Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:58 am BST

PDB ID	:	5I0I
Title	:	Crystal structure of myosin X motor domain with 2IQ motifs in pre-powerstroke state
Authors	:	Isabet, T.; Sweeney, H.L.; Houdusse, A.
Deposited on	:	2016-02-04
Resolution	:	3.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

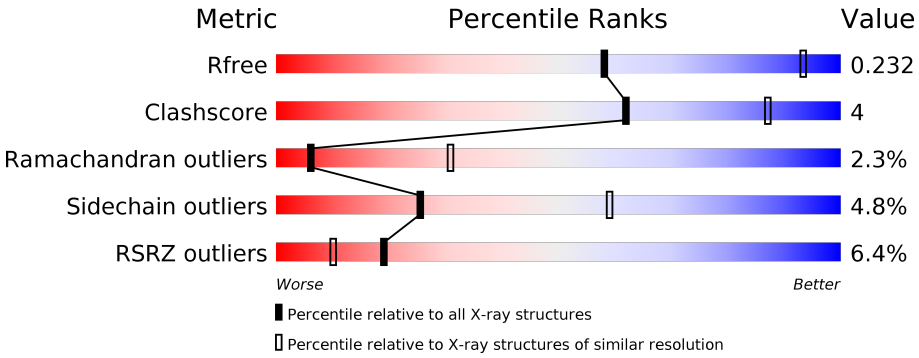
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 on 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 <=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	791	4% 88% 9%
1	B	791	6% 90% 9%
2	C	145	4% 74% 20% 5%
3	E	145	3% 74% 23%
4	G	43	35% 67% 28% 5%
5	I	64	33% 63% 25% 5% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	A	909	-	-	-	X
8	VO4	A	903	-	-	X	-
8	VO4	B	904	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15350 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 Unconventional myosin-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	784	Total	C	N	O	S	0	0	0
			6203	3935	1071	1169	28			
1	B	784	Total	C	N	O	S	0	1	0
			6159	3907	1060	1164	28			

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	145	Total	C	N	O	S	0	0	0
			1086	666	170	242	8			

- Molecule 3 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	145	Total	C	N	O	S	0	0	0
			1024	625	162	228	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	19	ALA	PHE	conflict	UNP P62158

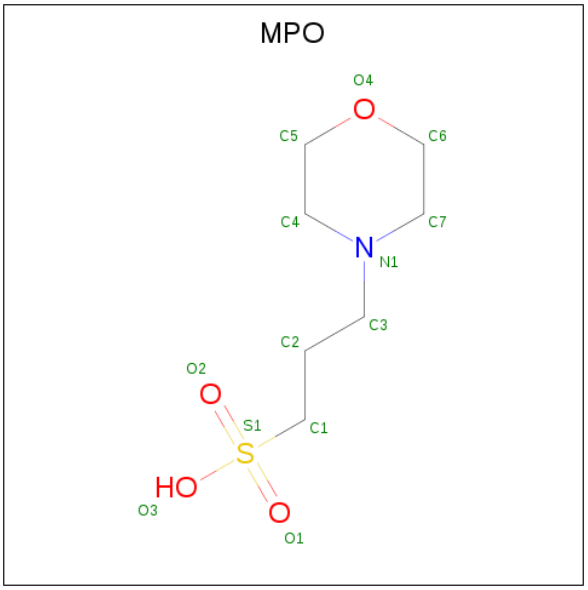
- Molecule 4 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	43	Total	C	N	O	S	0	0	0
			306	188	45	71	2			

- Molecule 5 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	59	Total	C	N	O	S	0	0	0
			424	254	68	99	3			

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).

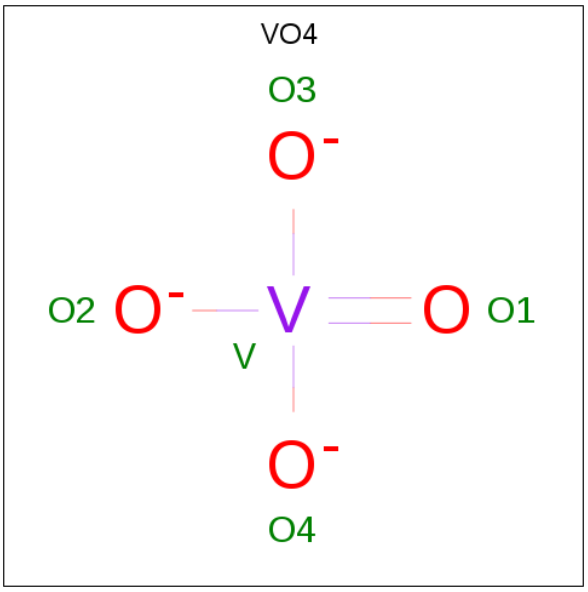


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

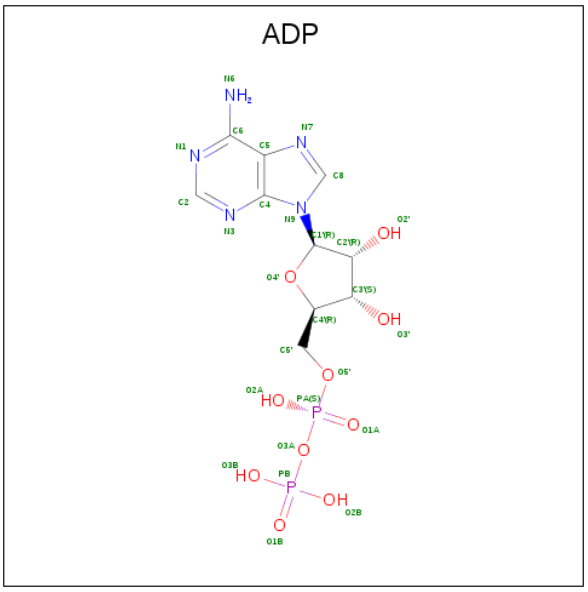
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O V 5 4 1	0	0
8	B	1	Total O V 5 4 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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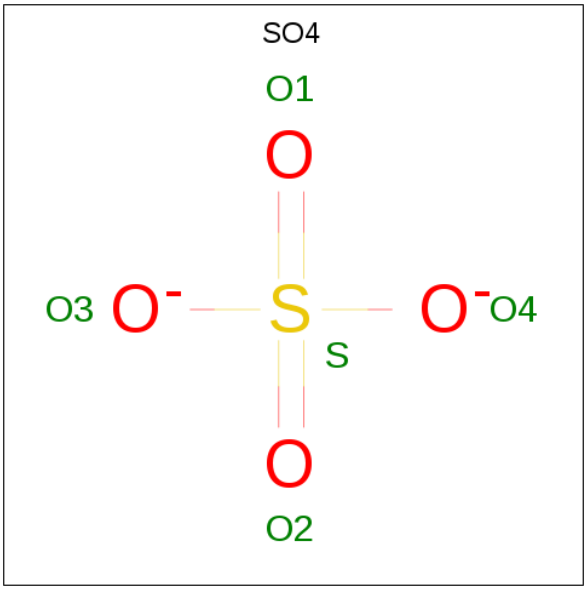
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is water.

