



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:55 AM EDT

PDB ID : 1DFL / pdb_00001dfL
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

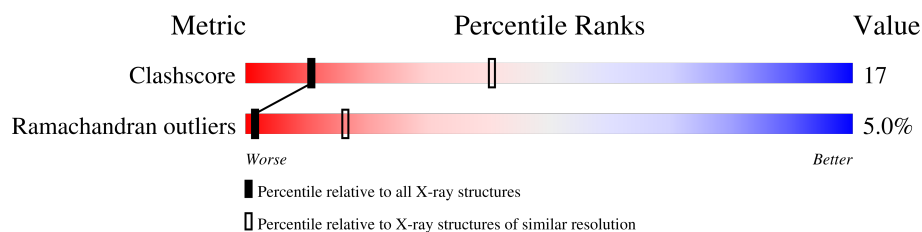
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	831	71% 18% • 7%
1	B	831	71% 18% • 8%
2	W	139	70% 24% • •
2	Y	139	71% 24% • •
3	X	152	70% 27% • •
3	Z	152	72% 25% • •

2 Entry composition

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
1	A	772	Total	C	N	O	0	0	0
			3816	2271	772	773			
1	B	766	Total	C	N	O	0	0	0
			3786	2253	766	767			

- Molecule 2 is a protein called MYOSIN HEAD.

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

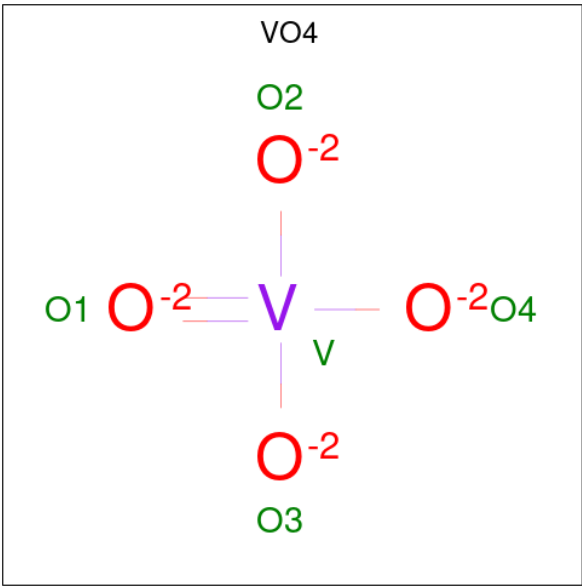
- Molecule 3 is a protein called MYOSIN HEAD.

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

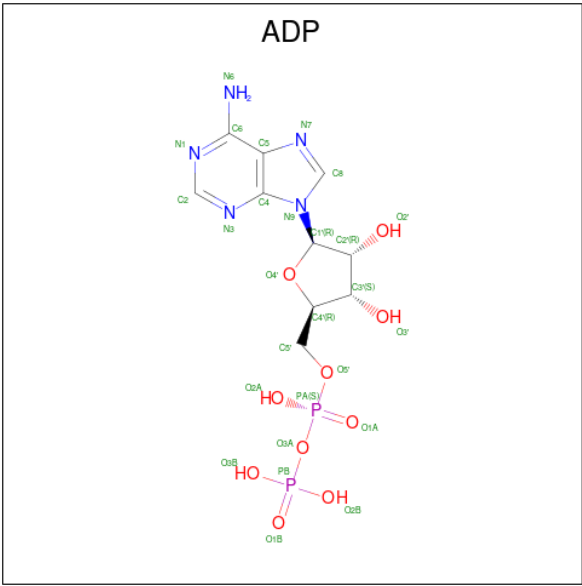
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	Y	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	W	1	Total	Mg	0	0
			1	1		

- Molecule 5 is VANADATE ION (CCD ID: VO4) (formula: O₄V).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

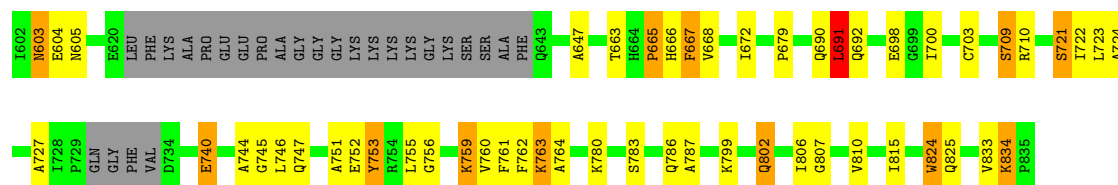
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

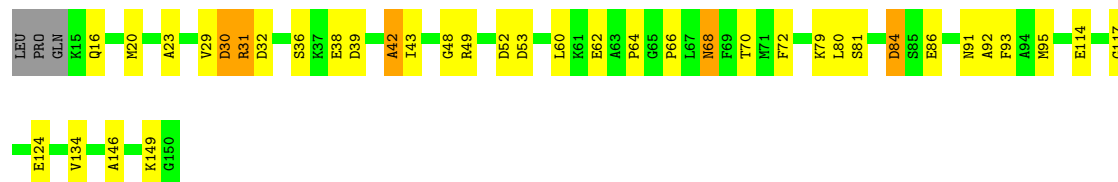
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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



