



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:22 AM UTC

PDB ID : 6JSJ / pdb_00006jsj
Title : Structural analysis of a trimeric assembly of the mitochondrial dynamin-like GTPase Mgm1
Authors : Yan, L.; Li, L.
Deposited on : 2019-04-08
Resolution : 3.20 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

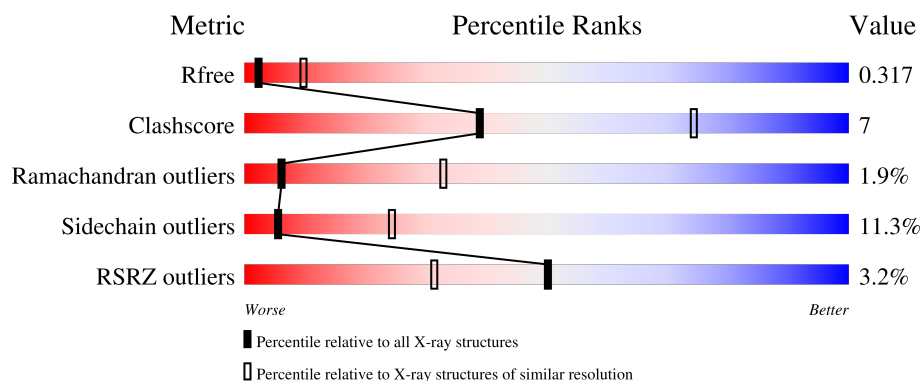
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	698	 64% 23% 10% 5%
1	B	698	 62% 24% 11% 5%
1	C	698	 66% 19% 11% 3%

2 Entry composition [i](#)

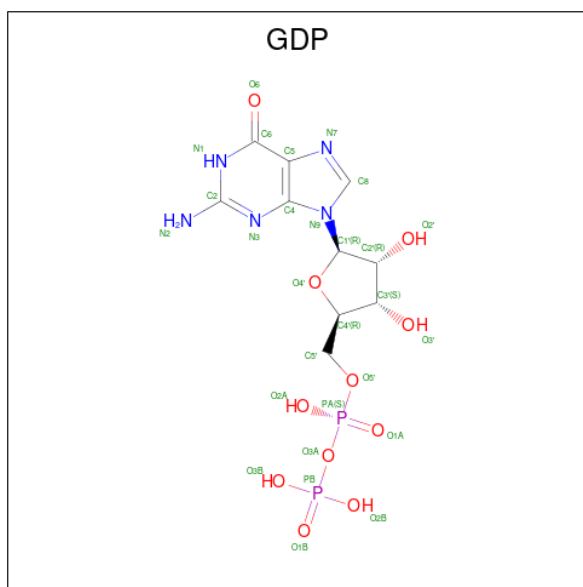
There are 3 unique types of molecules in this entry. The entry contains 15082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dynamin-like GTPase MGM1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			5014	3185	851	956	22			
1	B	624	Total	C	N	O	S	0	0	0
			5001	3178	848	953	22			
1	C	619	Total	C	N	O	S	0	0	0
			4958	3151	840	946	21			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

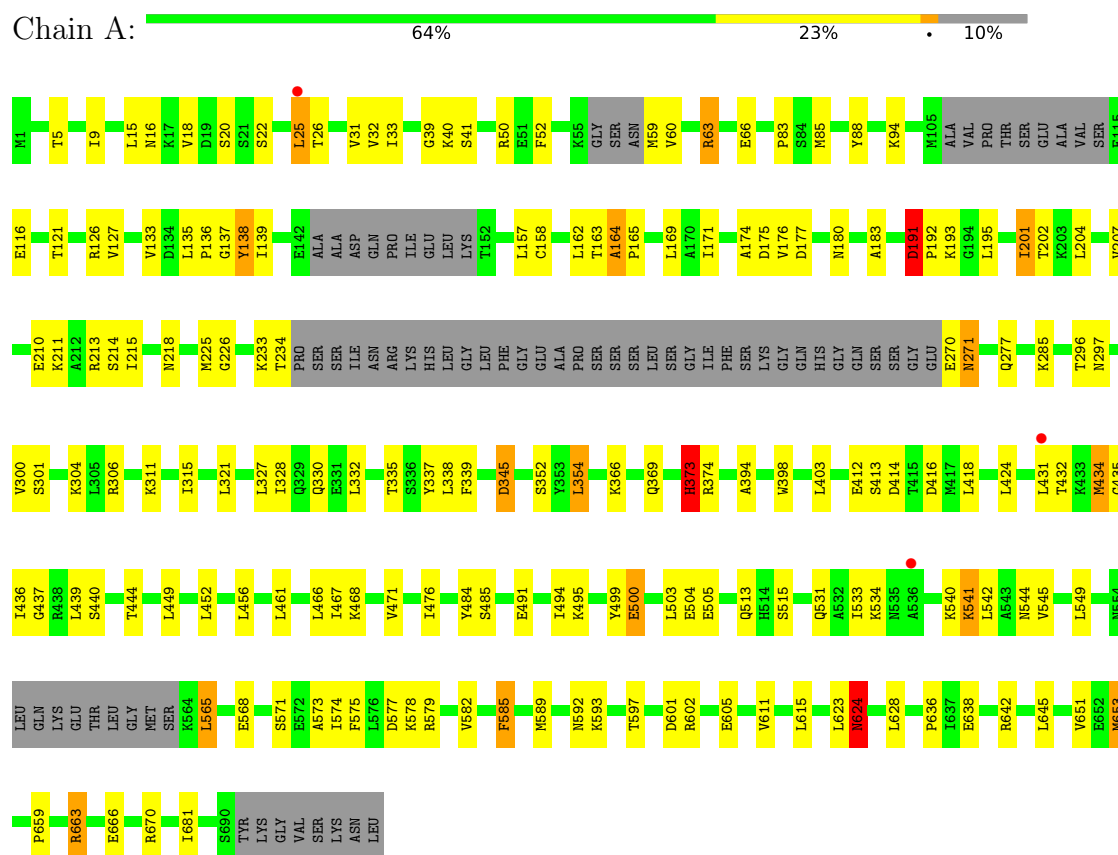
- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total I 9 9	0	0
3	B	10	Total I 10 10	0	0
3	C	6	Total I 6 6	0	0

