



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:32 AM UTC

PDB ID : 1OXU / pdb_00001oxu
Title : Crystal structure of GlcV, the ABC-ATPase of the glucose ABC transporter from *Sulfolobus solfataricus*
Authors : Verdon, G.; Albers, S.V.; Dijkstra, B.W.; Driessen, A.J.; Thunnissen, A.M.
Deposited on : 2003-04-03
Resolution : 2.10 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

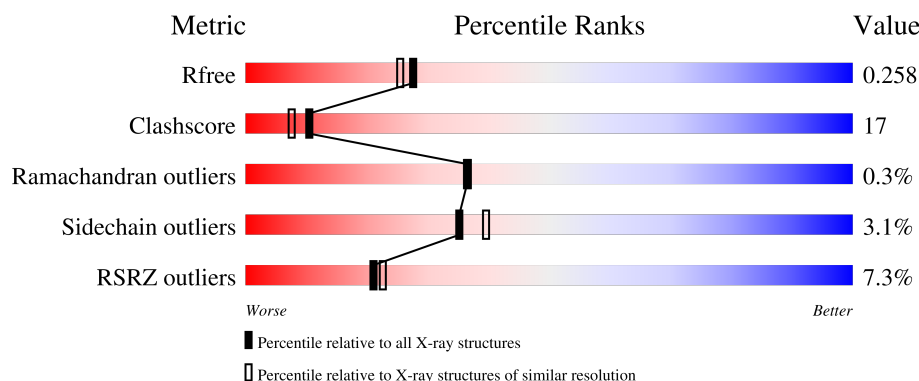
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	353	8% 80% 19% .
1	B	353	9% 71% 26% .
1	C	353	5% 80% 18% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	2016	-	-	X	-
3	IOD	A	2339	-	-	X	-
3	IOD	A	2387	-	-	X	-
3	IOD	B	2017	-	-	X	-
3	IOD	B	2037	-	-	X	-
3	IOD	B	2218	-	-	X	-
3	IOD	C	2004	-	-	X	-
3	IOD	C	2020	-	-	X	-
3	IOD	C	2233	-	-	X	-
3	IOD	C	2237	-	-	X	-
3	IOD	C	2541	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9045 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 ABC transporter, ATP binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2711	1737	468	500	6			
1	B	353	Total	C	N	O	S	0	1	0
			2697	1728	466	497	6			
1	C	353	Total	C	N	O	S	0	2	0
			2683	1715	462	500	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	I	0	0
			24	24		
3	B	15	Total	I	0	0
			15	15		
3	C	21	Total	I	0	0
			21	21		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

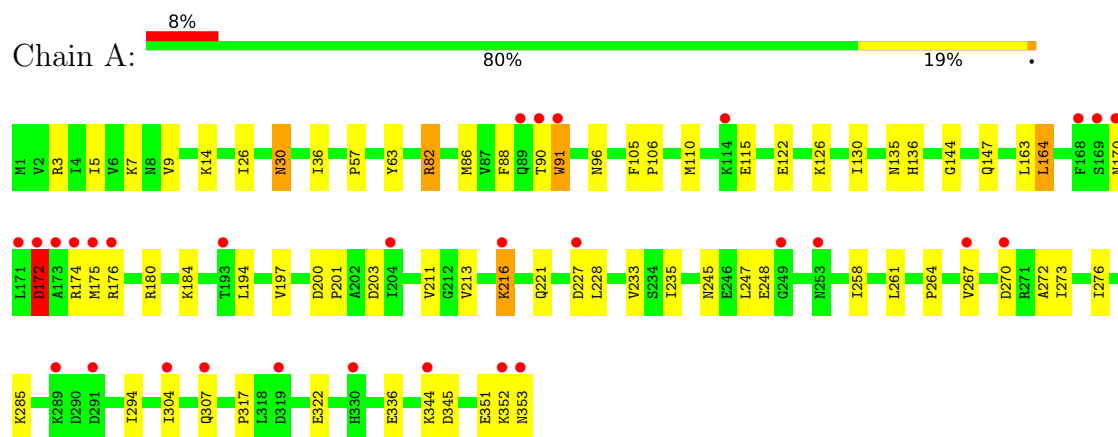
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total	O	0	0
			287	287		
5	B	226	Total	O	0	0
			226	226		
5	C	297	Total	O	0	0
			297	297		

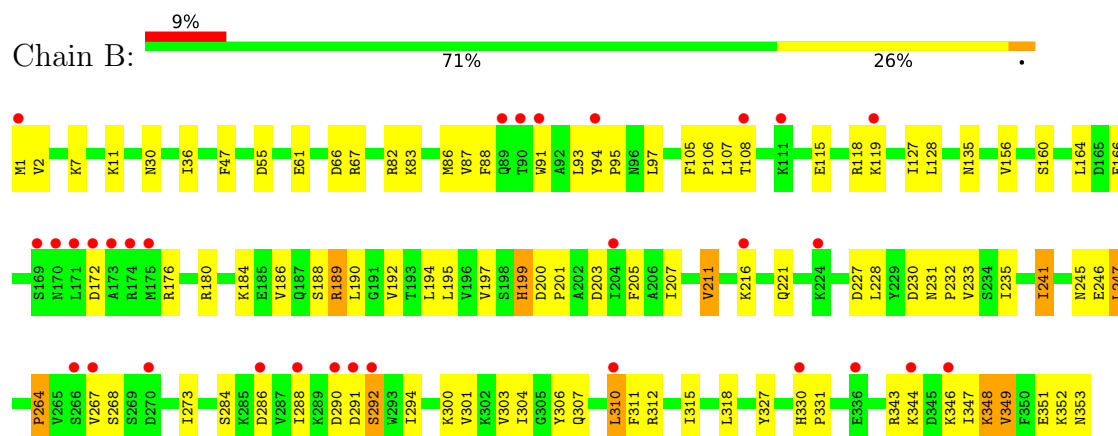
3 Residue-property plots [i](#)

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.

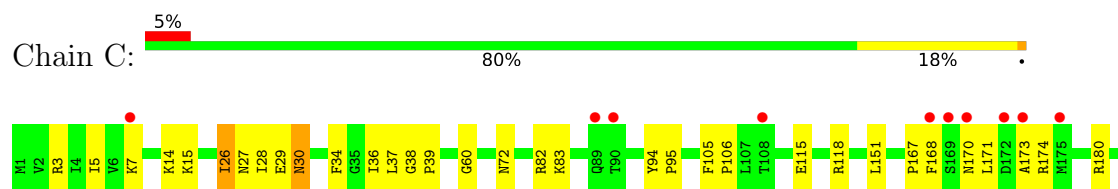
- Molecule 1: ABC transporter, ATP binding protein

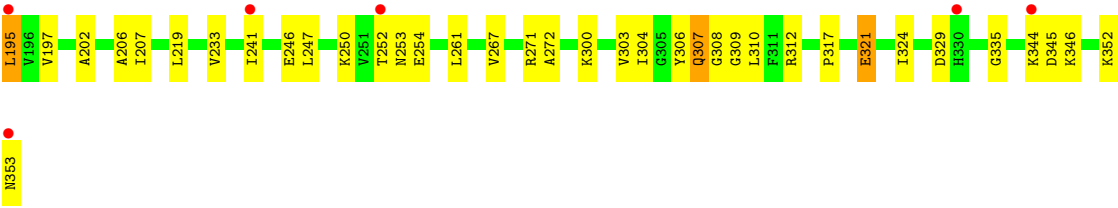


- Molecule 1: ABC transporter, ATP binding protein



- Molecule 1: ABC transporter, ATP binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.40Å 149.04Å 176.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.51 – 2.10 36.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.51-2.10) 98.9 (36.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.191 , 0.256 0.198 , 0.258	Depositor DCC
R_{free} test set	3749 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9045	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5829e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, 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	0.45	0/2756	0.89	3/3727 (0.1%)
1	B	0.39	0/2743	0.88	3/3712 (0.1%)
1	C	0.43	0/2729	0.90	2/3696 (0.1%)
All	All	0.43	0/8228	0.89	8/11135 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	PRO	N-CA-CB	8.34	108.08	102.25
1	C	174	ARG	N-CA-C	-6.53	104.25	111.36
1	C	207	ILE	N-CA-C	6.47	117.56	112.12
1	A	174	ARG	N-CA-C	-6.00	104.82	111.36
1	B	199	HIS	N-CA-C	-5.77	106.29	113.38
1	A	172	ASP	N-CA-C	-5.40	104.35	108.78
1	B	207	ILE	N-CA-C	5.26	118.22	112.96
1	A	82	ARG	CD-NE-CZ	-5.01	117.39	124.40

