



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 2Q3M / pdb_00002q3m
Title : Ensemble refinement of the protein crystal structure of an Arabidopsis thaliana putative steroid sulphotransferase
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-30
Resolution : 1.90 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
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

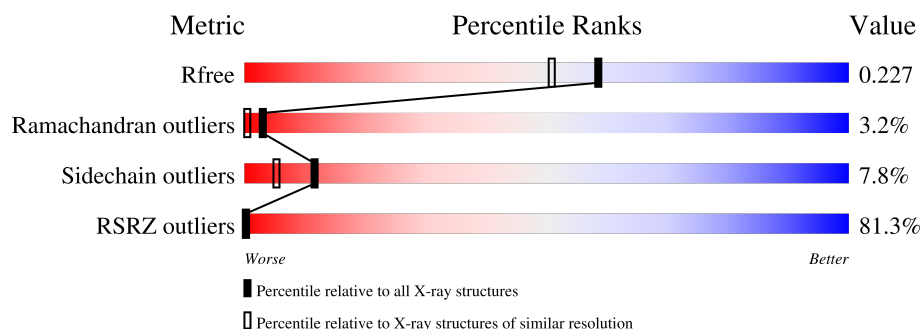
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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-A	326	71% 75% 12% • 13%
1	10-A	326	79% 8% 13%
1	11-A	326	77% 10% 13%
1	12-A	326	79% 8% 13%
1	13-A	326	76% 11% 13%
1	14-A	326	79% 8% 13%
1	15-A	326	79% 9% 13%

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Mol	Chain	Length	Quality of chain
1	16-A	326	 77% 10% 13%
1	2-A	326	 78% 9% 13%
1	3-A	326	 79% 7% 13%
1	4-A	326	 79% 7% 13%
1	5-A	326	 79% 8% 13%
1	6-A	326	 79% 8% 13%
1	7-A	326	 79% 8% 13%
1	8-A	326	 81% 6% 13%
1	9-A	326	 80% 7% 13%

2 Entry composition

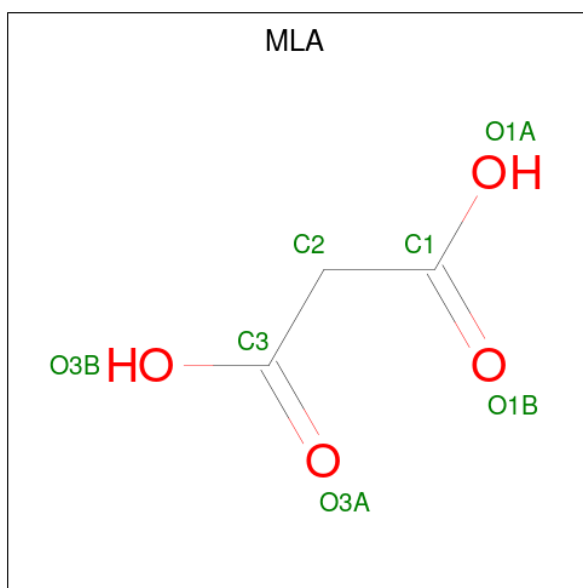
There are 3 unique types of molecules in this entry. The entry contains 40432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Flavonol sulfotransferase-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	2-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	3-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	4-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	5-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	6-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	7-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	8-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	9-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	10-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	11-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	12-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	13-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	14-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	15-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			
1	16-A	284	Total	C	N	O	S	0	0	0
			2306	1496	373	427	10			

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	C	O	0	0
			7	3	4		
2	2-A	1	Total	C	O	0	0
			7	3	4		
2	3-A	1	Total	C	O	0	0
			7	3	4		
2	4-A	1	Total	C	O	0	0
			7	3	4		
2	5-A	1	Total	C	O	0	0
			7	3	4		
2	6-A	1	Total	C	O	0	0
			7	3	4		
2	7-A	1	Total	C	O	0	0
			7	3	4		
2	8-A	1	Total	C	O	0	0
			7	3	4		
2	9-A	1	Total	C	O	0	0
			7	3	4		
2	10-A	1	Total	C	O	0	0
			7	3	4		
2	11-A	1	Total	C	O	0	0
			7	3	4		
2	12-A	1	Total	C	O	0	0
			7	3	4		
2	13-A	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	14-A	1	Total	C	O	0	0
			7	3	4		
2	15-A	1	Total	C	O	0	0
			7	3	4		
2	16-A	1	Total	C	O	0	0
			7	3	4		

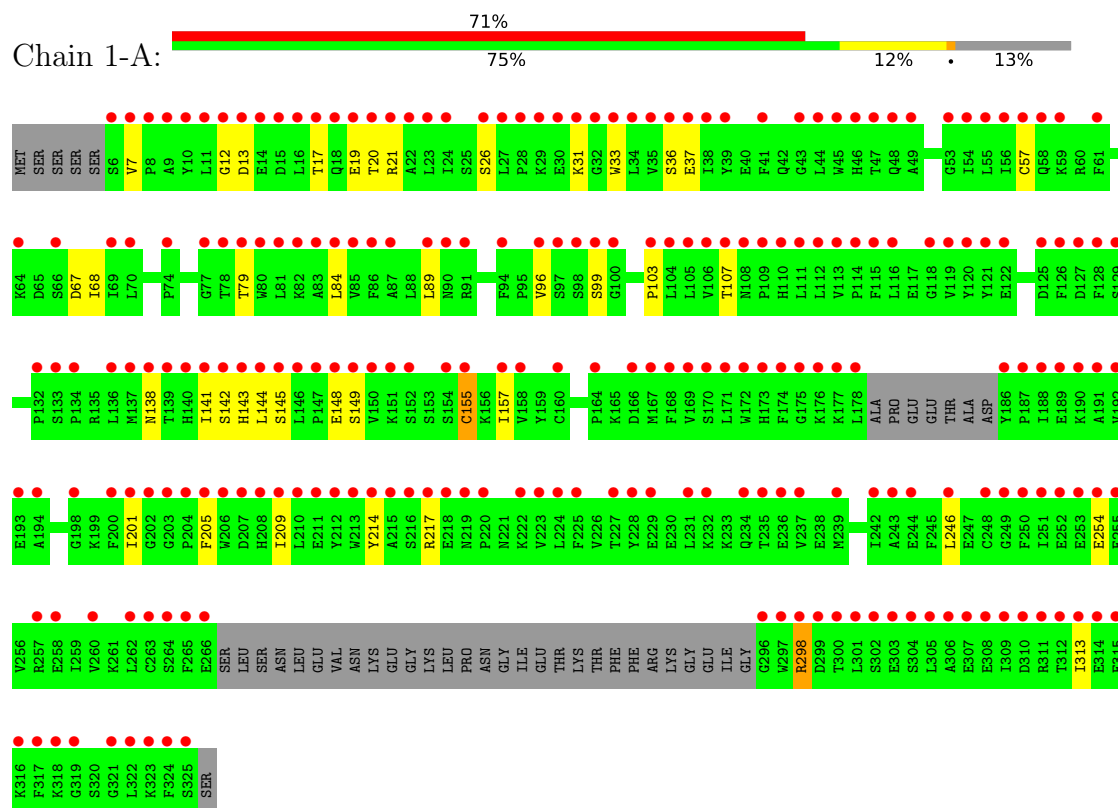
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	214	Total	O	0	0
			214	214		
3	2-A	214	Total	O	0	0
			214	214		
3	3-A	214	Total	O	0	0
			214	214		
3	4-A	214	Total	O	0	0
			214	214		
3	5-A	214	Total	O	0	0
			214	214		
3	6-A	214	Total	O	0	0
			214	214		
3	7-A	214	Total	O	0	0
			214	214		
3	8-A	214	Total	O	0	0
			214	214		
3	9-A	214	Total	O	0	0
			214	214		
3	10-A	214	Total	O	0	0
			214	214		
3	11-A	214	Total	O	0	0
			214	214		
3	12-A	214	Total	O	0	0
			214	214		
3	13-A	214	Total	O	0	0
			214	214		
3	14-A	214	Total	O	0	0
			214	214		
3	15-A	214	Total	O	0	0
			214	214		
3	16-A	214	Total	O	0	0
			214	214		

