



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:32 AM UTC

PDB ID : 7HK7 / pdb_00007hk7
Title : Crystal Structure of N-methylhydantoinase in complex with Mg-ADPNP
Authors : Stihle, M.; Benz, J.; Asztalos, P.; Rudolph, M.G.
Deposited on : 2024-10-10
Resolution : 3.13 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

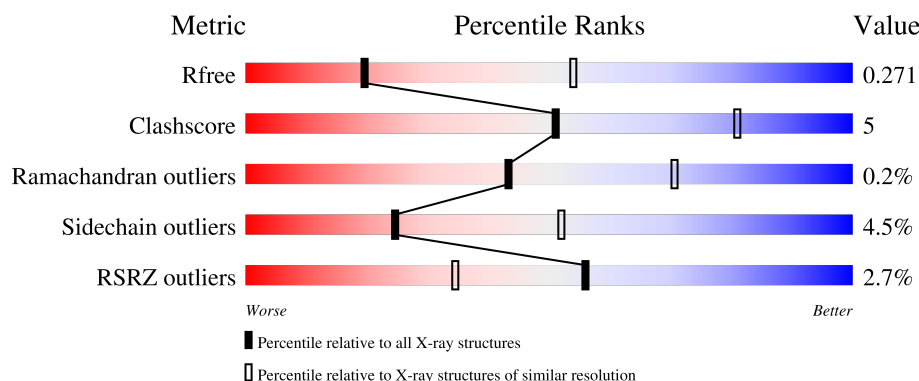
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	1288	 2% 84% 14% ..
1	B	1288	 3% 83% 15% ..
1	C	1288	 3% 83% 15% ..
1	D	1288	 3% 82% 16% ..

2 Entry composition [i](#)

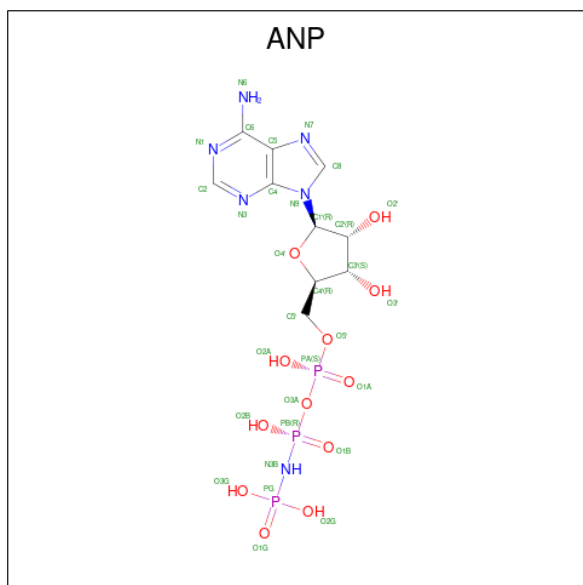
There are 5 unique types of molecules in this entry. The entry contains 39288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-methylhydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1280	Total	C	N	O	S	0	0	0
			9788	6143	1694	1911	40			
1	B	1278	Total	C	N	O	S	0	0	0
			9776	6135	1692	1909	40			
1	C	1280	Total	C	N	O	S	0	0	0
			9788	6143	1694	1911	40			
1	D	1280	Total	C	N	O	S	0	0	0
			9788	6143	1694	1911	40			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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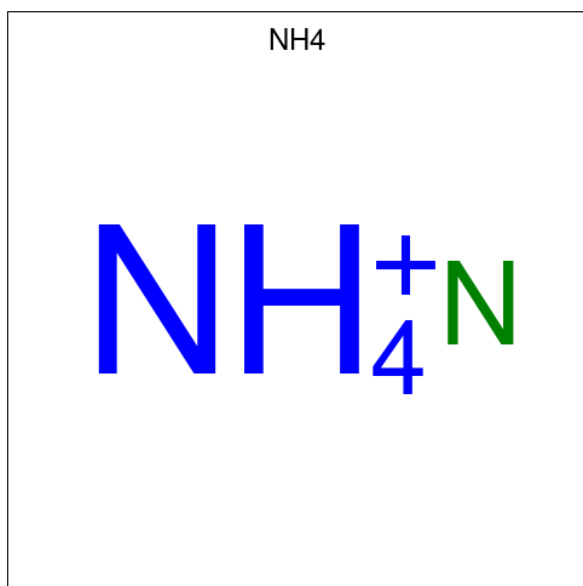
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 4 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total N 1 1	0	0

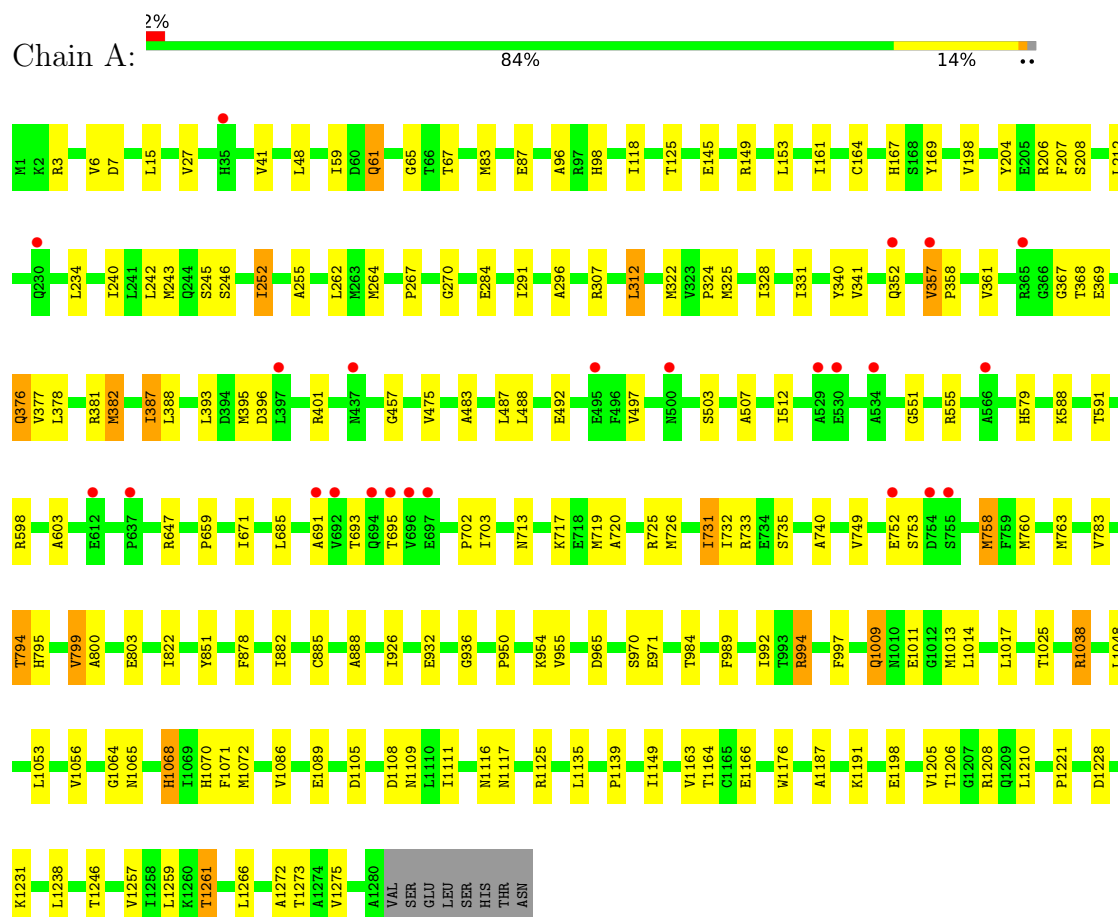
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	4	Total O 4 4	0	0
5	C	4	Total O 4 4	0	0
5	D	4	Total O 4 4	0	0

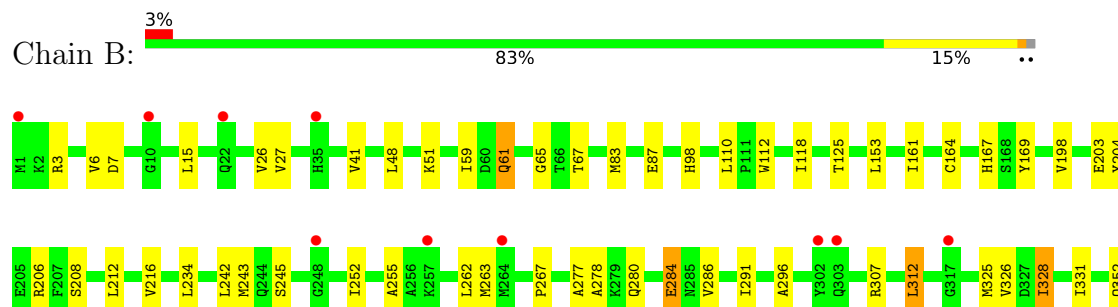
3 Residue-property plots

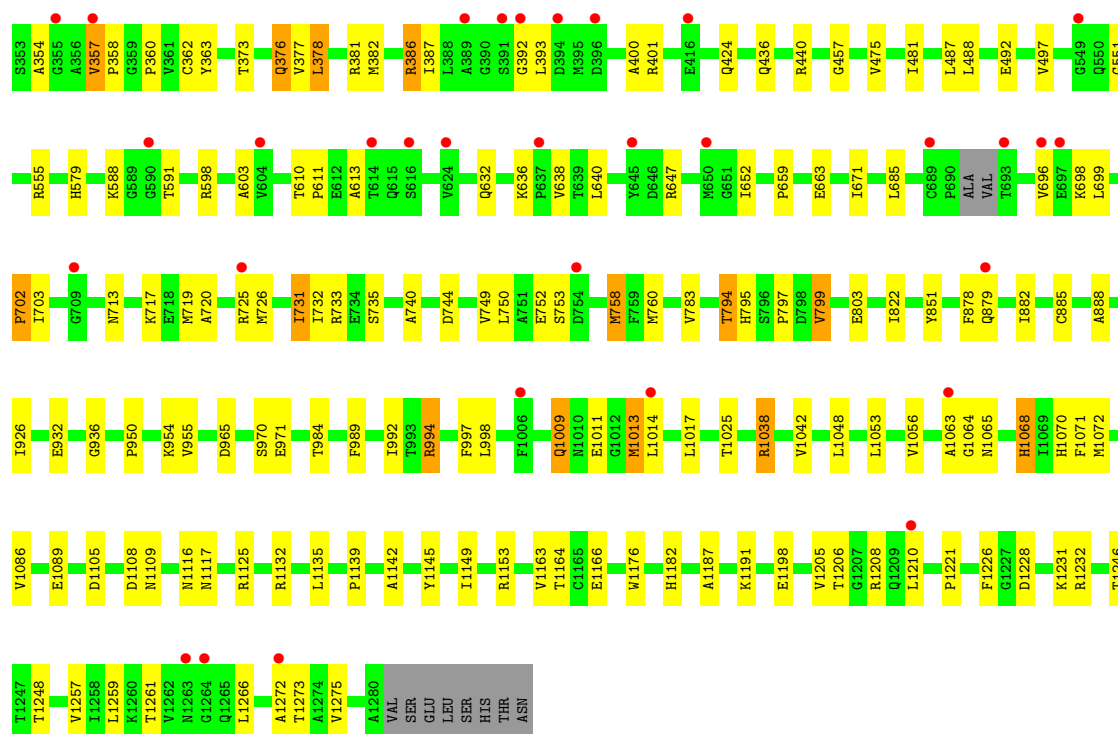
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

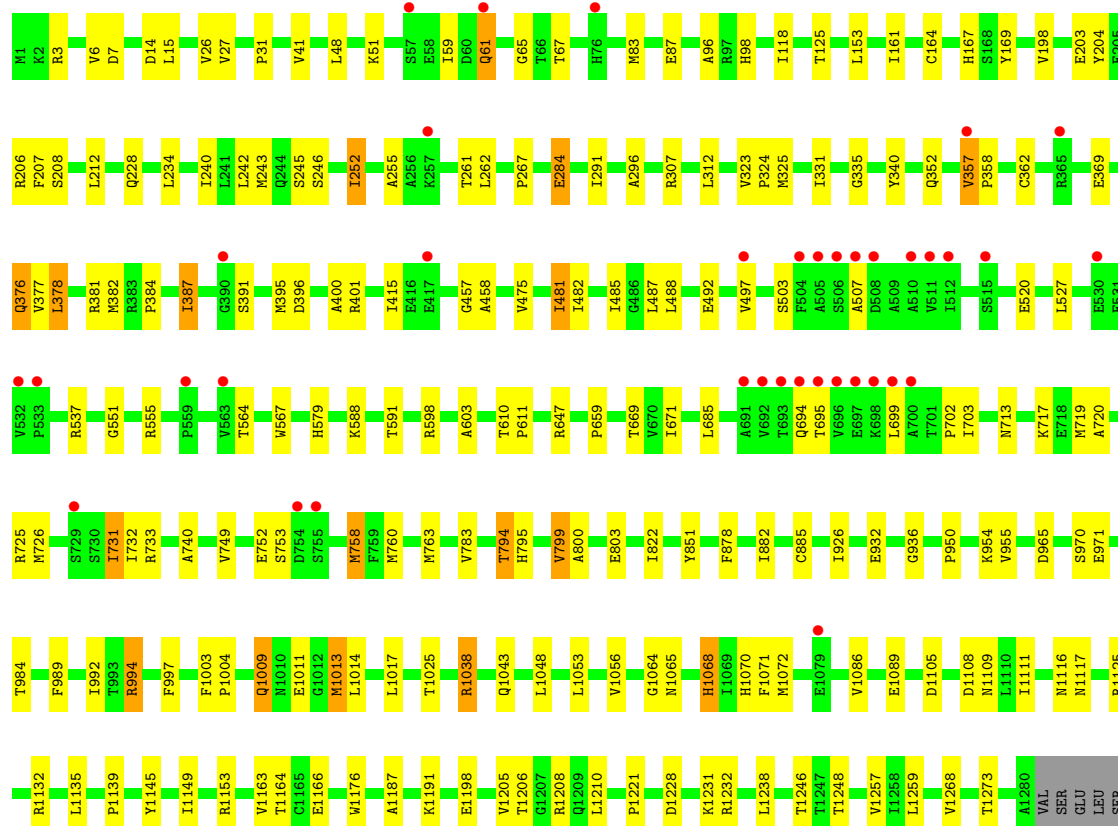
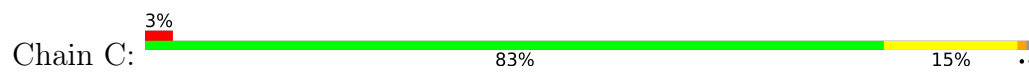


