:40:ASP:N	2.45	0.47
1:A:31:LEU:CD1	1:A:70:ARG:HD2	2.28	0.47
1:A:46:LEU:HD21	1:A:386:ALA:O	2.15	0.47
1:A:165:MET:HE1	1:A:201:PRO:HB3	1.97	0.47
2:D:67:ASP:O	2:D:68:THR:HG22	2.14	0.47
1:C:380:THR:OG1	1:C:381:PHE:N	2.46	0.47
1:A:189:ILE:HG22	1:A:189:ILE:O	2.15	0.47
1:C:189:ILE:HD13	1:C:217:PHE:HE1	1.79	0.47
2:D:102:PHE:HD1	2:D:132:LEU:HD21	1.80	0.47
1:A:207:ASP:C	1:A:209:SER:N	2.73	0.47
1:A:229:VAL:O	1:A:254:TYR:HA	2.15	0.47
1:A:258:GLU:HB3	1:A:323:ARG:HE	1.79	0.47
1:C:40:ASP:C	1:C:41:LEU:HG	2.40	0.47
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.80	0.46
1:A:249:GLN:NE2	2:B:67:ASP:OD1	2.49	0.46
1:A:363:ILE:O	1:A:363:ILE:HG13	2.14	0.46
1:C:34:LEU:O	1:C:35:ASP:C	2.58	0.46
1:A:21:PRO:C	1:A:23:SER:H	2.22	0.46
2:D:39:LEU:HD11	2:D:189:ILE:HD12	1.96	0.46
2:D:96:ASP:O	2:D:97:ALA:HB2	2.16	0.46
2:D:136:LYS:HG2	5:D:1201:GTP:C6	2.51	0.46
1:C:143:PHE:HA	1:C:398:THR:HG23	1.96	0.46
1:C:261:TRP:HA	1:C:261:TRP:CE3	2.50	0.46
1:A:70:ARG:O	1:A:72:LYS:N	2.49	0.46
2:D:36:LYS:HZ3	5:D:1201:GTP:PB	2.39	0.46
2:D:48:PHE:CD1	2:D:49:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:LYS:HG2	5:D:1201:GTP:C5	2.50	0.46
2:D:182:SER:O	2:D:185:SER:OG	2.31	0.46
1:A:41:LEU:HB3	1:A:52:ILE:HG23	1.98	0.46
1:C:363:ILE:HG13	1:C:363:ILE:O	2.15	0.46
2:B:67:ASP:O	2:B:68:THR:HG22	2.16	0.46
1:C:147:ARG:HH22	1:C:380:THR:CB	2.24	0.46
1:C:189:ILE:O	1:C:189:ILE:HG22	2.15	0.46
1:C:196:HIS:O	1:C:197:ARG:CB	2.63	0.46
1:C:331:GLU:HB3	1:C:334:ARG:NH2	2.31	0.46
1:A:109:LYS:HG2	1:A:394:PHE:CE2	2.50	0.46
1:A:146:ASP:OD1	1:A:147:ARG:HG3	2.16	0.46
2:B:92:TYR:O	2:B:93:PRO:C	2.59	0.46
1:C:31:LEU:O	1:C:32:ASP:C	2.58	0.46
2:B:155:THR:O	2:B:156:PRO:O	2.34	0.46
1:C:58:ARG:HH11	1:C:58:ARG:HG2	1.81	0.46
1:A:189:ILE:HD13	1:A:217:PHE:HE1	1.80	0.46
1:C:70:ARG:O	1:C:72:LYS:N	2.49	0.45
1:C:146:ASP:OD1	1:C:147:ARG:HG3	2.16	0.45
1:C:246:LEU:C	1:C:248:SER:H	2.24	0.45
1:A:120:PHE:C	1:A:120:PHE:CD1	2.94	0.45
2:B:48:PHE:CD1	2:B:49:PRO:HD2	2.52	0.45
1:C:40:ASP:HB3	1:C:387:PHE:CE2	2.51	0.45
1:C:159:GLY:HA2	1:C:368:PHE:CZ	2.51	0.45
1:C:392:LEU:O	1:C:395:VAL:HG23	2.16	0.45
2:D:177:CYS:O	2:D:177:CYS:SG	2.74	0.45
2:B:70:ARG:NH1	2:B:72:GLU:OE2	2.49	0.45
2:B:154:GLN:O	2:B:155:THR:CG2	2.62	0.45
1:C:172:GLU:O	1:C:173:LYS:C	2.59	0.45
1:C:335:HIS:CE1	1:C:336:LEU:HD12	2.50	0.45
2:B:136:LYS:HG2	5:B:1201:GTP:C5	2.51	0.45
1:C:10:ARG:O	1:C:11:PHE:C	2.60	0.45
1:C:109:LYS:CE	1:C:394:PHE:CD2	2.98	0.45
2:D:155:THR:O	2:D:156:PRO:O	2.34	0.45
1:A:354:PRO:HD2	1:A:355:VAL:H	1.81	0.45
1:C:207:ASP:C	1:C:209:SER:N	2.74	0.45
1:C:207:ASP:O	1:C:209:SER:N	2.50	0.45
2:B:136:LYS:HG2	5:B:1201:GTP:C6	2.52	0.45
1:C:233:THR:HG22	2:D:67:ASP:CB	2.45	0.45
2:D:27:VAL:HB	2:D:98:VAL:HG22	1.97	0.45
1:A:7:PHE:O	1:A:10:ARG:HB2	2.17	0.45
1:A:26:ASN:HD22	1:A:26:ASN:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:HA	2:B:113:VAL:CG1	2.41	0.45
2:D:33:GLN:HE21	2:D:33:GLN:HB2	1.62	0.45
2:D:112:SER:C	2:D:114:LEU:N	2.74	0.45
1:C:194:PHE:HB3	1:C:195:ILE:H	1.59	0.45
2:D:158:SER:O	2:D:159:TYR:C	2.58	0.45
2:D:178:SER:C	2:D:180:LEU:H	2.25	0.45
2:B:66:ILE:HG23	2:B:71:ILE:CD1	2.47	0.45
1:C:49:ASN:HD21	1:C:51:ASN:HB2	1.82	0.45
1:C:320:ARG:HB3	1:C:323:ARG:NH2	2.31	0.45
2:B:158:SER:O	2:B:159:TYR:C	2.60	0.45
1:C:117:ASP:HB3	1:C:120:PHE:HD2	1.81	0.45
1:C:123:GLU:HG3	1:C:220:CYS:HB2	1.99	0.45
1:C:137:VAL:O	1:C:137:VAL:HG12	2.17	0.45
1:C:180:ALA:HB2	1:C:338:PHE:CE2	2.52	0.45
1:C:258:GLU:HB3	1:C:323:ARG:HE	1.81	0.45
1:A:44:PRO:CD	1:A:45:ALA:H	2.29	0.44
1:A:180:ALA:HA	1:A:183:VAL:HG23	1.99	0.44
1:A:328:GLY:C	1:A:330:GLU:H	2.25	0.44
1:C:189:ILE:CD1	1:C:217:PHE:CE1	2.94	0.44
1:A:219:THR:HG22	1:A:235:VAL:CG1	2.47	0.44
2:B:129:LYS:HD3	2:B:196:ALA:HB1	1.99	0.44
2:B:198:VAL:O	2:B:199:ASN:C	2.59	0.44
1:C:120:PHE:CD1	1:C:120:PHE:C	2.95	0.44
1:C:249:GLN:HG3	2:D:67:ASP:OD1	2.17	0.44
1:C:388:VAL:HG23	1:C:389:GLY:N	2.32	0.44
1:A:133:SER:HA	1:A:134:PRO:HD3	1.76	0.44
1:A:300:PRO:C	1:A:302:ASP:H	2.26	0.44
2:B:102:PHE:HD1	2:B:132:LEU:HD21	1.82	0.44
1:C:165:MET:HE1	1:C:201:PRO:HB3	1.99	0.44
2:B:123:GLU:O	2:B:123:GLU:HG2	2.17	0.44
1:C:102:TYR:CB	1:C:152:VAL:HG12	2.45	0.44
1:C:149:LEU:HA	1:C:149:LEU:HD23	1.64	0.44
2:D:124:PHE:N	2:D:124:PHE:CD2	2.86	0.44
1:A:133:SER:HB3	1:A:136:VAL:HG23	1.99	0.44
2:B:178:SER:C	2:B:180:LEU:N	2.76	0.44
1:C:229:VAL:O	1:C:254:TYR:HA	2.18	0.44
1:C:261:TRP:HA	1:C:261:TRP:HE3	1.82	0.44
1:C:316:PHE:O	1:C:323:ARG:HD3	2.17	0.44
1:A:31:LEU:O	1:A:32:ASP:C	2.60	0.44
1:A:117:ASP:HB3	1:A:120:PHE:HD2	1.82	0.44
2:B:66:ILE:HD13	2:B:66:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:TRP:CH2	1:C:349:ARG:HB2	2.53	0.44
1:C:354:PRO:HD2	1:C:355:VAL:H	1.82	0.44
1:A:37:LEU:O	1:A:40:ASP:N	2.48	0.44
2:B:57:PHE:CZ	2:B:91:SER:HB3	2.53	0.44
1:A:312:LEU:C	1:A:312:LEU:CD2	2.91	0.44
2:B:51:ASN:ND2	2:B:51:ASN:N	2.66	0.44
2:B:112:SER:C	2:B:114:LEU:N	2.76	0.44
2:D:56:VAL:HB	2:D:57:PHE:H	1.61	0.44
2:B:27:VAL:HB	2:B:98:VAL:HG22	1.99	0.43
1:C:186:LEU:C	1:C:188:ALA:N	2.76	0.43
2:D:95:SER:HB2	2:D:125:CYS:SG	2.58	0.43
2:D:104:ILE:O	2:D:104:ILE:HG22	2.17	0.43
2:D:186:VAL:O	2:D:189:ILE:HB	2.17	0.43
1:A:383:ILE:HD12	1:A:383:ILE:H	1.82	0.43
1:C:284:VAL:CG2	2:D:192:VAL:HG13	2.44	0.43
1:C:324:LEU:HD12	1:C:325:GLY:N	2.34	0.43
1:C:328:GLY:C	1:C:330:GLU:H	2.26	0.43
1:A:302:ASP:HB3	1:A:304:ASP:OD1	2.17	0.43
1:C:38:VAL:HG22	1:C:56:LEU:HD23	2.00	0.43
1:C:248:SER:O	1:C:249:GLN:C	2.61	0.43
1:C:297:LEU:O	1:C:298:THR:HG23	2.18	0.43
1:C:392:LEU:C	1:C:394:PHE:N	2.71	0.43
2:D:162:GLY:O	2:D:165:MET:HB3	2.18	0.43
1:A:84:ARG:HD3	1:A:89:GLU:HB3	2.01	0.43
1:A:215:ALA:HA	1:A:217:PHE:HE2	1.83	0.43
1:C:175:ALA:HB2	1:C:272:LEU:HD21	2.01	0.43
1:C:237:THR:HA	1:C:238:PRO:HD3	1.81	0.43
1:C:308:GLU:HA	1:C:311:ASN:HB3	1.99	0.43
2:D:66:ILE:HG23	2:D:71:ILE:HD11	1.99	0.43
1:A:216:ASP:HB2	3:A:1480:ANP:O1A	2.18	0.43
2:B:123:GLU:C	2:B:124:PHE:CD2	2.97	0.43