• Molecule 2: MYOSIN HEAD

Chain Y: 71% 24%



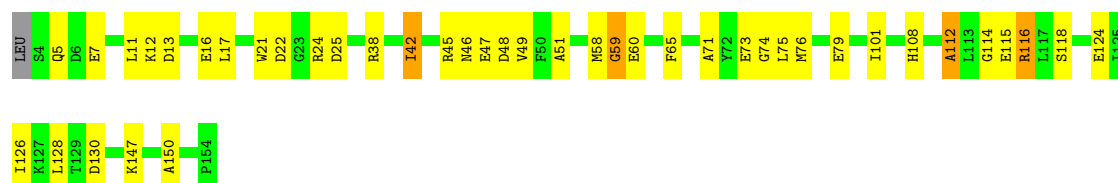
• Molecule 2: MYOSIN HEAD

Chain W: 70% 24%



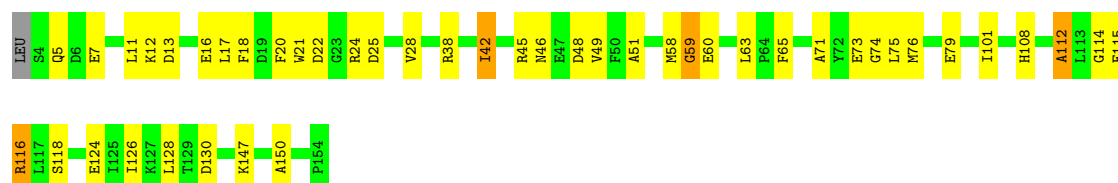
• Molecule 3: MYOSIN HEAD

Chain Z: 72% 25%



• Molecule 3: MYOSIN HEAD

Chain X: 70% 27%



4 Data and refinement statistics

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: MG, VO4, ADP, 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	1.64	15/3809 (0.4%)	1.69	72/5293 (1.4%)
1	B	1.66	18/3778 (0.5%)	1.86	88/5248 (1.7%)
2	W	0.73	2/672 (0.3%)	1.69	12/933 (1.3%)
2	Y	0.89	2/672 (0.3%)	1.36	10/933 (1.1%)
3	X	0.58	0/740	1.32	10/1024 (1.0%)
3	Z	0.58	0/740	1.32	10/1024 (1.0%)
All	All	1.45	37/10411 (0.4%)	1.69	202/14455 (1.4%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	ALA	C-N	47.04	1.92	1.33
1	A	709	SER	C-N	45.57	1.94	1.33
1	B	667	PHE	C-N	-43.92	0.75	1.33
1	B	709	SER	C-N	30.99	1.75	1.33
1	B	482	GLU	C-N	-27.83	0.94	1.33
1	A	482	GLU	C-N	-27.70	0.94	1.33
1	B	230	GLY	C-N	-26.79	1.00	1.33
1	A	445	THR	C-N	25.36	1.68	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	445	THR	C-N	25.34	1.68	1.33
1	B	371	GLN	C-N	-22.99	1.01	1.33
1	A	120	CYS	C-N	21.71	1.60	1.33
1	B	120	CYS	C-N	21.69	1.60	1.33
1	B	241	SER	C-N	-20.69	1.05	1.33
1	B	76	SER	C-N	-20.47	1.05	1.33
1	A	432	ASP	C-N	19.97	1.61	1.33
1	A	233	LYS	C-N	-18.41	1.09	1.33
1	B	233	LYS	C-N	-18.41	1.09	1.33
1	B	356	LEU	C-N	18.34	1.59	1.33
1	A	691	LEU	C-N	17.65	1.56	1.33
1	B	691	LEU	C-N	17.50	1.56	1.33
1	A	356	LEU	C-N	16.70	1.56	1.33
1	A	802	GLN	C-N	-16.50	1.10	1.33
2	Y	84	ASP	C-N	15.83	1.56	1.33
1	B	802	GLN	C-N	-13.80	1.14	1.33
1	B	235	THR	C-N	-12.49	1.17	1.33
1	A	235	THR	C-N	-12.46	1.17	1.33
1	B	462	ALA	C-N	11.48	1.47	1.33
1	A	76	SER	C-N	-11.10	1.19	1.33
1	B	115	TYR	C-N	9.51	1.45	1.33
1	A	115	TYR	C-N	9.03	1.44	1.33
2	W	84	ASP	C-N	8.51	1.45	1.33
1	A	775	ASP	C-N	-8.48	1.23	1.33
1	A	230	GLY	C-N	7.54	1.42	1.33
1	B	603	ASN	C-N	7.42	1.43	1.33
2	Y	149	LYS	CA-C	6.75	1.57	1.53
2	W	149	LYS	CA-C	6.69	1.57	1.53
1	B	592	THR	C-N	5.71	1.42	1.33

