



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:54 PM UTC

PDB ID : 5YU6 / pdb_00005yu6
Title : CRYSTAL STRUCTURE OF EXPORTIN-5:RANGTP COMPLEX
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Deposited on : 2017-11-20
Resolution : 3.00 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

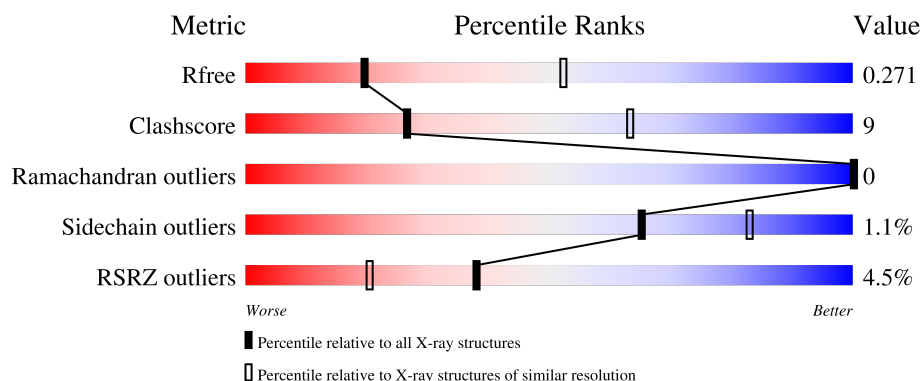
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



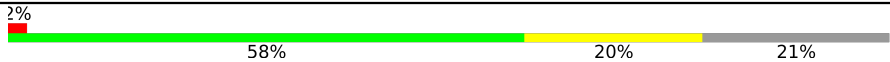
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1204	4% 70% 18% 11%
1	C	1204	5% 68% 21% 11%
2	E	13	100%
2	F	13	100%
3	B	216	2% 52% 27% 21%

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Mol	Chain	Length	Quality of chain
3	D	216	 A horizontal bar chart showing the quality of chain D. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a long green segment labeled '58%', a yellow segment labeled '20%', and a grey segment at the end labeled '21%'.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20096 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 Exportin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1069	Total	C	N	O	S	0	0	0
			8549	5468	1439	1569	73			
1	C	1073	Total	C	N	O	S	0	0	0
			8577	5486	1443	1574	74			

- Molecule 2 is a protein called 13-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	0	0	0
			66	39	13	14			
2	F	13	Total	C	N	O	0	0	0
			66	39	13	14			

- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	170	Total	C	N	O	S	0	0	0
			1386	900	244	238	4			
3	D	170	Total	C	N	O	S	0	0	0
			1386	900	244	238	4			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

Chain C: 5% 68% 21% 11%

Legend: 5% (Red), 68% (Yellow), 21% (Orange), 11% (Green)

Chain	Residue	Conservation
Chain A	1	5%
Chain A	2	5%
Chain A	3	5%
Chain A	4	5%
Chain A	5	5%
Chain A	6	5%
Chain A	7	5%
Chain A	8	5%
Chain A	9	5%
Chain A	10	5%
Chain A	11	5%
Chain A	12	5%
Chain A	13	5%
Chain A	14	5%
Chain A	15	5%
Chain A	16	5%
Chain A	17	5%
Chain A	18	5%
Chain A	19	5%
Chain A	20	5%
Chain A	21	5%
Chain A	22	5%
Chain A	23	5%
Chain A	24	5%
Chain A	25	5%
Chain A	26	5%
Chain A	27	5%
Chain A	28	5%
Chain A	29	5%
Chain A	30	5%
Chain A	31	5%
Chain A	32	5%
Chain A	33	5%
Chain A	34	5%
Chain A	35	5%
Chain A	36	5%
Chain A	37	5%
Chain A	38	5%
Chain A	39	5%
Chain A	40	5%
Chain A	41	5%
Chain A	42	5%
Chain A	43	5%
Chain A	44	5%
Chain A	45	5%
Chain A	46	5%
Chain A	47	5%
Chain A	48	5%
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Chain A	72	5%
Chain A	73	5%
Chain A	74	5%
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Chain A	76	5%
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Chain A	79	5%
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Chain A	132	5%
Chain A	133	5%
Chain A	134	5%
Chain A	135	5%
Chain A	136	5%
Chain A	137	5%
Chain A	138	5%
Chain A	139	5%
Chain A	140	5%
Chain A	141	5%
Chain A	142	5%
Chain A	143	5%
Chain A	144	5%
Chain A	145	5%
Chain A	146	5%
Chain A	147	5%
Chain A	148	5%
Chain A	149	5%
Chain A	150	5%
Chain A	151	

Chain E: 100%

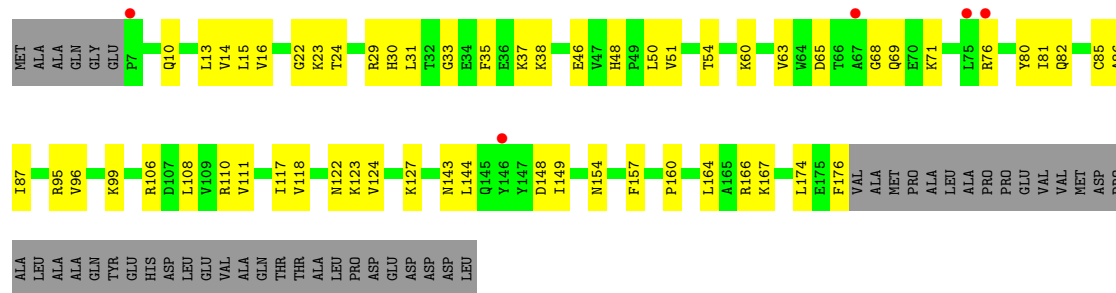
- Molecule 2: 13-mer peptide

Chain F:  100%

There are no outlier residues recorded for this chain.

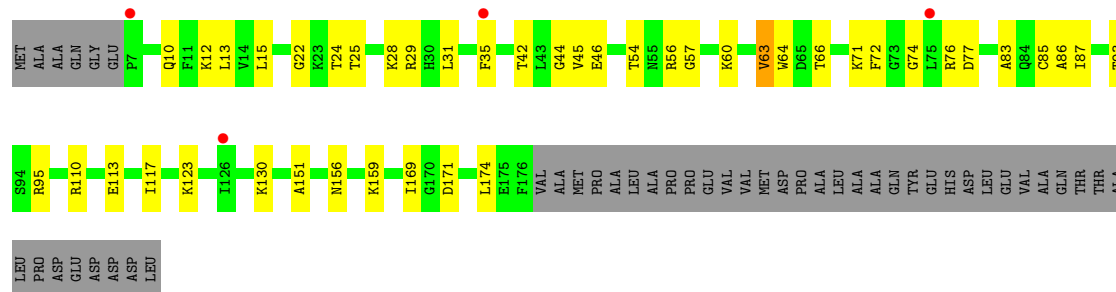
• Molecule 3: GTP-binding nuclear protein Ran

Chain B:  2% 52% 27% 21%



• Molecule 3: GTP-binding nuclear protein Ran

Chain D:  2% 58% 20% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.56Å 302.68Å 88.26Å 90.00° 109.24° 90.00°	Depositor
Resolution (Å)	48.98 – 3.00 48.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.9 (48.98-3.00) 82.0 (48.98-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.218 , 0.269 0.222 , 0.271	Depositor DCC
R_{free} test set	2875 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20096	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	0.11	0/8717	0.29	0/11803
1	C	0.11	0/8744	0.29	0/11838
3	B	0.11	0/1421	0.30	0/1918
3	D	0.12	0/1421	0.32	0/1918
All	All	0.11	0/20303	0.29	0/27477

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8549	0	8646	150	0
1	C	8577	0	8680	162	0
2	E	66	0	15	0	0
2	F	66	0	15	0	0
3	B	1386	0	1409	44	0
3	D	1386	0	1407	30	0
4	B	32	0	12	5	0
4	D	32	0	12	3	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	20096	0	20196	373	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 9.