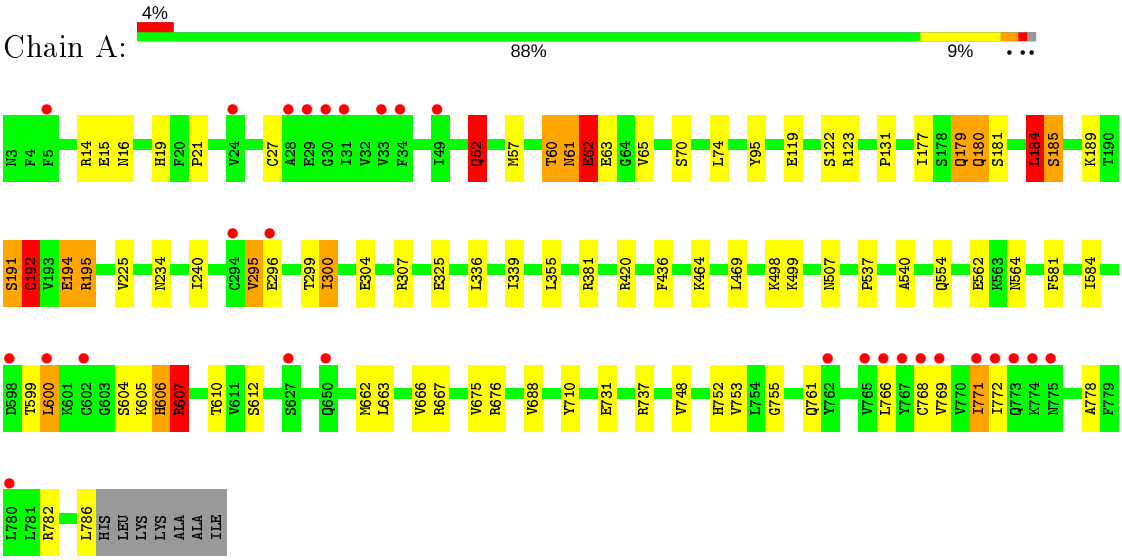
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	11	Total O 11 11	0	0
11	B	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

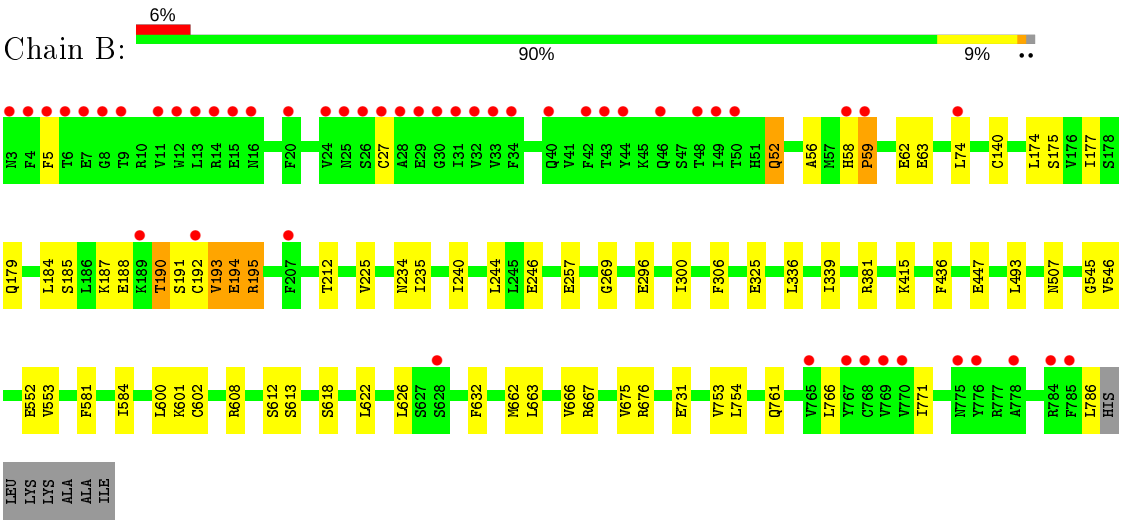
- Molecule 1: Unconventional myosin-X

Chain A:



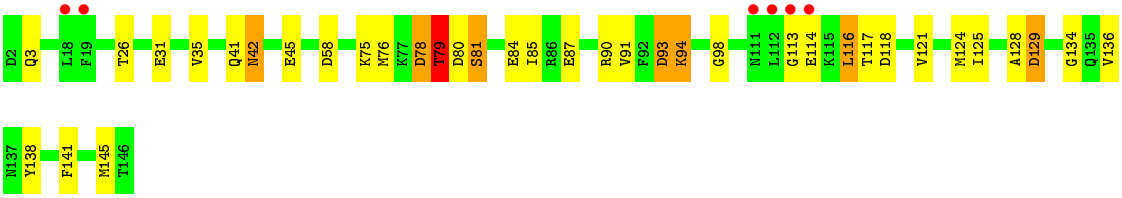
- Molecule 1: Unconventional myosin-X

Chain B:

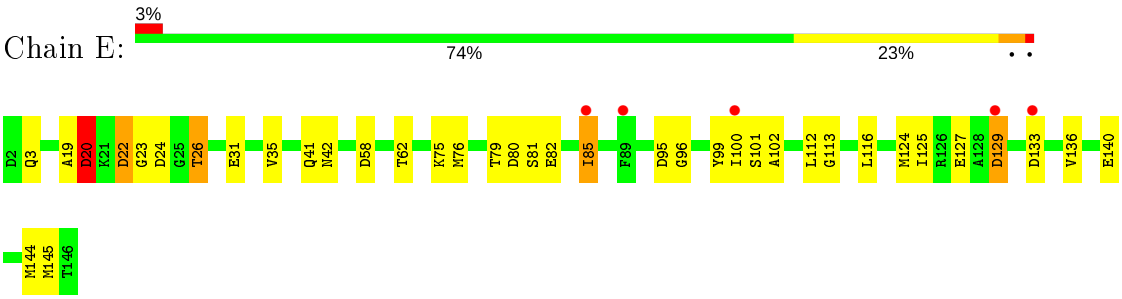


- Molecule 2: Calmodulin

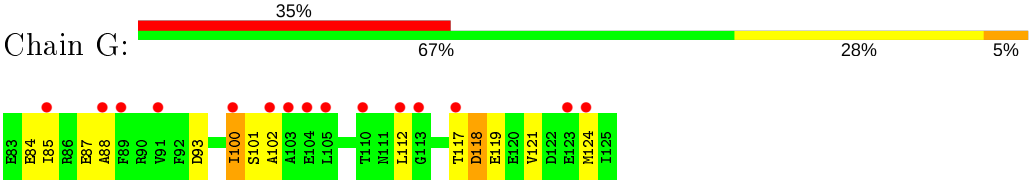
Chain C:



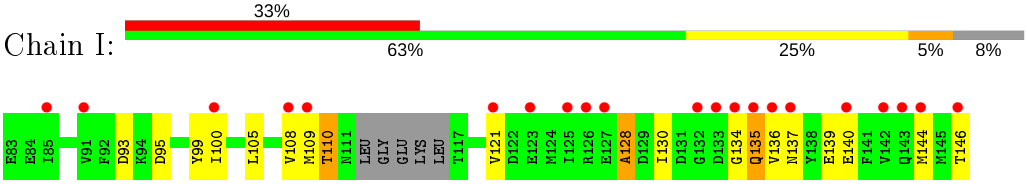
- Molecule 3: Calmodulin



- Molecule 4: Calmodulin



- Molecule 5: Calmodulin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.95Å 173.41Å 178.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.53 – 3.15 49.53 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.53-3.15) 99.9 (49.53-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.192 , 0.218 0.205 , 0.232	Depositor DCC
R_{free} test set	3082 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	103.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15350	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: VO4, MPO, MG, SO4, ADP

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	0.54	0/6330	0.74	10/8571 (0.1%)
1	B	0.48	0/6286	0.70	2/8519 (0.0%)
2	C	0.51	0/1098	0.80	1/1486 (0.1%)
3	E	0.58	0/1032	0.84	0/1401
4	G	0.60	0/307	0.86	0/417
5	I	0.54	0/425	0.74	0/576
All	All	0.52	0/15478	0.74	13/20970 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	GLN	C-N-CA	9.10	144.44	121.70
2	C	78	ASP	C-N-CA	6.96	139.10	121.70
1	A	52	GLN	C-N-CA	6.69	138.44	121.70
1	A	299	THR	C-N-CA	6.26	137.35	121.70
1	A	15	GLU	C-N-CA	6.13	137.02	121.70
1	A	15	GLU	CA-C-N	-6.09	103.81	117.20
1	A	62	GLU	C-N-CA	5.69	135.93	121.70
1	A	194	GLU	CA-CB-CG	5.43	125.35	113.40
1	B	52	GLN	C-N-CA	5.39	135.18	121.70
1	A	61	ASN	C-N-CA	5.35	135.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	LEU	C-N-CA	5.32	135.01	121.70
1	A	191	SER	C-N-CA	5.16	134.60	121.70
1	B	190	THR	C-N-CA	5.00	134.20	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6203	0	5954	49	0
1	B	6159	0	5853	32	0
2	C	1086	0	955	17	0
3	E	1024	0	869	17	0
4	G	306	0	257	3	0
5	I	424	0	347	8	0
6	A	13	0	14	0	0
6	B	13	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	5	0	0	3	0
8	B	5	0	0	3	0
9	A	27	0	12	1	0
9	B	27	0	12	0	0
10	A	25	0	0	0	0
10	B	5	0	0	0	0
10	C	5	0	0	0	0
10	E	5	0	0	0	0
11	A	11	0	0	0	0
11	B	5	0	0	0	0
All	All	15350	0	14287	129	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 4.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ARG:HH11	1:A:607:ARG:HG3	1.11	1.15
3:E:80:ASP:HA	3:E:81:SER:N	1.74	1.02
3:E:22:ASP:HB2	3:E:23:GLY:HA3	1.46	0.95
1:B:191:SER:HB3	1:B:195:ARG:HB2	1.52	0.89
1:A:65:VAL:HG11	1:A:70:SER:HB2	1.53	0.88
1:B:193:VAL:HG23	1:B:194:GLU:H	1.38	0.87
1:A:179:GLN:HA	1:A:180:GLN:O	1.74	0.86
1:A:122:SER:HB3	1:A:177:ILE:HD11	1.67	0.75
1:B:601:LYS:H	1:B:602:CYS:HA	1.52	0.72
2:C:80:ASP:HA	2:C:81:SER:HB2	1.72	0.71
3:E:100:ILE:HB	3:E:101:SER:HA	1.72	0.69
1:A:295:VAL:HG12	1:A:296:GLU:H	1.58	0.69
1:A:581:PHE:CD2	1:A:584:ILE:HG12	2.28	0.69
1:A:607:ARG:NH1	1:A:607:ARG:HG3	1.92	0.69
3:E:22:ASP:CB	3:E:23:GLY:HA3	2.23	0.68
1:B:581:PHE:CD2	1:B:584:ILE:HG12	2.29	0.68
1:A:607:ARG:HH11	1:A:607:ARG:CG	1.98	0.67
3:E:101:SER:HB2	3:E:136:VAL:H	1.60	0.66
5:I:105:LEU:O	5:I:109:MET:HG2	1.96	0.65
1:A:122:SER:CB	1:A:177:ILE:HD11	2.28	0.64
1:B:507:ASN:HD21	1:B:612:SER:HB2	1.62	0.64
2:C:78:ASP:HA	2:C:79:THR:HB	1.80	0.64
8:B:904:VO4:O3	8:B:904:VO4:V	1.56	0.63
8:A:903:VO4:O1	8:A:903:VO4:V	1.56	0.63
3:E:19:ALA:O	3:E:20:ASP:HB2	1.97	0.63
2:C:118:ASP:HA	2:C:121:VAL:HG22	1.80	0.62
1:A:599:THR:HB	1:A:600:LEU:HA	1.81	0.61
8:B:904:VO4:O1	8:B:904:VO4:V	1.57	0.61
8:A:903:VO4:O3	8:A:903:VO4:V	1.57	0.61
3:E:31:GLU:O	3:E:35:VAL:HG23	2.01	0.60
1:A:192:CYS:HB3	1:A:195:ARG:H	1.67	0.59
8:B:904:VO4:O2	8:B:904:VO4:V	1.58	0.59
1:B:188:GLU:C	1:B:190:THR:H	2.05	0.58
2:C:31:GLU:O	2:C:35:VAL:HG23	2.03	0.58
5:I:128:ALA:HB1	5:I:136:VAL:HG11	1.87	0.57
1:A:778:ALA:O	1:A:782:ARG:HG2	2.04	0.57
2:C:41:GLN:HE21	2:C:75:LYS:HG3	1.68	0.57
1:B:193:VAL:HG23	1:B:194:GLU:N	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LYS:HE2	1:A:469:LEU:HD11	1.88	0.55
1:A:599:THR:HB	1:A:600:LEU:CA	2.35	0.55
1:B:246:GLU:HG3	1:B:447:GLU:HG2	1.88	0.55
1:B:193:VAL:CG2	1:B:194:GLU:H	2.14	0.55
1:A:65:VAL:CG1	1:A:70:SER:HB2	2.34	0.55
1:B:336:LEU:O	1:B:339:ILE:HG12	2.06	0.55
2:C:87:GLU:O	2:C:90:ARG:HG2	2.07	0.54
