



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:20 PM UTC

PDB ID : 1EV1 / pdb_00001ev1
Title : ECHOVIRUS 1
Authors : Wien, M.W.; Filman, D.J.; Hogle, J.M.
Deposited on : 1997-12-02
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

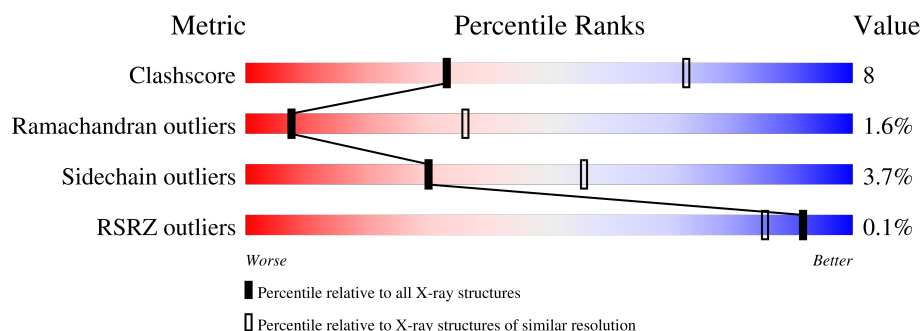
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	1	281	
2	2	254	
3	3	239	
4	4	68	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6575 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 ECHOVIRUS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	281	Total	C	N	O	S	0	0	0
			2227	1402	394	422	9			

- Molecule 2 is a protein called ECHOVIRUS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	254	Total	C	N	O	S	0	0	0
			1977	1250	336	376	15			

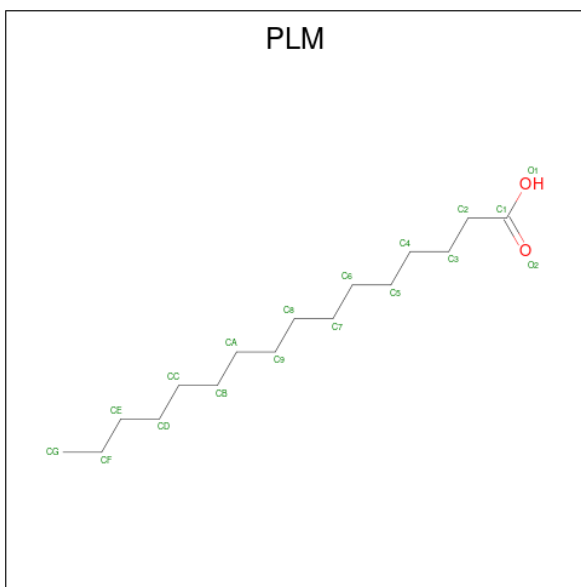
- Molecule 3 is a protein called ECHOVIRUS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	239	Total	C	N	O	S	0	0	0
			1849	1169	304	355	21			

- Molecule 4 is a protein called ECHOVIRUS 1.

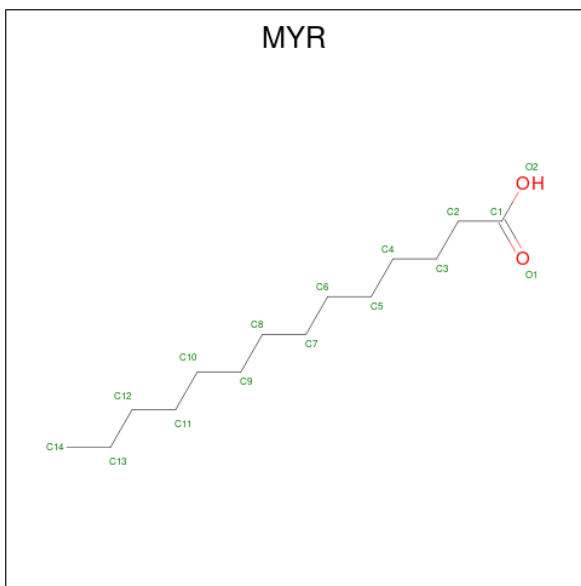
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	61	Total	C	N	O	S	0	0	0
			475	294	82	97	2			

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1	1	Total	C	O	0	0
			18	16	2		

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	4	1	Total	C	O	0	0
			15	14	1		

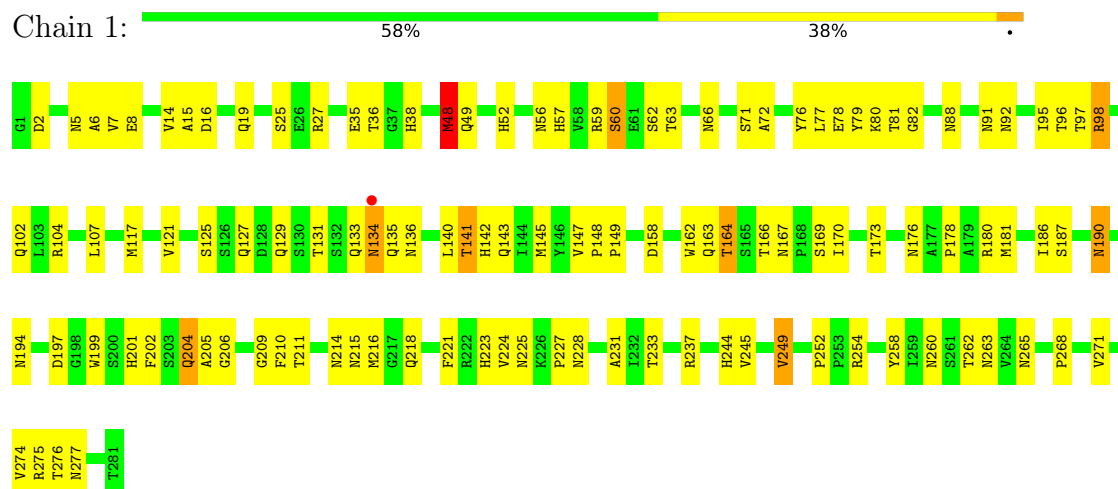
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	8	Total 8	O 8	3	0
7	2	3	Total 3	O 3	0	0
7	3	2	Total 2	O 2	0	0
7	4	1	Total 1	O 1	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