• Molecule 1: N-methylhydantoinase






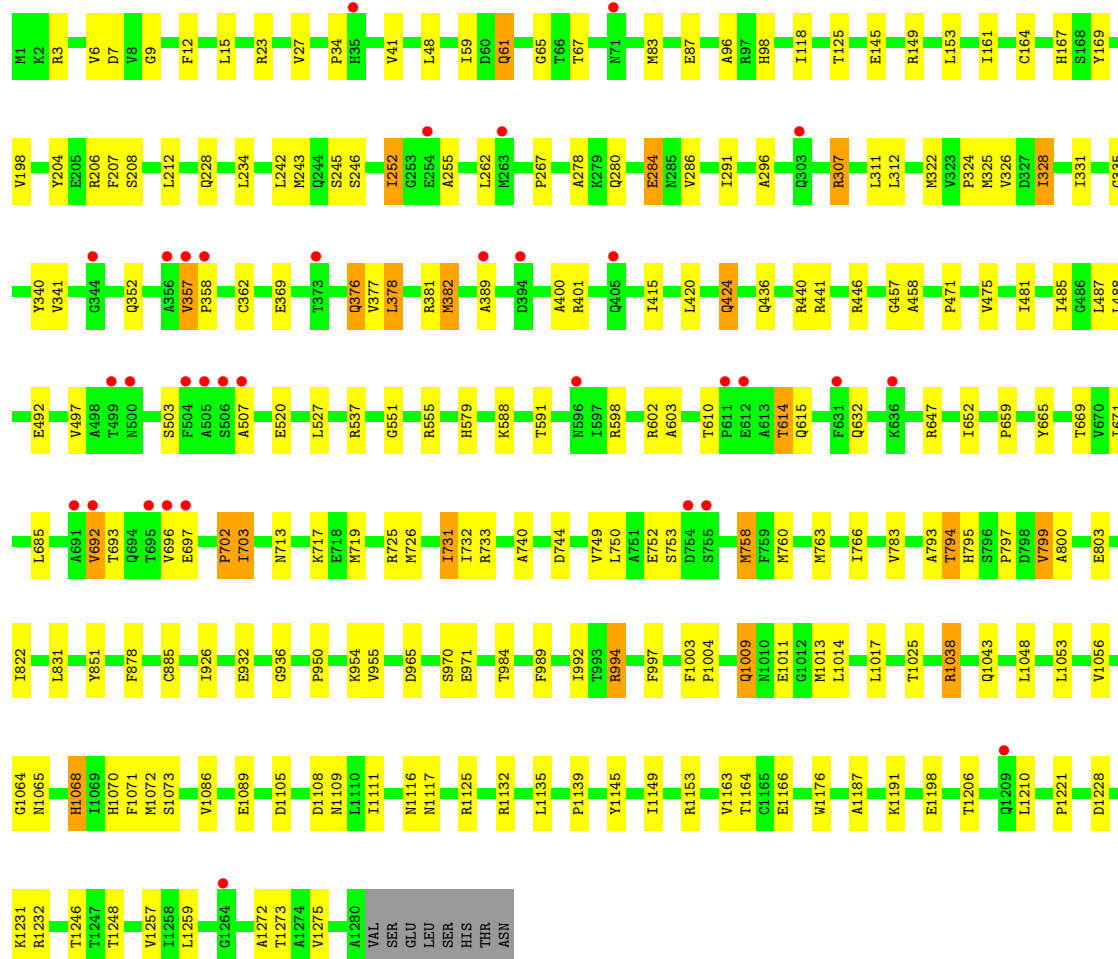
• Molecule 1: N-methylhydantoinase



HIS
THR
ASN

● Molecule 1: N-methylhydantoinase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.73Å 84.25Å 236.25Å 93.25° 94.82° 89.07°	Depositor
Resolution (Å)	49.38 – 3.13 49.38 – 3.13	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.38-3.13) 89.2 (49.38-3.13)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.223 , 0.265 0.233 , 0.271	Depositor DCC
R_{free} test set	4489 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	39288	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: ANP, NH4, 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	0.17	0/9982	0.43	0/13552
1	B	0.17	0/9969	0.42	0/13532
1	C	0.16	0/9982	0.42	0/13552
1	D	0.17	0/9982	0.42	0/13552
All	All	0.17	0/39915	0.42	0/54188

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	9788	0	9590	90	0
1	B	9776	0	9575	103	0
1	C	9788	0	9590	98	0
1	D	9788	0	9590	109	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	1	0
2	D	31	0	13	3	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
All	All	39288	0	38397	400	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 5.

