Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 08:59 PM EST

PDB ID	:	1DFL
Title	:	SCALLOP MYOSIN S1 COMPLEXED WITH MGADP:VANADATE-TRANSITION STATE
Authors	:	Houdusse, A.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on	:	1999-11-19
Resolution	:	4.20 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 (i) 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 (1)) were used in the production of this report:

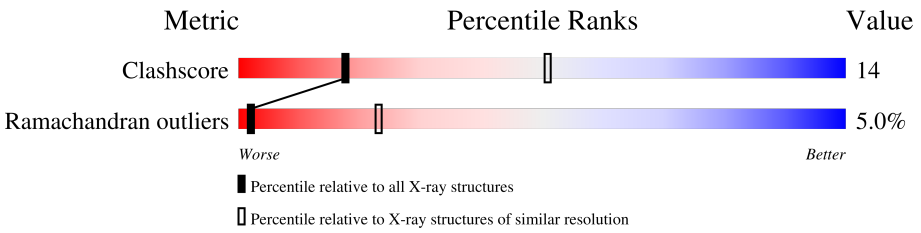
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	831	77% 13% • 7%
1	B	831	76% 14% • 8%
2	W	139	80% 15% • •
2	Y	139	80% 15% • •
3	X	152	80% 17% • •
3	Z	152	80% 17% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10500 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 MYOSIN HEAD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	772	3816	2271	772	773	0	0	0
1	B	766	3786	2253	766	767	0	0	0

- Molecule 2 is a protein called MYOSIN HEAD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	Y	136	673	400	136	137	0	0	0
2	W	136	673	400	136	137	0	0	0

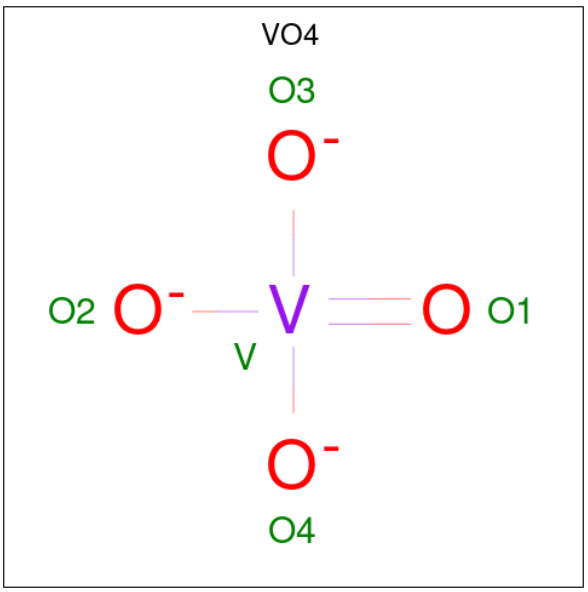
- Molecule 3 is a protein called MYOSIN HEAD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	Z	151	741	438	151	152	0	0	0
3	X	151	741	438	151	152	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

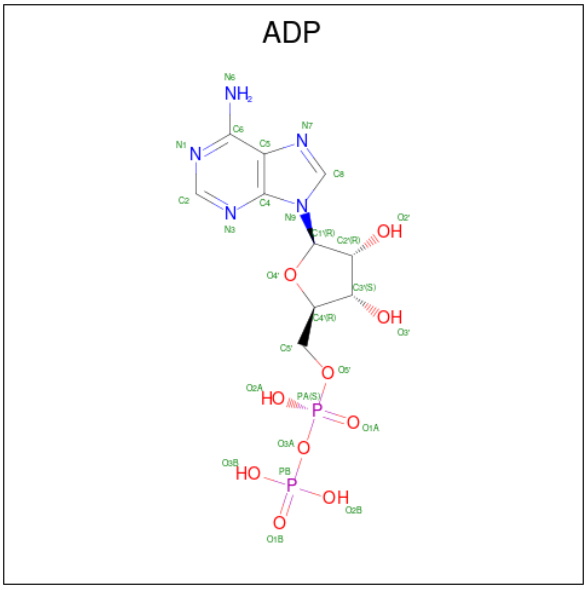
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	Y	1	1	1	0	0
4	B	1	1	1	0	0
4	W	1	1	1	0	0

- Molecule 5 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	Z	1	1	1	0	0
			Total	Ca		
7	X	1	1	1	0	0

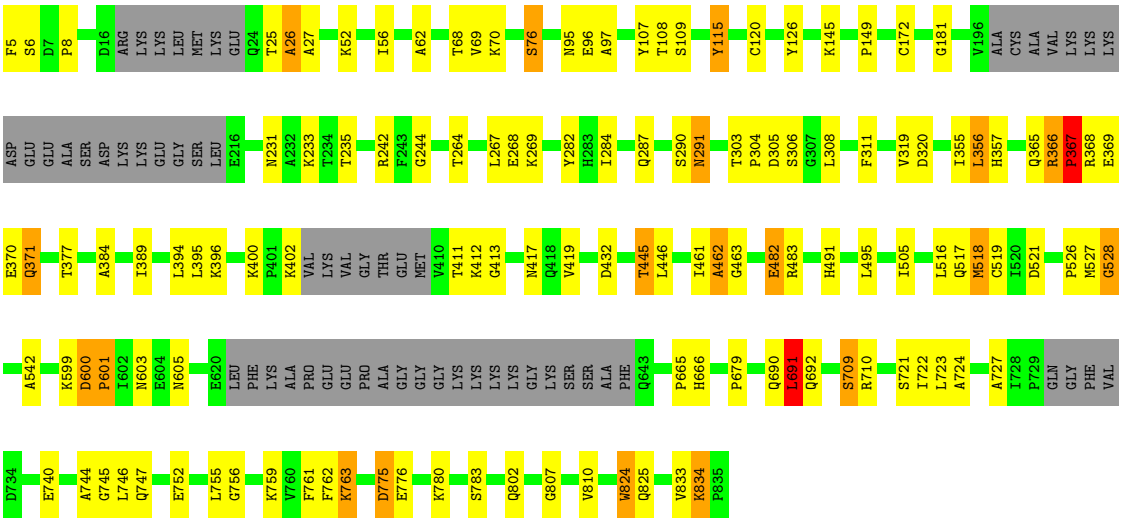
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

