



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:47 AM UTC

PDB ID : 1W0J / pdb_00001w0j
Title : Beryllium fluoride inhibited bovine F1-ATPase
Authors : Kagawa, R.; Montgomery, M.G.; Braig, K.; Walker, J.E.; Leslie, A.G.W.
Deposited on : 2004-06-08
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

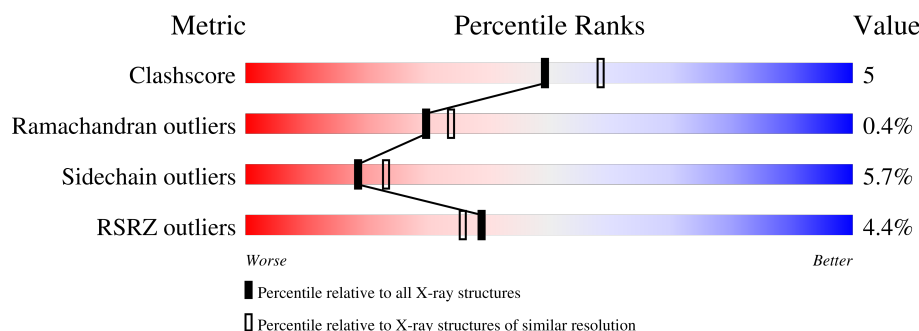
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	79% 14% • 5%
1	B	510	2% 80% 12% • 6%
1	C	510	80% 15% • •
2	D	482	86% 10% • •
2	E	482	9% 81% 14% • •
2	F	482	84% 11% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	272	21% 50% 17% • 29%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24480 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 ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	498	Total	C	N	O	S	0	0	0
			3797	2390	670	725	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	cloning artifact	UNP P19483
B	481	GLY	SER	cloning artifact	UNP P19483
C	481	GLY	SER	cloning artifact	UNP P19483

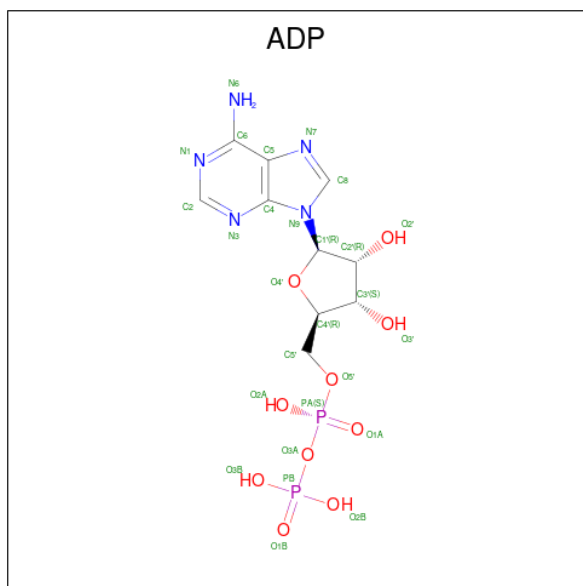
- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN, MITOCHONDRIAL PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	192	Total	C	N	O	S	0	0	0
			1492	942	268	275	7			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

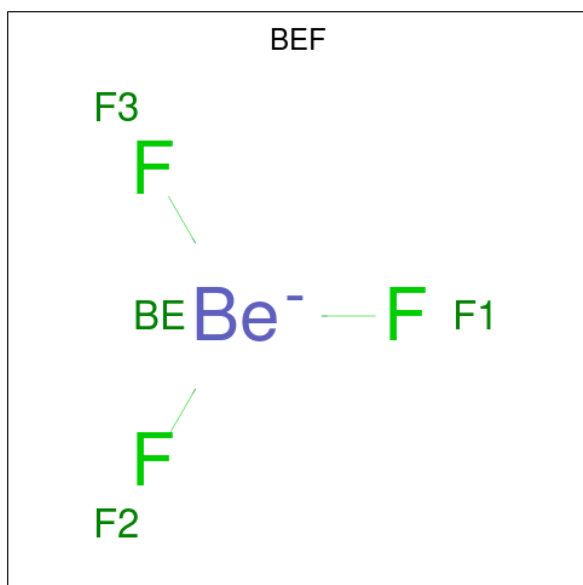
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



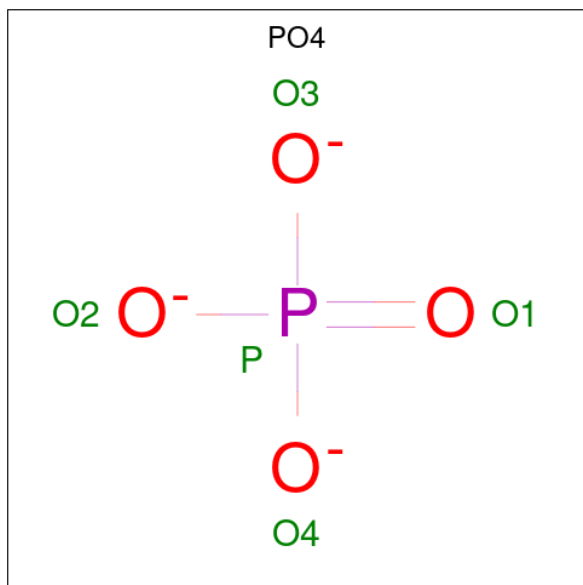
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	Be	F	0	0
			4	1	3		
7	F	1	Total	Be	F	0	0
			4	1	3		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		

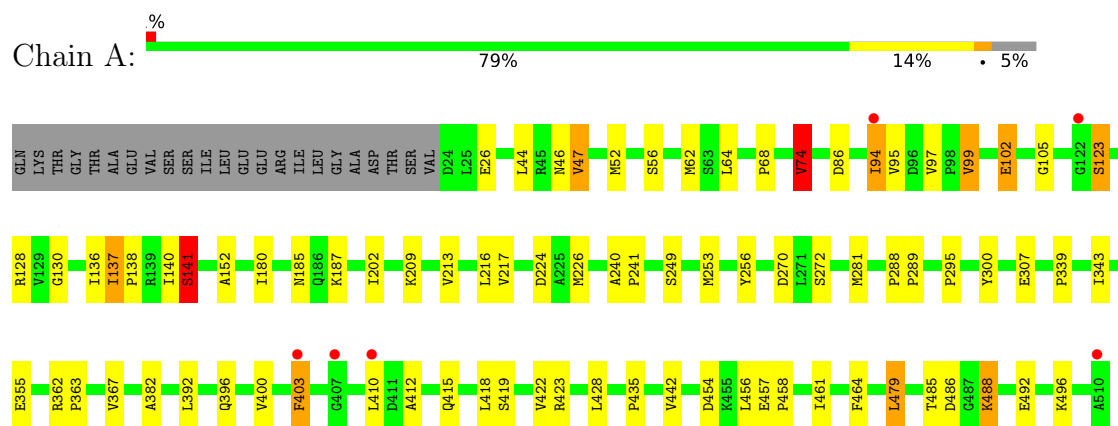
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	170	Total	O	0	0
			170	170		
9	B	167	Total	O	0	0
			167	167		
9	C	198	Total	O	0	0
			198	198		
9	D	187	Total	O	0	0
			187	187		
9	E	93	Total	O	0	0
			93	93		
9	F	194	Total	O	0	0
			194	194		
9	G	28	Total	O	0	0
			28	28		

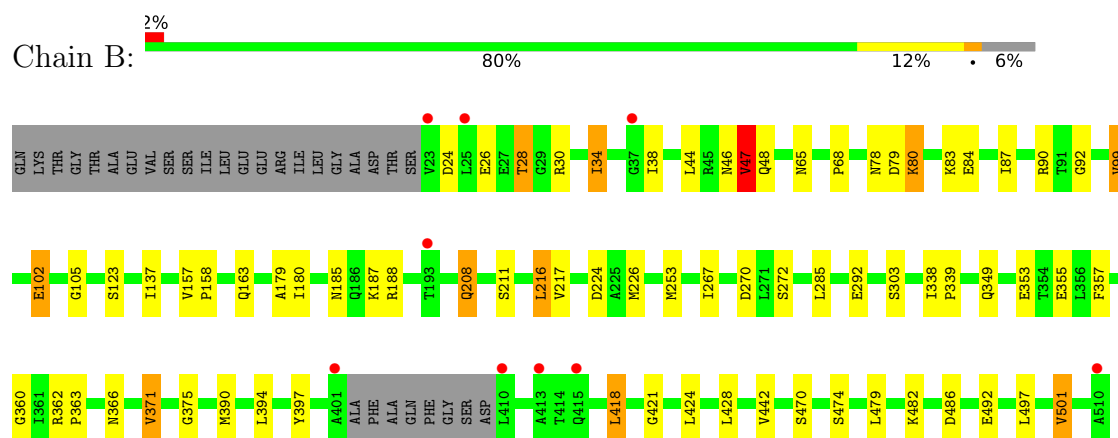
3 Residue-property plots

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.

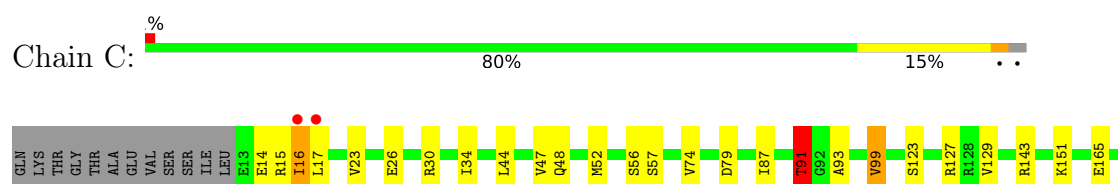
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

