



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 02:55 pm GMT

PDB ID : 1W0J  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

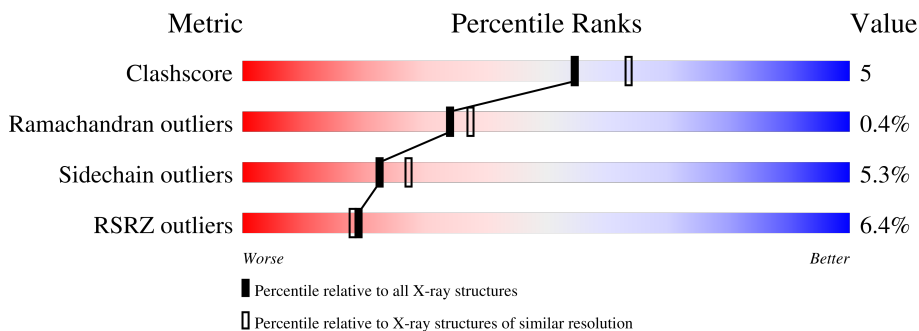
# 1 Overall quality at a glance

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	 2% 78% 15% • 5%
1	B	510	 4% 79% 13% • 6%
1	C	510	 2% 79% 17% • •
2	D	482	 % 86% 10% • •
2	E	482	 15% 79% 16% • •
2	F	482	 % 84% 11% • •

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Mol	Chain	Length	Quality of chain
3	G	272	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (26%), a green segment (50%), a yellow segment (18%), and a grey segment (29%). There are two small black dots on the yellow segment.</p>

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	487	Total 3715	C 2341	N 656	O 706	S 12	0	0	0
1	B	480	Total 3663	C 2308	N 648	O 695	S 12	0	0	0
1	C	498	Total 3797	C 2390	N 670	O 725	S 12	0	0	0

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
			Total	C	N	O	S			
2	D	467	Total 3539	C 2243	N 601	O 684	S 11	0	0	0
2	E	466	Total 3530	C 2238	N 600	O 681	S 11	0	0	0
2	F	466	Total 3530	C 2238	N 600	O 681	S 11	0	0	0

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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 (three-letter code: MG) (formula: Mg).

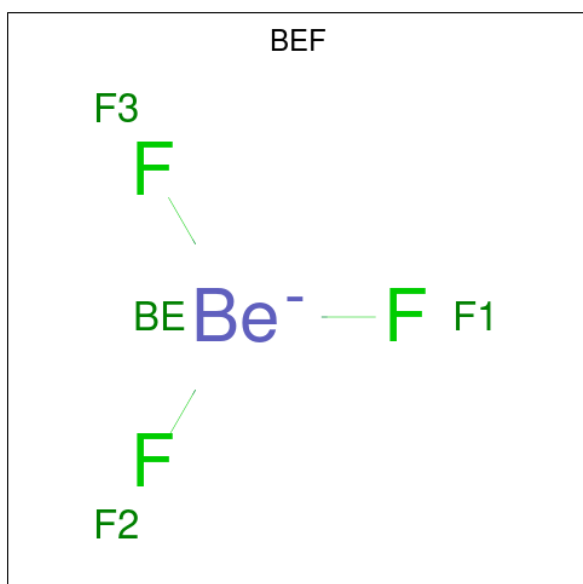
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



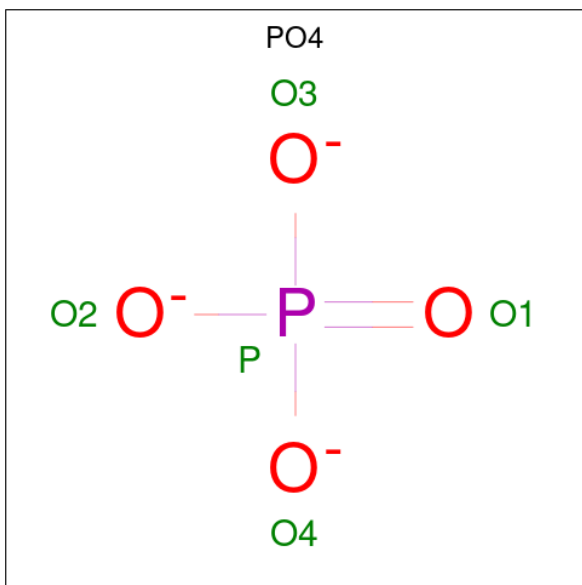
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula:  $BeF_3$ ).



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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

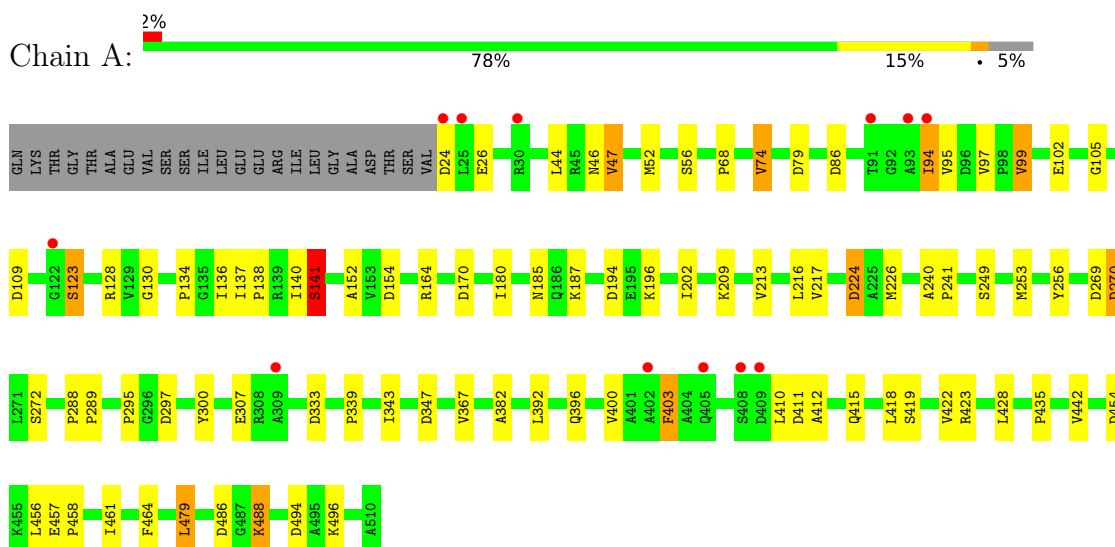
- Molecule 9 is water.