All (373) 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:39:GLU:O	1:C:43:LYS:HB2	1.69	0.92
1:A:890:PRO:O	1:A:894:VAL:HB	1.76	0.85
1:C:125:LYS:HB3	1:C:170:LEU:HD21	1.63	0.79
1:A:732:VAL:HG22	1:A:769:ILE:HD13	1.65	0.78
3:D:13:LEU:HD11	3:D:87:ILE:HG13	1.64	0.78
1:A:595:ARG:H	1:A:827:PRO:HB2	1.50	0.76
1:A:543:THR:HG22	1:A:545:ASP:H	1.52	0.75
1:C:927:LEU:O	1:C:931:TRP:HB2	1.87	0.75
1:A:39:GLU:HG3	1:A:43:LYS:HE3	1.70	0.74
3:B:29:ARG:HH21	3:B:35:PHE:HB2	1.53	0.72
1:A:1089:CYS:O	1:A:1093:LEU:HB2	1.90	0.71
1:C:642:GLN:HE22	1:C:722:SER:HB2	1.56	0.71
3:D:15:LEU:O	3:D:66:THR:HB	1.90	0.70
1:C:182:LEU:O	1:C:186:MET:HB2	1.92	0.70
1:A:163:ASP:OD1	3:B:106:ARG:NH1	2.25	0.70
1:A:858:MET:O	1:A:862:PHE:HB3	1.92	0.69
1:A:147:GLU:HB3	1:A:223:VAL:HG21	1.74	0.69
1:C:158:LEU:HD13	1:C:230:THR:HA	1.75	0.67
1:C:1105:ARG:HH12	1:C:1109:LEU:HD12	1.59	0.67
1:C:616:PRO:HB2	1:C:658:GLN:HG2	1.76	0.67
1:C:408:MET:HE3	1:C:416:SER:HB3	1.77	0.66
3:B:13:LEU:HD11	3:B:87:ILE:HG13	1.77	0.66
1:C:564:THR:HA	1:C:618:LEU:HD21	1.77	0.66
1:C:842:THR:O	1:C:846:ASN:HB2	1.96	0.66
1:C:1043:SER:O	1:C:1047:THR:HB	1.96	0.65
1:A:372:GLN:NE2	1:A:443:GLN:OE1	2.29	0.65
1:C:158:LEU:HB2	1:C:230:THR:HG22	1.78	0.65
1:A:5:GLN:OE1	1:A:7:ASN:N	2.29	0.64
1:A:805:MET:HE1	1:A:813:ILE:HD12	1.79	0.64
1:C:1086:HIS:HB3	1:C:1089:CYS:HB3	1.80	0.64
1:A:551:CYS:O	1:A:555:ASN:ND2	2.31	0.64
1:C:642:GLN:NE2	1:C:719:ALA:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:ARG:HD3	3:B:127:LYS:HE3	1.80	0.63
1:C:924:HIS:HE1	1:C:1030:ILE:HG22	1.62	0.63
1:C:1010:GLU:OE2	1:C:1057:LYS:NZ	2.28	0.63
1:A:880:LEU:HD23	1:A:883:ILE:HD12	1.80	0.63
1:A:536:GLN:NE2	1:A:540:ASN:OD1	2.32	0.62
1:A:291:PHE:HA	1:A:296:MET:HG2	1.81	0.61
1:C:541:PHE:O	1:C:576:LYS:NZ	2.33	0.61
1:A:787:TYR:OH	1:A:887:ARG:NH1	2.32	0.61
1:C:1024:VAL:O	1:C:1028:LEU:HB2	2.00	0.61
1:C:120:VAL:HB	1:C:156:ILE:HD12	1.83	0.60
1:C:312:VAL:HG23	1:C:315:HIS:HB2	1.83	0.60
1:A:313:GLU:OE1	3:B:167:LYS:NZ	2.34	0.60
3:B:81:ILE:HG22	3:B:82:GLN:HG2	1.84	0.60
1:C:1036:LEU:HD21	1:C:1044:CYS:HA	1.83	0.60
1:A:1018:LEU:HD22	1:A:1024:VAL:HG11	1.83	0.60
1:C:236:ASP:O	1:C:277:ARG:NH1	2.34	0.60
1:C:850:ILE:O	1:C:854:ALA:HB2	2.01	0.59
1:C:637:GLU:OE1	1:C:645:LYS:NZ	2.36	0.59
1:A:858:MET:O	1:A:862:PHE:CB	2.50	0.59
3:D:42:THR:HG23	3:D:46:GLU:HG3	1.86	0.58
1:C:128:TRP:HA	1:C:132:TRP:HB3	1.85	0.58
1:A:158:LEU:HB2	1:A:230:THR:HG22	1.86	0.58
1:C:98:ILE:HD11	1:C:120:VAL:HG21	1.85	0.58
1:C:293:ASP:O	1:C:297:HIS:HB2	2.03	0.58
1:A:124:ILE:HG23	1:A:128:TRP:HB2	1.86	0.58
1:C:120:VAL:O	1:C:124:ILE:HG12	2.02	0.58
1:A:541:PHE:O	1:A:576:LYS:NZ	2.29	0.57
1:A:883:ILE:O	1:A:926:ARG:NH2	2.32	0.57
1:A:958:GLU:O	1:A:962:VAL:HG23	2.05	0.57
1:A:1051:LEU:O	1:A:1055:LEU:HG	2.04	0.57
1:A:128:TRP:H	1:A:174:ARG:HH22	1.52	0.57
1:C:802:ALA:HB2	1:C:836:MET:HE3	1.87	0.57
1:C:225:VAL:O	1:C:229:ASN:ND2	2.32	0.57
1:C:1044:CYS:O	1:C:1048:THR:HB	2.05	0.57
1:A:111:HIS:HB3	3:B:111:VAL:HG13	1.87	0.56
1:A:698:TYR:CZ	1:A:717:ASN:HB3	2.40	0.56
1:A:250:LEU:O	1:A:254:LEU:HB2	2.05	0.56
3:B:29:ARG:NH2	3:B:35:PHE:HB2	2.20	0.56
1:A:906:GLU:OE2	1:A:906:GLU:N	2.36	0.56
1:A:1101:TYR:CZ	1:A:1105:ARG:HG3	2.40	0.56
1:C:620:LEU:HD22	1:C:658:GLN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:NH1	3:B:143:ASN:OD1	2.36	0.56
1:C:924:HIS:CE1	1:C:1030:ILE:HG22	2.40	0.56
1:A:868:LEU:HD12	1:A:869:ALA:N	2.21	0.55
1:A:139:LEU:HD13	1:A:153:VAL:HG13	1.88	0.55
1:C:1044:CYS:O	1:C:1048:THR:CB	2.54	0.55
1:A:154:MET:HB3	1:A:230:THR:HG21	1.89	0.55
3:B:124:VAL:HG21	3:B:148:ASP:HB3	1.89	0.55
3:B:24:THR:HG23	4:B:301:GTP:O2B	2.06	0.55
1:A:1065:LEU:HB2	1:A:1068:ALA:HB3	1.89	0.55
1:C:624:ASP:O	1:C:628:ASN:ND2	2.31	0.54
1:A:701:THR:HG22	1:A:799:PHE:HD2	1.72	0.54
1:C:72:GLU:HB3	1:C:119:ILE:HD13	1.89	0.54
1:C:678:SER:O	1:C:682:SER:OG	2.26	0.54
1:C:830:LYS:HB2	1:C:835:ARG:HG3	1.88	0.54
3:B:166:ARG:HG2	3:B:174:LEU:HB3	1.89	0.54
1:C:496:PHE:HA	1:C:500:PHE:HD2	1.73	0.54
3:D:13:LEU:O	3:D:63:VAL:HA	2.07	0.54
1:A:125:LYS:HB3	1:A:170:LEU:HD21	1.90	0.54
1:A:164:VAL:HG13	1:A:165:VAL:HG23	1.90	0.54
3:B:22:GLY:N	4:B:301:GTP:O1B	2.32	0.54
1:A:877:PHE:HB3	1:A:880:LEU:HD11	1.90	0.53
1:C:152:LEU:O	1:C:156:ILE:HG12	2.08	0.53
1:A:616:PRO:HB2	1:A:658:GLN:HG2	1.89	0.53
1:C:587:GLU:HG3	1:C:590:LYS:HD2	1.89	0.53
1:C:162:GLU:OE2	3:D:110:ARG:NH1	2.42	0.53
1:A:140:ASP:OD1	1:A:144:LYS:NZ	2.42	0.53
1:C:789:PRO:HD3	1:C:882:ASN:HD21	1.74	0.53
1:A:566:ARG:NH1	1:A:568:GLU:OE1	2.40	0.53
3:B:24:THR:HG22	3:B:65:ASP:OD2	2.08	0.53
1:A:1047:THR:HG23	1:A:1051:LEU:HD23	1.91	0.53
1:A:321:ARG:NH2	1:A:324:GLN:OE1	2.41	0.53
1:C:79:TRP:NE1	1:C:127:GLU:OE2	2.27	0.53
1:C:908:TYR:CZ	1:C:1014:LEU:HB2	2.45	0.52
1:A:162:GLU:OE2	3:B:110:ARG:NH2	2.43	0.52
1:A:977:CYS:SG	1:A:1028:LEU:HD21	2.50	0.52
3:B:29:ARG:HG3	3:B:157:PHE:CZ	2.45	0.52
3:D:171:ASP:HB3	3:D:174:LEU:HD13	1.91	0.52
1:A:689:LEU:HD22	1:A:779:LEU:HB2	1.89	0.52
1:A:1024:VAL:O	1:A:1028:LEU:HB2	2.10	0.52
1:C:443:GLN:HE21	1:C:447:MET:HB2	1.74	0.52
1:A:1020:LYS:NZ	1:A:1058:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:O	1:A:277:ARG:NH1	2.43	0.52
3:D:10:GLN:HG2	3:D:60:LYS:HD2	1.92	0.52
1:C:332:GLN:O	1:C:336:LEU:HB2	2.11	0.51
1:A:125:LYS:HD2	1:A:170:LEU:HD21	1.93	0.51
1:A:128:TRP:H	1:A:174:ARG:NH2	2.09	0.51
1:A:583:PHE:HD2	1:A:597:VAL:HG23	1.74	0.51
1:C:787:TYR:OH	1:C:887:ARG:NE	2.43	0.51
3:D:29:ARG:NH1	3:D:151:ALA:O	2.43	0.51
1:A:192:PHE:HD2	1:A:193:LEU:HD12	1.74	0.51
1:C:16:ALA:O	1:C:20:MET:HG3	2.10	0.51
1:C:885:ASP:OD1	1:C:926:ARG:NH2	2.37	0.51
1:A:105:ILE:HD11	1:A:147:GLU:HB2	1.92	0.51
1:C:311:LEU:HD22	1:C:420:GLU:HG3	1.93	0.51
1:A:406:VAL:HG22	1:A:408:MET:HG2	1.93	0.51
1:C:578:PHE:HE2	1:C:626:LEU:HD22	1.75	0.51
1:C:700:GLY:HA3	1:C:714:CYS:SG	2.51	0.51
1:A:284:ARG:HD2	1:A:332:GLN:HE22	1.75	0.51
3:B:117:ILE:HB	3:B:144:LEU:HD22	1.94	0.50
3:B:14:VAL:HG12	3:B:16:VAL:HG13	1.94	0.50
3:B:86:ALA:HB3	3:B:117:ILE:HG12	1.94	0.50
1:A:118:ARG:HH22	3:B:76:ARG:HH22	1.59	0.50
1:A:129:PRO:HD2	1:A:174:ARG:HH12	1.77	0.50
1:A:728:ILE:O	1:A:732:VAL:HG23	2.11	0.50
1:A:858:MET:HE3	1:A:862:PHE:HB2	1.93	0.50
3:D:13:LEU:HA	3:D:85:CYS:O	2.12	0.50
1:A:167:PHE:HE2	3:B:106:ARG:HD3	1.77	0.49
3:B:10:GLN:HG2	3:B:60:LYS:HD3	1.93	0.49
1:C:391:LEU:HA	1:C:394:ILE:HD12	1.94	0.49
1:C:1027:ALA:O	1:C:1031:THR:OG1	2.24	0.49
1:C:892:LEU:HA	1:C:896:VAL:HG22	1.95	0.49
1:C:1110:GLU:N	1:C:1110:GLU:OE2	2.45	0.49
3:D:54:THR:HG22	3:D:56:ARG:H	1.76	0.49
3:B:31:LEU:HD21	3:B:48:HIS:HB3	1.94	0.49
1:C:161:ALA:HB2	1:C:234:TYR:CZ	2.47	0.49
1:C:698:TYR:CZ	1:C:717:ASN:HB3	2.48	0.49
1:C:243:ILE:HG23	1:C:250:LEU:HD23	1.93	0.49
1:C:9:LEU:HD23	1:C:50:CYS:SG	2.52	0.49
3:D:12:LYS:HD2	3:D:83:ALA:HA	1.95	0.49
1:C:385:SER:HB3	1:C:453:LEU:HD21	1.94	0.48
3:D:25:THR:HG21	4:D:301:GTP:H3'	1.95	0.48
1:A:64:ARG:NH2	1:A:108:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:879:ASN:O	1:C:883:ILE:HG12	2.14	0.48
1:C:456:LYS:O	1:C:460:GLN:HG2	2.13	0.48
3:D:71:LYS:HE2	3:D:72:PHE:CE1	2.48	0.48
1:C:1105:ARG:HA	1:C:1111:ILE:HD11	1.95	0.48
3:D:86:ALA:HB3	3:D:117:ILE:HD13	1.95	0.48
1:A:613:ARG:HB2	1:A:654:LEU:HD13	1.95	0.48
3:B:118:VAL:HG11	3:B:160:PRO:HB3	1.95	0.48
1:A:542:ASP:OD2	1:A:544:LYS:NZ	2.46	0.48
1:A:880:LEU:O	1:A:922:TYR:OH	2.29	0.48
1:A:20:MET:O	1:A:30:ARG:NH1	2.46	0.48
1:A:865:VAL:N	1:A:868:LEU:HD23	2.28	0.48
1:C:151:GLU:HB2	1:C:223:VAL:HG12	1.96	0.48
1:C:858:MET:O	1:C:862:PHE:HB3	2.14	0.48
3:B:37:LYS:HB3	3:B:38:LYS:HZ2	1.78	0.48
1:C:958:GLU:O	1:C:962:VAL:HG23	2.12	0.48
1:A:430:GLU:OE1	1:A:430:GLU:N	2.43	0.47
1:A:1030:ILE:HA	1:A:1071:TRP:HH2	1.79	0.47
1:A:583:PHE:CD2	1:A:597:VAL:HG23	2.50	0.47
1:A:1039:LYS:NZ	1:A:1082:MET:SD	2.88	0.47
1:C:379:PHE:O	1:C:385:SER:OG	2.32	0.47
1:C:967:ARG:HE	1:C:1042:LEU:HD12	1.79	0.47
1:A:448:ARG:HG2	1:A:516:GLN:HE21	1.78	0.47
3:B:29:ARG:HH11	3:B:154:ASN:HD21	1.61	0.47
1:A:863:TYR:CE2	1:A:903:CYS:HA	2.49	0.47
1:C:698:TYR:CE2	1:C:717:ASN:HB3	2.50	0.47
1:C:1129:PHE:HA	1:C:1132:LYS:HB3	1.97	0.47
1:A:1041:THR:HA	1:A:1044:CYS:SG	2.55	0.47
1:C:44:CYS:O	1:C:78:ARG:NH1	2.36	0.47
3:D:169:ILE:HD12	3:D:174:LEU:HD21	1.97	0.47
1:C:72:GLU:O	1:C:76:LYS:HB2	2.14	0.47
1:C:443:GLN:O	1:C:443:GLN:NE2	2.48	0.47
3:B:123:LYS:HG2	4:B:301:GTP:C5	2.50	0.47
1:C:79:TRP:CD1	1:C:126:ARG:HD3	2.50	0.47
3:D:24:THR:O	3:D:28:LYS:HB2	2.14	0.47
3:D:156:ASN:HA	3:D:159:LYS:HD3	1.96	0.46
1:A:371:THR:HG22	1:A:375:TRP:CD1	2.51	0.46
1:C:194:LEU:HD11	1:C:250:LEU:HA	1.97	0.46
1:C:598:ARG:NH1	1:C:602:ARG:HH12	2.12	0.46
1:C:316:TYR:OH	1:C:425:ASP:OD2	2.32	0.46
1:C:470:LEU:HD23	1:C:503:TRP:HH2	1.81	0.46
1:C:846:ASN:O	1:C:850:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:O	1:A:538:VAL:HG23	2.15	0.46
1:A:553:LEU:HD22	1:A:577:LEU:HD23	1.98	0.46
1:A:574:PHE:CE1	1:A:626:LEU:HD21	2.50	0.46
3:D:45:VAL:HG21	3:D:64:TRP:HB3	1.98	0.46
1:A:161:ALA:HB2	1:A:234:TYR:CZ	2.51	0.46
1:A:560:PHE:CE1	1:A:611:MET:HE3	2.50	0.46