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	2711	0	2791	65	0
1	B	2697	0	2760	134	1
1	C	2683	0	2728	71	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	24	0	0	12	1
3	B	15	0	0	10	0
3	C	21	0	0	16	1
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
5	A	287	0	0	11	1
5	B	226	0	0	8	2
5	C	297	0	0	10	2
All	All	9045	0	8315	279	5

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 17.

All (279) 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:205:PHE:CE1	1:B:241:ILE:HD11	1.57	1.39
1:B:267:VAL:CG1	1:B:351:GLU:HG2	1.64	1.27
1:B:189:ARG:HB3	1:B:189:ARG:NH1	1.51	1.24
1:B:189:ARG:HH11	1:B:189:ARG:CB	1.52	1.22
1:B:246:GLU:C	1:B:247:LEU:HD13	1.64	1.21
3:C:2014:IOD:I	5:C:2929:HOH:O	2.35	1.12
1:B:273:ILE:HD11	1:B:352:LYS:CE	1.83	1.08
1:B:348:LYS:HE2	5:B:2932:HOH:O	1.51	1.07
1:C:252:THR:O	1:C:254:GLU:N	1.88	1.05
1:C:306:TYR:C	1:C:307:GLN:HG3	1.77	1.03
1:A:115:GLU:OE1	5:A:3251:HOH:O	1.74	1.03
1:B:273:ILE:HD11	1:B:352:LYS:HE2	1.40	1.03
1:B:221:GLN:OE1	1:B:233:VAL:HG23	1.58	1.03
1:B:135:ASN:OD1	5:B:3030:HOH:O	1.75	1.02
1:B:205:PHE:HE1	1:B:241:ILE:CD1	1.72	1.01
1:C:344:LYS:HD3	1:C:344:LYS:C	1.87	0.99
1:C:115:GLU:OE2	5:C:3071:HOH:O	1.77	0.99
1:B:205:PHE:CE1	1:B:241:ILE:CD1	2.46	0.98
1:C:14:LYS:NZ	3:C:2237:IOD:I	2.67	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2339:IOD:I	5:A:3193:HOH:O	2.53	0.97
1:B:273:ILE:HD11	1:B:352:LYS:NZ	1.79	0.97
1:B:205:PHE:CZ	1:B:241:ILE:HD11	2.00	0.96
1:B:267:VAL:HG11	1:B:351:GLU:HG2	1.48	0.95
1:B:189:ARG:HB3	1:B:189:ARG:HH11	0.78	0.94
1:A:270:ASP:OD1	5:A:3265:HOH:O	1.83	0.94
3:A:2288:IOD:I	5:A:3116:HOH:O	2.55	0.93
1:B:247:LEU:HD13	1:B:247:LEU:N	1.80	0.93
1:A:184:LYS:NZ	3:A:2016:IOD:I	2.73	0.91
1:C:27[A]:ASN:ND2	1:C:27[A]:ASN:OD1	2.03	0.91
1:B:205:PHE:HE1	1:B:241:ILE:HD11	0.97	0.91
1:B:127:ILE:HG21	1:B:189:ARG:HH21	1.34	0.90
1:B:211:VAL:HG13	1:B:228:LEU:HD11	1.51	0.90
1:B:221:GLN:CD	1:B:233:VAL:HG23	1.96	0.90
1:B:267:VAL:CG1	1:B:351:GLU:CG	2.50	0.89
1:B:246:GLU:C	1:B:247:LEU:CD1	2.46	0.89
3:A:2387:IOD:I	5:A:3151:HOH:O	2.61	0.87
1:B:267:VAL:HG13	1:B:351:GLU:HG2	1.55	0.86
1:C:344:LYS:HD3	1:C:344:LYS:O	1.75	0.86
1:B:105:PHE:O	1:B:108:THR:HG23	1.77	0.85
1:A:91:TRP:CZ2	1:A:147:GLN:OE1	2.31	0.84
1:B:294:ILE:HD13	1:B:344:LYS:HB2	1.58	0.84
1:B:93:LEU:O	1:B:95:PRO:HD3	1.80	0.82
1:B:273:ILE:CD1	1:B:352:LYS:HE2	2.10	0.82
1:C:344:LYS:C	1:C:344:LYS:CD	2.53	0.81
1:B:348:LYS:HD2	1:B:348:LYS:N	1.95	0.81
1:B:2:VAL:H	1:B:30[B]:ASN:ND2	1.80	0.79
3:C:2239:IOD:I	5:C:2927:HOH:O	2.71	0.78
1:A:30:ASN:HD22	1:A:30:ASN:H	1.32	0.77
1:A:294:ILE:HG13	1:A:344:LYS:HB2	1.66	0.76
1:C:261:LEU:HG	1:C:317:PRO:HB3	1.66	0.76
1:B:1:MET:HA	1:B:30[A]:ASN:ND2	2.00	0.76
1:C:82:ARG:O	3:C:2004:IOD:I	2.73	0.76
1:B:307:GLN:NE2	5:B:2868:HOH:O	2.12	0.76
1:C:30:ASN:HD22	1:C:30:ASN:H	1.33	0.76
1:C:202:ALA:HA	3:C:2233:IOD:I	2.56	0.76
1:A:82:ARG:O	3:A:2006:IOD:I	2.75	0.75
1:A:36:ILE:HB	1:A:197:VAL:HG12	1.68	0.75
1:A:175:MET:HE2	5:A:3139:HOH:O	1.86	0.75
1:A:285:LYS:NZ	1:A:336:GLU:OE1	2.20	0.74
1:C:28:ILE:HD13	1:C:195:LEU:CD2	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:TYR:O	1:B:307:GLN:HG3	1.86	0.74
1:C:170:ASN:O	1:C:171:LEU:HD23	1.87	0.74
1:C:94:TYR:HB3	3:C:2018:IOD:I	2.58	0.73
1:B:127:ILE:CG2	1:B:189:ARG:HH21	1.99	0.73
1:C:241:ILE:HD11	3:C:2253:IOD:I	2.59	0.73
1:B:105:PHE:HB3	1:B:106:PRO:HD3	1.71	0.72
3:B:2218:IOD:I	5:B:2992:HOH:O	2.77	0.72
1:A:172:ASP:O	1:A:176:ARG:HG3	1.90	0.72
1:C:306:TYR:O	1:C:307:GLN:HG3	1.90	0.72
1:B:82:ARG:O	3:B:2017:IOD:I	2.78	0.71
1:A:304:ILE:HG22	3:A:2011:IOD:I	2.60	0.71
1:B:346:LYS:O	1:B:348:LYS:HE3	1.90	0.71
1:A:216:LYS:HB2	1:A:216:LYS:NZ	2.06	0.70
1:B:211:VAL:HG13	1:B:228:LEU:CD1	2.21	0.69
1:A:105:PHE:HD2	3:A:2339:IOD:I	2.45	0.69
1:B:267:VAL:HG11	1:B:351:GLU:CG	2.18	0.69
1:C:28:ILE:HD13	1:C:195:LEU:HD23	1.75	0.69
1:B:267:VAL:HG13	1:B:351:GLU:CG	2.20	0.69
1:C:36:ILE:HB	1:C:197:VAL:HG12	1.75	0.68
1:A:184:LYS:CE	3:A:2016:IOD:I	3.11	0.68
1:B:30[B]:ASN:OD1	1:B:30[B]:ASN:ND2	2.25	0.68
1:B:267:VAL:CG2	1:B:349:VAL:HG22	2.23	0.68
1:B:310:LEU:C	1:B:310:LEU:HD12	2.18	0.68
1:B:7:LYS:HD2	1:B:61:GLU:OE2	1.94	0.68
1:A:30:ASN:H	1:A:30:ASN:ND2	1.89	0.68
1:A:216:LYS:HB2	1:A:216:LYS:HZ2	1.59	0.67