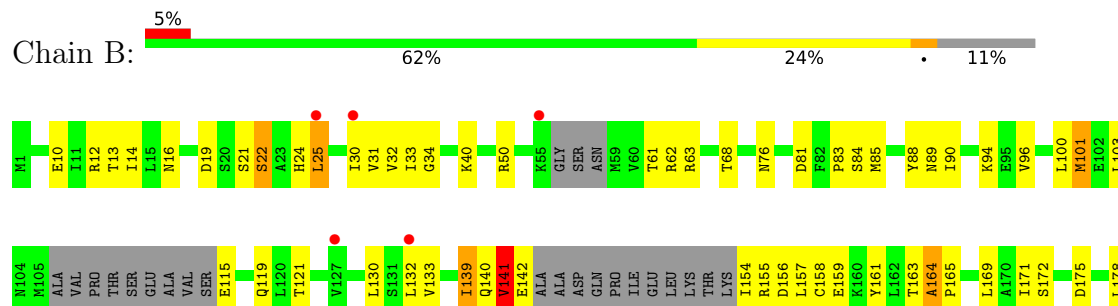
3 Residue-property plots

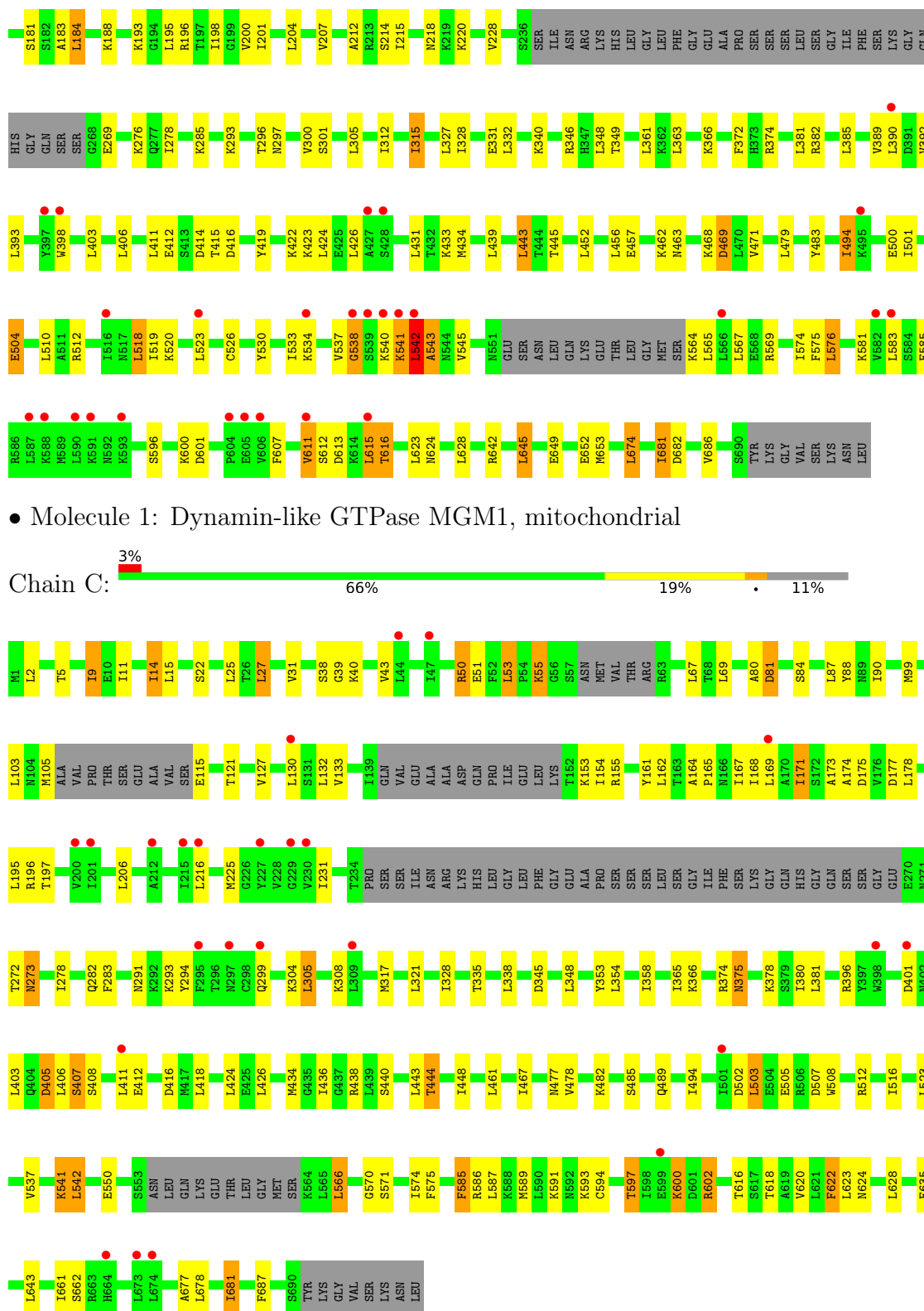
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dynamin-like GTPase MGM1, mitochondrial



- Molecule 1: Dynamin-like GTPase MGM1, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.94Å 152.94Å 236.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.20 49.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.17-3.20) 99.9 (49.17-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.19Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.243 , 0.306 0.267 , 0.317	Depositor DCC
R_{free} test set	2292 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	118.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 126.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15082	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: IOD, GDP

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	0.80	0/5078	1.48	43/6830 (0.6%)
1	B	0.82	1/5066 (0.0%)	1.49	41/6815 (0.6%)
1	C	0.81	0/5022	1.48	20/6754 (0.3%)
All	All	0.81	1/15166 (0.0%)	1.48	104/20399 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	ILE	CA-C	5.57	1.59	1.52

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	GLY	N-CA-C	17.17	153.88	113.18
1	C	602	ARG	CA-C-N	9.46	132.77	122.74
1	C	602	ARG	C-N-CA	9.46	132.77	122.74
1	B	585	PHE	CA-CB-CG	7.31	121.11	113.80
1	A	602	ARG	CA-C-N	7.09	132.70	122.98
1	A	602	ARG	C-N-CA	7.09	132.70	122.98
1	B	389	VAL	CA-C-N	7.05	129.73	120.28
1	B	389	VAL	C-N-CA	7.05	129.73	120.28
1	A	301	SER	CA-C-N	6.85	129.78	120.54
1	A	301	SER	C-N-CA	6.85	129.78	120.54
1	B	389	VAL	N-CA-C	-6.70	103.70	111.00
1	B	433	LYS	CA-C-N	6.62	129.44	120.38
1	B	433	LYS	C-N-CA	6.62	129.44	120.38
1	C	405	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	175	ASP	CA-CB-CG	6.38	118.97	112.60
1	A	352	SER	CA-C-N	6.37	129.14	120.54
1	A	352	SER	C-N-CA	6.37	129.14	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	PHE	CA-CB-CG	6.24	120.04	113.80
1	C	272	THR	N-CA-C	-6.15	105.04	112.54
1	C	305	LEU	CA-C-N	6.06	128.32	120.44
1	C	305	LEU	C-N-CA	6.06	128.32	120.44
1	A	544	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	24	HIS	CA-C-N	6.01	128.34	120.28
1	B	24	HIS	C-N-CA	6.01	128.34	120.28
1	A	636	PRO	CA-C-N	5.99	128.66	120.46
1	A	636	PRO	C-N-CA	5.99	128.66	120.46
1	A	653	MET	CA-C-N	5.94	128.16	120.44
1	A	653	MET	C-N-CA	5.94	128.16	120.44
1	B	276	LYS	CA-C-N	5.90	128.46	120.44
1	B	276	LYS	C-N-CA	5.90	128.46	120.44
1	B	681	ILE	N-CA-CB	5.90	117.05	110.62
1	A	541	LYS	CA-C-N	5.69	128.18	120.44
1	A	541	LYS	C-N-CA	5.69	128.18	120.44
1	B	315	ILE	N-CA-CB	5.67	116.81	110.51
1	B	81	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	18	VAL	N-CA-CB	5.60	117.03	110.82
1	A	373	HIS	CA-C-N	5.57	132.17	121.54
1	A	373	HIS	C-N-CA	5.57	132.17	121.54
1	A	271	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	306	ARG	N-CA-C	-5.54	104.46	111.11
1	A	577	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	153	LYS	CA-C-N	5.49	127.98	120.46
1	C	153	LYS	C-N-CA	5.49	127.98	120.46
1	B	22	SER	N-CA-C	-5.49	106.37	112.57
1	B	349	THR	CB-CA-C	5.47	116.25	110.17
1	B	469	ASP	CA-C-N	5.44	127.88	120.54
1	B	469	ASP	C-N-CA	5.44	127.88	120.54
1	B	443	LEU	CA-C-N	5.43	127.56	120.28
1	B	443	LEU	C-N-CA	5.43	127.56	120.28
1	B	296	THR	CB-CA-C	5.40	118.66	109.75
1	B	175	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	585	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	577	ASP	CA-C-N	5.32	127.41	120.28
1	A	577	ASP	C-N-CA	5.32	127.41	120.28
1	B	504	GLU	CA-C-N	5.32	127.84	120.29
1	B	504	GLU	C-N-CA	5.32	127.84	120.29
1	B	372	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	94	LYS	N-CA-C	-5.27	105.45	111.14
1	A	505	GLU	CA-C-N	5.27	127.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLU	C-N-CA	5.27	127.29	120.44
1	B	21	SER	N-CA-C	5.27	117.39	109.23
1	B	140	GLN	CA-C-N	5.26	131.44	121.97
1	B	140	GLN	C-N-CA	5.26	131.44	121.97
1	B	615	LEU	CA-C-N	5.25	127.32	120.28
1	B	615	LEU	C-N-CA	5.25	127.32	120.28
1	B	300	VAL	CA-C-N	5.23	131.53	121.54
1	B	300	VAL	C-N-CA	5.23	131.53	121.54
1	C	81	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	412	GLU	CA-C-N	5.16	131.39	121.54
1	A	412	GLU	C-N-CA	5.16	131.39	121.54
1	A	337	TYR	CA-C-N	5.16	127.44	120.38
1	A	337	TYR	C-N-CA	5.16	127.44	120.38
1	A	300	VAL	CA-C-N	5.14	131.36	121.54
1	A	300	VAL	C-N-CA	5.14	131.36	121.54
1	C	282	GLN	CA-C-N	5.13	127.41	120.38
1	C	282	GLN	C-N-CA	5.13	127.41	120.38
1	B	101	MET	CA-C-N	5.11	127.13	120.28
1	B	101	MET	C-N-CA	5.11	127.13	120.28
1	C	154	ILE	CA-C-N	5.10	127.07	120.44
1	C	154	ILE	C-N-CA	5.10	127.07	120.44
1	A	94	LYS	CA-C-N	5.10	127.11	120.28
1	A	94	LYS	C-N-CA	5.10	127.11	120.28
1	A	624	ASN	CA-C-N	5.09	126.98	120.56
1	A	624	ASN	C-N-CA	5.09	126.98	120.56
1	B	576	LEU	CA-C-N	5.08	127.09	120.28
1	B	576	LEU	C-N-CA	5.08	127.09	120.28
1	C	177	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	278	ILE	CA-C-N	5.08	126.95	120.56
1	B	278	ILE	C-N-CA	5.08	126.95	120.56
1	A	225	MET	N-CA-C	-5.07	99.50	108.23
1	B	96	VAL	CA-C-N	5.07	127.03	120.44
1	B	96	VAL	C-N-CA	5.07	127.03	120.44
1	A	565	LEU	CA-C-N	5.06	127.48	120.29
1	A	565	LEU	C-N-CA	5.06	127.48	120.29
1	A	592	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	175	ASP	CA-C-N	5.03	130.14	122.25
1	A	175	ASP	C-N-CA	5.03	130.14	122.25
1	C	407	SER	CA-C-N	5.02	131.12	121.54
1	C	407	SER	C-N-CA	5.02	131.12	121.54
1	C	9	ILE	N-CA-C	-5.02	105.81	110.53
1	A	88	TYR	CA-C-N	5.01	129.48	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TYR	C-N-CA	5.01	129.48	122.36
1	C	662	SER	CA-C-N	5.01	126.99	120.28
1	C	662	SER	C-N-CA	5.01	126.99	120.28

