



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2022 – 12:20 PM JST

PDB ID : 6IEG
Title : Crystal structure of human MTR4
Authors : Chen, J.Y.; Yun, C.H.
Deposited on : 2018-09-14
Resolution : 3.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

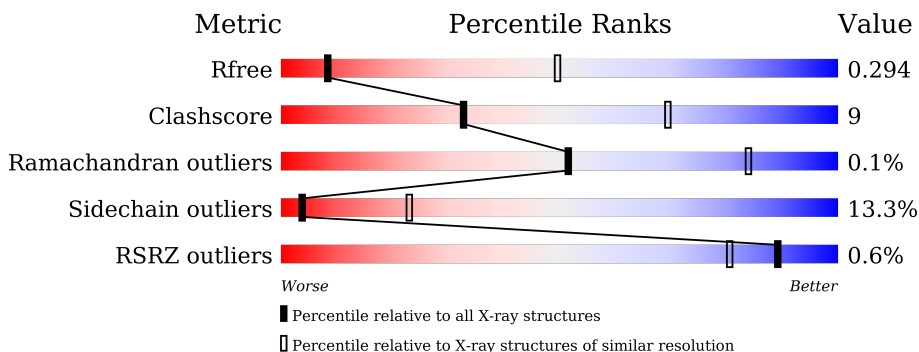
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.55 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}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	1002	
1	B	1002	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12978 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 Exosome RNA helicase MTR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	911	Total	C	N	O	S	0	0	0
			6617	4228	1110	1233	46			
1	A	872	Total	C	N	O	S	0	0	0
			6305	4028	1066	1169	42			

There are 60 discrepancies between the modelled and reference sequences:

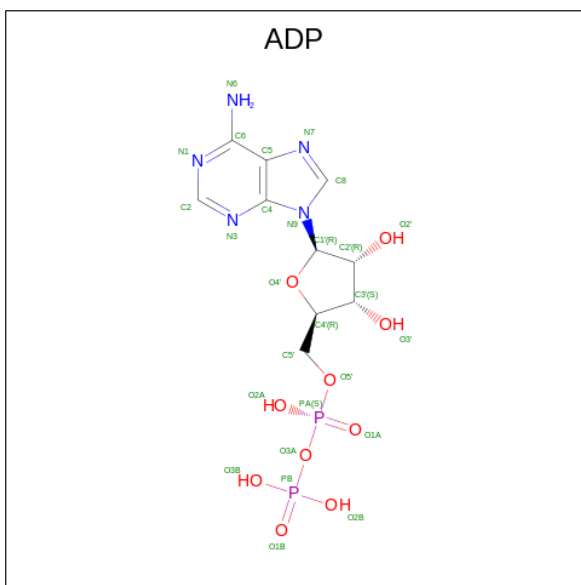
Chain	Residue	Modelled	Actual	Comment	Reference
B	41	MET	-	initiating methionine	UNP P42285
B	42	SER	-	expression tag	UNP P42285
B	43	TYR	-	expression tag	UNP P42285
B	44	TYR	-	expression tag	UNP P42285
B	45	HIS	-	expression tag	UNP P42285
B	46	HIS	-	expression tag	UNP P42285
B	47	HIS	-	expression tag	UNP P42285
B	48	HIS	-	expression tag	UNP P42285
B	49	HIS	-	expression tag	UNP P42285
B	50	HIS	-	expression tag	UNP P42285
B	51	ASP	-	expression tag	UNP P42285
B	52	TYR	-	expression tag	UNP P42285
B	53	ASP	-	expression tag	UNP P42285
B	54	ILE	-	expression tag	UNP P42285
B	55	PRO	-	expression tag	UNP P42285
B	56	THR	-	expression tag	UNP P42285
B	57	THR	-	expression tag	UNP P42285
B	58	GLU	-	expression tag	UNP P42285
B	59	ASN	-	expression tag	UNP P42285
B	60	LEU	-	expression tag	UNP P42285
B	61	TYR	-	expression tag	UNP P42285
B	62	PHE	-	expression tag	UNP P42285
B	63	GLN	-	expression tag	UNP P42285
B	64	GLY	-	expression tag	UNP P42285
B	65	ALA	-	expression tag	UNP P42285

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Chain	Residue	Modelled	Actual	Comment	Reference
B	66	MET	-	expression tag	UNP P42285
B	67	ASP	-	expression tag	UNP P42285
B	68	PRO	-	expression tag	UNP P42285
B	69	GLU	-	expression tag	UNP P42285
B	70	PHE	-	expression tag	UNP P42285
A	41	MET	-	initiating methionine	UNP P42285
A	42	SER	-	expression tag	UNP P42285
A	43	TYR	-	expression tag	UNP P42285
A	44	TYR	-	expression tag	UNP P42285
A	45	HIS	-	expression tag	UNP P42285
A	46	HIS	-	expression tag	UNP P42285
A	47	HIS	-	expression tag	UNP P42285
A	48	HIS	-	expression tag	UNP P42285
A	49	HIS	-	expression tag	UNP P42285
A	50	HIS	-	expression tag	UNP P42285
A	51	ASP	-	expression tag	UNP P42285
A	52	TYR	-	expression tag	UNP P42285
A	53	ASP	-	expression tag	UNP P42285
A	54	ILE	-	expression tag	UNP P42285
A	55	PRO	-	expression tag	UNP P42285
A	56	THR	-	expression tag	UNP P42285
A	57	THR	-	expression tag	UNP P42285
A	58	GLU	-	expression tag	UNP P42285
A	59	ASN	-	expression tag	UNP P42285
A	60	LEU	-	expression tag	UNP P42285
A	61	TYR	-	expression tag	UNP P42285
A	62	PHE	-	expression tag	UNP P42285
A	63	GLN	-	expression tag	UNP P42285
A	64	GLY	-	expression tag	UNP P42285
A	65	ALA	-	expression tag	UNP P42285
A	66	MET	-	expression tag	UNP P42285
A	67	ASP	-	expression tag	UNP P42285
A	68	PRO	-	expression tag	UNP P42285
A	69	GLU	-	expression tag	UNP P42285
A	70	PHE	-	expression tag	UNP P42285