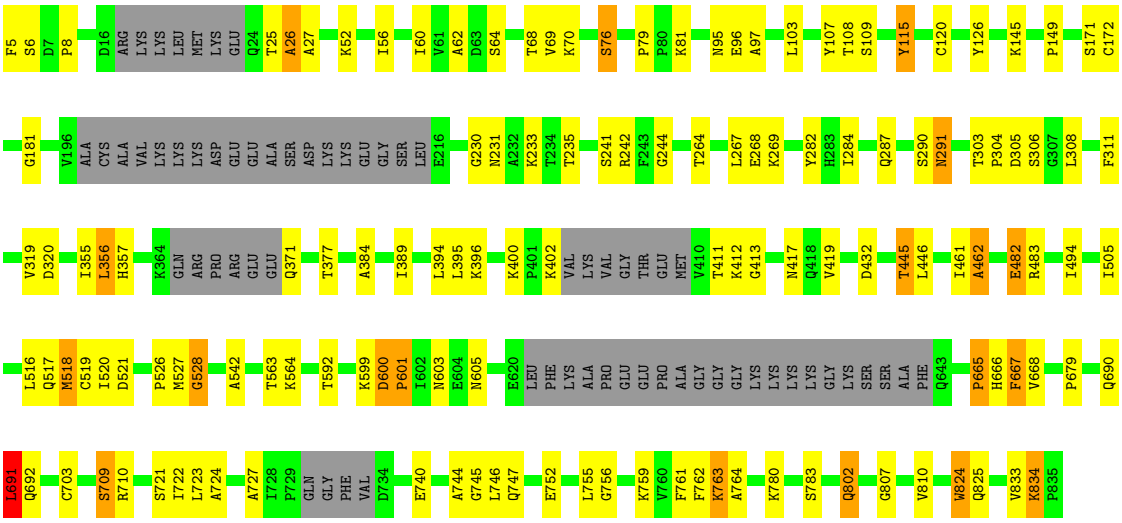
• Molecule 1: MYOSIN HEAD

Chain A: 77% 13% • 7%



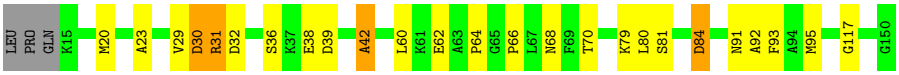
• Molecule 1: MYOSIN HEAD

Chain B: 76% 14% • 8%



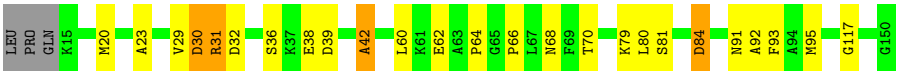
- Molecule 2: MYOSIN HEAD

Chain Y:



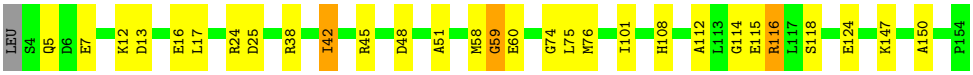
- Molecule 2: MYOSIN HEAD

Chain W:



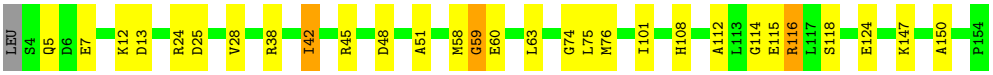
- Molecule 3: MYOSIN HEAD

Chain Z:



- Molecule 3: MYOSIN HEAD

Chain X:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.03Å 243.47Å 124.65Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	20.00 – 4.20	Depositor
% Data completeness (in resolution range)	95.0 (20.00-4.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.394 , 0.400	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10500	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

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: VO4, ADP, MG, CA

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	1.02	12/3809 (0.3%)	1.12	26/5293 (0.5%)
1	B	0.99	16/3778 (0.4%)	1.29	37/5248 (0.7%)
2	W	0.42	0/672	1.07	3/933 (0.3%)
2	Y	0.53	1/672 (0.1%)	0.72	0/933
3	X	0.38	0/740	0.74	0/1024
3	Z	0.38	0/740	0.74	0/1024
All	All	0.88	29/10411 (0.3%)	1.12	66/14455 (0.5%)

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	4
1	B	0	5
2	W	0	1
2	Y	0	1
All	All	0	11