1:A:26:ILE:HD12	3:A:2010:IOD:I	2.64	0.67
1:B:1:MET:HE3	1:B:192:VAL:HG12	1.77	0.67
1:B:304:ILE:HG22	3:B:2037:IOD:I	2.65	0.67
1:C:246[A]:GLU:OE1	1:C:246[A]:GLU:OE2	2.13	0.66
1:A:105:PHE:HB3	1:A:106:PRO:HD3	1.78	0.66
1:C:250:LYS:HD3	1:C:271:ARG:NH1	2.10	0.66
1:A:110:MET:HE1	5:A:3239:HOH:O	1.96	0.65
1:C:304:ILE:HG22	3:C:2020:IOD:I	2.66	0.65
1:B:310:LEU:HD11	1:B:327:TYR:CD2	2.31	0.65
1:B:306:TYR:C	1:B:307:GLN:HG3	2.21	0.65
1:B:83:LYS:HB2	3:B:2017:IOD:I	2.67	0.64
1:C:30:ASN:H	1:C:30:ASN:ND2	1.92	0.63
1:B:264:PRO:HB2	1:B:344:LYS:NZ	2.13	0.63
1:B:1:MET:CE	1:B:192:VAL:HG12	2.28	0.63
1:A:267:VAL:CG2	1:A:272:ALA:HB2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD13	1:B:327:TYR:HB3	1.81	0.62
1:A:247:LEU:HD12	1:A:322:GLU:HB3	1.80	0.61
1:B:241:ILE:HG13	1:B:241:ILE:O	1.99	0.61
1:B:267:VAL:HG12	1:B:351:GLU:HG2	1.77	0.60
1:B:343:ARG:HH11	1:B:343:ARG:HG2	1.66	0.60
1:C:3:ARG:NH1	1:C:29:GLU:OE2	2.35	0.60
1:C:352:LYS:O	1:C:353:ASN:C	2.43	0.60
1:B:186:VAL:HA	1:B:189:ARG:HH12	1.68	0.59
1:C:28:ILE:HD13	1:C:195:LEU:HD21	1.84	0.59
1:B:221:GLN:CD	1:B:233:VAL:CG2	2.74	0.59
1:B:294:ILE:HD13	1:B:344:LYS:CB	2.30	0.59
1:A:221:GLN:HE22	1:A:233:VAL:H	1.50	0.58
1:B:194:LEU:HD23	1:B:194:LEU:C	2.29	0.58
3:C:2049:IOD:I	5:C:3092:HOH:O	2.87	0.58
1:C:5:ILE:HG21	1:C:7:LYS:HE3	1.85	0.58
1:C:345:ASP:N	5:C:3006:HOH:O	2.24	0.58
1:A:91:TRP:HZ2	1:A:147:GLN:OE1	1.85	0.57
1:A:264:PRO:CG	1:A:344:LYS:HZ3	2.17	0.57
1:B:267:VAL:HG23	1:B:349:VAL:CG2	2.33	0.57
3:C:2541:IOD:I	5:C:3068:HOH:O	2.87	0.57
1:C:34:PHE:HB3	1:C:195:LEU:HD22	1.86	0.57
1:B:186:VAL:HA	1:B:189:ARG:NH1	2.20	0.57
1:A:264:PRO:HB2	1:A:344:LYS:NZ	2.20	0.56
1:B:189:ARG:NH1	1:B:189:ARG:CB	2.34	0.56
1:B:36:ILE:HB	1:B:197:VAL:HG12	1.88	0.56
1:A:176:ARG:HD2	1:A:180:ARG:NH2	2.21	0.55
1:B:205:PHE:CZ	1:B:241:ILE:CD1	2.85	0.55
1:C:309:GLY:C	1:C:310:LEU:HD12	2.32	0.55
1:B:216:LYS:HE3	5:B:3020:HOH:O	2.05	0.55
1:B:311:PHE:CZ	1:B:331:PRO:HG3	2.42	0.54
1:B:93:LEU:O	1:B:95:PRO:CD	2.53	0.54
1:C:303:VAL:HG23	3:C:2020:IOD:I	2.77	0.54
1:C:306:TYR:C	1:C:307:GLN:CG	2.64	0.54
1:C:151:LEU:HD21	3:C:2008:IOD:I	2.79	0.53
1:B:86:MET:N	3:B:2015:IOD:I	3.03	0.53
1:B:211:VAL:CG1	1:B:228:LEU:CD1	2.87	0.53
1:B:2:VAL:N	1:B:30[B]:ASN:ND2	2.53	0.53
1:B:303:VAL:HG23	3:B:2037:IOD:I	2.79	0.53
1:C:5:ILE:HG21	1:C:7:LYS:CE	2.38	0.53
1:A:264:PRO:HB2	1:A:344:LYS:HZ3	1.73	0.53
1:B:188:SER:OG	3:B:2218:IOD:I	2.95	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:VAL:HG23	1:A:228:LEU:HD21	1.91	0.52
1:C:167:PRO:HG2	1:C:168:PHE:CD1	2.44	0.52
1:A:135:ASN:OD1	1:A:136:HIS:HD2	1.92	0.52
1:B:1:MET:HE1	5:B:2913:HOH:O	2.09	0.52
1:B:190:LEU:HD11	3:B:2021:IOD:I	2.80	0.52
1:C:308:GLY:O	1:C:310:LEU:HD13	2.10	0.52
1:B:284:SER:OG	1:B:286:ASP:O	2.26	0.52
1:B:310:LEU:CD1	1:B:327:TYR:HB3	2.40	0.51
1:B:288:ILE:HG22	1:B:290:ASP:H	1.75	0.51
1:A:14:LYS:HE2	5:A:3176:HOH:O	2.09	0.51
1:B:30[A]:ASN:ND2	1:B:30[A]:ASN:OD1	2.44	0.51
1:A:122:GLU:O	1:A:126:LYS:HG3	2.10	0.51
1:B:88:PHE:O	1:B:91:TRP:HB3	2.10	0.51
1:A:267:VAL:HG21	1:A:272:ALA:HB2	1.93	0.51
1:C:247:LEU:HD21	1:C:324:ILE:HG13	1.93	0.51
1:C:321:GLU:HG2	5:C:3119:HOH:O	2.10	0.51
1:B:347:ILE:C	1:B:348:LYS:HD2	2.35	0.51
1:A:352:LYS:O	1:A:353:ASN:C	2.53	0.51
1:B:348:LYS:N	1:B:348:LYS:CD	2.71	0.51
1:B:352:LYS:HD3	1:B:353:ASN:N	2.26	0.50
1:A:144:GLY:HA3	3:A:2387:IOD:I	2.81	0.50
1:B:290:ASP:OD2	1:B:292:SER:CB	2.59	0.50
1:A:285:LYS:NZ	1:A:336:GLU:CD	2.69	0.50
1:C:105:PHE:HB3	1:C:106:PRO:HD3	1.94	0.50
1:B:301:VAL:HA	1:B:315:ILE:HG22	1.93	0.50
1:C:168:PHE:HB3	1:C:171:LEU:HD12	1.94	0.50
1:B:267:VAL:HG23	1:B:349:VAL:HG22	1.91	0.50
1:B:267:VAL:CG2	1:B:349:VAL:CG2	2.90	0.49
1:B:273:ILE:CG1	1:B:352:LYS:HE2	2.41	0.49
1:C:312:ARG:NH1	5:C:3039:HOH:O	2.37	0.49
1:B:211:VAL:CG1	1:B:228:LEU:HD11	2.33	0.49
1:B:267:VAL:HG21	1:B:349:VAL:HG22	1.93	0.48
1:A:3:ARG:CG	1:A:30:ASN:HD22	2.27	0.48
1:A:267:VAL:HG22	1:A:272:ALA:HB2	1.95	0.48
1:B:346:LYS:O	1:B:348:LYS:CE	2.59	0.48
1:A:164:LEU:HD22	1:A:194:LEU:HD11	1.95	0.48
1:C:28:ILE:CD1	1:C:195:LEU:HD21	2.43	0.48
1:B:246:GLU:CA	1:B:247:LEU:HD13	2.40	0.48
1:A:221:GLN:NE2	1:A:233:VAL:H	2.11	0.48
1:A:345:ASP:N	5:A:3161:HOH:O	2.36	0.48