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	824	TRP	O-C-N	-36.73	73.73	122.59
1	A	709	SER	O-C-N	34.79	166.03	123.24
1	B	709	SER	O-C-N	29.72	158.04	123.27
1	A	482	GLU	O-C-N	22.07	151.94	122.59
1	B	482	GLU	O-C-N	22.06	151.93	122.59
2	W	84	ASP	CA-C-N	-21.00	85.46	123.05
2	W	84	ASP	C-N-CA	-21.00	85.46	123.05
1	A	462	ALA	CA-C-N	-19.49	99.25	122.83
1	A	462	ALA	C-N-CA	-19.49	99.25	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	824	TRP	CA-C-N	19.11	158.04	121.54
1	B	824	TRP	C-N-CA	19.11	158.04	121.54
1	B	371	GLN	O-C-N	-18.88	92.79	123.00
1	B	76	SER	O-C-N	-18.73	97.01	122.48
1	B	667	PHE	O-C-N	16.80	144.33	123.16
1	A	709	SER	CA-C-N	-16.52	94.58	122.33
1	A	709	SER	C-N-CA	-16.52	94.58	122.33
1	B	667	PHE	CA-C-N	-16.07	100.65	122.99
1	B	667	PHE	C-N-CA	-16.07	100.65	122.99
1	B	462	ALA	CA-C-N	-15.51	104.06	122.83
1	B	462	ALA	C-N-CA	-15.51	104.06	122.83
1	B	76	SER	CA-C-N	15.09	150.36	121.54
1	B	76	SER	C-N-CA	15.09	150.36	121.54
1	A	824	TRP	O-C-N	-14.09	102.02	122.87
1	A	76	SER	O-C-N	-13.13	105.04	122.77
1	B	709	SER	CA-C-N	-12.87	104.85	122.99
1	B	709	SER	C-N-CA	-12.87	104.85	122.99
1	B	432	ASP	O-C-N	12.65	135.75	122.09
1	B	815	ILE	N-CA-C	-11.94	101.02	112.96
1	A	815	ILE	N-CA-C	-11.91	101.05	112.96
1	B	230	GLY	O-C-N	11.62	137.81	122.70
1	A	482	GLU	CA-C-N	-11.00	100.53	121.54
1	A	482	GLU	C-N-CA	-11.00	100.53	121.54
1	B	482	GLU	CA-C-N	-10.97	100.59	121.54
1	B	482	GLU	C-N-CA	-10.97	100.59	121.54
1	A	115	TYR	O-C-N	10.37	135.19	123.16
1	A	76	SER	CA-C-N	10.23	138.15	120.87
1	A	76	SER	C-N-CA	10.23	138.15	120.87
1	A	824	TRP	CA-C-N	9.95	140.54	121.54
1	A	824	TRP	C-N-CA	9.95	140.54	121.54
1	B	115	TYR	O-C-N	9.92	134.66	123.16
1	A	423	VAL	N-CA-C	-9.67	101.44	110.53
1	B	423	VAL	N-CA-C	-9.65	101.46	110.53
1	A	691	LEU	O-C-N	-9.59	109.84	122.59
2	W	84	ASP	O-C-N	9.54	135.27	122.59
1	B	691	LEU	O-C-N	-9.49	109.97	122.59
1	A	775	ASP	O-C-N	9.29	133.41	122.17
1	B	230	GLY	CA-C-N	-9.07	106.06	121.75
1	B	230	GLY	C-N-CA	-9.07	106.06	121.75
3	Z	73	GLU	N-CA-C	-9.07	101.48	111.36
1	A	775	ASP	CA-C-N	-9.04	106.81	121.19
1	A	775	ASP	C-N-CA	-9.04	106.81	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	73	GLU	N-CA-C	-8.96	101.59	111.36
1	A	115	TYR	CA-C-N	-8.85	110.98	123.20
1	A	115	TYR	C-N-CA	-8.85	110.98	123.20
1	B	115	TYR	CA-C-N	-8.45	111.54	123.20
1	B	115	TYR	C-N-CA	-8.45	111.54	123.20
1	B	432	ASP	CA-C-N	-8.40	109.02	120.28
1	B	432	ASP	C-N-CA	-8.40	109.02	120.28
1	B	462	ALA	O-C-N	-8.21	111.67	122.59
1	A	799	LYS	N-CA-C	-8.19	102.29	111.14
1	B	799	LYS	N-CA-C	-8.15	102.34	111.14
1	A	268	GLU	O-C-N	8.04	133.54	122.29
1	B	802	GLN	O-C-N	-8.02	110.98	122.36
1	B	268	GLU	O-C-N	7.90	133.35	122.29
1	B	270	SER	N-CA-C	7.89	120.78	111.71
1	A	270	SER	N-CA-C	7.87	120.76	111.71