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	ALA	C-N	33.12	1.92	1.33
1	A	709	SER	C-N	26.15	1.94	1.34
1	B	667	PHE	C-N	-25.43	0.75	1.34
1	B	709	SER	C-N	17.82	1.75	1.34
1	B	482	GLU	C-N	-17.10	0.94	1.34
1	A	482	GLU	C-N	-17.01	0.94	1.34
1	A	445	THR	C-N	14.82	1.68	1.34
1	B	445	THR	C-N	14.81	1.68	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	GLY	C-N	-14.42	1.00	1.34
1	B	371	GLN	C-N	-14.32	1.01	1.34
1	B	76	SER	C-N	-12.62	1.05	1.34
1	B	241	SER	C-N	-12.55	1.05	1.34
1	A	432	ASP	C-N	11.76	1.61	1.34
1	A	120	CYS	C-N	11.36	1.60	1.34
1	B	120	CYS	C-N	11.35	1.60	1.34
1	B	356	LEU	C-N	10.85	1.59	1.34
1	A	233	LYS	C-N	-10.85	1.09	1.34
1	B	233	LYS	C-N	-10.85	1.09	1.34
1	A	802	GLN	C-N	-10.33	1.10	1.34
1	A	691	LEU	C-N	9.91	1.56	1.34
1	B	691	LEU	C-N	9.82	1.56	1.34
1	A	356	LEU	C-N	9.71	1.56	1.34
2	Y	84	ASP	C-N	9.59	1.56	1.34
1	B	802	GLN	C-N	-8.66	1.14	1.34
1	B	462	ALA	C-N	8.23	1.47	1.33
1	B	235	THR	C-N	-7.30	1.17	1.34
1	A	235	THR	C-N	-7.28	1.17	1.34
1	A	76	SER	C-N	-6.46	1.19	1.34
1	B	592	THR	C-N	5.15	1.42	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	824	TRP	O-C-N	-30.60	73.73	122.70
1	A	709	SER	O-C-N	27.08	166.03	122.70
1	B	709	SER	O-C-N	22.09	158.04	122.70
1	A	709	SER	CA-C-N	-21.53	69.83	117.20
1	B	371	GLN	O-C-N	-18.70	92.79	122.70
1	B	709	SER	CA-C-N	-18.64	76.18	117.20
1	A	482	GLU	O-C-N	18.27	151.94	122.70
1	B	482	GLU	O-C-N	18.27	151.93	122.70
2	W	84	ASP	CA-C-N	-17.89	77.84	117.20
1	B	824	TRP	CA-C-N	17.12	154.86	117.20
1	B	76	SER	O-C-N	-16.05	97.01	122.70
1	A	482	GLU	CA-C-N	-14.87	84.50	117.20
1	B	482	GLU	CA-C-N	-14.83	84.56	117.20
1	B	824	TRP	C-N-CA	14.54	158.04	121.70
2	W	84	ASP	C-N-CA	-14.49	85.46	121.70
1	B	667	PHE	O-C-N	13.52	144.33	122.70
1	B	371	GLN	CA-C-N	13.11	146.05	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	824	TRP	O-C-N	-12.93	102.02	122.70
1	B	76	SER	C-N-CA	11.46	150.36	121.70
1	A	76	SER	O-C-N	-11.04	105.04	122.70
1	A	462	ALA	C-N-CA	-10.97	99.25	122.30
1	B	667	PHE	CA-C-N	-10.91	93.20	117.20
1	A	709	SER	C-N-CA	-10.85	94.58	121.70
1	B	76	SER	CA-C-N	9.59	138.31	117.20
1	B	230	GLY	O-C-N	9.44	137.81	122.70
1	A	115	TYR	CA-C-N	-8.82	97.79	117.20
1	B	462	ALA	C-N-CA	-8.68	104.06	122.30
1	B	115	TYR	CA-C-N	-8.57	98.35	117.20
1	A	482	GLU	C-N-CA	-8.47	100.53	121.70
1	B	482	GLU	C-N-CA	-8.44	100.59	121.70
1	B	667	PHE	C-N-CA	-8.42	100.65	121.70
1	B	432	ASP	O-C-N	8.16	135.75	122.70
1	A	691	LEU	O-C-N	-8.04	109.84	122.70
1	B	691	LEU	O-C-N	-7.96	109.97	122.70
2	W	84	ASP	O-C-N	7.86	135.27	122.70
1	A	115	TYR	O-C-N	7.81	135.19	122.70
1	A	824	TRP	CA-C-N	7.71	134.15	117.20
1	A	824	TRP	C-N-CA	7.53	140.54	121.70
1	B	115	TYR	O-C-N	7.48	134.66	122.70
1	B	802	GLN	O-C-N	-7.33	110.98	122.70
1	B	230	GLY	CA-C-N	-7.27	101.20	117.20
1	B	462	ALA	O-C-N	-6.78	111.67	123.20
1	A	268	GLU	O-C-N	6.78	133.54	122.70
1	B	709	SER	C-N-CA	-6.74	104.85	121.70
1	A	775	ASP	O-C-N	6.70	133.41	122.70
1	B	268	GLU	O-C-N	6.66	133.35	122.70
1	A	76	SER	C-N-CA	6.58	138.15	121.70
1	A	76	SER	CA-C-N	6.29	131.05	117.20
1	B	230	GLY	C-N-CA	-6.26	106.06	121.70
1	B	432	ASP	CA-C-N	-6.15	103.66	117.20
1	A	775	ASP	C-N-CA	-5.96	106.81	121.70
1	A	371	GLN	N-CA-C	-5.61	95.87	111.00
1	B	665	PRO	N-CA-CB	5.55	109.96	103.30
1	A	665	PRO	N-CA-CB	5.52	109.92	103.30
1	B	462	ALA	CA-C-N	5.51	127.21	116.20
1	B	241	SER	O-C-N	5.50	131.49	122.70
1	A	8	PRO	N-CA-CB	5.48	109.87	103.30
1	A	601	PRO	N-CA-CB	5.46	109.85	103.30
1	B	601	PRO	N-CA-CB	5.46	109.85	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	PRO	N-CA-CB	5.45	109.84	103.30
1	A	367	PRO	N-CA-CB	5.42	109.81	103.30
1	A	775	ASP	CA-C-N	-5.41	105.30	117.20
1	A	268	GLU	CA-C-N	-5.21	105.74	117.20
1	B	268	GLU	CA-C-N	-5.19	105.78	117.20
1	B	371	GLN	C-N-CA	5.17	134.62	121.70
1	B	432	ASP	C-N-CA	-5.07	109.02	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Mainchain
1	A	691	LEU	Mainchain
1	A	76	SER	Mainchain
1	A	824	TRP	Mainchain
1	B	115	TYR	Mainchain
1	B	691	LEU	Mainchain
1	B	76	SER	Mainchain
1	B	802	GLN	Mainchain
1	B	824	TRP	Mainchain
2	W	84	ASP	Mainchain
2	Y	84	ASP	Mainchain

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	3816	0	1691	72	0
1	B	3786	0	1675	78	0
2	W	673	0	302	16	0
2	Y	673	0	302	18	0
3	X	741	0	338	14	0
3	Z	741	0	338	14	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
7	X	1	0	0	0	0
7	Z	1	0	0	0	0
All	All	10500	0	4670	208	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 14.