3:B:14:VAL:HG11	3:B:80:TYR:CD1	2.51	0.46
1:C:296:MET:O	1:C:300:LEU:HG	2.16	0.46
1:A:596:ALA:O	1:A:600:VAL:HG23	2.15	0.46
3:B:29:ARG:HD3	3:B:33:GLY:HA2	1.98	0.46
1:C:32:GLU:O	1:C:36:PHE:HB3	2.14	0.46
1:C:213:GLN:HB3	1:C:216:LYS:HB3	1.98	0.46
1:C:873:LEU:HA	1:C:877:PHE:HB2	1.97	0.46
1:C:858:MET:HE3	1:C:862:PHE:HB2	1.96	0.46
1:C:689:LEU:HD22	1:C:779:LEU:HB2	1.98	0.45
1:A:120:VAL:HA	1:A:123:MET:HE2	1.97	0.45
1:A:643:MET:HG3	1:A:726:TYR:CZ	2.51	0.45
1:A:826:SER:N	1:A:827:PRO:HD3	2.31	0.45
3:B:123:LYS:HG2	4:B:301:GTP:C6	2.52	0.45
3:D:76:ARG:HG3	3:D:77:ASP:H	1.82	0.45
1:A:167:PHE:CE2	3:B:106:ARG:HD3	2.51	0.45
1:C:190:PHE:HZ	1:C:250:LEU:HB2	1.82	0.45
1:C:390:LEU:O	1:C:394:ILE:HG13	2.16	0.45
1:C:699:VAL:O	1:C:718:ARG:NH2	2.49	0.45
1:A:560:PHE:N	1:A:561:PRO:HD2	2.30	0.45
3:B:54:THR:HG22	3:B:176:PHE:HD1	1.82	0.45
3:D:93:THR:O	3:D:130:LYS:HE2	2.16	0.45
1:C:32:GLU:O	1:C:36:PHE:CB	2.65	0.45
1:A:231:LEU:O	1:A:235:ILE:HG13	2.17	0.45
1:A:963:ARG:O	1:A:967:ARG:HG2	2.17	0.45
1:A:288:MET:HE3	1:A:336:LEU:HD12	1.99	0.45
1:C:891:MET:O	1:C:895:PHE:HB3	2.17	0.45
3:B:13:LEU:HD23	3:B:63:VAL:HG12	1.99	0.45
1:C:297:HIS:O	1:C:301:SER:OG	2.34	0.45
1:C:444:GLY:O	1:C:448:ARG:HG3	2.17	0.45
1:A:669:LEU:HD13	1:A:765:CYS:HB3	1.98	0.45
1:A:158:LEU:HD13	1:A:230:THR:HA	1.99	0.44
1:A:972:LEU:O	1:A:976:CYS:HB2	2.17	0.44
1:C:210:ASP:CG	1:C:212:SER:HG	2.25	0.44
1:C:788:ALA:HA	1:C:882:ASN:HD22	1.83	0.44
1:A:408:MET:HE3	1:A:416:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:GLU:HG3	1:A:718:ARG:HH12	1.82	0.44
1:A:888:LEU:HD22	1:A:926:ARG:NH1	2.32	0.44
1:C:272:LEU:HD11	1:C:324:GLN:HB2	2.00	0.44
1:C:676:VAL:O	1:C:680:TRP:HB2	2.18	0.44
1:A:127:GLU:HB2	1:A:131:HIS:HB2	1.99	0.44
1:A:1045:GLN:HG3	1:A:1089:CYS:SG	2.56	0.44
3:B:15:LEU:HD21	3:B:23:LYS:HB2	1.99	0.44
3:B:29:ARG:NH1	3:B:154:ASN:OD1	2.51	0.44
1:C:443:GLN:NE2	1:C:447:MET:HB2	2.33	0.44
1:C:691:ASP:OD1	1:C:692:VAL:N	2.51	0.44
1:A:865:VAL:H	1:A:868:LEU:HD23	1.82	0.44
3:B:96:VAL:HA	3:B:99:LYS:HD2	2.00	0.44
1:C:48:VAL:HG13	1:C:90:LEU:HD13	2.00	0.44
1:C:513:VAL:O	1:C:517:MET:HB2	2.17	0.44
1:C:94:VAL:HG11	1:C:119:ILE:HG21	1.98	0.44
1:C:560:PHE:N	1:C:561:PRO:HD2	2.32	0.44
1:C:788:ALA:O	1:C:792:LEU:N	2.51	0.44
1:A:594:THR:OG1	1:A:597:VAL:HG12	2.17	0.44
1:A:616:PRO:HB2	1:A:658:GLN:CG	2.46	0.44
1:A:1035:SER:HA	1:A:1038:TRP:CE2	2.52	0.44
3:B:46:GLU:O	3:B:65:ASP:HB3	2.18	0.44
1:C:306:ALA:HB3	1:C:319:LEU:HD13	1.99	0.44
1:A:494:SER:HB3	1:A:545:ASP:OD2	2.18	0.44
1:A:873:LEU:HD11	1:A:915:ILE:HA	2.00	0.44
1:C:613:ARG:HB2	1:C:654:LEU:HD13	1.98	0.44
1:C:849:HIS:O	1:C:853:LYS:HB2	2.18	0.44
1:A:846:ASN:O	1:A:850:ILE:HG13	2.18	0.43
1:C:1082:MET:HG3	1:C:1083:HIS:CD2	2.53	0.43
1:A:466:LEU:HD23	1:A:534:LEU:HD22	1.99	0.43
1:A:806:LEU:HB3	1:A:809:GLU:HG3	2.00	0.43
1:C:240:MET:HG2	1:C:283:ASP:O	2.17	0.43
1:A:64:ARG:HH22	1:A:108:GLU:CD	2.26	0.43
1:A:285:LYS:HA	1:A:336:LEU:HD13	2.00	0.43
1:A:518:PHE:CE2	1:A:561:PRO:HB2	2.52	0.43
1:A:554:THR:OG1	1:A:603:HIS:NE2	2.41	0.43
1:A:680:TRP:NE1	1:A:775:ASN:HB2	2.33	0.43
1:C:595:ARG:HB3	1:C:827:PRO:HD2	2.00	0.43
1:A:830:LYS:HD2	1:A:830:LYS:HA	1.78	0.43
1:A:865:VAL:HB	1:A:868:LEU:HB3	2.01	0.43
1:C:316:TYR:CE2	1:C:320:LYS:HD2	2.53	0.43
1:C:498:PRO:HA	1:C:501:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:44:GLY:HA2	3:D:74:GLY:H	1.83	0.43
1:C:97:LEU:HA	1:C:101:GLY:HA3	2.01	0.43
1:C:192:PHE:O	1:C:196:THR:HG22	2.18	0.43
1:C:651:ALA:O	1:C:655:ILE:HG13	2.19	0.43
1:C:323:CYS:HB2	1:C:359:PHE:CE1	2.53	0.43
1:C:614:ASP:C	1:C:616:PRO:HD3	2.44	0.43
1:C:1044:CYS:O	1:C:1048:THR:OG1	2.35	0.43
3:B:30:HIS:HB3	3:B:50:LEU:HD21	2.01	0.43
1:A:321:ARG:HA	1:A:321:ARG:HH21	1.84	0.43
1:C:797:GLU:HG3	1:C:798:PRO:HD3	2.00	0.43
3:D:12:LYS:HE3	3:D:64:TRP:CD1	2.54	0.43
1:C:411:PRO:O	1:C:423:ARG:NH1	2.50	0.43
1:C:676:VAL:O	1:C:680:TRP:CB	2.67	0.43
1:A:264:GLN:HB2	1:A:318:PHE:CE1	2.53	0.43
1:A:216:LYS:O	1:A:219:ALA:HB3	2.19	0.42
3:B:69:GLN:NE2	3:B:71:LYS:HE2	2.34	0.42
1:C:48:VAL:HB	1:C:49:PRO:HD3	2.01	0.42
1:A:959:GLU:O	1:A:963:ARG:HG3	2.20	0.42
1:C:539:LEU:HD21	1:C:573:VAL:HG12	2.01	0.42
1:C:563:VAL:HG23	1:C:569:PHE:HB2	2.01	0.42
1:C:789:PRO:HD3	1:C:882:ASN:ND2	2.34	0.42
3:D:22:GLY:HA2	4:D:301:GTP:H5'	2.00	0.42
1:A:406:VAL:HG23	1:A:501:VAL:HG12	2.00	0.42
1:A:574:PHE:HZ	1:A:619:VAL:HG13	1.84	0.42
1:A:924:HIS:HB2	1:A:1031:THR:OG1	2.18	0.42
1:A:1056:LEU:HD23	1:A:1056:LEU:HA	1.91	0.42
1:A:48:VAL:HB	1:A:49:PRO:HD3	2.01	0.42
1:C:1043:SER:O	1:C:1047:THR:CB	2.66	0.42
1:A:356:PHE:CZ	1:A:371:THR:HG23	2.54	0.42
1:C:159:ARG:HH21	3:D:110:ARG:HG3	1.85	0.42
1:C:436:PHE:O	1:C:440:ARG:HB2	2.19	0.42
1:C:497:SER:HB3	1:C:498:PRO:HD2	2.02	0.42
1:C:631:LYS:HA	1:C:631:LYS:HD2	1.80	0.42
1:A:55:ALA:HA	1:A:64:ARG:HA	2.01	0.42
1:A:235:ILE:HG21	1:A:274:ALA:HB2	2.01	0.42
1:A:585:THR:OG1	1:A:587:GLU:O	2.35	0.42
1:A:928:SER:HA	1:A:1038:TRP:CH2	2.55	0.42
1:A:1070:THR:O	1:A:1074:THR:OG1	2.26	0.42
1:C:618:LEU:O	1:C:621:PRO:HD2	2.20	0.42
1:A:456:LYS:HA	1:A:456:LYS:HD2	1.85	0.41
1:A:624:ASP:N	1:A:624:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ASP:OD1	1:A:693:ASP:N	2.53	0.41
1:C:65:HIS:O	1:C:69:GLN:HB2	2.19	0.41
1:C:114:ASP:O	1:C:118:ARG:HG3	2.20	0.41
3:D:54:THR:HB	3:D:57:GLY:O	2.20	0.41
1:A:1085:GLN:OE1	3:B:95:ARG:NH1	2.53	0.41
3:B:68:GLY:N	4:B:301:GTP:O2G	2.38	0.41
1:C:680:TRP:CD1	1:C:772:LEU:HD22	2.55	0.41
1:C:716:LEU:O	1:C:720:ARG:HG3	2.21	0.41
1:C:930:LYS:HD3	1:C:962:VAL:HG22	2.02	0.41
1:C:1030:ILE:O	1:C:1034:ASN:HB2	2.21	0.41
1:A:889:ARG:HB3	1:A:890:PRO:HD3	2.02	0.41
1:C:91:LYS:HE2	1:C:132:TRP:CZ2	2.55	0.41
1:C:337:LEU:HD23	1:C:337:LEU:HA	1.94	0.41
1:C:801:LYS:HB2	1:C:833:LEU:HD21	2.02	0.41
1:A:22:ASP:O	1:A:30:ARG:NH2	2.53	0.41
1:A:381:HIS:HB3	1:A:384:LEU:HB2	2.02	0.41
1:C:379:PHE:CE1	1:C:390:LEU:HD21	2.56	0.41
1:C:601:ARG:NE	1:C:644:GLU:OE1	2.53	0.41
1:C:900:VAL:HG22	1:C:912:VAL:HG23	2.03	0.41
3:B:85:CYS:HB2	3:B:164:LEU:HD22	2.03	0.41
1:C:272:LEU:HD13	1:C:321:ARG:NH2	2.35	0.41
1:C:359:PHE:HD1	1:C:367:LEU:HD13	1.86	0.41
1:C:1115:MET:HE2	1:C:1115:MET:HB3	2.01	0.41
3:D:13:LEU:HB2	3:D:85:CYS:SG	2.61	0.41
3:D:123:LYS:HG2	4:D:301:GTP:C5	2.56	0.41
1:A:320:LYS:HG2	1:A:367:LEU:HD21	2.03	0.41
1:A:578:PHE:O	1:A:581:VAL:HB	2.20	0.41
1:A:1035:SER:HA	1:A:1038:TRP:NE1	2.36	0.41
1:A:1105:ARG:N	1:A:1106:PRO:HD2	2.36	0.41
1:C:124:ILE:HD13	1:C:132:TRP:CZ3	2.56	0.41
1:C:462:ALA:HB1	1:C:510:LEU:HD12	2.03	0.41
1:C:583:PHE:O	1:C:601:ARG:HD3	2.20	0.41
1:C:799:PHE:CD1	1:C:836:MET:HE1	2.56	0.41
1:C:850:ILE:O	1:C:854:ALA:CB	2.68	0.41
1:C:1073:PHE:HA	1:C:1076:VAL:HG12	2.02	0.41
3:D:29:ARG:NH1	3:D:35:PHE:HB2	2.36	0.41
1:A:31:LEU:O	1:A:35:LYS:HB2	2.20	0.41
1:A:786:LEU:HD12	1:A:786:LEU:HA	1.97	0.40
3:B:48:HIS:O	3:B:63:VAL:HG22	2.21	0.40
3:B:122:ASN:HA	3:B:149:ILE:HG13	2.02	0.40
1:C:1082:MET:HG3	1:C:1083:HIS:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ARG:H	1:A:827:PRO:CB	2.27	0.40
1:C:577:LEU:O	1:C:581:VAL:HG23	2.22	0.40
1:C:970:MET:HE3	1:C:1038:TRP:HZ3	1.86	0.40
3:D:95:ARG:CZ	3:D:130:LYS:HB3	2.51	0.40
1:C:877:PHE:HB3	1:C:880:LEU:HD11	2.03	0.40
1:A:273:ILE:HD12	1:A:273:ILE:HA	2.00	0.40
1:A:545:ASP:OD2	1:A:548:ILE:HG12	2.22	0.40
1:A:1065:LEU:HD22	1:A:1065:LEU:H	1.86	0.40
1:C:699:VAL:HG23	1:C:701:THR:HG23	2.03	0.40
1:C:745:LYS:HA	1:C:750:VAL:HG22	2.04	0.40
1:C:1101:TYR:CZ	1:C:1105:ARG:HD3	2.56	0.40
1:A:571:PRO:HG2	1:C:572:GLN:HA	2.04	0.40
3:D:86:ALA:O	3:D:117:ILE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1059/1204 (88%)	1036 (98%)	23 (2%)	0	100	100
1	C	1063/1204 (88%)	1036 (98%)	27 (2%)	0	100	100
3	B	168/216 (78%)	166 (99%)	2 (1%)	0	100	100
3	D	168/216 (78%)	160 (95%)	8 (5%)	0	100	100
All	All	2458/2840 (86%)	2398 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	965/1073 (90%)	954 (99%)	11 (1%)	65	83
1	C	968/1073 (90%)	959 (99%)	9 (1%)	70	85
3	B	150/185 (81%)	148 (99%)	2 (1%)	61	81
3	D	150/185 (81%)	147 (98%)	3 (2%)	48	76
All	All	2233/2516 (89%)	2208 (99%)	25 (1%)	65	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ILE
1	A	186	MET
1	A	207	VAL
1	A	254	LEU
1	A	343	VAL
1	A	356	PHE
1	A	568	GLU
1	A	570	LEU
1	A	1069	VAL
1	A	1115	MET
1	A	1134	LEU
3	B	51	VAL
3	B	108	LEU
1	C	72	GLU
1	C	119	ILE
1	C	466	LEU
1	C	658	GLN
1	C	663	GLU
1	C	816	LEU
1	C	1028	LEU
1	C	1059	VAL
1	C	1121	ILE
3	D	31	LEU
3	D	63	VAL
3	D	113	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	242	HIS
1	A	264	GLN
1	A	372	GLN
1	A	443	GLN
1	A	516	GLN
1	A	658	GLN
1	A	665	GLN
1	A	768	GLN
1	A	775	ASN
1	A	1045	GLN
1	A	1086	HIS
1	A	1099	GLN
1	A	1135	ASN
3	B	30	HIS
3	B	62	ASN
1	C	24	ASN
1	C	27	GLN
1	C	220	ASN
1	C	442	GLN
1	C	516	GLN
1	C	632	GLN
1	C	642	GLN
1	C	882	ASN
1	C	1095	HIS
1	C	1099	GLN
3	D	62	ASN
3	D	114	ASN
3	D	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
4	GTP	D	301	5	33,34,34	0.97	2 (6%)	50,54,54	1.62	9 (18%)
4	GTP	B	301	5	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)