All (400) 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:D:693:THR:HB	1:D:696:VAL:HG21	1.57	0.87
1:C:694:GLN:HB3	1:C:699:LEU:HD21	1.56	0.86
1:B:387:ILE:HG23	1:B:392:GLY:HA2	1.70	0.72
1:C:492:GLU:HB2	1:C:603:ALA:HB3	1.72	0.70
1:D:291:ILE:HD12	1:D:457:GLY:HA2	1.75	0.68
1:D:245:SER:HB3	1:D:325:MET:HG3	1.77	0.67
1:B:497:VAL:HG12	1:B:598:ARG:HB3	1.76	0.67
1:D:492:GLU:HB2	1:D:603:ALA:HB3	1.76	0.67
1:C:6:VAL:HG21	1:C:41:VAL:HG13	1.76	0.67
1:C:245:SER:HB3	1:C:325:MET:HG3	1.76	0.66
1:C:497:VAL:HG12	1:C:598:ARG:HB3	1.76	0.66
1:A:971:GLU:HA	1:A:1025:THR:HA	1.79	0.65
1:C:67:THR:HG22	1:C:267:PRO:HD3	1.77	0.65
1:B:492:GLU:HB2	1:B:603:ALA:HB3	1.79	0.65
1:A:67:THR:HG22	1:A:267:PRO:HD3	1.79	0.65
1:A:245:SER:HB3	1:A:325:MET:HG3	1.77	0.65
1:B:245:SER:HB3	1:B:325:MET:HG3	1.79	0.64
1:D:6:VAL:HG21	1:D:41:VAL:HG13	1.80	0.64
1:D:758:MET:HG3	1:D:794:THR:HG21	1.80	0.64
1:D:497:VAL:HG12	1:D:598:ARG:HB3	1.80	0.64
1:A:291:ILE:HD12	1:A:457:GLY:HA2	1.80	0.63
1:B:971:GLU:HA	1:B:1025:THR:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:HD12	1:C:457:GLY:HA2	1.79	0.63
1:B:424:GLN:HE21	1:B:632:GLN:HG2	1.63	0.63
1:C:255:ALA:HB1	1:C:262:LEU:HD11	1.80	0.63
1:A:6:VAL:HG21	1:A:41:VAL:HG13	1.82	0.62
1:B:291:ILE:HD12	1:B:457:GLY:HA2	1.82	0.62
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.82	0.62
1:B:3:ARG:HG2	1:B:61:GLN:HB3	1.82	0.62
1:A:492:GLU:HB2	1:A:603:ALA:HB3	1.82	0.61
1:A:497:VAL:HG12	1:A:598:ARG:HB3	1.82	0.61
1:D:971:GLU:HA	1:D:1025:THR:HA	1.83	0.61
1:A:783:VAL:HB	1:A:851:TYR:HB2	1.82	0.61
1:C:357:VAL:HB	1:C:358:PRO:HD3	1.83	0.60
1:D:296:ALA:HB3	1:D:331:ILE:HG13	1.84	0.60
1:A:1191:LYS:O	1:A:1198:GLU:HA	2.02	0.59
1:B:6:VAL:HG21	1:B:41:VAL:HG13	1.84	0.59
1:A:3:ARG:HG2	1:A:61:GLN:HB3	1.84	0.59
1:B:255:ALA:HB1	1:B:262:LEU:HD11	1.85	0.59
1:D:362:CYS:HB3	1:D:400:ALA:HB2	1.84	0.59
1:A:1164:THR:HG23	1:A:1206:THR:HA	1.85	0.59
1:C:971:GLU:HA	1:C:1025:THR:HA	1.84	0.59
1:A:1257:VAL:HA	1:A:1273:THR:HG23	1.85	0.58
1:D:280:GLN:HE21	1:D:610:THR:HG22	1.69	0.58
1:B:378:LEU:HD21	1:B:401:ARG:HD3	1.84	0.58
1:D:1043:GLN:HG2	1:D:1111:ILE:HD12	1.86	0.58
1:A:932:GLU:HG2	1:A:954:LYS:HG3	1.85	0.58
1:B:822:ILE:HG23	1:B:1086:VAL:HB	1.85	0.58
1:D:255:ALA:HB1	1:D:262:LEU:HD11	1.86	0.57
1:C:932:GLU:HG2	1:C:954:LYS:HG3	1.86	0.57
1:D:3:ARG:HG2	1:D:61:GLN:HB3	1.85	0.57
1:A:296:ALA:HB3	1:A:331:ILE:HG13	1.87	0.57
1:B:357:VAL:HB	1:B:358:PRO:HD3	1.85	0.57
1:C:822:ILE:HG23	1:C:1086:VAL:HB	1.86	0.57
1:B:67:THR:HG22	1:B:267:PRO:HD3	1.86	0.57
1:C:296:ALA:HB3	1:C:331:ILE:HG13	1.86	0.57
1:D:357:VAL:HB	1:D:358:PRO:HD3	1.86	0.57
1:A:377:VAL:HG22	1:A:382:MET:HB2	1.87	0.57
1:C:1043:GLN:HG2	1:C:1111:ILE:HD12	1.87	0.57
1:A:822:ILE:HG23	1:A:1086:VAL:HB	1.88	0.56
1:D:551:GLY:N	1:D:733:ARG:HD2	2.20	0.56
1:D:420:LEU:HD22	1:D:632:GLN:HB2	1.86	0.56
1:D:822:ILE:HG23	1:D:1086:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:HIS:HE1	1:A:726:MET:HE3	1.71	0.56
1:D:783:VAL:HB	1:D:851:TYR:HB2	1.87	0.56
1:D:932:GLU:HG2	1:D:954:LYS:HG3	1.88	0.56
1:B:83:MET:HB2	1:B:118:ILE:HG21	1.87	0.55
1:B:932:GLU:HG2	1:B:954:LYS:HG3	1.88	0.55
1:B:475:VAL:HB	1:B:685:LEU:HB2	1.89	0.55
1:D:87:GLU:HA	1:D:125:THR:HB	1.89	0.55
1:C:1135:LEU:HD22	1:C:1149:ILE:HB	1.89	0.55
1:D:15:LEU:HB3	1:D:48:LEU:HD22	1.89	0.55
1:D:1191:LYS:O	1:D:1198:GLU:HA	2.06	0.55
1:D:475:VAL:HB	1:D:685:LEU:HB2	1.88	0.55
1:D:243:MET:HE2	1:D:487:LEU:HD23	1.89	0.54
1:B:296:ALA:HB3	1:B:331:ILE:HG13	1.89	0.54
1:D:389:ALA:HB2	1:D:665:TYR:O	2.07	0.54
1:B:758:MET:HG3	1:B:794:THR:HG21	1.89	0.54
1:C:3:ARG:HG2	1:C:61:GLN:HB3	1.88	0.54
1:B:1191:LYS:O	1:B:1198:GLU:HA	2.08	0.54
1:D:377:VAL:HG22	1:D:382:MET:HB2	1.90	0.54
1:D:67:THR:HG22	1:D:267:PRO:HD3	1.89	0.54
1:B:87:GLU:HA	1:B:125:THR:HB	1.88	0.54
1:C:83:MET:HB2	1:C:118:ILE:HG21	1.89	0.54
1:C:362:CYS:HB3	1:C:400:ALA:HB2	1.90	0.54
1:C:475:VAL:HB	1:C:685:LEU:HB2	1.90	0.54
1:C:1072:MET:HB2	1:C:1089:GLU:HB3	1.91	0.53
1:D:335:GLY:HA3	2:D:1301:ANP:O3'	2.08	0.53
1:D:752:GLU:HB2	1:D:760:MET:HG3	1.91	0.53
1:D:1072:MET:HB2	1:D:1089:GLU:HB3	1.90	0.53
1:D:1164:THR:HG23	1:D:1206:THR:HA	1.89	0.53
1:B:783:VAL:HB	1:B:851:TYR:HB2	1.90	0.53
1:B:1072:MET:HB2	1:B:1089:GLU:HB3	1.90	0.53
1:D:955:VAL:HG11	1:D:1053:LEU:HD11	1.90	0.53
1:A:1072:MET:HB2	1:A:1089:GLU:HB3	1.90	0.53
1:B:198:VAL:HG13	1:B:206:ARG:HG3	1.91	0.53
1:A:1228:ASP:HB3	1:A:1231:LYS:HD3	1.90	0.53
1:B:362:CYS:HB3	1:B:400:ALA:HB2	1.90	0.53
1:B:1071:PHE:HB3	1:B:1166:GLU:HB3	1.91	0.53
1:C:579:HIS:HE1	1:C:726:MET:HE3	1.74	0.53
1:D:1139:PRO:HB3	1:D:1246:THR:HA	1.91	0.53
1:B:551:GLY:N	1:B:733:ARG:HD2	2.24	0.52
1:C:955:VAL:HG11	1:C:1053:LEU:HD11	1.90	0.52
1:D:98:HIS:CD2	1:D:1116:ASN:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ALA:O	1:B:280:GLN:HG2	2.09	0.52
1:C:198:VAL:HG13	1:C:206:ARG:HG3	1.90	0.52
1:A:83:MET:HB2	1:A:118:ILE:HG21	1.92	0.52
1:A:243:MET:HE2	1:A:487:LEU:HD23	1.90	0.52
1:D:1257:VAL:HA	1:D:1273:THR:HG23	1.91	0.52
1:A:475:VAL:HB	1:A:685:LEU:HB2	1.90	0.52
1:A:1163:VAL:HG21	1:A:1210:LEU:HD12	1.91	0.52
1:B:98:HIS:CD2	1:B:1116:ASN:HB3	2.45	0.52
1:C:87:GLU:HA	1:C:125:THR:HB	1.90	0.52
1:B:613:ALA:HB1	1:B:652:ILE:HD11	1.92	0.52
1:B:1228:ASP:HB3	1:B:1231:LYS:HD3	1.92	0.52
1:A:198:VAL:HG13	1:A:206:ARG:HG3	1.92	0.52
1:A:955:VAL:HG11	1:A:1053:LEU:HD11	1.92	0.52
1:A:989:PHE:HA	1:A:992:ILE:HG22	1.91	0.52
1:D:83:MET:HB2	1:D:118:ILE:HG21	1.91	0.52
1:A:87:GLU:HA	1:A:125:THR:HB	1.91	0.52
1:C:243:MET:HE2	1:C:487:LEU:HD23	1.91	0.52
1:A:758:MET:HG3	1:A:794:THR:HG21	1.92	0.52
1:A:1065:ASN:HB3	1:A:1109:ASN:HD21	1.75	0.51
1:C:950:PRO:HD2	1:C:970:SER:HB2	1.93	0.51
1:B:1257:VAL:HA	1:B:1273:THR:HG23	1.91	0.51
1:B:1065:ASN:HB3	1:B:1109:ASN:HD21	1.75	0.51
1:B:994:ARG:HH11	1:B:1009:GLN:HG2	1.76	0.51
1:C:1139:PRO:HB3	1:C:1246:THR:HA	1.92	0.51
1:C:376:GLN:HG3	1:C:381:ARG:HB2	1.93	0.51
1:A:98:HIS:CD2	1:A:1116:ASN:HB3	2.46	0.50
1:B:243:MET:HE2	1:B:487:LEU:HD23	1.92	0.50
1:C:1065:ASN:HB3	1:C:1109:ASN:HD21	1.76	0.50
1:D:758:MET:HE3	1:D:984:THR:HG23	1.93	0.50
1:C:1228:ASP:HB3	1:C:1231:LYS:HD3	1.93	0.50
1:C:15:LEU:HB3	1:C:48:LEU:HD22	1.94	0.50
1:B:1135:LEU:HD22	1:B:1149:ILE:HB	1.94	0.50
1:D:1272:ALA:HA	1:D:1275:VAL:HG12	1.93	0.50
1:C:758:MET:HG3	1:C:794:THR:HG21	1.94	0.50
1:C:384:PRO:HA	1:C:395:MET:HB2	1.93	0.50
1:D:198:VAL:HG13	1:D:206:ARG:HG3	1.92	0.50
1:D:763:MET:HE3	1:D:800:ALA:HB1	1.93	0.50
1:D:1071:PHE:HB3	1:D:1166:GLU:HB3	1.93	0.50
1:B:83:MET:HE2	1:B:164:CYS:HB2	1.93	0.50
1:B:1272:ALA:HA	1:B:1275:VAL:HG22	1.93	0.50
1:C:31:PRO:HD3	1:C:391:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1228:ASP:HB3	1:D:1231:LYS:HD3	1.94	0.49
1:A:61:GLN:HE22	1:A:492:GLU:CD	2.20	0.49
1:A:1135:LEU:HD22	1:A:1149:ILE:HB	1.94	0.49
1:C:98:HIS:CD2	1:C:1116:ASN:HB3	2.46	0.49
1:D:83:MET:HE2	1:D:164:CYS:HB2	1.95	0.49
1:A:376:GLN:HG3	1:A:381:ARG:HB2	1.93	0.49
1:B:579:HIS:HE1	1:B:726:MET:HE3	1.77	0.49
1:B:1187:ALA:HB2	1:B:1221:PRO:HD3	1.94	0.49
1:C:61:GLN:HE22	1:C:492:GLU:CD	2.20	0.49
1:C:1257:VAL:HA	1:C:1273:THR:HG23	1.94	0.49
1:D:1135:LEU:HD22	1:D:1149:ILE:HB	1.95	0.49
1:C:551:GLY:N	1:C:733:ARG:HD2	2.27	0.49
1:D:659:PRO:HA	1:D:671:ILE:O	2.13	0.49
1:B:955:VAL:HG11	1:B:1053:LEU:HD11	1.95	0.49
1:B:1164:THR:HG23	1:B:1206:THR:HA	1.94	0.49
1:B:61:GLN:HE22	1:B:492:GLU:CD	2.20	0.48
1:C:783:VAL:HB	1:C:851:TYR:HB2	1.95	0.48
1:C:1071:PHE:HB3	1:C:1166:GLU:HB3	1.95	0.48
1:D:696:VAL:HG12	1:D:696:VAL:O	2.14	0.48
1:A:7:ASP:HA	1:A:65:GLY:O	2.14	0.48
1:A:994:ARG:HH11	1:A:1009:GLN:HG2	1.78	0.48
1:B:7:ASP:HA	1:B:65:GLY:O	2.14	0.48
1:D:614:THR:O	1:D:652:ILE:HG13	2.13	0.48
1:C:713:ASN:O	1:C:717:LYS:HG2	2.13	0.48
1:C:1187:ALA:HB2	1:C:1221:PRO:HD3	1.96	0.48
1:D:153:LEU:HD13	1:D:161:ILE:HG12	1.96	0.48
1:B:15:LEU:HB3	1:B:48:LEU:HD22	1.95	0.48
1:C:1248:THR:HG23	1:C:1259:LEU:HD12	1.96	0.48
1:D:527:LEU:HD22	1:D:537:ARG:HG2	1.95	0.48
1:A:1139:PRO:HB3	1:A:1246:THR:HA	1.94	0.48
1:C:752:GLU:HB2	1:C:760:MET:HG3	1.95	0.48
1:B:752:GLU:HB2	1:B:760:MET:HG3	1.95	0.48
1:D:1163:VAL:HG21	1:D:1210:LEU:HD12	1.95	0.47
1:C:989:PHE:HA	1:C:992:ILE:HG22	1.96	0.47
1:B:588:LYS:H	1:B:588:LYS:HD2	1.79	0.47
1:C:758:MET:HE3	1:C:984:THR:HG23	1.95	0.47
1:B:1139:PRO:HB3	1:B:1246:THR:HA	1.96	0.47
1:A:731:ILE:HG22	1:A:732:ILE:HG13	1.96	0.47
1:A:758:MET:HG2	1:A:1038:ARG:HH12	1.78	0.47
1:A:1272:ALA:HA	1:A:1275:VAL:HG12	1.97	0.47
1:C:1191:LYS:O	1:C:1198:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLN:HE22	1:D:492:GLU:CD	2.22	0.47
1:A:1261:THR:HA	1:A:1266:LEU:HA	1.97	0.47
1:B:1163:VAL:HG21	1:B:1210:LEU:HD12	1.97	0.47
1:D:9:GLY:HA3	2:D:1301:ANP:O1B	2.15	0.47
1:A:1071:PHE:HB3	1:A:1166:GLU:HB3	1.97	0.47
1:C:240:ILE:HB	1:C:252:ILE:HG13	1.97	0.47
1:D:588:LYS:H	1:D:588:LYS:HD2	1.80	0.47
1:B:758:MET:HE3	1:B:984:THR:HG23	1.96	0.46
1:D:1065:ASN:HB3	1:D:1109:ASN:HD21	1.80	0.46
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.81	0.46
1:D:376:GLN:HG3	1:D:381:ARG:HB2	1.97	0.46
1:D:731:ILE:HG22	1:D:732:ILE:HG13	1.96	0.46
1:A:164:CYS:HB3	1:A:207:PHE:CD1	2.50	0.46
1:C:246:SER:HB3	1:C:324:PRO:HB2	1.98	0.46
1:C:458:ALA:HB1	1:C:669:THR:HG23	1.98	0.46
1:C:659:PRO:HA	1:C:671:ILE:O	2.14	0.46
1:C:1163:VAL:HG21	1:C:1210:LEU:HD12	1.97	0.46
1:A:255:ALA:HB1	1:A:262:LEU:HD11	1.97	0.46