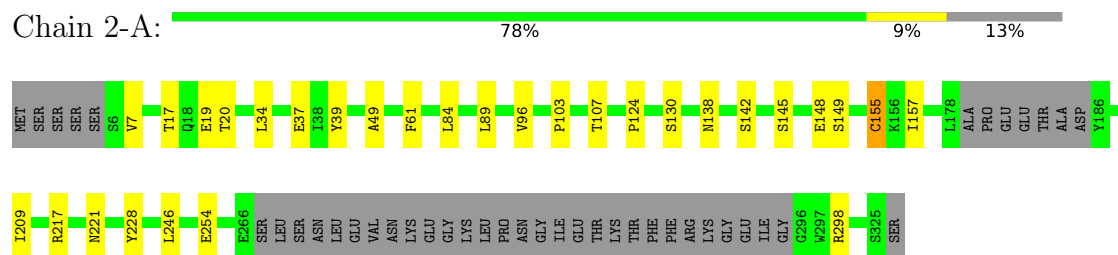
3 Residue-property plots

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.

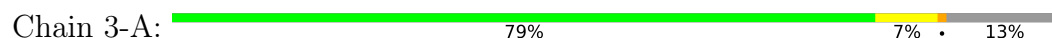
- Molecule 1: Flavonol sulfotransferase-like

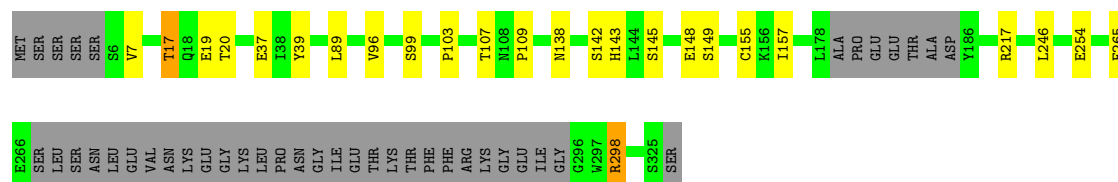


- Molecule 1: Flavonol sulfotransferase-like



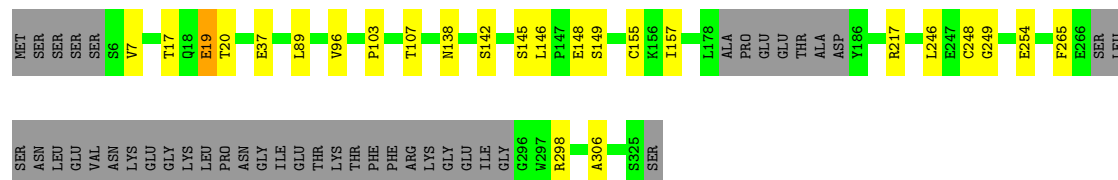
- Molecule 1: Flavonol sulfotransferase-like





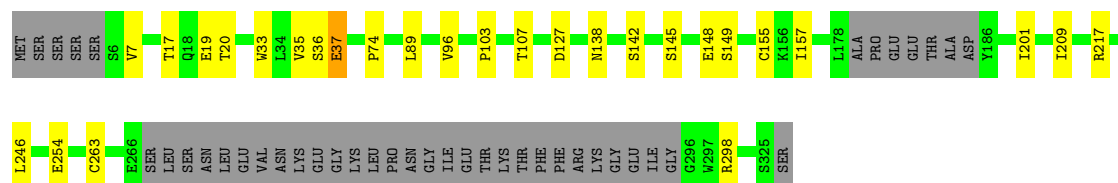
- Molecule 1: Flavonol sulfotransferase-like

Chain 4-A: 79% 7% 13%



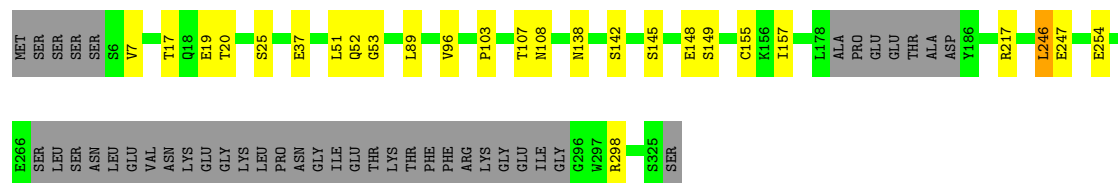
- Molecule 1: Flavonol sulfotransferase-like

Chain 5-A: 79% 8% 13%



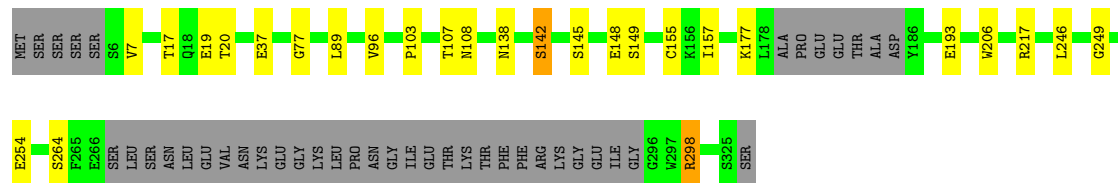
- Molecule 1: Flavonol sulfotransferase-like