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
4	GTP	D	301	5	-	1/22/38/38	0/3/3/3
4	GTP	B	301	5	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	GTP	C2-N3	2.27	1.38	1.33
4	D	301	GTP	C2-N3	2.23	1.38	1.33
4	B	301	GTP	PA-O3A	2.10	1.61	1.59
4	D	301	GTP	PB-O3A	2.06	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	GTP	C5-C4-N3	-5.07	120.32	128.39
4	B	301	GTP	C5-C4-N3	-5.01	120.41	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	GTP	C2-N3-C4	4.63	120.27	112.30
4	B	301	GTP	C2-N3-C4	4.61	120.24	112.30
4	B	301	GTP	N9-C4-N3	3.30	132.56	125.95
4	D	301	GTP	N9-C4-N3	3.23	132.41	125.95
4	D	301	GTP	C2-N1-C6	-2.92	119.81	125.11
4	B	301	GTP	C2-N1-C6	-2.85	119.94	125.11
4	B	301	GTP	N9-C8-N7	-2.65	108.48	113.40
4	D	301	GTP	N9-C8-N7	-2.53	108.72	113.40
4	B	301	GTP	C5-C6-N1	2.51	119.65	113.25
4	B	301	GTP	C8-N7-C5	2.51	108.73	104.26
4	D	301	GTP	C5-C6-N1	2.50	119.61	113.25
4	D	301	GTP	C8-N7-C5	2.46	108.65	104.26
4	D	301	GTP	O6-C6-C5	-2.40	120.19	126.53
4	B	301	GTP	O6-C6-C5	-2.40	120.20	126.53
4	D	301	GTP	C3'-C2'-C1'	2.30	105.81	101.46
4	B	301	GTP	C3'-C2'-C1'	2.15	105.54	101.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GTP	O4'-C4'-C5'-O5'
4	B	301	GTP	C3'-C4'-C5'-O5'
4	B	301	GTP	PB-O3B-PG-O2G
4	B	301	GTP	C5'-O5'-PA-O1A
4	D	301	GTP	O4'-C4'-C5'-O5'