1:B:376:GLN:HG3	1:B:381:ARG:HB2	1.98	0.46
1:A:1068:HIS:CE1	1:A:1221:PRO:HD2	2.50	0.46
1:C:1164:THR:HG23	1:C:1206:THR:HA	1.96	0.46
1:D:527:LEU:HD13	1:D:537:ARG:HD3	1.96	0.46
1:C:719:MET:HE2	1:C:740:ALA:HB1	1.98	0.46
1:C:994:ARG:HH11	1:C:1009:GLN:HG2	1.81	0.46
1:D:994:ARG:HH11	1:D:1009:GLN:HG2	1.81	0.46
1:A:475:VAL:HG12	1:A:647:ARG:HH12	1.80	0.46
1:A:950:PRO:HD2	1:A:970:SER:HB2	1.96	0.46
1:D:7:ASP:HA	1:D:65:GLY:O	2.15	0.46
1:B:989:PHE:HA	1:B:992:ILE:HG22	1.97	0.46
1:D:167:HIS:HA	1:D:169:TYR:CE1	2.51	0.46
1:D:278:ALA:HB1	1:D:286:VAL:HG11	1.98	0.46
1:D:744:ASP:HB3	1:D:750:LEU:HD21	1.98	0.46
1:A:719:MET:SD	1:A:888:ALA:HB2	2.55	0.45
1:B:1261:THR:HA	1:B:1266:LEU:HA	1.97	0.45
1:C:749:VAL:HG12	1:C:1011:GLU:OE1	2.16	0.45
1:D:12:PHE:HB2	2:D:1301:ANP:O1A	2.16	0.45
1:A:758:MET:HE3	1:A:984:THR:HG23	1.99	0.45
1:B:436:GLN:HA	1:B:440:ARG:HG3	1.97	0.45
1:C:731:ILE:HG22	1:C:732:ILE:HG13	1.98	0.45
1:B:26:VAL:HG11	1:B:51:LYS:HB3	1.99	0.45
1:B:167:HIS:HA	1:B:169:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:SER:O	1:C:507:ALA:HB2	2.17	0.45
1:D:1248:THR:HG23	1:D:1259:LEU:HD12	1.98	0.45
1:A:551:GLY:N	1:A:733:ARG:HD2	2.31	0.45
1:B:638:VAL:HG12	1:B:640:LEU:HG	1.99	0.45
1:C:482:ILE:HA	1:C:485:ILE:HD12	1.99	0.45
1:C:926:ILE:HG13	1:C:997:PHE:HE1	1.81	0.45
1:A:713:ASN:O	1:A:717:LYS:HG2	2.17	0.45
1:B:659:PRO:HA	1:B:671:ILE:O	2.16	0.45
1:B:713:ASN:O	1:B:717:LYS:HG2	2.17	0.45
1:C:803:GLU:HB2	1:C:885:CYS:HB3	1.99	0.45
1:D:926:ILE:HG13	1:D:997:PHE:HE1	1.82	0.45
1:A:720:ALA:HB2	1:A:753:SER:HB2	1.99	0.45
1:C:26:VAL:HG11	1:C:51:LYS:HB3	1.98	0.45
1:B:153:LEU:HD13	1:B:161:ILE:HG12	1.98	0.44
1:A:145:GLU:O	1:A:149:ARG:HG2	2.17	0.44
1:B:360:PRO:HD2	1:B:363:TYR:CG	2.52	0.44
1:A:588:LYS:H	1:A:588:LYS:HD2	1.81	0.44
1:B:731:ILE:HG22	1:B:732:ILE:HG13	2.00	0.44
1:B:950:PRO:HD2	1:B:970:SER:HB2	1.99	0.44
1:C:1145:TYR:HA	1:C:1232:ARG:NH1	2.32	0.44
1:A:752:GLU:HB2	1:A:760:MET:HG3	1.99	0.44
1:A:926:ILE:HG13	1:A:997:PHE:HE1	1.82	0.44
1:B:360:PRO:O	1:B:363:TYR:HB2	2.18	0.44
1:C:228:GLN:HB2	1:C:252:ILE:HG21	1.99	0.44
1:A:167:HIS:HA	1:A:169:TYR:CE1	2.52	0.44
1:B:719:MET:HE2	1:B:740:ALA:HB1	1.99	0.44
1:B:1063:ALA:HB2	1:B:1226:PHE:CD2	2.53	0.44
1:B:1065:ASN:HB3	1:B:1109:ASN:ND2	2.33	0.44
1:A:15:LEU:HB3	1:A:48:LEU:HD22	1.99	0.44
1:A:1187:ALA:HB2	1:A:1221:PRO:HD3	1.99	0.44
1:B:278:ALA:CB	1:B:286:VAL:HG11	2.47	0.44
1:D:424:GLN:HE21	1:D:424:GLN:HB3	1.52	0.44
1:D:719:MET:HE2	1:D:740:ALA:HB1	1.98	0.44
1:A:659:PRO:HA	1:A:671:ILE:O	2.18	0.44
1:B:354:ALA:O	1:B:358:PRO:HD2	2.17	0.44
1:D:246:SER:HB3	1:D:324:PRO:HB2	1.99	0.44
1:D:702:PRO:HB2	1:D:703:ILE:H	1.71	0.44
1:D:1145:TYR:HA	1:D:1232:ARG:NH1	2.32	0.44
1:A:264:MET:HG3	1:A:267:PRO:HB2	1.99	0.44
1:D:713:ASN:O	1:D:717:LYS:HG2	2.17	0.44
1:D:795:HIS:CE1	1:D:1038:ARG:HH21	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:989:PHE:HA	1:D:992:ILE:HG22	2.00	0.44
1:D:1064:GLY:HA3	1:D:1176:TRP:O	2.18	0.44
1:B:475:VAL:HG12	1:B:647:ARG:HH12	1.82	0.43
1:B:926:ILE:HG13	1:B:997:PHE:HE1	1.83	0.43
1:C:387:ILE:HD11	1:C:391:SER:O	2.17	0.43
1:C:1132:ARG:O	1:C:1153:ARG:HA	2.18	0.43
1:D:749:VAL:HG12	1:D:1011:GLU:OE1	2.18	0.43
1:A:954:LYS:HB3	1:A:965:ASP:HB3	2.00	0.43
1:D:1068:HIS:CE1	1:D:1221:PRO:HD2	2.53	0.43
1:B:799:VAL:HG11	1:B:878:PHE:HE1	1.82	0.43
1:B:954:LYS:HB3	1:B:965:ASP:HB3	2.00	0.43
1:B:731:ILE:HD13	1:B:735:SER:HB2	2.01	0.43
1:C:799:VAL:HG11	1:C:878:PHE:HE1	1.83	0.43
1:A:731:ILE:HD13	1:A:735:SER:HB2	2.00	0.43
1:B:373:THR:HG23	1:B:382:MET:HE2	2.01	0.43
1:B:758:MET:HG2	1:B:1038:ARG:HH12	1.83	0.43
1:C:795:HIS:CE1	1:C:1038:ARG:HH21	2.37	0.43
1:C:1068:HIS:CE1	1:C:1221:PRO:HD2	2.54	0.43
1:D:34:PRO:HG2	1:D:357:VAL:HG22	2.01	0.43
1:D:278:ALA:CB	1:D:286:VAL:HG11	2.48	0.43
1:D:950:PRO:HD2	1:D:970:SER:HB2	1.99	0.43
1:D:1132:ARG:O	1:D:1153:ARG:HA	2.19	0.43
1:D:1187:ALA:HB2	1:D:1221:PRO:HD3	2.00	0.43
1:A:795:HIS:CE1	1:A:1038:ARG:HH21	2.37	0.43
1:C:378:LEU:HD21	1:C:415:ILE:HG12	2.01	0.43
1:C:564:THR:H	1:C:567:TRP:CB	2.32	0.43
1:D:766:ILE:HD11	1:D:793:ALA:HA	2.00	0.43
1:D:803:GLU:HB2	1:D:885:CYS:HB3	2.01	0.43
1:A:1205:VAL:HB	1:A:1208:ARG:HG3	2.00	0.43
1:C:164:CYS:HB3	1:C:207:PHE:CD1	2.54	0.43
1:A:691:ALA:O	1:A:693:THR:HG23	2.18	0.43
1:A:361:VAL:HA	1:A:367:GLY:HA3	2.00	0.43
1:D:326:VAL:HB	1:D:328:ILE:HD11	2.00	0.43
1:D:936:GLY:HA3	1:D:1048:LEU:HD11	2.01	0.43
1:C:610:THR:HA	1:C:611:PRO:HD3	1.94	0.42
1:C:1009:GLN:OE1	1:C:1013:MET:HG2	2.19	0.42
1:D:307:ARG:HH22	1:D:441:ARG:HH11	1.66	0.42
1:D:311:LEU:HG	1:D:322:MET:HG2	2.01	0.42
1:C:475:VAL:HG12	1:C:647:ARG:HH12	1.83	0.42
1:D:145:GLU:O	1:D:149:ARG:HG2	2.19	0.42
1:D:164:CYS:HB3	1:D:207:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:ILE:HG22	1:C:485:ILE:HG13	2.00	0.42
1:C:1205:VAL:HB	1:C:1208:ARG:HG3	2.01	0.42
1:D:475:VAL:HG12	1:D:647:ARG:HH12	1.84	0.42
1:B:795:HIS:CE1	1:B:797:PRO:HG2	2.54	0.42
1:C:7:ASP:HA	1:C:65:GLY:O	2.19	0.42
1:A:246:SER:HB3	1:A:324:PRO:HB2	2.01	0.42
1:B:879:GLN:HA	1:B:882:ILE:HD12	2.00	0.42
1:B:984:THR:HG22	1:B:1042:VAL:HG11	2.02	0.42
1:C:377:VAL:HG22	1:C:382:MET:HB2	2.01	0.42
1:C:588:LYS:H	1:C:588:LYS:HD2	1.84	0.42
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.86	0.42
1:A:749:VAL:HG12	1:A:1011:GLU:OE1	2.20	0.42
1:A:936:GLY:HA3	1:A:1048:LEU:HD11	2.01	0.42
1:B:749:VAL:HG12	1:B:1011:GLU:OE1	2.19	0.42
1:B:1068:HIS:CE1	1:B:1221:PRO:HD2	2.54	0.42
1:B:1205:VAL:HB	1:B:1208:ARG:HG3	2.00	0.42
1:C:153:LEU:HD13	1:C:161:ILE:HG12	2.01	0.42
1:A:270:GLY:HA2	1:A:483:ALA:HA	2.01	0.42
1:A:1065:ASN:HB3	1:A:1109:ASN:ND2	2.34	0.42
1:B:998:LEU:HD12	1:B:1013:MET:HE2	2.02	0.42
1:C:936:GLY:HA3	1:C:1048:LEU:HD11	2.01	0.42
1:A:388:LEU:HD13	1:A:395:MET:HE3	2.01	0.42
1:A:719:MET:HE2	1:A:740:ALA:HB1	2.02	0.42
1:C:1065:ASN:HB3	1:C:1109:ASN:ND2	2.35	0.42
1:D:284:GLU:H	1:D:284:GLU:HG2	1.72	0.42
1:A:799:VAL:HG11	1:A:878:PHE:HE1	1.84	0.42
1:B:1064:GLY:HA3	1:B:1176:TRP:O	2.18	0.42
1:C:261:THR:HA	1:C:323:VAL:HG11	2.02	0.42
1:C:783:VAL:HG11	1:C:882:ILE:HG12	2.02	0.42
1:D:831:LEU:HD12	1:D:1073:SER:HB2	2.02	0.42
1:A:763:MET:HE3	1:A:800:ALA:HB1	2.00	0.41
1:B:720:ALA:HB2	1:B:753:SER:HB2	2.02	0.41
1:B:803:GLU:HB2	1:B:885:CYS:HB3	2.01	0.41
1:B:1248:THR:HG23	1:B:1259:LEU:HD12	2.01	0.41
1:A:164:CYS:HB3	1:A:207:PHE:CE1	2.55	0.41
1:A:1238:LEU:HD13	1:A:1259:LEU:HD22	2.02	0.41
1:B:719:MET:SD	1:B:888:ALA:HB2	2.60	0.41
1:A:153:LEU:HD13	1:A:161:ILE:HG12	2.02	0.41
1:A:312:LEU:HD23	1:A:322:MET:HE3	2.03	0.41
1:B:744:ASP:HB3	1:B:750:LEU:HD21	2.01	0.41
1:C:527:LEU:HD13	1:C:537:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HA	1:A:393:LEU:O	2.21	0.41
1:A:803:GLU:HB2	1:A:885:CYS:HB3	2.02	0.41
1:C:167:HIS:HA	1:C:169:TYR:CE1	2.55	0.41
1:C:335:GLY:HA3	2:C:1301:ANP:O3'	2.20	0.41
1:C:763:MET:HE3	1:C:800:ALA:HB1	2.02	0.41
1:A:240:ILE:HB	1:A:252:ILE:HG13	2.02	0.41
1:A:507:ALA:HB1	1:A:512:ILE:HD11	2.02	0.41
1:B:386:ARG:HD2	1:B:663:GLU:CD	2.45	0.41
1:B:698:LYS:O	1:B:702:PRO:HA	2.20	0.41
1:C:203:GLU:HG2	1:C:204:TYR:N	2.34	0.41
1:D:228:GLN:HB2	1:D:252:ILE:HG21	2.03	0.41
1:A:503:SER:O	1:A:507:ALA:HB2	2.19	0.41
1:C:1064:GLY:HA3	1:C:1176:TRP:O	2.21	0.41
1:C:1238:LEU:HD22	1:C:1268:VAL:HG23	2.03	0.41
1:D:446:ARG:HA	1:D:471:PRO:HD3	2.01	0.41
1:D:954:LYS:HB3	1:D:965:ASP:HB3	2.02	0.41
1:A:96:ALA:HA	1:A:204:TYR:CE1	2.55	0.41
1:A:783:VAL:HG11	1:A:882:ILE:HG12	2.01	0.41
1:A:1064:GLY:HA3	1:A:1176:TRP:O	2.21	0.41
1:C:720:ALA:HB2	1:C:753:SER:HB2	2.03	0.41
1:B:1145:TYR:HA	1:B:1232:ARG:NH1	2.35	0.41
1:C:954:LYS:HB3	1:C:965:ASP:HB3	2.02	0.41
1:C:1003:PHE:HA	1:C:1004:PRO:HD3	1.96	0.41
1:D:1003:PHE:HA	1:D:1004:PRO:HD3	1.95	0.41
1:A:1111:ILE:H	1:A:1111:ILE:HG12	1.74	0.41
1:B:216:VAL:HG21	1:B:263:MET:HE2	2.03	0.41
1:B:284:GLU:H	1:B:284:GLU:HG2	1.70	0.41
1:C:96:ALA:HA	1:C:204:TYR:CE1	2.56	0.41
1:C:284:GLU:H	1:C:284:GLU:HG2	1.74	0.41
1:D:436:GLN:HA	1:D:440:ARG:HG3	2.02	0.41
1:D:481:ILE:HG22	1:D:485:ILE:HG13	2.03	0.41
1:B:1132:ARG:O	1:B:1153:ARG:HA	2.21	0.41
1:D:458:ALA:HB1	1:D:669:THR:HG23	2.02	0.41
1:D:579:HIS:HE1	1:D:726:MET:HE3	1.86	0.41
1:D:692:VAL:O	1:D:693:THR:C	2.64	0.41
1:D:717:LYS:HD3	1:D:753:SER:O	2.21	0.41
1:B:110:LEU:HD22	1:B:112:TRP:CZ2	2.56	0.40
1:B:326:VAL:HB	1:B:328:ILE:HD11	2.02	0.40
1:B:1142:ALA:HB3	1:B:1182:HIS:CG	2.56	0.40
1:D:378:LEU:HD21	1:D:415:ILE:HG12	2.03	0.40
1:D:96:ALA:HA	1:D:204:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:VAL:HG22	1:B:382:MET:HB2	2.03	0.40
1:D:503:SER:O	1:D:507:ALA:HB2	2.21	0.40
1:D:795:HIS:CE1	1:D:797:PRO:HG2	2.56	0.40
1:D:822:ILE:HD13	1:D:822:ILE:HA	1.97	0.40
1:B:610:THR:HA	1:B:611:PRO:HD3	1.97	0.40
1:C:357:VAL:CB	1:C:358:PRO:HD3	2.49	0.40
1:B:203:GLU:HG2	1:B:204:TYR:N	2.36	0.40
1:B:936:GLY:HA3	1:B:1048:LEU:HD11	2.04	0.40
1:D:799:VAL:HG11	1:D:878:PHE:HE1	1.85	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	1278/1288 (99%)	1225 (96%)	51 (4%)	2 (0%)	43	70
1	B	1274/1288 (99%)	1227 (96%)	45 (4%)	2 (0%)	43	70
1	C	1278/1288 (99%)	1224 (96%)	52 (4%)	2 (0%)	43	70
1	D	1278/1288 (99%)	1224 (96%)	52 (4%)	2 (0%)	43	70
All	All	5108/5152 (99%)	4900 (96%)	200 (4%)	8 (0%)	43	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	702	PRO
1	D	702	PRO
1	A	702	PRO
1	C	702	PRO
1	B	703	ILE
1	C	703	ILE