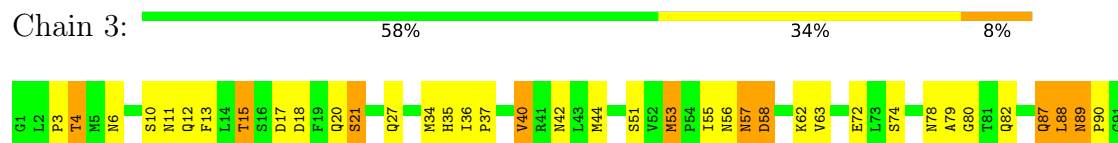
• Molecule 1: ECHOVIRUS 1

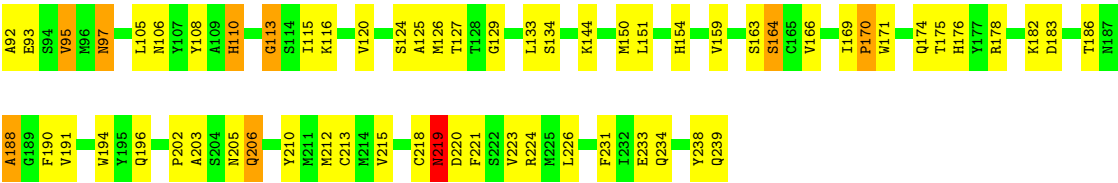


• Molecule 2: ECHOVIRUS 1

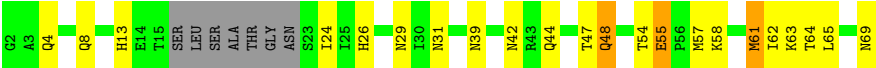


• Molecule 3: ECHOVIRUS 1





● Molecule 4: ECHOVIRUS 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	472.15Å 483.20Å 352.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 50.00 – 3.56	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.55) 45.6 (50.00-3.56)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 3.56Å)	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.263 , (Not available) 0.543 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.07	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3615e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, PLM

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	1	0.99	11/2286 (0.5%)	2.06	86/3123 (2.8%)
2	2	0.98	11/2034 (0.5%)	1.94	75/2781 (2.7%)
3	3	0.93	6/1897 (0.3%)	1.97	70/2579 (2.7%)
4	4	0.97	2/483 (0.4%)	2.03	19/651 (2.9%)
All	All	0.97	30/6700 (0.4%)	2.00	250/9134 (2.7%)

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	1	0	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	35	HIS	CD2-NE2	-7.48	1.29	1.37
1	1	244	HIS	CD2-NE2	-7.37	1.29	1.37
1	1	134	ASN	CG-OD1	7.23	1.37	1.23
1	1	57	HIS	CD2-NE2	-6.88	1.30	1.37
1	1	38	HIS	CD2-NE2	-6.73	1.30	1.37
3	3	154	HIS	CD2-NE2	-6.71	1.30	1.37
2	2	216	HIS	CD2-NE2	-6.66	1.30	1.37
3	3	110	HIS	CD2-NE2	-6.53	1.30	1.37
1	1	142	HIS	CD2-NE2	-6.52	1.30	1.37
3	3	176	HIS	CD2-NE2	-6.44	1.30	1.37
2	2	187	HIS	CD2-NE2	-6.41	1.30	1.37
1	1	52	HIS	CD2-NE2	-6.37	1.30	1.37
2	2	99	HIS	CD2-NE2	-6.27	1.30	1.37
4	4	26	HIS	CD2-NE2	-6.14	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	109	HIS	CD2-NE2	-6.10	1.31	1.37
2	2	260	HIS	CD2-NE2	-6.07	1.31	1.37
2	2	164	HIS	CD2-NE2	-5.82	1.31	1.37
1	1	201	HIS	CD2-NE2	-5.81	1.31	1.37
2	2	164	HIS	CG-ND1	-5.68	1.31	1.38
2	2	118	HIS	CD2-NE2	-5.67	1.31	1.37
1	1	38	HIS	CG-ND1	-5.57	1.32	1.38
2	2	145	HIS	CD2-NE2	-5.55	1.31	1.37
4	4	13	HIS	CD2-NE2	-5.53	1.31	1.37
1	1	223	HIS	CD2-NE2	-5.50	1.31	1.37
2	2	217	HIS	CD2-NE2	-5.47	1.31	1.37
3	3	4	THR	CB-OG1	5.46	1.52	1.43
1	1	244	HIS	CG-ND1	-5.40	1.32	1.38
3	3	4	THR	CA-CB	5.18	1.61	1.53
2	2	99	HIS	CG-ND1	-5.13	1.32	1.38
1	1	57	HIS	CG-ND1	-5.04	1.32	1.38