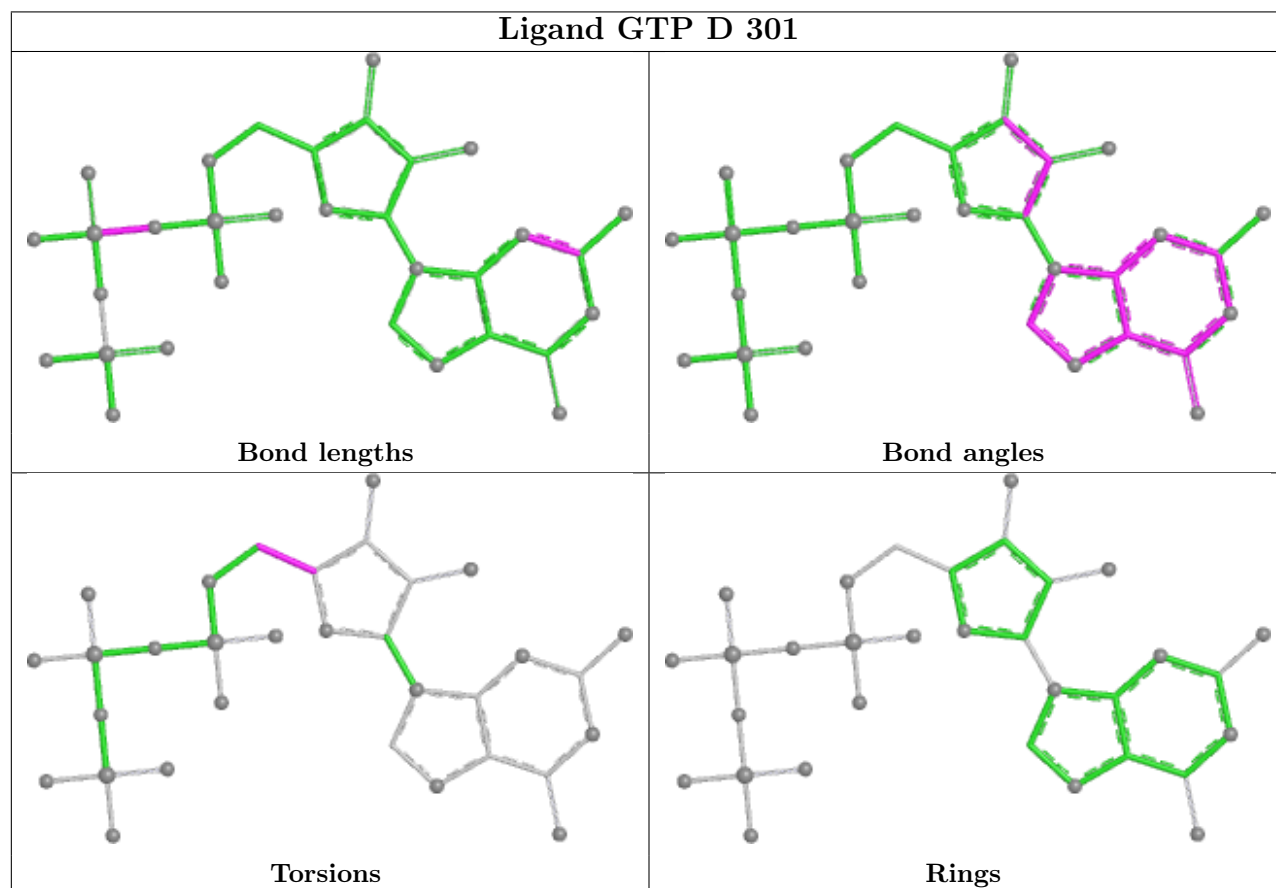
There are no ring outliers.