All (208) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:PHE:C	1:B:668:VAL:CA	1.77	1.50
1:B:667:PHE:CA	1:B:668:VAL:N	1.73	1.49
1:B:445:THR:C	1:B:446:LEU:N	1.68	1.48
1:A:445:THR:C	1:A:446:LEU:N	1.68	1.45
1:B:709:SER:C	1:B:710:ARG:N	1.75	1.41
1:B:709:SER:CA	1:B:710:ARG:N	2.01	1.23
1:A:709:SER:CA	1:A:710:ARG:N	2.00	1.23
1:A:462:ALA:C	1:A:463:GLY:N	1.92	1.21
1:A:709:SER:C	1:A:710:ARG:N	1.94	1.19
1:A:709:SER:HA	1:A:710:ARG:N	1.59	1.13
1:B:709:SER:HA	1:B:710:ARG:N	1.62	1.11
1:A:599:LYS:O	1:A:600:ASP:O	1.71	1.09
1:B:599:LYS:O	1:B:600:ASP:O	1.71	1.09
1:B:667:PHE:O	1:B:668:VAL:N	1.89	1.06
1:A:461:ILE:C	1:A:462:ALA:N	2.12	1.02
1:B:461:ILE:C	1:B:462:ALA:N	2.12	1.02
1:B:667:PHE:O	1:B:668:VAL:CA	2.16	0.93
1:A:461:ILE:HA	1:A:462:ALA:N	1.85	0.92
1:B:461:ILE:CA	1:B:462:ALA:N	2.32	0.92
1:A:461:ILE:CA	1:A:462:ALA:N	2.32	0.92
1:B:461:ILE:HA	1:B:462:ALA:N	1.85	0.92
1:B:171:SER:O	1:B:665:PRO:HA	1.69	0.91
1:B:667:PHE:O	1:B:668:VAL:HA	1.74	0.87
1:A:518:MET:O	1:A:521:ASP:N	2.09	0.86
1:B:667:PHE:C	1:B:668:VAL:HA	1.96	0.85
1:B:518:MET:O	1:B:521:ASP:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:PHE:C	1:B:668:VAL:N	0.75	0.80
1:B:667:PHE:HA	1:B:668:VAL:N	1.93	0.79
1:A:709:SER:C	1:A:710:ARG:CA	2.52	0.77
1:B:709:SER:C	1:B:710:ARG:CA	2.55	0.75
1:B:482:GLU:O	1:B:483:ARG:C	2.21	0.73
1:A:482:GLU:O	1:A:483:ARG:C	2.21	0.73
1:A:462:ALA:C	1:A:463:GLY:CA	2.59	0.71
2:W:29:VAL:C	2:W:31:ARG:H	1.95	0.70
2:Y:29:VAL:C	2:Y:31:ARG:H	1.95	0.70
1:B:667:PHE:CB	1:B:668:VAL:N	2.58	0.66
1:B:518:MET:O	1:B:519:CYS:C	2.36	0.63
1:A:518:MET:O	1:A:519:CYS:C	2.36	0.63
1:A:365:GLN:O	1:A:366:ARG:CB	2.47	0.62
1:B:517:GLN:O	1:B:521:ASP:N	2.33	0.60
2:W:117:GLY:O	3:X:24:ARG:N	2.33	0.60
1:A:244:GLY:O	1:A:264:THR:HA	2.01	0.59
1:A:709:SER:O	1:A:761:PHE:HA	2.02	0.59
1:B:244:GLY:O	1:B:264:THR:HA	2.01	0.59
1:B:703:CYS:O	1:B:764:ALA:HB2	2.03	0.59
2:Y:29:VAL:O	2:Y:31:ARG:N	2.36	0.58
3:X:58:MET:O	3:X:60:GLU:N	2.32	0.58
1:A:517:GLN:O	1:A:521:ASP:N	2.36	0.58
2:W:29:VAL:O	2:W:31:ARG:N	2.36	0.58
1:A:709:SER:C	1:A:710:ARG:HA	2.24	0.58
3:Z:58:MET:O	3:Z:60:GLU:N	2.32	0.58
1:A:740:GLU:O	1:A:744:ALA:HB2	2.03	0.57
1:B:740:GLU:O	1:B:744:ALA:HB2	2.03	0.57
1:A:690:GLN:C	1:A:692:GLN:H	2.08	0.57
1:B:690:GLN:C	1:B:692:GLN:H	2.08	0.56
1:A:400:LYS:HA	1:A:413:GLY:HA2	1.87	0.56
1:B:599:LYS:C	1:B:600:ASP:O	2.43	0.56
1:B:400:LYS:HA	1:B:413:GLY:HA2	1.87	0.56
1:A:603:ASN:C	1:A:605:ASN:H	2.08	0.55
1:B:172:CYS:HA	1:B:666:HIS:O	2.07	0.55
1:B:807:GLY:O	2:W:92:ALA:HB1	2.08	0.54
1:A:284:ILE:O	1:A:287:GLN:N	2.41	0.54
1:A:603:ASN:C	1:A:605:ASN:N	2.61	0.54
1:A:306:SER:C	1:A:308:LEU:H	2.12	0.53
1:A:319:VAL:O	1:A:320:ASP:C	2.47	0.53
1:B:306:SER:C	1:B:308:LEU:H	2.12	0.53
1:A:745:GLY:C	1:A:747:GLN:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:ASP:O	1:A:776:GLU:C	2.44	0.53
1:B:126:TYR:O	1:B:679:PRO:CB	2.57	0.53
1:A:126:TYR:O	1:A:679:PRO:CB	2.57	0.53
1:A:807:GLY:O	2:Y:92:ALA:HB1	2.08	0.53
1:A:780:LYS:O	1:A:783:SER:N	2.42	0.53
1:A:690:GLN:C	1:A:692:GLN:N	2.63	0.52
1:B:745:GLY:C	1:B:747:GLN:H	2.11	0.52
1:B:709:SER:O	1:B:761:PHE:HA	2.10	0.52
1:B:690:GLN:C	1:B:692:GLN:N	2.63	0.52
3:X:147:LYS:O	3:X:150:ALA:HB3	2.10	0.52
3:Z:108:HIS:O	3:Z:112:ALA:HB3	2.10	0.52
3:Z:147:LYS:O	3:Z:150:ALA:HB3	2.10	0.51
1:B:284:ILE:O	1:B:287:GLN:N	2.41	0.51
1:B:319:VAL:O	1:B:320:ASP:C	2.47	0.51
2:W:29:VAL:C	2:W:31:ARG:N	2.64	0.51
1:A:462:ALA:O	1:A:463:GLY:HA2	2.11	0.51
1:A:599:LYS:C	1:A:600:ASP:O	2.43	0.51
1:B:516:LEU:O	1:B:517:GLN:C	2.49	0.51
1:B:709:SER:O	1:B:762:PHE:N	2.41	0.51
1:B:599:LYS:O	1:B:600:ASP:C	2.47	0.50
1:A:516:LEU:O	1:A:517:GLN:C	2.49	0.50
3:X:114:GLY:O	3:X:116:ARG:N	2.44	0.50
3:X:108:HIS:O	3:X:112:ALA:HB3	2.11	0.50
1:A:690:GLN:O	1:A:692:GLN:N	2.45	0.50
1:B:690:GLN:O	1:B:692:GLN:N	2.45	0.50
1:B:780:LYS:O	1:B:783:SER:N	2.42	0.49
1:A:745:GLY:O	1:A:747:GLN:N	2.45	0.49
3:Z:114:GLY:O	3:Z:116:ARG:N	2.44	0.49
2:Y:20:MET:O	2:Y:23:ALA:HB3	2.13	0.49
1:B:745:GLY:O	1:B:747:GLN:N	2.45	0.49
1:A:95:ASN:O	1:A:97:ALA:N	2.46	0.49
2:Y:29:VAL:C	2:Y:31:ARG:N	2.64	0.48
1:B:603:ASN:C	1:B:605:ASN:H	2.16	0.48
1:B:95:ASN:O	1:B:97:ALA:N	2.46	0.48
2:W:20:MET:O	2:W:23:ALA:HB3	2.13	0.48
1:B:402:LYS:HA	1:B:411:THR:HA	1.96	0.48
1:B:107:TYR:C	1:B:109:SER:H	2.18	0.48
2:W:36:SER:O	2:W:39:ASP:N	2.47	0.47
2:W:38:GLU:O	2:W:42:ALA:HB2	2.14	0.47
1:A:107:TYR:C	1:A:109:SER:H	2.18	0.47