1:C:47:ARG:C	1:C:49:ASN:N	2.71	0.43
1:C:128:MET:HB3	1:C:139:LEU:HB2	2.01	0.43
2:D:37:THR:HG21	2:D:55:THR:HG21	2.00	0.43
1:A:123:GLU:HG3	1:A:220:CYS:HB2	2.00	0.43
1:C:26:ASN:HD22	1:C:26:ASN:H	1.66	0.43
2:D:195:LEU:O	2:D:199:ASN:HB2	2.19	0.43
1:A:63:ILE:HA	1:A:63:ILE:HD12	1.70	0.43
1:A:189:ILE:O	1:A:189:ILE:CG2	2.66	0.43
1:A:201:PRO:HA	1:A:204:MET:HG3	2.00	0.43
1:C:348:LEU:HD12	1:C:348:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:C	1:A:12:GLU:H	2.27	0.43
1:A:25:VAL:O	1:A:26:ASN:C	2.60	0.43
1:A:35:ASP:OD2	1:A:67:ARG:NE	2.51	0.43
1:A:243:PRO:HD2	1:A:244:GLU:OE2	2.19	0.43
1:C:390:ASN:C	1:C:392:LEU:N	2.76	0.43
1:A:159:GLY:HA2	1:A:368:PHE:CZ	2.54	0.43
1:C:31:LEU:O	1:C:33:GLY:N	2.52	0.43
1:A:66:ILE:HG23	1:A:67:ARG:N	2.33	0.42
1:C:288:SER:CB	2:D:175:ILE:HG22	2.49	0.42
2:D:59:ASN:ND2	2:D:76:TRP:CE2	2.87	0.42
2:D:123:GLU:O	2:D:123:GLU:HG2	2.19	0.42
1:A:131:ALA:O	1:A:132:ASN:C	2.61	0.42
1:A:237:THR:HA	1:A:238:PRO:HD3	1.82	0.42
2:B:36:LYS:HZ3	5:B:1201:GTP:PB	2.42	0.42
1:C:46:LEU:HD21	1:C:386:ALA:C	2.44	0.42
1:C:183:VAL:HG11	1:C:332:ILE:CG2	2.49	0.42
1:C:287:TYR:O	1:C:291:MET:HG2	2.19	0.42
2:D:24:CYS:HB2	2:D:197:CYS:SG	2.59	0.42
2:B:71:ILE:HD12	2:B:71:ILE:H	1.81	0.42
2:B:59:ASN:ND2	2:B:76:TRP:CE2	2.87	0.42
1:C:110:PHE:CD1	1:C:110:PHE:C	2.98	0.42
1:C:133:SER:HA	1:C:134:PRO:HD3	1.77	0.42
1:A:84:ARG:NH2	1:A:371:LEU:HB3	2.34	0.42
1:A:172:GLU:O	1:A:173:LYS:C	2.63	0.42
1:A:246:LEU:C	1:A:248:SER:N	2.77	0.42
1:A:248:SER:O	1:A:249:GLN:C	2.62	0.42
2:D:180:LEU:O	2:D:180:LEU:HD12	2.19	0.42
1:A:26:ASN:O	1:A:27:SER:C	2.63	0.42
1:A:47:ARG:C	1:A:49:ASN:N	2.75	0.42
1:A:186:LEU:C	1:A:188:ALA:N	2.76	0.42
1:C:244:GLU:OE2	1:C:323:ARG:NH2	2.53	0.42
1:A:165:MET:HE1	1:A:201:PRO:CB	2.50	0.42
1:A:183:VAL:HG11	1:A:332:ILE:HG21	2.00	0.42
1:A:261:TRP:HA	1:A:261:TRP:CE3	2.53	0.42
1:C:324:LEU:CD1	1:C:331:GLU:HG3	2.49	0.42
1:C:383:ILE:HD12	1:C:383:ILE:H	1.85	0.42
2:B:57:PHE:HE2	2:B:88:ARG:HA	1.84	0.42
1:A:110:PHE:CD1	1:A:110:PHE:C	2.98	0.42
1:C:213:LYS:HE2	1:C:349:ARG:NH2	2.35	0.42
1:C:323:ARG:O	1:C:326:ARG:HB3	2.20	0.42
1:A:66:ILE:HD13	1:A:66:ILE:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:HD23	2:B:145:THR:HG21	2.01	0.41
1:C:35:ASP:OD2	1:C:67:ARG:NE	2.53	0.41
2:D:114:LEU:HD13	2:D:169:ILE:HG22	2.02	0.41
1:A:323:ARG:O	1:A:326:ARG:HB3	2.20	0.41
2:B:104:ILE:O	2:B:104:ILE:CG2	2.68	0.41
1:C:84:ARG:HD3	1:C:89:GLU:HB3	2.02	0.41
2:D:51:ASN:ND2	2:D:51:ASN:N	2.68	0.41
1:A:31:LEU:O	1:A:33:GLY:N	2.54	0.41
1:A:34:LEU:O	1:A:35:ASP:C	2.63	0.41
1:A:95:HIS:CG	1:A:98:THR:HG23	2.56	0.41
1:A:175:ALA:HB2	1:A:272:LEU:HD21	2.02	0.41
1:A:181:GLU:HG3	1:A:348:LEU:CD2	2.49	0.41
1:C:189:ILE:O	1:C:189:ILE:CG2	2.67	0.41
1:A:198:ASP:HB2	1:A:219:THR:HG21	2.02	0.41
1:A:336:LEU:H	1:A:336:LEU:HG	1.68	0.41
1:A:137:VAL:O	1:A:137:VAL:HG12	2.21	0.41
1:A:196:HIS:O	1:A:197:ARG:CB	2.69	0.41
1:A:244:GLU:OE1	1:A:323:ARG:NH2	2.54	0.41
1:A:316:PHE:O	1:A:323:ARG:HD3	2.20	0.41
1:C:47:ARG:CD	1:C:53:ASP:OD1	2.62	0.41
1:C:145:ASP:OD1	1:C:145:ASP:C	2.64	0.41
1:C:180:ALA:HB1	1:C:345:TRP:CZ3	2.55	0.41
1:C:210:GLY:HA2	1:C:357:PRO:HD3	2.02	0.41
1:A:388:VAL:HG23	1:A:389:GLY:N	2.35	0.41
2:B:180:LEU:HD12	2:B:180:LEU:O	2.21	0.41
2:B:191:HIS:CD2	2:B:191:HIS:C	2.99	0.41
2:D:66:ILE:O	2:D:67:ASP:C	2.62	0.41
1:A:381:PHE:HA	1:A:382:PRO:HD3	1.76	0.41
1:C:66:ILE:HG23	1:C:67:ARG:N	2.35	0.41
1:A:266:VAL:HG22	1:A:317:LEU:HD11	2.01	0.41
1:A:301:ASP:O	1:A:301:ASP:CG	2.64	0.41
1:A:383:ILE:HD12	1:A:383:ILE:N	2.36	0.41
1:C:131:ALA:O	1:C:132:ASN:C	2.61	0.41
1:C:177:PHE:CG	1:C:354:PRO:HG3	2.56	0.41
1:C:181:GLU:HG3	1:C:348:LEU:CD2	2.50	0.41
1:C:286:THR:O	1:C:286:THR:CG2	2.69	0.41
2:D:70:ARG:NH1	2:D:72:GLU:OE2	2.53	0.41
1:A:40:ASP:HB3	1:A:387:PHE:CE2	2.56	0.41
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.36	0.41
1:A:64:ASN:C	1:A:66:ILE:H	2.29	0.41
1:A:114:LYS:C	1:A:116:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HH22	1:A:380:THR:CB	2.28	0.41
1:A:266:VAL:O	1:A:266:VAL:HG12	2.19	0.41
1:C:197:ARG:HB2	1:C:219:THR:HB	2.03	0.41
1:C:198:ASP:HB2	1:C:219:THR:HG21	2.03	0.41
1:C:301:ASP:C	1:C:303:ASN:H	2.29	0.41
2:D:102:PHE:CD1	2:D:132:LEU:HD21	2.56	0.41
1:A:199:VAL:HB	1:A:263:SER:HB3	2.02	0.41
2:B:186:VAL:O	2:B:189:ILE:HB	2.21	0.41
1:C:318:THR:O	1:C:319:ASP:C	2.64	0.41
1:A:309:ALA:C	1:A:311:ASN:N	2.77	0.40
1:A:312:LEU:HA	1:A:335:HIS:HE2	1.85	0.40
2:B:84:TYR:HD1	2:B:87:VAL:HG11	1.85	0.40
1:C:383:ILE:HD12	1:C:383:ILE:N	2.36	0.40
1:A:26:ASN:ND2	1:A:29:CYS:SG	2.94	0.40
1:A:318:THR:O	1:A:319:ASP:C	2.64	0.40
2:B:182:SER:O	2:B:185:SER:OG	2.32	0.40
1:C:66:ILE:HD13	1:C:66:ILE:C	2.47	0.40
1:C:147:ARG:NH2	1:C:379:GLU:O	2.54	0.40
1:C:286:THR:O	1:C:286:THR:HG22	2.22	0.40
1:C:356:VAL:HA	1:C:357:PRO:HD3	1.88	0.40
1:C:381:PHE:HA	1:C:382:PRO:HD3	1.77	0.40
1:A:31:LEU:C	1:A:33:GLY:N	2.78	0.40
1:A:155:TYR:OH	1:A:365:THR:HG22	2.21	0.40
2:B:95:SER:HB2	2:B:125:CYS:SG	2.61	0.40
1:C:109:LYS:HG2	1:C:394:PHE:CE2	2.55	0.40
1:A:39:TYR:CE1	1:A:146:ASP:HB3	2.56	0.40
2:B:24:CYS:HB2	2:B:197:CYS:SG	2.61	0.40
2:B:56:VAL:HB	2:B:57:PHE:H	1.58	0.40
1:C:8:GLU:C	1:C:10:ARG:H	2.29	0.40
1:C:33:GLY:O	1:C:34:LEU:C	2.64	0.40
1:C:58:ARG:HG2	1:C:58:ARG:NH1	2.36	0.40
1:C:85:GLY:O	1:C:86:ALA:C	2.65	0.40
1:C:99:ARG:HA	1:C:99:ARG:HD2	1.84	0.40
1:A:392:LEU:O	1:A:395:VAL:HG23	2.21	0.40
2:B:36:LYS:HZ1	5:B:1201:GTP:PG	2.44	0.40
2:B:110:LEU:HD21	2:B:165:MET:HG2	2.03	0.40
1:C:31:LEU:CD1	1:C:70:ARG:HD2	2.23	0.40
1:C:164:LEU:C	1:C:164:LEU:HD23	2.47	0.40
1:C:199:VAL:HB	1:C:263:SER:HB3	2.03	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	389/406 (96%)	291 (75%)	74 (19%)	24 (6%)	1	14
1	C	392/406 (97%)	295 (75%)	74 (19%)	23 (6%)	1	15
2	B	179/200 (90%)	147 (82%)	26 (14%)	6 (3%)	3	25
2	D	180/200 (90%)	147 (82%)	27 (15%)	6 (3%)	3	25
All	All	1140/1212 (94%)	880 (77%)	201 (18%)	59 (5%)	1	17