1:B:273:ILE:HD11	1:B:352:LYS:HZ3	1.76	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PHE:CE1	1:B:331:PRO:HG3	2.49	0.47
1:C:27[B]:ASN:OD1	1:C:27[B]:ASN:ND2	2.47	0.47
1:A:216:LYS:NZ	1:A:216:LYS:CB	2.76	0.47
1:A:264:PRO:CB	1:A:344:LYS:HZ3	2.26	0.47
1:C:118:ARG:HG2	1:C:118:ARG:HH11	1.79	0.47
1:B:352:LYS:HD3	1:B:353:ASN:H	1.79	0.47
1:A:90:THR:O	1:A:91:TRP:C	2.58	0.46
1:C:118:ARG:HG2	1:C:118:ARG:NH1	2.31	0.46
1:A:276:ILE:HG23	1:A:276:ILE:O	2.15	0.46
1:A:345:ASP:HB2	5:A:3161:HOH:O	2.15	0.46
1:A:7:LYS:HG3	5:A:3053:HOH:O	2.15	0.46
1:B:235:ILE:HD11	1:B:246:GLU:HG2	1.97	0.46
1:A:88:PHE:O	1:A:91:TRP:HB3	2.16	0.46
1:B:189:ARG:HH11	1:B:189:ARG:CG	2.20	0.46
1:C:83:LYS:HB2	3:C:2004:IOD:I	2.86	0.46
1:C:252:THR:C	1:C:254:GLU:N	2.68	0.46
1:C:306:TYR:O	1:C:307:GLN:CG	2.61	0.46
1:B:67:ARG:NE	3:B:2019:IOD:I	3.12	0.46
1:B:184:LYS:HG2	3:B:2218:IOD:I	2.85	0.46
1:B:343:ARG:HG2	1:B:343:ARG:NH1	2.30	0.46
1:A:213:VAL:HG23	1:A:228:LEU:CD2	2.46	0.45
1:B:94:TYR:HB3	1:B:97:LEU:HG	1.98	0.45
1:C:60:GLY:H	1:C:72:ASN:ND2	2.14	0.45
1:A:245:ASN:HB2	1:A:276:ILE:HG23	1.98	0.45
1:B:273:ILE:HD11	1:B:352:LYS:HZ1	1.72	0.45
1:B:310:LEU:C	1:B:310:LEU:CD1	2.89	0.45
1:B:343:ARG:NE	5:B:2845:HOH:O	2.49	0.45
1:A:261:LEU:HG	1:A:317:PRO:HB3	1.97	0.45
1:C:241:ILE:O	1:C:241:ILE:HG13	2.15	0.45
1:B:246:GLU:O	1:B:247:LEU:CD1	2.63	0.45
1:B:94:TYR:HB2	1:B:97:LEU:HB2	1.99	0.45
1:B:115:GLU:O	1:B:119:LYS:HG3	2.17	0.45
1:A:96:ASN:HB2	3:A:2153:IOD:I	2.87	0.45
1:B:180:ARG:NH2	1:B:203:ASP:OD2	2.45	0.45
1:C:344:LYS:C	1:C:346:LYS:H	2.25	0.44
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.79	0.44
1:A:245:ASN:HB2	1:A:276:ILE:CG2	2.48	0.44
1:B:200:ASP:HA	1:B:201:PRO:HD3	1.85	0.44
1:C:202:ALA:CA	3:C:2233:IOD:I	3.33	0.44
1:A:200:ASP:HA	1:A:201:PRO:HD3	1.84	0.43
1:B:189:ARG:NH1	1:B:189:ARG:CG	2.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:PRO:HG2	1:C:168:PHE:H	1.83	0.43
1:A:285:LYS:HZ3	1:A:336:GLU:CD	2.22	0.43
1:B:87:VAL:HB	1:B:164:LEU:CD2	2.47	0.43
1:B:230:ASP:C	1:B:232:PRO:HD3	2.43	0.43
1:B:330:HIS:HA	1:B:331:PRO:HD3	1.81	0.43
1:A:267:VAL:HB	1:A:351:GLU:HG2	2.00	0.43
1:C:5:ILE:CG2	1:C:7:LYS:HE3	2.49	0.43
1:A:248:GLU:HG2	1:A:273:ILE:HD13	2.00	0.43
1:B:346:LYS:O	1:B:348:LYS:CD	2.67	0.43
3:C:2541:IOD:I	5:C:2882:HOH:O	2.91	0.43
1:B:47:PHE:HE2	1:B:195:LEU:HD21	1.84	0.42
1:B:107:LEU:HD11	1:B:156:VAL:HG22	2.01	0.42
1:C:233:VAL:HG22	1:C:233:VAL:O	2.19	0.42
1:A:247:LEU:HB3	1:A:258:ILE:HD13	2.01	0.42
1:C:30:ASN:ND2	5:C:2948:HOH:O	2.42	0.42
1:B:127:ILE:CG2	1:B:189:ARG:NH2	2.75	0.42
1:B:346:LYS:O	1:B:348:LYS:HD2	2.20	0.42
1:B:303:VAL:HG22	1:B:304:ILE:N	2.35	0.42
1:B:245:ASN:HB3	1:B:247:LEU:HD11	2.02	0.41
1:A:5:ILE:HB	1:A:63:TYR:HB2	2.02	0.41
1:A:86:MET:N	3:A:2023:IOD:I	3.15	0.41
1:B:172:ASP:O	1:B:176:ARG:HG3	2.19	0.41
1:C:247:LEU:HD21	1:C:324:ILE:CG1	2.50	0.41
1:C:300:LYS:HE3	1:C:335:GLY:HA2	2.03	0.41
1:C:352:LYS:O	1:C:353:ASN:O	2.39	0.41
1:C:26:ILE:HG12	1:C:219:LEU:CD2	2.50	0.41
1:B:166:GLU:OE1	1:B:199:HIS:ND1	2.49	0.41
1:B:1:MET:HE3	1:B:160:SER:HA	2.03	0.41
1:B:290:ASP:OD2	1:B:292:SER:N	2.48	0.41
1:C:38:GLY:HA2	1:C:39:PRO:HD3	1.90	0.41
1:C:267:VAL:CG2	1:C:272:ALA:HB2	2.51	0.41
1:B:11:LYS:HE2	1:B:55:ASP:OD2	2.20	0.41
1:B:231:ASN:N	1:B:232:PRO:HD3	2.35	0.41
1:C:30:ASN:ND2	1:C:30:ASN:N	2.65	0.41
1:C:94:TYR:HA	1:C:95:PRO:HD3	1.88	0.41
1:A:180:ARG:NH2	1:A:203:ASP:OD1	2.49	0.41
1:A:163:LEU:O	1:A:164:LEU:HD12	2.21	0.40
1:C:15:LYS:N	3:C:2823:IOD:I	3.22	0.40
1:C:344:LYS:C	1:C:346:LYS:N	2.79	0.40
1:B:267:VAL:CG1	1:B:268:SER:N	2.85	0.40
1:B:294:ILE:CD1	1:B:344:LYS:HB2	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:HD3	1:C:206:ALA:CB	2.51	0.40
1:A:211:VAL:HG13	1:A:228:LEU:HD22	2.03	0.40
1:A:235:ILE:HD12	1:A:235:ILE:HA	1.99	0.40
1:B:221:GLN:HG2	1:B:228:LEU:CD2	2.51	0.40
1:B:233:VAL:HG21	5:B:2860:HOH:O	2.22	0.40
1:B:312:ARG:HG3	1:B:327:TYR:CE2	2.57	0.40
1:A:9:VAL:HG13	1:A:57:PRO:HB3	2.04	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:OD1	5:B:3046:HOH:O[4_566]	1.48	0.72
5:B:3015:HOH:O	5:C:3067:HOH:O[1_565]	1.82	0.38
5:C:3028:HOH:O	5:C:3047:HOH:O[1_455]	1.91	0.29
3:A:2845:IOD:I	5:A:3222:HOH:O[1_655]	1.97	0.23
1:C:329:ASP:OD2	3:C:2237:IOD:I[1_455]	1.97	0.23