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Mol	Chain	Res	Type
1	A	703	ILE
1	D	703	ILE

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	1031/1039 (99%)	984 (95%)	47 (5%)	24	51
1	B	1030/1039 (99%)	987 (96%)	43 (4%)	26	54
1	C	1031/1039 (99%)	986 (96%)	45 (4%)	25	52
1	D	1031/1039 (99%)	981 (95%)	50 (5%)	23	50
All	All	4123/4156 (99%)	3938 (96%)	185 (4%)	24	52

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	59	ILE
1	A	61	GLN
1	A	208	SER
1	A	212	LEU
1	A	234	LEU
1	A	242	LEU
1	A	252	ILE
1	A	284	GLU
1	A	307	ARG
1	A	312	LEU
1	A	328	ILE
1	A	340	TYR
1	A	341	VAL
1	A	352	GLN
1	A	357	VAL
1	A	368	THR
1	A	369	GLU
1	A	376	GLN

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Mol	Chain	Res	Type
1	A	378	LEU
1	A	382	MET
1	A	387	ILE
1	A	396	ASP
1	A	401	ARG
1	A	488	LEU
1	A	555	ARG
1	A	591	THR
1	A	695	THR
1	A	725	ARG
1	A	731	ILE
1	A	758	MET
1	A	794	THR
1	A	799	VAL
1	A	994	ARG
1	A	1009	GLN
1	A	1013	MET
1	A	1014	LEU
1	A	1017	LEU
1	A	1038	ARG
1	A	1056	VAL
1	A	1068	HIS
1	A	1070	HIS
1	A	1105	ASP
1	A	1108	ASP
1	A	1117	ASN
1	A	1125	ARG
1	A	1261	THR
1	B	27	VAL
1	B	59	ILE
1	B	61	GLN
1	B	208	SER
1	B	212	LEU
1	B	234	LEU
1	B	242	LEU
1	B	252	ILE
1	B	284	GLU
1	B	307	ARG
1	B	312	LEU
1	B	328	ILE
1	B	352	GLN
1	B	357	VAL

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Mol	Chain	Res	Type
1	B	376	GLN
1	B	378	LEU
1	B	386	ARG
1	B	393	LEU
1	B	481	ILE
1	B	488	LEU
1	B	555	ARG
1	B	591	THR
1	B	636	LYS
1	B	696	VAL
1	B	699	LEU
1	B	725	ARG
1	B	731	ILE
1	B	758	MET
1	B	794	THR
1	B	799	VAL
1	B	994	ARG
1	B	1009	GLN
1	B	1013	MET
1	B	1014	LEU
1	B	1017	LEU
1	B	1038	ARG
1	B	1056	VAL
1	B	1068	HIS
1	B	1070	HIS
1	B	1105	ASP
1	B	1108	ASP
1	B	1117	ASN
1	B	1125	ARG
1	C	14	ASP
1	C	27	VAL
1	C	59	ILE
1	C	61	GLN
1	C	208	SER
1	C	212	LEU
1	C	234	LEU
1	C	242	LEU
1	C	252	ILE
1	C	284	GLU
1	C	307	ARG
1	C	312	LEU
1	C	340	TYR

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Mol	Chain	Res	Type
1	C	352	GLN
1	C	357	VAL
1	C	369	GLU
1	C	376	GLN
1	C	378	LEU
1	C	387	ILE
1	C	396	ASP
1	C	401	ARG
1	C	481	ILE
1	C	488	LEU
1	C	520	GLU
1	C	555	ARG
1	C	591	THR
1	C	695	THR
1	C	725	ARG
1	C	731	ILE
1	C	758	MET
1	C	794	THR
1	C	799	VAL
1	C	994	ARG
1	C	1009	GLN
1	C	1013	MET
1	C	1014	LEU
1	C	1017	LEU
1	C	1038	ARG
1	C	1056	VAL
1	C	1068	HIS
1	C	1070	HIS
1	C	1105	ASP
1	C	1108	ASP
1	C	1117	ASN
1	C	1125	ARG
1	D	23	ARG
1	D	27	VAL
1	D	59	ILE
1	D	61	GLN
1	D	208	SER
1	D	212	LEU
1	D	234	LEU
1	D	242	LEU
1	D	252	ILE
1	D	284	GLU

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Mol	Chain	Res	Type
1	D	307	ARG
1	D	312	LEU
1	D	328	ILE
1	D	340	TYR
1	D	341	VAL
1	D	352	GLN
1	D	357	VAL
1	D	369	GLU
1	D	376	GLN
1	D	378	LEU
1	D	382	MET
1	D	401	ARG
1	D	424	GLN
1	D	488	LEU
1	D	520	GLU
1	D	555	ARG
1	D	591	THR
1	D	602	ARG
1	D	614	THR
1	D	615	GLN
1	D	692	VAL
1	D	697	GLU
1	D	725	ARG
1	D	731	ILE
1	D	758	MET
1	D	794	THR
1	D	799	VAL
1	D	994	ARG
1	D	1009	GLN
1	D	1013	MET
1	D	1014	LEU
1	D	1017	LEU
1	D	1038	ARG
1	D	1056	VAL
1	D	1068	HIS
1	D	1070	HIS
1	D	1105	ASP
1	D	1108	ASP
1	D	1117	ASN
1	D	1125	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	102	HIS
1	A	107	GLN
1	A	134	HIS
1	A	633	GLN
1	A	748	ASN
1	A	857	GLN
1	A	1091	ASN
1	B	22	GLN
1	B	102	HIS
1	B	107	GLN
1	B	134	HIS
1	B	280	GLN
1	B	500	ASN
1	B	596	ASN
1	B	632	GLN
1	B	684	ASN
1	B	748	ASN
1	B	857	GLN
1	B	1091	ASN
1	C	22	GLN
1	C	102	HIS
1	C	107	GLN
1	C	134	HIS
1	C	500	ASN
1	C	596	ASN
1	C	632	GLN
1	C	748	ASN
1	C	857	GLN
1	C	863	HIS
1	C	879	GLN
1	C	1091	ASN
1	D	22	GLN
1	D	102	HIS
1	D	107	GLN
1	D	134	HIS
1	D	148	GLN
1	D	280	GLN
1	D	424	GLN
1	D	478	HIS
1	D	500	ASN
1	D	596	ASN
1	D	632	GLN

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Mol	Chain	Res	Type
1	D	694	GLN
1	D	857	GLN
1	D	879	GLN
1	D	1091	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic and 4 are modelled with single atom - leaving 4 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	ANP	B	1301	3	33,33,33	2.27	5 (15%)	45,52,52	1.02	4 (8%)
2	ANP	D	1301	3	33,33,33	2.19	5 (15%)	45,52,52	1.13	3 (6%)
2	ANP	C	1301	3	33,33,33	2.22	5 (15%)	45,52,52	1.13	3 (6%)
2	ANP	A	1301	3	33,33,33	2.20	5 (15%)	45,52,52	1.27	4 (8%)

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	ANP	B	1301	3	-	8/18/38/38	0/3/3/3
2	ANP	D	1301	3	-	8/18/38/38	0/3/3/3
2	ANP	C	1301	3	-	8/18/38/38	0/3/3/3
2	ANP	A	1301	3	-	8/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	ANP	PB-O3A	8.71	1.69	1.59
2	C	1301	ANP	PB-O3A	8.51	1.69	1.59
2	D	1301	ANP	PB-O3A	8.35	1.69	1.59
2	A	1301	ANP	PB-O3A	8.27	1.69	1.59
2	B	1301	ANP	PG-N3B	6.52	1.80	1.63
2	D	1301	ANP	PG-N3B	6.37	1.80	1.63
2	A	1301	ANP	PG-N3B	6.27	1.79	1.63
2	C	1301	ANP	PG-N3B	6.23	1.79	1.63
2	C	1301	ANP	PG-O1G	4.53	1.53	1.46
2	A	1301	ANP	PG-O1G	4.45	1.52	1.46
2	B	1301	ANP	PG-O1G	4.40	1.52	1.46
2	D	1301	ANP	PG-O1G	4.35	1.52	1.46
2	A	1301	ANP	PB-O1B	3.00	1.50	1.46
2	C	1301	ANP	PB-O1B	2.72	1.50	1.46
2	B	1301	ANP	PB-O1B	2.67	1.50	1.46
2	D	1301	ANP	PB-O1B	2.34	1.49	1.46
2	C	1301	ANP	PB-O2B	-2.24	1.50	1.56
2	D	1301	ANP	PB-O2B	-2.22	1.50	1.56
2	A	1301	ANP	PB-O2B	-2.16	1.51	1.56
2	B	1301	ANP	PB-O2B	-2.11	1.51	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	ANP	O1G-PG-N3B	-5.10	104.26	111.77
2	A	1301	ANP	O2B-PB-O1B	4.59	119.72	109.87
2	C	1301	ANP	O1G-PG-N3B	-4.14	105.68	111.77
2	D	1301	ANP	O2B-PB-O1B	4.00	118.44	109.87
2	D	1301	ANP	O1G-PG-N3B	-3.98	105.91	111.77
2	C	1301	ANP	O2B-PB-O1B	3.91	118.25	109.87
2	B	1301	ANP	O2B-PB-O1B	3.86	118.15	109.87
2	D	1301	ANP	O2G-PG-O3G	2.92	115.45	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	ANP	O1G-PG-N3B	-2.70	107.80	111.77
2	C	1301	ANP	O2G-PG-O3G	2.50	114.32	107.59
2	B	1301	ANP	O2G-PG-O3G	2.23	113.57	107.59
2	A	1301	ANP	O2G-PG-O3G	2.20	113.49	107.59
2	B	1301	ANP	O5'-C5'-C4'	2.11	116.18	108.99
2	A	1301	ANP	O5'-C5'-C4'	2.04	115.95	108.99

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ANP	PB-N3B-PG-O1G
2	A	1301	ANP	PA-O3A-PB-O2B
2	A	1301	ANP	C5'-O5'-PA-O1A
2	A	1301	ANP	C5'-O5'-PA-O3A
2	B	1301	ANP	PB-N3B-PG-O1G
2	B	1301	ANP	PG-N3B-PB-O3A
2	B	1301	ANP	PA-O3A-PB-O2B
2	B	1301	ANP	C5'-O5'-PA-O1A
2	B	1301	ANP	C5'-O5'-PA-O3A
2	C	1301	ANP	PB-N3B-PG-O1G
2	C	1301	ANP	PG-N3B-PB-O3A
2	C	1301	ANP	PA-O3A-PB-O2B
2	C	1301	ANP	C5'-O5'-PA-O1A
2	C	1301	ANP	C5'-O5'-PA-O3A
2	D	1301	ANP	PB-N3B-PG-O1G
2	D	1301	ANP	PG-N3B-PB-O3A
2	D	1301	ANP	PA-O3A-PB-O2B
2	D	1301	ANP	C5'-O5'-PA-O1A
2	D	1301	ANP	C5'-O5'-PA-O3A
2	A	1301	ANP	O4'-C4'-C5'-O5'
2	B	1301	ANP	O4'-C4'-C5'-O5'
2	C	1301	ANP	O4'-C4'-C5'-O5'
2	D	1301	ANP	O4'-C4'-C5'-O5'
2	A	1301	ANP	C3'-C4'-C5'-O5'
2	B	1301	ANP	C3'-C4'-C5'-O5'
2	C	1301	ANP	C3'-C4'-C5'-O5'
2	D	1301	ANP	C3'-C4'-C5'-O5'
2	A	1301	ANP	PG-N3B-PB-O3A
2	A	1301	ANP	O4'-C1'-N9-C8
2	B	1301	ANP	O4'-C1'-N9-C8
2	C	1301	ANP	O4'-C1'-N9-C8