Chain 6-A: 79% 8% 13%



- Molecule 1: Flavonol sulfotransferase-like

Chain 7-A: 79% 8% 13%



- Molecule 1: Flavonol sulfotransferase-like

Chain 8-A: 81% 6% 13%

- Molecule 1: Flavonol sulfotransferase-like

Chain 9-A: 80% 7% 13%

- Molecule 1: Flavonol sulfotransferase-like

Chain 10-A:  79% 8% 13%

- Molecule 1: Flavonol sulfotransferase-like

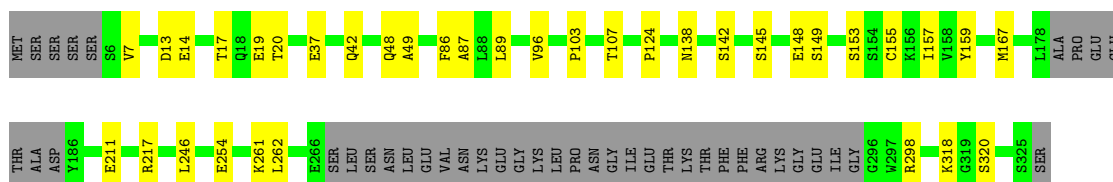
Chain 11-A: 77% 10% 13%

- Molecule 1: Flavonol sulfotransferase-like

Chain 12-A: 

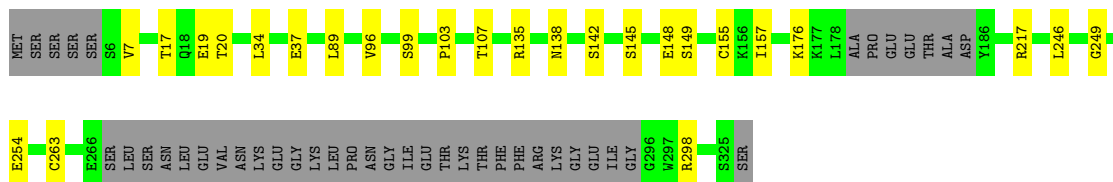
- Molecule 1: Flavonol sulfotransferase-like

Chain 13-A: 



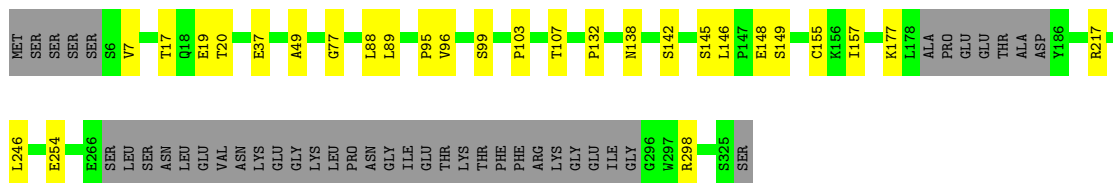
- Molecule 1: Flavonol sulfotransferase-like

Chain 14-A: 79% 8% 13%



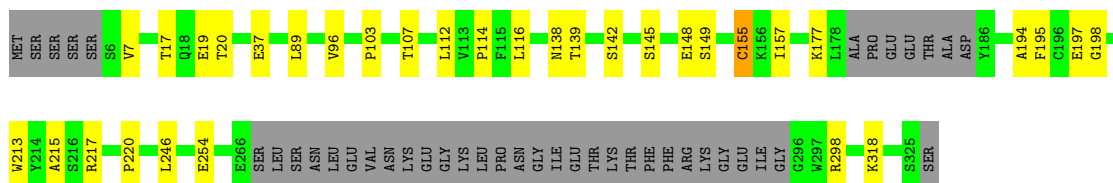
- Molecule 1: Flavonol sulfotransferase-like

Chain 15-A: 79% 9% 13%



- Molecule 1: Flavonol sulfotransferase-like

Chain 16-A: 77% 10% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.48Å 120.90Å 74.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 1.90 19.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.79-1.90) 99.2 (19.79-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.157 , 0.217 0.170 , 0.227	Depositor DCC
R_{free} test set	1654 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	40432	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MLA

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-A	0.25	0/2367	0.26	0/3201
1	2-A	0.25	0/2367	0.26	0/3201
1	3-A	0.25	0/2367	0.26	0/3201
1	4-A	0.25	0/2367	0.26	0/3201
1	5-A	0.25	0/2367	0.26	0/3201
1	6-A	0.25	0/2367	0.26	0/3201
1	7-A	0.25	0/2367	0.26	0/3201
1	8-A	0.25	0/2367	0.26	0/3201
1	9-A	0.25	0/2367	0.26	0/3201
1	10-A	0.25	0/2367	0.26	0/3201
1	11-A	0.25	0/2367	0.26	0/3201
1	12-A	0.25	0/2367	0.26	0/3201
1	13-A	0.25	0/2367	0.26	0/3201
1	14-A	0.25	0/2367	0.26	0/3201
1	15-A	0.25	0/2367	0.26	0/3201
1	16-A	0.25	0/2367	0.26	0/3201
All	All	0.25	0/37872	0.26	0/51216

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-A	0	1
1	2-A	0	1
1	3-A	0	1
1	12-A	0	1
1	13-A	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	214	TYR	Sidechain
1	12-A	120	TYR	Sidechain
1	13-A	159	TYR	Sidechain
1	2-A	39	TYR	Sidechain
1	3-A	39	TYR	Sidechain