1:A:402:LYS:HA	1:A:411:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:36:SER:O	2:Y:39:ASP:N	2.47	0.47
3:Z:48:ASP:O	3:Z:51:ALA:HB3	2.14	0.47
1:B:384:ALA:HB1	1:B:389:ILE:O	2.15	0.47
2:W:91:ASN:C	2:W:93:PHE:N	2.68	0.47
1:B:527:MET:O	1:B:528:GLY:O	2.32	0.47
1:B:709:SER:C	1:B:710:ARG:HA	2.34	0.47
1:A:833:VAL:O	1:A:834:LYS:C	2.53	0.47
1:B:5:PHE:O	1:B:6:SER:CB	2.62	0.47
2:Y:38:GLU:O	2:Y:42:ALA:HB2	2.14	0.47
3:X:38:ARG:HA	3:X:42:ILE:O	2.15	0.47
3:Z:38:ARG:HA	3:Z:42:ILE:O	2.15	0.46
1:B:833:VAL:O	1:B:834:LYS:C	2.53	0.46
1:A:527:MET:O	1:A:528:GLY:O	2.32	0.46
1:A:5:PHE:O	1:A:6:SER:CB	2.62	0.46
2:Y:60:LEU:C	2:Y:62:GLU:N	2.69	0.46
3:X:12:LYS:O	3:X:13:ASP:C	2.53	0.46
3:X:48:ASP:O	3:X:51:ALA:HB3	2.14	0.46
3:Z:12:LYS:O	3:Z:13:ASP:C	2.53	0.46
1:A:231:ASN:O	1:A:282:TYR:HA	2.16	0.46
1:A:384:ALA:HB1	1:A:389:ILE:O	2.15	0.46
3:X:147:LYS:O	3:X:150:ALA:N	2.49	0.46
1:A:267:LEU:O	1:A:269:LYS:N	2.49	0.46
1:A:756:GLY:HA3	1:A:759:LYS:O	2.16	0.46
2:Y:91:ASN:C	2:Y:93:PHE:N	2.68	0.46
1:B:25:THR:O	1:B:26:ALA:HB3	2.16	0.46
2:W:60:LEU:C	2:W:62:GLU:N	2.69	0.46
1:A:709:SER:CB	1:A:710:ARG:N	2.73	0.45
3:Z:147:LYS:O	3:Z:150:ALA:N	2.49	0.45
1:B:756:GLY:HA3	1:B:759:LYS:O	2.16	0.45
1:A:56:ILE:O	1:A:68:THR:HA	2.17	0.45
1:B:56:ILE:O	1:B:68:THR:HA	2.16	0.45
1:B:355:ILE:O	1:B:357:HIS:N	2.49	0.45
2:W:93:PHE:C	2:W:95:MET:H	2.20	0.45
1:B:721:SER:C	1:B:723:LEU:H	2.20	0.45
2:W:60:LEU:C	2:W:62:GLU:H	2.20	0.45
1:A:394:LEU:O	1:A:396:LYS:N	2.50	0.45
1:B:394:LEU:O	1:B:396:LYS:N	2.50	0.45
1:A:366:ARG:O	1:A:367:PRO:C	2.55	0.45
1:A:516:LEU:C	1:A:518:MET:N	2.69	0.45
1:A:599:LYS:O	1:A:600:ASP:C	2.47	0.45
1:B:603:ASN:C	1:B:605:ASN:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:C	1:A:357:HIS:N	2.71	0.45
2:Y:93:PHE:C	2:Y:95:MET:H	2.20	0.45
1:A:721:SER:C	1:A:723:LEU:H	2.20	0.44
2:W:68:ASN:C	2:W:70:THR:H	2.21	0.44
1:A:745:GLY:C	1:A:747:GLN:N	2.70	0.44
2:Y:30:ASP:O	2:Y:32:ASP:N	2.50	0.44
1:B:290:SER:O	1:B:291:ASN:CB	2.66	0.44
3:X:74:GLY:C	3:X:76:MET:H	2.21	0.44
1:A:290:SER:O	1:A:291:ASN:CB	2.66	0.44
3:Z:74:GLY:C	3:Z:76:MET:H	2.21	0.44
1:B:355:ILE:C	1:B:357:HIS:N	2.71	0.44
1:A:355:ILE:O	1:A:357:HIS:N	2.50	0.44
2:Y:60:LEU:C	2:Y:62:GLU:H	2.20	0.44
1:B:267:LEU:O	1:B:269:LYS:N	2.49	0.44
2:W:30:ASP:O	2:W:32:ASP:N	2.50	0.44
2:Y:117:GLY:O	3:Z:24:ARG:N	2.49	0.43
1:B:745:GLY:C	1:B:747:GLN:N	2.71	0.43
1:A:516:LEU:O	1:A:518:MET:N	2.52	0.43
1:A:762:PHE:O	1:A:763:LYS:O	2.37	0.43
1:A:303:THR:O	1:A:305:ASP:N	2.44	0.43
1:A:462:ALA:C	1:A:463:GLY:HA2	2.35	0.43
2:Y:68:ASN:C	2:Y:70:THR:H	2.21	0.43
1:B:516:LEU:O	1:B:518:MET:N	2.52	0.43
1:B:762:PHE:O	1:B:763:LYS:O	2.37	0.43
1:B:231:ASN:O	1:B:282:TYR:HA	2.19	0.42
1:B:303:THR:O	1:B:305:ASP:N	2.44	0.42
1:A:242:ARG:O	1:A:267:LEU:HA	2.20	0.42
1:A:25:THR:O	1:A:26:ALA:HB3	2.19	0.42
1:A:369:GLU:O	1:A:370:GLU:CB	2.68	0.42
1:A:394:LEU:C	1:A:396:LYS:N	2.73	0.42
2:Y:68:ASN:C	2:Y:70:THR:N	2.73	0.42
3:X:5:GLN:C	3:X:7:GLU:N	2.73	0.42
2:Y:79:LYS:C	2:Y:81:SER:H	2.23	0.42
1:B:516:LEU:C	1:B:518:MET:N	2.69	0.42
1:A:491:HIS:HA	1:A:495:LEU:CB	2.50	0.41
3:Z:5:GLN:C	3:Z:7:GLU:N	2.73	0.41
1:B:69:VAL:O	1:B:70:LYS:C	2.58	0.41
2:W:79:LYS:C	2:W:81:SER:H	2.23	0.41
3:Z:59:GLY:O	3:Z:60:GLU:C	2.59	0.41
1:B:60:ILE:O	1:B:64:SER:HA	2.21	0.41
1:B:417:ASN:C	1:B:419:VAL:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:C	1:A:419:VAL:N	2.74	0.41
2:W:68:ASN:C	2:W:70:THR:N	2.73	0.41
3:Z:16:GLU:O	3:Z:17:LEU:C	2.60	0.41
1:B:242:ARG:O	1:B:267:LEU:HA	2.20	0.41
1:B:563:THR:O	1:B:564:LYS:C	2.60	0.41
1:A:762:PHE:C	1:A:763:LYS:O	2.58	0.41
3:X:28:VAL:O	3:X:63:LEU:N	2.52	0.41
1:A:172:CYS:HA	1:A:666:HIS:O	2.21	0.40
2:Y:93:PHE:C	2:Y:95:MET:N	2.74	0.40
3:X:59:GLY:O	3:X:60:GLU:C	2.59	0.40
1:A:69:VAL:O	1:A:70:LYS:C	2.58	0.40
1:B:518:MET:O	1:B:520:ILE:N	2.54	0.40
3:X:45:ARG:O	3:X:48:ASP:N	2.54	0.40
3:Z:45:ARG:O	3:Z:48:ASP:N	2.54	0.40
1:B:79:PRO:O	1:B:81:LYS:N	2.55	0.40
1:B:394:LEU:C	1:B:396:LYS:N	2.73	0.40
2:Y:91:ASN:C	2:Y:93:PHE:H	2.25	0.40
1:B:762:PHE:C	1:B:763:LYS:O	2.58	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	758/831 (91%)	606 (80%)	114 (15%)	38 (5%)	2 23
1	B	750/831 (90%)	606 (81%)	108 (14%)	36 (5%)	2 24
2	W	134/139 (96%)	94 (70%)	34 (25%)	6 (4%)	2 25
2	Y	134/139 (96%)	95 (71%)	33 (25%)	6 (4%)	2 25
3	X	149/152 (98%)	104 (70%)	36 (24%)	9 (6%)	1 20
3	Z	149/152 (98%)	104 (70%)	36 (24%)	9 (6%)	1 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2074/2244 (92%)	1609 (78%)	361 (17%)	104 (5%)	2 23