1	B	371	GLN	CA-C-N	7.67	134.62	122.59
1	B	371	GLN	C-N-CA	7.67	134.62	122.59
1	B	116	SER	CA-C-N	-7.56	111.88	120.42
1	B	116	SER	C-N-CA	-7.56	111.88	120.42
1	A	116	SER	CA-C-N	-7.56	111.88	120.42
1	A	116	SER	C-N-CA	-7.56	111.88	120.42
2	Y	114	GLU	N-CA-C	7.36	119.00	110.97
2	W	114	GLU	N-CA-C	7.29	118.92	110.97
1	B	802	GLN	N-CA-C	-7.16	104.67	113.41
1	A	802	GLN	N-CA-C	-7.15	104.69	113.41
1	B	665	PRO	N-CA-CB	7.13	109.96	103.19
1	A	665	PRO	N-CA-CB	7.08	109.92	103.19
1	A	371	GLN	N-CA-C	-7.01	95.87	110.80
2	W	124	GLU	N-CA-C	-6.98	103.67	111.28
2	Y	124	GLU	N-CA-C	-6.97	103.69	111.28
3	X	126	ILE	N-CA-C	-6.89	103.62	110.30
1	B	346	GLN	N-CA-C	-6.89	105.15	113.97
1	A	347	SER	N-CA-C	-6.87	103.87	111.36
1	B	347	SER	N-CA-C	-6.84	103.90	111.36
1	A	346	GLN	N-CA-C	-6.83	105.23	113.97
3	Z	126	ILE	N-CA-C	-6.81	103.69	110.30
1	B	241	SER	CA-C-N	-6.73	111.69	122.66
1	B	241	SER	C-N-CA	-6.73	111.69	122.66
1	B	241	SER	O-C-N	6.67	131.49	122.82
1	B	268	GLU	CA-C-N	-6.54	111.42	120.38
1	B	268	GLU	C-N-CA	-6.54	111.42	120.38
1	A	268	GLU	CA-C-N	-6.54	111.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	GLU	C-N-CA	-6.54	111.42	120.38
1	B	524	GLU	N-CA-C	6.49	121.47	112.45
3	Z	11	LEU	N-CA-C	-6.48	104.14	111.07
3	X	11	LEU	N-CA-C	-6.47	104.14	111.07
1	A	524	GLU	N-CA-C	6.46	121.42	112.45
2	W	16	GLN	N-CA-C	-6.42	104.13	112.23
2	Y	16	GLN	N-CA-C	-6.42	104.14	112.23
1	A	601	PRO	N-CA-CB	6.29	109.85	103.25
1	B	601	PRO	N-CA-CB	6.28	109.85	103.25
1	B	118	LEU	N-CA-C	6.25	120.51	113.01
1	A	367	PRO	N-CA-CB	6.25	109.81	103.25
1	A	118	LEU	N-CA-C	6.22	120.48	113.01
1	B	252	GLY	CA-C-N	6.15	127.52	119.84
1	B	252	GLY	C-N-CA	6.15	127.52	119.84
3	Z	65	PHE	N-CA-C	-6.14	105.62	113.23
1	A	252	GLY	CA-C-N	6.12	127.49	119.84
1	A	252	GLY	C-N-CA	6.12	127.49	119.84
3	X	65	PHE	N-CA-C	-6.09	105.67	113.23
2	Y	43	ILE	N-CA-C	6.06	116.81	110.62
1	A	786	GLN	N-CA-C	-6.06	104.96	112.90
1	A	422	SER	N-CA-C	-6.06	105.72	113.23
2	W	43	ILE	N-CA-C	6.06	116.80	110.62
1	B	786	GLN	N-CA-C	-6.02	105.01	112.90
3	X	79	GLU	N-CA-C	5.99	119.05	110.24
3	Z	79	GLU	N-CA-C	5.99	119.04	110.24
2	Y	86	GLU	N-CA-C	-5.98	105.48	112.89
1	B	740	GLU	N-CA-C	-5.98	104.76	111.28
1	A	740	GLU	N-CA-C	-5.96	104.78	111.28
1	B	422	SER	N-CA-C	-5.92	105.89	113.23
2	W	86	GLU	N-CA-C	-5.91	105.56	112.89
1	A	554	ASN	N-CA-C	5.90	120.61	113.41
1	B	554	ASN	N-CA-C	5.89	120.48	113.12
1	A	281	ASN	N-CA-C	-5.88	101.24	110.36
1	A	8	PRO	N-CA-CB	5.87	109.87	103.30
2	Y	68	ASN	N-CA-C	-5.87	102.96	110.53
2	W	68	ASN	N-CA-C	-5.86	102.97	110.53
1	B	8	PRO	N-CA-CB	5.84	109.84	103.30
1	B	281	ASN	N-CA-C	-5.82	101.35	110.36
1	A	303	THR	N-CA-C	-5.81	100.21	109.04
1	A	587	VAL	N-CA-C	5.79	116.85	107.71
1	B	233	LYS	CA-C-N	5.78	131.61	122.36