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	351/353 (99%)	339 (97%)	11 (3%)	1 (0%)	36	36
1	B	352/353 (100%)	343 (97%)	9 (3%)	0	100	100
1	C	353/353 (100%)	342 (97%)	9 (2%)	2 (1%)	21	18
All	All	1056/1059 (100%)	1024 (97%)	29 (3%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	173	ALA
1	A	91	TRP

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	296/307 (96%)	288 (97%)	8 (3%)	39	45
1	B	291/307 (95%)	278 (96%)	13 (4%)	24	25
1	C	288/307 (94%)	282 (98%)	6 (2%)	47	54
All	All	875/921 (95%)	848 (97%)	27 (3%)	35	39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	130	ILE
1	A	164	LEU
1	A	170	ASN
1	A	172	ASP
1	A	216	LYS
1	A	227	ASP
1	A	307	GLN
1	B	118	ARG
1	B	128	LEU
1	B	189	ARG
1	B	211	VAL
1	B	227	ASP
1	B	241	ILE
1	B	247	LEU
1	B	291	ASP
1	B	292	SER
1	B	300	LYS
1	B	310	LEU
1	B	348	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	349	VAL
1	C	26	ILE
1	C	30	ASN
1	C	37	LEU
1	C	195	LEU
1	C	307	GLN
1	C	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	136	HIS
1	A	146	GLN
1	A	147	GLN
1	A	170	ASN
1	A	221	GLN
1	B	23	ASN
1	B	89	GLN
1	B	135	ASN
1	B	146	GLN
1	B	170	ASN
1	C	30	ASN
1	C	72	ASN
1	C	146	GLN
1	C	231	ASN
1	C	307	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 66 ligands modelled in this entry, 63 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
4	ADP	C	1487	2	28,29,29	1.09	5 (17%)	43,45,45	1.76	9 (20%)
4	ADP	B	1488	2	28,29,29	1.16	4 (14%)	43,45,45	1.81	9 (20%)
4	ADP	A	1486	2	28,29,29	1.07	5 (17%)	43,45,45	1.77	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	C	1487	2	-	2/16/32/32	0/3/3/3
4	ADP	B	1488	2	-	3/16/32/32	0/3/3/3
4	ADP	A	1486	2	-	2/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1488	ADP	PA-O3A	3.03	1.62	1.59
4	C	1487	ADP	C2-N1	2.72	1.38	1.33
4	A	1486	ADP	C2-N1	2.57	1.38	1.33
4	B	1488	ADP	C2-N1	2.51	1.38	1.33
4	C	1487	ADP	C2-N3	2.46	1.38	1.33
4	B	1488	ADP	C2-N3	2.44	1.38	1.33
4	A	1486	ADP	PA-O3A	2.29	1.62	1.59
4	A	1486	ADP	C2-N3	2.25	1.37	1.33
4	C	1487	ADP	PA-O3A	2.16	1.61	1.59
4	C	1487	ADP	C8-N7	2.12	1.35	1.31
4	A	1486	ADP	C8-N7	2.07	1.35	1.31
4	B	1488	ADP	C8-N7	2.06	1.35	1.31
4	C	1487	ADP	C5-N7	-2.03	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1486	ADP	C5-N7	-2.01	1.35	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1486	ADP	N3-C2-N1	-5.77	119.85	128.58
4	B	1488	ADP	N3-C2-N1	-5.61	120.08	128.58
4	C	1487	ADP	N3-C2-N1	-5.58	120.14	128.58
4	B	1488	ADP	C5-C4-N3	-4.34	120.74	126.72
4	C	1487	ADP	C5-C4-N3	-4.32	120.77	126.72
4	A	1486	ADP	N9-C8-N7	-4.10	108.12	113.94
4	B	1488	ADP	N9-C8-N7	-4.00	108.26	113.94
4	C	1487	ADP	N9-C8-N7	-3.92	108.38	113.94
4	A	1486	ADP	C5-C4-N3	-3.80	121.49	126.72
4	B	1488	ADP	C5-N7-C8	3.42	108.83	103.45
4	B	1488	ADP	C2-N3-C4	3.39	120.12	111.83
4	A	1486	ADP	C5-N7-C8	3.39	108.78	103.45
4	C	1487	ADP	C2-N3-C4	3.32	119.94	111.83
4	C	1487	ADP	C5-N7-C8	3.30	108.64	103.45
4	A	1486	ADP	C2-N3-C4	3.12	119.44	111.83
4	C	1487	ADP	N3-C4-N9	2.84	131.99	127.17
4	B	1488	ADP	N3-C4-N9	2.78	131.90	127.17
4	A	1486	ADP	O2B-PB-O3A	2.69	113.65	104.64
4	A	1486	ADP	N3-C4-N9	2.49	131.40	127.17
4	A	1486	ADP	O2A-PA-O3A	2.46	113.92	107.27
4	A	1486	ADP	C4-C5-N7	-2.37	107.87	110.58
4	B	1488	ADP	C4-C5-N7	-2.36	107.88	110.58
4	B	1488	ADP	O2A-PA-O3A	2.32	113.55	107.27
4	C	1487	ADP	C4-C5-N7	-2.31	107.95	110.58
4	A	1486	ADP	C4-N9-C8	2.27	108.12	105.74
4	C	1487	ADP	O2B-PB-O3A	2.23	112.11	104.64
4	B	1488	ADP	O2B-PB-O3A	2.13	111.79	104.64
4	C	1487	ADP	O3B-PB-O3A	2.02	111.40	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1486	ADP	PA-O3A-PB-O2B
4	B	1488	ADP	PA-O3A-PB-O2B
4	C	1487	ADP	PA-O3A-PB-O2B
4	A	1486	ADP	PA-O3A-PB-O1B

Continued on next page...