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

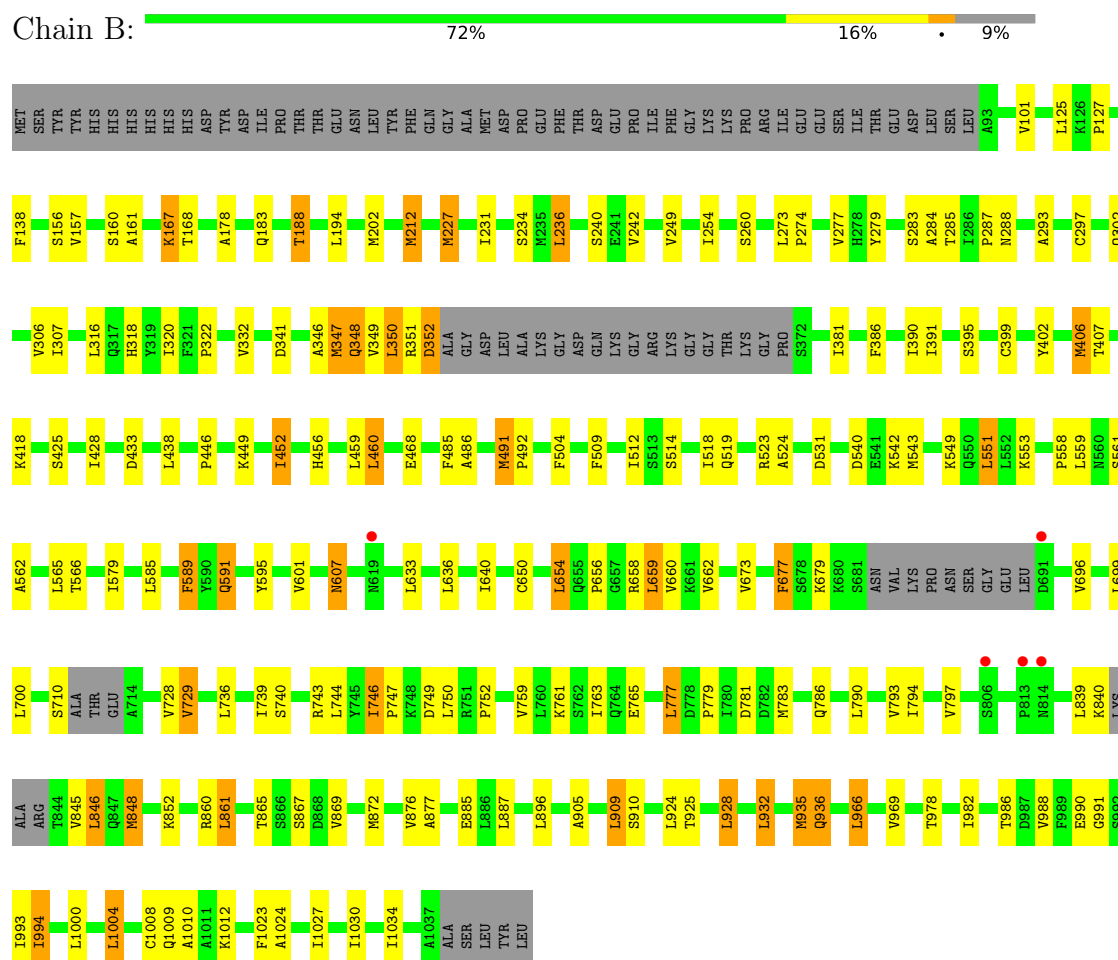
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

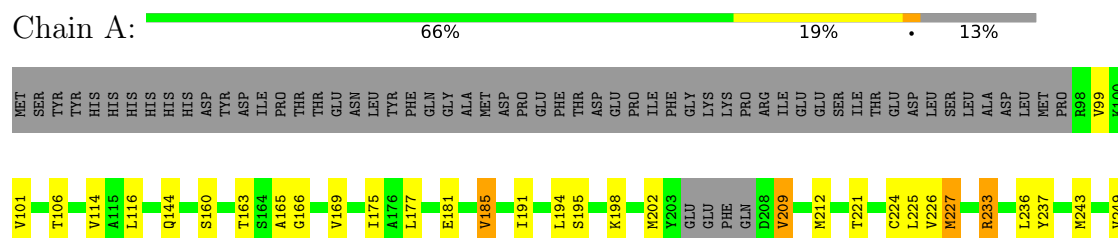
3 Residue-property plots

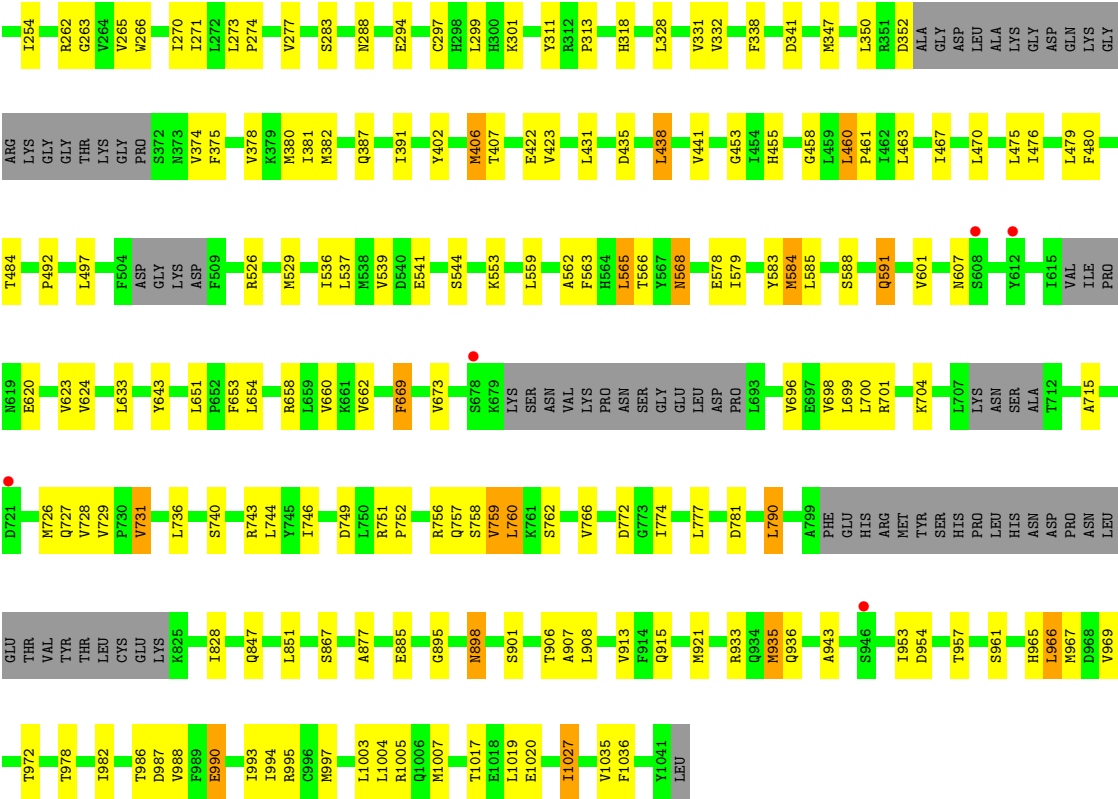
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Exosome RNA helicase MTR4