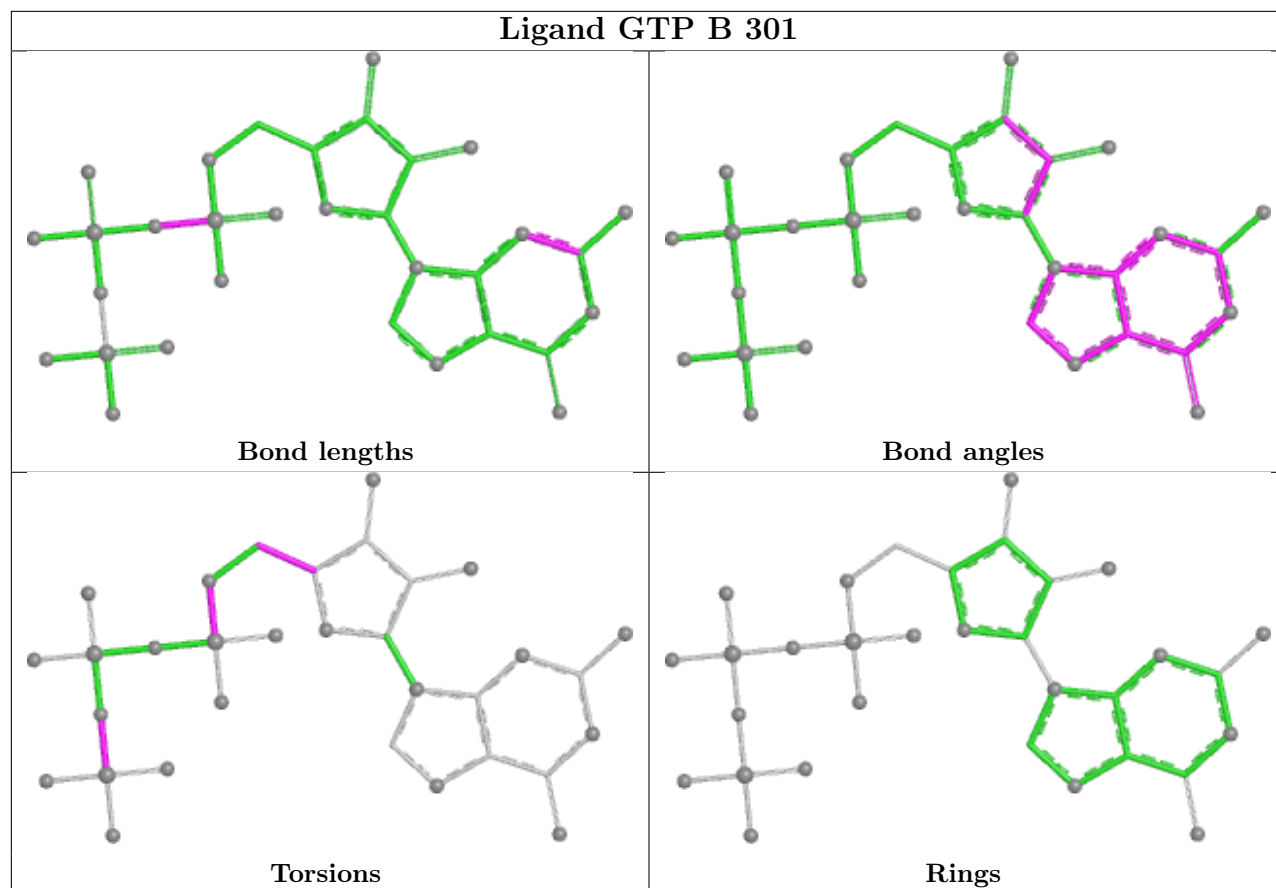
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	GTP	3	0
4	B	301	GTP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1069/1204 (88%)	0.27	47 (4%) 39 21	23, 57, 121, 215	0
1	C	1073/1204 (89%)	0.52	56 (5%) 33 17	27, 74, 139, 249	0
2	E	0/13	-	-	-	-
2	F	0/13	-	-	-	-
3	B	170/216 (78%)	0.14	5 (2%) 53 31	28, 49, 80, 109	0
3	D	170/216 (78%)	0.22	4 (2%) 59 36	27, 52, 91, 122	0
All	All	2482/2866 (86%)	0.37	112 (4%) 38 20	23, 63, 129, 249	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	940	LEU	5.0
1	C	1073	PHE	4.4
3	B	7	PRO	4.4
1	C	827	PRO	4.3
1	C	1065	LEU	4.2
1	C	828	VAL	4.1
1	A	829	PHE	4.1
1	A	1060	LEU	4.0
1	C	1032	ALA	3.9
1	C	625	MET	3.8
1	C	1036	LEU	3.8
1	C	805	MET	3.8
1	C	1104	LEU	3.6
1	C	1100	ILE	3.5
1	C	1025	CYS	3.5
1	A	819	PRO	3.4
1	A	473	PHE	3.3
1	A	956	MET	3.3
1	A	1097	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1069	VAL	3.2
1	A	496	PHE	3.2
1	A	711	GLU	3.2
1	A	1089	CYS	3.2
1	C	453	LEU	3.2
3	D	75	LEU	3.2
1	C	494	SER	3.1
1	A	339	ALA	3.1
1	A	495	VAL	3.1
1	A	860	GLN	3.1
1	C	1080	LEU	3.0
1	C	310	GLY	3.0
3	B	75	LEU	3.0
1	A	708	PRO	3.0
3	D	7	PRO	3.0
1	A	492	LEU	2.9
1	C	842	THR	2.9
1	C	811	SER	2.8
1	A	816	LEU	2.8
1	C	604	ALA	2.8
1	C	496	PHE	2.8
1	A	828	VAL	2.8
1	C	586	VAL	2.8
1	A	134	ASP	2.7
1	A	712	ASP	2.7
1	A	1064	LEU	2.7
1	C	820	LEU	2.7
1	A	710	LEU	2.7
1	A	827	PRO	2.6
1	A	699	VAL	2.6
1	C	637	GLU	2.6
1	A	1066	ALA	2.6
1	A	1094	VAL	2.5
1	C	1041	THR	2.5
1	C	806	LEU	2.5
1	C	939	LEU	2.5
1	A	586	VAL	2.5
1	A	642	GLN	2.5
1	A	1067	ASP	2.5
1	A	1065	LEU	2.5
1	C	129	PRO	2.5
1	C	646	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1029	LEU	2.4
3	D	126	ILE	2.4
3	B	76	ARG	2.4
3	B	67	ALA	2.4
1	A	908	TYR	2.4
1	C	595	ARG	2.4
1	A	1134	LEU	2.4
1	C	1084	GLY	2.4
1	C	341	SER	2.4
1	A	962	VAL	2.3
1	C	311	LEU	2.3
1	C	823	LEU	2.3
1	C	1083	HIS	2.3
1	C	495	VAL	2.3
1	C	1037	ALA	2.3
1	A	173	GLN	2.3
1	A	826	SER	2.3
1	A	1074	THR	2.3
1	C	1074	THR	2.3
1	A	1111	ILE	2.3
1	C	190	PHE	2.3
1	A	692	VAL	2.3
1	A	713	PRO	2.3
1	C	338	GLY	2.3
3	D	35	PHE	2.2
1	C	795	MET	2.2
1	A	767	GLU	2.2
1	C	5	GLN	2.2
1	C	1030	ILE	2.2
1	C	230	THR	2.2
1	C	509	PHE	2.2
1	C	369	SER	2.2
1	C	1033	PHE	2.2
1	A	1086	HIS	2.2
1	A	820	LEU	2.2
1	C	1136	PRO	2.2
1	A	1108	TYR	2.2
1	C	491	SER	2.2
1	C	712	ASP	2.1
1	C	803	LEU	2.1
1	A	1044	CYS	2.1
1	A	1093	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	952	GLU	2.1
1	C	933	VAL	2.1
1	C	170	LEU	2.1
1	A	603	HIS	2.0
1	A	415	ASP	2.0
1	C	711	GLU	2.0
3	B	146	TYR	2.0
1	C	1044	CYS	2.0
1	A	1051	LEU	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](#)