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-A	2306	0	2277	0	0
1	2-A	2306	0	2277	0	0
1	3-A	2306	0	2277	0	0
1	4-A	2306	0	2277	0	0
1	5-A	2306	0	2277	0	0
1	6-A	2306	0	2277	0	0
1	7-A	2306	0	2277	0	0
1	8-A	2306	0	2277	0	0
1	9-A	2306	0	2277	0	0
1	10-A	2306	0	2277	0	0
1	11-A	2306	0	2277	0	0
1	12-A	2306	0	2277	0	0
1	13-A	2306	0	2277	0	0
1	14-A	2306	0	2277	0	0
1	15-A	2306	0	2277	0	0
1	16-A	2306	0	2277	0	0
2	1-A	7	0	2	0	0
2	2-A	7	0	2	0	0
2	3-A	7	0	2	0	0
2	4-A	7	0	2	0	0
2	5-A	7	0	2	0	0
2	6-A	7	0	2	0	0
2	7-A	7	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	8-A	7	0	2	0	0
2	9-A	7	0	2	0	0
2	10-A	7	0	2	0	0
2	11-A	7	0	3	0	0
2	12-A	7	0	2	0	0
2	13-A	7	0	2	0	0
2	14-A	7	0	2	0	0
2	15-A	7	0	2	0	0
2	16-A	7	0	2	0	0
3	1-A	214	0	0	0	0
3	2-A	214	0	0	0	0
3	3-A	214	0	0	0	0
3	4-A	214	0	0	0	0
3	5-A	214	0	0	0	0
3	6-A	214	0	0	0	0
3	7-A	214	0	0	0	0
3	8-A	214	0	0	0	0
3	9-A	214	0	0	0	0
3	10-A	214	0	0	0	0
3	11-A	214	0	0	0	0
3	12-A	214	0	0	0	0
3	13-A	214	0	0	0	0
3	14-A	214	0	0	0	0
3	15-A	214	0	0	0	0
3	16-A	214	0	0	0	0
All	All	40432	0	36465	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	278/326 (85%)	217 (78%)	39 (14%)	22 (8%)	1	0
1	2-A	278/326 (85%)	242 (87%)	26 (9%)	10 (4%)	2	0
1	3-A	278/326 (85%)	253 (91%)	19 (7%)	6 (2%)	5	1
1	4-A	278/326 (85%)	258 (93%)	14 (5%)	6 (2%)	5	1
1	5-A	278/326 (85%)	244 (88%)	25 (9%)	9 (3%)	3	0
1	6-A	278/326 (85%)	256 (92%)	15 (5%)	7 (2%)	4	1
1	7-A	278/326 (85%)	252 (91%)	17 (6%)	9 (3%)	3	0
1	8-A	278/326 (85%)	263 (95%)	14 (5%)	1 (0%)	30	22
1	9-A	278/326 (85%)	245 (88%)	28 (10%)	5 (2%)	6	1
1	10-A	278/326 (85%)	239 (86%)	33 (12%)	6 (2%)	5	1
1	11-A	278/326 (85%)	239 (86%)	26 (9%)	13 (5%)	2	0
1	12-A	278/326 (85%)	253 (91%)	19 (7%)	6 (2%)	5	1
1	13-A	278/326 (85%)	238 (86%)	25 (9%)	15 (5%)	1	0
1	14-A	278/326 (85%)	240 (86%)	32 (12%)	6 (2%)	5	1
1	15-A	278/326 (85%)	236 (85%)	34 (12%)	8 (3%)	3	0
1	16-A	278/326 (85%)	240 (86%)	24 (9%)	14 (5%)	1	0
All	All	4448/5216 (85%)	3915 (88%)	390 (9%)	143 (3%)	3	0

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	13	ASP
1	1-A	33	TRP
1	1-A	67	ASP
1	1-A	79	THR
1	1-A	84	LEU
1	1-A	141	ILE
1	1-A	144	LEU
1	1-A	155	CYS
1	1-A	201	ILE
1	1-A	209	ILE
1	2-A	34	LEU
1	2-A	61	PHE
1	2-A	124	PRO
1	2-A	228	TYR
1	3-A	99	SER
1	4-A	306	ALA

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Mol	Chain	Res	Type
1	5-A	37	GLU
1	6-A	51	LEU
1	6-A	247	GLU
1	9-A	210	LEU
1	10-A	61	PHE
1	11-A	99	SER
1	12-A	87	ALA
1	12-A	88	LEU
1	13-A	48	GLN
1	13-A	211	GLU
1	13-A	318	LYS
1	14-A	34	LEU
1	14-A	99	SER
1	14-A	249	GLY
1	14-A	263	CYS
1	15-A	49	ALA
1	15-A	99	SER
1	15-A	132	PRO
1	16-A	155	CYS
1	16-A	195	PHE
1	16-A	215	ALA
1	16-A	220	PRO
1	1-A	12	GLY
1	1-A	21	ARG
1	1-A	99	SER
1	1-A	143	HIS
1	1-A	298	ARG
1	2-A	49	ALA
1	2-A	130	SER
1	2-A	221	ASN
1	3-A	298	ARG
1	4-A	19	GLU
1	4-A	248	CYS
1	4-A	265	PHE
1	5-A	127	ASP
1	5-A	263	CYS
1	6-A	108	ASN
1	7-A	193	GLU
1	7-A	249	GLY
1	9-A	20	THR
1	9-A	201	ILE
1	11-A	33	TRP

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Mol	Chain	Res	Type
1	11-A	127	ASP
1	11-A	264	SER
1	12-A	34	LEU
1	12-A	237	VAL
1	13-A	87	ALA
1	13-A	153	SER
1	13-A	261	LYS
1	13-A	262	LEU
1	14-A	135	ARG
1	14-A	176	LYS
1	15-A	177	LYS
1	1-A	31	LYS
1	1-A	36	SER
1	1-A	57	CYS
1	1-A	313	ILE
1	2-A	155	CYS
1	3-A	109	PRO
1	6-A	53	GLY
1	6-A	246	LEU
1	7-A	142	SER
1	7-A	264	SER
1	8-A	306	ALA
1	9-A	206	TRP
1	9-A	209	ILE
1	10-A	58	GLN
1	10-A	207	ASP
1	11-A	32	GLY
1	11-A	177	LYS
1	11-A	191	ALA
1	11-A	237	VAL
1	12-A	99	SER
1	12-A	238	GLU
1	13-A	13	ASP
1	16-A	116	LEU
1	16-A	213	TRP
1	16-A	318	LYS
1	1-A	26	SER
1	2-A	84	LEU
1	3-A	17	THR
1	3-A	143	HIS
1	3-A	265	PHE
1	5-A	33	TRP

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Mol	Chain	Res	Type
1	6-A	25	SER
1	7-A	177	LYS
1	7-A	206	TRP
1	7-A	298	ARG
1	11-A	49	ALA
1	11-A	108	ASN
1	13-A	86	PHE
1	13-A	124	PRO
1	13-A	320	SER
1	15-A	88	LEU
1	15-A	95	PRO
1	16-A	139	THR
1	16-A	177	LYS
1	16-A	197	GLU
1	1-A	68	ILE
1	1-A	205	PHE
1	5-A	35	VAL
1	5-A	74	PRO
1	6-A	52	GLN
1	10-A	318	LYS
1	13-A	167	MET
1	16-A	112	LEU
1	16-A	194	ALA
1	5-A	36	SER
1	5-A	201	ILE
1	7-A	77	GLY
1	7-A	108	ASN
1	11-A	192	VAL
1	13-A	14	GLU
1	13-A	42	GLN
1	13-A	49	ALA
1	15-A	77	GLY
1	4-A	249	GLY
1	10-A	201	ILE
1	15-A	146	LEU
1	2-A	209	ILE
1	4-A	146	LEU
1	5-A	209	ILE
1	11-A	220	PRO
1	16-A	198	GLY
1	10-A	198	GLY
1	16-A	114	PRO

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Mol	Chain	Res	Type
1	11-A	204	PRO

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-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	2-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	3-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	4-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	5-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	6-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	7-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	8-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	9-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	10-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	11-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	12-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	13-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	14-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	15-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
1	16-A	258/294 (88%)	238 (92%)	20 (8%)	11	5
All	All	4128/4704 (88%)	3808 (92%)	320 (8%)	11	5

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	7	VAL
1	1-A	17	THR
1	1-A	19	GLU