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	5014	0	5214	58	0
1	B	5001	0	5198	90	0
1	C	4958	0	5155	67	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
3	A	9	0	0	1	0
3	B	10	0	0	3	0
3	C	6	0	0	3	0
All	All	15082	0	15603	209	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 7.

All (209) 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:B:541:LYS:HA	1:B:542:LEU:CB	1.69	1.22
1:B:541:LYS:HA	1:B:542:LEU:HB3	1.18	1.16
1:B:541:LYS:CA	1:B:542:LEU:CB	2.30	1.06
1:B:542:LEU:HD13	1:B:542:LEU:O	1.55	1.04
1:B:541:LYS:N	1:B:542:LEU:HB2	1.74	1.03
1:B:537:VAL:HG22	1:B:538:GLY:N	1.74	1.02
1:B:541:LYS:H	1:B:542:LEU:HB2	1.23	1.01
1:B:537:VAL:CG2	1:B:538:GLY:H	1.74	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:LYS:CA	1:B:542:LEU:HB2	1.94	0.98
1:B:540:LYS:O	1:B:541:LYS:HD3	1.68	0.94
1:B:541:LYS:O	1:B:541:LYS:HG2	1.65	0.93
1:B:537:VAL:CG2	1:B:538:GLY:N	2.30	0.88
1:A:191:ASP:HB3	1:A:192:PRO:HA	1.57	0.84
1:C:403:LEU:HB3	1:C:585:PHE:HZ	1.43	0.84
1:B:542:LEU:O	1:B:542:LEU:HD22	1.79	0.82
1:B:541:LYS:O	1:B:541:LYS:CG	2.30	0.80
1:B:542:LEU:O	1:B:542:LEU:CD1	2.30	0.80
1:B:540:LYS:O	1:B:541:LYS:CG	2.30	0.79
1:B:540:LYS:O	1:B:541:LYS:CD	2.30	0.79
1:B:542:LEU:O	1:B:543:ALA:CB	2.32	0.77
1:C:174:ALA:HA	1:C:178:LEU:HD21	1.68	0.75
1:B:541:LYS:HA	1:B:542:LEU:HB2	1.58	0.75
1:B:541:LYS:O	1:B:545:VAL:HG23	1.87	0.74
1:B:537:VAL:HG23	1:B:538:GLY:H	1.51	0.73
1:B:542:LEU:HD22	1:B:542:LEU:C	2.14	0.72
1:B:530:TYR:HA	1:C:293:LYS:HE2	1.72	0.70
1:B:613:ASP:HA	1:B:616:THR:HB	1.72	0.70
1:A:440:SER:O	1:A:444:THR:HG22	1.92	0.69
1:A:191:ASP:HB3	1:A:192:PRO:CA	2.22	0.69
1:C:407:SER:HB3	1:C:589:MET:SD	2.34	0.68
1:B:624:ASN:HA	1:B:628:LEU:HB2	1.77	0.66
1:A:484:TYR:H	1:B:76:ASN:HD21	1.44	0.65
1:A:164:ALA:HB1	1:A:165:PRO:HD2	1.77	0.65
1:B:84:SER:HB3	3:B:705:IOD:I	2.66	0.65
1:A:138:TYR:HD1	1:A:139:ILE:H	1.44	0.64
1:C:440:SER:O	1:C:444:THR:HG22	1.98	0.63
1:C:566:LEU:HD13	1:C:566:LEU:H	1.63	0.63
1:B:141:VAL:HA	1:B:155:ARG:HG3	1.80	0.63
1:B:142:GLU:HB3	1:B:154:ILE:HG21	1.80	0.62
1:A:164:ALA:HB1	1:A:165:PRO:CD	2.29	0.62
1:A:271:ASN:HB3	1:C:477:ASN:OD1	1.99	0.62
1:A:461:LEU:HD22	1:A:467:ILE:HG21	1.82	0.62
1:A:452:LEU:HD21	1:A:471:VAL:HG12	1.82	0.61
1:B:542:LEU:O	1:B:542:LEU:CD2	2.47	0.61
1:B:540:LYS:O	1:B:541:LYS:HG2	2.00	0.61
1:C:678:LEU:HA	1:C:681:ILE:HG22	1.82	0.61
1:B:542:LEU:O	1:B:543:ALA:HB2	1.99	0.61
1:C:537:VAL:HG12	1:C:541:LYS:HD2	1.83	0.59
1:B:163:THR:HA	1:B:196:ARG:HH22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:HD11	1:A:476:ILE:HD13	1.85	0.59
1:A:624:ASN:HA	1:A:628:LEU:HB2	1.83	0.58
1:A:589:MET:HE3	1:A:593:LYS:HD3	1.83	0.58
1:C:461:LEU:HD22	1:C:467:ILE:HG21	1.85	0.58
1:B:22:SER:HA	1:B:25:LEU:HD13	1.87	0.56
1:B:155:ARG:HB3	1:B:158:CYS:HB2	1.87	0.56
1:A:311:LYS:O	1:A:315:ILE:HG12	2.05	0.56
1:B:607:PHE:O	1:B:611:VAL:HB	2.04	0.56
1:C:624:ASN:HA	1:C:628:LEU:HB2	1.86	0.56
1:B:457:GLU:HA	1:B:462:LYS:HB3	1.87	0.56
1:C:403:LEU:HB3	1:C:585:PHE:CZ	2.32	0.56
1:B:172:SER:O	1:B:201:ILE:HA	2.06	0.56
1:C:14:ILE:HD11	1:C:677:ALA:HB2	1.88	0.56
1:B:534:LYS:HE3	1:B:540:LYS:HZ1	1.71	0.55
1:B:542:LEU:O	1:B:542:LEU:CG	2.52	0.55
1:C:81:ASP:HB2	1:C:121:THR:HB	1.87	0.55
1:B:452:LEU:HD21	1:B:471:VAL:HG12	1.88	0.55
1:A:174:ALA:C	1:A:176:VAL:H	2.15	0.54
1:B:439:LEU:O	1:B:443:LEU:HB2	2.08	0.54
1:B:534:LYS:HE3	1:B:540:LYS:NZ	2.22	0.54
1:A:31:VAL:HG12	1:A:133:VAL:HB	1.91	0.53
1:B:381:LEU:HD23	1:B:616:THR:HG23	1.90	0.53
1:B:31:VAL:HG12	1:B:133:VAL:HB	1.90	0.53
1:A:193:LYS:HD3	1:A:195:LEU:HD11	1.90	0.53
1:C:537:VAL:HG11	1:C:542:LEU:HD23	1.90	0.53
1:A:444:THR:HG21	1:A:623:LEU:HD22	1.91	0.53
1:C:15:LEU:HD11	1:C:328:ILE:HD11	1.92	0.52
1:B:537:VAL:HG22	1:B:538:GLY:H	1.42	0.52
1:A:663:ARG:HG2	3:A:704:IOD:I	2.80	0.52
1:C:38:SER:HB2	1:C:173:ALA:HB2	1.91	0.52
1:A:138:TYR:OH	1:A:183:ALA:HA	2.10	0.52
1:B:596:SER:HB3	1:B:600:LYS:H	1.75	0.52
1:B:181:SER:OG	1:B:184:LEU:HB2	2.10	0.51
1:B:542:LEU:O	1:B:543:ALA:HB3	2.10	0.51
1:A:32:VAL:HG12	1:A:169:LEU:HB3	1.91	0.51
1:B:412:GLU:H	1:B:416:ASP:HB3	1.75	0.51
1:C:358:ILE:HG21	1:C:643:LEU:HD11	1.93	0.50
1:B:611:VAL:O	1:B:615:LEU:HG	2.11	0.50
1:C:31:VAL:HG12	1:C:133:VAL:HB	1.94	0.50
1:C:53:LEU:HB3	1:C:55:LYS:HD2	1.93	0.50
1:A:158:CYS:O	1:A:162:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD22	1:A:681:ILE:HG23	1.93	0.49
1:C:51:GLU:HB2	1:C:273:ASN:HD21	1.76	0.49
1:A:332:LEU:HA	1:A:335:THR:HG22	1.94	0.49
1:C:434:MET:HE3	1:C:436:ILE:HG13	1.93	0.49
1:C:412:GLU:H	1:C:416:ASP:HB2	1.78	0.49
1:B:61:THR:HG23	3:B:710:IOD:I	2.83	0.49
1:C:434:MET:CE	1:C:436:ILE:HG13	2.42	0.49
1:C:505:GLU:HA	1:C:508:TRP:HB3	1.95	0.49
1:A:575:PHE:CZ	1:B:297:ASN:HB2	2.48	0.49
1:C:5:THR:O	1:C:9:ILE:HG12	2.13	0.49
1:A:515:SER:HB2	1:A:605:GLU:HB3	1.95	0.49
1:B:540:LYS:O	1:B:541:LYS:CB	2.61	0.49
1:A:373:HIS:HD1	1:A:628:LEU:HD23	1.78	0.48
1:C:69:LEU:HB3	1:C:127:VAL:HG13	1.96	0.48