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	134	ASN	OD1-CG-ND2	13.54	136.14	122.60
1	1	134	ASN	CB-CG-ND2	-13.02	96.88	116.40
1	1	136	ASN	OD1-CG-ND2	-12.21	110.39	122.60
3	3	219	ASN	OD1-CG-ND2	-10.15	112.45	122.60
4	4	29	ASN	OD1-CG-ND2	-9.53	113.07	122.60
4	4	31	ASN	OD1-CG-ND2	-9.51	113.09	122.60
2	2	261	GLN	OE1-CD-NE2	-9.41	113.19	122.60
3	3	58	ASP	N-CA-C	9.33	122.62	111.33
1	1	134	ASN	N-CA-C	9.31	123.90	112.54
1	1	205	ALA	N-CA-C	9.30	120.17	108.45
3	3	82	GLN	OE1-CD-NE2	-9.28	113.32	122.60
3	3	17	ASP	CA-CB-CG	9.23	121.83	112.60
3	3	206	GLN	OE1-CD-NE2	-9.14	113.46	122.60
1	1	263	ASN	OD1-CG-ND2	-9.12	113.48	122.60
1	1	135	GLN	N-CA-C	9.08	123.63	110.10
1	1	91	ASN	OD1-CG-ND2	-9.05	113.55	122.60
1	1	102	GLN	OE1-CD-NE2	-9.04	113.56	122.60
3	3	42	ASN	OD1-CG-ND2	-8.96	113.64	122.60
2	2	70	GLN	OE1-CD-NE2	-8.44	114.16	122.60
1	1	19	GLN	OE1-CD-NE2	-8.34	114.26	122.60
1	1	245	VAL	N-CA-C	8.29	120.28	109.58
2	2	172	ASN	OD1-CG-ND2	-8.24	114.36	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	134	ASN	O-C-N	8.08	133.25	122.43
2	2	253	ASN	OD1-CG-ND2	-8.04	114.56	122.60
3	3	35	HIS	N-CA-C	7.99	119.77	111.14
4	4	4	GLN	OE1-CD-NE2	-7.98	114.62	122.60
2	2	52	GLN	OE1-CD-NE2	-7.95	114.65	122.60
2	2	63	PHE	N-CA-C	7.91	121.83	108.23
1	1	215	ASN	OD1-CG-ND2	-7.84	114.76	122.60
3	3	239	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	1	204	GLN	OE1-CD-NE2	-7.78	114.82	122.60
2	2	181	ASN	OD1-CG-ND2	-7.78	114.82	122.60
4	4	24	ILE	N-CA-C	7.71	119.75	107.73
2	2	26	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	1	57	HIS	CB-CG-CD2	-7.58	121.35	131.20
2	2	37	GLU	N-CA-C	7.54	120.80	108.52
2	2	125	VAL	N-CA-C	7.47	119.59	108.46
1	1	56	ASN	OD1-CG-ND2	-7.45	115.15	122.60
3	3	6	ASN	CB-CG-ND2	7.42	127.53	116.40
3	3	154	HIS	N-CA-C	7.36	120.55	108.99
4	4	69	ASN	OD1-CG-ND2	-7.33	115.27	122.60
3	3	57	ASN	N-CA-CB	-7.26	99.94	110.47
1	1	218	GLN	N-CA-C	7.22	120.04	109.07
3	3	97	ASN	OD1-CG-ND2	-7.22	115.38	122.60
3	3	219	ASN	CB-CG-ND2	7.12	127.08	116.40
1	1	25	SER	N-CA-C	7.12	117.99	108.38
3	3	213	CYS	N-CA-C	7.09	119.97	108.41
1	1	197	ASP	CA-CB-CG	7.03	119.63	112.60
2	2	136	GLN	OE1-CD-NE2	-7.00	115.60	122.60
2	2	55	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	1	167	ASN	OD1-CG-ND2	-6.96	115.64	122.60
3	3	12	GLN	OE1-CD-NE2	-6.96	115.64	122.60
3	3	163	SER	N-CA-C	6.95	119.73	111.33
1	1	218	GLN	OE1-CD-NE2	-6.94	115.66	122.60
3	3	134	SER	N-CA-C	6.91	120.94	109.95
2	2	206	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	1	194	ASN	OD1-CG-ND2	-6.88	115.72	122.60
2	2	50	GLU	N-CA-C	6.88	121.12	112.87
1	1	190	ASN	OD1-CG-ND2	-6.87	115.73	122.60
3	3	27	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	1	187	SER	N-CA-C	6.83	119.55	110.53
3	3	106	ASN	OD1-CG-ND2	-6.81	115.79	122.60
2	2	215	ARG	CB-CG-CD	-6.81	95.64	111.30
4	4	42	ASN	OD1-CG-ND2	-6.79	115.81	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	191	ASN	OD1-CG-ND2	-6.78	115.83	122.60
3	3	234	GLN	OE1-CD-NE2	-6.78	115.82	122.60
2	2	81	LYS	N-CA-C	6.72	119.47	108.52
3	3	171	TRP	CG-CD2-CE3	6.70	140.60	133.90
1	1	15	ALA	N-CA-C	6.69	120.39	109.76
3	3	10	SER	N-CA-C	6.67	120.30	110.30
2	2	73	ASN	OD1-CG-ND2	-6.63	115.97	122.60
2	2	195	ASN	OD1-CG-ND2	-6.62	115.98	122.60
3	3	106	ASN	CA-CB-CG	-6.61	105.99	112.60
3	3	110	HIS	CA-CB-CG	6.59	120.39	113.80
2	2	208	VAL	N-CA-CB	-6.59	101.98	111.21
2	2	45	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	1	210	PHE	N-CA-C	6.55	120.13	111.75
2	2	175	MET	N-CA-C	6.52	118.76	110.61
1	1	214	ASN	OD1-CG-ND2	-6.51	116.09	122.60
2	2	68	SER	N-CA-C	6.49	119.89	110.28
2	2	41	TYR	N-CA-C	6.49	119.65	110.50
1	1	260	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	1	223	HIS	CB-CG-CD2	-6.47	122.78	131.20
1	1	225	ASN	N-CA-C	6.47	119.37	110.24