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ALA
1	A	366	ARG
1	A	368	ARG
1	A	371	GLN
1	A	542	ALA
1	A	600	ASP
1	A	601	PRO
1	A	722	ILE
1	A	752	GLU
1	A	755	LEU
1	A	834	LYS
2	Y	31	ARG
3	Z	42	ILE
3	Z	75	LEU
3	Z	116	ARG
1	B	27	ALA
1	B	542	ALA
1	B	600	ASP
1	B	601	PRO
1	B	722	ILE
1	B	752	GLU
1	B	755	LEU
1	B	825	GLN
1	B	834	LYS
2	W	31	ARG
3	X	42	ILE
3	X	75	LEU
3	X	116	ARG
1	A	26	ALA
1	A	62	ALA
1	A	96	GLU
1	A	145	LYS
1	A	291	ASN
1	A	367	PRO
1	A	518	MET
1	A	528	GLY
1	A	746	LEU

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Mol	Chain	Res	Type
1	A	763	LYS
1	A	825	GLN
2	Y	30	ASP
2	Y	66	PRO
2	Y	80	LEU
3	Z	115	GLU
1	B	26	ALA
1	B	62	ALA
1	B	96	GLU
1	B	145	LYS
1	B	291	ASN
1	B	505	ILE
1	B	518	MET
1	B	528	GLY
1	B	746	LEU
1	B	763	LYS
2	W	30	ASP
2	W	66	PRO
2	W	80	LEU
3	X	115	GLU
1	A	52	LYS
1	A	149	PRO
1	A	395	LEU
1	A	505	ILE
1	A	691	LEU
1	A	727	ALA
3	Z	25	ASP
3	Z	59	GLY
3	Z	124	GLU
1	B	52	LYS
1	B	149	PRO
1	B	395	LEU
1	B	691	LEU
1	B	727	ALA
3	X	25	ASP
3	X	59	GLY
3	X	124	GLU
1	A	311	PHE
1	A	356	LEU
1	A	377	THR
2	Y	42	ALA
1	B	311	PHE