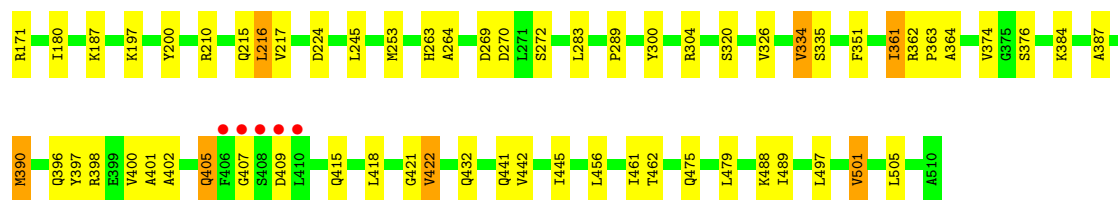


• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

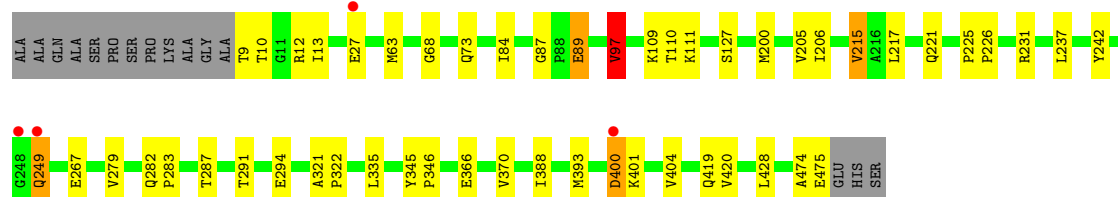
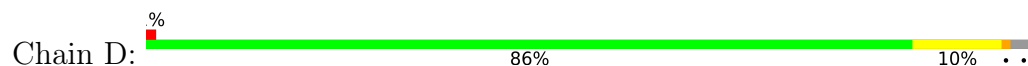


• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

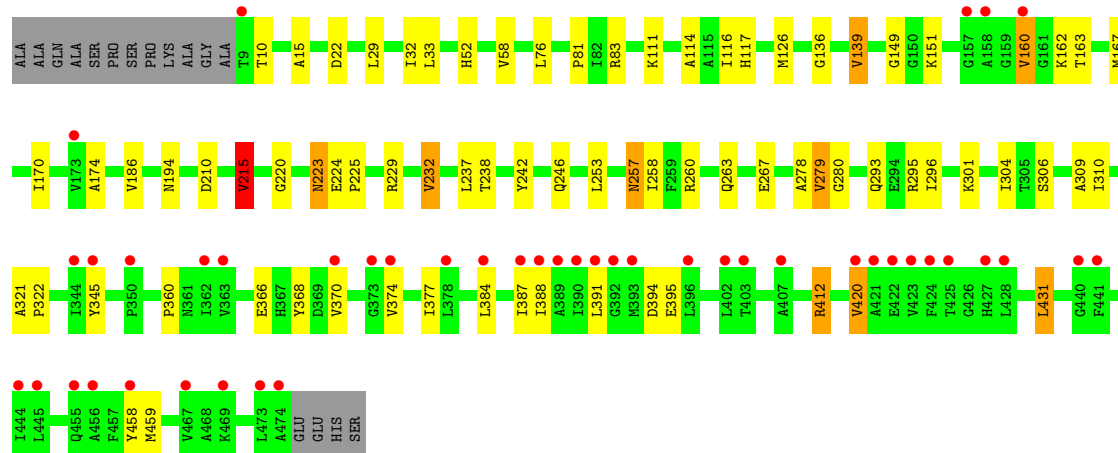
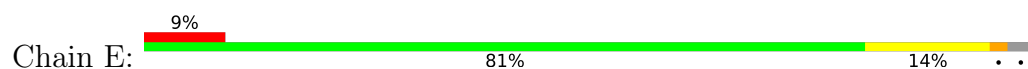




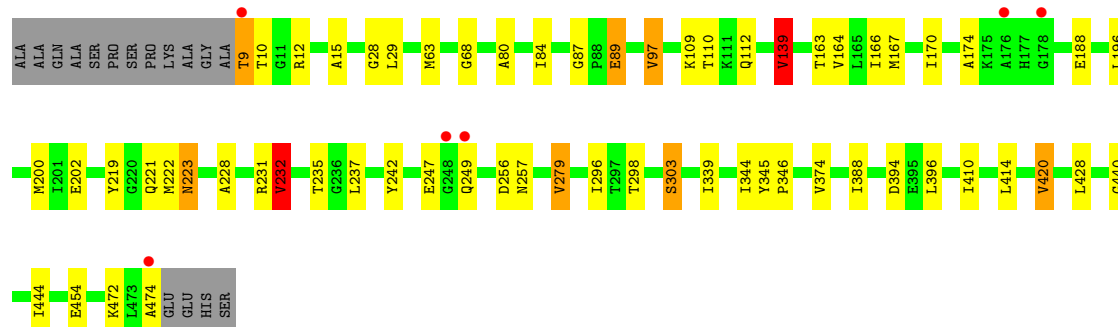
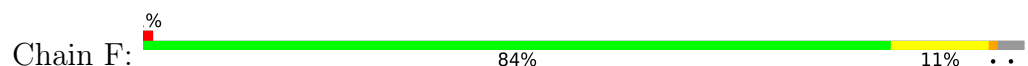
• Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR



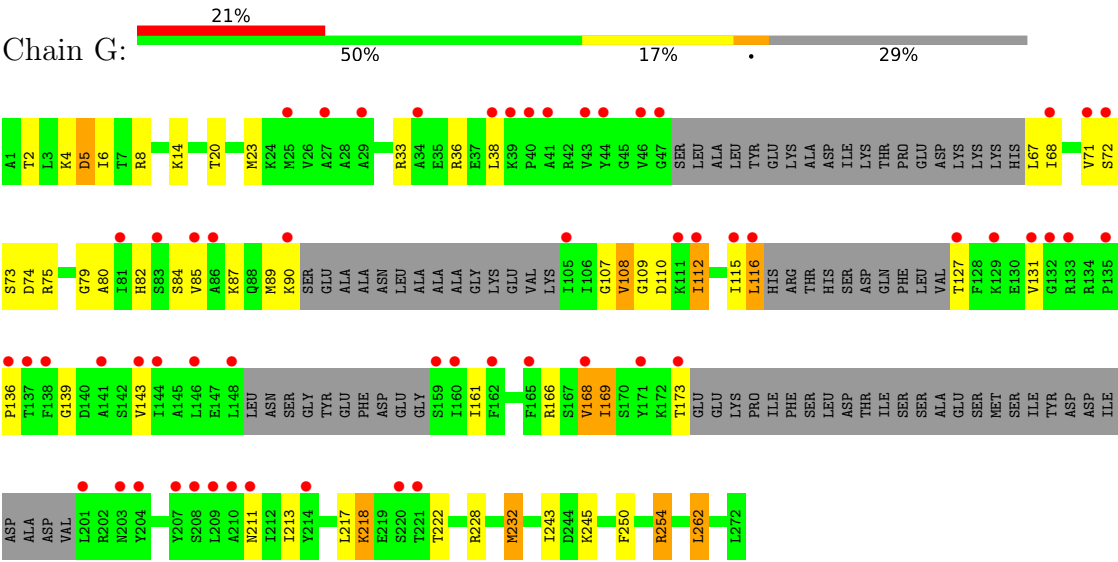
• Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR



• Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR



● Molecule 3: ATP SYNTHASE GAMMA CHAIN, MITOCHONDRIAL PRECURSOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	283.52Å 107.37Å 137.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.8 (20.00-2.20) 86.7 (20.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.184 , 0.236 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24480	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: MG, ADP, PO4, BEF, GOL

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	0.69	1/3766 (0.0%)	0.98	2/5080 (0.0%)
1	B	0.69	1/3711 (0.0%)	0.96	2/5005 (0.0%)
1	C	0.73	0/3848	0.97	3/5191 (0.1%)
2	D	0.72	0/3596	0.95	1/4879 (0.0%)
2	E	0.64	0/3587	0.94	5/4867 (0.1%)
2	F	0.72	0/3587	0.96	5/4867 (0.1%)
3	G	0.58	0/1502	0.95	0/2006
All	All	0.69	2/23597 (0.0%)	0.96	18/31895 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	ILE	CA-CB	6.21	1.58	1.53
1	A	137	ILE	CA-CB	5.10	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-9.15	99.79	112.14
2	F	139	VAL	CB-CA-C	-8.54	100.95	111.88
2	F	97	VAL	CB-CA-C	-7.75	101.95	111.88
1	B	371	VAL	CB-CA-C	-7.28	101.68	111.80
2	F	249	GLN	N-CA-C	6.93	120.61	109.86
2	F	232	VAL	CB-CA-C	-6.78	102.15	112.05
2	E	210	ASP	N-CA-C	5.72	113.47	108.78
2	E	215	VAL	CB-CA-C	-5.66	102.06	110.33
2	F	80	ALA	N-CA-C	5.50	112.97	108.07
1	B	47	VAL	CB-CA-C	-5.44	103.08	111.08
1	C	374	VAL	N-CA-C	-5.37	107.59	112.96
2	E	139	VAL	CB-CA-C	-5.35	105.12	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	VAL	N-CA-CB	-5.35	104.90	111.00
2	E	160	VAL	N-CA-C	5.31	117.22	112.17
1	C	374	VAL	CB-CA-C	5.25	115.68	111.06
1	C	91	THR	N-CA-C	-5.18	107.62	114.04
2	E	232	VAL	N-CA-C	5.09	115.81	110.62
1	A	74	VAL	CB-CA-C	5.03	117.04	110.96