• Molecule 1: Exosome RNA helicase MTR4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.32Å 119.14Å 124.57Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	46.95 – 3.55 46.95 – 3.55	Depositor EDS
% Data completeness (in resolution range)	88.9 (46.95-3.55) 88.9 (46.95-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.268 , 0.305 0.278 , 0.294	Depositor DCC
R_{free} test set	1358 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 26.7	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	0.78	EDS
Total number of atoms	12978	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: ADP, 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	0.62	0/6417	0.84	0/8746
1	B	0.64	0/6738	0.85	0/9187
All	All	0.63	0/13155	0.85	0/17933

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

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	6305	0	5826	105	0
1	B	6617	0	6151	113	0
2	A	27	0	12	2	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	12978	0	12001	218	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 (218) 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:348:GLN:HE21	1:B:348:GLN:CA	1.54	1.15
1:B:348:GLN:HA	1:B:348:GLN:NE2	1.49	1.13
1:B:351:ARG:O	1:B:352:ASP:HB2	1.47	1.08
1:B:654:LEU:HD12	1:B:696:VAL:HG21	1.47	0.95
1:B:350:LEU:O	1:B:350:LEU:HD22	1.70	0.91
1:B:348:GLN:HE21	1:B:348:GLN:HA	0.74	0.88
1:B:969:VAL:HG13	1:B:982:ILE:HG23	1.57	0.85
1:B:260:SER:HA	1:B:562:ALA:HB1	1.63	0.80
1:A:921:MET:HB3	1:A:965:HIS:HD2	1.47	0.79
1:B:350:LEU:O	1:B:350:LEU:CD2	2.30	0.78
1:B:212:MET:HG2	1:B:231:ILE:HG21	1.68	0.76
1:A:271:ILE:HA	1:A:299:LEU:HD21	1.68	0.75
1:A:701:ARG:HA	1:A:726:MET:HG2	1.68	0.74
1:B:865:THR:HG23	1:B:867:SER:H	1.55	0.72
1:B:779:PRO:HA	1:B:783:MET:HB3	1.71	0.72
1:B:249:VAL:HG23	1:B:277:VAL:HG11	1.74	0.70
1:A:441:VAL:HG22	1:A:463:LEU:HD21	1.74	0.69
1:A:669:PHE:CE2	1:A:715:ALA:HB3	2.27	0.69
1:B:274:PRO:HG2	1:B:277:VAL:HG23	1.74	0.69
1:A:191:ILE:HB	1:A:194:LEU:HD13	1.75	0.69
1:B:601:VAL:HG22	1:B:839:LEU:HD11	1.74	0.69
1:B:260:SER:HA	1:B:562:ALA:CB	2.23	0.68
1:B:347:MET:HE2	1:B:543:MET:H	1.56	0.68
1:B:876:VAL:HG13	1:B:1010:ALA:HB1	1.74	0.67
1:B:288:ASN:HD21	1:B:559:LEU:HB3	1.58	0.67
1:B:351:ARG:O	1:B:352:ASP:CB	2.33	0.67
1:A:455:HIS:HB2	1:A:479:LEU:HD21	1.78	0.66
1:A:461:PRO:HD2	1:A:994:ILE:HD12	1.78	0.66
1:A:698:VAL:HG12	1:A:700:LEU:HG	1.77	0.65
1:B:318:HIS:HB2	1:B:332:VAL:HB	1.80	0.64
1:B:512:ILE:HG13	1:B:551:LEU:HD21	1.80	0.64
1:B:486:ALA:O	1:B:523:ARG:NH1	2.31	0.63
1:B:673:VAL:HG21	1:B:744:LEU:HD11	1.82	0.62
1:A:565:LEU:HD11	1:A:585:LEU:HD21	1.82	0.61
1:A:328:LEU:HD21	1:A:536:ILE:HG12	1.82	0.61
1:B:425:SER:HA	1:B:428:ILE:HG22	1.83	0.61
1:A:202:MET:HB2	1:A:209:VAL:HG21	1.83	0.61
1:B:561:SER:HB3	1:B:589:PHE:HB3	1.83	0.60
1:B:935:MET:HG3	1:B:936:GLN:N	2.16	0.60
1:B:865:THR:HG22	1:B:869:VAL:H	1.67	0.60
1:B:877:ALA:HB1	1:B:885:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HA	1:B:227:MET:O	2.02	0.59
1:B:460:LEU:HG	1:B:1034:ILE:HD11	1.85	0.59
1:A:198:LYS:O	1:A:202:MET:HG2	2.02	0.59
1:A:378:VAL:O	1:A:382:MET:HG2	2.02	0.59
1:A:673:VAL:HG11	1:A:759:VAL:HG11	1.85	0.58
1:A:492:PRO:HB2	1:A:526:ARG:HG2	1.86	0.58
1:B:991:GLY:HA2	1:B:994:ILE:HG23	1.86	0.57
1:B:406:MET:HB2	1:B:452:ILE:HD12	1.86	0.57
1:B:236:LEU:HD21	1:B:273:LEU:HG	1.86	0.57
1:B:640:ILE:HD11	1:B:797:VAL:HG11	1.88	0.56
1:B:178:ALA:HA	1:B:183:GLN:HG3	1.88	0.55
1:B:212:MET:HB3	1:B:227:MET:HG3	1.88	0.55
1:B:565:LEU:HD21	1:B:585:LEU:HD21	1.89	0.55
1:B:1004:LEU:HB3	1:B:1027:ILE:HG22	1.88	0.54
1:A:751:ARG:HA	1:A:756:ARG:HH21	1.70	0.54
1:B:350:LEU:CD2	1:B:350:LEU:C	2.74	0.54
1:B:390:ILE:HD13	1:B:485:PHE:HE2	1.73	0.54
1:A:969:VAL:HG13	1:A:982:ILE:HB	1.90	0.54