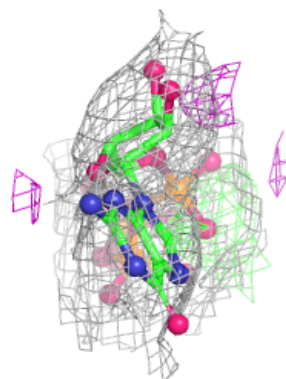
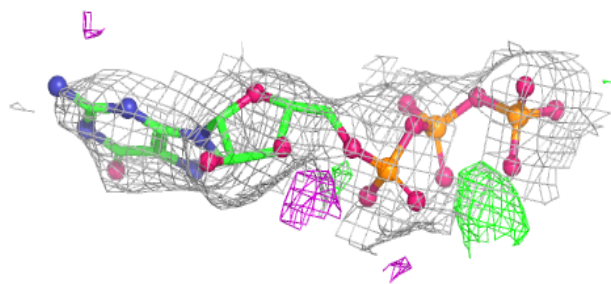
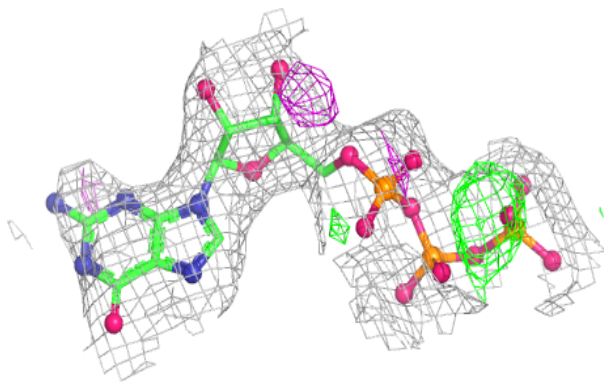
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	302	1/1	0.82	0.18	54,54,54,54	0
5	MG	B	302	1/1	0.90	0.14	41,41,41,41	0
4	GTP	B	301	32/32	0.93	0.09	33,55,63,71	0
4	GTP	D	301	32/32	0.95	0.09	38,61,81,85	0