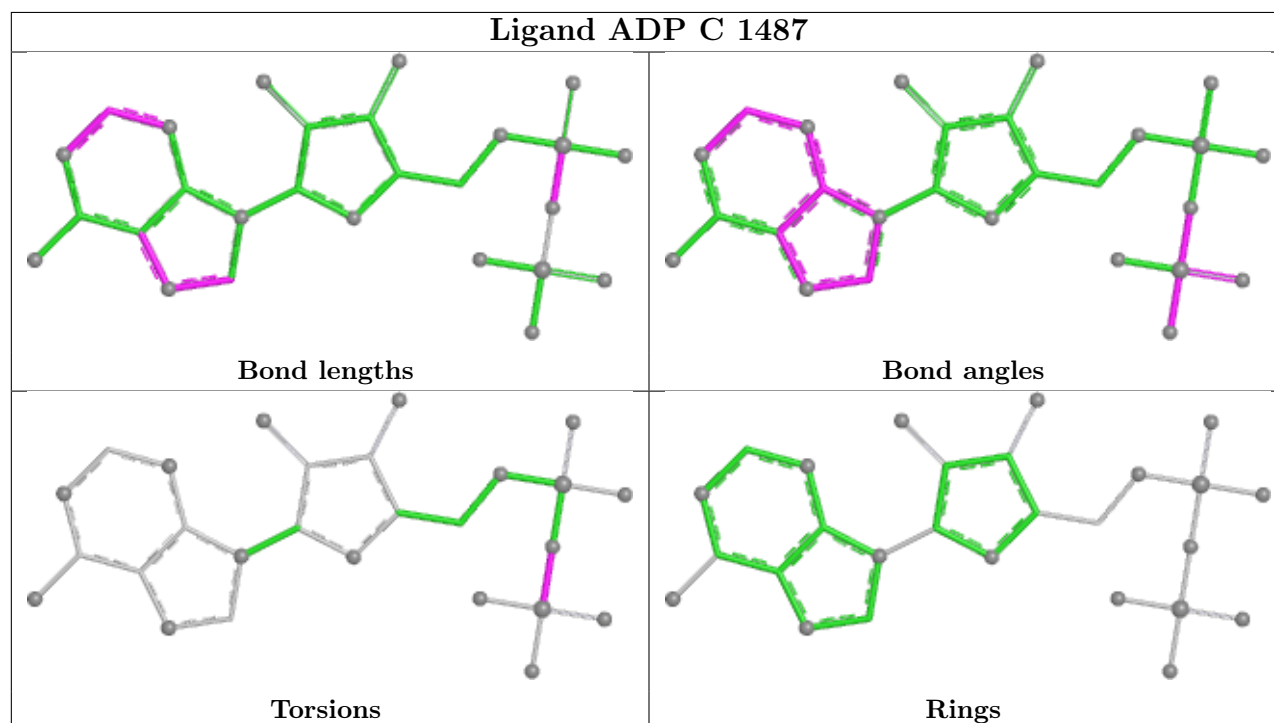
Continued from previous page...

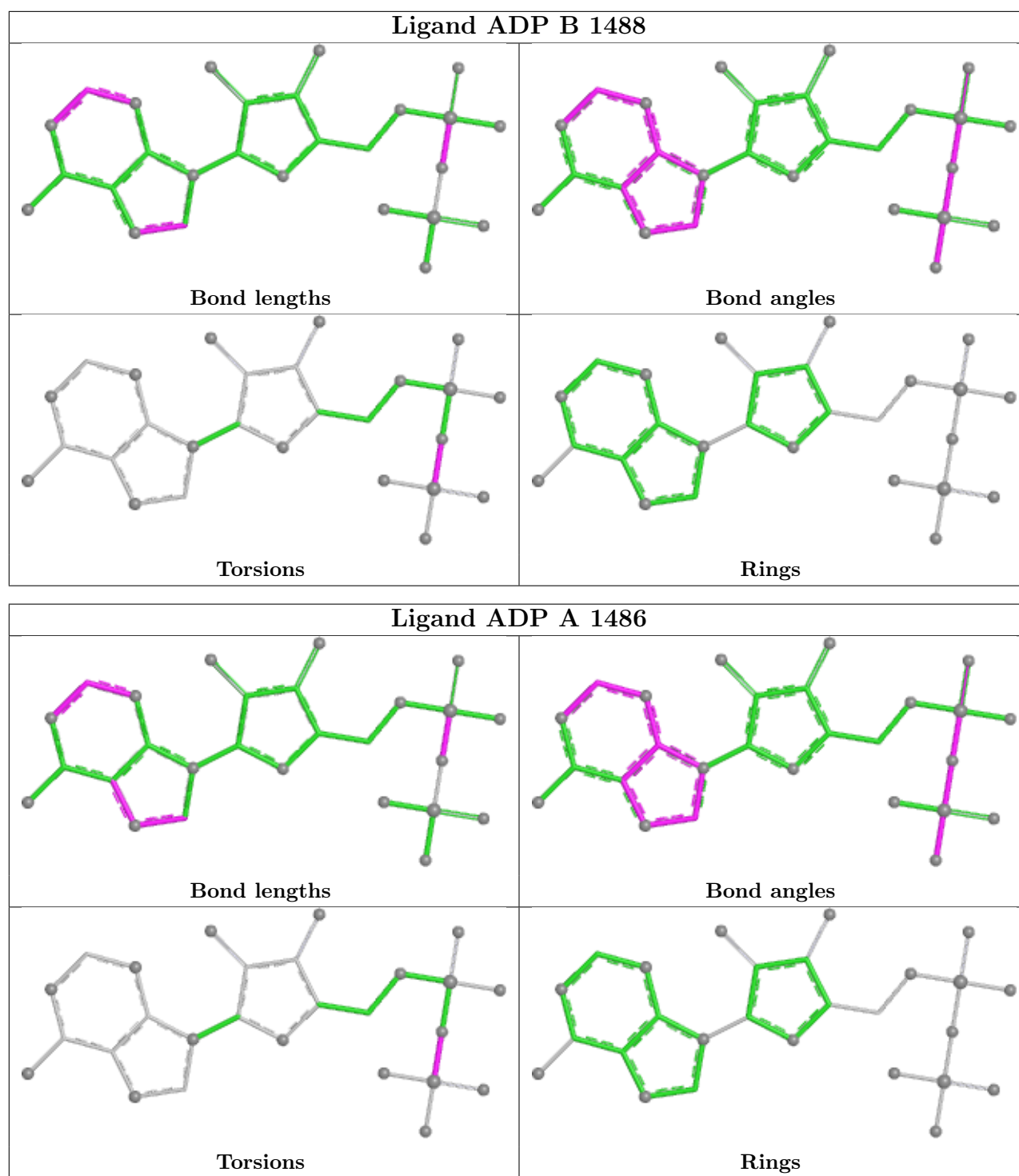
Mol	Chain	Res	Type	Atoms
4	B	1488	ADP	PA-O3A-PB-O1B
4	B	1488	ADP	PA-O3A-PB-O3B
4	C	1487	ADP	PA-O3A-PB-O1B