1:B:932:LEU:HD22	1:B:935:MET:HG2	1.90	0.53
1:B:793:VAL:O	1:B:797:VAL:HG13	2.09	0.53
1:B:658:ARG:HA	1:B:743:ARG:HG2	1.91	0.53
1:A:460:LEU:CD1	1:A:990:GLU:HB2	2.38	0.53
1:A:288:ASN:HD21	1:A:559:LEU:HB3	1.74	0.53
1:A:877:ALA:HB1	1:A:885:GLU:HB2	1.91	0.52
1:A:654:LEU:HD13	1:A:696:VAL:HG11	1.90	0.52
1:B:468:GLU:HA	1:B:491:MET:HE1	1.92	0.52
1:A:470:LEU:HD22	1:A:475:LEU:HD12	1.91	0.52
1:B:746:ILE:HD13	1:B:746:ILE:H	1.75	0.52
1:B:160:SER:HA	1:B:283:SER:O	2.10	0.52
1:B:591:GLN:HG2	1:B:846:LEU:HD11	1.92	0.52
1:B:591:GLN:HG2	1:B:846:LEU:HD21	1.90	0.51
1:B:161:ALA:HB3	1:B:167:LYS:HD3	1.92	0.51
1:B:350:LEU:HD22	1:B:350:LEU:C	2.29	0.51
1:A:236:LEU:HD11	1:A:273:LEU:HG	1.92	0.51
1:B:254:ILE:HG22	1:B:283:SER:HB2	1.93	0.51
1:A:669:PHE:CD2	1:A:715:ALA:HB3	2.46	0.51
1:A:740:SER:HB2	1:A:774:ILE:CG2	2.41	0.51
1:A:906:THR:HG22	1:A:1004:LEU:HD21	1.92	0.51
1:B:348:GLN:CA	1:B:348:GLN:NE2	2.31	0.50
1:A:662:VAL:HG11	1:A:731:VAL:HG11	1.92	0.50
1:B:293:ALA:HB2	1:B:306:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:PRO:HG3	1:A:994:ILE:HG21	1.94	0.50
1:A:160:SER:HA	1:A:283:SER:O	2.11	0.50
1:A:175:ILE:HA	1:A:185:VAL:HG11	1.96	0.48
1:A:563:PHE:CZ	1:A:584:MET:HG2	2.49	0.48
1:A:658:ARG:HA	1:A:743:ARG:HB3	1.96	0.48
1:B:654:LEU:HD11	1:B:736:LEU:HD11	1.94	0.48
1:B:287:PRO:HD2	1:B:558:PRO:HA	1.96	0.47
1:A:375:PHE:HA	1:A:406:MET:SD	2.54	0.47
1:B:542:LYS:O	1:B:710:SER:HB3	2.14	0.47
1:A:144:GLN:OE1	1:A:169:VAL:HG21	2.14	0.47
1:B:966:LEU:HD21	1:B:993:ILE:HG23	1.96	0.47
1:A:374:VAL:HG11	1:A:402:TYR:CD2	2.49	0.47
1:A:458:GLY:O	1:A:990:GLU:HG3	2.14	0.47
1:A:966:LEU:HD11	1:A:993:ILE:HG12	1.95	0.47
1:B:553:LYS:HE3	1:B:553:LYS:HB3	1.67	0.47
1:B:794:ILE:O	1:B:797:VAL:HG22	2.14	0.47
1:A:406:MET:HG3	1:A:480:PHE:CZ	2.49	0.47
1:A:885:GLU:CD	1:A:885:GLU:H	2.17	0.47
1:B:491:MET:HB3	1:B:491:MET:HE3	1.61	0.47
1:B:845:VAL:HG12	1:B:848:MET:HB2	1.97	0.47
1:B:491:MET:N	1:B:492:PRO:HD3	2.30	0.47
1:A:993:ILE:O	1:A:997:MET:HG2	2.15	0.47
1:B:273:LEU:HD13	1:B:279:TYR:HE2	1.80	0.46
1:A:453:GLY:HA3	1:A:476:ILE:HD13	1.95	0.46
1:A:620:GLU:O	1:A:623:VAL:HG12	2.14	0.46
1:A:757:GLN:HE21	1:A:757:GLN:HB3	1.51	0.46
1:B:839:LEU:O	1:B:840:LYS:C	2.53	0.46
1:A:195:SER:HB3	1:A:226:VAL:HG12	1.97	0.46
1:A:696:VAL:HG23	1:A:698:VAL:HG23	1.97	0.46
1:A:328:LEU:HD11	1:A:536:ILE:HG23	1.97	0.46
1:A:461:PRO:CD	1:A:994:ILE:HD12	2.44	0.46
1:B:662:VAL:HG22	1:B:736:LEU:HD23	1.97	0.46
1:B:969:VAL:HG21	1:B:986:THR:HG22	1.98	0.46
1:A:460:LEU:HD11	1:A:990:GLU:HB2	1.97	0.46
1:B:350:LEU:O	1:B:350:LEU:HD23	2.15	0.46
1:B:322:PRO:HB3	1:B:346:ALA:O	2.15	0.45
1:B:747:PRO:O	1:B:750:LEU:HG	2.16	0.45
1:A:762:SER:O	1:A:766:VAL:HG23	2.15	0.45
1:A:185:VAL:O	1:A:224:CYS:HA	2.17	0.45
1:A:908:LEU:HD11	1:A:935:MET:HB2	1.97	0.45
1:B:381:ILE:HG23	1:B:386:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:LEU:HG	1:A:1007:MET:HE3	1.99	0.45
1:B:607:ASN:HD22	1:B:607:ASN:HA	1.53	0.45
1:B:699:LEU:HD12	1:B:728:VAL:HG22	1.98	0.45
1:A:579:ILE:HG23	1:A:583:TYR:HB3	1.98	0.45
1:B:905:ALA:O	1:B:909:LEU:HD12	2.17	0.45
1:A:99:VAL:HG11	1:A:294:GLU:HB3	1.97	0.45
1:A:699:LEU:HA	1:A:728:VAL:HA	1.98	0.45
1:A:166:GLY:HA3	2:A:2101:ADP:H8	1.81	0.45
1:A:254:ILE:HG22	1:A:283:SER:HB3	1.97	0.45
1:B:759:VAL:O	1:B:763:ILE:HG23	2.16	0.45
1:A:727:GLN:HA	1:A:756:ARG:HD3	1.99	0.45
1:A:274:PRO:HG2	1:A:277:VAL:HG23	1.99	0.44
1:B:700:LEU:HD12	1:B:729:VAL:CG1	2.47	0.44
1:A:585:LEU:O	1:A:591:GLN:HG3	2.17	0.44
1:B:446:PRO:HA	1:B:449:LYS:HE2	1.99	0.44
1:B:504:PHE:HA	1:B:509:PHE:HA	1.98	0.44
1:B:677:PHE:CD1	1:B:677:PHE:N	2.85	0.44
1:B:523:ARG:HD3	1:B:523:ARG:HA	1.59	0.44
1:A:318:HIS:HB2	1:A:332:VAL:HB	2.00	0.44
1:A:969:VAL:HG21	1:A:986:THR:HG23	1.99	0.44