1:A:211:LYS:HE3	1:A:215:ILE:HD11	1.96	0.48
1:B:382:ARG:HG3	1:B:616:THR:HG21	1.94	0.48
1:C:485:SER:O	1:C:489:GLN:HB2	2.13	0.48
1:C:348:LEU:HD21	1:C:661:ILE:HG23	1.94	0.48
1:A:339:PHE:CD2	1:A:345:ASP:HA	2.49	0.48
1:B:494:ILE:HD11	1:B:615:LEU:HB3	1.96	0.48
1:C:155:ARG:H	1:C:155:ARG:HD2	1.79	0.48
1:A:431:LEU:O	1:A:434:MET:HB3	2.13	0.47
1:A:574:ILE:HG22	1:A:578:LYS:HE2	1.97	0.47
1:C:381:LEU:HD23	1:C:616:THR:HG23	1.96	0.47
1:A:174:ALA:HB2	1:A:201:ILE:HG22	1.95	0.47
1:B:164:ALA:HB1	1:B:165:PRO:CD	2.45	0.47
1:A:22:SER:HA	1:A:25:LEU:HD23	1.97	0.47
1:B:30:ILE:HB	1:B:132:LEU:HD23	1.95	0.47
1:A:83:PRO:C	1:A:85:MET:H	2.22	0.47
1:C:162:LEU:HD22	1:C:168:ILE:HD12	1.97	0.47
1:B:228:VAL:HG11	1:B:305:LEU:HB2	1.97	0.47
1:C:571:SER:HA	1:C:574:ILE:HD12	1.97	0.47
1:A:32:VAL:HG23	1:A:40:LYS:HE2	1.97	0.47
1:C:622:PHE:HD1	1:C:622:PHE:N	2.13	0.47
1:A:394:ALA:HA	1:A:398:TRP:HB2	1.97	0.47
1:A:432:THR:HG22	1:A:615:LEU:HD11	1.96	0.47
1:A:571:SER:HA	1:A:574:ILE:HD12	1.97	0.46
1:B:642:ARG:HA	1:B:645:LEU:HD12	1.97	0.46
1:B:682:ASP:O	1:B:686:VAL:HG23	2.16	0.46
1:C:168:ILE:HG23	1:C:197:THR:HG23	1.97	0.46
1:C:622:PHE:N	1:C:622:PHE:CD1	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:VAL:HA	1:A:585:PHE:CE2	2.50	0.46
1:C:27:LEU:HD12	1:C:317:MET:HE2	1.97	0.46
1:C:444:THR:HG21	1:C:623:LEU:HD22	1.98	0.46
1:B:34:GLY:HA2	1:B:183:ALA:HB2	1.96	0.46
1:B:541:LYS:N	1:B:542:LEU:CB	2.56	0.46
1:C:353:TYR:HA	3:C:706:IOD:I	2.86	0.46
1:B:68:THR:HB	1:B:121:THR:HG22	1.98	0.45
1:A:15:LEU:HD11	1:A:328:ILE:HD11	1.99	0.45
1:C:512:ARG:O	1:C:516:ILE:HG12	2.16	0.45
1:A:177:ASP:HB3	1:A:180:ASN:HD22	1.80	0.45
1:C:478:VAL:HG21	1:C:635:PHE:HA	1.98	0.45
1:B:332:LEU:HD13	1:B:674:LEU:HB3	1.99	0.45
1:C:31:VAL:HG11	1:C:161:TYR:HB3	1.98	0.45
1:C:587:LEU:HG	1:C:591:LYS:HE2	1.97	0.45
1:A:466:LEU:HD13	1:A:653:MET:HE3	1.99	0.45
1:B:212:ALA:HA	1:B:215:ILE:HD12	1.98	0.45
1:C:67:LEU:HD23	1:C:132:LEU:HD13	1.98	0.45
1:B:220:LYS:HG3	3:B:711:IOD:I	2.87	0.44
1:B:518:LEU:HD23	1:B:519:ILE:HG13	1.99	0.44
1:B:519:ILE:O	1:B:523:LEU:HB2	2.17	0.44
1:C:43:VAL:HG21	1:C:171:ILE:HG12	1.99	0.44
1:A:531:GLN:HA	1:A:534:LYS:HB2	1.99	0.44
1:C:542:LEU:HD11	1:C:570:GLY:HA2	1.99	0.44
1:A:456:LEU:HD22	1:A:468:LYS:HG2	2.00	0.44
1:C:403:LEU:HD22	1:C:586:ARG:HD3	1.99	0.44
1:A:354:LEU:HG	1:A:651:VAL:HG13	1.98	0.44
1:B:193:LYS:HE3	1:B:195:LEU:HD21	1.99	0.44
1:A:437:GLY:HA3	1:A:491:GLU:HG2	2.00	0.44
1:C:22:SER:HA	1:C:25:LEU:HD12	2.00	0.44
1:C:50:ARG:HG3	1:C:273:ASN:HB3	1.99	0.44
1:A:541:LYS:O	1:A:545:VAL:HG23	2.18	0.44
1:B:171:ILE:HG13	1:B:200:VAL:HG13	2.00	0.44
1:A:158:CYS:HA	1:A:162:LEU:HD23	2.00	0.43
1:A:659:PRO:O	1:A:663:ARG:HB2	2.18	0.43
1:C:299:GLN:HE21	1:C:308:LYS:HD2	1.83	0.43
1:B:10:GLU:O	1:B:14:ILE:HG12	2.17	0.43
1:B:84:SER:HB2	1:B:119:GLN:HB2	1.99	0.43
1:A:50:ARG:HH12	1:A:270:GLU:CD	2.26	0.43
1:B:156:ASP:HA	1:B:159:GLU:HG2	2.01	0.43
1:C:291:ASN:HB2	1:C:294:TYR:HB2	2.01	0.43
1:C:512:ARG:HD2	1:C:594:CYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HH22	1:A:157:LEU:HD11	1.84	0.42
1:B:88:TYR:O	1:B:90:ILE:HG13	2.20	0.42
1:B:63:ARG:HH21	1:B:103:LEU:HD12	1.84	0.42
1:C:2:LEU:HD13	1:C:687:PHE:HZ	1.85	0.42
1:C:11:ILE:HG21	1:C:681:ILE:HD12	2.01	0.42
1:A:213:ARG:HH21	1:A:296:THR:HG23	1.85	0.42
1:B:83:PRO:C	1:B:85:MET:H	2.28	0.42
1:B:198:ILE:HD11	1:B:312:ILE:HG21	2.01	0.42
1:A:642:ARG:HH22	1:B:269:GLU:CD	2.28	0.41
1:B:31:VAL:HG11	1:B:161:TYR:HB3	2.02	0.41
1:A:215:ILE:O	1:A:218:ASN:HB2	2.20	0.41
1:C:396:ARG:HD3	3:C:702:IOD:I	2.90	0.41
1:B:346:ARG:HH12	1:B:348:LEU:HD12	1.84	0.41
1:C:594:CYS:HA	1:C:600:LYS:HG2	2.02	0.41
1:B:431:LEU:HD21	1:B:612:SER:HB3	2.02	0.41
1:B:63:ARG:HB3	1:B:115:GLU:HG3	2.02	0.41
1:C:378:LYS:HA	1:C:620:VAL:HG11	2.02	0.41
1:A:39:GLY:HA3	1:A:202:THR:HG21	2.03	0.41
1:B:445:THR:HG23	1:B:479:LEU:HD13	2.02	0.41
1:B:456:LEU:HD22	1:B:468:LYS:HG2	2.03	0.41
1:C:434:MET:HE2	1:C:434:MET:HB3	1.96	0.41
1:A:297:ASN:HB2	1:C:575:PHE:CE2	2.56	0.41
1:A:494:ILE:HB	1:A:615:LEU:HD23	2.03	0.41
1:B:419:TYR:HA	1:B:422:LYS:HE2	2.03	0.41
1:C:164:ALA:HB1	1:C:165:PRO:HD2	2.03	0.41
1:C:374:ARG:HG3	1:C:375:ASN:H	1.85	0.41
1:C:537:VAL:HB	1:C:542:LEU:HB2	2.03	0.41
1:C:537:VAL:HG13	3:C:707:IOD:I	2.91	0.41
1:B:564:LYS:HD2	1:B:565:LEU:HG	2.03	0.41
1:C:197:THR:H	1:C:225:MET:HG3	1.85	0.41
1:A:533:ILE:HG21	1:A:573:ALA:HB2	2.03	0.40
1:C:566:LEU:H	1:C:566:LEU:CD1	2.30	0.40
1:B:530:TYR:CE1	1:B:576:LEU:HD13	2.57	0.40
1:C:99:MET:O	1:C:103:LEU:HB2	2.22	0.40
1:B:540:LYS:HB3	1:B:541:LYS:H	1.59	0.40
1:B:32:VAL:HG12	1:B:169:LEU:HB3	2.03	0.40
1:C:80:ALA:HB3	1:C:90:ILE:HB	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	613/698 (88%)	561 (92%)	37 (6%)	15 (2%)	4	28
1	B	612/698 (88%)	554 (90%)	46 (8%)	12 (2%)	6	31
1	C	607/698 (87%)	556 (92%)	44 (7%)	7 (1%)	10	42
All	All	1832/2094 (88%)	1671 (91%)	127 (7%)	34 (2%)	6	33