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	MET
1	A	86	ALA
1	A	402	ASN
2	B	156	PRO
1	C	71	MET
1	C	86	ALA
1	C	303	ASN
1	C	402	ASN
2	D	156	PRO
1	A	13	LYS
1	A	249	GLN
1	A	252	ASP
1	A	391	GLN
1	C	13	LYS
1	C	249	GLN
1	C	252	ASP
1	C	351	THR
1	C	362	ASP
1	C	391	GLN
1	A	33	GLY
1	A	197	ARG
1	A	208	LYS

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Mol	Chain	Res	Type
1	A	216	ASP
1	A	351	THR
2	B	97	ALA
1	C	22	LYS
1	C	33	GLY
1	C	197	ARG
1	C	208	LYS
1	C	216	ASP
1	C	224	ASN
2	D	21	ASN
2	D	97	ALA
1	A	31	LEU
1	A	32	ASP
1	A	301	ASP
1	A	385	LYS
1	A	392	LEU
2	B	67	ASP
1	C	31	LEU
1	C	32	ASP
1	C	392	LEU
2	D	67	ASP
1	A	224	ASN
1	A	319	ASP
1	A	362	ASP
1	A	386	ALA
1	C	247	LYS
1	C	319	ASP
2	D	31	ASP
2	B	31	ASP
2	B	93	PRO
1	A	354	PRO
2	D	93	PRO
1	A	305	ILE
1	A	353	ALA
1	C	354	PRO
1	C	300	PRO
2	B	89	PRO