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		

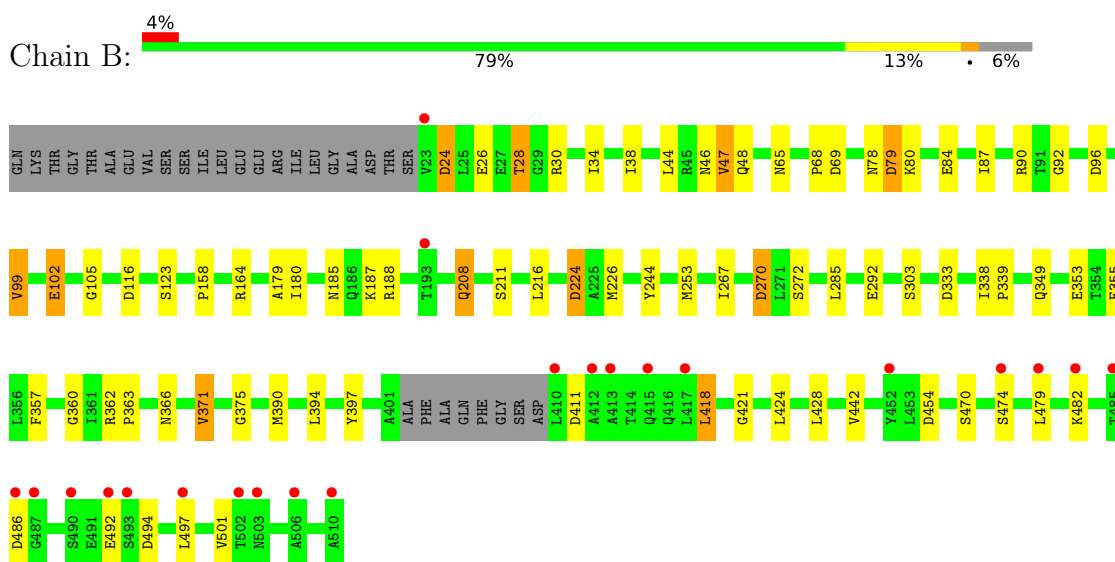
### 3 Residue-property plots i

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

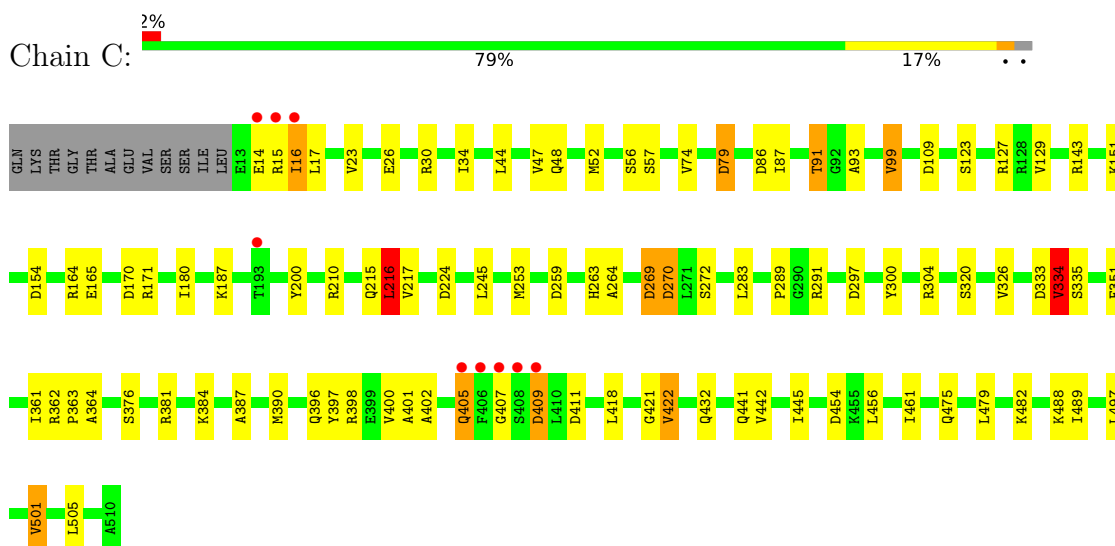


- Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRE-CURSOR

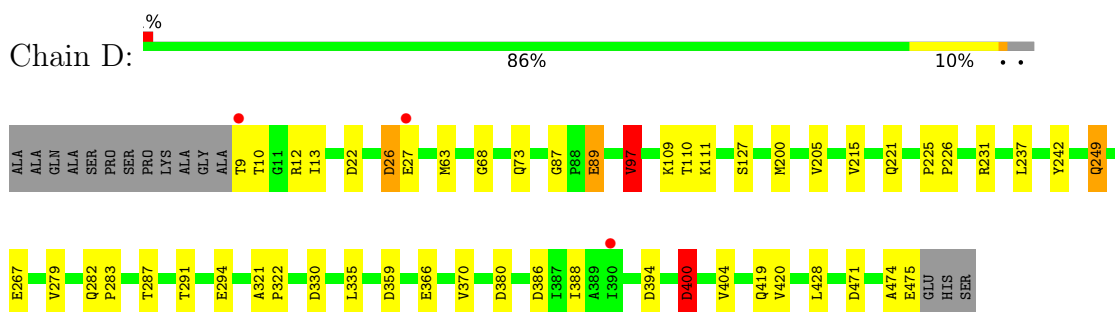




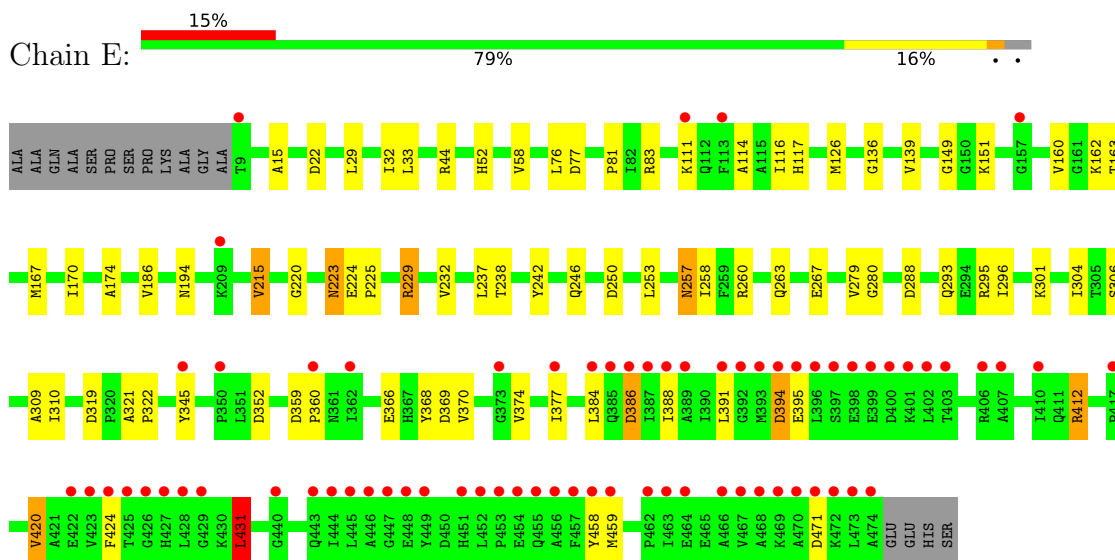
- Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM, MITOCHONDRIAL PRECURSOR



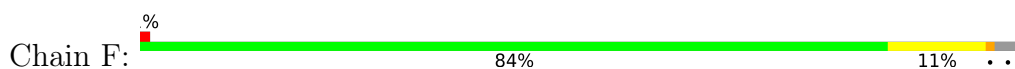
- Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR

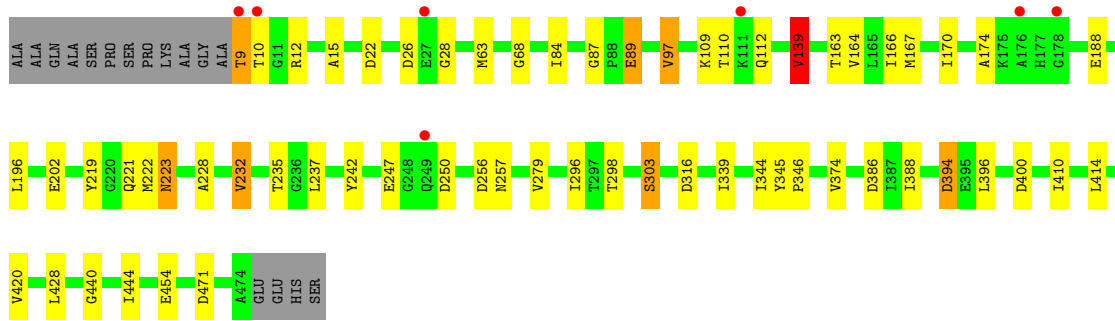


- Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR

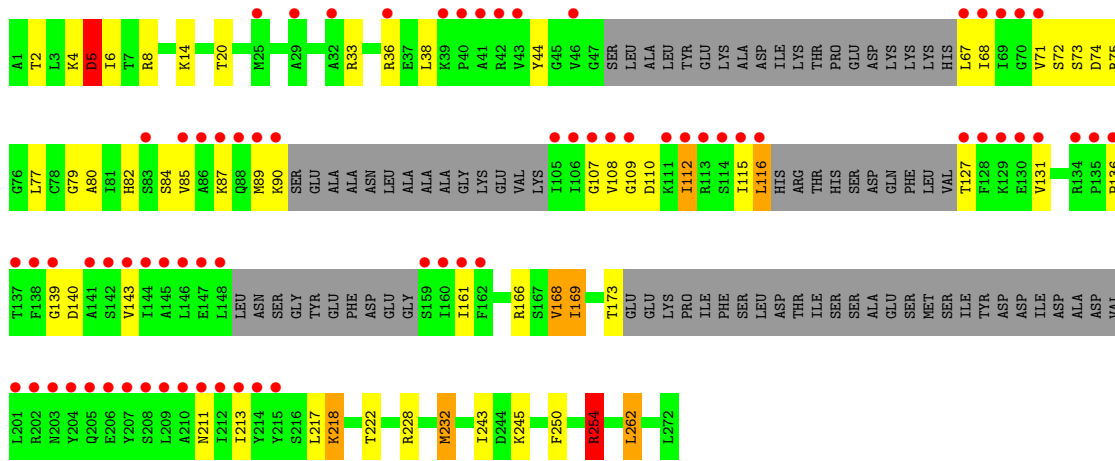


- Molecule 2: ATP SYNTHASE BETA CHAIN, MITOCHONDRIAL PRECURSOR





● 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, $\alpha$ , $\beta$ , $\gamma$	283.52Å 107.37Å 137.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 45.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.8 (20.00-2.20) 86.8 (45.39-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.20Å)	Xtrriage
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 <sup>2</sup> )	37.5	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, BEF, GOL, 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	0.53	0/3766	0.79	14/5080 (0.3%)
1	B	0.53	0/3711	0.79	12/5005 (0.2%)
1	C	0.57	0/3848	0.84	16/5191 (0.3%)
2	D	0.55	0/3596	0.79	10/4879 (0.2%)
2	E	0.48	0/3587	0.77	11/4867 (0.2%)
2	F	0.56	0/3587	0.80	8/4867 (0.2%)
3	G	0.44	0/1502	0.71	4/2006 (0.2%)
All	All	0.53	0/23597	0.79	75/31895 (0.2%)

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	229	ARG	NE-CZ-NH2	-7.76	116.42	120.30
3	G	254	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	96	ASP	CB-CG-OD2	7.26	124.83	118.30
1	C	411	ASP	CB-CG-OD2	7.00	124.60	118.30
2	D	400	ASP	CB-CG-OD2	6.97	124.57	118.30
1	C	79	ASP	CB-CG-OD2	6.93	124.54	118.30
3	G	5	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	24	ASP	CB-CG-OD2	6.78	124.40	118.30
2	E	359	ASP	CB-CG-OD2	6.73	124.36	118.30
2	D	22	ASP	CB-CG-OD2	6.70	124.33	118.30
1	C	170	ASP	CB-CG-OD2	6.50	124.15	118.30
2	F	22	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	109	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	494	ASP	CB-CG-OD2	6.26	123.94	118.30
2	F	316	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	333	ASP	CB-CG-OD2	6.19	123.87	118.30
2	D	26	ASP	CB-CG-OD2	6.15	123.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-6.11	99.79	111.40
1	B	69	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	291	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	216	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	24	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	270	ASP	CB-CG-OD2	6.02	123.72	118.30
2	D	359	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	109	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	409	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	454	ASP	CB-CG-OD2	5.89	123.61	118.30
1	A	170	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	86	ASP	CB-CG-OD2	5.85	123.57	118.30
2	E	431	LEU	CA-CB-CG	5.82	128.68	115.30
3	G	254	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	D	471	ASP	CB-CG-OD2	5.77	123.50	118.30
2	E	369	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	333	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	333	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	297	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	224	ASP	CB-CG-OD2	5.61	123.35	118.30
2	F	471	ASP	CB-CG-OD2	5.58	123.32	118.30
3	G	140	ASP	CB-CG-OD2	5.56	123.30	118.30
1	C	259	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	79	ASP	CB-CG-OD2	5.50	123.25	118.30
2	F	139	VAL	CB-CA-C	-5.50	100.95	111.40
1	B	454	ASP	CB-CG-OD2	5.48	123.23	118.30
2	D	330	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	270	ASP	CB-CG-OD2	5.43	123.19	118.30
2	F	400	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	224	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	79	ASP	CB-CG-OD2	5.38	123.14	118.30
2	F	26	ASP	CB-CG-OD2	5.37	123.13	118.30
2	E	250	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	347	ASP	CB-CG-OD2	5.32	123.08	118.30
2	F	394	ASP	CB-CG-OD2	5.31	123.08	118.30
2	D	386	ASP	CB-CG-OD2	5.29	123.06	118.30
2	E	288	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	297	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	411	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	154	ASP	CB-CG-OD2	5.23	123.01	118.30
2	E	77	ASP	CB-CG-OD2	5.23	123.00	118.30
2	F	386	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ASP	CB-CG-OD2	5.18	122.97	118.30
2	D	380	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	116	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	270	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	371	VAL	CB-CA-C	-5.12	101.68	111.40
1	A	411	ASP	CB-CG-OD2	5.12	122.90	118.30
2	E	394	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	269	ASP	CB-CG-OD2	5.09	122.88	118.30
2	E	319	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	494	ASP	CB-CG-OD2	5.08	122.87	118.30
2	E	386	ASP	CB-CG-OD2	5.05	122.85	118.30
2	E	471	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	194	ASP	CB-CG-OD2	5.04	122.84	118.30
2	D	394	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	154	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	334	VAL	CB-CA-C	-5.01	101.88	111.40

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	3715	0	3814	44	0
1	B	3663	0	3774	39	0
1	C	3797	0	3894	41	0
2	D	3539	0	3592	27	0
2	E	3530	0	3587	42	0
2	F	3530	0	3586	38	0
3	G	1492	0	1587	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	246	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 (246) 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: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
1:B:180:ILE:HD12	1:B:216:LEU:HD21	1.62	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:94:ILE:CD1	1:A:128:ARG:HG2	2.15	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
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
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:F:63:MET:HE3	2:F:97:VAL:HG11	1.84	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:B:390:MET:HG3	1:B:424:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:77:LEU:HD13	3:G:232:MET:HE1	1.88	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:D:63:MET:HE1	2:D:231:ARG:HB2	1.90	0.53
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
1:B:211:SER:HB3	2:E:126:MET:HE1	1.90	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:283:LEU:HD21	1:C:289:PRO:HB3	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:HA	2:D:249:GLN:OE1	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:63:MET:HE1	2:D:97:VAL:HG11	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:167:MET:HE1	2:F:196:LEU:HD13	1.95	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: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:F:345:TYR:HA	2:F:346:PRO:C	2.34	0.47
2:D:226:PRO:HB3	2:D:267:GLU:OE1	2.13	0.47
2:F:167:MET:CE	2:F:196:LEU:HD13	2.44	0.47
2:E:366:GLU:O	2:E:370:VAL:HG23	2.14	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:2:THR:HG22	3:G:4:LYS:H	1.79	0.47
1:B:362:ARG:HA	1:B:363:PRO:C	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:362:ARG:HA	1:C:363:PRO:C	2.37	0.45
2:E:345:TYR:H	2:E:459:MET:HE1	1.80	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
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:A:99:VAL:HG22	1:A:253:MET:HA	2.00	0.43
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:387:ALA:HA	1:C:390:MET:HE2	2.01	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
3:G:20:THR:HG22	3:G:232:MET:HE2	2.01	0.42
2:D:200:MET:HB2	2:D:200:MET:HE2	1.61	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: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
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
3:G:74:ASP:CG	3:G:110:ASP:HB2	2.40	0.41
2:E:174:ALA:HB2	9:E:2039:HOH:O	2.20	0.41
1:B:482:LYS:O	1:B:486:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:464:PHE:C	1:A:464:PHE:CD2	2.93	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:A:486:ASP:C	1:A:488:LYS:H	2.25	0.40
1:B:338:ILE:HB	1:B:339:PRO:HD3	2.03	0.40
2:D:63:MET:CE	2:D:231:ARG:HB2	2.49	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
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%)	47	55
1	B	476/510 (93%)	458 (96%)	18 (4%)	0	100	100
1	C	496/510 (97%)	480 (97%)	12 (2%)	4 (1%)	19	19
2	D	465/482 (96%)	440 (95%)	24 (5%)	1 (0%)	47	55
2	E	464/482 (96%)	433 (93%)	29 (6%)	2 (0%)	34	37
2	F	464/482 (96%)	448 (97%)	14 (3%)	2 (0%)	34	37
3	G	180/272 (66%)	169 (94%)	10 (6%)	1 (1%)	25	26
All	All	3030/3248 (93%)	2893 (96%)	126 (4%)	11 (0%)	34	37