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	PRO
1	A	191	ASP
1	A	226	GLY
1	A	374	ARG
1	A	597	THR
1	B	89	ASN
1	B	141	VAL
1	B	374	ARG
1	B	542	LEU
1	C	196	ARG
1	C	597	THR
1	A	137	GLY
1	A	164	ALA
1	A	373	HIS
1	A	500	GLU
1	B	19	ASP
1	B	301	SER
1	B	543	ALA
1	C	408	SER
1	A	413	SER
1	A	601	ASP
1	B	164	ALA
1	B	500	GLU
1	A	52	PHE

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Mol	Chain	Res	Type
1	B	483	TYR
1	B	520	LYS
1	C	195	LEU
1	C	503	LEU
1	A	20	SER
1	C	88	TYR
1	A	63	ARG
1	B	218	ASN
1	C	39	GLY
1	A	435	GLY

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	579/638 (91%)	515 (89%)	64 (11%)	6	25
1	B	577/638 (90%)	505 (88%)	72 (12%)	4	21
1	C	572/638 (90%)	512 (90%)	60 (10%)	6	28
All	All	1728/1914 (90%)	1532 (89%)	196 (11%)	5	24

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

Mol	Chain	Res	Type
1	A	5	THR
1	A	9	ILE
1	A	16	ASN
1	A	25	LEU
1	A	26	THR
1	A	33	ILE
1	A	41	SER
1	A	59	MET
1	A	60	VAL
1	A	66	GLU
1	A	116	GLU
1	A	121	THR

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Mol	Chain	Res	Type
1	A	126	ARG
1	A	127	VAL
1	A	135	LEU
1	A	138	TYR
1	A	163	THR
1	A	171	ILE
1	A	191	ASP
1	A	201	ILE
1	A	204	LEU
1	A	207	VAL
1	A	210	GLU
1	A	214	SER
1	A	233	LYS
1	A	234	THR
1	A	277	GLN
1	A	285	LYS
1	A	304	LYS
1	A	327	LEU
1	A	330	GLN
1	A	338	LEU
1	A	345	ASP
1	A	354	LEU
1	A	366	LYS
1	A	369	GLN
1	A	403	LEU
1	A	414	ASP
1	A	416	ASP
1	A	418	LEU
1	A	424	LEU
1	A	434	MET
1	A	436	ILE
1	A	439	LEU
1	A	485	SER
1	A	495	LYS
1	A	499	TYR
1	A	500	GLU
1	A	503	LEU
1	A	504	GLU
1	A	513	GLN
1	A	540	LYS
1	A	542	LEU
1	A	549	LEU

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Mol	Chain	Res	Type
1	A	565	LEU
1	A	568	GLU
1	A	579	ARG
1	A	611	VAL
1	A	624	ASN
1	A	638	GLU
1	A	645	LEU
1	A	663	ARG
1	A	666	GLU
1	A	670	ARG
1	B	12	ARG
1	B	13	THR
1	B	16	ASN
1	B	25	LEU
1	B	33	ILE
1	B	40	LYS
1	B	50	ARG
1	B	62	ARG
1	B	100	LEU
1	B	101	MET
1	B	130	LEU
1	B	139	ILE
1	B	141	VAL
1	B	157	LEU
1	B	178	LEU
1	B	184	LEU
1	B	188	LYS
1	B	204	LEU
1	B	207	VAL
1	B	214	SER
1	B	285	LYS
1	B	293	LYS
1	B	315	ILE
1	B	327	LEU
1	B	328	ILE
1	B	331	GLU
1	B	340	LYS
1	B	361	LEU
1	B	363	LEU
1	B	366	LYS
1	B	385	LEU
1	B	390	LEU

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Mol	Chain	Res	Type
1	B	392	VAL
1	B	393	LEU
1	B	398	TRP
1	B	403	LEU
1	B	406	LEU
1	B	411	LEU
1	B	414	ASP
1	B	415	THR
1	B	423	LYS
1	B	424	LEU
1	B	426	LEU
1	B	434	MET
1	B	463	ASN
1	B	469	ASP
1	B	494	ILE
1	B	501	ILE
1	B	504	GLU
1	B	510	LEU
1	B	512	ARG
1	B	518	LEU
1	B	526	CYS
1	B	533	ILE
1	B	541	LYS
1	B	542	LEU
1	B	567	LEU
1	B	569	ARG
1	B	574	ILE
1	B	575	PHE
1	B	581	LYS
1	B	583	LEU
1	B	601	ASP
1	B	611	VAL
1	B	616	THR
1	B	623	LEU
1	B	645	LEU
1	B	649	GLU
1	B	652	GLU
1	B	653	MET
1	B	674	LEU
1	B	681	ILE
1	C	14	ILE
1	C	27	LEU