5.3.2 Protein sidechains [i](#)

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	334/361 (92%)	270 (81%)	64 (19%)	1	9
1	C	334/361 (92%)	267 (80%)	67 (20%)	1	8
2	B	155/181 (86%)	131 (84%)	24 (16%)	2	15
2	D	154/181 (85%)	131 (85%)	23 (15%)	3	16
All	All	977/1084 (90%)	799 (82%)	178 (18%)	2	11

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	14	MET
1	A	25	VAL
1	A	26	ASN
1	A	30	LEU
1	A	34	LEU
1	A	37	LEU
1	A	40	ASP
1	A	58	ARG
1	A	60	LYS
1	A	63	ILE
1	A	66	ILE
1	A	78	VAL
1	A	91	GLN
1	A	98	THR
1	A	101	VAL
1	A	113	ILE
1	A	132	ASN
1	A	137	VAL
1	A	138	GLN
1	A	139	LEU
1	A	152	VAL
1	A	156	MET
1	A	160	ASP
1	A	161	LEU
1	A	179	THR
1	A	182	VAL
1	A	192	MET

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Mol	Chain	Res	Type
1	A	199	VAL
1	A	204	MET
1	A	208	LYS
1	A	212	LEU
1	A	219	THR
1	A	232	ASP
1	A	233	THR
1	A	235	VAL
1	A	239	ASP
1	A	242	SER
1	A	257	ARG
1	A	262	TRP
1	A	268	LEU
1	A	273	VAL
1	A	281	ASP
1	A	290	ILE
1	A	291	MET
1	A	297	LEU
1	A	298	THR
1	A	308	GLU
1	A	312	LEU
1	A	313	ILE
1	A	317	LEU
1	A	321	GLU
1	A	329	VAL
1	A	332	ILE
1	A	336	LEU
1	A	340	ASN
1	A	341	ASP
1	A	342	GLN
1	A	346	GLU
1	A	351	THR
1	A	371	LEU
1	A	392	LEU
1	A	398	THR
1	A	403	ARG
2	B	22	VAL
2	B	33	GLN
2	B	42	VAL
2	B	50	GLU
2	B	51	ASN
2	B	56	VAL

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Mol	Chain	Res	Type
2	B	66	ILE
2	B	68	THR
2	B	69	GLN
2	B	73	LEU
2	B	113	VAL
2	B	122	GLN
2	B	124	PHE
2	B	125	CYS
2	B	132	LEU
2	B	146	LEU
2	B	147	VAL
2	B	148	GLU
2	B	175	ILE
2	B	184	ASN
2	B	186	VAL
2	B	189	ILE
2	B	195	LEU
2	B	198	VAL
1	C	9	THR
1	C	14	MET
1	C	25	VAL
1	C	26	ASN
1	C	30	LEU
1	C	34	LEU
1	C	37	LEU
1	C	40	ASP
1	C	47	ARG
1	C	58	ARG
1	C	60	LYS
1	C	63	ILE
1	C	66	ILE
1	C	72	LYS
1	C	78	VAL
1	C	91	GLN
1	C	98	THR
1	C	101	VAL
1	C	113	ILE
1	C	132	ASN
1	C	138	GLN
1	C	139	LEU
1	C	152	VAL
1	C	156	MET

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Mol	Chain	Res	Type
1	C	160	ASP
1	C	161	LEU
1	C	179	THR
1	C	182	VAL
1	C	192	MET
1	C	199	VAL
1	C	204	MET
1	C	208	LYS
1	C	212	LEU
1	C	214	LEU
1	C	219	THR
1	C	232	ASP
1	C	233	THR
1	C	235	VAL
1	C	239	ASP
1	C	242	SER
1	C	257	ARG
1	C	262	TRP
1	C	264	VAL
1	C	268	LEU
1	C	273	VAL
1	C	281	ASP
1	C	284	VAL
1	C	290	ILE
1	C	291	MET
1	C	297	LEU
1	C	298	THR
1	C	308	GLU
1	C	312	LEU
1	C	313	ILE
1	C	317	LEU
1	C	321	GLU
1	C	329	VAL
1	C	332	ILE
1	C	336	LEU
1	C	340	ASN
1	C	341	ASP
1	C	342	GLN
1	C	346	GLU
1	C	351	THR
1	C	371	LEU
1	C	392	LEU

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Mol	Chain	Res	Type
1	C	398	THR
2	D	33	GLN
2	D	42	VAL
2	D	50	GLU
2	D	51	ASN
2	D	56	VAL
2	D	66	ILE
2	D	68	THR
2	D	69	GLN
2	D	73	LEU
2	D	113	VAL
2	D	122	GLN
2	D	124	PHE
2	D	125	CYS
2	D	132	LEU
2	D	146	LEU
2	D	147	VAL
2	D	148	GLU
2	D	175	ILE
2	D	184	ASN
2	D	186	VAL
2	D	189	ILE
2	D	195	LEU
2	D	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	91	GLN
1	A	132	ASN
1	A	144	GLN
1	A	167	ASN
1	A	211	HIS
1	A	293	HIS
1	A	327	ASN
1	A	340	ASN
1	A	342	GLN
2	B	33	GLN
2	B	51	ASN
2	B	59	ASN
2	B	69	GLN

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Mol	Chain	Res	Type
2	B	122	GLN
2	B	168	GLN
2	B	191	HIS
1	C	26	ASN
1	C	91	GLN
1	C	132	ASN
1	C	144	GLN
1	C	167	ASN
1	C	292	ASN
1	C	311	ASN
1	C	327	ASN
1	C	340	ASN
1	C	342	GLN
2	D	33	GLN
2	D	51	ASN
2	D	59	ASN
2	D	69	GLN
2	D	122	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
6	SO4	D	1203	-	4,4,4	0.25	0	6,6,6	0.09	0
5	GTP	D	1201	4	33,34,34	1.11	2 (6%)	50,54,54	1.73	11 (22%)
5	GTP	B	1201	4	33,34,34	0.96	1 (3%)	50,54,54	1.75	12 (24%)
3	ANP	A	1480	-	33,33,33	4.90	21 (63%)	45,52,52	1.81	9 (20%)
3	ANP	C	1480	-	33,33,33	4.84	21 (63%)	45,52,52	1.84	10 (22%)

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
5	GTP	D	1201	4	-	12/22/38/38	0/3/3/3
5	GTP	B	1201	4	-	12/22/38/38	0/3/3/3
3	ANP	A	1480	-	-	8/18/38/38	0/3/3/3
3	ANP	C	1480	-	-	8/18/38/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1480	ANP	PB-O1B	12.79	1.65	1.46
3	C	1480	ANP	PB-O1B	12.75	1.65	1.46
3	A	1480	ANP	C2-N1	9.75	1.51	1.33
3	C	1480	ANP	C2-N1	9.64	1.51	1.33
3	A	1480	ANP	C2-N3	8.72	1.49	1.33
3	C	1480	ANP	C2-N3	8.62	1.49	1.33
3	C	1480	ANP	C8-N7	7.97	1.47	1.31
3	A	1480	ANP	C8-N7	7.94	1.46	1.31
3	A	1480	ANP	C8-N9	7.68	1.50	1.37
3	A	1480	ANP	C4-N3	7.65	1.48	1.34
3	C	1480	ANP	C8-N9	7.57	1.50	1.37
3	C	1480	ANP	C4-N3	7.45	1.48	1.34
3	A	1480	ANP	C5-C4	6.00	1.49	1.39
3	A	1480	ANP	PA-O3A	5.98	1.66	1.59
3	C	1480	ANP	PA-O3A	5.84	1.65	1.59
3	C	1480	ANP	C5-C4	5.82	1.49	1.39
3	A	1480	ANP	PB-O3A	5.54	1.66	1.59
3	C	1480	ANP	PB-O3A	5.31	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1480	ANP	C4-N9	4.98	1.48	1.37
3	A	1480	ANP	C5-N7	4.88	1.48	1.39
3	C	1480	ANP	C4-N9	4.82	1.47	1.37
3	C	1480	ANP	C5-N7	4.72	1.47	1.39
3	C	1480	ANP	C6-N6	4.68	1.46	1.34
3	A	1480	ANP	C6-N6	4.61	1.46	1.34
3	A	1480	ANP	PB-O2B	-3.88	1.46	1.56
3	C	1480	ANP	PB-O2B	-3.86	1.46	1.56
3	A	1480	ANP	C5-C6	3.84	1.51	1.41
3	C	1480	ANP	C5-C6	3.81	1.51	1.41
3	A	1480	ANP	C6-N1	3.54	1.45	1.35
3	C	1480	ANP	C6-N1	3.51	1.45	1.35
3	C	1480	ANP	PG-O3G	3.47	1.66	1.56
3	A	1480	ANP	PG-O3G	3.41	1.65	1.56
3	A	1480	ANP	PB-N3B	3.41	1.72	1.63
5	D	1201	GTP	PB-O3A	3.38	1.63	1.59
3	A	1480	ANP	PG-N3B	3.35	1.72	1.63
3	C	1480	ANP	PG-N3B	3.26	1.71	1.63
3	C	1480	ANP	PG-O2G	3.22	1.65	1.56
3	A	1480	ANP	PG-O2G	3.21	1.65	1.56
3	C	1480	ANP	PB-N3B	3.11	1.71	1.63
5	D	1201	GTP	PA-O3A	2.46	1.62	1.59
3	C	1480	ANP	O4'-C1'	2.26	1.47	1.42
3	C	1480	ANP	PA-O2A	2.25	1.65	1.55
3	A	1480	ANP	PA-O2A	2.21	1.65	1.55
5	B	1201	GTP	PB-O3A	2.19	1.61	1.59
3	A	1480	ANP	O4'-C1'	2.03	1.46	1.42