1:B:600:LEU:N	1:B:601:LYS:HA	2.23	0.54
1:A:507:ASN:HD21	1:A:612:SER:HB2	1.73	0.54
3:E:41:GLN:HE21	3:E:75:LYS:HG3	1.73	0.54
3:E:22:ASP:HB2	3:E:23:GLY:CA	2.30	0.53
1:B:58:HIS:O	1:B:59:PRO:C	2.47	0.53
5:I:137:ASN:HD21	5:I:139:GLU:HB3	1.74	0.52
1:A:336:LEU:O	1:A:339:ILE:HG12	2.08	0.52
5:I:93:ASP:HB2	5:I:100:ILE:HG23	1.91	0.51
3:E:112:LEU:HA	3:E:113:GLY:C	2.31	0.51
1:B:140:CYS:HA	1:B:632:PHE:CE2	2.44	0.51
1:B:622:LEU:O	1:B:626:LEU:HG	2.12	0.50
1:A:604:SER:HB3	1:A:606:HIS:CE1	2.47	0.50
2:C:98:GLY:HA2	2:C:138:TYR:CE2	2.46	0.50
5:I:137:ASN:HD22	5:I:140:GLU:HG3	1.77	0.50
4:G:93:ASP:HB3	4:G:100:ILE:HG22	1.93	0.49
1:A:675:VAL:HG11	1:A:731:GLU:HG3	1.95	0.49
2:C:81:SER:HB3	2:C:84:GLU:HB2	1.94	0.49
2:C:125:ILE:O	2:C:129:ASP:HB3	2.13	0.49
1:A:119:GLU:HB3	1:A:123:ARG:HH12	1.77	0.48
1:A:74:LEU:HD21	1:A:666:VAL:HG11	1.95	0.48
3:E:82:GLU:HA	3:E:85:ILE:HD12	1.96	0.48
1:A:19:HIS:HE1	1:A:52:GLN:OE1	1.97	0.48
1:A:755:GLY:HA3	2:C:42:ASN:HD22	1.79	0.48
3:E:140:GLU:O	3:E:144:MET:HB2	2.13	0.48
1:B:675:VAL:HG11	1:B:731:GLU:HG3	1.95	0.48
5:I:110:THR:HG23	5:I:121:VAL:HG21	1.96	0.47
8:A:903:VO4:O3	9:A:904:ADP:O3B	2.33	0.47
1:A:537:PRO:HG3	1:A:554:GLN:HE22	1.80	0.47
1:A:21:PRO:HA	1:A:57:MET:CE	2.45	0.46
1:A:60:THR:C	1:A:62:GLU:HA	2.36	0.46
1:B:74:LEU:HD21	1:B:666:VAL:HG11	1.98	0.45
1:A:304:GLU:OE2	1:A:307:ARG:NH1	2.48	0.45
2:C:129:ASP:HA	2:C:136:VAL:HG23	1.99	0.45
1:A:184:LEU:CD2	1:A:185:SER:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.84	0.45
1:B:545:GLY:HA2	1:B:553:VAL:O	2.16	0.45
1:A:599:THR:CB	1:A:600:LEU:HA	2.46	0.45
1:A:191:SER:O	1:A:420:ARG:NH2	2.49	0.44
1:A:179:GLN:CA	1:A:180:GLN:O	2.58	0.44
3:E:127:GLU:C	3:E:129:ASP:H	2.21	0.43
1:A:507:ASN:ND2	1:A:610:THR:OG1	2.51	0.43
1:A:119:GLU:HB3	1:A:123:ARG:NH1	2.34	0.43
1:A:771:ILE:HD11	4:G:88:ALA:HB2	1.99	0.43
1:B:174:LEU:HA	1:B:177:ILE:HG22	2.01	0.43
1:B:225:VAL:HG22	1:B:240:ILE:HG12	2.00	0.43
1:B:546:VAL:O	1:B:552:GLU:HA	2.18	0.43
1:B:175:SER:O	1:B:179:GLN:HG2	2.19	0.43
1:B:601:LYS:H	1:B:602:CYS:CA	2.26	0.43
5:I:99:TYR:HD2	5:I:135:GLN:HB2	1.83	0.43
1:A:507:ASN:ND2	1:A:564:ASN:HD21	2.16	0.43
1:B:325:GLU:HG2	1:B:581:PHE:HE1	1.84	0.43
1:B:663:LEU:HD21	1:B:667:ARG:NH2	2.34	0.43
1:A:225:VAL:HG22	1:A:240:ILE:HG12	2.01	0.42
1:A:769:VAL:HA	1:A:772:ILE:HG13	2.01	0.42
1:B:269:GLY:HA3	1:B:306:PHE:CG	2.55	0.42
1:A:325:GLU:HG2	1:A:581:PHE:HE1	1.84	0.42
1:A:663:LEU:HD21	1:A:667:ARG:NH2	2.34	0.42
2:C:80:ASP:HA	2:C:81:SER:CB	2.40	0.42
1:A:21:PRO:HA	1:A:57:MET:HE1	2.02	0.42
1:A:61:ASN:N	1:A:62:GLU:HA	2.34	0.42
1:A:748:VAL:O	1:A:752:HIS:HD2	2.01	0.42
1:B:212:THR:HA	1:B:257:GLU:HG2	2.01	0.42
2:C:124:MET:O	2:C:128:ALA:HB3	2.19	0.42
1:B:192:CYS:O	1:B:193:VAL:HG22	2.20	0.42
1:A:95:TYR:CZ	1:A:131:PRO:HA	2.55	0.41
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.86	0.41
1:A:498:LYS:HG3	1:A:499:LYS:O	2.20	0.41
2:C:141:PHE:O	2:C:145:MET:HG3	2.20	0.41
1:A:19:HIS:HE1	1:A:52:GLN:CD	2.24	0.41
2:C:116:LEU:HD22	2:C:117:THR:H	1.86	0.41
2:C:93:ASP:HA	2:C:94:LYS:CB	2.51	0.41
5:I:130:ILE:HG23	5:I:134:GLY:HA2	2.03	0.41
1:B:185:SER:C	1:B:187:LYS:H	2.24	0.41
1:A:184:LEU:HG	1:A:189:LYS:NZ	2.36	0.41
1:A:710:TYR:OH	1:A:737:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:26:THR:HB	3:E:62:THR:HB	2.03	0.41
2:C:87:GLU:HA	2:C:90:ARG:HG2	2.03	0.40
3:E:20:ASP:OD2	3:E:24:ASP:OD1	2.39	0.40
4:G:121:VAL:HA	4:G:124:MET:HG2	2.03	0.40
1:A:295:VAL:HG12	1:A:296:GLU:N	2.32	0.40
1:B:5:PHE:CE1	1:B:56:ALA:HB2	2.57	0.40
1:B:754:LEU:HD11	3:E:116:LEU:HD11	2.04	0.40
3:E:99:TYR:HA	3:E:136:VAL:O	2.20	0.40
1:B:193:VAL:HG21	1:B:235:ILE:O	2.22	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	782/791 (99%)	738 (94%)	29 (4%)	15 (2%)	8 36
1	B	783/791 (99%)	735 (94%)	37 (5%)	11 (1%)	11 43
2	C	143/145 (99%)	124 (87%)	13 (9%)	6 (4%)	3 17
3	E	141/145 (97%)	122 (86%)	13 (9%)	6 (4%)	2 17
4	G	41/43 (95%)	32 (78%)	4 (10%)	5 (12%)	0 1
5	I	55/64 (86%)	50 (91%)	4 (7%)	1 (2%)	8 37
All	All	1945/1979 (98%)	1801 (93%)	100 (5%)	44 (2%)	6 31