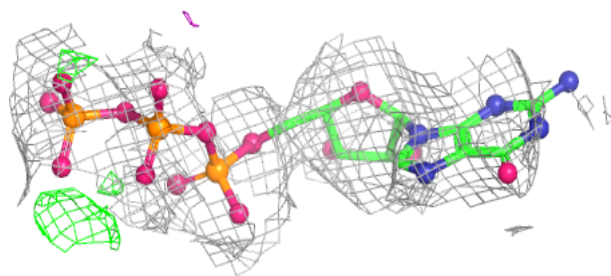
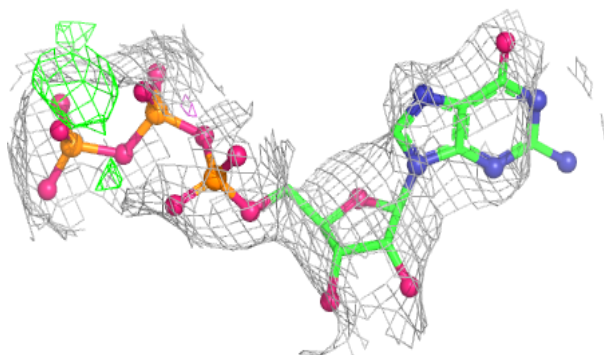
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP B 301:

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

**Electron density around GTP D 301:**

$2mF_o-DF_c$ (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.