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1480	ANP	C5-C4-N3	-5.68	118.90	126.72
3	A	1480	ANP	C5-C4-N3	-5.58	119.04	126.72
3	C	1480	ANP	N3-C2-N1	-5.52	120.22	128.58
5	B	1201	GTP	C5-C4-N3	-5.40	119.79	128.39
5	D	1201	GTP	C5-C4-N3	-5.37	119.84	128.39
3	A	1480	ANP	N3-C2-N1	-5.29	120.58	128.58
5	B	1201	GTP	C2-N3-C4	5.03	120.96	112.30
5	D	1201	GTP	C2-N3-C4	4.70	120.39	112.30
5	D	1201	GTP	N9-C4-N3	3.64	133.22	125.95
5	B	1201	GTP	N9-C4-N3	3.60	133.15	125.95
3	C	1480	ANP	C2-N3-C4	3.57	120.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	ANP	N9-C8-N7	-3.46	109.03	113.94
3	A	1480	ANP	C2-N3-C4	3.40	120.14	111.83
3	C	1480	ANP	N9-C8-N7	-3.40	109.11	113.94
3	C	1480	ANP	N3-C4-N9	3.26	132.71	127.17
5	D	1201	GTP	C2-N1-C6	-3.22	119.27	125.11
5	D	1201	GTP	O2B-PB-O3A	3.16	115.81	107.27
3	A	1480	ANP	N3-C4-N9	3.14	132.51	127.17
5	B	1201	GTP	C2-N1-C6	-2.98	119.71	125.11
3	A	1480	ANP	C5-N7-C8	2.86	107.94	103.45
5	B	1201	GTP	O6-C6-C5	-2.76	119.25	126.53
3	C	1480	ANP	C5-N7-C8	2.67	107.64	103.45
5	D	1201	GTP	O6-C6-C5	-2.65	119.54	126.53
5	B	1201	GTP	O2B-PB-O3A	2.60	114.30	107.27
5	B	1201	GTP	C5-C6-N1	2.55	119.74	113.25
5	B	1201	GTP	N9-C8-N7	-2.54	108.69	113.40
5	D	1201	GTP	C5-C6-N1	2.48	119.56	113.25
3	A	1480	ANP	C6-C5-C4	2.46	120.54	117.18
3	C	1480	ANP	C6-C5-C4	2.44	120.51	117.18
5	D	1201	GTP	N9-C8-N7	-2.44	108.88	113.40
3	A	1480	ANP	C5-C4-N9	2.42	108.44	105.81
5	B	1201	GTP	C8-N7-C5	2.37	108.48	104.26
3	C	1480	ANP	C5-C4-N9	2.37	108.39	105.81
5	D	1201	GTP	O3'-C3'-C2'	-2.31	104.41	111.82
3	A	1480	ANP	C4-C5-N7	-2.29	107.97	110.58
5	D	1201	GTP	C3'-C2'-C1'	2.24	105.70	101.46
5	B	1201	GTP	C3'-C2'-C1'	2.21	105.64	101.46
5	B	1201	GTP	O3'-C3'-C2'	-2.20	104.77	111.82
5	D	1201	GTP	C8-N7-C5	2.19	108.17	104.26
3	C	1480	ANP	C4-C5-N7	-2.05	108.24	110.58
3	C	1480	ANP	O4'-C1'-N9	2.03	111.99	108.09
5	B	1201	GTP	O2G-PG-O3B	2.01	111.37	104.64

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1480	ANP	PB-N3B-PG-O1G
3	A	1480	ANP	PG-N3B-PB-O1B
3	A	1480	ANP	PA-O3A-PB-O2B
3	C	1480	ANP	PB-N3B-PG-O1G
3	C	1480	ANP	PG-N3B-PB-O1B
3	C	1480	ANP	PA-O3A-PB-O2B