1:A:262:ARG:O	1:A:265:VAL:HG22	2.18	0.44
1:B:845:VAL:HG12	1:B:848:MET:CB	2.47	0.44
1:A:227:MET:HE2	1:A:227:MET:HB2	1.69	0.44
1:A:453:GLY:O	1:A:479:LEU:HA	2.18	0.44
1:A:907:ALA:O	1:A:967:MET:HG2	2.17	0.44
1:A:643:TYR:HD2	1:A:790:LEU:HG	1.82	0.44
1:B:1004:LEU:HD12	1:B:1004:LEU:HA	1.84	0.43
1:A:1017:THR:O	1:A:1020:GLU:HB3	2.18	0.43
1:A:653:PHE:O	1:A:658:ARG:HD2	2.17	0.43
1:B:852:LYS:HD3	1:B:852:LYS:HA	1.79	0.43
1:A:1019:LEU:HD23	1:A:1019:LEU:HA	1.83	0.43
1:B:777:LEU:HD12	1:B:783:MET:HB2	2.00	0.43
1:A:591:GLN:HE21	1:A:591:GLN:HB3	1.53	0.43
1:B:636:LEU:HB3	1:B:797:VAL:HG12	2.00	0.43
1:A:435:ASP:O	1:A:438:LEU:HB2	2.18	0.43
1:B:486:ALA:O	1:B:523:ARG:NH2	2.51	0.43
1:B:700:LEU:HD12	1:B:729:VAL:HG13	1.99	0.43
1:A:943:ALA:HA	1:A:953:ILE:HD11	2.01	0.43
1:B:1024:ALA:O	1:B:1027:ILE:HG12	2.19	0.43
1:B:761:LYS:O	1:B:765:GLU:HG2	2.19	0.43
1:B:1023:PHE:O	1:B:1027:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:MET:HG3	1:A:480:PHE:HZ	1.84	0.43
1:B:659:LEU:HG	1:B:744:LEU:HD21	2.00	0.43
1:B:254:ILE:HD12	1:B:254:ILE:HA	1.88	0.43
1:B:656:PRO:HD3	1:B:677:PHE:CE2	2.54	0.42
1:A:1007:MET:HE3	1:A:1007:MET:HB2	1.89	0.42
1:A:986:THR:HB	1:A:988:VAL:H	1.83	0.42
1:A:378:VAL:HB	1:A:406:MET:SD	2.59	0.42
1:B:293:ALA:HB2	1:B:306:VAL:CG2	2.50	0.42
1:B:297:CYS:HA	1:B:302:GLN:O	2.20	0.42
1:B:739:ILE:HG22	1:B:777:LEU:HD21	1.99	0.42
1:A:933:ARG:HD2	1:A:936:GLN:HE22	1.85	0.42
1:B:986:THR:CG2	1:B:988:VAL:HG22	2.50	0.42
1:A:460:LEU:HD13	1:A:990:GLU:HB2	2.00	0.42
1:A:704:LYS:HD3	1:A:704:LYS:HA	1.77	0.42
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.78	0.42
1:B:460:LEU:HD13	1:B:460:LEU:HA	1.82	0.42
1:A:936:GLN:HE21	1:A:936:GLN:HB2	1.49	0.42
1:B:273:LEU:HD23	1:B:274:PRO:HD2	2.02	0.42
1:B:749:ASP:O	1:B:752:PRO:HD2	2.20	0.42
1:A:380:MET:HG3	1:A:381:ILE:N	2.34	0.42
1:B:969:VAL:HG21	1:B:986:THR:CG2	2.50	0.42
1:A:263:GLY:HA3	1:A:562:ALA:HB3	2.02	0.42
1:A:1004:LEU:HD23	1:A:1027:ILE:HG22	2.00	0.41
1:A:1035:VAL:HG23	1:A:1036:PHE:CD2	2.55	0.41
1:B:227:MET:HE2	1:B:227:MET:HB2	1.83	0.41
1:B:549:LYS:O	1:B:553:LYS:HB2	2.19	0.41
1:B:861:LEU:HD12	1:B:861:LEU:HA	1.90	0.41
1:A:254:ILE:HD12	1:A:266:TRP:CE3	2.55	0.41
1:B:659:LEU:HA	1:B:659:LEU:HD23	1.85	0.41
1:A:166:GLY:HA2	2:A:2101:ADP:O5'	2.19	0.41
1:A:423:VAL:HB	1:A:470:LEU:HD21	2.03	0.41
1:A:539:VAL:HG22	1:A:541:GLU:O	2.20	0.41
1:A:699:LEU:HD12	1:A:728:VAL:HG22	2.03	0.41
1:B:591:GLN:HE21	1:B:591:GLN:HB3	1.55	0.41
1:A:177:LEU:O	1:A:181:GLU:HG2	2.20	0.41
1:A:701:ARG:HE	1:A:760:LEU:HD21	1.86	0.41
1:A:749:ASP:O	1:A:752:PRO:HD2	2.20	0.41
1:B:316:LEU:HD11	1:B:524:ALA:O	2.21	0.41
1:B:928:LEU:HA	1:B:928:LEU:HD12	1.84	0.41
1:A:225:LEU:HA	1:A:225:LEU:HD12	1.82	0.41
1:A:249:VAL:HG23	1:A:277:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PHE:HB2	1:A:553:LYS:HD3	2.01	0.41
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.84	0.41
1:A:957:THR:O	1:A:961:SER:N	2.54	0.41
1:B:161:ALA:O	1:B:284:ALA:HA	2.21	0.41
1:B:986:THR:HG23	1:B:988:VAL:HG22	2.03	0.41
1:B:1009:GLN:O	1:B:1012:LYS:HB2	2.20	0.41
1:A:165:ALA:HA	1:A:313:PRO:HG2	2.02	0.41
1:A:266:TRP:O	1:A:270:ILE:HG13	2.21	0.41
1:B:456:HIS:H	1:B:459:LEU:HD12	1.86	0.41
1:A:895:GLY:HA2	1:A:898:ASN:OD1	2.21	0.41
1:B:654:LEU:HD13	1:B:696:VAL:HG11	2.02	0.40
1:A:990:GLU:H	1:A:990:GLU:HG2	1.14	0.40
1:A:233:ARG:HH22	1:A:568:ASN:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	856/1002 (85%)	836 (98%)	20 (2%)	0	100	100
1	B	901/1002 (90%)	879 (98%)	21 (2%)	1 (0%)	51	84
All	All	1757/2004 (88%)	1715 (98%)	41 (2%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	597/883 (68%)	519 (87%)	78 (13%)	4	23
1	B	639/883 (72%)	553 (86%)	86 (14%)	4	22
All	All	1236/1766 (70%)	1072 (87%)	164 (13%)	4	23