1	B	233	LYS	C-N-CA	5.78	131.61	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	THR	N-CA-C	-5.78	100.26	109.04
1	B	587	VAL	N-CA-C	5.78	116.84	107.71
1	B	647	ALA	CA-C-N	-5.78	113.17	120.56
1	B	647	ALA	C-N-CA	-5.78	113.17	120.56
1	A	647	ALA	CA-C-N	-5.77	113.18	120.56
1	A	647	ALA	C-N-CA	-5.77	113.18	120.56
1	A	233	LYS	CA-C-N	5.76	131.58	122.36
1	A	233	LYS	C-N-CA	5.76	131.58	122.36
1	A	245	LYS	N-CA-C	5.75	117.77	108.34
1	B	787	ALA	N-CA-C	-5.73	104.95	111.14
1	B	245	LYS	N-CA-C	5.67	117.63	108.34
3	Z	112	ALA	N-CA-C	5.66	120.32	112.45
1	B	604	GLU	N-CA-C	-5.66	106.08	112.87
1	B	760	VAL	CB-CA-C	-5.64	103.49	111.21
1	A	787	ALA	N-CA-C	-5.62	105.08	111.14
3	X	112	ALA	N-CA-C	5.59	120.22	112.45
3	Z	49	VAL	N-CA-C	5.58	116.22	110.36
1	B	663	THR	O-C-N	5.55	129.89	123.17
3	X	49	VAL	N-CA-C	5.55	116.18	110.36
1	A	760	VAL	CB-CA-C	-5.54	103.62	111.21
1	B	806	ILE	N-CA-C	-5.53	105.71	110.74
3	X	21	TRP	N-CA-C	5.51	119.11	112.38
1	A	663	THR	O-C-N	5.50	129.83	123.17
1	A	806	ILE	N-CA-C	-5.49	105.74	110.74
2	W	134	VAL	N-CA-C	5.49	115.69	107.51
1	B	363	PHE	N-CA-C	5.49	115.53	108.34
1	A	444	LYS	N-CA-C	-5.45	105.23	111.07
1	B	444	LYS	N-CA-C	-5.45	105.23	111.07
2	Y	134	VAL	N-CA-C	5.45	115.62	107.51
1	A	287	GLN	N-CA-C	-5.43	105.27	111.14
1	A	759	LYS	N-CA-C	5.43	117.32	109.07
3	Z	21	TRP	N-CA-C	5.43	119.01	112.38
1	B	759	LYS	N-CA-C	5.39	117.27	109.07
3	Z	71	ALA	N-CA-C	-5.37	105.51	111.36
1	B	287	GLN	N-CA-C	-5.37	105.34	111.14
3	X	71	ALA	N-CA-C	-5.36	105.52	111.36
1	A	443	ASN	N-CA-C	-5.34	106.61	113.23
2	Y	84	ASP	N-CA-C	5.33	117.57	109.63
2	Y	146	ALA	N-CA-C	-5.33	105.12	111.03
2	W	146	ALA	N-CA-C	-5.32	105.12	111.03
1	B	443	ASN	N-CA-C	-5.31	106.64	113.23
2	Y	149	LYS	O-C-N	5.29	126.04	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	LYS	CA-C-N	5.28	126.44	119.84
1	A	525	LYS	C-N-CA	5.28	126.44	119.84
3	Z	22	ASP	N-CA-C	-5.26	103.71	111.81
1	B	135	SER	N-CA-C	-5.26	105.44	111.07
2	W	149	LYS	O-C-N	5.25	126.00	121.65
3	X	22	ASP	N-CA-C	-5.25	103.73	111.81
1	A	563	THR	N-CA-C	5.20	117.54	108.76
1	A	672	ILE	CA-C-N	5.17	124.97	119.28
1	A	672	ILE	C-N-CA	5.17	124.97	119.28
1	A	332	ASP	N-CA-C	-5.16	105.57	111.14
1	B	525	LYS	CA-C-N	5.16	126.29	119.84
1	B	525	LYS	C-N-CA	5.16	126.29	119.84
1	B	753	TYR	N-CA-C	5.16	115.97	108.14
1	B	563	THR	N-CA-C	5.15	117.47	108.76
1	B	332	ASP	N-CA-C	-5.15	105.58	111.14
1	A	135	SER	N-CA-C	-5.12	105.59	111.07
1	B	672	ILE	CA-C-N	5.12	124.91	119.28
1	B	672	ILE	C-N-CA	5.12	124.91	119.28
1	A	753	TYR	N-CA-C	5.12	115.92	108.14
1	A	721	SER	N-CA-C	-5.08	105.44	111.69
1	B	802	GLN	CA-C-N	5.05	129.21	120.58
1	B	802	GLN	C-N-CA	5.05	129.21	120.58
1	A	292	ALA	N-CA-C	-5.01	106.01	111.82
1	B	292	ALA	N-CA-C	-5.01	106.01	111.82
1	B	721	SER	N-CA-C	-5.00	105.53	111.69