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Mol	Chain	Res	Type
1	B	356	LEU
1	B	377	THR
2	W	42	ALA
1	A	108	THR
1	A	412	LYS
1	A	526	PRO
3	Z	118	SER
1	B	108	THR
1	B	412	LYS
1	B	526	PRO
3	X	118	SER
1	B	103	LEU
1	A	304	PRO
3	Z	101	ILE
1	B	304	PRO
1	A	810	VAL
1	B	810	VAL
2	W	64	PRO
3	X	101	ILE
1	A	181	GLY
2	Y	64	PRO
1	B	494	ILE
1	B	181	GLY
1	A	724	ALA
1	B	724	ALA

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	VO4	A	1998	6,4	1,4,4	0.72	0	-		
5	VO4	B	2998	6,4	1,4,4	0.71	0	-		
6	ADP	A	1999	4,5	24,29,29	0.91	0	29,45,45	1.21	3 (10%)
6	ADP	B	2999	4,5	24,29,29	0.92	0	29,45,45	1.20	3 (10%)

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
6	ADP	B	2999	4,5	-	3/12/32/32	0/3/3/3
6	ADP	A	1999	4,5	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1999	ADP	C5-C6-N6	3.03	124.95	120.35
6	B	2999	ADP	C5-C6-N6	3.02	124.94	120.35
6	B	2999	ADP	C4-C5-N7	2.76	112.27	109.40
6	A	1999	ADP	C4-C5-N7	2.74	112.25	109.40
6	A	1999	ADP	C2'-C3'-C4'	-2.14	98.49	102.64
6	B	2999	ADP	C2'-C3'-C4'	-2.13	98.50	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

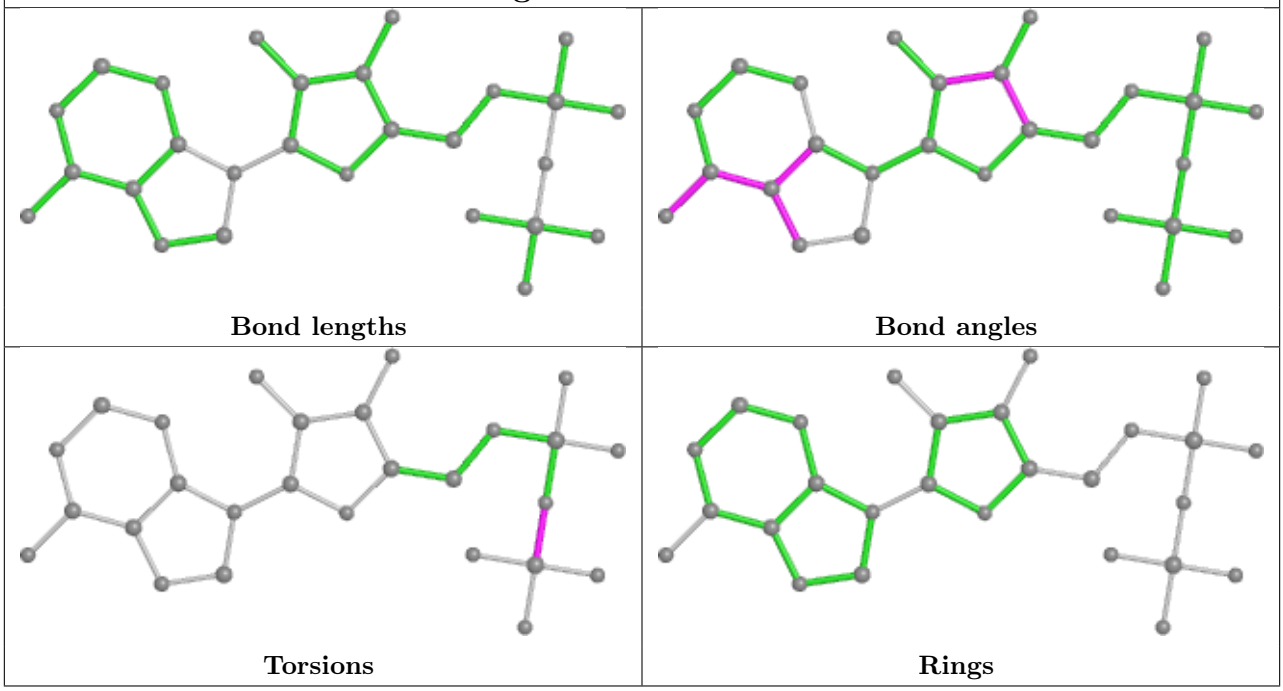
Mol	Chain	Res	Type	Atoms
6	A	1999	ADP	PA-O3A-PB-O1B
6	B	2999	ADP	PA-O3A-PB-O1B
6	A	1999	ADP	PA-O3A-PB-O2B
6	A	1999	ADP	PA-O3A-PB-O3B
6	B	2999	ADP	PA-O3A-PB-O2B
6	B	2999	ADP	PA-O3A-PB-O3B