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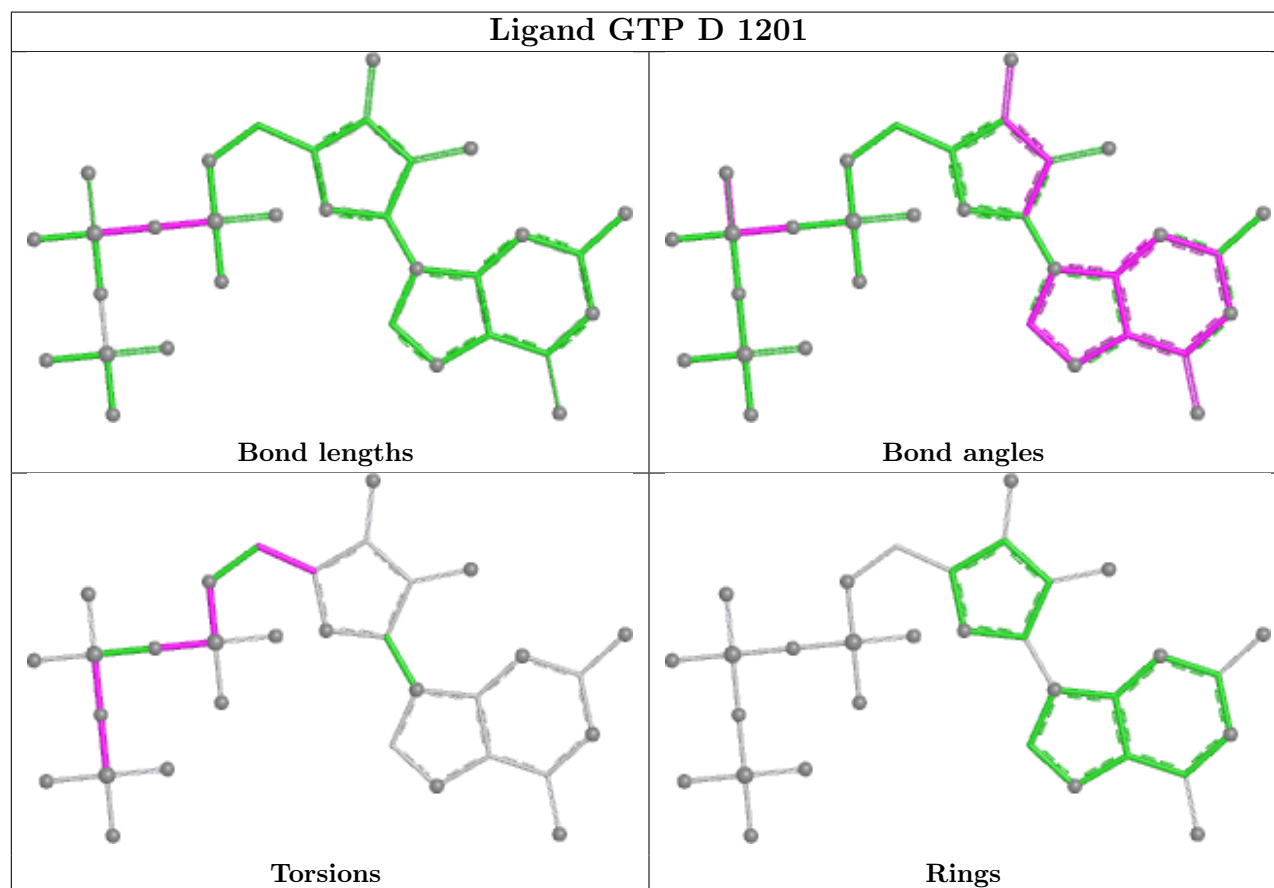
Mol	Chain	Res	Type	Atoms
5	B	1201	GTP	PB-O3B-PG-O2G
5	B	1201	GTP	C5'-O5'-PA-O1A
5	B	1201	GTP	C5'-O5'-PA-O2A
5	D	1201	GTP	PB-O3B-PG-O2G
5	D	1201	GTP	C5'-O5'-PA-O1A
5	D	1201	GTP	C5'-O5'-PA-O2A
3	A	1480	ANP	O4'-C4'-C5'-O5'
3	C	1480	ANP	O4'-C4'-C5'-O5'
3	A	1480	ANP	C3'-C4'-C5'-O5'
3	C	1480	ANP	C3'-C4'-C5'-O5'
5	B	1201	GTP	O4'-C4'-C5'-O5'
5	D	1201	GTP	O4'-C4'-C5'-O5'
5	B	1201	GTP	C3'-C4'-C5'-O5'
5	D	1201	GTP	C3'-C4'-C5'-O5'
3	A	1480	ANP	C5'-O5'-PA-O1A
3	A	1480	ANP	C5'-O5'-PA-O2A
3	A	1480	ANP	C5'-O5'-PA-O3A
3	C	1480	ANP	C5'-O5'-PA-O1A
3	C	1480	ANP	C5'-O5'-PA-O2A
3	C	1480	ANP	C5'-O5'-PA-O3A
5	B	1201	GTP	C5'-O5'-PA-O3A
5	D	1201	GTP	C5'-O5'-PA-O3A
5	B	1201	GTP	PG-O3B-PB-O2B
5	D	1201	GTP	PG-O3B-PB-O2B
5	B	1201	GTP	PB-O3A-PA-O2A
5	B	1201	GTP	PB-O3B-PG-O1G
5	D	1201	GTP	PB-O3B-PG-O1G
5	B	1201	GTP	PB-O3B-PG-O3G
5	D	1201	GTP	PB-O3B-PG-O3G
5	B	1201	GTP	PG-O3B-PB-O1B
5	B	1201	GTP	PB-O3A-PA-O1A
5	D	1201	GTP	PG-O3B-PB-O1B
5	D	1201	GTP	PB-O3A-PA-O1A
5	D	1201	GTP	PB-O3A-PA-O2A

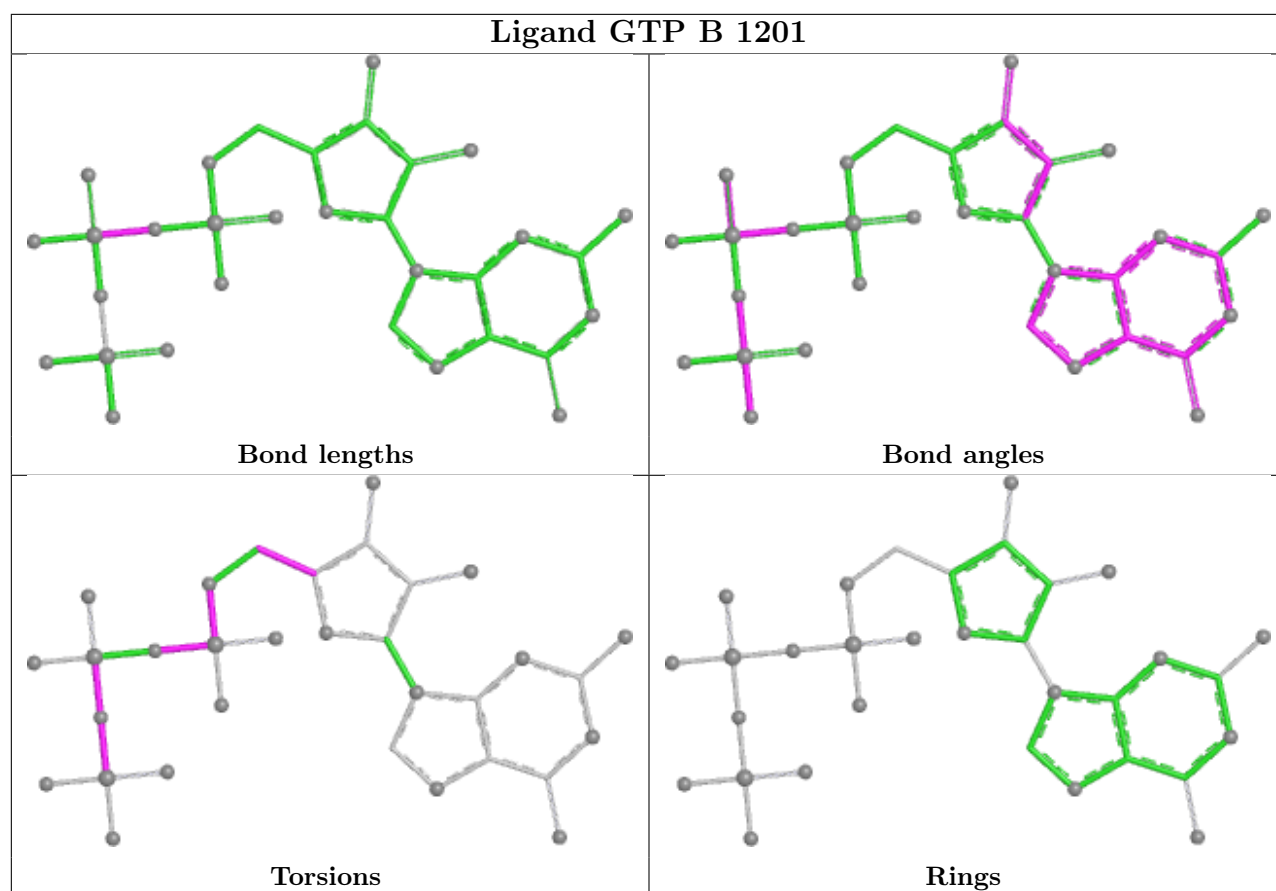
There are no ring outliers.