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 ⓘ

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	88	0
1	B	3786	0	1675	89	0
2	W	673	0	302	22	0
2	Y	673	0	302	21	0
3	X	741	0	338	18	0
3	Z	741	0	338	18	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	W	1	0	0	0	0
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	252	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 17.

All (252) 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:445:THR:C	1:B:446:LEU:N	1.68	1.52
1:B:667:PHE:C	1:B:668:VAL:CA	1.77	1.51
1:A:445:THR:C	1:A:446:LEU:N	1.68	1.49
1:B:667:PHE:CA	1:B:668:VAL:N	1.73	1.49
1:B:709:SER:C	1:B:710:ARG:N	1.75	1.45
1:A:462:ALA:C	1:A:463:GLY:N	1.92	1.27
1:A:709:SER:C	1:A:710:ARG:N	1.94	1.23
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:461:ILE:C	1:B:462:ALA:N	2.12	1.08
1:A:461:ILE:C	1:A:462:ALA:N	2.12	1.07
1:B:667:PHE:O	1:B:668:VAL:N	1.89	1.06
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:B:461:ILE:HA	1:B:462:ALA:N	1.85	0.92
1:A:461:ILE:CA	1:A:462:ALA:N	2.32	0.91
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:667:PHE:C	1:B:668:VAL:N	0.75	0.85
1:A:709:SER:C	1:A:710:ARG:CA	2.52	0.82
1:B:518:MET:O	1:B:521:ASP:N	2.12	0.82
1:B:709:SER:C	1:B:710:ARG:CA	2.55	0.80
1:B:667:PHE:HA	1:B:668:VAL:N	1.93	0.79
1:A:482:GLU:O	1:A:483:ARG:C	2.21	0.78
1:B:482:GLU:O	1:B:483:ARG:C	2.21	0.78
1:A:462:ALA:C	1:A:463:GLY:CA	2.59	0.76
2:Y:29:VAL:C	2:Y:31:ARG:H	1.95	0.74
2:W:29:VAL:C	2:W:31:ARG:H	1.95	0.74
1:B:518:MET:O	1:B:519:CYS:C	2.36	0.68
1:A:518:MET:O	1:A:519:CYS:C	2.36	0.67
1:B:667:PHE:CB	1:B:668:VAL:N	2.58	0.66
1:A:709:SER:C	1:A:710:ARG:HA	2.24	0.62
1:A:365:GLN:O	1:A:366:ARG:CB	2.47	0.62
1:A:599:LYS:C	1:A:600:ASP:O	2.43	0.62
1:A:690:GLN:C	1:A:692:GLN:H	2.08	0.61
1:B:690:GLN:C	1:B:692:GLN:H	2.08	0.61
1:B:599:LYS:C	1:B:600:ASP:O	2.43	0.61
1:A:603:ASN:C	1:A:605:ASN:H	2.08	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:603:ASN:C	1:A:605:ASN:N	2.61	0.58
1:A:306:SER:C	1:A:308:LEU:H	2.12	0.58
1:A:319:VAL:O	1:A:320:ASP:C	2.47	0.58
1:B:306:SER:C	1:B:308:LEU:H	2.12	0.58
1:A:599:LYS:O	1:A:600:ASP:C	2.47	0.58
1:A:775:ASP:O	1:A:776:GLU:C	2.44	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:A:745:GLY:C	1:A:747:GLN:H	2.11	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:N	2.63	0.57
1:B:599:LYS:O	1:B:600:ASP:C	2.47	0.57
1:B:690:GLN:C	1:B:692:GLN:N	2.63	0.57
1:B:745:GLY:C	1:B:747:GLN:H	2.11	0.57
1:B:319:VAL:O	1:B:320:ASP:C	2.47	0.56
2:W:29:VAL:C	2:W:31:ARG:N	2.64	0.56
1:A:400:LYS:HA	1:A:413:GLY:HA2	1.87	0.56
1:B:400:LYS:HA	1:B:413:GLY:HA2	1.87	0.56
1:B:516:LEU:O	1:B:517:GLN:C	2.49	0.55
1:B:172:CYS:HA	1:B:666:HIS:O	2.07	0.55
1:A:516:LEU:O	1:A:517:GLN:C	2.49	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:B:603:ASN:C	1:B:605:ASN:H	2.16	0.54
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:B:107:TYR:C	1:B:109:SER:H	2.18	0.52
1:B:709:SER:O	1:B:761:PHE:HA	2.10	0.52
1:A:107:TYR:C	1:A:109:SER:H	2.18	0.52
1:A:462:ALA:C	1:A:463:GLY:HA2	2.35	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
1:A:833:VAL:O	1:A:834:LYS:C	2.53	0.51
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:709:SER:C	1:B:710:ARG:HA	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:VAL:O	1:B:834:LYS:C	2.53	0.51
1:A:462:ALA:O	1:A:463:GLY:HA2	2.11	0.51
2:Y:60:LEU:C	2:Y:62:GLU:N	2.69	0.51
3:X:12:LYS:O	3:X:13:ASP:C	2.53	0.51
1:B:709:SER:O	1:B:762:PHE:N	2.41	0.51
3:Z:12:LYS:O	3:Z:13:ASP:C	2.53	0.50
2:W:60:LEU:C	2:W:62:GLU:N	2.69	0.50
2:Y:91:ASN:C	2:Y:93:PHE:N	2.68	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:721:SER:C	1:B:723:LEU:H	2.20	0.50
1:B:780:LYS:O	1:B:783:SER:N	2.42	0.49
2:W:60:LEU:C	2:W:62:GLU:H	2.20	0.49
2:W:91:ASN:C	2:W:93:PHE:N	2.68	0.49
2:W:93:PHE:C	2:W:95:MET:H	2.20	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
1:A:366:ARG:O	1:A:367:PRO:C	2.55	0.49
1:A:516:LEU:C	1:A:518:MET:N	2.69	0.49
1:A:355:ILE:C	1:A:357:HIS:N	2.71	0.49
1:A:721:SER:C	1:A:723:LEU:H	2.20	0.49
2:Y:93:PHE:C	2:Y:95:MET:H	2.20	0.49
2:Y:20:MET:O	2:Y:23:ALA:HB3	2.13	0.49
2:W:68:ASN:C	2:W:70:THR:H	2.21	0.49
3:X:74:GLY:C	3:X:76:MET:H	2.21	0.49
1:A:745:GLY:C	1:A:747:GLN:N	2.70	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:60:LEU:C	2:Y:62:GLU:H	2.20	0.49
3:Z:74:GLY:C	3:Z:76:MET:H	2.21	0.49
1:B:355:ILE:C	1:B:357:HIS:N	2.71	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:745:GLY:C	1:B:747:GLN:N	2.71	0.48