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 ⓘ

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

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	353/353 (100%)	0.25	30 (8%)	16 17	5, 15, 41, 92	0
1	B	353/353 (100%)	0.43	31 (8%)	15 16	0, 15, 43, 78	1 (0%)
1	C	353/353 (100%)	0.14	16 (4%)	38 40	5, 14, 39, 78	2 (0%)
All	All	1059/1059 (100%)	0.28	77 (7%)	21 22	0, 15, 41, 92	3 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	4.9
1	B	344	LYS	4.6
1	B	310	LEU	4.4
1	B	94	TYR	4.3
1	C	169	SER	3.9
1	A	169	SER	3.9
1	A	170	ASN	3.8
1	B	330	HIS	3.7
1	A	173	ALA	3.7
1	B	216	LYS	3.6
1	A	172	ASP	3.5
1	A	344	LYS	3.5
1	A	90	THR	3.3
1	C	173	ALA	3.3
1	C	175	MET	3.3
1	A	168	PHE	3.2
1	C	7	LYS	3.2
1	A	89	GLN	3.2
1	C	89	GLN	3.2
1	B	1	MET	3.1
1	A	353	ASN	3.1
1	A	304	ILE	3.1
1	B	291	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	216	LYS	3.0
1	C	241	ILE	3.0
1	A	176	ARG	3.0
1	B	288	ILE	3.0
1	B	290	ASP	2.9
1	B	169	SER	2.9
1	B	89	GLN	2.8
1	B	204	ILE	2.8
1	B	267	VAL	2.8
1	C	195	LEU	2.8
1	B	173	ALA	2.7
1	B	175	MET	2.7
1	B	224	LYS	2.7
1	C	344	LYS	2.7
1	B	170	ASN	2.7
1	C	168	PHE	2.6
1	B	174	ARG	2.6
1	C	170	ASN	2.6
1	A	174	ARG	2.6
1	B	336	GLU	2.5
1	B	108	THR	2.5
1	A	91	TRP	2.5
1	A	291	ASP	2.5
1	A	249	GLY	2.5
1	C	353	ASN	2.5
1	C	108	THR	2.4
1	B	171	LEU	2.4
1	A	270	ASP	2.4
1	A	267	VAL	2.4
1	A	114	LYS	2.4
1	B	292	SER	2.4
1	A	330	HIS	2.4
1	A	307	GLN	2.3
1	A	227	ASP	2.3
1	A	319	ASP	2.3
1	B	286	ASP	2.3
1	B	270	ASP	2.3
1	C	172	ASP	2.3
1	B	266	SER	2.3
1	A	204	ILE	2.3
1	B	119	LYS	2.3
1	B	172	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	90	THR	2.2
1	C	90	THR	2.2
1	C	252	THR	2.1
1	A	289	LYS	2.1
1	A	253	ASN	2.1
1	B	91	TRP	2.1
1	A	175	MET	2.1
1	A	352	LYS	2.1
1	C	330	HIS	2.0
1	B	111	LYS	2.0
1	B	346	LYS	2.0
1	A	193	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IOD	C	2237	1/1	0.71	0.27	213,213,213,213	1
3	IOD	C	2253	1/1	0.74	0.23	113,113,113,113	1
3	IOD	A	2016	1/1	0.79	0.12	59,59,59,59	1
3	IOD	B	2218	1/1	0.79	0.19	141,141,141,141	1
3	IOD	B	2078	1/1	0.84	0.15	66,66,66,66	1
3	IOD	A	2165	1/1	0.84	0.20	89,89,89,89	1
3	IOD	C	2233	1/1	0.88	0.13	53,53,53,53	1
3	IOD	C	2823	1/1	0.89	0.11	38,38,38,38	1
3	IOD	A	2288	1/1	0.89	0.21	68,68,68,68	1
3	IOD	B	2198	1/1	0.89	0.18	72,72,72,72	1
3	IOD	C	2438	1/1	0.89	0.10	38,38,38,38	1

Continued on next page...

Continued from previous page...

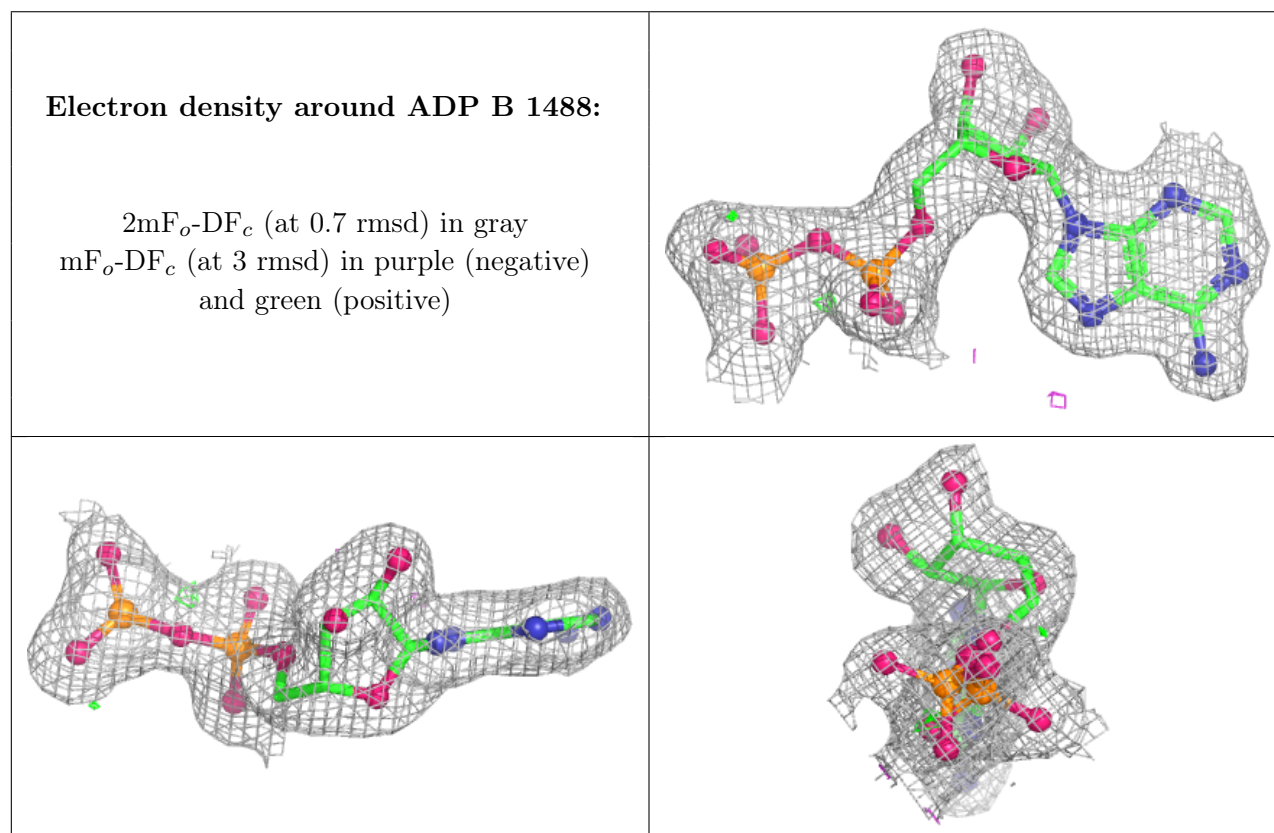
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IOD	C	2258	1/1	0.89	0.17	80,80,80,80	1
3	IOD	B	2831	1/1	0.90	0.12	39,39,39,39	1
3	IOD	A	2683	1/1	0.90	0.10	42,42,42,42	1
3	IOD	B	2337	1/1	0.91	0.09	41,41,41,41	1
3	IOD	C	2813	1/1	0.92	0.11	27,27,27,27	1
3	IOD	A	2832	1/1	0.92	0.09	41,41,41,41	1
2	MG	B	1503	1/1	0.93	0.05	28,28,28,28	0
3	IOD	A	2153	1/1	0.93	0.08	53,53,53,53	1
3	IOD	B	2012	1/1	0.93	0.11	31,31,31,31	1
3	IOD	C	2018	1/1	0.94	0.17	33,33,33,33	1
3	IOD	B	2386	1/1	0.94	0.08	32,32,32,32	1
3	IOD	A	2116	1/1	0.94	0.14	47,47,47,47	1
3	IOD	B	2015	1/1	0.94	0.06	36,36,36,36	1
3	IOD	C	2049	1/1	0.95	0.08	36,36,36,36	1
3	IOD	B	2017	1/1	0.95	0.06	28,28,28,28	1
3	IOD	B	2019	1/1	0.95	0.05	29,29,29,29	1
2	MG	A	1502	1/1	0.95	0.04	21,21,21,21	0
3	IOD	C	2137	1/1	0.95	0.19	52,52,52,52	1
3	IOD	A	2528	1/1	0.95	0.07	35,35,35,35	1
3	IOD	C	2536	1/1	0.96	0.07	37,37,37,37	1
3	IOD	C	2682	1/1	0.96	0.07	33,33,33,33	1
3	IOD	C	2014	1/1	0.96	0.05	31,31,31,31	1
3	IOD	A	2986	1/1	0.96	0.06	35,35,35,35	1
3	IOD	B	2037	1/1	0.96	0.06	40,40,40,40	1
3	IOD	A	2830	1/1	0.97	0.05	36,36,36,36	1
3	IOD	A	2023	1/1	0.97	0.04	37,37,37,37	1
3	IOD	A	2339	1/1	0.97	0.04	38,38,38,38	1
3	IOD	A	2050	1/1	0.97	0.04	32,32,32,32	1
3	IOD	C	2239	1/1	0.97	0.07	38,38,38,38	1
3	IOD	A	2010	1/1	0.97	0.06	32,32,32,32	1
3	IOD	C	2541	1/1	0.97	0.05	39,39,39,39	1
3	IOD	A	2006	1/1	0.97	0.07	30,30,30,30	1
3	IOD	C	2809	1/1	0.97	0.07	27,27,27,27	1
4	ADP	B	1488	27/27	0.97	0.06	17,28,41,46	0
3	IOD	B	2021	1/1	0.98	0.05	26,26,26,26	1
3	IOD	A	2011	1/1	0.98	0.07	34,34,34,34	1
3	IOD	C	2020	1/1	0.98	0.04	36,36,36,36	1
3	IOD	A	2816	1/1	0.98	0.09	32,32,32,32	1
3	IOD	A	2828	1/1	0.98	0.05	31,31,31,31	1
4	ADP	A	1486	27/27	0.98	0.05	15,21,28,35	0
3	IOD	C	2004	1/1	0.98	0.04	26,26,26,26	1
4	ADP	C	1487	27/27	0.98	0.06	11,21,34,37	0