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	63	GLU
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	192	CYS
1	A	295	VAL
1	A	300	ILE
1	A	605	LYS
1	B	59	PRO
1	B	184	LEU
1	B	194	GLU
1	B	296	GLU
1	B	300	ILE
3	E	20	ASP
3	E	22	ASP
3	E	96	GLY
3	E	102	ALA
4	G	101	SER
4	G	102	ALA
1	A	16	ASN
1	B	608	ARG
2	C	79	THR
2	C	94	LYS
4	G	117	THR
1	A	52	GLN
1	A	185	SER
1	B	52	GLN
1	B	193	VAL
1	B	244	LEU
1	B	381	ARG
2	C	134	GLY
3	E	79	THR
4	G	118	ASP
1	A	184	LEU
1	A	381	ARG
1	A	540	ALA
1	B	62	GLU
4	G	84	GLU
1	A	607	ARG
2	C	93	ASP
3	E	129	ASP
1	A	181	SER
2	C	81	SER
5	I	128	ALA
2	C	113	GLY

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	657/704 (93%)	633 (96%)	24 (4%)	34 66
1	B	644/704 (92%)	628 (98%)	16 (2%)	47 75
2	C	111/125 (89%)	99 (89%)	12 (11%)	6 25
3	E	97/124 (78%)	85 (88%)	12 (12%)	4 20
4	G	29/37 (78%)	23 (79%)	6 (21%)	1 5
5	I	40/55 (73%)	34 (85%)	6 (15%)	3 13
All	All	1578/1749 (90%)	1502 (95%)	76 (5%)	25 59

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	27	CYS
1	A	62	GLU
1	A	184	LEU
1	A	192	CYS
1	A	194	GLU
1	A	195	ARG
1	A	234	ASN
1	A	300	ILE
1	A	355	LEU
1	A	436	PHE
1	A	562	GLU
1	A	600	LEU
1	A	606	HIS
1	A	607	ARG
1	A	662	MET
1	A	676	ARG
1	A	688	VAL
1	A	753	VAL
1	A	761	GLN
1	A	766	LEU
1	A	768	CYS

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Mol	Chain	Res	Type
1	A	771	ILE
1	A	786	LEU
1	B	27	CYS
1	B	63	GLU
1	B	195	ARG
1	B	234	ASN
1	B	415	LYS
1	B	436	PHE
1	B	493	LEU
1	B	613	SER
1	B	618	SER
1	B	662	MET
1	B	676	ARG
1	B	753	VAL
1	B	761	GLN
1	B	766	LEU
1	B	771	ILE
1	B	786	LEU
2	C	3	GLN
2	C	26	THR
2	C	42	ASN
2	C	45	GLU
2	C	58	ASP
2	C	76	MET
2	C	79	THR
2	C	85	ILE
2	C	91	VAL
2	C	114	GLU
2	C	116	LEU
2	C	129	ASP
3	E	3	GLN
3	E	20	ASP
3	E	26	THR
3	E	42	ASN
3	E	58	ASP
3	E	76	MET
3	E	85	ILE
3	E	95	ASP
3	E	124	MET
3	E	125	ILE
3	E	133	ASP
3	E	145	MET

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Mol	Chain	Res	Type
4	G	85	ILE
4	G	87	GLU
4	G	100	ILE
4	G	112	LEU
4	G	118	ASP
4	G	119	GLU
5	I	95	ASP
5	I	108	VAL
5	I	110	THR
5	I	135	GLN
5	I	144	MET
5	I	146	THR

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

Mol	Chain	Res	Type
1	A	19	HIS
1	A	40	GLN
1	A	46	GLN
1	A	507	ASN
1	A	554	GLN
1	A	752	HIS
1	A	773	GLN
1	B	40	GLN
1	B	46	GLN
1	B	85	GLN
1	B	138	ASN
1	B	507	ASN
2	C	41	GLN
2	C	42	ASN
2	C	107	HIS
3	E	41	GLN
5	I	137	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
6	MPO	B	901	-	13,13,13	1.02	1 (7%)	17,17,17	0.79	0
6	MPO	A	901	-	13,13,13	1.16	1 (7%)	17,17,17	0.39	0
10	SO4	A	908	-	4,4,4	0.18	0	6,6,6	0.11	0
10	SO4	A	909	-	4,4,4	0.29	0	6,6,6	0.17	0
9	ADP	A	904	8,7	24,29,29	0.95	1 (4%)	29,45,45	1.16	4 (13%)
10	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.20	0
10	SO4	A	905	-	4,4,4	0.42	0	6,6,6	0.46	0
9	ADP	B	903	8,7	24,29,29	0.77	1 (4%)	29,45,45	0.99	3 (10%)
10	SO4	A	906	-	4,4,4	0.24	0	6,6,6	0.35	0
8	VO4	A	903	9,7	1,4,4	1.18	0	-		
10	SO4	A	907	-	4,4,4	0.26	0	6,6,6	0.29	0
10	SO4	E	201	-	4,4,4	0.18	0	6,6,6	0.32	0
8	VO4	B	904	9,7	1,4,4	0.89	0	-		
10	SO4	B	905	-	4,4,4	0.22	0	6,6,6	0.22	0

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
9	ADP	B	903	8,7	-	3/12/32/32	0/3/3/3
6	MPO	B	901	-	-	1/7/15/15	0/1/1/1
6	MPO	A	901	-	-	3/7/15/15	0/1/1/1
9	ADP	A	904	8,7	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	901	MPO	C1-S1	-4.15	1.71	1.77
6	B	901	MPO	C1-S1	-3.47	1.72	1.77
9	A	904	ADP	PB-O3B	-3.07	1.43	1.54
9	B	903	ADP	PB-O3B	-2.34	1.45	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	904	ADP	O3B-PB-O3A	-2.78	95.32	104.64
9	A	904	ADP	O2B-PB-O3A	2.61	113.40	104.64
9	A	904	ADP	O3'-C3'-C2'	2.47	119.83	111.82
9	A	904	ADP	O3'-C3'-C4'	2.40	118.00	111.05
9	B	903	ADP	O2B-PB-O3A	2.37	112.60	104.64
9	B	903	ADP	O5'-PA-O1A	2.09	117.25	109.07
9	B	903	ADP	C5-C6-N6	2.06	123.48	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	903	ADP	PA-O3A-PB-O2B
6	A	901	MPO	C2-C3-N1-C4
6	A	901	MPO	C2-C3-N1-C7
6	A	901	MPO	C1-C2-C3-N1
6	B	901	MPO	S1-C1-C2-C3
9	B	903	ADP	PA-O3A-PB-O1B
9	B	903	ADP	PA-O3A-PB-O3B