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	372 (95%)	21 (5%)	22	27
1	B	389/412 (94%)	373 (96%)	16 (4%)	30	39
1	C	402/412 (98%)	374 (93%)	28 (7%)	15	16
2	D	377/386 (98%)	360 (96%)	17 (4%)	27	34
2	E	376/386 (97%)	356 (95%)	20 (5%)	22	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	376/386 (97%)	362 (96%)	14 (4%)	34	43
3	G	162/230 (70%)	146 (90%)	16 (10%)	8	7
All	All	2475/2624 (94%)	2343 (95%)	132 (5%)	22	27

All (132) 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	123	SER
1	A	134	PRO
1	A	136	ILE
1	A	141	SER
1	A	164	ARG
1	A	196	LYS
1	A	202	ILE
1	A	217	VAL
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	488	LYS
1	B	28	THR
1	B	30	ARG
1	B	47	VAL
1	B	65	ASN
1	B	87	ILE
1	B	99	VAL
1	B	102	GLU
1	B	164	ARG
1	B	208	GLN
1	B	244	TYR
1	B	355	GLU
1	B	371	VAL
1	B	418	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	442	VAL
1	B	479	LEU
1	B	492	GLU
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	164	ARG
1	C	165	GLU
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	381	ARG
1	C	398	ARG
1	C	422	VAL
1	C	475	GLN
1	C	479	LEU
1	C	482	LYS
1	C	501	VAL
1	C	505	LEU
2	D	9	THR
2	D	10	THR
2	D	12	ARG
2	D	26	ASP
2	D	27	GLU
2	D	89	GLU
2	D	97	VAL
2	D	109	LYS
2	D	111	LYS
2	D	127	SER
2	D	237	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	44	ARG
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	352	ASP
2	E	386	ASP
2	E	394	ASP
2	E	412	ARG
2	E	420	VAL
2	E	424	PHE
2	E	431	LEU
2	F	9	THR
2	F	12	ARG
2	F	89	GLU
2	F	97	VAL
2	F	109	LYS
2	F	112	GLN
2	F	139	VAL
2	F	202	GLU
2	F	223	ASN
2	F	232	VAL
2	F	247	GLU
2	F	250	ASP
2	F	303	SER
2	F	428	LEU
3	G	44	TYR
3	G	67	LEU

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Mol	Chain	Res	Type
3	G	87	LYS
3	G	89	MET
3	G	90	LYS
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 (28) 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	C	263	HIS
1	C	416	GLN
1	C	432	GLN
2	D	130	GLN
2	D	194	ASN
2	D	221	GLN
2	D	379	GLN
2	D	411	GLN
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	455	GLN
2	F	177	HIS
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN

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Mol	Chain	Res	Type
2	F	223	ASN
2	F	419	GLN
2	F	443	GLN
3	G	211	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	24,29,29	0.90	1 (4%)	29,45,45	1.19	1 (3%)
6	GOL	C	1513	-	5,5,5	0.35	0	5,5,5	0.39	0
8	PO4	E	1475	-	4,4,4	0.90	0	6,6,6	0.59	0
4	ADP	D	1476	5,7	24,29,29	1.12	3 (12%)	29,45,45	1.47	5 (17%)
4	ADP	A	1511	5	24,29,29	0.91	1 (4%)	29,45,45	1.34	3 (10%)
4	ADP	F	1475	5,7	24,29,29	0.94	2 (8%)	29,45,45	1.27	4 (13%)
6	GOL	D	1475	-	5,5,5	0.46	0	5,5,5	0.58	0
6	GOL	A	1513	-	5,5,5	0.21	0	5,5,5	0.58	0
4	ADP	B	1511	5	24,29,29	1.02	1 (4%)	29,45,45	1.36	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BEF	F	1477	4,5	0,3,3	-	-	-		
6	GOL	B	1513	-	5,5,5	0.42	0	5,5,5	0.29	0
7	BEF	D	1478	4,5	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	C	1511	5	-	1/12/32/32	0/3/3/3
6	GOL	C	1513	-	-	0/4/4/4	-
4	ADP	D	1476	5,7	-	2/12/32/32	0/3/3/3
4	ADP	A	1511	5	-	0/12/32/32	0/3/3/3
4	ADP	F	1475	5,7	-	2/12/32/32	0/3/3/3
6	GOL	D	1475	-	-	2/4/4/4	-
6	GOL	A	1513	-	-	3/4/4/4	-
4	ADP	B	1511	5	-	0/12/32/32	0/3/3/3
6	GOL	B	1513	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1511	ADP	C5-C4	2.59	1.47	1.40
4	A	1511	ADP	C5-C4	2.57	1.47	1.40
4	D	1476	ADP	O4'-C1'	2.35	1.44	1.41
4	D	1476	ADP	C5-C4	2.34	1.47	1.40
4	D	1476	ADP	C2-N3	2.25	1.35	1.32
4	F	1475	ADP	C5-C4	2.19	1.46	1.40
4	C	1511	ADP	C5-C4	2.17	1.46	1.40
4	F	1475	ADP	O4'-C1'	2.03	1.43	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1476	ADP	N3-C2-N1	-4.14	122.20	128.68
4	A	1511	ADP	N3-C2-N1	-3.53	123.16	128.68
4	C	1511	ADP	N3-C2-N1	-3.49	123.22	128.68
4	B	1511	ADP	N3-C2-N1	-3.18	123.71	128.68
4	F	1475	ADP	N3-C2-N1	-3.16	123.73	128.68
4	B	1511	ADP	C4-C5-N7	-3.03	106.24	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1511	ADP	C4-C5-N7	-2.97	106.31	109.40
4	D	1476	ADP	C2-N1-C6	2.81	123.56	118.75
4	F	1475	ADP	O3A-PB-O1B	-2.45	97.59	111.19
4	D	1476	ADP	O3B-PB-O2B	2.44	116.98	107.64
4	D	1476	ADP	O3B-PB-O3A	-2.34	96.78	104.64
4	D	1476	ADP	N6-C6-N1	2.14	123.02	118.57
4	B	1511	ADP	O3A-PB-O1B	-2.14	99.31	111.19
4	B	1511	ADP	PA-O3A-PB	-2.09	125.65	132.83
4	A	1511	ADP	C2-N1-C6	2.09	122.32	118.75
4	F	1475	ADP	C4-C5-N7	-2.05	107.26	109.40
4	F	1475	ADP	C2-N1-C6	2.05	122.25	118.75