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	3715	0	3814	47	0
1	B	3663	0	3774	40	0
1	C	3797	0	3894	41	0
2	D	3539	0	3592	29	0
2	E	3530	0	3587	44	0
2	F	3530	0	3586	40	0
3	G	1492	0	1587	29	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	F	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	6	0	8	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	D	4	0	0	0	0
7	F	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	5	0	0	1	0
9	A	170	0	0	1	0
9	B	167	0	0	3	0
9	C	198	0	0	3	0
9	D	187	0	0	3	0
9	E	93	0	0	1	0
9	F	194	0	0	1	0
9	G	28	0	0	1	0
All	All	24480	0	23926	256	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 (256) 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)
2:F:237:LEU:HD11	2:F:296:ILE:HG12	1.40	1.01
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.41	0.99
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.46	0.98
2:F:167:MET:HE1	2:F:196:LEU:HD13	1.52	0.90
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.51	0.89
2:E:257:ASN:HD21	2:E:260:ARG:HG3	1.36	0.89
2:D:366:GLU:O	2:D:370:VAL:HG23	1.74	0.87
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.57	0.85
1:C:23:VAL:HG12	1:C:23:VAL:O	1.77	0.85
1:A:99:VAL:HG13	1:A:256:TYR:HB2	1.61	0.83
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.61	0.82
1:B:180:ILE:HD12	1:B:216:LEU:HD21	1.62	0.82
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.59	0.81
1:C:52:MET:O	1:C:91:THR:HB	1.81	0.80
3:G:80:ALA:O	3:G:84:SER:HB2	1.83	0.79
2:F:237:LEU:HD11	2:F:296:ILE:CG1	2.14	0.78
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.65	0.77
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.14	0.76
2:F:388:ILE:HD11	2:F:396:LEU:HD11	1.68	0.75
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.22	0.75
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.67	0.74
1:A:94:ILE:CD1	1:A:128:ARG:HG2	2.15	0.74
3:G:20:THR:HG22	3:G:232:MET:HE3	1.68	0.74
2:D:205:VAL:HG12	2:D:215:VAL:CG2	2.18	0.73
1:C:418:LEU:O	1:C:422:VAL:HG23	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:47:VAL:HG22	1.89	0.72
1:B:187:LYS:HE3	1:B:224:ASP:HB3	1.71	0.71
2:F:237:LEU:CD1	2:F:296:ILE:HG12	2.19	0.70
2:E:257:ASN:ND2	2:E:260:ARG:HG3	2.07	0.69
1:A:102:GLU:HG3	1:A:123:SER:HA	1.74	0.69
1:A:456:LEU:HD23	1:A:461:ILE:HD13	1.73	0.69
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.75	0.67
2:F:223:ASN:HD22	2:F:223:ASN:H	1.42	0.67
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.77	0.67
1:C:15:ARG:HG2	1:C:16:ILE:N	2.11	0.66
1:A:382:ALA:HB2	1:A:488:LYS:HA	1.75	0.66
2:E:149:GLY:HA2	2:E:304:ILE:O	1.96	0.65
1:A:295:PRO:HD3	9:A:2105:HOH:O	1.94	0.65
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.79	0.65
1:B:292:GLU:OE2	9:B:2107:HOH:O	2.14	0.65
1:A:479:LEU:HG	1:A:496:LYS:HG2	1.79	0.64
1:B:497:LEU:O	1:B:501:VAL:HG23	1.98	0.64
1:A:412:ALA:HA	1:A:415:GLN:HE21	1.61	0.63
1:B:44:LEU:O	1:B:47:VAL:HG22	1.98	0.63
1:C:91:THR:HG22	1:C:93:ALA:H	1.63	0.62
2:F:196:LEU:HD11	2:F:200:MET:HE3	1.81	0.62
1:B:349:GLN:NE2	9:B:2139:HOH:O	2.27	0.62
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.81	0.62
1:B:102:GLU:HG3	1:B:123:SER:HA	1.82	0.61
2:E:223:ASN:HD22	2:E:223:ASN:H	1.48	0.61
2:E:224:GLU:O	2:E:229:ARG:HD3	2.01	0.60
1:B:470:SER:O	1:B:474:SER:HB2	2.02	0.59
2:E:263:GLN:NE2	2:E:267:GLU:OE2	2.25	0.59
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.85	0.59
1:A:270:ASP:OD1	1:A:272:SER:HB2	2.01	0.59
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.32	0.59
1:A:105:GLY:HA2	1:A:226:MET:O	2.03	0.59
3:G:136:PRO:O	3:G:218:LYS:NZ	2.36	0.59
2:D:205:VAL:CG1	2:D:215:VAL:CG2	2.81	0.58
1:C:44:LEU:O	1:C:47:VAL:HG22	2.02	0.58
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.86	0.58
1:B:390:MET:HG3	1:B:424:LEU:HD13	1.85	0.58
1:B:397:TYR:HD1	1:B:418:LEU:HA	1.69	0.58
2:D:63:MET:CE	2:D:97:VAL:HG11	2.33	0.58
1:B:24:ASP:O	1:B:28:THR:HB	2.04	0.57
1:B:360:GLY:HA2	1:B:362:ARG:HE	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.38	0.56
2:F:223:ASN:HD22	2:F:223:ASN:N	1.97	0.56
3:G:23:MET:HE3	3:G:75:ARG:HH21	1.70	0.56
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.34	0.55
2:D:225:PRO:HB2	9:D:2011:HOH:O	2.05	0.55
2:D:474:ALA:O	2:D:475:GLU:HB2	2.06	0.55
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.87	0.55
1:B:353:GLU:OE1	1:B:366:ASN:ND2	2.25	0.54
2:E:257:ASN:HB2	2:E:309:ALA:O	2.08	0.54
1:C:23:VAL:O	1:C:23:VAL:CG1	2.50	0.54
1:C:99:VAL:HG22	1:C:253:MET:HA	1.90	0.54
1:C:187:LYS:HE2	1:C:224:ASP:HB3	1.90	0.54
3:G:33:ARG:HD2	3:G:36:ARG:HH12	1.73	0.54
3:G:75:ARG:O	3:G:82:HIS:NE2	2.36	0.54
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.91	0.53
1:A:307:GLU:HG3	2:E:223:ASN:HB3	1.90	0.53
2:E:186:VAL:HG22	2:E:232:VAL:HG23	1.91	0.53
2:D:388:ILE:HG13	9:D:2159:HOH:O	2.09	0.53
3:G:85:VAL:HG23	3:G:112:ILE:HD11	1.91	0.53
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.33	0.53
1:C:497:LEU:O	1:C:501:VAL:HG13	2.09	0.52
2:F:223:ASN:H	2:F:223:ASN:ND2	2.07	0.52
2:E:32:ILE:O	2:E:33:LEU:HB2	2.10	0.52
1:B:26:GLU:O	1:B:46:ASN:HB2	2.09	0.52
1:B:78:ASN:OD1	1:B:80:LYS:HB3	2.09	0.52
1:B:362:ARG:HA	1:B:363:PRO:C	2.34	0.52
2:D:287:THR:O	2:D:291:THR:HG23	2.10	0.52
1:C:397:TYR:CD1	1:C:421:GLY:HA3	2.45	0.52
2:F:164:VAL:HG13	2:F:420:VAL:HG12	1.92	0.52
3:G:109:GLY:HA2	3:G:131:VAL:CG2	2.41	0.51
1:A:52:MET:HG3	1:A:95:VAL:CG2	2.31	0.51
2:F:345:TYR:HA	2:F:346:PRO:C	2.34	0.51
1:A:423:ARG:HD3	1:A:454:ASP:HA	1.93	0.51
1:C:171:ARG:HD3	9:C:2059:HOH:O	2.11	0.51
1:C:441:GLN:O	1:C:445:ILE:HG12	2.10	0.51
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.92	0.51
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.92	0.51
3:G:254:ARG:NH2	9:G:2019:HOH:O	2.41	0.51
2:F:339:ILE:HG23	2:F:344:ILE:HB	1.93	0.50
1:A:130:GLY:HA2	6:A:1513:GOL:H11	1.93	0.50
2:D:89:GLU:CG	2:D:110:THR:HG22	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.93	0.50
1:C:362:ARG:HA	1:C:363:PRO:C	2.37	0.50
2:D:63:MET:HE3	2:D:97:VAL:HG11	1.93	0.50
1:C:361:ILE:O	1:C:364:ALA:HA	2.12	0.50
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.47	0.49
2:F:9:THR:HG22	2:F:10:THR:H	1.76	0.49
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.47	0.49
1:C:171:ARG:NE	9:C:2059:HOH:O	2.44	0.49
2:D:249:GLN:OE1	2:D:249:GLN:HA	2.10	0.49
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.42	0.49
1:B:48:GLN:HB3	2:F:68:GLY:HA2	1.94	0.49
2:D:97:VAL:HG22	9:D:2079:HOH:O	2.12	0.49
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.95	0.49
2:E:83:ARG:HA	2:E:114:ALA:O	2.13	0.49
3:G:168:VAL:HG23	3:G:169:ILE:HG13	1.94	0.49
2:F:188:GLU:O	2:F:222:MET:HG2	2.13	0.48
3:G:139:GLY:O	3:G:143:VAL:HG23	2.13	0.48
1:A:403:PHE:N	1:A:403:PHE:CD2	2.78	0.48