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Mol	Chain	Res	Type
1	1-A	20	THR
1	1-A	37	GLU
1	1-A	89	LEU
1	1-A	96	VAL
1	1-A	103	PRO
1	1-A	107	THR
1	1-A	138	ASN
1	1-A	142	SER
1	1-A	145	SER
1	1-A	148	GLU
1	1-A	149	SER
1	1-A	155	CYS
1	1-A	157	ILE
1	1-A	217	ARG
1	1-A	246	LEU
1	1-A	254	GLU
1	1-A	298	ARG
1	2-A	7	VAL
1	2-A	17	THR
1	2-A	19	GLU
1	2-A	20	THR
1	2-A	37	GLU
1	2-A	89	LEU
1	2-A	96	VAL
1	2-A	103	PRO
1	2-A	107	THR
1	2-A	138	ASN
1	2-A	142	SER
1	2-A	145	SER
1	2-A	148	GLU
1	2-A	149	SER
1	2-A	155	CYS
1	2-A	157	ILE
1	2-A	217	ARG
1	2-A	246	LEU
1	2-A	254	GLU
1	2-A	298	ARG
1	3-A	7	VAL
1	3-A	17	THR
1	3-A	19	GLU
1	3-A	20	THR
1	3-A	37	GLU

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Mol	Chain	Res	Type
1	3-A	89	LEU
1	3-A	96	VAL
1	3-A	103	PRO
1	3-A	107	THR
1	3-A	138	ASN
1	3-A	142	SER
1	3-A	145	SER
1	3-A	148	GLU
1	3-A	149	SER
1	3-A	155	CYS
1	3-A	157	ILE
1	3-A	217	ARG
1	3-A	246	LEU
1	3-A	254	GLU
1	3-A	298	ARG
1	4-A	7	VAL
1	4-A	17	THR
1	4-A	19	GLU
1	4-A	20	THR
1	4-A	37	GLU
1	4-A	89	LEU
1	4-A	96	VAL
1	4-A	103	PRO
1	4-A	107	THR
1	4-A	138	ASN
1	4-A	142	SER
1	4-A	145	SER
1	4-A	148	GLU
1	4-A	149	SER
1	4-A	155	CYS
1	4-A	157	ILE
1	4-A	217	ARG
1	4-A	246	LEU
1	4-A	254	GLU
1	4-A	298	ARG
1	5-A	7	VAL
1	5-A	17	THR
1	5-A	19	GLU
1	5-A	20	THR
1	5-A	37	GLU
1	5-A	89	LEU
1	5-A	96	VAL

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Mol	Chain	Res	Type
1	5-A	103	PRO
1	5-A	107	THR
1	5-A	138	ASN
1	5-A	142	SER
1	5-A	145	SER
1	5-A	148	GLU
1	5-A	149	SER
1	5-A	155	CYS
1	5-A	157	ILE
1	5-A	217	ARG
1	5-A	246	LEU
1	5-A	254	GLU
1	5-A	298	ARG
1	6-A	7	VAL
1	6-A	17	THR
1	6-A	19	GLU
1	6-A	20	THR
1	6-A	37	GLU
1	6-A	89	LEU
1	6-A	96	VAL
1	6-A	103	PRO
1	6-A	107	THR
1	6-A	138	ASN
1	6-A	142	SER
1	6-A	145	SER
1	6-A	148	GLU
1	6-A	149	SER
1	6-A	155	CYS
1	6-A	157	ILE
1	6-A	217	ARG
1	6-A	246	LEU
1	6-A	254	GLU
1	6-A	298	ARG
1	7-A	7	VAL
1	7-A	17	THR
1	7-A	19	GLU
1	7-A	20	THR
1	7-A	37	GLU
1	7-A	89	LEU
1	7-A	96	VAL
1	7-A	103	PRO
1	7-A	107	THR

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Mol	Chain	Res	Type
1	7-A	138	ASN
1	7-A	142	SER
1	7-A	145	SER
1	7-A	148	GLU
1	7-A	149	SER
1	7-A	155	CYS
1	7-A	157	ILE
1	7-A	217	ARG
1	7-A	246	LEU
1	7-A	254	GLU
1	7-A	298	ARG
1	8-A	7	VAL
1	8-A	17	THR
1	8-A	19	GLU
1	8-A	20	THR
1	8-A	37	GLU
1	8-A	89	LEU
1	8-A	96	VAL
1	8-A	103	PRO
1	8-A	107	THR
1	8-A	138	ASN
1	8-A	142	SER
1	8-A	145	SER
1	8-A	148	GLU
1	8-A	149	SER
1	8-A	155	CYS
1	8-A	157	ILE
1	8-A	217	ARG
1	8-A	246	LEU
1	8-A	254	GLU
1	8-A	298	ARG
1	9-A	7	VAL
1	9-A	17	THR
1	9-A	19	GLU
1	9-A	20	THR
1	9-A	37	GLU
1	9-A	89	LEU
1	9-A	96	VAL
1	9-A	103	PRO
1	9-A	107	THR
1	9-A	138	ASN
1	9-A	142	SER

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Mol	Chain	Res	Type
1	9-A	145	SER
1	9-A	148	GLU
1	9-A	149	SER
1	9-A	155	CYS
1	9-A	157	ILE
1	9-A	217	ARG
1	9-A	246	LEU
1	9-A	254	GLU
1	9-A	298	ARG
1	10-A	7	VAL
1	10-A	17	THR
1	10-A	19	GLU
1	10-A	20	THR
1	10-A	37	GLU
1	10-A	89	LEU
1	10-A	96	VAL
1	10-A	103	PRO
1	10-A	107	THR
1	10-A	138	ASN
1	10-A	142	SER
1	10-A	145	SER
1	10-A	148	GLU
1	10-A	149	SER
1	10-A	155	CYS
1	10-A	157	ILE
1	10-A	217	ARG
1	10-A	246	LEU
1	10-A	254	GLU
1	10-A	298	ARG
1	11-A	7	VAL
1	11-A	17	THR
1	11-A	19	GLU
1	11-A	20	THR
1	11-A	37	GLU
1	11-A	89	LEU
1	11-A	96	VAL
1	11-A	103	PRO
1	11-A	107	THR
1	11-A	138	ASN
1	11-A	142	SER
1	11-A	145	SER
1	11-A	148	GLU

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Mol	Chain	Res	Type
1	11-A	149	SER
1	11-A	155	CYS
1	11-A	157	ILE
1	11-A	217	ARG
1	11-A	246	LEU
1	11-A	254	GLU
1	11-A	298	ARG
1	12-A	7	VAL
1	12-A	17	THR
1	12-A	19	GLU
1	12-A	20	THR
1	12-A	37	GLU
1	12-A	89	LEU
1	12-A	96	VAL
1	12-A	103	PRO
1	12-A	107	THR
1	12-A	138	ASN
1	12-A	142	SER
1	12-A	145	SER
1	12-A	148	GLU
1	12-A	149	SER
1	12-A	155	CYS
1	12-A	157	ILE
1	12-A	217	ARG
1	12-A	246	LEU
1	12-A	254	GLU
1	12-A	298	ARG
1	13-A	7	VAL
1	13-A	17	THR
1	13-A	19	GLU
1	13-A	20	THR
1	13-A	37	GLU
1	13-A	89	LEU
1	13-A	96	VAL
1	13-A	103	PRO
1	13-A	107	THR
1	13-A	138	ASN
1	13-A	142	SER
1	13-A	145	SER
1	13-A	148	GLU
1	13-A	149	SER
1	13-A	155	CYS