Continued on next page...

Continued from previous page...

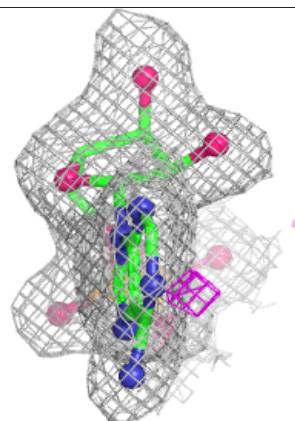
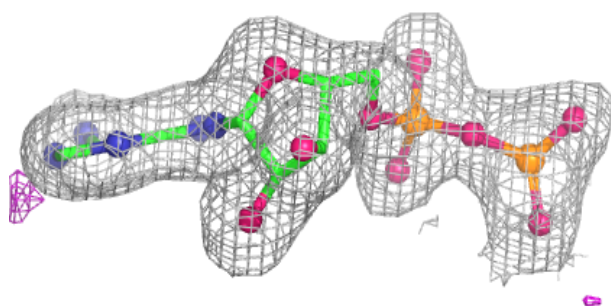
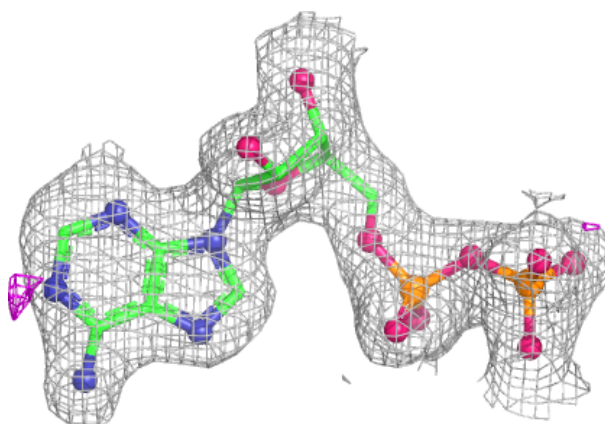
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	1501	1/1	0.99	0.03	20,20,20,20	0
3	IOD	A	2007	1/1	0.99	0.05	26,26,26,26	1
3	IOD	C	2001	1/1	0.99	0.03	25,25,25,25	1
3	IOD	A	2022	1/1	0.99	0.04	23,23,23,23	1
3	IOD	C	2008	1/1	0.99	0.05	27,27,27,27	1
3	IOD	C	2013	1/1	0.99	0.02	23,23,23,23	1
3	IOD	A	2009	1/1	0.99	0.04	31,31,31,31	1
3	IOD	A	2003	1/1	0.99	0.04	29,29,29,29	1
3	IOD	B	2808	1/1	0.99	0.05	30,30,30,30	1
3	IOD	A	2387	1/1	0.99	0.12	34,34,34,34	1
3	IOD	B	2002	1/1	0.99	0.04	30,30,30,30	1
3	IOD	B	2005	1/1	0.99	0.04	25,25,25,25	1
3	IOD	A	2845	1/1	0.99	0.07	38,38,38,38	1

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.

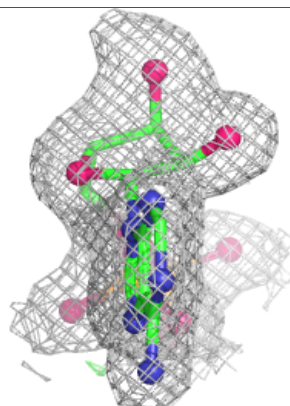
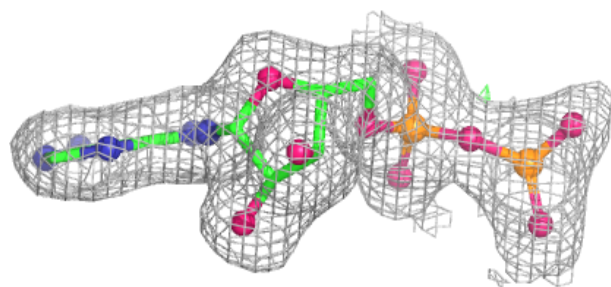
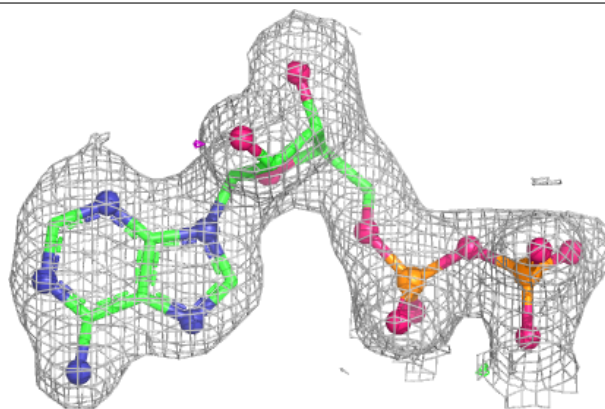


Electron density around ADP A 1486:

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

**Electron density around ADP C 1487:**

$2mF_o-DF_c$ (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.