2:F:170:ILE:O	2:F:174:ALA:HB3	2.13	0.48
2:F:454:GLU:HG3	9:F:2184:HOH:O	2.12	0.48
2:E:384:LEU:O	2:E:388:ILE:HG12	2.14	0.48
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.95	0.48
1:A:185:ASN:OD1	1:A:435:PRO:HB2	2.14	0.48
1:B:211:SER:HA	2:E:126:MET:HE2	1.96	0.48
2:E:345:TYR:H	2:E:459:MET:HE1	1.77	0.48
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.48	0.48
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.96	0.48
3:G:38:LEU:HD22	3:G:222:THR:HG21	1.95	0.48
2:D:226:PRO:HB3	2:D:267:GLU:OE1	2.13	0.47
1:A:64:LEU:HD11	1:A:281:MET:HE3	1.96	0.47
2:E:366:GLU:O	2:E:370:VAL:HG23	2.14	0.47
2:D:200:MET:HE3	2:D:206:ILE:CD1	2.44	0.47
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.45	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
1:B:90:ARG:HH21	1:B:92:GLY:HA2	1.80	0.47
2:E:374:VAL:O	2:E:377:ILE:HG22	2.15	0.47
2:F:196:LEU:HD23	2:F:219:TYR:OH	2.15	0.47
3:G:74:ASP:CG	3:G:110:ASP:HB2	2.40	0.47
3:G:2:THR:HG22	3:G:4:LYS:H	1.79	0.47
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.50	0.46
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.97	0.46
3:G:73:SER:HA	3:G:131:VAL:HG23	1.97	0.46
1:A:339:PRO:O	1:A:343:ILE:HG13	2.15	0.46
1:A:464:PHE:CD2	1:A:464:PHE:C	2.93	0.46
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.98	0.46
2:E:242:TYR:CD1	2:E:246:GLN:HG3	2.51	0.46
1:A:418:LEU:O	1:A:422:VAL:HG13	2.15	0.45
2:E:167:MET:HB3	2:E:420:VAL:HG21	1.98	0.45
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.74	0.45
1:A:486:ASP:C	1:A:488:LYS:H	2.25	0.45
1:B:208:GLN:OE1	9:B:2069:HOH:O	2.21	0.45
1:C:401:ALA:HA	1:C:418:LEU:HD21	1.97	0.45
3:G:72:SER:OG	3:G:73:SER:N	2.49	0.45
2:F:394:ASP:HB3	3:G:79:GLY:HA2	1.99	0.45
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.98	0.45
1:B:158:PRO:O	1:B:375:GLY:HA3	2.16	0.45
1:C:432:GLN:NE2	4:C:1511:ADP:O2'	2.48	0.45
2:F:388:ILE:CD1	2:F:396:LEU:HD11	2.43	0.45
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.17	0.45
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.82	0.45
1:C:270:ASP:OD1	1:C:272:SER:HB2	2.17	0.45
1:A:400:VAL:HG13	1:A:403:PHE:CD1	2.51	0.44
2:F:298:THR:HG23	2:F:303:SER:HA	1.99	0.44
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.52	0.44
1:C:187:LYS:CE	1:C:224:ASP:HB3	2.47	0.44
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.47	0.44
1:B:303:SER:HB2	2:F:222:MET:HB2	1.98	0.44
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.52	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.81	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB3	1.99	0.44
1:A:140:ILE:HG13	1:A:141:SER:N	2.33	0.44
3:G:107:GLY:O	3:G:127:THR:HA	2.18	0.44
1:A:52:MET:CG	1:A:95:VAL:HG22	2.32	0.44
1:C:402:ALA:O	1:C:405:GLN:HB2	2.18	0.44
2:D:393:MET:HE3	2:D:401:LYS:HB2	2.00	0.44
3:G:85:VAL:HG12	3:G:173:THR:HG23	2.00	0.44
1:B:38:ILE:HG13	1:B:285:LEU:HD21	1.98	0.43
1:C:151:LYS:HA	1:C:441:GLN:OE1	2.18	0.43
1:B:211:SER:CB	2:E:126:MET:HE2	2.49	0.43
2:E:278:ALA:C	2:E:279:VAL:HG23	2.43	0.43
1:A:99:VAL:HG22	1:A:253:MET:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.99	0.43
2:D:400:ASP:O	2:D:404:VAL:HG23	2.19	0.43
3:G:71:VAL:HA	3:G:108:VAL:HG13	2.01	0.43
1:B:394:LEU:HD11	1:B:428:LEU:HD11	2.01	0.43
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.48	0.43
1:C:456:LEU:HD23	1:C:461:ILE:HD13	2.00	0.43
2:E:136:GLY:HA3	2:E:431:LEU:HD13	2.00	0.43
2:F:139:VAL:HG13	2:F:414:LEU:HD22	2.00	0.43
2:F:472:LYS:C	2:F:474:ALA:H	2.26	0.43
1:C:23:VAL:HG11	1:C:30:ARG:HH21	1.83	0.43
1:C:171:ARG:CD	9:C:2059:HOH:O	2.66	0.43
2:E:163:THR:HG23	8:E:1475:PO4:O2	2.18	0.43
2:E:167:MET:HA	2:E:170:ILE:HD12	1.99	0.43
2:E:237:LEU:HD21	2:E:295:ARG:HB2	2.00	0.43
2:E:253:LEU:O	2:E:306:SER:HA	2.19	0.43
2:E:52:HIS:CD2	2:E:58:VAL:HG12	2.54	0.43
1:C:270:ASP:HB2	1:C:326:VAL:O	2.19	0.43
1:B:68:PRO:HD3	2:F:15:ALA:HB2	2.00	0.43
2:E:280:GLY:HA2	3:G:262:LEU:HD23	2.01	0.43
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.48	0.43
1:A:137:ILE:N	1:A:138:PRO:CD	2.82	0.42
1:A:152:ALA:HA	1:A:428:LEU:HD22	2.00	0.42
1:A:392:LEU:O	1:A:396:GLN:HG3	2.19	0.42
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.42
3:G:115:ILE:HG22	3:G:116:LEU:HD13	2.01	0.42
1:C:376:SER:HB2	1:C:384:LYS:HG3	2.01	0.42
2:D:345:TYR:HA	2:D:346:PRO:C	2.44	0.42
2:E:391:LEU:HB3	2:E:395:GLU:HG3	2.01	0.42
1:C:488:LYS:HB2	1:C:488:LYS:HE3	1.78	0.42
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.01	0.42
1:A:213:VAL:O	1:A:216:LEU:HB3	2.20	0.42
1:A:300:TYR:CZ	2:E:225:PRO:HG3	2.55	0.42
1:C:396:GLN:O	1:C:400:VAL:HG23	2.20	0.42
1:A:26:GLU:HB3	1:A:46:ASN:ND2	2.35	0.42
1:A:362:ARG:HA	1:A:363:PRO:C	2.45	0.42
2:F:440:GLY:O	2:F:444:ILE:HG13	2.19	0.42
2:F:228:ALA:O	2:F:232:VAL:HG22	2.20	0.41
2:E:111:LYS:H	2:E:111:LYS:HG2	1.62	0.41
2:E:412:ARG:HG2	2:E:458:TYR:HB2	2.01	0.41
2:E:174:ALA:HB2	9:E:2039:HOH:O	2.20	0.41
3:G:5:ASP:O	3:G:6:ILE:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LYS:O	1:B:486:ASP:HB2	2.20	0.41
3:G:213:ILE:O	3:G:217:LEU:HB2	2.20	0.41
1:B:99:VAL:HG22	1:B:253:MET:HA	2.01	0.41
1:C:263:HIS:HD2	1:C:320:SER:OG	2.02	0.41
2:D:282:GLN:HA	2:D:283:PRO:HD3	1.91	0.41
1:A:457:GLU:HA	1:A:458:PRO:HD3	1.90	0.41
1:C:200:TYR:O	1:C:264:ALA:HA	2.20	0.41
3:G:68:ILE:HG23	3:G:161:ILE:HD13	2.03	0.41
1:A:307:GLU:CG	2:E:223:ASN:HB3	2.50	0.41
1:B:84:GLU:HB3	2:E:29:LEU:HD12	2.03	0.41
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.86	0.41
2:F:89:GLU:HG2	2:F:110:THR:HG23	1.98	0.41
2:F:163:THR:O	2:F:166:ILE:HG22	2.20	0.41
1:A:187:LYS:CE	1:A:224:ASP:HB3	2.51	0.41
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.55	0.41
1:B:105:GLY:HA2	1:B:226:MET:O	2.21	0.40
1:B:270:ASP:OD1	1:B:272:SER:HB2	2.21	0.40
2:F:139:VAL:HG13	2:F:414:LEU:HB3	2.03	0.40
1:B:338:ILE:HB	1:B:339:PRO:HD3	2.03	0.40
2:F:196:LEU:HD23	2:F:219:TYR:HH	1.86	0.40
1:C:300:TYR:O	1:C:304:ARG:HG2	2.20	0.40
3:G:228:ARG:O	3:G:232:MET:HB2	2.22	0.40
1:A:240:ALA:N	1:A:241:PRO:CD	2.85	0.40
1:C:269:ASP:HA	1:C:270:ASP:HA	1.83	0.40
1:C:387:ALA:HA	1:C:390:MET:HE2	2.04	0.40
3:G:5:ASP:O	3:G:8:ARG:N	2.52	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	485/510 (95%)	465 (96%)	19 (4%)	1 (0%)	43	51
1	B	476/510 (93%)	458 (96%)	18 (4%)	0	100	100
1	C	496/510 (97%)	480 (97%)	12 (2%)	4 (1%)	16	16
2	D	465/482 (96%)	440 (95%)	24 (5%)	1 (0%)	43	51
2	E	464/482 (96%)	433 (93%)	29 (6%)	2 (0%)	30	34
2	F	464/482 (96%)	448 (97%)	14 (3%)	2 (0%)	30	34
3	G	180/272 (66%)	169 (94%)	10 (6%)	1 (1%)	21	23
All	All	3030/3248 (93%)	2893 (96%)	126 (4%)	11 (0%)	30	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	C	16	ILE
1	C	407	GLY
1	C	409	ASP
2	F	28	GLY
2	E	81	PRO
2	E	279	VAL
1	C	405	GLN
3	G	5	ASP
2	F	279	VAL
2	D	279	VAL