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Mol	Chain	Res	Type
1	C	40	LYS
1	C	50	ARG
1	C	53	LEU
1	C	55	LYS
1	C	84	SER
1	C	87	LEU
1	C	105	MET
1	C	115	GLU
1	C	130	LEU
1	C	167	ILE
1	C	169	LEU
1	C	171	ILE
1	C	175	ASP
1	C	206	LEU
1	C	216	LEU
1	C	231	ILE
1	C	273	ASN
1	C	278	ILE
1	C	283	PHE
1	C	304	LYS
1	C	305	LEU
1	C	321	LEU
1	C	335	THR
1	C	338	LEU
1	C	345	ASP
1	C	354	LEU
1	C	365	ILE
1	C	366	LYS
1	C	375	ASN
1	C	380	ILE
1	C	401	ASP
1	C	405	ASP
1	C	406	LEU
1	C	411	LEU
1	C	418	LEU
1	C	424	LEU
1	C	426	LEU
1	C	438	ARG
1	C	443	LEU
1	C	444	THR
1	C	448	ILE
1	C	482	LYS

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Mol	Chain	Res	Type
1	C	494	ILE
1	C	502	ASP
1	C	503	LEU
1	C	507	ASP
1	C	523	LEU
1	C	541	LYS
1	C	542	LEU
1	C	550	GLU
1	C	566	LEU
1	C	593	LYS
1	C	597	THR
1	C	600	LYS
1	C	602	ARG
1	C	618	THR
1	C	622	PHE
1	C	681	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	89	ASN
1	A	180	ASN
1	A	277	GLN
1	A	330	GLN
1	A	369	GLN
1	A	387	GLN
1	A	473	ASN
1	A	489	GLN
1	A	527	ASN
1	A	531	GLN
1	B	3	ASN
1	B	76	ASN
1	B	104	ASN
1	B	273	ASN
1	B	282	GLN
1	B	297	ASN
1	B	329	GLN
1	B	517	ASN
1	B	551	ASN
1	C	217	ASN
1	C	273	ASN

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Mol	Chain	Res	Type
1	C	277	GLN
1	C	291	ASN
1	C	297	ASN
1	C	299	GLN
1	C	329	GLN
1	C	446	ASN
1	C	463	ASN
1	C	480	ASN
1	C	535	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 25 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GDP	C	701	-	29,30,30	1.92	4 (13%)	45,47,47	1.86	10 (22%)
2	GDP	B	701	-	29,30,30	1.82	5 (17%)	45,47,47	1.74	10 (22%)
2	GDP	A	701	-	29,30,30	1.95	5 (17%)	45,47,47	1.76	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	C	701	-	-	7/16/32/32	0/3/3/3
2	GDP	B	701	-	-	5/16/32/32	0/3/3/3
2	GDP	A	701	-	-	7/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	GDP	O6-C6	6.87	1.36	1.23
2	A	701	GDP	O6-C6	6.77	1.36	1.23
2	B	701	GDP	O6-C6	6.77	1.36	1.23
2	A	701	GDP	PA-O3A	4.95	1.64	1.59
2	C	701	GDP	PA-O3A	4.08	1.63	1.59
2	C	701	GDP	C5-N7	-2.84	1.33	1.39
2	A	701	GDP	C5-C6	-2.82	1.34	1.44
2	C	701	GDP	C5-C6	-2.79	1.34	1.44
2	B	701	GDP	C5-C6	-2.78	1.34	1.44
2	B	701	GDP	C5-N7	-2.72	1.33	1.39
2	A	701	GDP	C5-N7	-2.62	1.33	1.39
2	B	701	GDP	PA-O3A	2.46	1.62	1.59
2	B	701	GDP	C6-N1	-2.16	1.34	1.38
2	A	701	GDP	C6-N1	-2.04	1.35	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	GDP	C5-C4-N3	-5.57	119.53	128.39
2	B	701	GDP	C5-C4-N3	-5.10	120.27	128.39
2	A	701	GDP	C5-C4-N3	-5.08	120.30	128.39
2	C	701	GDP	C2-N3-C4	4.72	120.43	112.30
2	B	701	GDP	C2-N3-C4	4.61	120.24	112.30
2	A	701	GDP	C2-N3-C4	4.59	120.21	112.30
2	C	701	GDP	O6-C6-C5	-3.82	116.45	126.53
2	A	701	GDP	O6-C6-C5	-3.57	117.10	126.53
2	B	701	GDP	O6-C6-C5	-3.55	117.17	126.53
2	C	701	GDP	N9-C4-N3	3.52	133.00	125.95
2	C	701	GDP	C2-N1-C6	-3.18	119.34	125.11
2	B	701	GDP	N9-C4-N3	3.17	132.29	125.95
2	A	701	GDP	N9-C4-N3	3.10	132.16	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	GDP	C5-C6-N1	3.10	121.13	113.25
2	B	701	GDP	C5-C6-N1	3.00	120.88	113.25
2	A	701	GDP	C5-C6-N1	2.93	120.72	113.25
2	B	701	GDP	N9-C8-N7	-2.87	108.07	113.40
2	A	701	GDP	N9-C8-N7	-2.78	108.24	113.40
2	C	701	GDP	N9-C8-N7	-2.76	108.28	113.40
2	A	701	GDP	C2-N1-C6	-2.71	120.19	125.11
2	B	701	GDP	C2-N1-C6	-2.70	120.21	125.11
2	B	701	GDP	N1-C2-N3	-2.35	119.02	123.32
2	A	701	GDP	N1-C2-N3	-2.27	119.17	123.32
2	C	701	GDP	C8-N7-C5	2.15	108.09	104.26
2	B	701	GDP	C8-N7-C5	2.06	107.93	104.26
2	B	701	GDP	O3B-PB-O2B	2.04	115.45	107.80
2	A	701	GDP	C8-N7-C5	2.03	107.89	104.26
2	C	701	GDP	N1-C2-N3	-2.03	119.60	123.32
2	C	701	GDP	O3B-PB-O2B	2.01	115.35	107.80

There are no chirality outliers.

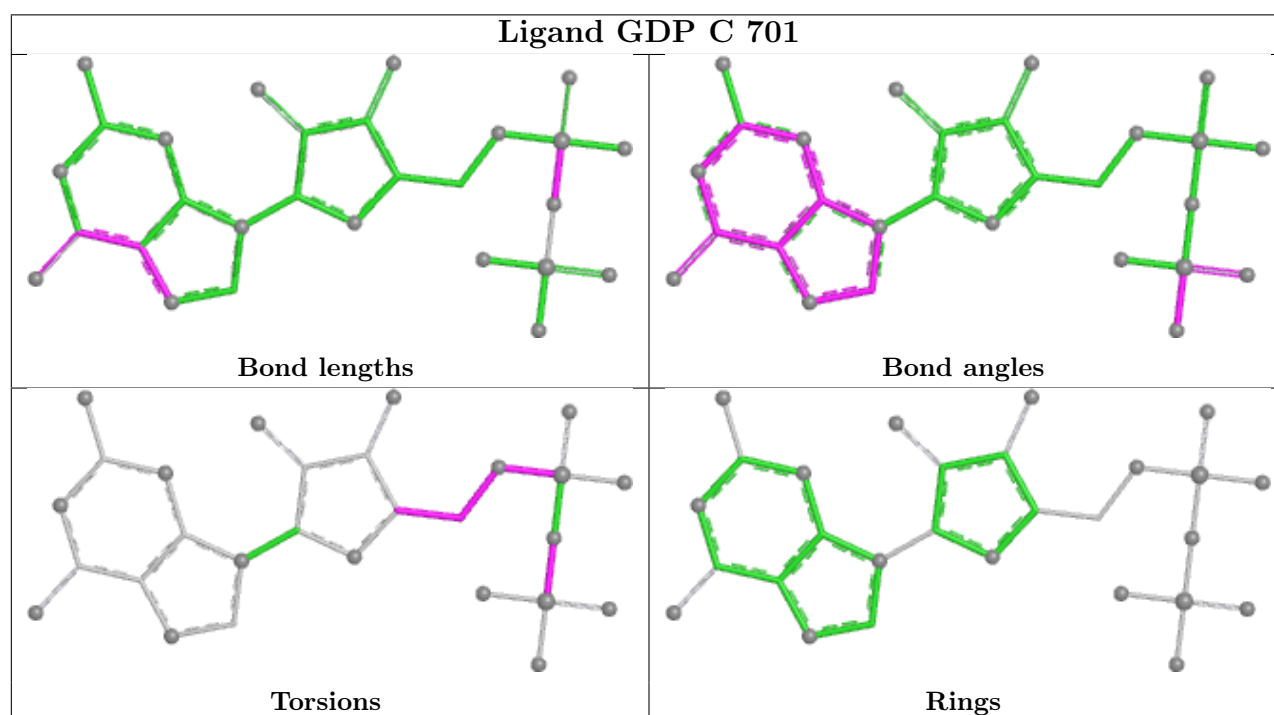
All (19) torsion outliers are listed below:

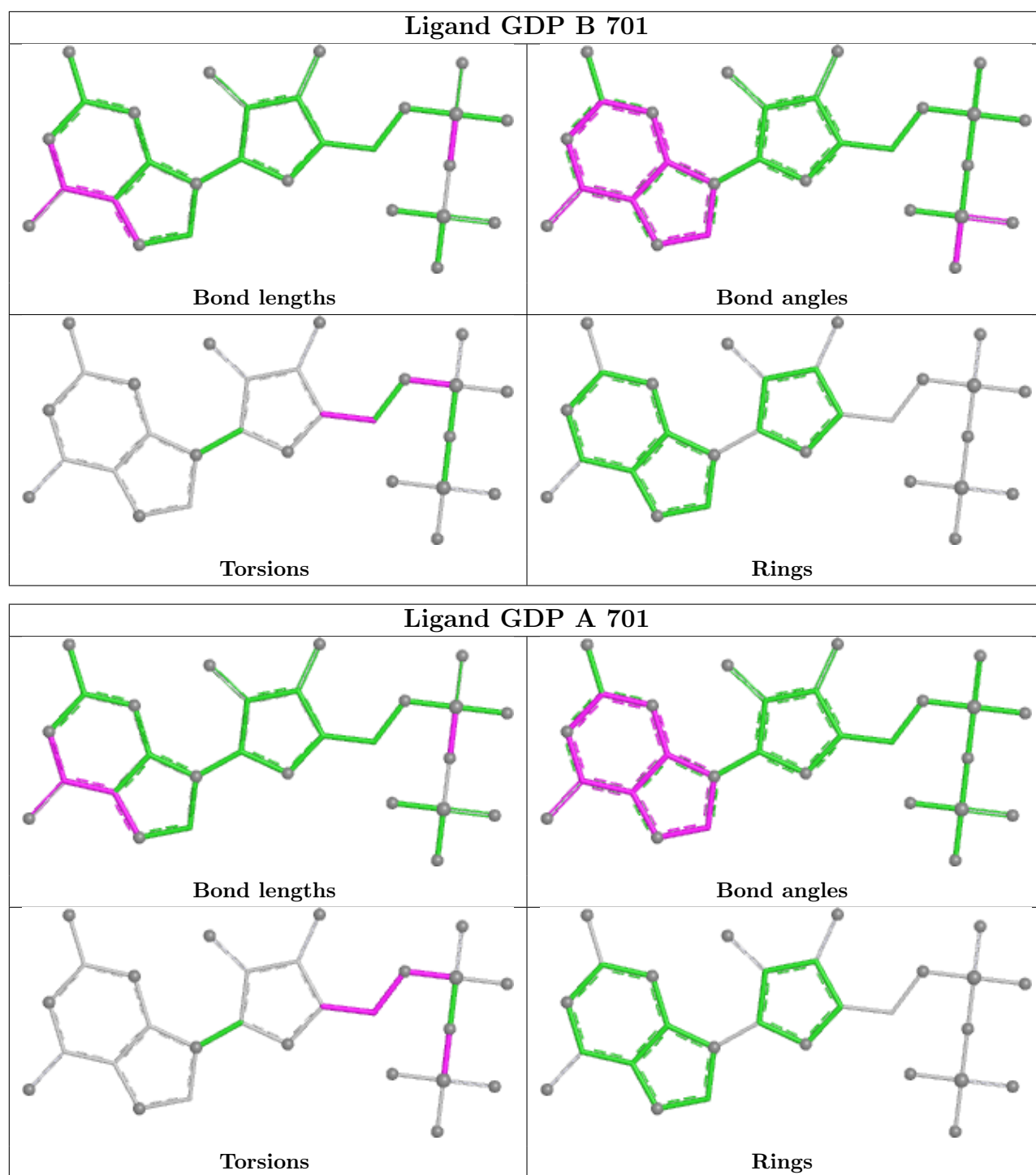
Mol	Chain	Res	Type	Atoms
2	A	701	GDP	PA-O3A-PB-O2B
2	A	701	GDP	C5'-O5'-PA-O3A
2	B	701	GDP	C5'-O5'-PA-O3A
2	B	701	GDP	C5'-O5'-PA-O1A
2	C	701	GDP	PA-O3A-PB-O3B
2	C	701	GDP	C5'-O5'-PA-O3A
2	C	701	GDP	C5'-O5'-PA-O2A
2	C	701	GDP	O4'-C4'-C5'-O5'
2	A	701	GDP	O4'-C4'-C5'-O5'
2	B	701	GDP	O4'-C4'-C5'-O5'
2	C	701	GDP	C3'-C4'-C5'-O5'
2	A	701	GDP	C3'-C4'-C5'-O5'
2	B	701	GDP	C3'-C4'-C5'-O5'
2	A	701	GDP	C5'-O5'-PA-O1A
2	B	701	GDP	C5'-O5'-PA-O2A
2	C	701	GDP	PA-O3A-PB-O1B
2	A	701	GDP	C4'-C5'-O5'-PA
2	C	701	GDP	C4'-C5'-O5'-PA
2	A	701	GDP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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	625/698 (89%)	-0.03	3 (0%) 87 76	79, 118, 163, 200	0
1	B	624/698 (89%)	0.21	32 (5%) 33 21	24, 130, 196, 224	0
1	C	619/698 (88%)	0.15	24 (3%) 43 27	85, 144, 188, 217	0
All	All	1868/2094 (89%)	0.11	59 (3%) 50 31	24, 130, 188, 224	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	538	GLY	6.7
1	B	539	SER	5.3
1	C	398	TRP	4.4
1	B	397	TYR	4.0
1	B	540	LYS	3.8
1	C	44	LEU	3.7
1	B	611	VAL	3.7
1	B	566	LEU	3.4
1	B	541	LYS	3.4
1	C	216	LEU	3.3
1	C	169	LEU	3.2
1	B	127	VAL	3.2
1	B	523	LEU	3.1
1	B	605	GLU	3.1
1	C	227	TYR	3.1
1	A	431	LEU	3.0
1	B	591	LYS	2.9
1	C	200	VAL	2.9
1	B	615	LEU	2.9
1	C	47	ILE	2.8
1	C	673	LEU	2.8
1	B	132	LEU	2.8
1	B	582	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	516	ILE	2.8
1	B	587	LEU	2.7
1	B	604	PRO	2.7
1	B	534	LYS	2.7
1	B	606	VAL	2.6
1	B	495	LYS	2.6
1	C	295	PHE	2.6
1	B	427	ALA	2.6
1	B	428	SER	2.5
1	C	299	GLN	2.5
1	C	411	LEU	2.5
1	C	674	LEU	2.5
1	B	390	LEU	2.4
1	C	230	VAL	2.4
1	C	664	HIS	2.4
1	B	398	TRP	2.4
1	B	588	LYS	2.3
1	C	201	ILE	2.3
1	C	215	ILE	2.3
1	B	30	ILE	2.3
1	C	297	ASN	2.2
1	C	229	GLY	2.2
1	C	130	LEU	2.2
1	C	401	ASP	2.2
1	B	542	LEU	2.2
1	C	599	GLU	2.2
1	C	309	LEU	2.2
1	C	212	ALA	2.2
1	B	55	LYS	2.1
1	B	25	LEU	2.1
1	B	590	LEU	2.1
1	A	536	ALA	2.1
1	B	593	LYS	2.0
1	A	25	LEU	2.0
1	B	583	LEU	2.0
1	C	501	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