3	3	169	ILE	N-CA-C	6.46	113.44	107.56
4	4	31	ASN	CB-CG-ND2	6.41	126.02	116.40
3	3	183	ASP	CA-CB-CG	6.41	119.01	112.60
3	3	205	ASN	OD1-CG-ND2	-6.41	116.19	122.60
3	3	21	SER	O-C-N	-6.38	116.31	121.80
1	1	134	ASN	CA-C-N	6.38	129.81	120.82
1	1	134	ASN	C-N-CA	6.38	129.81	120.82
2	2	113	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	1	228	ASN	OD1-CG-ND2	-6.36	116.24	122.60
2	2	30	ASN	CA-CB-CG	6.34	118.94	112.60
1	1	6	ALA	N-CA-C	6.33	118.99	111.33
1	1	5	ASN	OD1-CG-ND2	-6.33	116.27	122.60
4	4	63	LYS	N-CA-C	6.32	118.97	111.33
1	1	66	ASN	OD1-CG-ND2	-6.29	116.31	122.60
3	3	113	GLY	N-CA-C	6.29	118.45	112.04
4	4	39	ASN	N-CA-C	6.26	118.79	110.53
2	2	9	TYR	N-CA-C	6.24	124.09	110.80
3	3	82	GLN	CG-CD-NE2	6.22	125.74	116.40
2	2	260	HIS	CA-C-N	6.22	132.89	121.70
2	2	260	HIS	C-N-CA	6.22	132.89	121.70
2	2	127	VAL	N-CA-C	6.19	113.19	107.56
1	1	163	GLN	OE1-CD-NE2	-6.17	116.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	217	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	1	88	ASN	OD1-CG-ND2	-6.14	116.46	122.60
4	4	8	GLN	OE1-CD-NE2	-6.12	116.48	122.60
2	2	119	GLN	OE1-CD-NE2	-6.10	116.50	122.60
2	2	172	ASN	CB-CG-ND2	6.10	125.55	116.40
3	3	97	ASN	N-CA-C	6.10	121.43	111.37
3	3	210	TYR	N-CA-C	6.09	119.41	109.24
1	1	209	GLY	N-CA-C	6.08	120.68	112.17
3	3	120	VAL	N-CA-C	6.06	116.65	108.17
3	3	176	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	1	201	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	1	277	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	1	49	GLN	OE1-CD-NE2	-6.00	116.60	122.60
2	2	187	HIS	N-CA-C	6.00	118.18	109.07
2	2	142	ASN	OD1-CG-ND2	-5.96	116.64	122.60
4	4	13	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	1	133	GLN	OE1-CD-NE2	-5.96	116.64	122.60
3	3	53	MET	N-CA-C	5.95	118.24	109.50
3	3	166	VAL	N-CA-C	5.95	116.50	108.17
3	3	72	GLU	N-CA-C	5.94	118.34	109.25
3	3	56	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	1	102	GLN	N-CA-C	5.89	117.57	111.03
2	2	43	SER	N-CA-C	5.89	119.19	110.48
2	2	212	ASN	OD1-CG-ND2	-5.87	116.73	122.60
2	2	188	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	1	143	GLN	OE1-CD-NE2	-5.86	116.75	122.60
1	1	186	ILE	N-CA-C	5.86	120.20	112.76
3	3	97	ASN	CB-CG-ND2	5.83	125.15	116.40
3	3	78	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	1	72	ALA	N-CA-C	5.75	119.43	110.17
1	1	92	ASN	OD1-CG-ND2	-5.75	116.85	122.60
2	2	47	ALA	N-CA-C	5.75	118.11	110.53
3	3	234	GLN	CG-CD-NE2	5.72	124.98	116.40
1	1	231	ALA	N-CA-C	5.71	118.12	110.35
3	3	40	VAL	CB-CA-C	-5.69	104.07	110.96
1	1	129	GLN	OE1-CD-NE2	-5.67	116.93	122.60
3	3	164	SER	N-CA-C	5.65	118.68	109.24
2	2	11	ASP	CA-CB-CG	5.65	118.25	112.60
1	1	265	ASN	N-CA-C	5.64	118.45	110.50
2	2	152	ALA	N-CA-C	5.63	118.74	110.30
3	3	188	ALA	N-CA-C	5.62	120.12	112.88
1	1	147	VAL	CA-C-N	5.61	123.76	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	147	VAL	C-N-CA	5.61	123.76	119.66
2	2	161	ALA	N-CA-C	5.58	117.33	108.79
2	2	235	ALA	N-CA-C	5.58	116.41	108.54
1	1	136	ASN	CB-CG-ND2	5.57	124.76	116.40
1	1	263	ASN	CB-CG-ND2	5.57	124.75	116.40
2	2	157	THR	CA-C-O	5.57	126.36	119.79
2	2	218	ASN	OD1-CG-ND2	-5.55	117.05	122.60
3	3	144	LYS	N-CA-C	5.54	118.25	111.82
1	1	78	GLU	N-CA-C	5.54	118.43	109.40
1	1	127	GLN	OE1-CD-NE2	-5.54	117.06	122.60
2	2	195	ASN	N-CA-C	5.54	117.61	109.24
3	3	154	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	1	262	THR	N-CA-C	5.50	117.35	111.36
3	3	219	ASN	N-CA-C	5.50	122.51	110.80
1	1	140	LEU	N-CA-C	5.48	117.67	108.96
1	1	135	GLN	OE1-CD-NE2	-5.48	117.12	122.60
3	3	106	ASN	N-CA-C	5.48	119.71	113.19
3	3	190	PHE	N-CA-C	5.47	118.00	108.76
1	1	176	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	1	63	THR	CA-CB-OG1	-5.46	101.41	109.60
2	2	109	HIS	CB-CG-CD2	-5.46	124.11	131.20
3	3	11	ASN	OD1-CG-ND2	-5.46	117.14	122.60