2:Y:68:ASN:C	2:Y:70:THR:H	2.21	0.47
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: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
1:B:527:MET:O	1:B:528:GLY:O	2.32	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
2:Y:68:ASN:C	2:Y:70:THR:N	2.73	0.46
2:Y:79:LYS:C	2:Y:81:SER:H	2.23	0.46
3:Z:38:ARG:HA	3:Z:42:ILE:O	2.15	0.46
1:B:516:LEU:C	1:B:518:MET:N	2.69	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
1:A:461:ILE:C	1:A:462:ALA:C	2.84	0.46
1:B:603:ASN:C	1:B:605:ASN:N	2.70	0.46
3:X:5:GLN:C	3:X:7:GLU:N	2.73	0.46
1:A:394:LEU:C	1:A:396:LYS:N	2.73	0.46
1:B:69:VAL:O	1:B:70:LYS:C	2.58	0.46
3:X:48:ASP:O	3:X:51:ALA:HB3	2.14	0.46
3:Z:59:GLY:O	3:Z:60:GLU:C	2.59	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
2:W:79:LYS:C	2:W:81:SER:H	2.23	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
1:B:25:THR:O	1:B:26:ALA:HB3	2.16	0.46
2:Y:29:VAL:C	2:Y:31:ARG:N	2.64	0.45
3:Z:16:GLU:O	3:Z:17:LEU:C	2.60	0.45
2:W:68:ASN:C	2:W:70:THR:N	2.73	0.45
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:563:THR:O	1:B:564:LYS:C	2.60	0.45
1:A:762:PHE:C	1:A:763:LYS:O	2.58	0.45
3:X:59:GLY:O	3:X:60:GLU:C	2.59	0.45
1:A:69:VAL:O	1:A:70:LYS:C	2.58	0.45
2:Y:93:PHE:C	2:Y:95:MET:N	2.74	0.45
1:B:461:ILE:C	1:B:462:ALA:C	2.84	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
3:Z:5:GLN:C	3:Z:7:GLU:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:394:LEU:C	1:B:396:LYS:N	2.73	0.45
1:B:762:PHE:C	1:B:763:LYS:O	2.58	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:563:THR:O	1:A:564:LYS:C	2.60	0.45
2:Y:91:ASN:C	2:Y:93:PHE:H	2.25	0.45
3:X:16:GLU:O	3:X:17:LEU:C	2.60	0.44
3:Z:128:LEU:C	3:Z:130:ASP:H	2.26	0.44
2:W:91:ASN:C	2:W:93:PHE:H	2.25	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
1:A:290:SER:O	1:A:291:ASN:CB	2.66	0.44
2:W:48:GLY:O	2:W:49:ARG:C	2.60	0.44
2:W:93:PHE:C	2:W:95:MET:N	2.74	0.44
2:Y:48:GLY:O	2:Y:49:ARG:C	2.60	0.44
1:A:355:ILE:O	1:A:357:HIS:N	2.50	0.44
1:A:417:ASN:C	1:A:419:VAL:N	2.74	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
1:B:79:PRO:C	1:B:81:LYS:H	2.26	0.44
1:A:582:HIS:O	1:A:583:TYR:C	2.62	0.43
1:A:355:ILE:C	1:A:357:HIS:H	2.27	0.43
1:A:518:MET:C	1:A:520:ILE:N	2.77	0.43
2:Y:117:GLY:O	3:Z:24:ARG:N	2.49	0.43
1:A:79:PRO:C	1:A:81:LYS:H	2.26	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:B:417:ASN:C	1:B:419:VAL:N	2.74	0.43
1:A:303:THR:O	1:A:305:ASP:N	2.44	0.43
1:B:582:HIS:O	1:B:583:TYR:C	2.62	0.43
1:B:516:LEU:O	1:B:518:MET:N	2.52	0.43
1:A:396:LYS:C	1:A:398:LEU:H	2.27	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:355:ILE:C	1:B:357:HIS:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ALA:O	1:B:27:ALA:C	2.62	0.42
2:Y:52:ASP:O	2:Y:53:ASP:C	2.63	0.42
3:X:128:LEU:C	3:X:130:ASP:H	2.26	0.42
1:B:448:THR:C	1:B:450:ALA:H	2.28	0.42
1:B:79:PRO:C	1:B:81:LYS:N	2.77	0.41
2:W:70:THR:C	2:W:72:PHE:N	2.77	0.41
1:A:491:HIS:HA	1:A:495:LEU:CB	2.50	0.41
3:Z:45:ARG:O	3:Z:46:ASN:C	2.63	0.41
1:B:284:ILE:O	1:B:285:PHE:C	2.63	0.41
1:B:396:LYS:C	1:B:398:LEU:H	2.27	0.41
1:A:448:THR:C	1:A:450:ALA:H	2.28	0.41
1:B:751:ALA:C	1:B:753:TYR:H	2.29	0.41
3:X:45:ARG:O	3:X:46:ASN:C	2.63	0.41
1:B:698:GLU:C	1:B:700:ILE:N	2.78	0.41
1:B:60:ILE:O	1:B:64:SER:HA	2.21	0.41
3:X:18:PHE:C	3:X:20:PHE:N	2.78	0.41
1:A:26:ALA:O	1:A:27:ALA:C	2.64	0.41
1:A:284:ILE:O	1:A:285:PHE:C	2.63	0.41
1:A:751:ALA:C	1:A:753:TYR:H	2.29	0.41
3:Z:46:ASN:O	3:Z:47:GLU:C	2.64	0.41
2:W:52:ASP:O	2:W:53:ASP:C	2.63	0.41
1:B:242:ARG:O	1:B:267:LEU:HA	2.20	0.41
1:A:780:LYS:O	1:A:781:ILE:C	2.64	0.41
3:Z:128:LEU:C	3:Z:130:ASP:N	2.79	0.41
3:X:28:VAL:O	3:X:63:LEU:N	2.52	0.41
1:A:79:PRO:C	1:A:81:LYS:N	2.77	0.40
1:A:172:CYS:HA	1:A:666:HIS:O	2.21	0.40
1:A:696:VAL:O	1:A:697:LEU:C	2.65	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
1:A:306:SER:C	1:A:308:LEU:N	2.79	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
2:W:23:ALA:O	2:W:24:PHE:C	2.65	0.40
2:Y:70:THR:C	2:Y:72:PHE:N	2.77	0.40
1:A:698:GLU:C	1:A:700:ILE:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	1	16
1	B	750/831 (90%)	606 (81%)	108 (14%)	36 (5%)	2	17
2	W	134/139 (96%)	94 (70%)	34 (25%)	6 (4%)	2	18
2	Y	134/139 (96%)	95 (71%)	33 (25%)	6 (4%)	2	18
3	X	149/152 (98%)	104 (70%)	36 (24%)	9 (6%)	1	14
3	Z	149/152 (98%)	104 (70%)	36 (24%)	9 (6%)	1	14
All	All	2074/2244 (92%)	1609 (78%)	361 (17%)	104 (5%)	1	16