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Mol	Chain	Res	Type
1	13-A	157	ILE
1	13-A	217	ARG
1	13-A	246	LEU
1	13-A	254	GLU
1	13-A	298	ARG
1	14-A	7	VAL
1	14-A	17	THR
1	14-A	19	GLU
1	14-A	20	THR
1	14-A	37	GLU
1	14-A	89	LEU
1	14-A	96	VAL
1	14-A	103	PRO
1	14-A	107	THR
1	14-A	138	ASN
1	14-A	142	SER
1	14-A	145	SER
1	14-A	148	GLU
1	14-A	149	SER
1	14-A	155	CYS
1	14-A	157	ILE
1	14-A	217	ARG
1	14-A	246	LEU
1	14-A	254	GLU
1	14-A	298	ARG
1	15-A	7	VAL
1	15-A	17	THR
1	15-A	19	GLU
1	15-A	20	THR
1	15-A	37	GLU
1	15-A	89	LEU
1	15-A	96	VAL
1	15-A	103	PRO
1	15-A	107	THR
1	15-A	138	ASN
1	15-A	142	SER
1	15-A	145	SER
1	15-A	148	GLU
1	15-A	149	SER
1	15-A	155	CYS
1	15-A	157	ILE
1	15-A	217	ARG

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Mol	Chain	Res	Type
1	15-A	246	LEU
1	15-A	254	GLU
1	15-A	298	ARG
1	16-A	7	VAL
1	16-A	17	THR
1	16-A	19	GLU
1	16-A	20	THR
1	16-A	37	GLU
1	16-A	89	LEU
1	16-A	96	VAL
1	16-A	103	PRO
1	16-A	107	THR
1	16-A	138	ASN
1	16-A	142	SER
1	16-A	145	SER
1	16-A	148	GLU
1	16-A	149	SER
1	16-A	155	CYS
1	16-A	157	ILE
1	16-A	217	ARG
1	16-A	246	LEU
1	16-A	254	GLU
1	16-A	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	48	GLN
1	1-A	101	ASN
1	1-A	108	ASN
1	1-A	138	ASN
1	1-A	219	ASN
1	2-A	42	GLN
1	2-A	101	ASN
1	2-A	108	ASN
1	2-A	110	HIS
1	2-A	140	HIS
1	3-A	108	ASN
1	3-A	138	ASN
1	3-A	143	HIS
1	3-A	173	HIS
1	3-A	219	ASN

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Mol	Chain	Res	Type
1	3-A	221	ASN
1	4-A	42	GLN
1	4-A	46	HIS
1	4-A	108	ASN
1	4-A	110	HIS
1	4-A	173	HIS
1	4-A	219	ASN
1	4-A	221	ASN
1	5-A	42	GLN
1	5-A	73	ASN
1	5-A	108	ASN
1	5-A	110	HIS
1	5-A	173	HIS
1	5-A	219	ASN
1	5-A	221	ASN
1	5-A	234	GLN
1	6-A	42	GLN
1	6-A	52	GLN
1	6-A	101	ASN
1	6-A	108	ASN
1	6-A	110	HIS
1	6-A	219	ASN
1	6-A	221	ASN
1	6-A	234	GLN
1	7-A	42	GLN
1	7-A	73	ASN
1	7-A	108	ASN
1	7-A	110	HIS
1	7-A	143	HIS
1	7-A	219	ASN
1	7-A	221	ASN
1	8-A	42	GLN
1	8-A	90	ASN
1	8-A	108	ASN
1	8-A	110	HIS
1	8-A	219	ASN
1	8-A	221	ASN
1	9-A	42	GLN
1	9-A	46	HIS
1	9-A	101	ASN
1	9-A	108	ASN
1	9-A	110	HIS

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Mol	Chain	Res	Type
1	9-A	138	ASN
1	9-A	219	ASN
1	9-A	221	ASN
1	10-A	58	GLN
1	10-A	101	ASN
1	10-A	108	ASN
1	10-A	110	HIS
1	10-A	138	ASN
1	10-A	143	HIS
1	10-A	219	ASN
1	10-A	221	ASN
1	11-A	73	ASN
1	11-A	101	ASN
1	11-A	110	HIS
1	11-A	138	ASN
1	11-A	219	ASN
1	11-A	221	ASN
1	12-A	18	GLN
1	12-A	42	GLN
1	12-A	138	ASN
1	12-A	143	HIS
1	12-A	219	ASN
1	12-A	221	ASN
1	13-A	42	GLN
1	13-A	58	GLN
1	13-A	90	ASN
1	13-A	108	ASN
1	13-A	143	HIS
1	13-A	163	ASN
1	13-A	234	GLN
1	14-A	42	GLN
1	14-A	48	GLN
1	14-A	52	GLN
1	14-A	101	ASN
1	14-A	108	ASN
1	14-A	110	HIS
1	14-A	140	HIS
1	14-A	173	HIS
1	14-A	234	GLN
1	15-A	18	GLN
1	15-A	42	GLN
1	15-A	46	HIS

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Mol	Chain	Res	Type
1	15-A	52	GLN
1	15-A	90	ASN
1	15-A	101	ASN
1	15-A	108	ASN
1	15-A	219	ASN
1	15-A	234	GLN
1	16-A	42	GLN
1	16-A	52	GLN
1	16-A	108	ASN
1	16-A	110	HIS
1	16-A	140	HIS
1	16-A	143	HIS
1	16-A	221	ASN
1	16-A	234	GLN

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](#)