3	3	57	ASN	N-CA-C	5.45	119.56	113.02
1	1	199	TRP	CE2-CD2-CG	-5.45	100.66	107.20
3	3	15	THR	CA-CB-OG1	-5.44	101.44	109.60
1	1	158	ASP	CA-CB-CG	5.41	118.01	112.60
3	3	95	VAL	N-CA-C	5.40	115.60	110.42
3	3	171	TRP	CE2-CD2-CG	-5.40	100.72	107.20
4	4	55	GLU	O-C-N	-5.39	116.67	121.20
2	2	213	MET	N-CA-C	5.38	117.90	111.71
3	3	4	THR	O-C-N	-5.38	117.04	123.06
2	2	75	SER	CA-C-N	5.37	124.70	118.85
2	2	75	SER	C-N-CA	5.37	124.70	118.85
3	3	233	GLU	N-CA-C	5.37	117.23	109.07
1	1	96	THR	N-CA-C	5.36	117.23	108.55
4	4	61	MET	N-CA-C	5.35	117.41	107.99
1	1	8	GLU	CA-CB-CG	-5.34	103.41	114.10
3	3	169	ILE	CA-C-N	5.34	125.11	119.76
3	3	169	ILE	C-N-CA	5.34	125.11	119.76
2	2	44	ASP	N-CA-C	5.34	119.28	112.34
1	1	82	GLY	N-CA-C	5.33	120.18	111.27
1	1	125	SER	N-CA-C	5.33	118.25	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	143	TYR	N-CA-C	5.30	120.12	111.37
3	3	18	ASP	CA-CB-CG	5.30	117.90	112.60
1	1	16	ASP	N-CA-C	5.30	117.97	110.50
3	3	87	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	1	38	HIS	CB-CG-CD2	-5.29	124.33	131.20
2	2	70	GLN	CG-CD-NE2	5.28	124.33	116.40
2	2	171	TRP	CE2-CD2-CG	-5.28	100.87	107.20
4	4	26	HIS	CB-CG-CD2	-5.27	124.35	131.20
4	4	29	ASN	CB-CG-ND2	5.26	124.30	116.40
1	1	265	ASN	OD1-CG-ND2	-5.25	117.35	122.60
2	2	162	GLU	N-CA-C	5.25	117.48	110.35
2	2	111	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	1	98	ARG	N-CA-C	5.23	119.53	113.20
2	2	261	GLN	CG-CD-NE2	5.23	124.25	116.40
1	1	180	ARG	N-CA-C	5.23	117.94	108.69
1	1	95	ILE	N-CA-C	5.22	115.98	108.93
3	3	89	ASN	OD1-CG-ND2	-5.22	117.38	122.60
4	4	44	GLN	N-CA-C	5.21	118.66	112.72
2	2	132	MET	N-CA-C	5.21	118.60	110.32
3	3	196	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	1	162	TRP	CG-CD2-CE3	5.20	139.10	133.90
2	2	122	ILE	N-CA-C	5.19	116.05	108.53
1	1	206	GLY	O-C-N	-5.19	119.21	123.41
4	4	47	THR	CA-CB-OG1	-5.19	101.82	109.60
1	1	148	PRO	N-CA-C	5.18	115.44	110.47
3	3	127	THR	O-C-N	-5.17	117.12	122.96
3	3	171	TRP	CB-CG-CD1	-5.17	119.15	126.90
2	2	215	ARG	N-CA-C	5.16	117.58	111.33
1	1	79	TYR	N-CA-C	5.16	116.78	108.32
2	2	196	ASN	OD1-CG-ND2	-5.16	117.44	122.60
2	2	52	GLN	CG-CD-NE2	5.16	124.14	116.40
3	3	116	LYS	CG-CD-CE	-5.16	99.44	111.30
2	2	147	SER	N-CA-C	5.15	117.75	108.48
1	1	141	THR	O-C-N	-5.15	117.30	123.06
1	1	7	VAL	N-CA-CB	-5.14	102.75	111.23
2	2	156	THR	N-CA-C	5.14	117.86	109.59
2	2	82	PHE	N-CA-C	5.12	117.73	110.40
3	3	218	CYS	O-C-N	-5.11	117.02	122.85
2	2	78	TRP	CE2-CD2-CG	-5.11	101.07	107.20
3	3	20	GLN	OE1-CD-NE2	-5.11	117.49	122.60
4	4	48	GLN	N-CA-C	5.11	116.60	108.79
2	2	64	TYR	N-CA-C	5.10	116.62	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	154	ARG	N-CA-C	5.10	118.53	109.96
3	3	194	TRP	CE2-CD2-CG	-5.10	101.08	107.20
4	4	55	GLU	N-CA-C	5.09	116.88	109.30
2	2	88	ASP	CA-CB-CG	-5.08	107.52	112.60
1	1	121	VAL	N-CA-C	5.07	115.27	107.77
1	1	117	MET	N-CA-C	5.06	117.67	109.06
2	2	73	ASN	CB-CG-ND2	5.05	123.98	116.40
1	1	164	THR	N-CA-C	5.05	118.36	111.39
2	2	192	LEU	N-CA-C	5.05	118.91	112.34
3	3	74	SER	N-CA-C	5.05	117.06	109.23
3	3	170	PRO	N-CA-CB	5.05	108.03	103.34
1	1	48	MET	CB-CA-C	-5.04	99.87	109.66
2	2	44	ASP	CA-CB-CG	5.04	117.64	112.60
2	2	259	GLY	N-CA-C	5.04	125.12	113.18
1	1	2	ASP	CA-CB-CG	5.04	117.64	112.60
2	2	106	TYR	N-CA-C	5.03	117.35	108.75
1	1	216	MET	N-CA-C	5.02	119.49	113.17
2	2	163	ASP	N-CA-C	5.01	121.46	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	134	ASN	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	1	2227	0	2161	37	0
2	2	1977	0	1861	43	0
3	3	1849	0	1781	43	0
4	4	475	0	456	8	0
5	1	18	0	31	0	0
6	4	15	0	27	0	0
7	1	8	0	0	0	0
7	2	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	3	2	0	0	0	0
7	4	1	0	0	0	0
All	All	6575	0	6317	100	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 8.