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

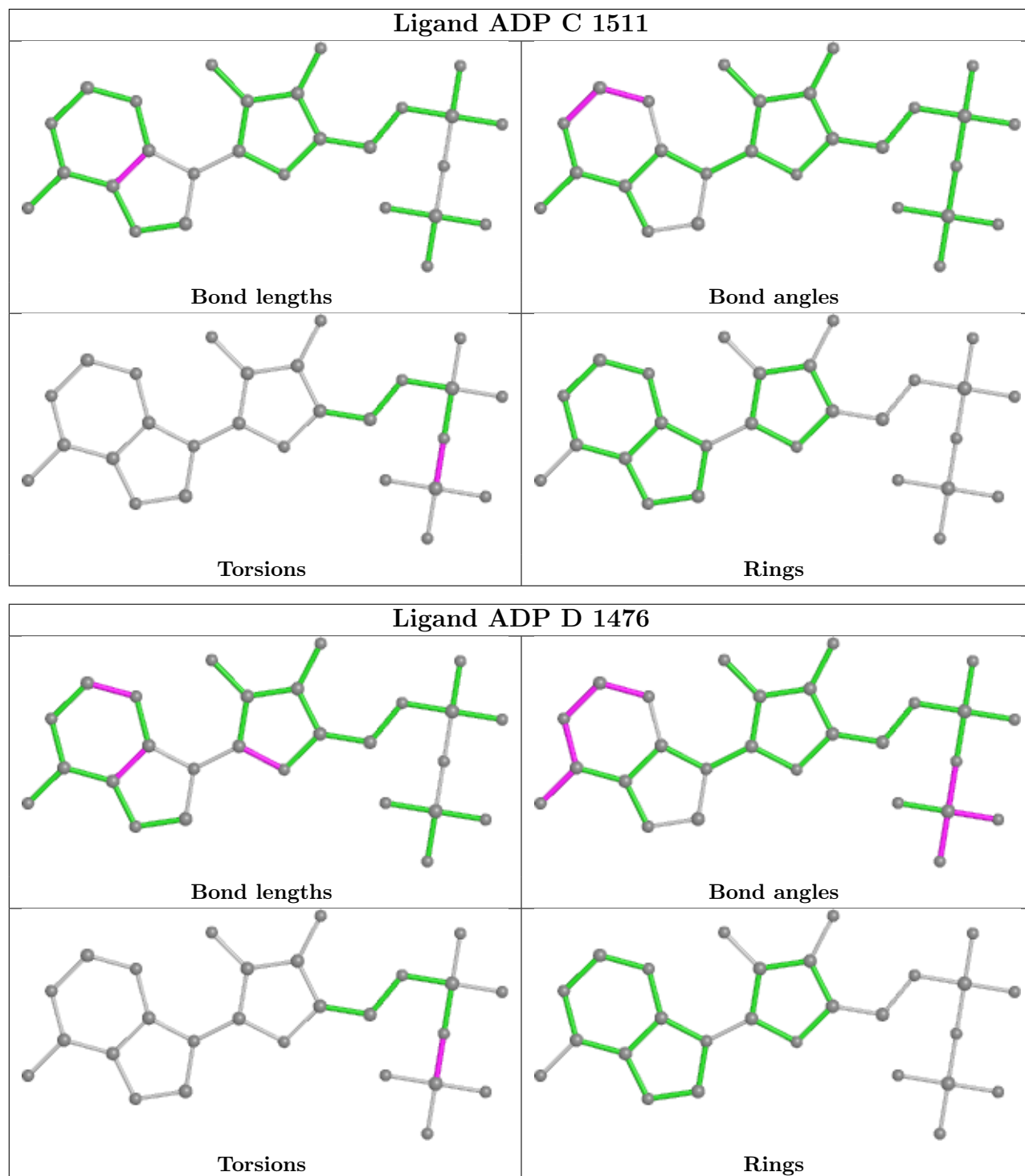
There are no ring outliers.

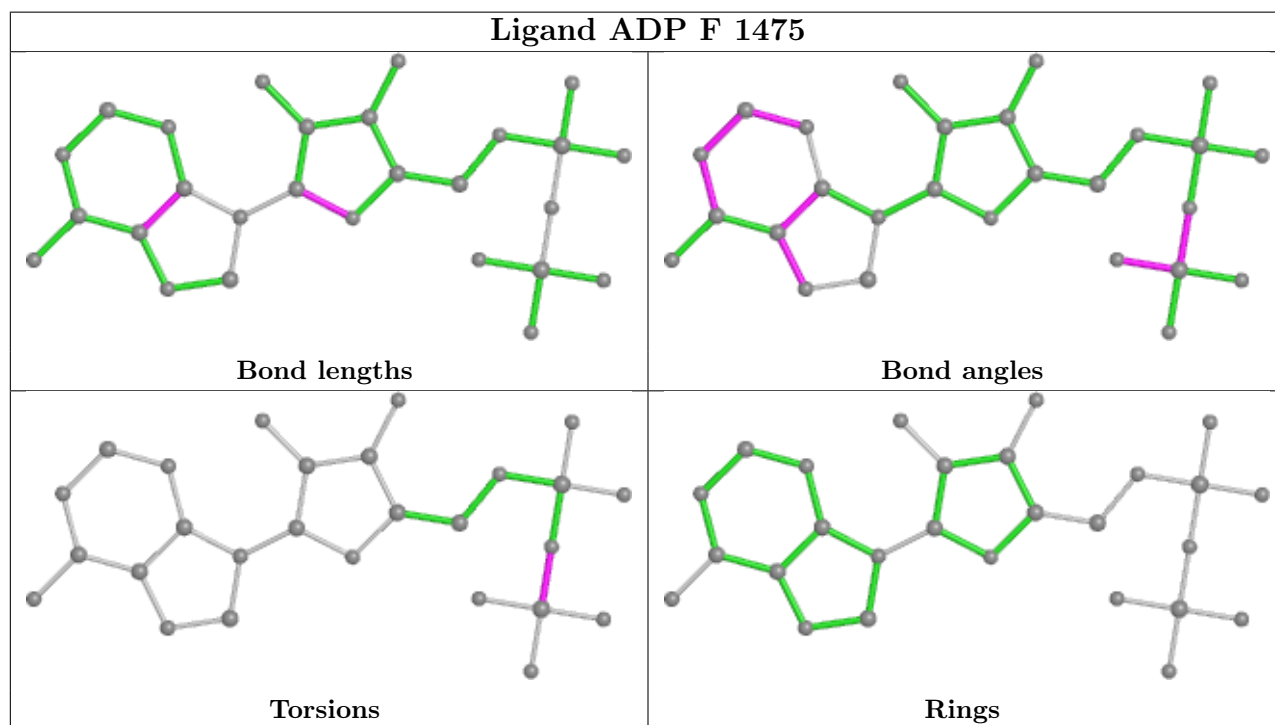
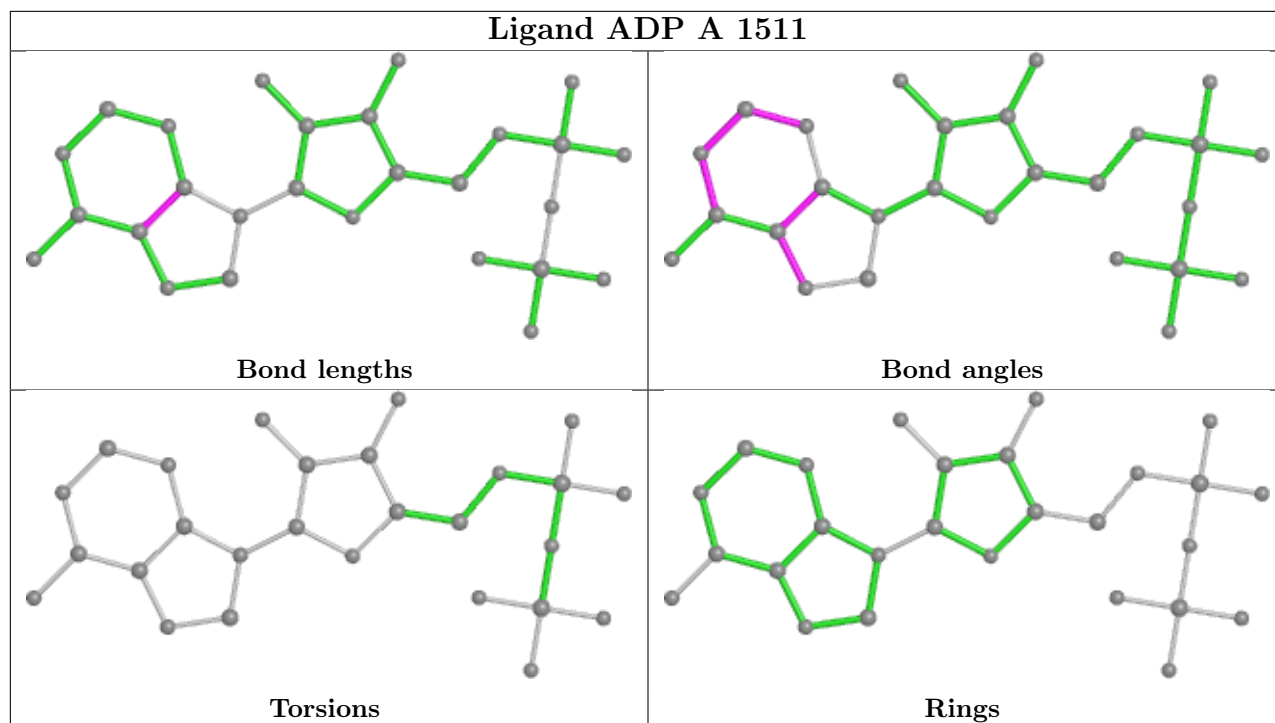
3 monomers are involved in 3 short contacts:

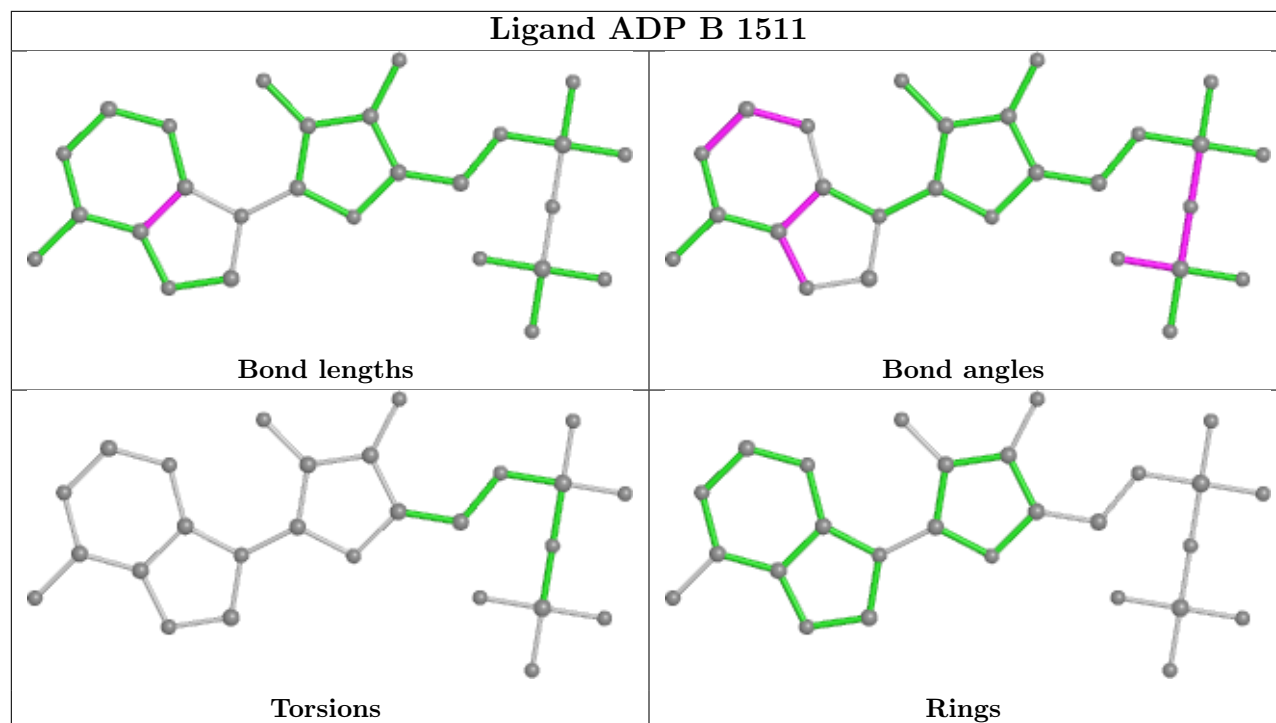
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1511	ADP	1	0
8	E	1475	PO4	1	0
6	A	1513	GOL	1	0

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.







## 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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	487/510 (95%)	-0.09	12 (2%) 57 55	25, 43, 72, 105	0
1	B	480/510 (94%)	0.04	22 (4%) 32 31	23, 43, 85, 111	0
1	C	498/510 (97%)	-0.28	9 (1%) 68 66	22, 36, 62, 116	0
2	D	467/482 (96%)	-0.22	3 (0%) 89 88	20, 37, 70, 98	0
2	E	466/482 (96%)	0.48	71 (15%) 2 2	24, 57, 109, 135	0
2	F	466/482 (96%)	-0.25	7 (1%) 73 72	21, 37, 67, 84	0
3	G	192/272 (70%)	1.78	71 (36%) 0 0	27, 89, 125, 138	0
All	All	3056/3248 (94%)	0.06	195 (6%) 19 18	20, 42, 96, 138	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	201	LEU	11.0
3	G	144	ILE	10.8
3	G	67	LEU	10.4
3	G	106	ILE	8.4
2	E	388	ILE	8.1
3	G	204	TYR	7.8
1	B	412	ALA	7.5
3	G	143	VAL	7.0
3	G	146	LEU	6.9
3	G	69	ILE	6.9
2	E	473	LEU	6.7
3	G	148	LEU	6.4
2	E	425	THR	6.3
3	G	202	ARG	6.3
3	G	207	TYR	6.2
3	G	128	PHE	6.2
1	C	407	GLY	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	142	SER	5.9
3	G	68	ILE	5.8
3	G	215	TYR	5.7
1	B	510	ALA	5.6
3	G	203	ASN	5.6
2	E	457	PHE	5.5
2	E	453	PRO	5.5
1	B	506	ALA	5.5
2	E	446	ALA	5.4
3	G	212	ILE	5.3
3	G	105	ILE	5.2
3	G	86	ALA	5.1
2	E	467	VAL	4.9
3	G	43	VAL	4.9
2	E	452	LEU	4.9
2	E	423	VAL	4.9
2	E	426	GLY	4.9
1	B	193	THR	4.8
3	G	87	LYS	4.8
3	G	159	SER	4.7
2	E	474	ALA	4.7
3	G	161	ILE	4.6
3	G	85	VAL	4.6
3	G	205	GLN	4.5
3	G	115	ILE	4.5
3	G	89	MET	4.5
3	G	206	GLU	4.5
2	E	395	GLU	4.4
2	E	468	ALA	4.4
2	E	451	HIS	4.4
2	E	396	LEU	4.4
2	F	9	THR	4.4
3	G	210	ALA	4.4
3	G	145	ALA	4.3
2	E	472	LYS	4.3
3	G	42	ARG	4.2
1	B	413	ALA	4.2
1	C	406	PHE	4.2
3	G	213	ILE	4.2
1	C	409	ASP	4.1
3	G	39	LYS	4.1
2	E	389	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	40	PRO	4.0
3	G	29	ALA	4.0
2	E	455	GLN	4.0
3	G	214	TYR	4.0
3	G	36	ARG	3.9
2	E	471	ASP	3.9
2	E	454	GLU	3.9
3	G	112	ILE	3.9
1	C	16	ILE	3.9
3	G	138	PHE	3.8
2	E	456	ALA	3.8
2	E	407	ALA	3.8
2	E	424	PHE	3.8
3	G	208	SER	3.7
1	B	485	THR	3.7
2	E	447	GLY	3.7
2	E	449	TYR	3.7
2	E	427	HIS	3.6
2	E	458	TYR	3.6
3	G	141	ALA	3.6
2	E	445	LEU	3.5
1	B	492	GLU	3.5
2	E	410	ILE	3.5
3	G	160	ILE	3.4
3	G	131	VAL	3.4
3	G	90	LYS	3.4
2	E	463	ILE	3.4
2	E	399	GLU	3.4
3	G	32	ALA	3.4
2	E	403	THR	3.4
2	E	402	LEU	3.4
3	G	147	GLU	3.4
2	E	113	PHE	3.4
3	G	134	ARG	3.4
2	E	350	PRO	3.3
1	C	15	ARG	3.3
3	G	209	LEU	3.3
2	E	466	ALA	3.3
3	G	113	ARG	3.3
2	E	417	PRO	3.3
3	G	70	GLY	3.3
1	B	410	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	116	LEU	3.2
2	E	397	SER	3.2
2	E	391	LEU	3.2
2	E	470	ALA	3.2
1	A	408	SER	3.2
2	D	9	THR	3.1
3	G	137	THR	3.1
1	A	122	GLY	3.1
2	E	464	GLU	3.1
2	E	440	GLY	3.1
3	G	130	GLU	3.1
2	E	392	GLY	3.0
1	B	23	VAL	3.0
3	G	108	VAL	3.0
1	B	415	GLN	3.0
2	E	345	TYR	2.9
2	F	178	GLY	2.9
1	B	482	LYS	2.9
2	E	385	GLN	2.9
3	G	211	ASN	2.9
1	A	24	ASP	2.9
1	A	30	ARG	2.9
2	F	249	GLN	2.9
1	B	452	TYR	2.9
2	F	176	ALA	2.8
3	G	135	PRO	2.8
3	G	127	THR	2.8
2	E	393	MET	2.8
2	E	462	PRO	2.8
1	B	474	SER	2.8
1	B	497	LEU	2.8
1	A	94	ILE	2.8
2	E	398	GLU	2.8
2	E	428	LEU	2.8
2	E	394	ASP	2.8
2	E	443	GLN	2.7
2	D	390	ILE	2.7
2	E	422	GLU	2.7
2	E	448	GLU	2.7
1	A	405	GLN	2.7
2	E	157	GLY	2.7
2	E	373	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	400	ASP	2.7
1	C	408	SER	2.7
1	B	503	ASN	2.7
2	E	386	ASP	2.7
3	G	109	GLY	2.7
2	E	387	ILE	2.6
3	G	139	GLY	2.6
1	C	405	GLN	2.6
3	G	129	LYS	2.6
2	E	429	GLY	2.6
1	B	417	LEU	2.6
2	E	384	LEU	2.6
3	G	114	SER	2.5
2	E	9	THR	2.5
3	G	107	GLY	2.5
1	C	193	THR	2.5
2	E	377	ILE	2.5
1	A	402	ALA	2.4
2	D	27	GLU	2.4
3	G	88	GLN	2.4
2	F	111	LYS	2.4
1	B	486	ASP	2.4
1	C	14	GLU	2.4
2	E	362	ILE	2.4
2	E	360	PRO	2.4
2	E	444	ILE	2.4
2	E	469	LYS	2.4
1	B	493	SER	2.4
2	E	111	LYS	2.3
3	G	162	PHE	2.3
1	A	25	LEU	2.3
3	G	25	MET	2.3
1	A	91	THR	2.2
2	F	10	THR	2.2
1	B	490	SER	2.2
2	E	401	LYS	2.2
1	B	502	THR	2.2
3	G	83	SER	2.2
1	B	479	LEU	2.2
2	E	459	MET	2.2
3	G	136	PRO	2.2
3	G	71	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	111	LYS	2.2
1	A	409	ASP	2.2
1	B	487	GLY	2.2
1	A	309	ALA	2.1
3	G	41	ALA	2.1
2	E	209	LYS	2.1
1	A	93	ALA	2.1
2	F	27	GLU	2.0
3	G	46	VAL	2.0
2	E	406	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> 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.