16 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
2	MLA	6-A	901	-	6,6,6	0.93	0	7,7,7	1.34	1 (14%)
2	MLA	3-A	901	-	6,6,6	1.32	1 (16%)	7,7,7	1.32	0
2	MLA	1-A	901	-	6,6,6	0.84	0	7,7,7	1.16	0
2	MLA	9-A	901	-	6,6,6	0.92	0	7,7,7	1.21	0
2	MLA	4-A	901	-	6,6,6	1.66	1 (16%)	7,7,7	1.33	1 (14%)
2	MLA	7-A	901	-	6,6,6	0.90	0	7,7,7	1.08	0
2	MLA	12-A	901	-	6,6,6	1.16	1 (16%)	7,7,7	1.02	0
2	MLA	14-A	901	-	6,6,6	1.38	1 (16%)	7,7,7	1.53	2 (28%)
2	MLA	15-A	901	-	6,6,6	0.90	0	7,7,7	1.02	0
2	MLA	13-A	901	-	6,6,6	1.59	1 (16%)	7,7,7	1.28	1 (14%)
2	MLA	5-A	901	-	6,6,6	1.06	1 (16%)	7,7,7	1.21	0
2	MLA	8-A	901	-	6,6,6	1.32	1 (16%)	7,7,7	1.28	0
2	MLA	16-A	901	-	6,6,6	1.90	2 (33%)	7,7,7	1.50	1 (14%)
2	MLA	11-A	901	-	6,6,6	1.77	2 (33%)	7,7,7	1.43	1 (14%)
2	MLA	10-A	901	-	6,6,6	1.32	1 (16%)	7,7,7	1.23	1 (14%)
2	MLA	2-A	901	-	6,6,6	1.07	1 (16%)	7,7,7	1.21	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
2	MLA	6-A	901	-	-	0/4/4/4	-
2	MLA	3-A	901	-	-	0/4/4/4	-
2	MLA	1-A	901	-	-	0/4/4/4	-
2	MLA	9-A	901	-	-	0/4/4/4	-
2	MLA	4-A	901	-	-	0/4/4/4	-
2	MLA	7-A	901	-	-	0/4/4/4	-
2	MLA	12-A	901	-	-	0/4/4/4	-
2	MLA	14-A	901	-	-	0/4/4/4	-
2	MLA	15-A	901	-	-	0/4/4/4	-
2	MLA	13-A	901	-	-	0/4/4/4	-
2	MLA	5-A	901	-	-	0/4/4/4	-
2	MLA	8-A	901	-	-	0/4/4/4	-
2	MLA	16-A	901	-	-	0/4/4/4	-
2	MLA	11-A	901	-	-	0/4/4/4	-
2	MLA	10-A	901	-	-	0/4/4/4	-
2	MLA	2-A	901	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	16-A	901	MLA	C2-C3	3.71	1.56	1.51
2	13-A	901	MLA	C2-C1	3.67	1.56	1.51
2	11-A	901	MLA	C2-C3	3.04	1.55	1.51
2	8-A	901	MLA	C2-C1	2.86	1.55	1.51
2	11-A	901	MLA	O1A-C1	2.82	1.40	1.30
2	4-A	901	MLA	C2-C1	2.82	1.55	1.51
2	12-A	901	MLA	C2-C3	-2.48	1.47	1.51
2	10-A	901	MLA	C2-C1	2.42	1.54	1.51
2	14-A	901	MLA	C2-C1	2.41	1.54	1.51
2	2-A	901	MLA	C2-C3	2.32	1.54	1.51
2	3-A	901	MLA	C2-C3	2.21	1.54	1.51
2	5-A	901	MLA	C2-C1	2.20	1.54	1.51
2	16-A	901	MLA	C2-C1	2.06	1.54	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-A	901	MLA	O1A-C1-O1B	-2.31	117.39	123.33
2	14-A	901	MLA	O1A-C1-O1B	-2.21	117.65	123.33
2	6-A	901	MLA	O1A-C1-O1B	-2.21	117.66	123.33
2	11-A	901	MLA	O3B-C3-O3A	-2.18	117.73	123.33
2	13-A	901	MLA	O1A-C1-O1B	-2.15	117.81	123.33
2	4-A	901	MLA	O3B-C3-C2	2.11	121.06	114.51
2	10-A	901	MLA	O3B-C3-O3A	-2.03	118.11	123.33
2	14-A	901	MLA	O3B-C3-C2	2.02	120.78	114.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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-A	284/326 (87%)	3.69	231 (81%) 0 0	1, 2, 3, 4	284 (100%)
1	2-A	0/326	-	-	-	-
1	3-A	0/326	-	-	-	-
1	4-A	0/326	-	-	-	-
1	5-A	0/326	-	-	-	-
1	6-A	0/326	-	-	-	-
1	7-A	0/326	-	-	-	-
1	8-A	0/326	-	-	-	-
1	9-A	0/326	-	-	-	-
1	10-A	0/326	-	-	-	-
1	11-A	0/326	-	-	-	-
1	12-A	0/326	-	-	-	-
1	13-A	0/326	-	-	-	-
1	14-A	0/326	-	-	-	-
1	15-A	0/326	-	-	-	-
1	16-A	0/326	-	-	-	-
All	All	284/5216 (5%)	3.69	231 (81%) 0 0	1, 2, 3, 4	284 (100%)