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	393/412 (95%)	371 (94%)	22 (6%)	19	24
1	B	389/412 (94%)	367 (94%)	22 (6%)	18	23
1	C	402/412 (98%)	372 (92%)	30 (8%)	12	14
2	D	377/386 (98%)	359 (95%)	18 (5%)	23	30
2	E	376/386 (97%)	358 (95%)	18 (5%)	23	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	376/386 (97%)	360 (96%)	16 (4%)	26	35
3	G	162/230 (70%)	146 (90%)	16 (10%)	7	8
All	All	2475/2624 (94%)	2333 (94%)	142 (6%)	18	23

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	56	SER
1	A	74	VAL
1	A	86	ASP
1	A	94	ILE
1	A	99	VAL
1	A	102	GLU
1	A	123	SER
1	A	136	ILE
1	A	141	SER
1	A	202	ILE
1	A	217	VAL
1	A	355	GLU
1	A	367	VAL
1	A	403	PHE
1	A	410	LEU
1	A	419	SER
1	A	442	VAL
1	A	479	LEU
1	A	485	THR
1	A	488	LYS
1	A	492	GLU
1	B	28	THR
1	B	30	ARG
1	B	34	ILE
1	B	47	VAL
1	B	65	ASN
1	B	80	LYS
1	B	83	LYS
1	B	87	ILE
1	B	99	VAL
1	B	102	GLU
1	B	157	VAL
1	B	163	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	208	GLN
1	B	216	LEU
1	B	217	VAL
1	B	355	GLU
1	B	371	VAL
1	B	418	LEU
1	B	442	VAL
1	B	479	LEU
1	B	492	GLU
1	B	501	VAL
1	C	14	GLU
1	C	17	LEU
1	C	26	GLU
1	C	56	SER
1	C	57	SER
1	C	74	VAL
1	C	87	ILE
1	C	91	THR
1	C	99	VAL
1	C	123	SER
1	C	127	ARG
1	C	143	ARG
1	C	165	GLU
1	C	197	LYS
1	C	210	ARG
1	C	215	GLN
1	C	216	LEU
1	C	217	VAL
1	C	334	VAL
1	C	335	SER
1	C	361	ILE
1	C	390	MET
1	C	398	ARG
1	C	415	GLN
1	C	422	VAL
1	C	462	THR
1	C	475	GLN
1	C	479	LEU
1	C	501	VAL
1	C	505	LEU
2	D	9	THR
2	D	10	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	12	ARG
2	D	27	GLU
2	D	84	ILE
2	D	89	GLU
2	D	97	VAL
2	D	109	LYS
2	D	111	LYS
2	D	127	SER
2	D	215	VAL
2	D	237	LEU
2	D	249	GLN
2	D	335	LEU
2	D	400	ASP
2	D	419	GLN
2	D	420	VAL
2	D	428	LEU
2	E	10	THR
2	E	76	LEU
2	E	139	VAL
2	E	160	VAL
2	E	162	LYS
2	E	194	ASN
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	258	ILE
2	E	293	GLN
2	E	301	LYS
2	E	310	ILE
2	E	387	ILE
2	E	394	ASP
2	E	412	ARG
2	E	420	VAL
2	E	431	LEU
2	F	9	THR
2	F	12	ARG
2	F	29	LEU
2	F	89	GLU
2	F	97	VAL
2	F	109	LYS
2	F	112	GLN
2	F	139	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	202	GLU
2	F	223	ASN
2	F	232	VAL
2	F	247	GLU
2	F	279	VAL
2	F	303	SER
2	F	420	VAL
2	F	428	LEU
3	G	67	LEU
3	G	87	LYS
3	G	89	MET
3	G	90	LYS
3	G	108	VAL
3	G	112	ILE
3	G	116	LEU
3	G	166	ARG
3	G	168	VAL
3	G	169	ILE
3	G	211	ASN
3	G	218	LYS
3	G	232	MET
3	G	245	LYS
3	G	254	ARG
3	G	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	172	GLN
1	A	396	GLN
1	A	415	GLN
1	B	42	HIS
1	B	186	GLN
1	B	330	GLN
1	B	415	GLN
1	B	503	ASN
1	C	48	GLN
1	C	186	GLN
1	C	263	HIS
1	C	415	GLN
1	C	416	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	432	GLN
1	C	471	HIS
2	D	24	GLN
2	D	130	GLN
2	D	221	GLN
2	D	249	GLN
2	D	379	GLN
2	D	411	GLN
2	D	419	GLN
2	D	427	HIS
2	E	171	ASN
2	E	194	ASN
2	E	223	ASN
2	E	257	ASN
2	E	293	GLN
2	E	308	GLN
2	E	367	HIS
2	E	379	GLN
2	E	385	GLN
2	F	177	HIS
2	F	221	GLN
2	F	223	ASN
2	F	249	GLN
2	F	367	HIS
2	F	419	GLN
2	F	443	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	1511	5	28,29,29	1.57	6 (21%)	43,45,45	1.81	8 (18%)
7	BEF	D	1478	5,4	0,3,3	-	-	-		
6	GOL	B	1513	-	5,5,5	0.43	0	5,5,5	0.30	0
7	BEF	F	1477	5,4	0,3,3	-	-	-		
4	ADP	B	1511	5	28,29,29	1.65	5 (17%)	43,45,45	1.88	11 (25%)
6	GOL	D	1475	-	5,5,5	0.47	0	5,5,5	0.64	0
4	ADP	D	1476	5,7	28,29,29	1.68	5 (17%)	43,45,45	1.96	13 (30%)
8	PO4	E	1475	-	4,4,4	0.95	0	6,6,6	0.62	0
6	GOL	A	1513	-	5,5,5	0.21	0	5,5,5	0.62	0
4	ADP	A	1511	5	28,29,29	1.57	5 (17%)	43,45,45	1.83	10 (23%)
6	GOL	C	1513	-	5,5,5	0.35	0	5,5,5	0.40	0
4	ADP	F	1475	5,7	28,29,29	1.28	4 (14%)	43,45,45	1.81	11 (25%)

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	1511	5	-	1/16/32/32	0/3/3/3
6	GOL	B	1513	-	-	0/4/4/4	-
4	ADP	B	1511	5	-	0/16/32/32	0/3/3/3
6	GOL	D	1475	-	-	2/4/4/4	-
4	ADP	D	1476	5,7	-	2/16/32/32	0/3/3/3
6	GOL	A	1513	-	-	3/4/4/4	-
4	ADP	A	1511	5	-	0/16/32/32	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	-
4	ADP	F	1475	5,7	-	2/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1476	ADP	PA-O3A	5.08	1.65	1.59
4	B	1511	ADP	C5-C4	4.88	1.47	1.39
4	A	1511	ADP	C5-C4	4.85	1.47	1.39
4	D	1476	ADP	C5-C4	4.50	1.47	1.39
4	B	1511	ADP	PA-O3A	4.41	1.64	1.59
4	C	1511	ADP	PA-O3A	4.31	1.64	1.59
4	F	1475	ADP	C5-C4	4.28	1.46	1.39
4	C	1511	ADP	C5-C4	4.25	1.46	1.39
4	A	1511	ADP	PA-O3A	4.01	1.63	1.59
4	B	1511	ADP	C5-C6	3.02	1.49	1.41
4	C	1511	ADP	C5-C6	2.83	1.48	1.41
4	F	1475	ADP	C5-C6	2.71	1.48	1.41
4	A	1511	ADP	C5-C6	2.68	1.48	1.41
4	D	1476	ADP	C5-C6	2.65	1.48	1.41
4	A	1511	ADP	C8-N7	2.50	1.36	1.31
4	D	1476	ADP	C8-N7	2.37	1.36	1.31
4	C	1511	ADP	C4-N9	-2.36	1.32	1.37
4	B	1511	ADP	C5-N7	-2.28	1.34	1.39
4	F	1475	ADP	C8-N7	2.16	1.35	1.31
4	B	1511	ADP	C8-N7	2.14	1.35	1.31
4	D	1476	ADP	C5-N7	-2.13	1.35	1.39
4	A	1511	ADP	C5-N7	-2.10	1.35	1.39
4	C	1511	ADP	C8-N7	2.04	1.35	1.31
4	C	1511	ADP	C5-N7	-2.03	1.35	1.39
4	F	1475	ADP	C5-N7	-2.01	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1476	ADP	C5-C4-N3	-5.59	119.02	126.72
4	B	1511	ADP	C5-C4-N3	-5.58	119.04	126.72
4	F	1475	ADP	C5-C4-N3	-5.42	119.25	126.72
4	A	1511	ADP	C5-C4-N3	-5.36	119.33	126.72
4	C	1511	ADP	C5-C4-N3	-5.36	119.34	126.72
4	D	1476	ADP	N3-C4-N9	4.82	135.36	127.17
4	C	1511	ADP	N3-C4-N9	4.58	134.96	127.17
4	F	1475	ADP	N3-C4-N9	4.58	134.95	127.17
4	B	1511	ADP	N3-C4-N9	4.50	134.83	127.17
4	D	1476	ADP	N3-C2-N1	-4.21	122.20	128.58
4	A	1511	ADP	N3-C4-N9	4.21	134.33	127.17
4	C	1511	ADP	C2-N3-C4	3.82	121.15	111.83
4	B	1511	ADP	C4-C5-N7	-3.79	106.24	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1511	ADP	C4-C5-N7	-3.74	106.31	110.58
4	A	1511	ADP	C2-N3-C4	3.63	120.69	111.83
4	D	1476	ADP	C2-N3-C4	3.62	120.66	111.83
4	B	1511	ADP	C2-N3-C4	3.61	120.65	111.83
4	A	1511	ADP	N3-C2-N1	-3.58	123.16	128.58
4	C	1511	ADP	N3-C2-N1	-3.54	123.22	128.58
4	F	1475	ADP	C2-N3-C4	3.37	120.06	111.83
4	D	1476	ADP	C2'-C1'-N9	-3.23	105.27	113.30
4	B	1511	ADP	N3-C2-N1	-3.22	123.71	128.58
4	F	1475	ADP	N3-C2-N1	-3.20	123.73	128.58
4	C	1511	ADP	C4-N9-C8	3.10	108.99	105.74
4	A	1511	ADP	C4-N9-C8	3.06	108.95	105.74
4	B	1511	ADP	C5-N7-C8	3.02	108.19	103.45
4	B	1511	ADP	C4-N9-C8	2.98	108.87	105.74
4	D	1476	ADP	C2-N1-C6	2.94	123.56	118.73
4	F	1475	ADP	C4-C5-N7	-2.90	107.26	110.58
4	F	1475	ADP	C4-N9-C8	2.86	108.74	105.74
4	D	1476	ADP	C4-N9-C8	2.75	108.62	105.74
4	A	1511	ADP	C5-N7-C8	2.75	107.77	103.45
4	D	1476	ADP	C4-C5-N7	-2.74	107.44	110.58
4	A	1511	ADP	C6-C5-N7	2.68	137.26	132.09
4	C	1511	ADP	C4-C5-N7	-2.64	107.56	110.58
4	F	1475	ADP	O3A-PB-O1B	-2.56	97.59	111.04
4	F	1475	ADP	C5-N7-C8	2.54	107.44	103.45
4	C	1511	ADP	O4'-C1'-N9	2.47	112.83	108.09
4	D	1476	ADP	O3B-PB-O2B	2.45	116.98	107.80
4	D	1476	ADP	C5-N7-C8	2.43	107.27	103.45
4	B	1511	ADP	C6-C5-N7	2.39	136.69	132.09
4	B	1511	ADP	N9-C8-N7	-2.37	110.57	113.94
4	C	1511	ADP	C6-C5-N7	2.36	136.65	132.09
4	D	1476	ADP	O3B-PB-O3A	-2.34	96.78	104.64
4	A	1511	ADP	N9-C8-N7	-2.32	110.64	113.94
4	B	1511	ADP	O3A-PB-O1B	-2.23	99.31	111.04
4	F	1475	ADP	N9-C8-N7	-2.22	110.78	113.94
4	A	1511	ADP	C2-N1-C6	2.19	122.32	118.73
4	F	1475	ADP	C2-N1-C6	2.15	122.25	118.73
4	F	1475	ADP	C2'-C1'-N9	-2.10	108.08	113.30
4	D	1476	ADP	N6-C6-N1	2.08	123.02	118.38
4	B	1511	ADP	C2-N1-C6	2.04	122.08	118.73
4	D	1476	ADP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1476	ADP	PA-O3A-PB-O2B
4	F	1475	ADP	PA-O3A-PB-O2B
6	A	1513	GOL	C1-C2-C3-O3
6	A	1513	GOL	O2-C2-C3-O3
6	D	1475	GOL	O1-C1-C2-C3
4	C	1511	ADP	PA-O3A-PB-O1B
6	D	1475	GOL	O1-C1-C2-O2
6	A	1513	GOL	O1-C1-C2-O2
4	D	1476	ADP	PA-O3A-PB-O1B
4	F	1475	ADP	PA-O3A-PB-O1B