All (100) 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)
1:1:141:THR:HG22	1:1:173:THR:HG22	1.68	0.74
1:1:48:MET:SD	3:3:170:PRO:HG3	2.30	0.72
1:1:36:THR:HG21	4:4:61:MET:SD	2.31	0.71
2:2:226:PHE:HB3	3:3:212:MET:HE1	1.73	0.70
2:2:193:ARG:HA	3:3:125:ALA:HB2	1.74	0.69
3:3:174:GLN:HG3	3:3:175:THR:HG23	1.74	0.67
2:2:142:ASN:HD21	2:2:144:GLU:HG2	1.59	0.67
2:2:183:THR:HG21	3:3:51:SER:HA	1.76	0.67
2:2:155:PHE:HB3	2:2:170:VAL:HG22	1.78	0.66
1:1:164:THR:HG21	1:1:169:SER:OG	2.00	0.62
2:2:156:THR:HG22	2:2:168:ALA:HB3	1.82	0.62
2:2:103:ARG:HB2	2:2:210:MET:HG2	1.83	0.61
2:2:205:VAL:HG22	3:3:37:PRO:HG2	1.82	0.60
3:3:53:MET:HE2	3:3:215:VAL:HB	1.83	0.60
2:2:96:MET:HE3	2:2:213:MET:HB3	1.83	0.59
2:2:108:ILE:HD12	2:2:126:CYS:SG	2.42	0.58
3:3:58:ASP:HB2	3:3:62:LYS:HD3	1.86	0.57
4:4:62:ILE:HB	4:4:65:LEU:HD12	1.86	0.57
2:2:116:LYS:HA	3:3:125:ALA:HB3	1.88	0.56
1:1:59:ARG:HD2	4:4:48:GLN:HE22	1.71	0.56
1:1:274:VAL:HG22	3:3:63:VAL:HG21	1.87	0.56
2:2:156:THR:O	2:2:169:ALA:HA	2.06	0.55
2:2:66:LEU:HD23	2:2:89:MET:HE2	1.89	0.55
2:2:116:LYS:HB2	3:3:126:MET:HE2	1.89	0.55
2:2:257:LEU:H	2:2:257:LEU:HD23	1.72	0.54
3:3:89:ASN:HD21	3:3:182:LYS:HE2	1.73	0.54
2:2:135:ALA:HA	2:2:167:GLN:HB2	1.89	0.53
1:1:178:PRO:HG2	3:3:13:PHE:HB2	1.90	0.52
2:2:60:THR:HG23	2:2:92:PHE:HD1	1.73	0.52
1:1:141:THR:HG22	1:1:173:THR:CG2	2.38	0.52
2:2:69:VAL:HG21	2:2:78:TRP:NE1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:254:ARG:HH21	1:1:258:TYR:HA	1.74	0.52
1:1:275:ARG:HE	3:3:57:ASN:HB3	1.75	0.52
3:3:150:MET:HE2	3:3:151:LEU:HG	1.91	0.52
1:1:170:ILE:HD11	1:1:181:MET:HG3	1.91	0.52
1:1:145:MET:SD	1:1:164:THR:CG2	2.98	0.51
3:3:55:ILE:HG12	3:3:95:VAL:HG13	1.93	0.51
4:4:54:THR:HG23	4:4:55:GLU:HG3	1.94	0.50
2:2:31:VAL:HG13	4:4:58:LYS:HB3	1.93	0.50
1:1:36:THR:HG22	4:4:57:MET:SD	2.52	0.50
1:1:97:THR:HG21	1:1:107:LEU:HD12	1.94	0.50
1:1:62:SER:HA	3:3:108:TYR:OH	2.12	0.50
1:1:252:PRO:HD3	2:2:184:ILE:HG21	1.92	0.50
3:3:89:ASN:HB3	3:3:92:ALA:HB3	1.94	0.50
3:3:126:MET:HG3	3:3:202:PRO:HG2	1.95	0.49
1:1:145:MET:SD	1:1:164:THR:HG22	2.52	0.49
2:2:80:TRP:CZ2	2:2:152:ALA:HB2	2.48	0.49
3:3:89:ASN:ND2	3:3:182:LYS:HE2	2.27	0.49
3:3:110:HIS:HB2	3:3:224:ARG:HB2	1.96	0.48
2:2:231:PHE:CZ	2:2:237:THR:HA	2.50	0.47
3:3:108:TYR:CE2	3:3:226:LEU:HD13	2.50	0.46
2:2:155:PHE:HA	2:2:168:ALA:HB1	1.97	0.46
2:2:40:GLU:HA	2:2:249:CYS:SG	2.56	0.46
1:1:76:TYR:HB3	1:1:237:ARG:HG2	1.97	0.46
2:2:37:GLU:O	2:2:203:PRO:HG3	2.16	0.46
3:3:87:GLN:HG3	3:3:89:ASN:ND2	2.31	0.45
1:1:14:VAL:HG13	3:3:220:ASP:HA	1.98	0.45
3:3:90:PRO:HG3	3:3:115:ILE:HD11	1.98	0.45
3:3:97:ASN:ND2	3:3:231:PHE:HZ	2.14	0.45
2:2:172:ASN:HA	2:2:177:VAL:O	2.16	0.45
1:1:80:LYS:HE2	1:1:233:THR:OG1	2.18	0.44
1:1:190:ASN:HD22	3:3:34:MET:HB3	1.81	0.44
2:2:142:ASN:ND2	2:2:144:GLU:HG2	2.30	0.44
1:1:35:GLU:HA	2:2:189:TRP:HB2	1.99	0.44
1:1:71:SER:O	3:3:15:THR:HG23	2.18	0.44
2:2:69:VAL:HG21	2:2:78:TRP:CD1	2.52	0.44
1:1:190:ASN:ND2	3:3:34:MET:HB3	2.33	0.44
2:2:209:PRO:HA	3:3:34:MET:HE1	1.98	0.44
1:1:27:ARG:HB2	4:4:64:THR:HB	2.00	0.44
1:1:97:THR:CG2	1:1:107:LEU:HD12	2.48	0.44
1:1:14:VAL:CG1	3:3:220:ASP:HA	2.48	0.44
2:2:16:ILE:HD12	2:2:23:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:126:MET:HG3	3:3:202:PRO:CG	2.47	0.44
2:2:117:PHE:CE2	3:3:126:MET:HE3	2.53	0.43
2:2:145:HIS:HB3	2:2:165:GLY:HA2	1.99	0.43
3:3:93:GLU:O	3:3:97:ASN:HB2	2.18	0.43
1:1:81:THR:HG22	1:1:227:PRO:HA	2.01	0.43
3:3:178:ARG:HG2	3:3:186:THR:HB	2.00	0.43
2:2:27:GLU:HB2	2:2:196:ASN:ND2	2.34	0.43
1:1:141:THR:OG1	1:1:224:VAL:HB	2.18	0.42
2:2:213:MET:HA	2:2:213:MET:HE2	2.01	0.42
1:1:170:ILE:HD11	1:1:181:MET:CG	2.50	0.42
2:2:32:VAL:HG22	4:4:57:MET:HE1	2.02	0.42
2:2:81:LYS:HE3	2:2:146:ILE:HG23	2.02	0.42
1:1:77:LEU:HD23	1:1:221:PHE:CD1	2.55	0.42
3:3:44:MET:HE3	3:3:223:VAL:HG22	2.02	0.42
1:1:258:TYR:HB2	3:3:238:TYR:CZ	2.55	0.41
2:2:116:LYS:CB	3:3:126:MET:HE2	2.50	0.41
3:3:88:LEU:O	3:3:188:ALA:HB3	2.20	0.41
3:3:90:PRO:HB2	3:3:105:LEU:CD1	2.51	0.41
1:1:98:ARG:HA	1:1:104:ARG:HD2	2.02	0.41
1:1:181:MET:HE3	1:1:181:MET:HB2	1.97	0.41
1:1:249:VAL:HG13	2:2:35:TYR:OH	2.21	0.41
1:1:268:PRO:HD3	2:2:167:GLN:NE2	2.36	0.41
3:3:129:GLY:O	3:3:159:VAL:HG12	2.21	0.41
2:2:114:ALA:O	2:2:115:SER:HB3	2.21	0.41
1:1:202:PHE:HA	2:2:215:ARG:HG3	2.02	0.40
2:2:87:ARG:HA	2:2:96:MET:SD	2.61	0.40
3:3:113:GLY:HA3	3:3:221:PHE:HA	2.02	0.40
3:3:206:GLN:HA	3:3:206:GLN:OE1	2.21	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	1	279/281 (99%)	252 (90%)	24 (9%)	3 (1%)	11	43
2	2	252/254 (99%)	215 (85%)	34 (14%)	3 (1%)	10	42
3	3	237/239 (99%)	214 (90%)	16 (7%)	7 (3%)	3	25
4	4	57/68 (84%)	51 (90%)	6 (10%)	0	100	100
All	All	825/842 (98%)	732 (89%)	80 (10%)	13 (2%)	7	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	236	SER
2	2	233	ALA
3	3	36	ILE
3	3	203	ALA
3	3	219	ASN
2	2	9	TYR
3	3	79	ALA
1	1	60	SER
3	3	3	PRO
3	3	88	LEU
1	1	149	PRO
1	1	249	VAL
3	3	80	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	250/250 (100%)	242 (97%)	8 (3%)	34	58
2	2	212/212 (100%)	201 (95%)	11 (5%)	21	48
3	3	208/208 (100%)	200 (96%)	8 (4%)	29	55
4	4	52/57 (91%)	52 (100%)	0	100	100
All	All	722/727 (99%)	695 (96%)	27 (4%)	30	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	48	MET
1	1	60	SER
1	1	131	THR
1	1	166	THR
1	1	204	GLN
1	1	211	THR
1	1	271	VAL
1	1	276	THR
2	2	31	VAL
2	2	45	ASN
2	2	88	ASP
2	2	96	MET
2	2	141	VAL
2	2	142	ASN
2	2	164	HIS
2	2	175	MET
2	2	237	THR
2	2	239	VAL
2	2	261	GLN
3	3	4	THR
3	3	21	SER
3	3	40	VAL
3	3	124	SER
3	3	133	LEU
3	3	164	SER
3	3	191	VAL
3	3	219	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	56	ASN
1	1	92	ASN
1	1	102	GLN
1	1	134	ASN
1	1	176	ASN
1	1	218	GLN
2	2	94	GLN
2	2	261	GLN
3	3	42	ASN
3	3	76	ASN
3	3	89	ASN
3	3	219	ASN