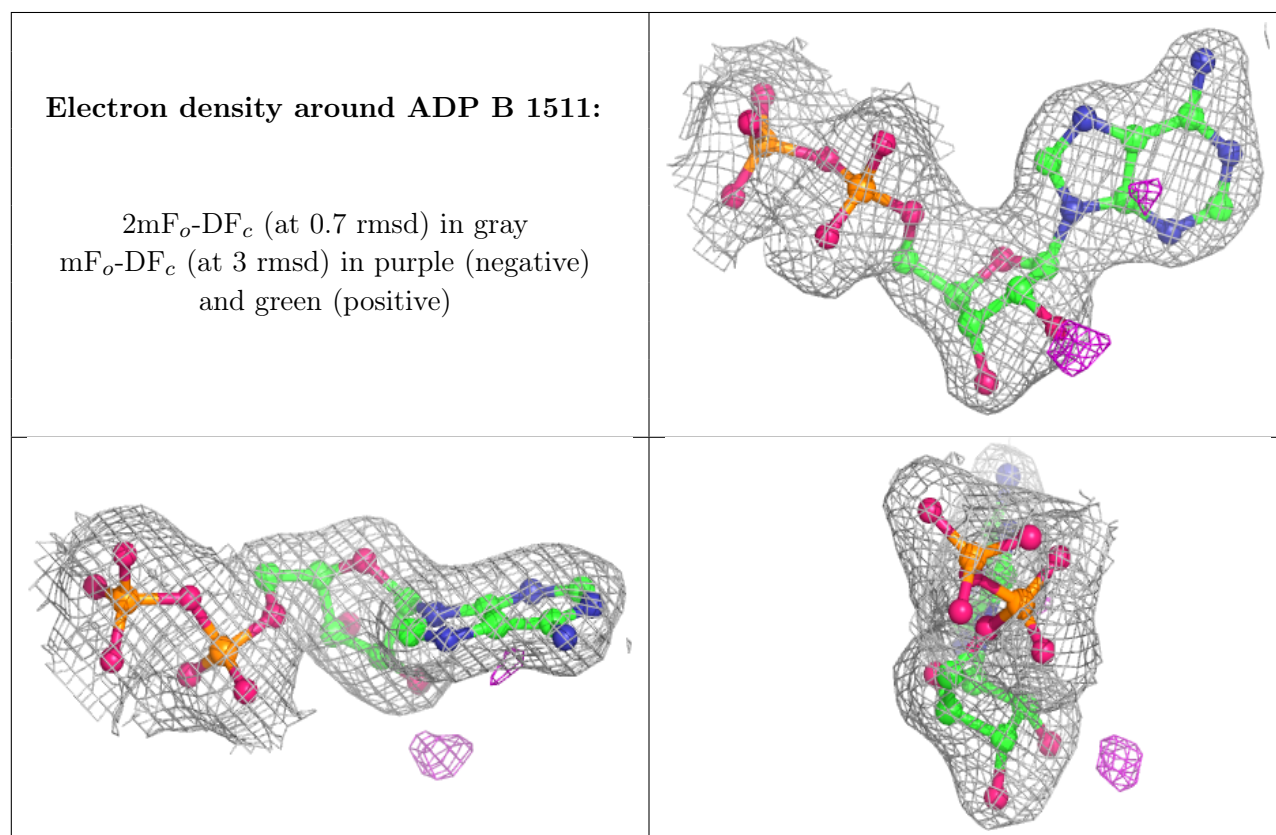
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	PO4	E	1475	5/5	0.87	0.15	87,87,90,92	0
6	GOL	D	1475	6/6	0.93	0.24	59,61,62,62	0
5	MG	D	1477	1/1	0.94	0.17	30,30,30,30	0
5	MG	A	1512	1/1	0.95	0.13	28,28,28,28	0
6	GOL	A	1513	6/6	0.95	0.16	45,47,49,57	0
7	BEF	D	1478	4/4	0.96	0.14	17,20,23,25	0
6	GOL	B	1513	6/6	0.96	0.13	34,37,38,39	0
7	BEF	F	1477	4/4	0.97	0.11	23,27,28,31	0
5	MG	F	1476	1/1	0.97	0.14	25,25,25,25	0
5	MG	B	1512	1/1	0.98	0.08	31,31,31,31	0
5	MG	C	1512	1/1	0.98	0.12	24,24,24,24	0
4	ADP	B	1511	27/27	0.98	0.11	26,45,49,54	0
6	GOL	C	1513	6/6	0.98	0.16	32,36,40,43	0

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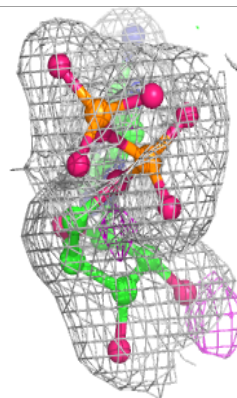
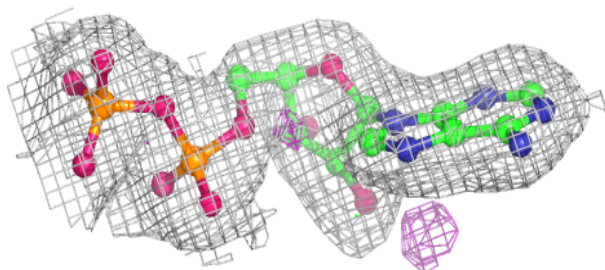
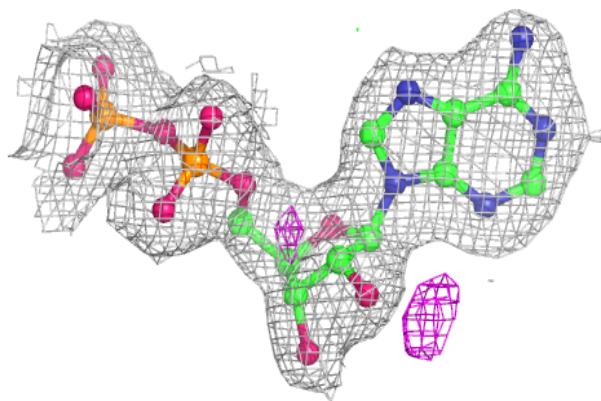
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	A	1511	27/27	0.99	0.11	20,37,42,47	0
4	ADP	C	1511	27/27	0.99	0.12	22,27,32,36	0
4	ADP	D	1476	27/27	0.99	0.14	18,25,30,34	0
4	ADP	F	1475	27/27	0.99	0.14	23,29,35,38	0

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.