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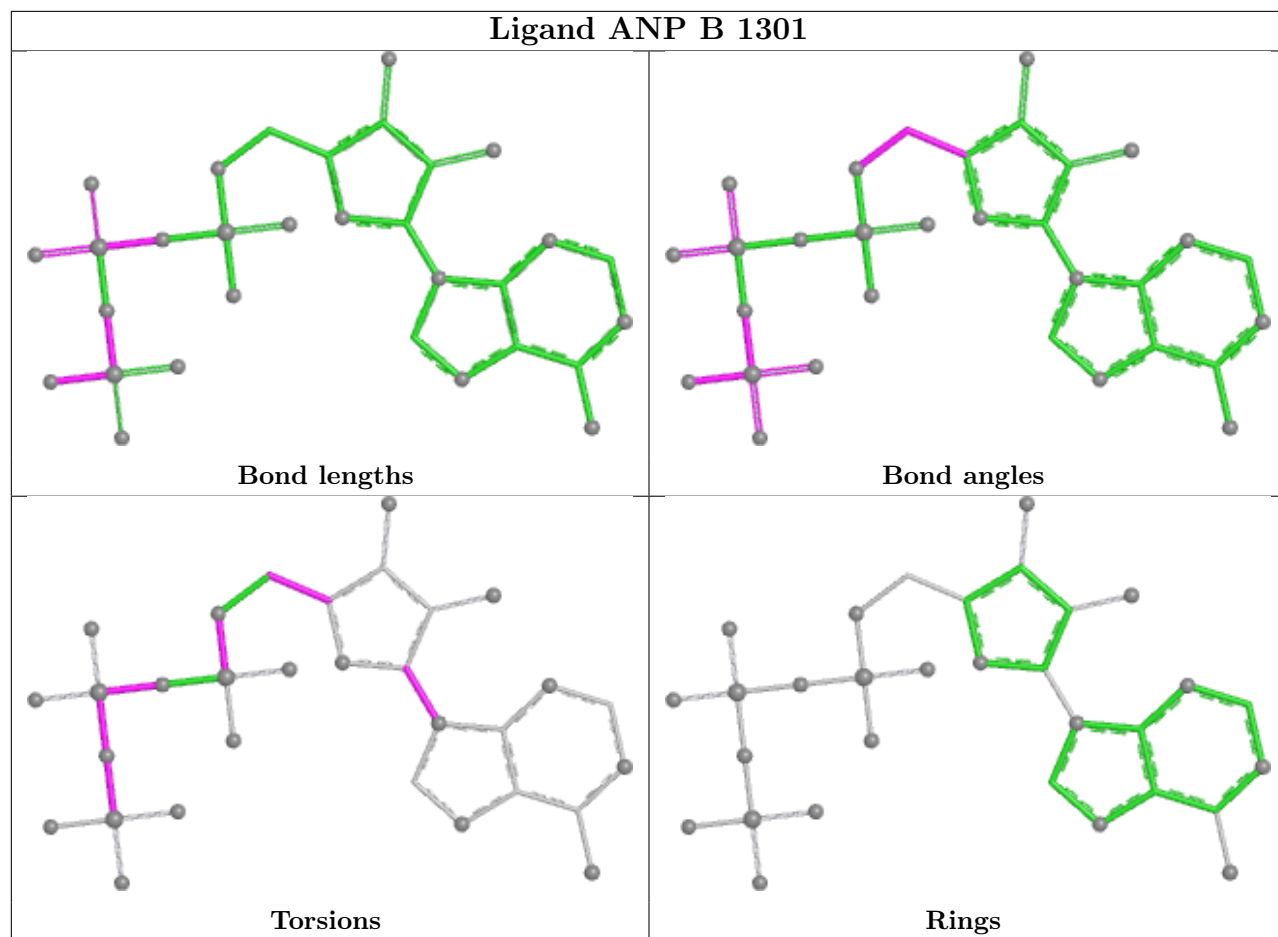
Mol	Chain	Res	Type	Atoms
2	D	1301	ANP	O4'-C1'-N9-C8

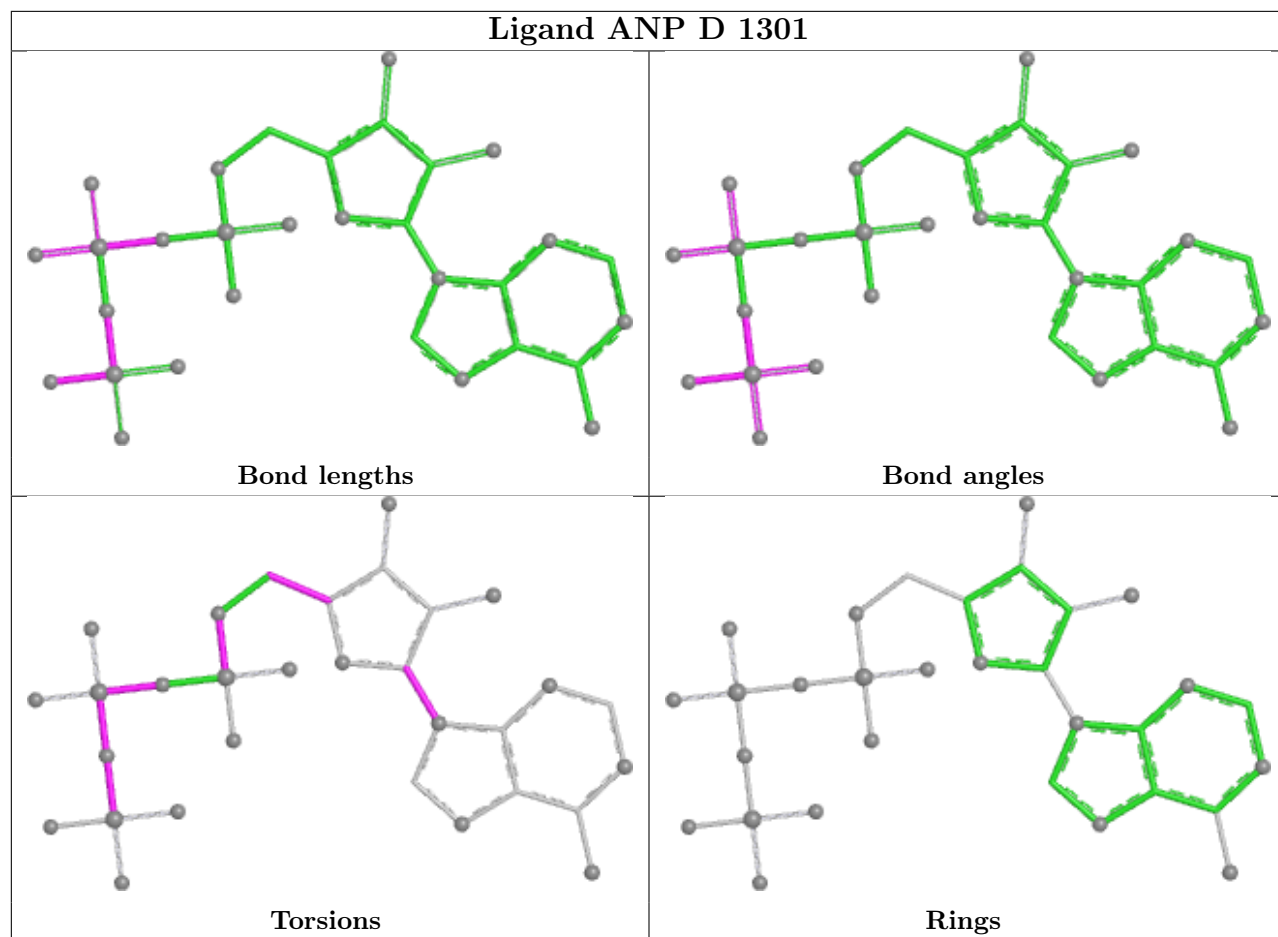
There are no ring outliers.

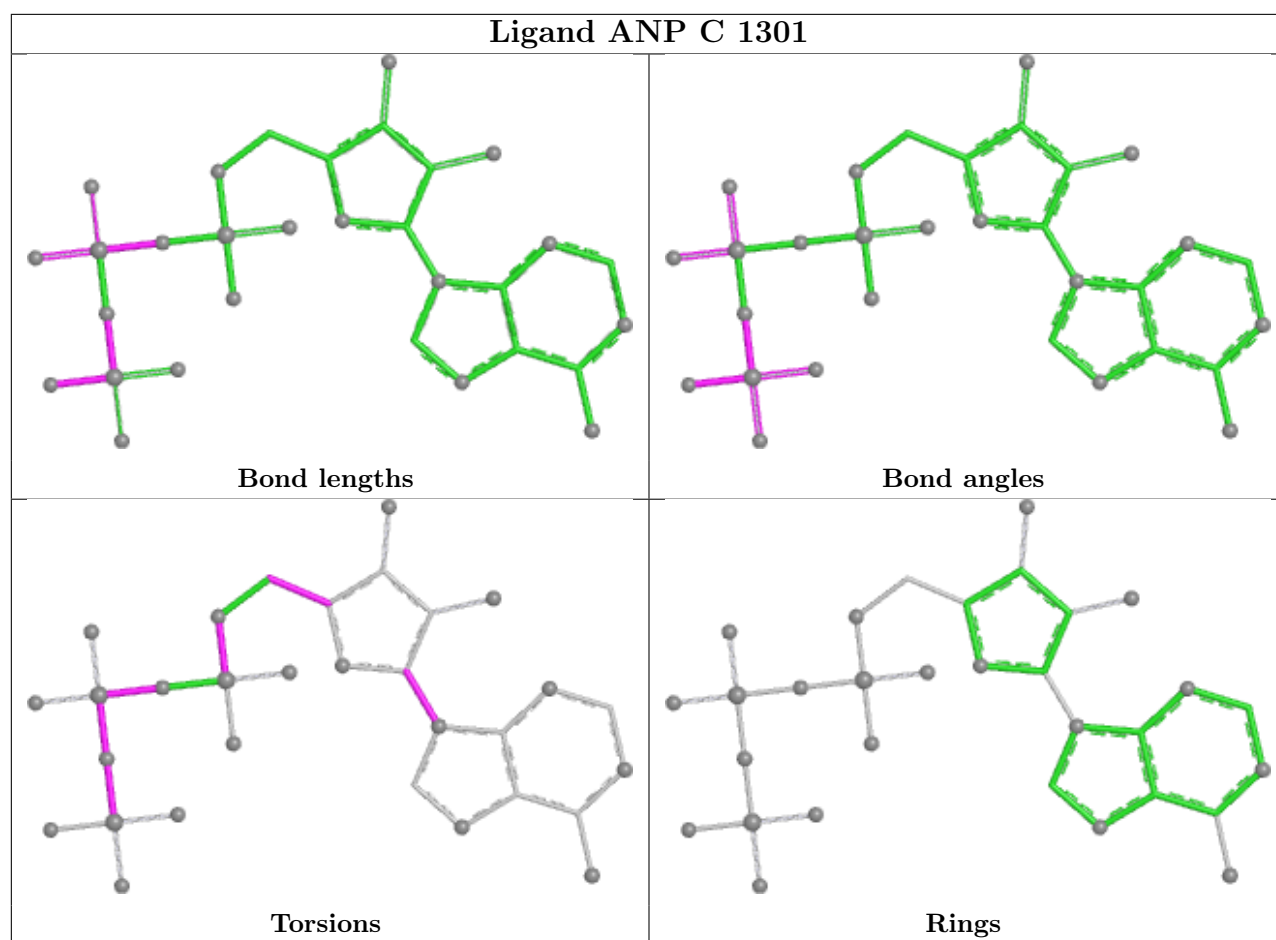
2 monomers are involved in 4 short contacts:

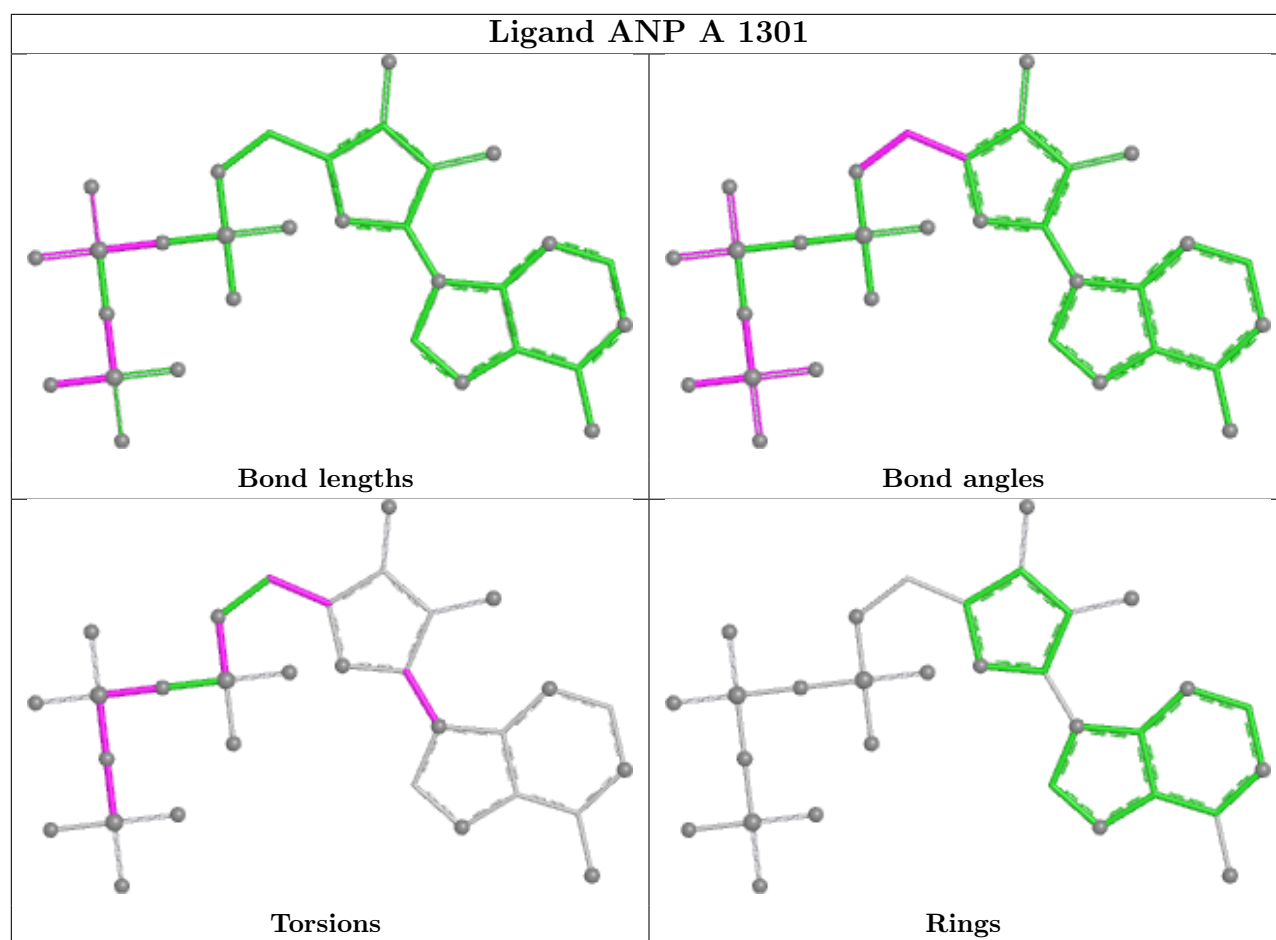
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301	ANP	3	0
2	C	1301	ANP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	1280/1288 (99%)	0.32	24 (1%)	66	45	28, 45, 83, 168	0
1	B	1278/1288 (99%)	0.47	42 (3%)	49	28	29, 52, 93, 149	0
1	C	1280/1288 (99%)	0.50	37 (2%)	53	32	34, 52, 102, 191	0
1	D	1280/1288 (99%)	0.45	33 (2%)	57	35	31, 52, 89, 141	0
All	All	5118/5152 (99%)	0.44	136 (2%)	56	34	28, 50, 92, 191	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	692	VAL	4.6
1	A	692	VAL	4.3
1	D	692	VAL	4.3
1	B	391	SER	4.0
1	B	754	ASP	3.9
1	D	754	ASP	3.9
1	B	697	GLU	3.8
1	C	506	SER	3.7
1	C	510	ALA	3.6
1	C	530	GLU	3.3
1	D	755	SER	3.2
1	C	694	GLN	3.2
1	D	691	ALA	3.2
1	A	500	ASN	3.2
1	A	437	ASN	3.2
1	D	695	THR	3.2
1	C	76	HIS	3.1
1	C	61	GLN	3.1
1	C	695	THR	3.1
1	A	530	GLU	3.1
1	B	709	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	754	ASP	3.0
1	C	696	VAL	3.0
1	C	563	VAL	3.0
1	D	1264	GLY	3.0
1	C	257	LYS	2.9
1	C	505	ALA	2.9
1	C	700	ALA	2.9
1	B	10	GLY	2.9
1	A	695	THR	2.9
1	A	755	SER	2.9
1	B	590	GLY	2.9
1	B	1263	ASN	2.9
1	B	614	THR	2.9
1	D	500	ASN	2.9
1	B	693	THR	2.8
1	A	697	GLU	2.8
1	B	725	ARG	2.8
1	C	508	ASP	2.8
1	C	754	ASP	2.8
1	C	1079	GLU	2.8
1	D	611	PRO	2.8
1	C	512	ILE	2.8
1	B	355	GLY	2.7
1	B	257	LYS	2.7
1	C	691	ALA	2.7
1	C	357	VAL	2.7
1	C	699	LEU	2.7
1	B	549	GLY	2.7
1	B	616	SER	2.7
1	B	1	MET	2.7
1	B	689	CYS	2.7
1	D	357	VAL	2.7
1	A	694	GLN	2.7
1	B	357	VAL	2.6
1	C	515	SER	2.6
1	D	373	THR	2.6
1	D	696	VAL	2.6
1	D	636	LYS	2.6
1	D	596	ASN	2.6
1	A	357	VAL	2.6
1	C	365	ARG	2.6
1	C	533	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	729	SER	2.5
1	A	566	ALA	2.5
1	D	1209	GLN	2.5
1	D	356	ALA	2.5
1	B	696	VAL	2.5
1	C	532	VAL	2.5
1	B	303	GLN	2.5
1	D	505	ALA	2.4
1	C	559	PRO	2.4
1	A	529	ALA	2.4
1	B	624	VAL	2.4
1	C	390	GLY	2.4
1	C	755	SER	2.4
1	B	317	GLY	2.4
1	C	507	ALA	2.4
1	D	506	SER	2.4
1	B	35	HIS	2.4
1	A	691	ALA	2.4
1	B	302	TYR	2.3
1	B	389	ALA	2.3
1	D	405	GLN	2.3
1	A	534	ALA	2.3
1	D	35	HIS	2.3
1	B	396	ASP	2.3
1	D	631	PHE	2.3
1	D	71	ASN	2.3
1	B	879	GLN	2.3
1	C	417	GLU	2.3
1	D	303	GLN	2.3
1	B	637	PRO	2.3
1	B	392	GLY	2.3
1	B	1272	ALA	2.3
1	C	57	SER	2.3
1	C	504	PHE	2.3
1	B	1264	GLY	2.2
1	A	35	HIS	2.2
1	A	230	GLN	2.2
1	B	248	GLY	2.2
1	B	1006	PHE	2.2
1	A	352	GLN	2.2
1	B	394	ASP	2.2
1	D	394	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	645	TYR	2.2
1	C	697	GLU	2.2
1	D	697	GLU	2.2
1	A	637	PRO	2.2
1	B	604	VAL	2.2
1	C	497	VAL	2.1
1	D	254	GLU	2.1
1	A	397	LEU	2.1
1	B	650	MET	2.1
1	D	263	MET	2.1
1	D	389	ALA	2.1
1	D	612	GLU	2.1
1	C	698	LYS	2.1
1	A	365	ARG	2.1
1	B	264	MET	2.1
1	A	495	GLU	2.1
1	A	696	VAL	2.1
1	B	1014	LEU	2.1
1	B	1210	LEU	2.1
1	C	693	THR	2.1
1	D	499	THR	2.1
1	B	22	GLN	2.1
1	D	344	GLY	2.1
1	D	358	PRO	2.1
1	B	1063	ALA	2.0
1	D	504	PHE	2.0
1	A	612	GLU	2.0
1	D	507	ALA	2.0
1	A	752	GLU	2.0
1	B	416	GLU	2.0
1	C	511	VAL	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

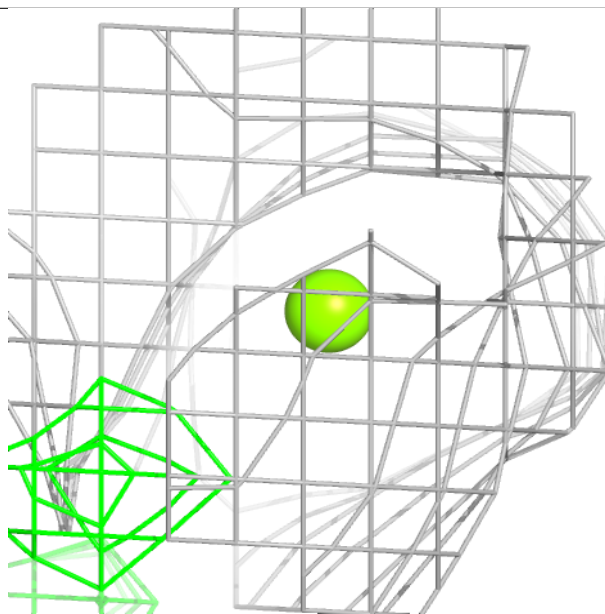
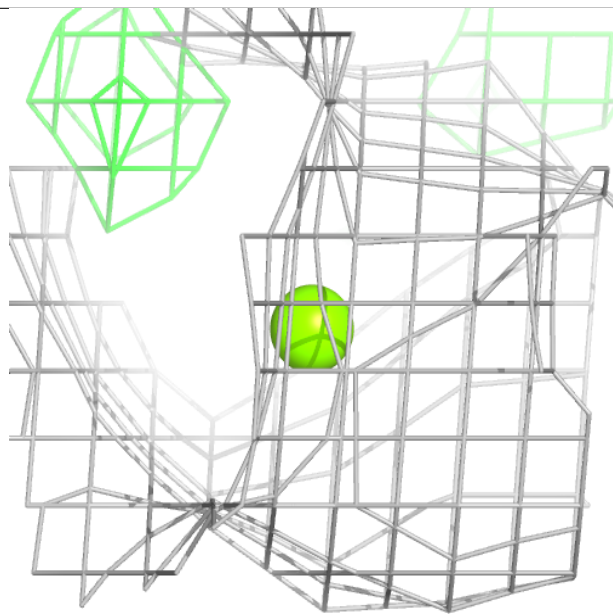
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NH4	C	1303	1/1	0.26	0.25	51,51,51,51	0
4	NH4	D	1303	1/1	0.55	0.18	55,55,55,55	0
4	NH4	A	1303	1/1	0.67	0.24	38,38,38,38	0
4	NH4	B	1303	1/1	0.73	0.17	48,48,48,48	0
3	MG	D	1302	1/1	0.89	0.08	59,59,59,59	0
2	ANP	D	1301	31/31	0.90	0.11	41,54,64,65	0
2	ANP	B	1301	31/31	0.90	0.12	45,60,68,69	0
2	ANP	C	1301	31/31	0.90	0.10	46,52,60,64	0
2	ANP	A	1301	31/31	0.94	0.08	38,43,47,52	0
3	MG	C	1302	1/1	0.95	0.06	47,47,47,47	0
3	MG	B	1302	1/1	0.95	0.05	64,64,64,64	0
3	MG	A	1302	1/1	0.97	0.05	50,50,50,50	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.

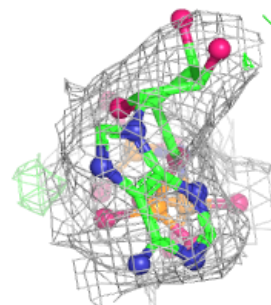
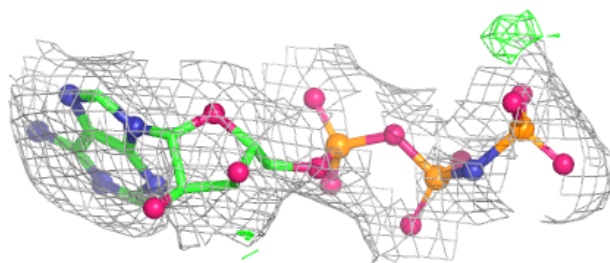
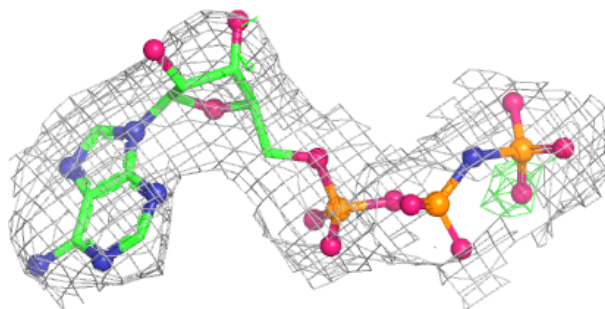
Electron density around MG D 1302:

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

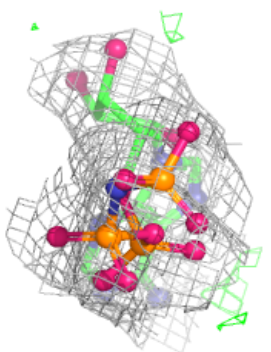
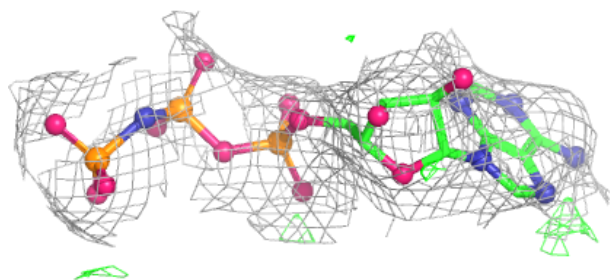
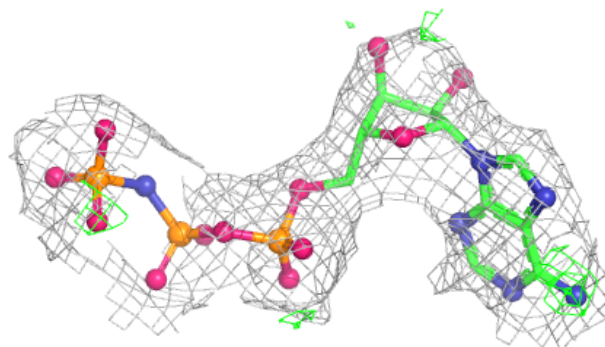


Electron density around ANP D 1301:

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

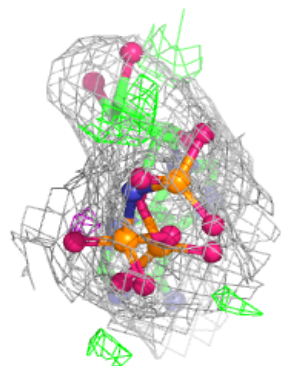
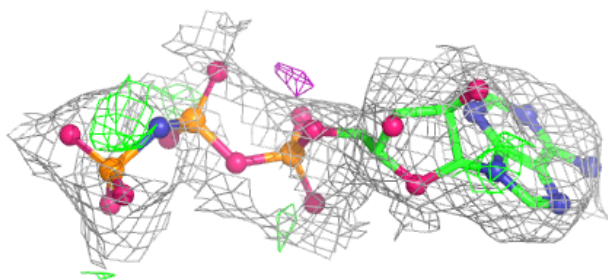
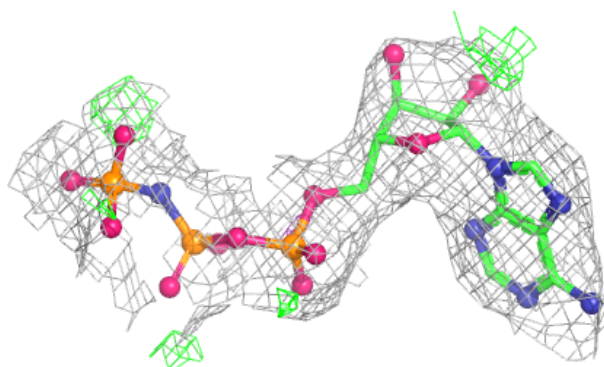
**Electron density around ANP B 1301:**

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

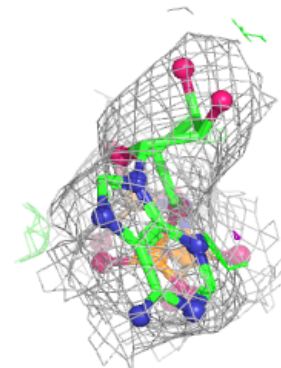
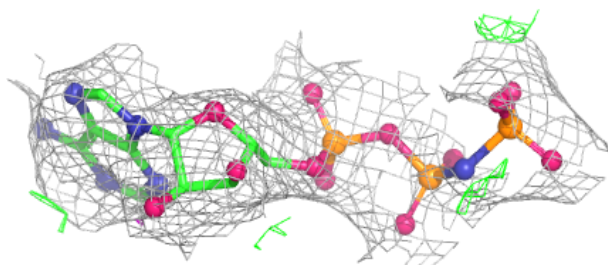
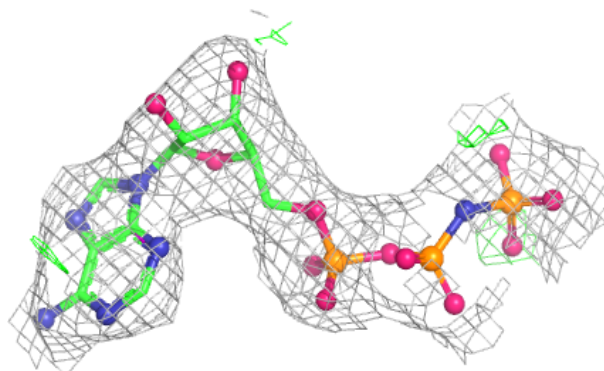


Electron density around ANP C 1301:

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

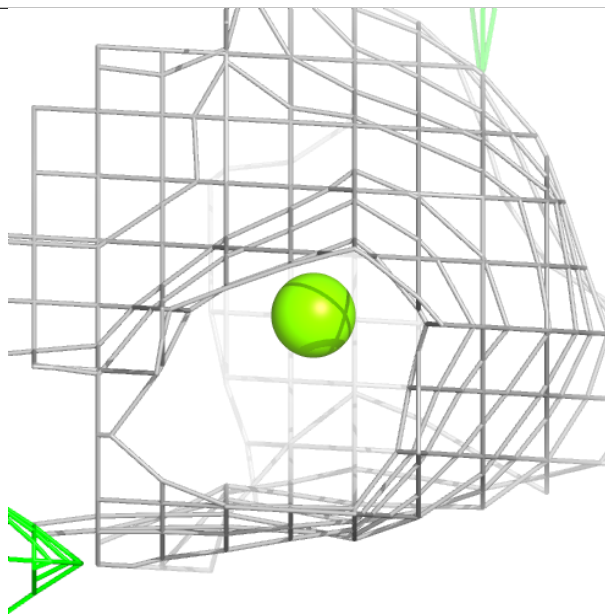
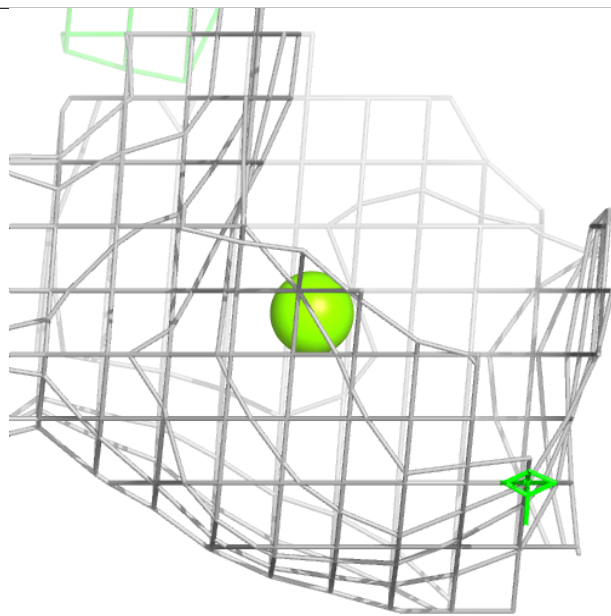
**Electron density around ANP A 1301:**

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



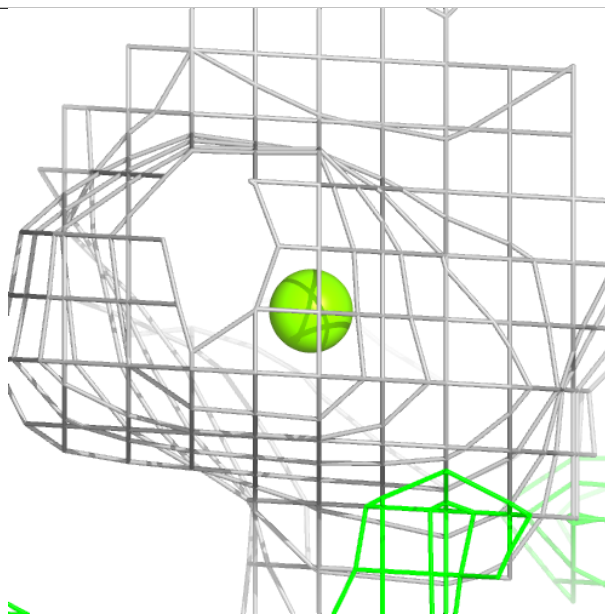
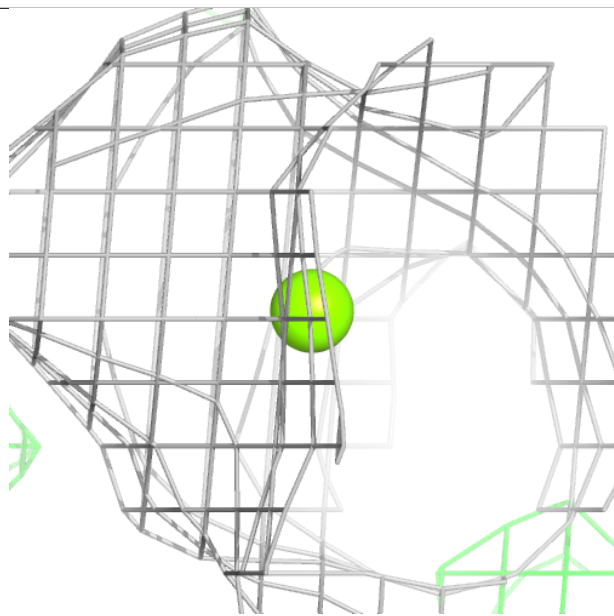
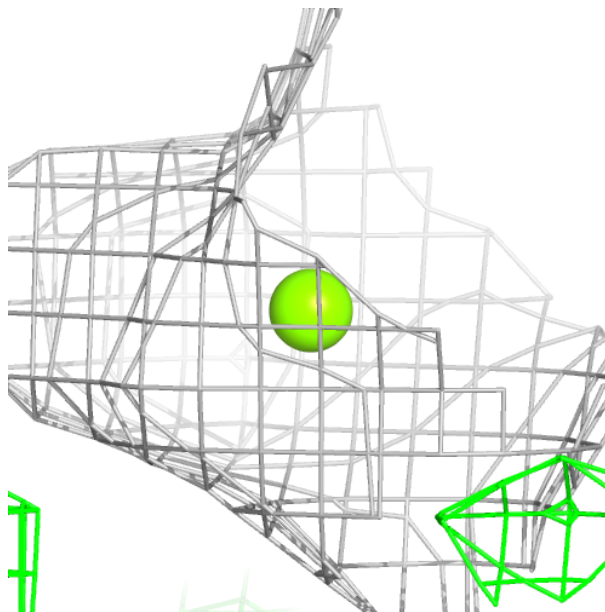
Electron density around MG C 1302:

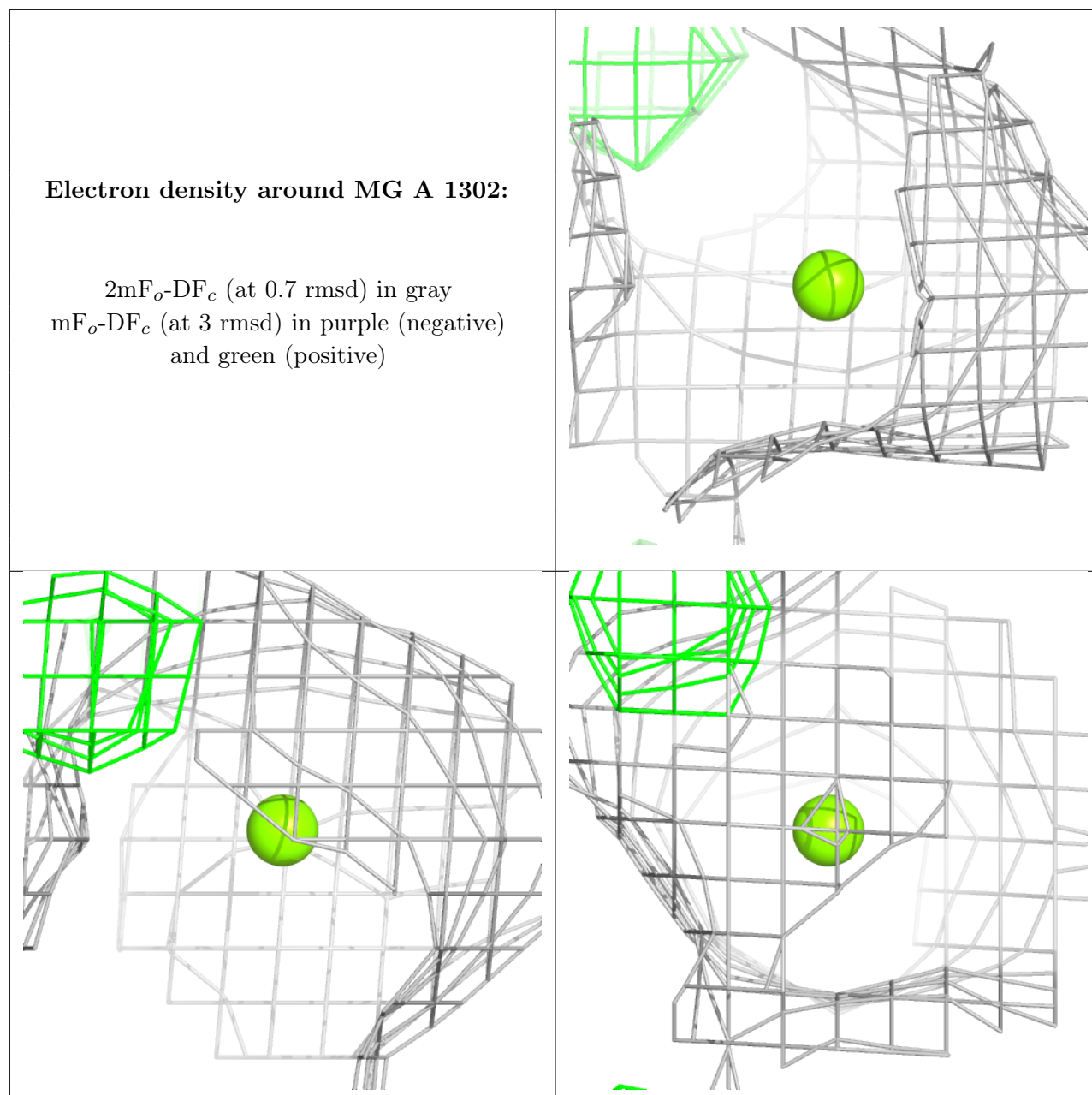
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 1302:

$2mF_o-DF_c$ (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.