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Mol	Chain	Res	Type
4	4	8	GLN
4	4	31	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	MYR	4	1	4	13,14,15	0.27	0	12,13,15	1.12	2 (16%)
5	PLM	1	0	-	17,17,17	0.65	1 (5%)	17,17,17	1.08	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
6	MYR	4	1	4	-	3/12/12/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	1	0	-	-	2/15/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	0	PLM	O1-C1	-2.13	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	4	1	MYR	C7-C6-C5	-2.61	101.16	114.37
6	4	1	MYR	C12-C11-C10	-2.28	102.84	114.37

There are no chirality outliers.

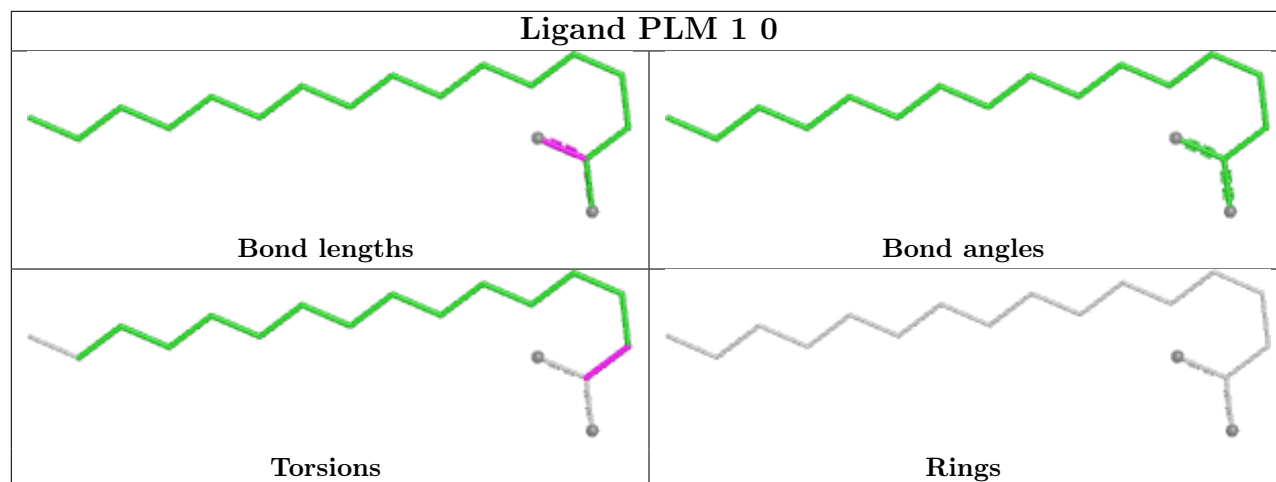
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	4	1	MYR	C1-C2-C3-C4
6	4	1	MYR	C7-C8-C9-C10
6	4	1	MYR	C6-C7-C8-C9
5	1	0	PLM	O1-C1-C2-C3
5	1	0	PLM	O2-C1-C2-C3