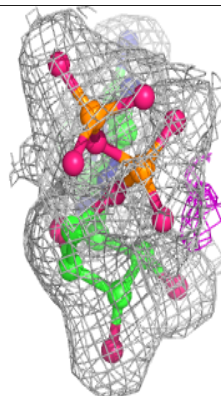
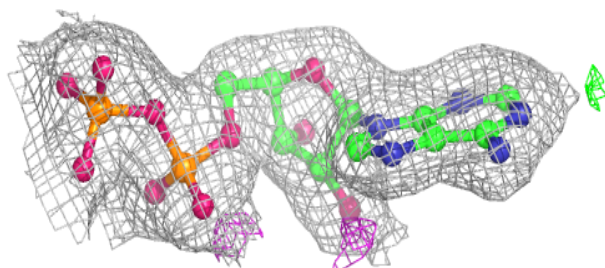
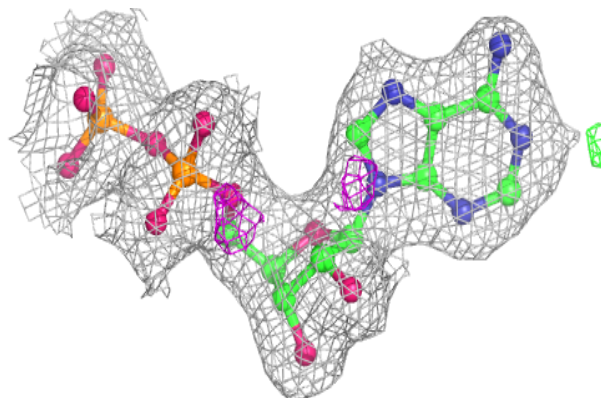


**Electron density around ADP A 1511:**

$2mF_o-DF_c$  (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:**

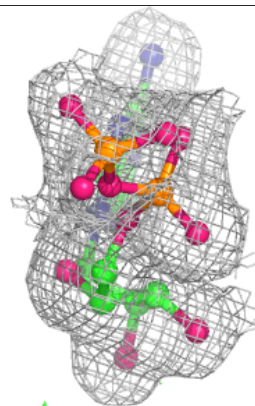
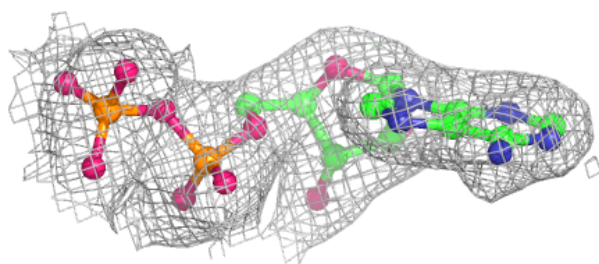
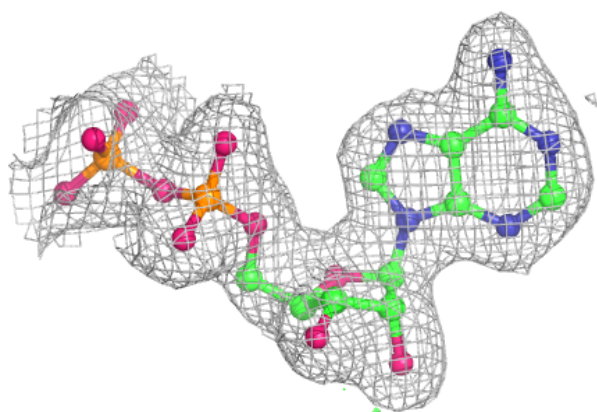
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

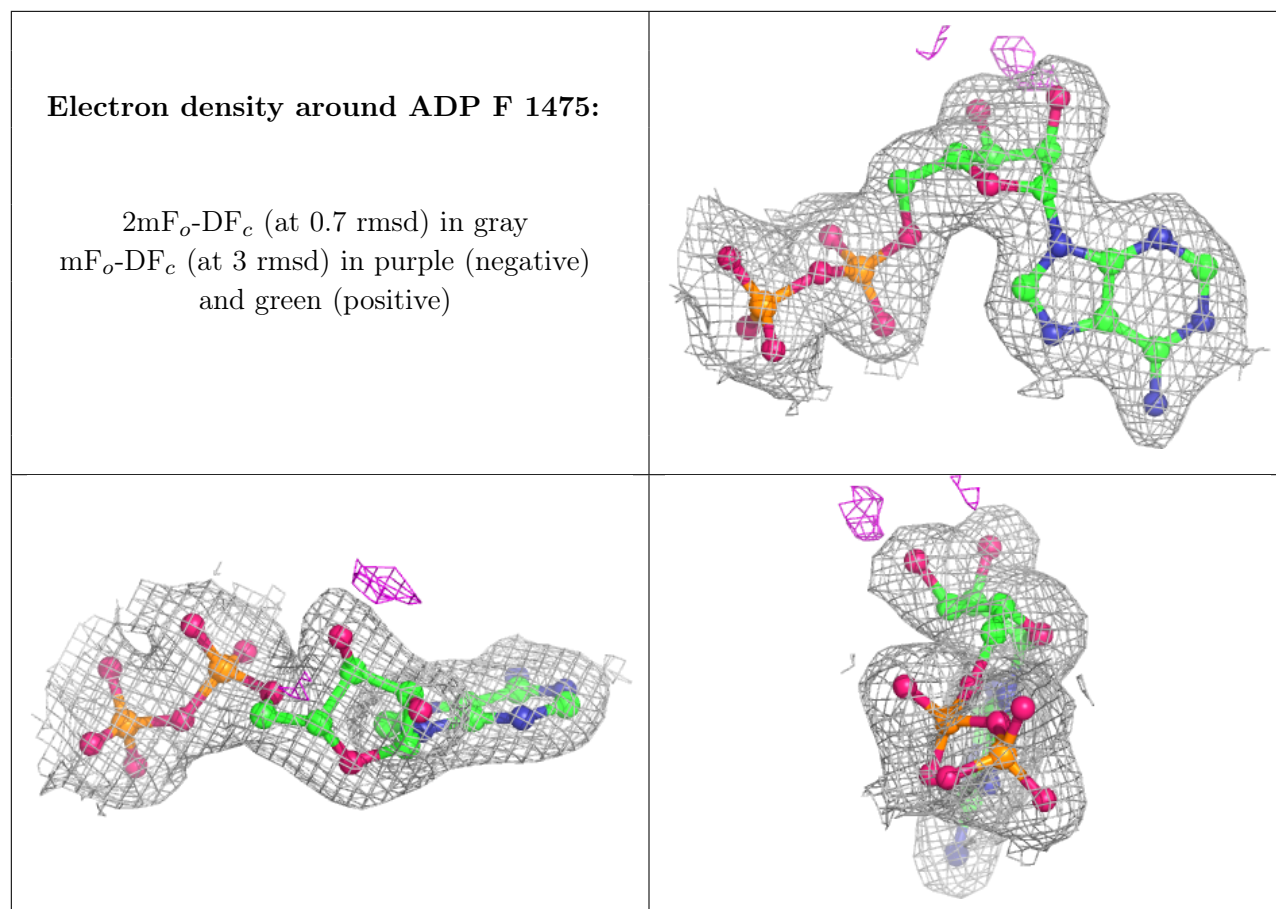




**Electron density around ADP D 1476:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.