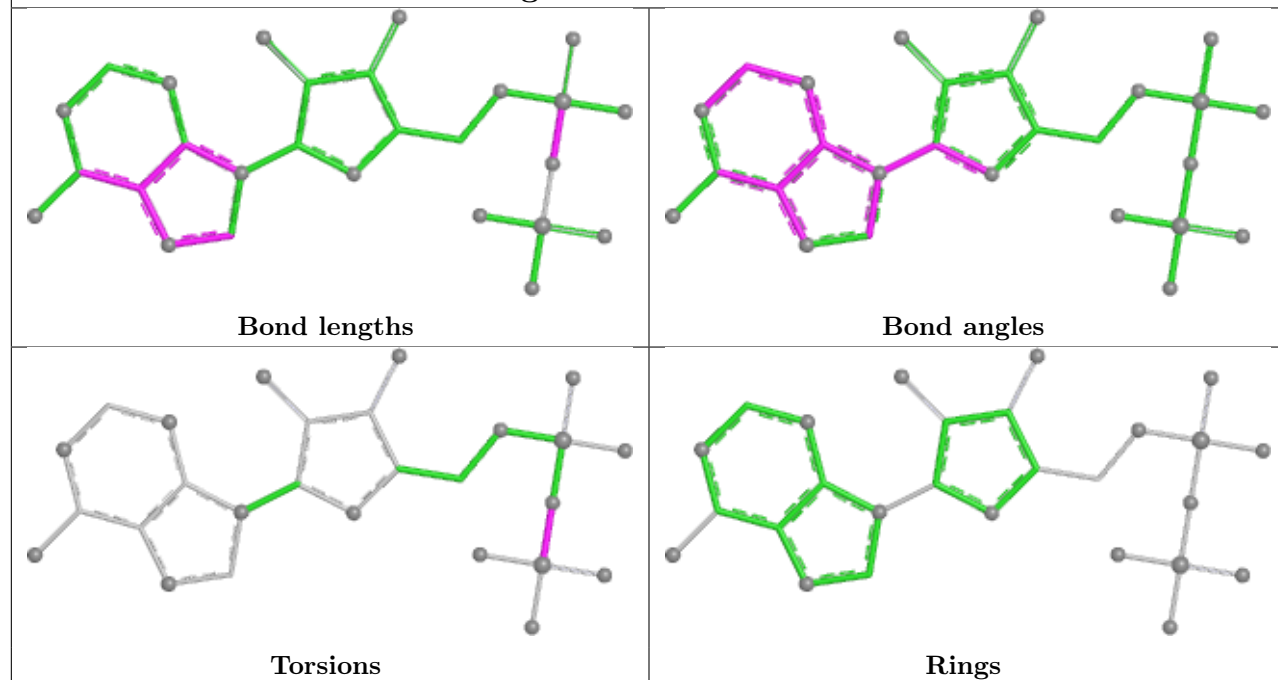
There are no ring outliers.

3 monomers are involved in 3 short contacts:

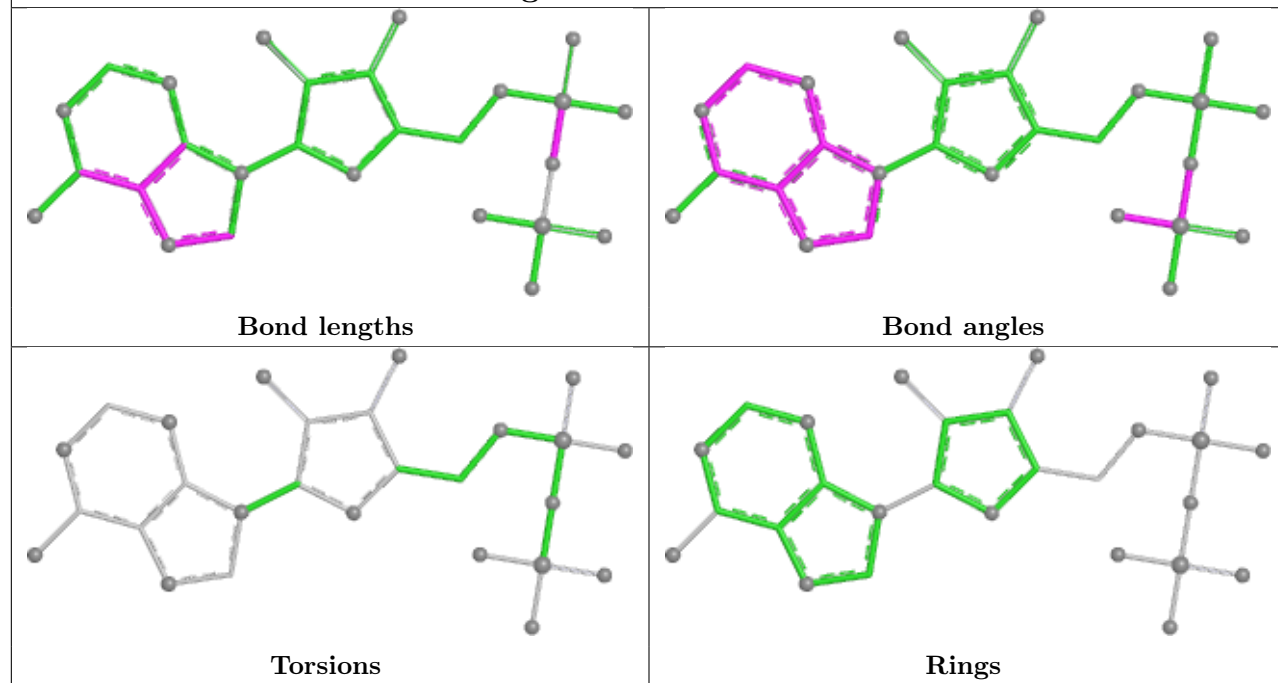
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1511	ADP	1	0
8	E	1475	PO4	1	0
6	A	1513	GOL	1	0

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.