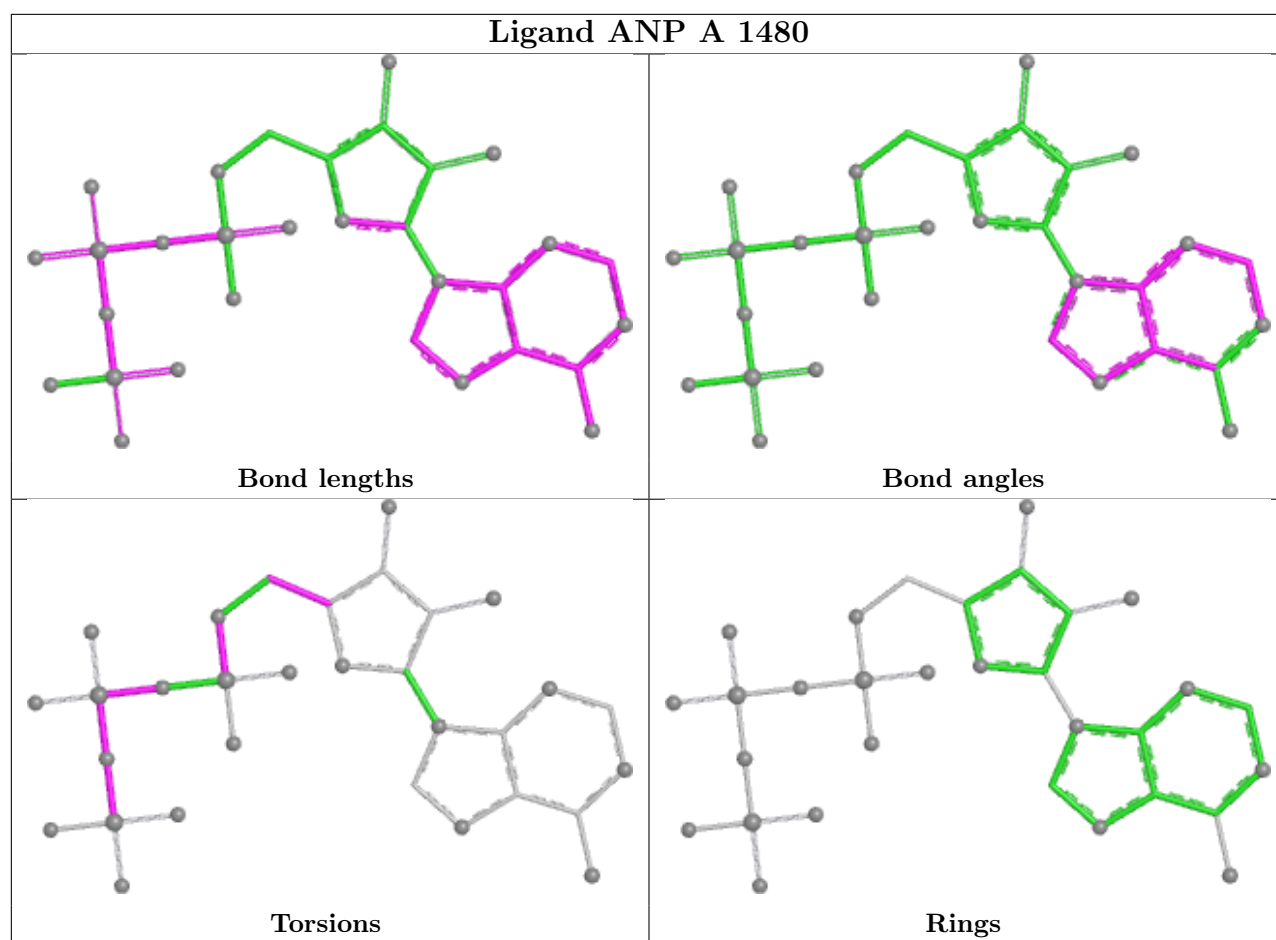
3 monomers are involved in 14 short contacts:

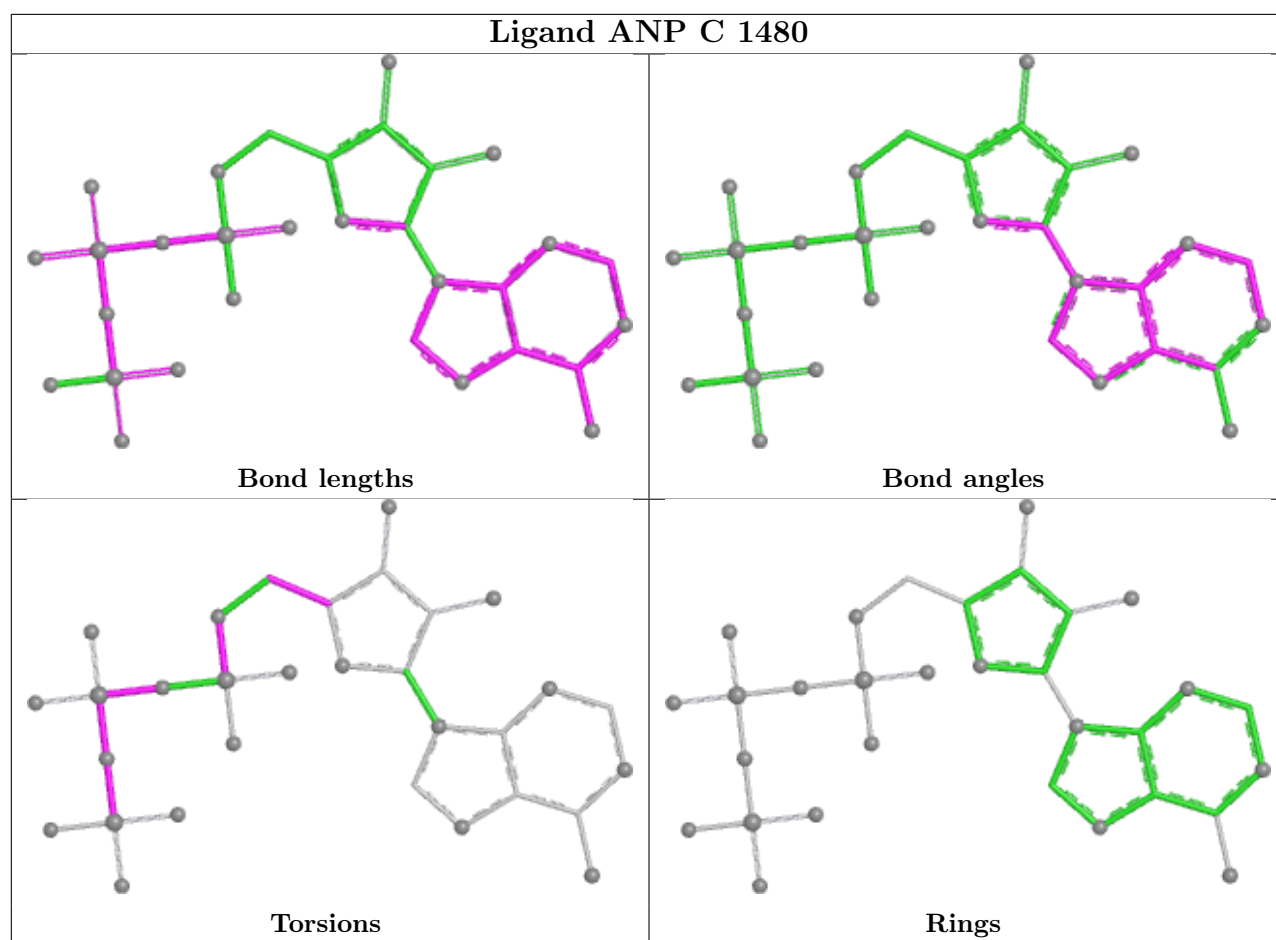
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1201	GTP	6	0
5	B	1201	GTP	7	0
3	A	1480	ANP	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	393/406 (96%)	-0.19	0 100 100	49, 80, 116, 149	1 (0%)
1	C	396/406 (97%)	-0.22	2 (0%) 87 69	49, 80, 116, 150	4 (1%)
2	B	181/200 (90%)	-0.26	0 100 100	52, 75, 110, 144	1 (0%)
2	D	182/200 (91%)	-0.34	0 100 100	51, 72, 106, 143	1 (0%)
All	All	1152/1212 (95%)	-0.24	2 (0%) 91 80	49, 78, 113, 150	7 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	LYS	3.3
1	C	294	LYS	2.8

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](#)