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	101	VAL
1	B	125	LEU
1	B	138	PHE
1	B	156	SER
1	B	157	VAL
1	B	167	LYS
1	B	168	THR
1	B	188	THR
1	B	194	LEU
1	B	202	MET
1	B	212	MET
1	B	227	MET
1	B	234	SER
1	B	236	LEU
1	B	240	SER
1	B	242	VAL
1	B	285	THR
1	B	307	ILE
1	B	320	ILE
1	B	341	ASP
1	B	347	MET
1	B	348	GLN
1	B	349	VAL
1	B	350	LEU
1	B	352	ASP
1	B	391	ILE
1	B	395	SER

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Mol	Chain	Res	Type
1	B	399	CYS
1	B	402	TYR
1	B	406	MET
1	B	407	THR
1	B	418	LYS
1	B	433	ASP
1	B	438	LEU
1	B	452	ILE
1	B	460	LEU
1	B	491	MET
1	B	514	SER
1	B	518	ILE
1	B	519	GLN
1	B	531	ASP
1	B	540	ASP
1	B	551	LEU
1	B	566	THR
1	B	579	ILE
1	B	589	PHE
1	B	591	GLN
1	B	595	TYR
1	B	607	ASN
1	B	633	LEU
1	B	650	CYS
1	B	654	LEU
1	B	659	LEU
1	B	660	VAL
1	B	677	PHE
1	B	679	LYS
1	B	729	VAL
1	B	740	SER
1	B	746	ILE
1	B	777	LEU
1	B	781	ASP
1	B	786	GLN
1	B	790	LEU
1	B	846	LEU
1	B	848	MET
1	B	860	ARG
1	B	861	LEU
1	B	872	MET
1	B	887	LEU

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Mol	Chain	Res	Type
1	B	896	LEU
1	B	909	LEU
1	B	910	SER
1	B	924	LEU
1	B	925	THR
1	B	928	LEU
1	B	932	LEU
1	B	935	MET
1	B	936	GLN
1	B	966	LEU
1	B	978	THR
1	B	990	GLU
1	B	994	ILE
1	B	1000	LEU
1	B	1004	LEU
1	B	1008	CYS
1	B	1030	ILE
1	A	101	VAL
1	A	106	THR
1	A	114	VAL
1	A	116	LEU
1	A	163	THR
1	A	185	VAL
1	A	209	VAL
1	A	212	MET
1	A	221	THR
1	A	227	MET
1	A	233	ARG
1	A	237	TYR
1	A	243	MET
1	A	297	CYS
1	A	301	LYS
1	A	311	TYR
1	A	331	VAL
1	A	341	ASP
1	A	347	MET
1	A	350	LEU
1	A	352	ASP
1	A	387	GLN
1	A	391	ILE
1	A	406	MET
1	A	407	THR

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Mol	Chain	Res	Type
1	A	422	GLU
1	A	438	LEU
1	A	460	LEU
1	A	467	ILE
1	A	484	THR
1	A	497	LEU
1	A	529	MET
1	A	537	LEU
1	A	544	SER
1	A	565	LEU
1	A	566	THR
1	A	568	ASN
1	A	578	GLU
1	A	584	MET
1	A	588	SER
1	A	591	GLN
1	A	601	VAL
1	A	607	ASN
1	A	624	VAL
1	A	633	LEU
1	A	651	LEU
1	A	660	VAL
1	A	669	PHE
1	A	729	VAL
1	A	731	VAL
1	A	736	LEU
1	A	744	LEU
1	A	746	ILE
1	A	758	SER
1	A	759	VAL
1	A	760	LEU
1	A	772	ASP
1	A	777	LEU
1	A	781	ASP
1	A	790	LEU
1	A	828	ILE
1	A	847	GLN
1	A	851	LEU
1	A	867	SER
1	A	898	ASN
1	A	901	SER
1	A	913	VAL

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Mol	Chain	Res	Type
1	A	915	GLN
1	A	935	MET
1	A	954	ASP
1	A	966	LEU
1	A	972	THR
1	A	978	THR
1	A	987	ASP
1	A	990	GLU
1	A	995	ARG
1	A	1005	ARG
1	A	1027	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	196	ASN
1	B	302	GLN
1	B	348	GLN
1	B	519	GLN
1	B	591	GLN
1	B	607	ASN
1	B	611	GLN
1	B	788	GLN
1	B	1016	ASN
1	A	149	GLN
1	A	317	GLN
1	A	329	HIS
1	A	335	ASN
1	A	591	GLN
1	A	757	GLN
1	A	936	GLN
1	A	965	HIS

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 monosaccharides 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	$\# Z > 2$
2	ADP	A	2101	3	24,29,29	0.71	0	29,45,45	0.80	1 (3%)
2	ADP	B	1101	3	24,29,29	0.73	0	29,45,45	0.90	1 (3%)

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	ADP	A	2101	3	-	6/12/32/32	0/3/3/3
2	ADP	B	1101	3	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ADP	C5-C6-N6	2.26	123.79	120.35
2	A	2101	ADP	C5-C6-N6	2.16	123.64	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	ADP	C5'-O5'-PA-O1A