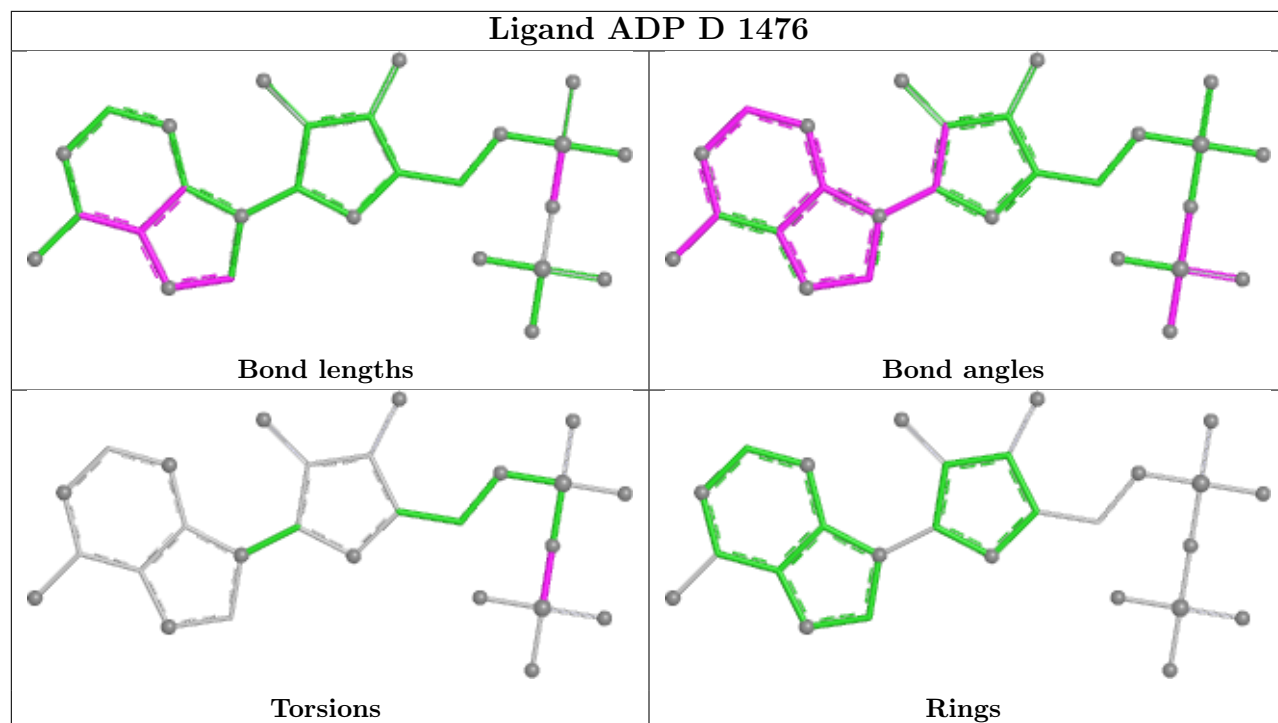
Ligand ADP C 1511



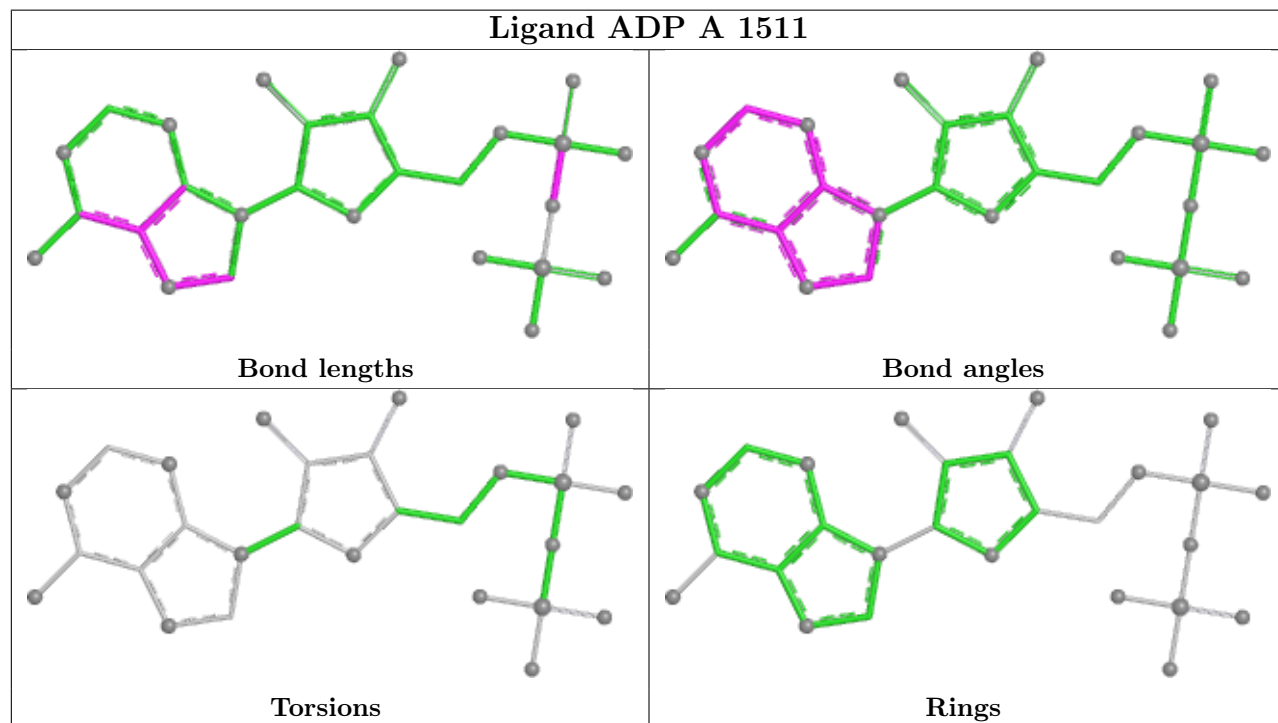
Ligand ADP B 1511

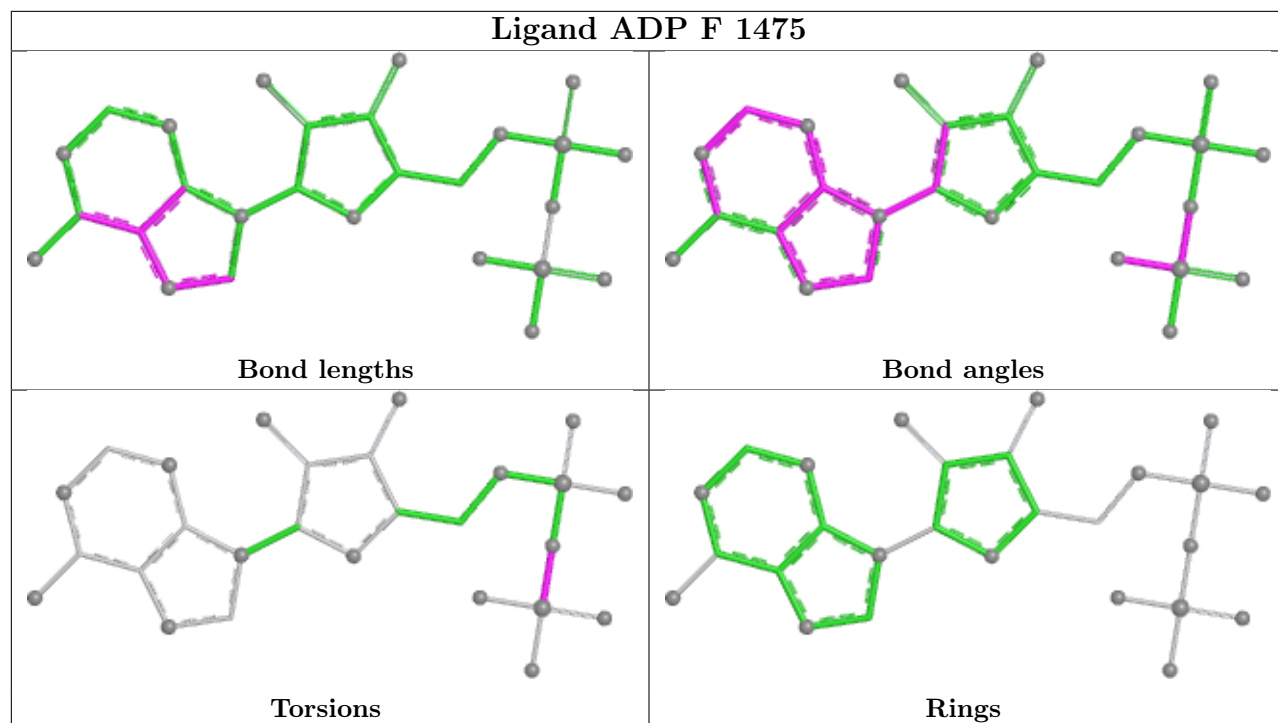


Ligand ADP D 1476



Ligand ADP A 1511





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	487/510 (95%)	-0.10	6 (1%) 76 74	25, 43, 72, 105	0
1	B	480/510 (94%)	-0.07	9 (1%) 66 63	23, 43, 85, 111	0
1	C	498/510 (97%)	-0.36	7 (1%) 73 71	22, 36, 62, 116	0
2	D	467/482 (96%)	-0.36	4 (0%) 81 79	20, 37, 70, 98	0
2	E	466/482 (96%)	0.59	45 (9%) 13 10	24, 57, 109, 135	0
2	F	466/482 (96%)	-0.33	6 (1%) 75 73	21, 37, 67, 84	0
3	G	192/272 (70%)	1.42	57 (29%) 1 1	27, 89, 125, 138	0
All	All	3056/3248 (94%)	-0.01	134 (4%) 39 36	20, 42, 96, 138	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	43	VAL	5.7
3	G	47	GLY	5.2
1	B	410	LEU	4.6
3	G	105	ILE	4.5
2	E	424	PHE	4.5
2	E	396	LEU	4.5
3	G	116	LEU	4.5
2	E	389	ALA	4.2
3	G	115	ILE	4.1
3	G	44	TYR	4.1
3	G	204	TYR	4.1
3	G	144	ILE	4.1
2	E	473	LEU	4.0
2	F	474	ALA	4.0
3	G	148	LEU	4.0
2	E	407	ALA	3.9
1	C	406	PHE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	83	SER	3.9
3	G	210	ALA	3.8
3	G	207	TYR	3.7
2	E	423	VAL	3.7
3	G	135	PRO	3.6
3	G	201	LEU	3.6
2	E	391	LEU	3.6
1	B	23	VAL	3.5
1	B	510	ALA	3.5
3	G	40	PRO	3.5
1	C	407	GLY	3.5
1	C	409	ASP	3.5
3	G	141	ALA	3.4
1	C	17	LEU	3.4
1	A	403	PHE	3.3
2	E	469	LYS	3.3
3	G	146	LEU	3.3
3	G	46	VAL	3.2
3	G	143	VAL	3.2
3	G	68	ILE	3.2
2	E	157	GLY	3.2
2	F	9	THR	3.2
3	G	173	THR	3.2
3	G	29	ALA	3.1
3	G	138	PHE	3.1
2	F	249	GLN	3.1
1	B	193	THR	3.1
3	G	39	LYS	3.1
2	E	362	ILE	3.1
2	E	387	ILE	3.1
2	E	390	ILE	3.1
2	F	178	GLY	3.1
1	B	401	ALA	3.1
2	E	388	ILE	3.0
3	G	86	ALA	3.0
3	G	168	VAL	3.0
2	E	345	TYR	3.0
2	F	176	ALA	2.9
2	E	427	HIS	2.9
3	G	90	LYS	2.9
3	G	208	SER	2.9
2	E	392	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	403	THR	2.8
3	G	209	LEU	2.8
3	G	132	GLY	2.8
3	G	159	SER	2.8
2	E	158	ALA	2.8
2	E	344	ILE	2.8
3	G	131	VAL	2.8
3	G	160	ILE	2.7
1	A	122	GLY	2.7
3	G	34	ALA	2.7
3	G	133	ARG	2.7
3	G	71	VAL	2.7
2	E	445	LEU	2.7
1	B	37	GLY	2.6
1	A	410	LEU	2.6
2	E	428	LEU	2.6
3	G	27	ALA	2.6
2	D	27	GLU	2.6
3	G	165	PHE	2.6
1	C	408	SER	2.6
2	E	402	LEU	2.5
2	E	474	ALA	2.5
2	E	444	ILE	2.5
3	G	221	THR	2.5
3	G	112	ILE	2.5
2	E	422	GLU	2.5
3	G	214	TYR	2.5
1	B	413	ALA	2.5
3	G	137	THR	2.5
1	C	410	LEU	2.5
3	G	25	MET	2.5
2	E	455	GLN	2.5
1	C	16	ILE	2.4
3	G	129	LYS	2.4
2	F	248	GLY	2.4
3	G	72	SER	2.4
2	E	420	VAL	2.4
2	D	248	GLY	2.4
2	E	393	MET	2.4
2	E	467	VAL	2.4
3	G	85	VAL	2.4
2	E	384	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	249	GLN	2.4
2	E	421	ALA	2.3
2	E	374	VAL	2.3
3	G	81	ILE	2.3
3	G	38	LEU	2.3
2	E	458	TYR	2.3
3	G	171	TYR	2.3
2	E	456	ALA	2.3
3	G	136	PRO	2.3
1	A	94	ILE	2.3
2	E	160	VAL	2.3
2	E	373	GLY	2.3
2	E	425	THR	2.3
2	E	173	VAL	2.2
2	E	441	PHE	2.2
2	E	350	PRO	2.2
3	G	127	THR	2.2
2	E	378	LEU	2.2
2	D	400	ASP	2.2
1	B	415	GLN	2.2
2	E	9	THR	2.2
3	G	41	ALA	2.2
3	G	220	SER	2.2
2	E	440	GLY	2.2
3	G	203	ASN	2.1
1	A	510	ALA	2.1
3	G	162	PHE	2.1
1	A	407	GLY	2.1
3	G	111	LYS	2.1
2	E	363	VAL	2.1
2	E	370	VAL	2.1
1	B	25	LEU	2.0
3	G	211	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