There are no ring outliers.

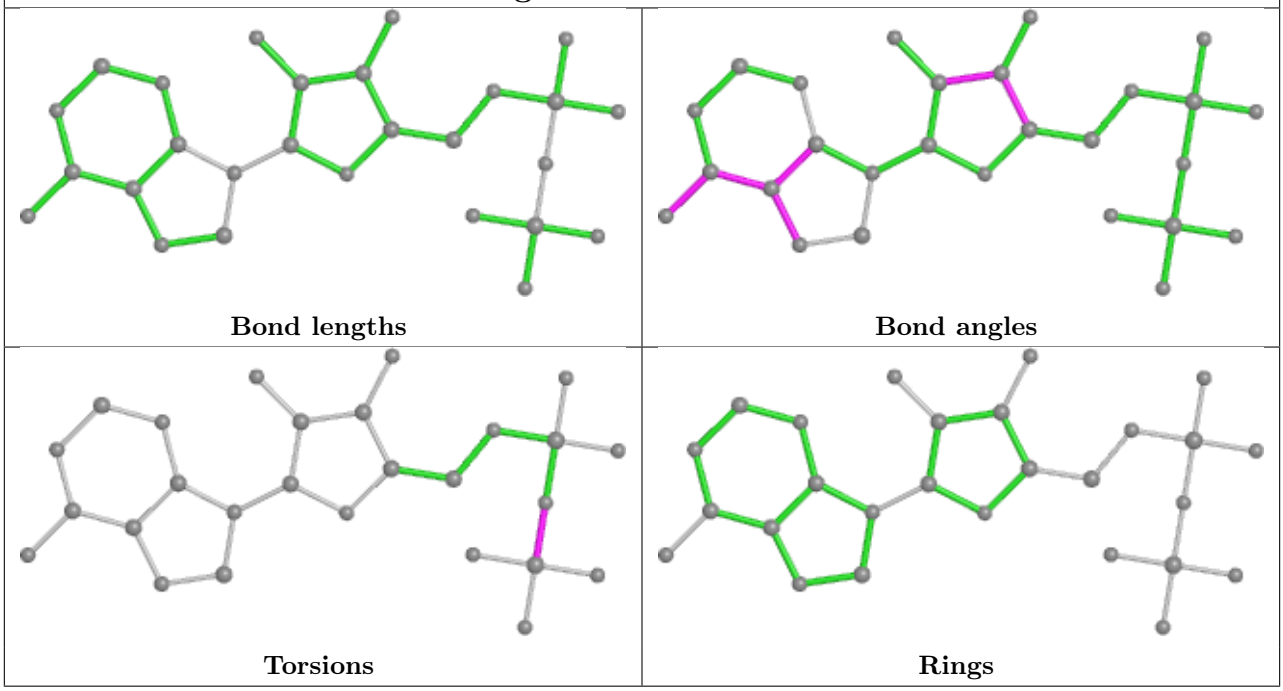
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 1999



Ligand ADP B 2999



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	12
1	A	10

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	461:ILE	C	462:ALA	N	2.12
1	B	461:ILE	C	462:ALA	N	2.12
1	A	709:SER	C	710:ARG	N	1.94
1	A	462:ALA	C	463:GLY	N	1.92
1	B	709:SER	C	710:ARG	N	1.75
1	A	445:THR	C	446:LEU	N	1.68
1	B	445:THR	C	446:LEU	N	1.68
1	A	432:ASP	C	433:ARG	N	1.61
1	A	76:SER	C	77:MET	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	235:THR	C	236:ARG	N	1.17
1	B	235:THR	C	236:ARG	N	1.17
1	B	802:GLN	C	803:ASP	N	1.14
1	A	802:GLN	C	803:ASP	N	1.10
1	A	233:LYS	C	234:THR	N	1.09
1	B	233:LYS	C	234:THR	N	1.09
1	B	76:SER	C	77:MET	N	1.05
1	B	241:SER	C	242:ARG	N	1.05
1	B	371:GLN	C	372:ALA	N	1.01
1	B	230:GLY	C	231:ASN	N	1.00
1	A	482:GLU	C	483:ARG	N	0.94
1	B	482:GLU	C	483:ARG	N	0.94
1	B	667:PHE	C	668:VAL	N	0.75

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.