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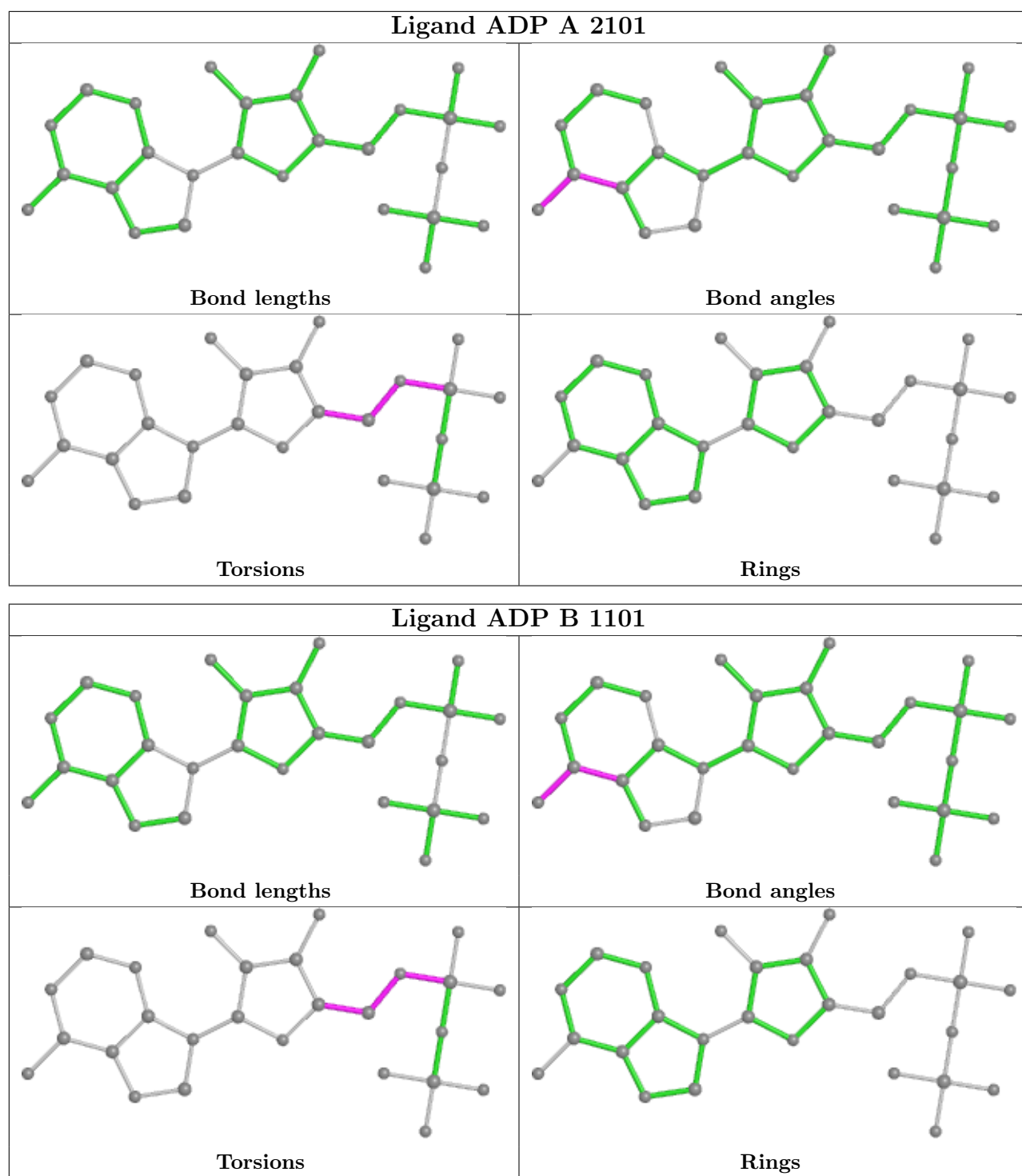
Mol	Chain	Res	Type	Atoms
2	B	1101	ADP	C4'-C5'-O5'-PA
2	B	1101	ADP	C3'-C4'-C5'-O5'
2	A	2101	ADP	C5'-O5'-PA-O1A
2	B	1101	ADP	O4'-C4'-C5'-O5'
2	A	2101	ADP	O4'-C4'-C5'-O5'
2	A	2101	ADP	C3'-C4'-C5'-O5'
2	A	2101	ADP	C5'-O5'-PA-O3A
2	A	2101	ADP	C5'-O5'-PA-O2A
2	A	2101	ADP	C4'-C5'-O5'-PA
2	B	1101	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2101	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	872/1002 (87%)	-0.28	5 (0%) 89 80	6, 32, 65, 99	0
1	B	911/1002 (90%)	-0.36	5 (0%) 91 83	5, 21, 59, 117	0
All	All	1783/2004 (88%)	-0.32	10 (0%) 89 80	5, 26, 64, 117	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	813	PRO	3.6
1	A	721	ASP	3.1
1	A	608	SER	2.6
1	B	619	ASN	2.4
1	B	691	ASP	2.3
1	B	806	SER	2.1
1	B	814	ASN	2.1
1	A	612	TYR	2.1
1	A	946	SER	2.0
1	A	678	SER	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 monosaccharides in this entry.

6.4 Ligands

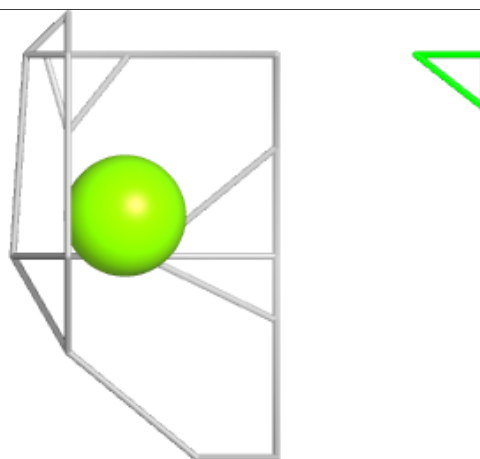
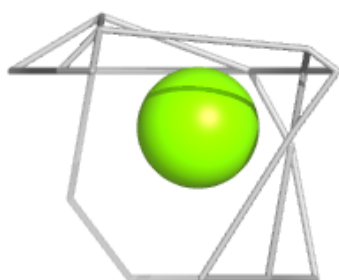
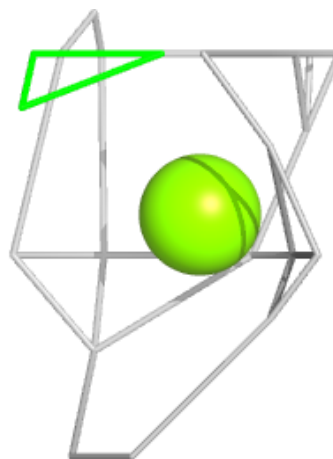
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	2102	1/1	0.81	0.42	30,30,30,30	0
2	ADP	A	2101	27/27	0.86	0.26	21,36,48,75	0
2	ADP	B	1101	27/27	0.90	0.19	21,36,48,75	0
3	MG	B	1102	1/1	0.92	0.43	48,48,48,48	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.