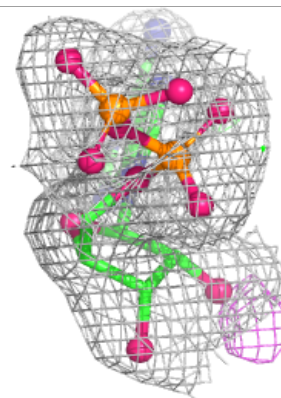
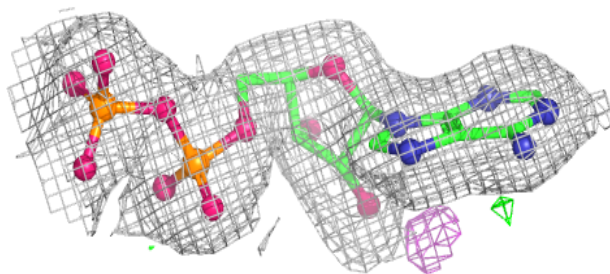
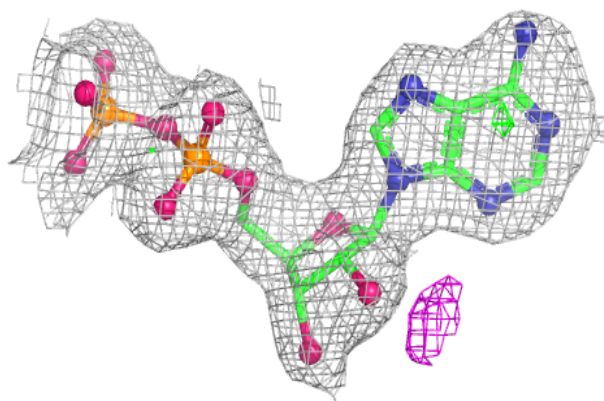
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PO4	E	1475	5/5	0.72	0.13	87,87,90,92	0
6	GOL	D	1475	6/6	0.84	0.16	59,61,62,62	0
6	GOL	A	1513	6/6	0.93	0.08	45,47,49,57	0
6	GOL	C	1513	6/6	0.96	0.06	32,36,40,43	0
5	MG	C	1512	1/1	0.96	0.03	24,24,24,24	0
6	GOL	B	1513	6/6	0.96	0.07	34,37,38,39	0
7	BEF	D	1478	4/4	0.97	0.04	17,20,23,25	0
5	MG	A	1512	1/1	0.98	0.03	28,28,28,28	0
4	ADP	A	1511	27/27	0.98	0.05	20,37,42,47	0
7	BEF	F	1477	4/4	0.98	0.05	23,27,28,31	0
5	MG	D	1477	1/1	0.98	0.03	30,30,30,30	0
5	MG	B	1512	1/1	0.99	0.04	31,31,31,31	0
4	ADP	C	1511	27/27	0.99	0.04	22,27,32,36	0
4	ADP	D	1476	27/27	0.99	0.04	18,25,30,34	0
4	ADP	F	1475	27/27	0.99	0.04	23,29,35,38	0
4	ADP	B	1511	27/27	0.99	0.05	26,45,49,54	0
5	MG	F	1476	1/1	1.00	0.01	25,25,25,25	0

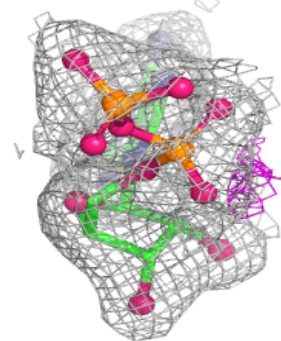
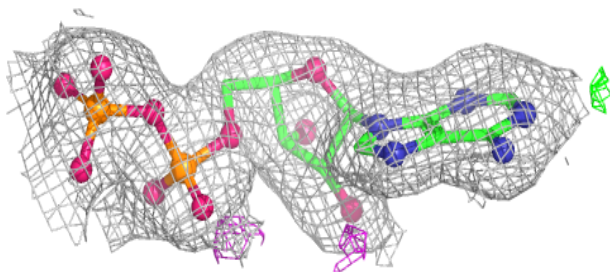
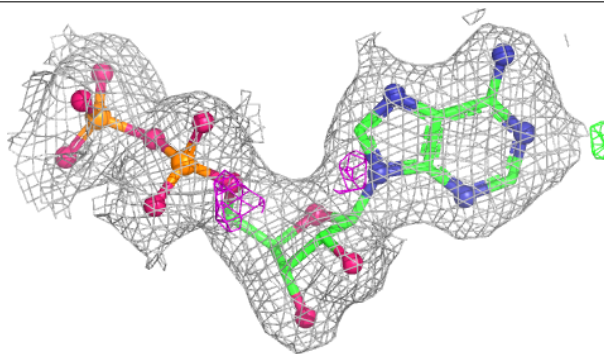
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1511:

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

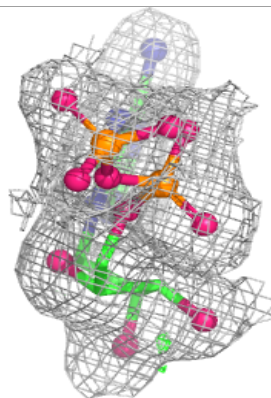
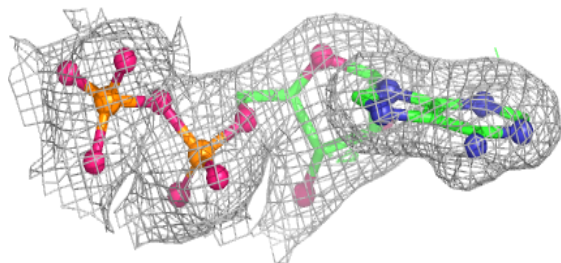
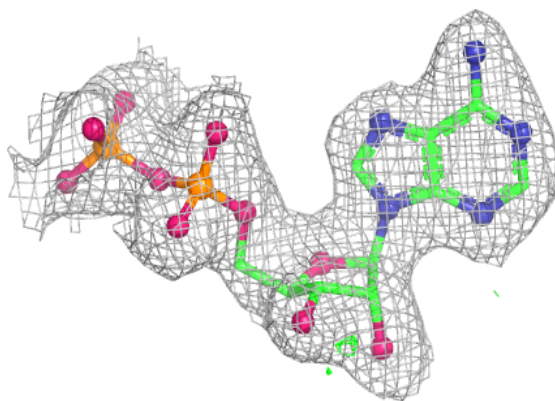
**Electron density around ADP C 1511:**

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

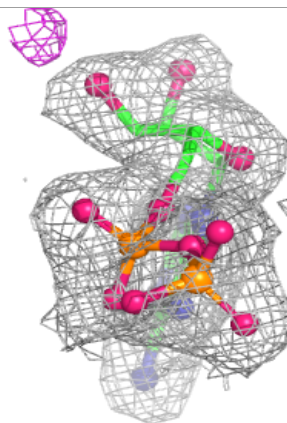
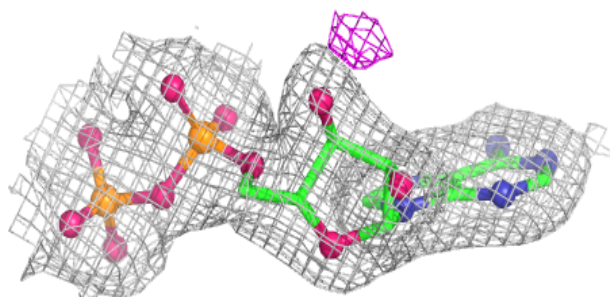
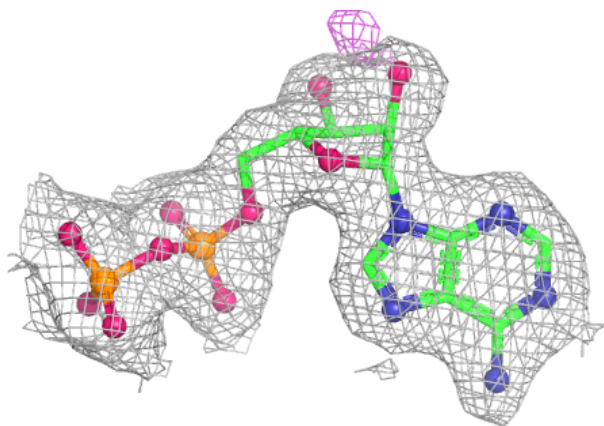


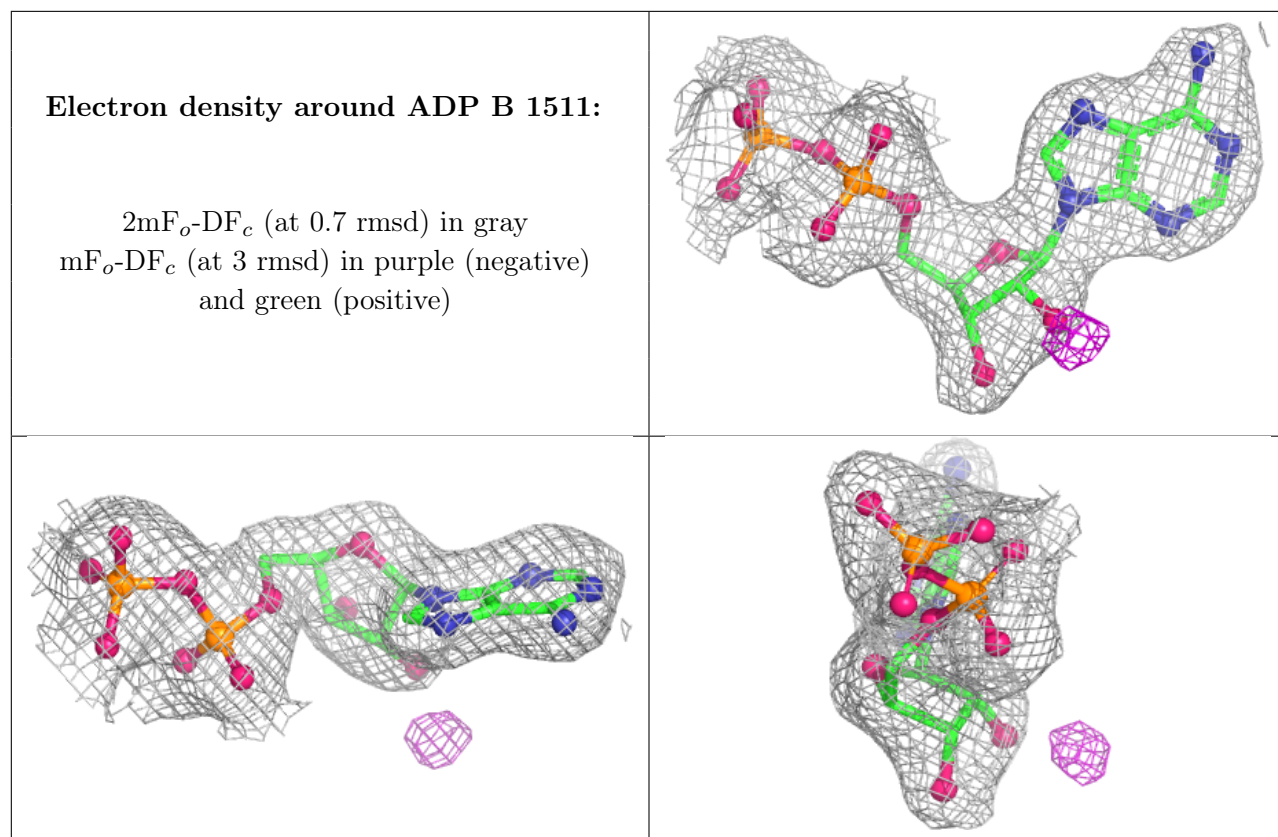
Electron density around ADP D 1476:

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

**Electron density around ADP F 1475:**

$2mF_o-DF_c$ (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.