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 oligosaccharides 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	B	2998	4,6	0,4,4	-	-	-		
6	ADP	B	2999	5,4	28,29,29	0.95	1 (3%)	43,45,45	0.84	1 (2%)
6	ADP	A	1999	5,4	28,29,29	0.95	0	43,45,45	0.84	1 (2%)
5	VO4	A	1998	4,6	0,4,4	-	-	-		

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	5,4	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	1999	5,4	-	3/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2999	ADP	C2'-N1	2.01	1.37	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1999	ADP	C2'-C3'-C4'	-2.13	98.49	102.61
6	B	2999	ADP	C2'-C3'-C4'	-2.13	98.50	102.61

There are no chirality outliers.

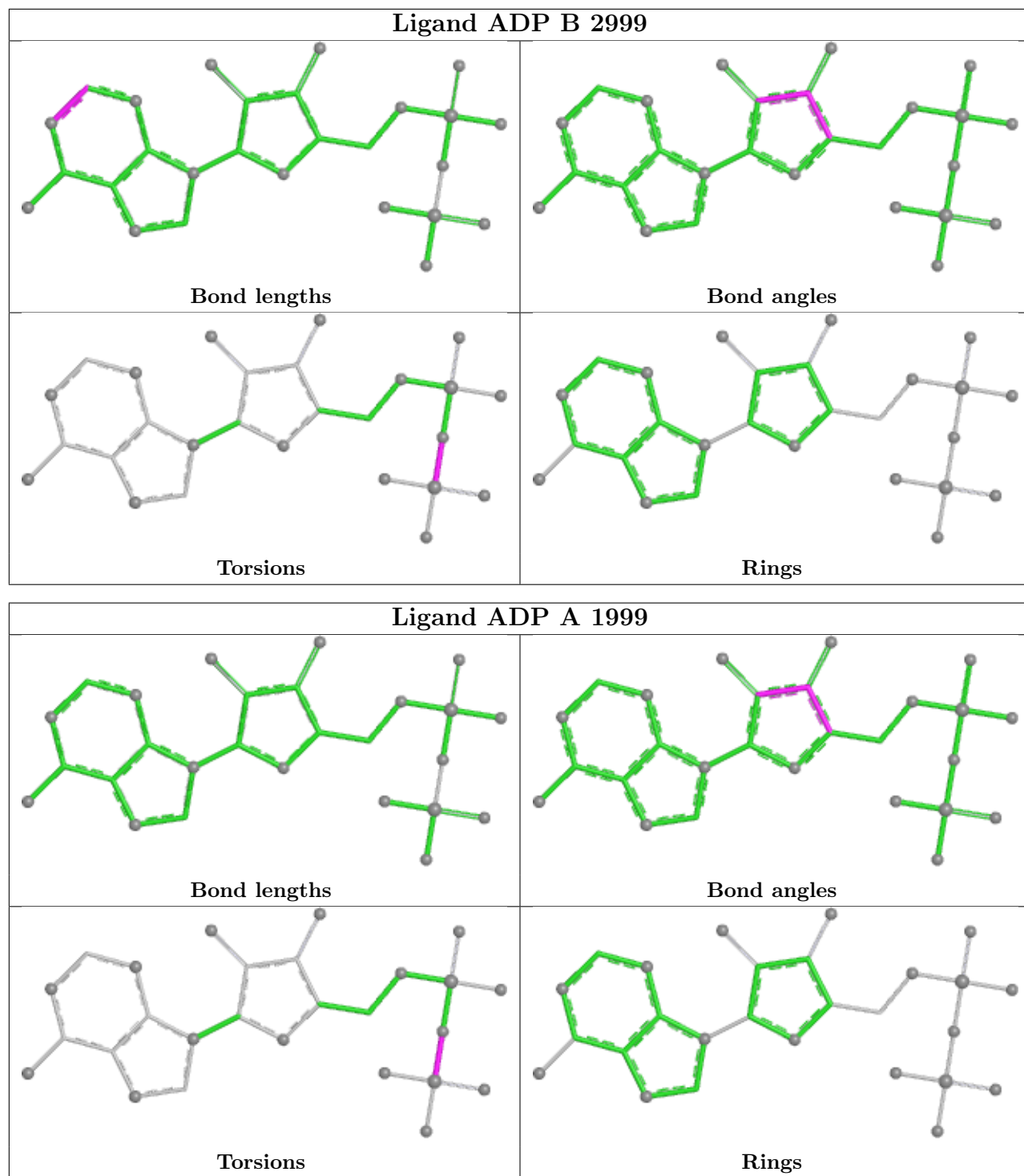
All (6) torsion outliers are listed below:

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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
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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.