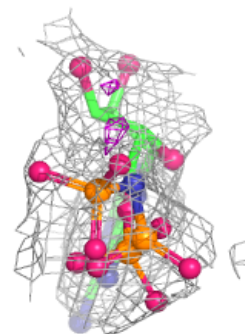
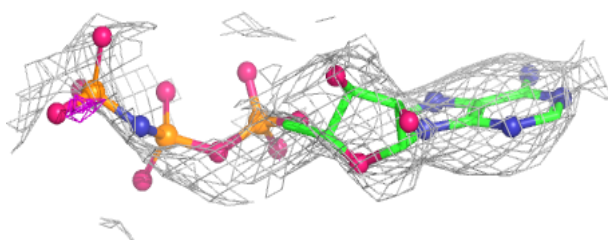
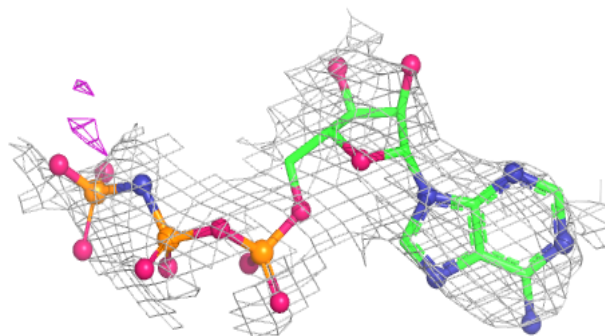
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	1203	5/5	0.82	0.21	128,142,143,150	0
3	ANP	A	1480	31/31	0.90	0.14	76,141,253,269	0
3	ANP	C	1480	31/31	0.93	0.13	77,140,253,269	0
4	MG	C	1481	1/1	0.95	0.09	99,99,99,99	0
4	MG	A	1481	1/1	0.95	0.15	106,106,106,106	0
5	GTP	B	1201	32/32	0.98	0.07	49,63,94,117	0
5	GTP	D	1201	32/32	0.98	0.06	29,61,95,115	0
4	MG	B	1202	1/1	0.98	0.09	50,50,50,50	0
4	MG	D	1202	1/1	0.99	0.05	34,34,34,34	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.

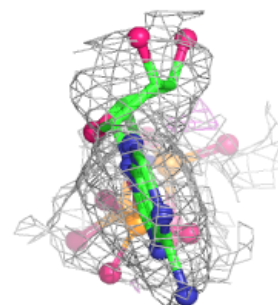
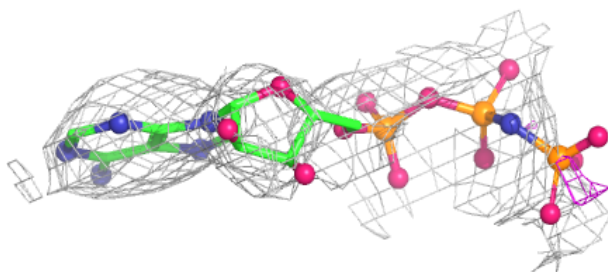
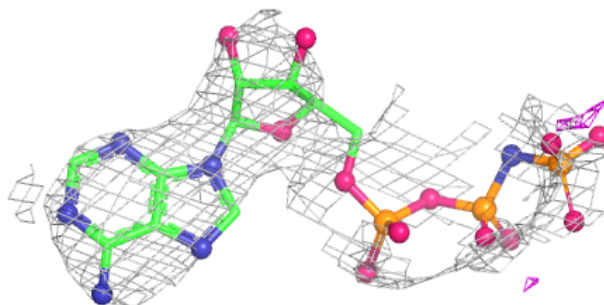
Electron density around ANP A 1480:

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

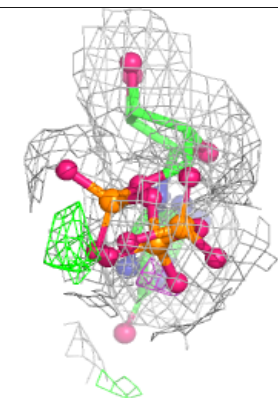
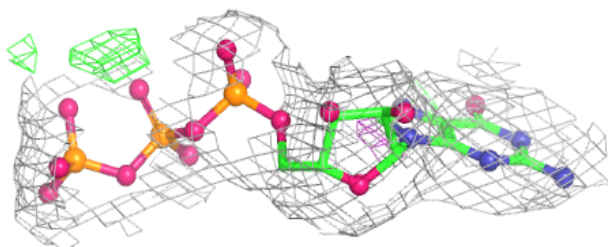
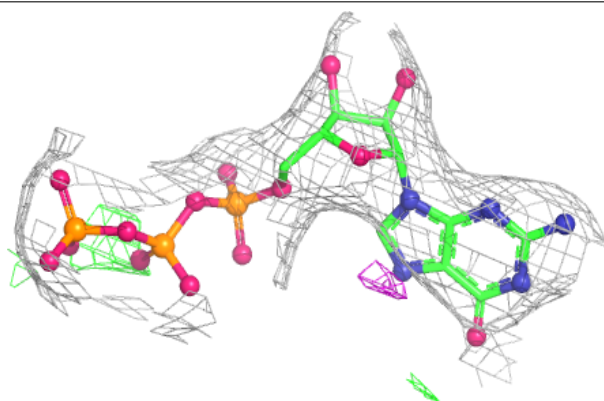


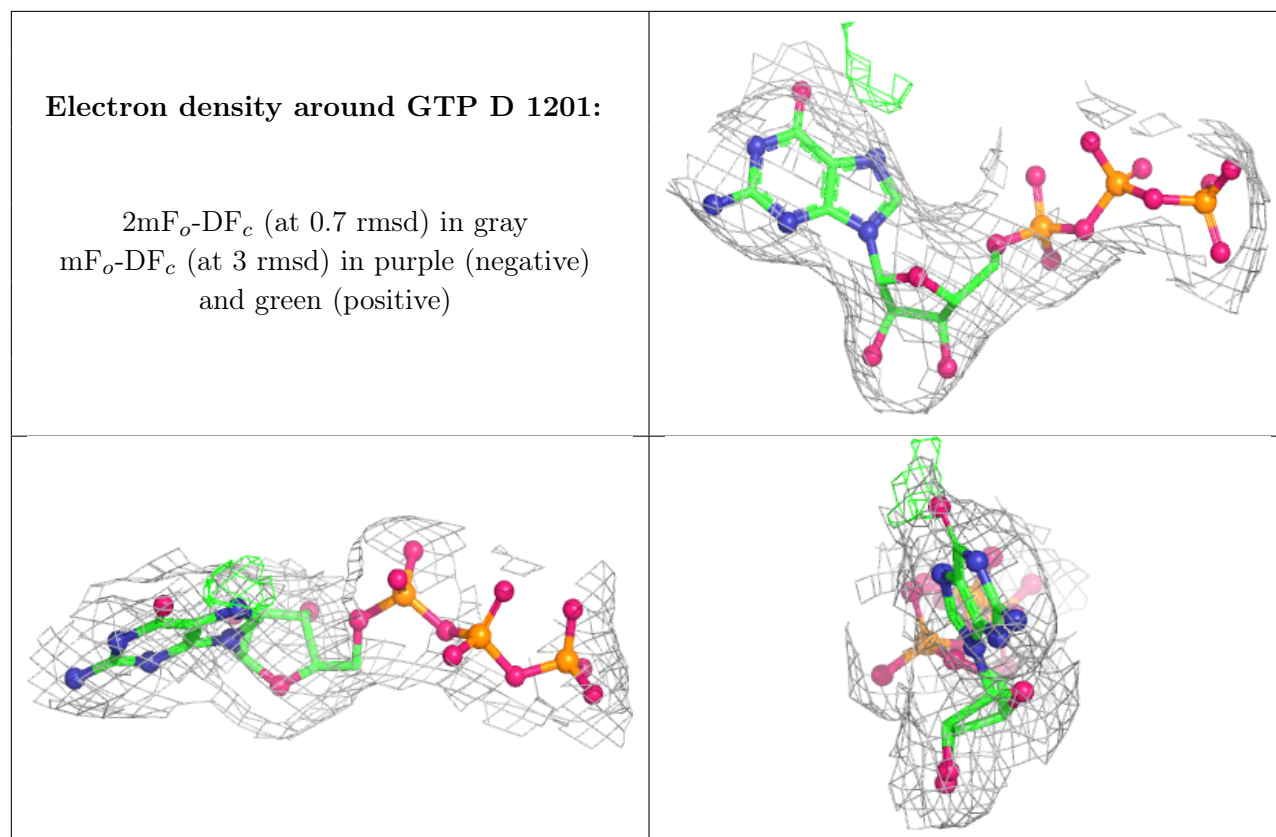
Electron density around ANP C 1480:

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

**Electron density around GTP B 1201:**

$2mF_o-DF_c$ (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.