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	904	ADP	1	0

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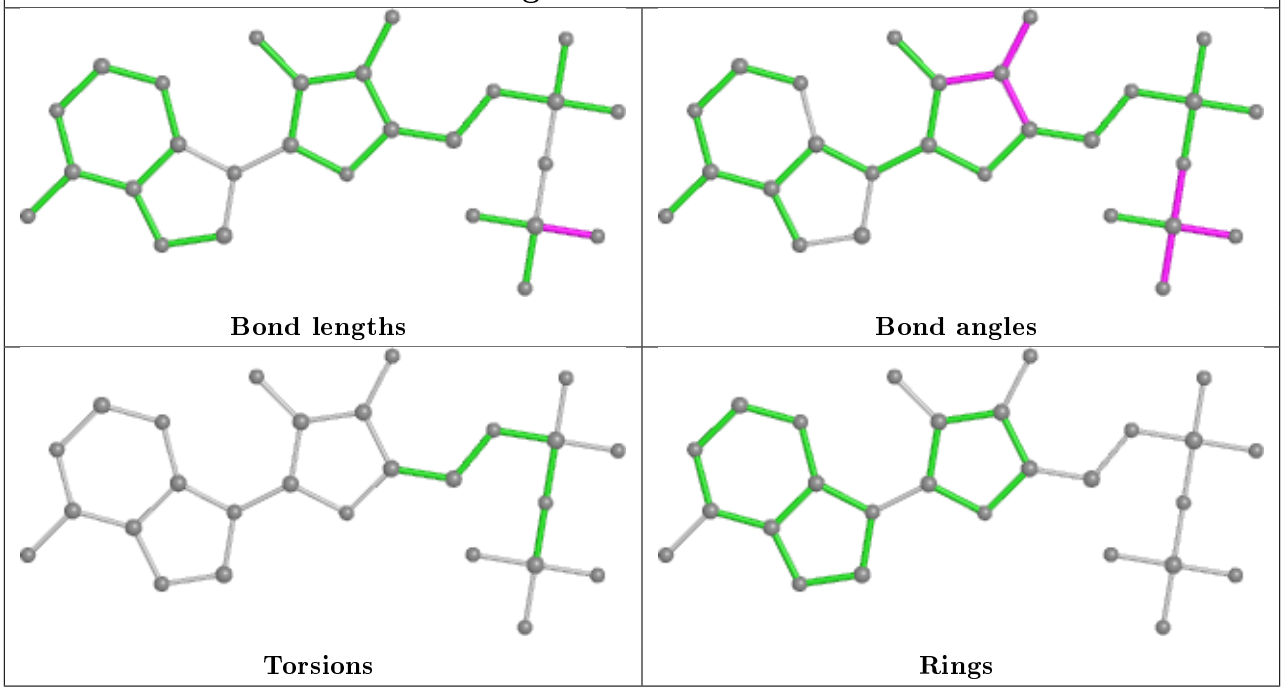
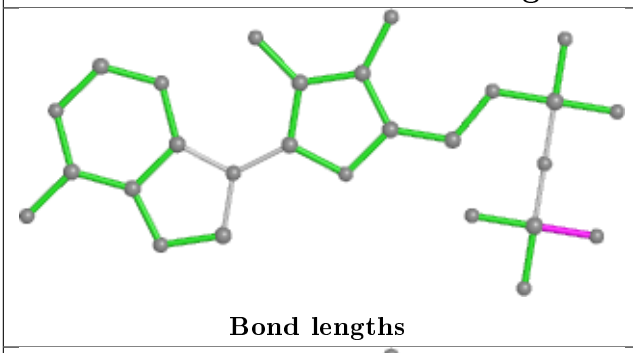
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	903	VO4	3	0
8	B	904	VO4	3	0

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 then 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.

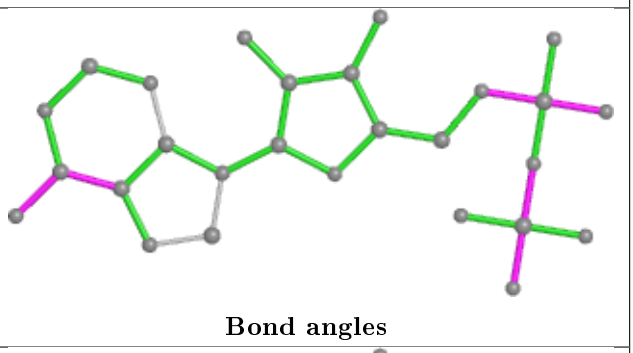
Ligand ADP A 904



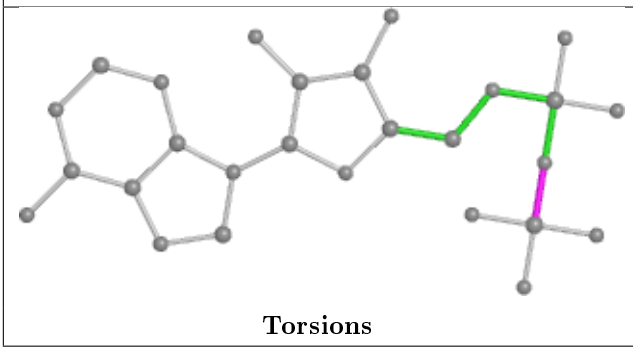
Ligand ADP B 903



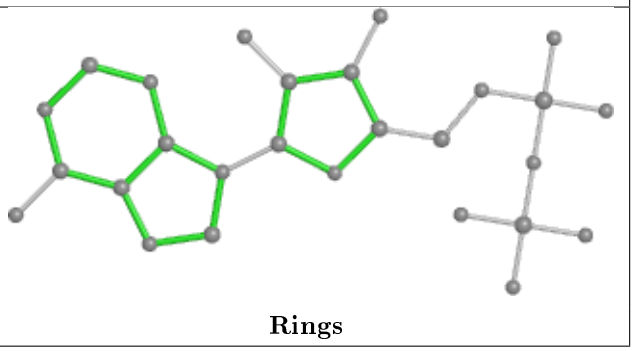
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	80:ASP	C	81:SER	N	3.33