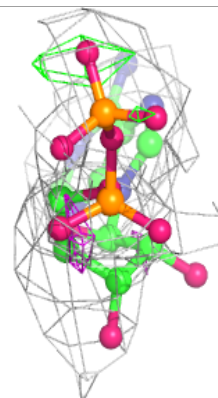
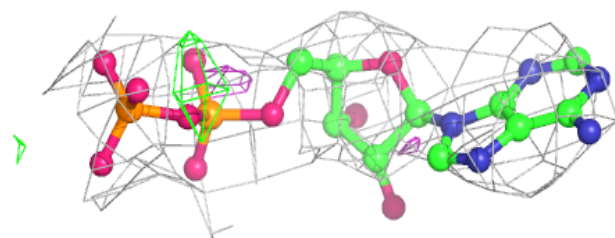
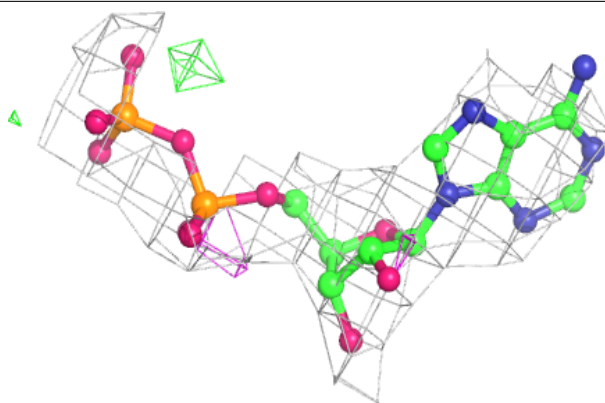
Electron density around MG A 2102:

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

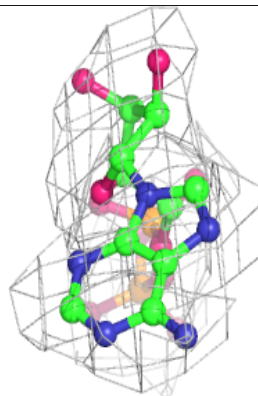
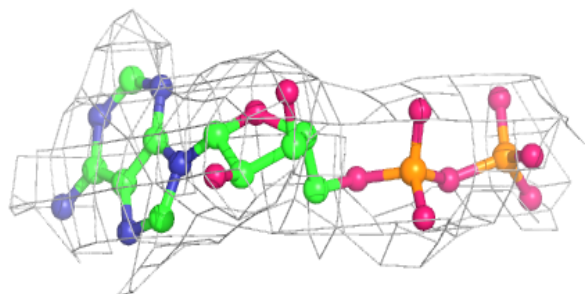
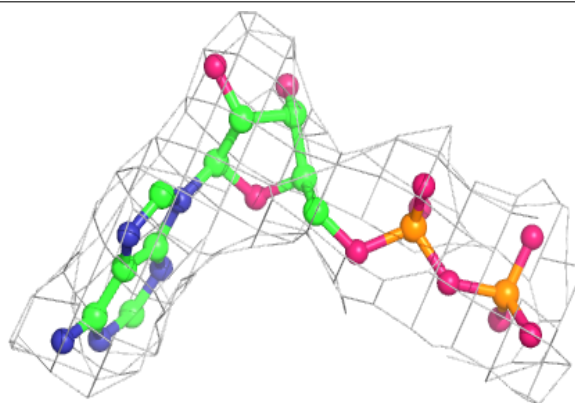


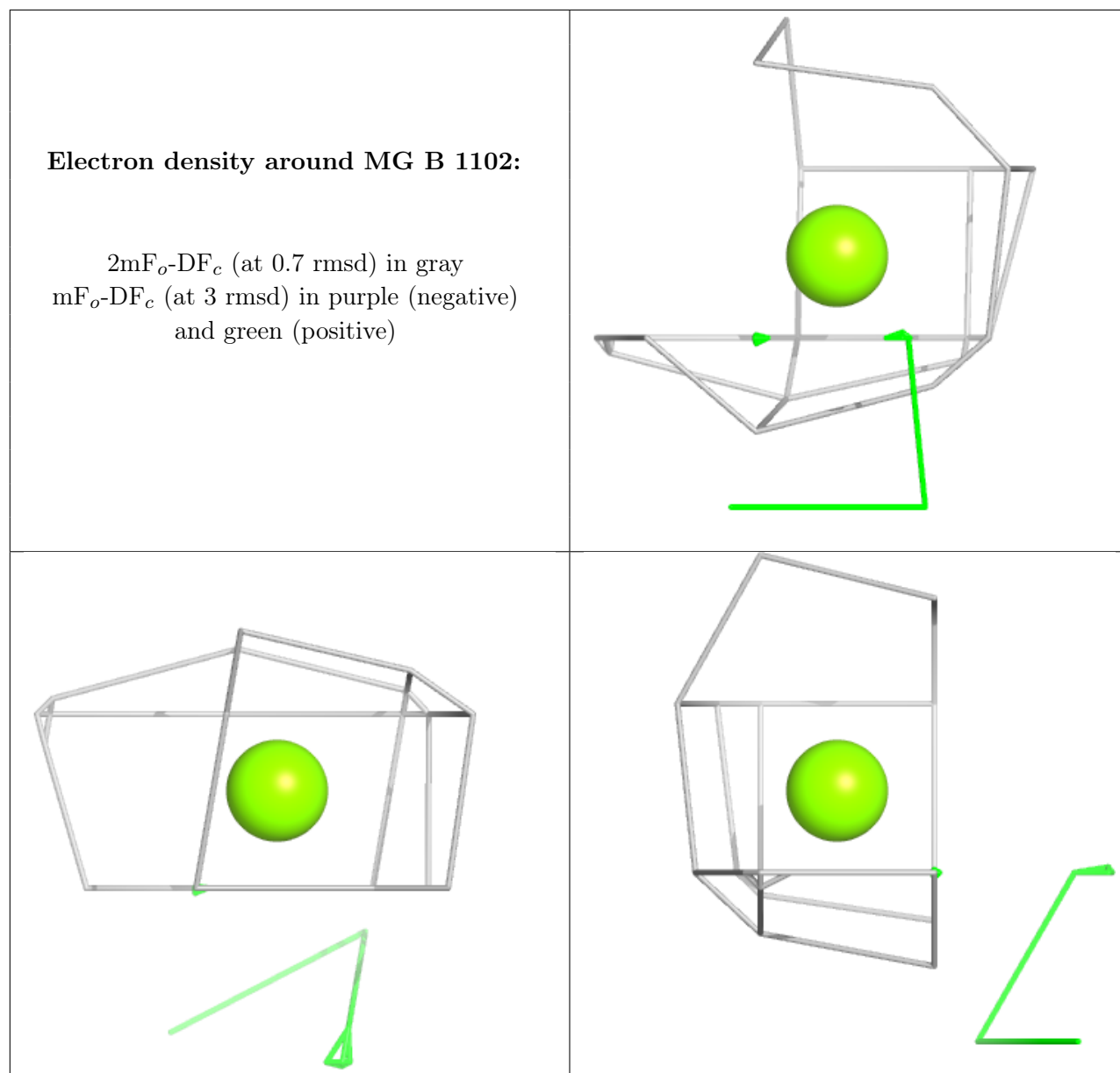
Electron density around ADP A 2101:

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

**Electron density around ADP B 1101:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.