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	281/281 (100%)	-0.58	1 (0%) 88 70	15, 15, 15, 15	0
2	2	254/254 (100%)	-0.63	0 100 100	15, 15, 15, 15	0
3	3	239/239 (100%)	-0.57	0 100 100	15, 15, 15, 15	0
4	4	61/68 (89%)	-0.52	0 100 100	15, 15, 15, 15	0
All	All	835/842 (99%)	-0.59	1 (0%) 92 85	15, 15, 15, 15	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	134	ASN	2.3

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

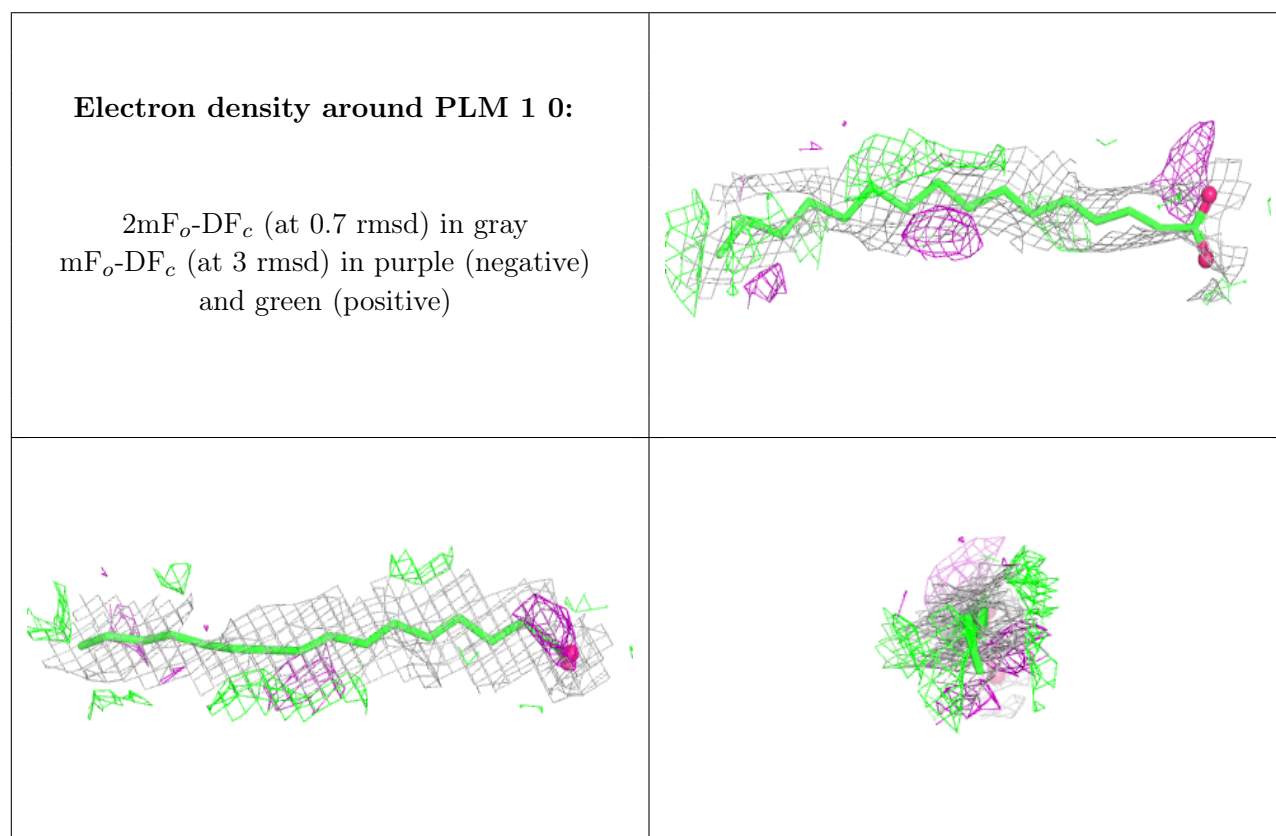
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MYR	4	1	15/16	0.97	0.12	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PLM	1	0	18/18	0.98	0.10	15,15,15,15	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.