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, 95^{th} 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	784/791 (99%)	0.07	28 (3%) 42 26	62, 88, 196, 246	3 (0%)
1	B	784/791 (99%)	0.21	50 (6%) 19 10	79, 121, 232, 258	6 (0%)
2	C	145/145 (100%)	0.04	6 (4%) 37 22	109, 153, 217, 228	0
3	E	145/145 (100%)	0.01	5 (3%) 45 28	88, 144, 211, 234	0
4	G	43/43 (100%)	1.83	15 (34%) 0 0	191, 215, 230, 238	0
5	I	59/64 (92%)	1.58	21 (35%) 0 0	165, 214, 248, 253	0
All	All	1960/1979 (99%)	0.21	125 (6%) 19 10	62, 116, 225, 258	9 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	GLU	9.3
1	B	28	ALA	9.3
1	B	3	ASN	8.2
1	B	31	ILE	7.8
1	A	600	LEU	7.6
1	B	5	PHE	6.6
2	C	113	GLY	6.5
1	B	30	GLY	6.2
4	G	89	PHE	5.9
1	B	9	THR	5.9
1	A	775	ASN	5.6
1	B	26	SER	5.5
1	B	27	CYS	5.5
4	G	100	ILE	5.5
1	B	25	ASN	5.4
5	I	132	GLY	5.3
1	B	767	TYR	5.3
5	I	133	ASP	5.0
4	G	105	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	768	CYS	4.7
5	I	109	MET	4.6
5	I	108	VAL	4.5
2	C	114	GLU	4.4
1	B	49	ILE	4.4
1	B	44	TYR	4.3
1	B	785	PHE	4.2
1	B	33	VAL	4.2
4	G	112	LEU	4.2
1	A	30	GLY	4.0
1	B	40	GLN	4.0
5	I	144	MET	4.0
1	A	780	LEU	4.0
5	I	85	ILE	3.9
1	B	43	THR	3.9
1	A	762	TYR	3.8
1	B	776	TYR	3.8
4	G	124	MET	3.8
1	B	765	VAL	3.8
1	B	12	TRP	3.7
1	A	598	ASP	3.7
1	B	769	VAL	3.7
1	A	774	LYS	3.7
1	B	13	LEU	3.6
1	B	11	VAL	3.6
4	G	117	THR	3.5
5	I	100	ILE	3.5
1	B	4	PHE	3.4
5	I	143	GLN	3.4
4	G	113	GLY	3.4
2	C	18	LEU	3.4
1	B	6	THR	3.3
1	B	8	GLY	3.3
2	C	112	LEU	3.2
1	B	34	PHE	3.2
1	B	189	LYS	3.2
4	G	102	ALA	3.1
5	I	91	VAL	3.1
1	A	769	VAL	3.1
2	C	111	ASN	3.1
3	E	133	ASP	3.0
1	A	766	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	129	ASP	3.0
1	A	28	ALA	3.0
1	A	49	ILE	3.0
1	A	767	TYR	3.0
1	B	48	THR	3.0
1	A	31	ILE	2.9
4	G	103	ALA	2.9
1	B	58	HIS	2.9
1	B	42	PHE	2.8
5	I	121	VAL	2.8
1	B	24	VAL	2.8
1	A	296	GLU	2.7
5	I	136	VAL	2.7
1	B	770	VAL	2.7
1	B	59	PRO	2.6
1	B	775	ASN	2.6
1	A	771	ILE	2.6
3	E	85	ILE	2.6
3	E	89	PHE	2.6
5	I	137	ASN	2.6
5	I	146	THR	2.6
1	B	784	ARG	2.6
2	C	19	PHE	2.6
1	B	7	GLU	2.6
1	B	74	LEU	2.6
1	B	46	GLN	2.5
1	A	34	PHE	2.5
1	A	602	CYS	2.5
4	G	85	ILE	2.4
1	A	29	GLU	2.4
5	I	135	GLN	2.4
4	G	91	VAL	2.4
5	I	142	VAL	2.4
1	A	773	GLN	2.3
5	I	125	ILE	2.3
1	B	16	ASN	2.3
1	B	50	THR	2.3
1	A	24	VAL	2.3
4	G	123	GLU	2.3
1	B	32	VAL	2.3
1	A	33	VAL	2.3
1	B	15	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	100	ILE	2.2
1	A	650	GLN	2.2
1	B	778	ALA	2.2
1	B	20	PHE	2.2
4	G	88	ALA	2.2
1	A	294	CYS	2.2
4	G	110	THR	2.2
5	I	123	GLU	2.1
1	A	627	SER	2.1
1	A	772	ILE	2.1
1	A	5	PHE	2.1
1	A	765	VAL	2.1
5	I	140	GLU	2.1
1	B	14	ARG	2.1
5	I	127	GLU	2.1
1	B	207	PHE	2.1
1	B	628	SER	2.1
5	I	134	GLY	2.0
4	G	104	GLU	2.0
5	I	126	ARG	2.0
1	B	192	CYS	2.0
1	B	768	CYS	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 carbohydrates 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^{th} 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
10	SO4	A	908	5/5	0.64	0.40	217,217,217,218	0