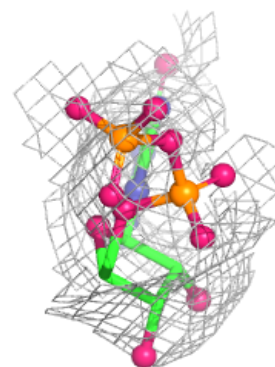
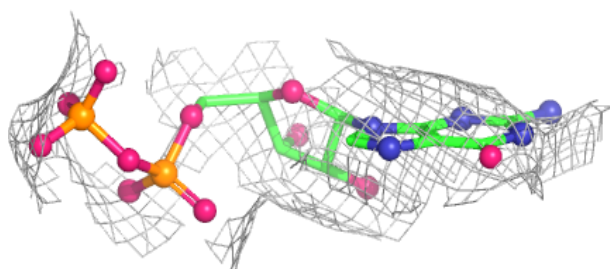
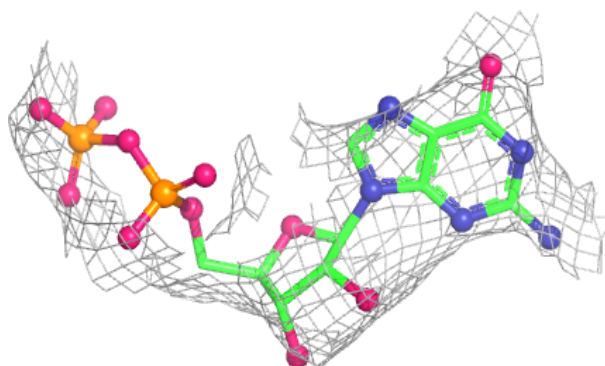
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IOD	B	709	1/1	0.66	0.11	300,300,300,300	0
3	IOD	B	708	1/1	0.70	0.15	275,275,275,275	0
2	GDP	C	701	28/28	0.74	0.07	223,226,228,229	0
3	IOD	B	706	1/1	0.74	0.11	300,300,300,300	0
3	IOD	A	704	1/1	0.81	0.22	255,255,255,255	0
3	IOD	B	710	1/1	0.81	0.09	291,291,291,291	0
3	IOD	B	711	1/1	0.83	0.07	294,294,294,294	0
3	IOD	C	706	1/1	0.84	0.13	240,240,240,240	0
3	IOD	C	707	1/1	0.84	0.10	229,229,229,229	0
3	IOD	B	702	1/1	0.85	0.09	222,222,222,222	0
3	IOD	A	707	1/1	0.85	0.14	262,262,262,262	0
3	IOD	B	704	1/1	0.86	0.23	250,250,250,250	0
3	IOD	C	704	1/1	0.86	0.19	242,242,242,242	0
3	IOD	B	703	1/1	0.86	0.07	241,241,241,241	0
3	IOD	B	707	1/1	0.86	0.08	285,285,285,285	0
2	GDP	A	701	28/28	0.88	0.07	122,133,148,149	0
3	IOD	A	708	1/1	0.88	0.10	231,231,231,231	0
3	IOD	A	706	1/1	0.89	0.09	216,216,216,216	0
3	IOD	C	703	1/1	0.90	0.12	219,219,219,219	0
3	IOD	A	703	1/1	0.90	0.09	216,216,216,216	0
3	IOD	A	709	1/1	0.93	0.11	189,189,189,189	0
2	GDP	B	701	28/28	0.93	0.07	125,131,140,141	0
3	IOD	A	710	1/1	0.94	0.06	194,194,194,194	0
3	IOD	C	705	1/1	0.94	0.09	215,215,215,215	0
3	IOD	B	705	1/1	0.95	0.06	165,165,165,165	0
3	IOD	A	705	1/1	0.96	0.07	173,173,173,173	0
3	IOD	A	702	1/1	0.97	0.04	135,135,135,135	0
3	IOD	C	702	1/1	0.98	0.04	139,139,139,139	0

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

orientation to approximate a three-dimensional view.

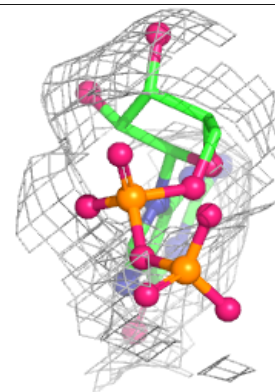
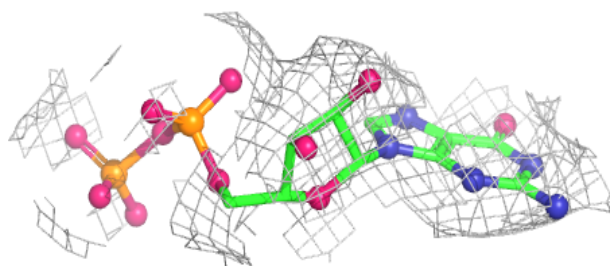
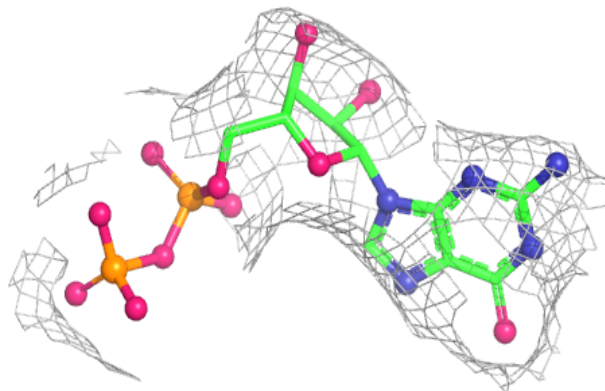
Electron density around GDP C 701:

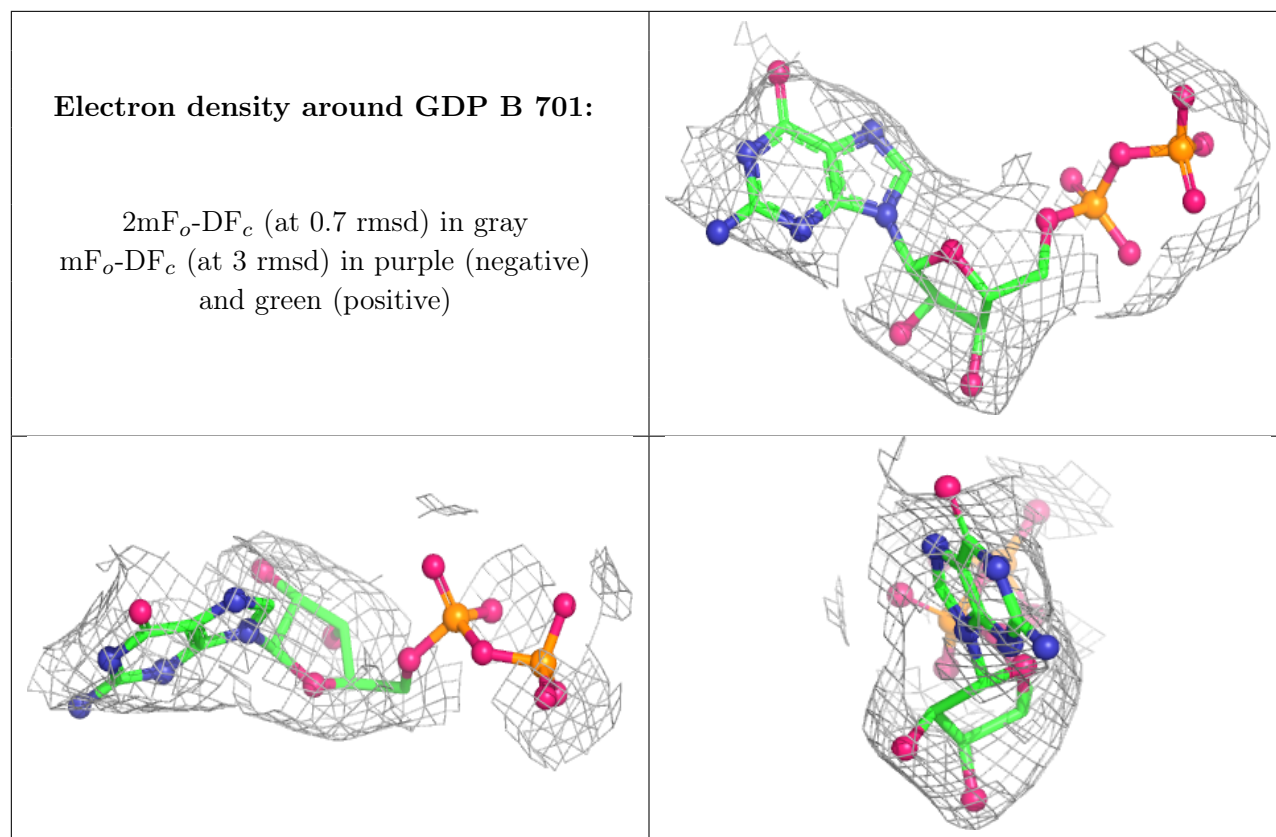
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP A 701:

$2mF_o-DF_c$ (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.