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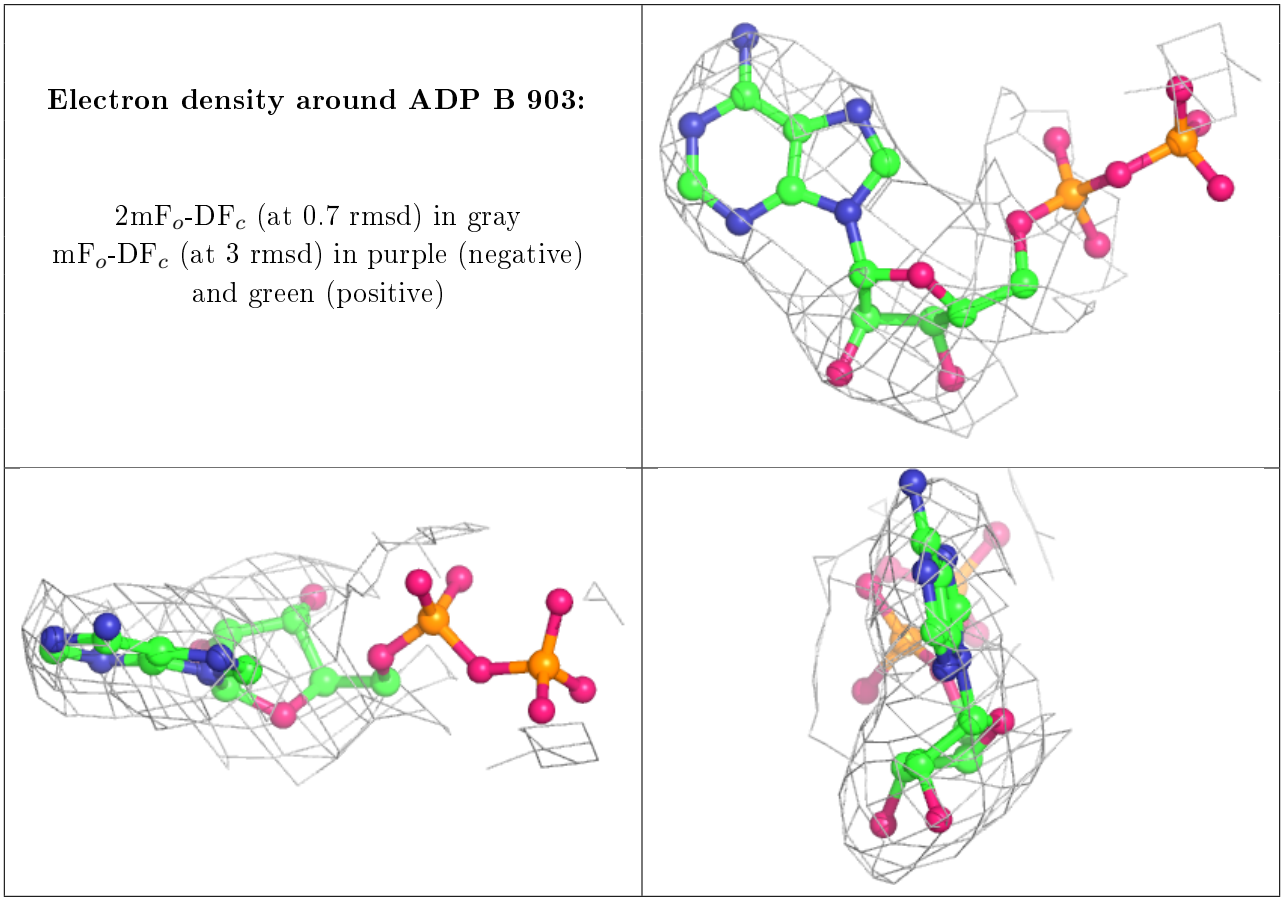
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	SO4	A	909	5/5	0.64	0.83	191,192,193,193	0
6	MPO	B	901	13/13	0.75	0.36	163,167,188,190	0
6	MPO	A	901	13/13	0.80	0.25	132,139,176,178	0
10	SO4	A	906	5/5	0.82	0.24	144,148,149,150	0
10	SO4	A	907	5/5	0.83	0.44	168,168,171,172	0
10	SO4	B	905	5/5	0.85	0.30	159,160,161,161	0
10	SO4	E	201	5/5	0.86	0.26	171,171,172,173	0
10	SO4	C	201	5/5	0.92	0.22	181,182,182,182	0
10	SO4	A	905	5/5	0.94	0.28	121,122,123,124	0
7	MG	B	902	1/1	0.97	0.25	101,101,101,101	0
9	ADP	B	903	27/27	0.97	0.21	103,119,126,129	0
9	ADP	A	904	27/27	0.98	0.21	69,78,85,87	0
8	VO4	B	904	5/5	0.99	0.23	109,110,111,111	0
7	MG	A	902	1/1	0.99	0.19	69,69,69,69	0
8	VO4	A	903	5/5	0.99	0.18	72,75,77,77	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.

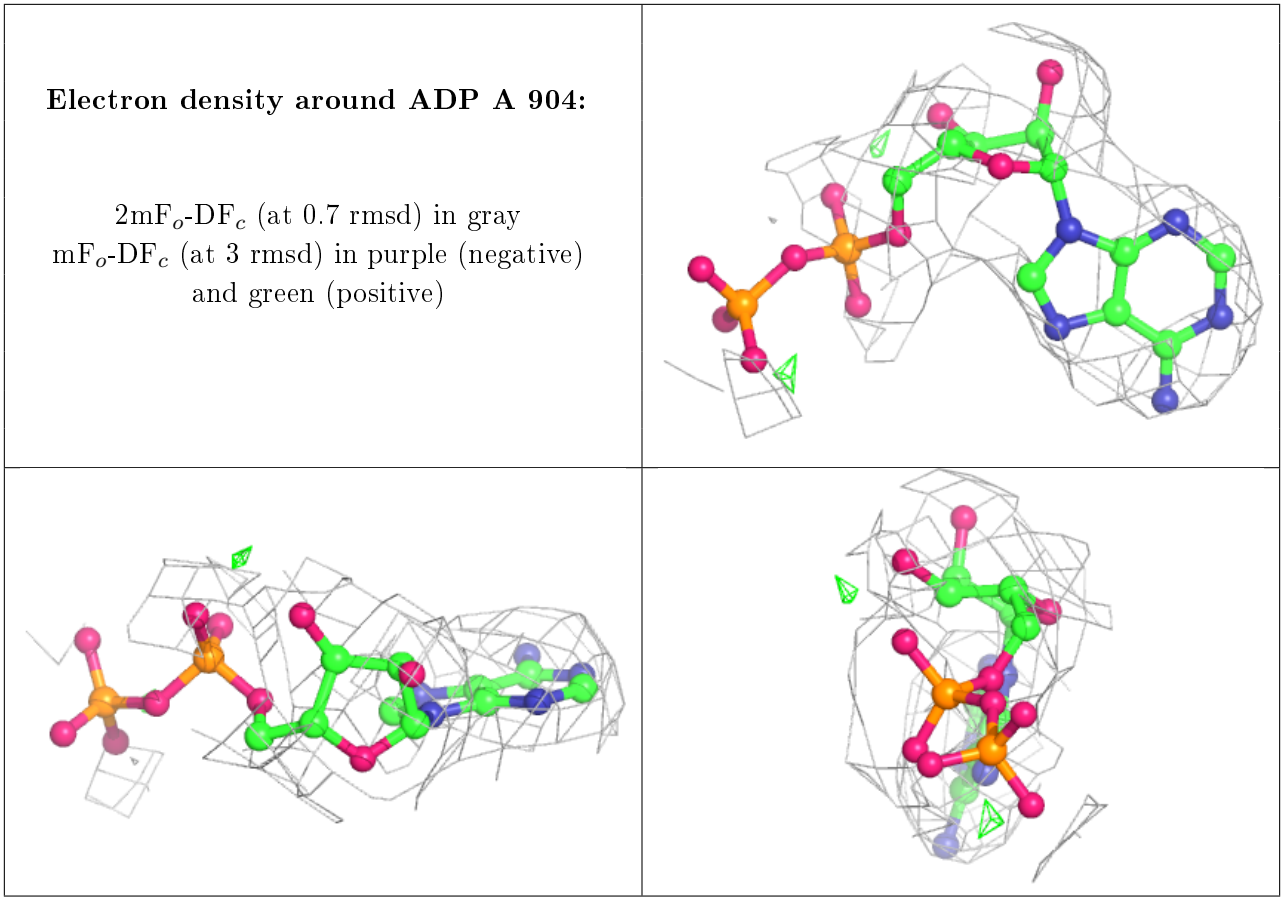
Electron density around ADP B 903:

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



Electron density around ADP A 904:

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



6.5 Other polymers

There are no such residues in this entry.