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	32	GLY	16.2
1	1-A	6	SER	15.9
1	1-A	248	CYS	13.4
1	1-A	35	VAL	11.5
1	1-A	33	TRP	10.8
1	1-A	178	LEU	9.8
1	1-A	16	LEU	9.3
1	1-A	214	TYR	8.5
1	1-A	34	LEU	8.5
1	1-A	10	TYR	8.4
1	1-A	20	THR	8.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	174	PHE	8.2
1	1-A	147	PRO	8.1
1	1-A	57	CYS	7.8
1	1-A	187	PRO	7.6
1	1-A	134	PRO	7.4
1	1-A	19	GLU	7.2
1	1-A	173	HIS	7.1
1	1-A	143	HIS	6.8
1	1-A	17	THR	6.7
1	1-A	15	ASP	6.6
1	1-A	12	GLY	6.6
1	1-A	81	LEU	6.6
1	1-A	142	SER	6.6
1	1-A	14	GLU	6.5
1	1-A	141	ILE	6.4
1	1-A	324	PHE	6.3
1	1-A	7	VAL	6.3
1	1-A	186	TYR	6.3
1	1-A	210	LEU	6.0
1	1-A	206	TRP	6.0
1	1-A	9	ALA	5.9
1	1-A	208	HIS	5.8
1	1-A	246	LEU	5.8
1	1-A	138	ASN	5.7
1	1-A	99	SER	5.7
1	1-A	237	VAL	5.7
1	1-A	305	LEU	5.7
1	1-A	314	GLU	5.6
1	1-A	170	SER	5.6
1	1-A	296	GLY	5.6
1	1-A	84	LEU	5.5
1	1-A	56	ILE	5.5
1	1-A	37	GLU	5.5
1	1-A	22	ALA	5.5
1	1-A	137	MET	5.5
1	1-A	36	SER	5.4
1	1-A	98	SER	5.3
1	1-A	13	ASP	5.3
1	1-A	44	LEU	5.2
1	1-A	204	PRO	5.2
1	1-A	48	GLN	5.2
1	1-A	188	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	23	LEU	5.1
1	1-A	150	VAL	5.1
1	1-A	38	ILE	5.1
1	1-A	228	TYR	5.1
1	1-A	306	ALA	5.0
1	1-A	140	HIS	5.0
1	1-A	325	SER	4.9
1	1-A	307	GLU	4.8
1	1-A	190	LYS	4.8
1	1-A	144	LEU	4.8
1	1-A	309	ILE	4.8
1	1-A	27	LEU	4.8
1	1-A	265	PHE	4.8
1	1-A	11	LEU	4.8
1	1-A	249	GLY	4.8
1	1-A	211	GLU	4.7
1	1-A	85	VAL	4.7
1	1-A	118	GLY	4.7
1	1-A	166	ASP	4.7
1	1-A	89	LEU	4.7
1	1-A	24	ILE	4.6
1	1-A	215	ALA	4.6
1	1-A	91	ARG	4.6
1	1-A	45	TRP	4.6
1	1-A	171	LEU	4.5
1	1-A	297	TRP	4.4
1	1-A	164	PRO	4.4
1	1-A	175	GLY	4.4
1	1-A	189	GLU	4.4
1	1-A	53	GLY	4.3
1	1-A	231	LEU	4.3
1	1-A	28	PRO	4.3
1	1-A	107	THR	4.2
1	1-A	29	LYS	4.1
1	1-A	312	THR	4.1
1	1-A	207	ASP	4.1
1	1-A	304	SER	4.0
1	1-A	317	PHE	4.0
1	1-A	257	ARG	4.0
1	1-A	303	GLU	4.0
1	1-A	323	LYS	4.0
1	1-A	264	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	18	GLN	3.9
1	1-A	255	GLU	3.9
1	1-A	299	ASP	3.9
1	1-A	116	LEU	3.9
1	1-A	318	LYS	3.9
1	1-A	21	ARG	3.9
1	1-A	55	LEU	3.9
1	1-A	300	THR	3.9
1	1-A	315	GLU	3.9
1	1-A	177	LYS	3.9
1	1-A	212	TYR	3.8
1	1-A	201	ILE	3.8
1	1-A	319	GLY	3.8
1	1-A	148	GLU	3.8
1	1-A	176	LYS	3.8
1	1-A	316	LYS	3.8
1	1-A	235	THR	3.7
1	1-A	104	LEU	3.7
1	1-A	194	ALA	3.6
1	1-A	298	ARG	3.6
1	1-A	168	PHE	3.6
1	1-A	155	CYS	3.5
1	1-A	154	SER	3.5
1	1-A	169	VAL	3.5
1	1-A	172	TRP	3.5
1	1-A	47	THR	3.5
1	1-A	79	THR	3.5
1	1-A	216	SER	3.5
1	1-A	311	ARG	3.5
1	1-A	113	VAL	3.4
1	1-A	244	GLU	3.4
1	1-A	149	SER	3.4
1	1-A	114	PRO	3.4
1	1-A	31	LYS	3.4
1	1-A	30	GLU	3.4
1	1-A	111	LEU	3.4
1	1-A	70	LEU	3.4
1	1-A	200	PHE	3.4
1	1-A	157	ILE	3.3
1	1-A	219	ASN	3.3
1	1-A	49	ALA	3.3
1	1-A	90	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	145	SER	3.3
1	1-A	152	SER	3.3
1	1-A	83	ALA	3.3
1	1-A	94	PHE	3.3
1	1-A	310	ASP	3.2
1	1-A	96	VAL	3.2
1	1-A	103	PRO	3.2
1	1-A	122	GLU	3.2
1	1-A	253	GLU	3.2
1	1-A	308	GLU	3.2
1	1-A	213	TRP	3.2
1	1-A	133	SER	3.1
1	1-A	251	ILE	3.1
1	1-A	236	GLU	3.1
1	1-A	220	PRO	3.1
1	1-A	209	ILE	3.0
1	1-A	61	PHE	3.0
1	1-A	26	SER	3.0
1	1-A	198	GLY	3.0
1	1-A	222	LYS	3.0
1	1-A	136	LEU	3.0
1	1-A	217	ARG	3.0
1	1-A	39	TYR	3.0
1	1-A	158	VAL	3.0
1	1-A	266	GLU	3.0
1	1-A	69	ILE	3.0
1	1-A	192	VAL	2.9
1	1-A	224	LEU	2.9
1	1-A	262	LEU	2.9
1	1-A	8	PRO	2.9
1	1-A	151	LYS	2.9
1	1-A	301	LEU	2.9
1	1-A	100	GLY	2.9
1	1-A	105	LEU	2.8
1	1-A	87	ALA	2.8
1	1-A	202	GLY	2.8
1	1-A	322	LEU	2.7
1	1-A	243	ALA	2.7
1	1-A	46	HIS	2.7
1	1-A	115	PHE	2.7
1	1-A	125	ASP	2.7
1	1-A	97	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	86	PHE	2.7
1	1-A	127	ASP	2.7
1	1-A	250	PHE	2.7
1	1-A	232	LYS	2.7
1	1-A	225	PHE	2.6
1	1-A	106	VAL	2.6
1	1-A	77	GLY	2.6
1	1-A	191	ALA	2.6
1	1-A	260	VAL	2.6
1	1-A	160	CYS	2.6
1	1-A	242	ILE	2.6
1	1-A	54	ILE	2.5
1	1-A	119	VAL	2.5
1	1-A	139	THR	2.5
1	1-A	313	ILE	2.5
1	1-A	58	GLN	2.5
1	1-A	205	PHE	2.5
1	1-A	129	SER	2.5
1	1-A	254	GLU	2.5
1	1-A	80	TRP	2.5
1	1-A	227	THR	2.4
1	1-A	43	GLY	2.4
1	1-A	146	LEU	2.4
1	1-A	64	LYS	2.4
1	1-A	126	PHE	2.4
1	1-A	66	SER	2.4
1	1-A	112	LEU	2.3
1	1-A	74	PRO	2.3
1	1-A	302	SER	2.3
1	1-A	234	GLN	2.3
1	1-A	108	ASN	2.3
1	1-A	110	HIS	2.3
1	1-A	78	THR	2.3
1	1-A	203	GLY	2.2
1	1-A	167	MET	2.2
1	1-A	193	GLU	2.2
1	1-A	82	LYS	2.2
1	1-A	229	GLU	2.2
1	1-A	121	TYR	2.2
1	1-A	223	VAL	2.2
1	1-A	41	PHE	2.1
1	1-A	120	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	218	GLU	2.1
1	1-A	109	PRO	2.1
1	1-A	128	PHE	2.1
1	1-A	59	LYS	2.1
1	1-A	258	GLU	2.1
1	1-A	252	GLU	2.0
1	1-A	321	GLY	2.0
1	1-A	263	CYS	2.0
1	1-A	239	MET	2.0
1	1-A	132	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	MLA	1-A	901	7/7	0.78	0.39	0,10,27,29	7
2	MLA	2-A	901	7/7	-	-	15,20,25,27	7
2	MLA	3-A	901	7/7	-	-	15,21,27,30	7
2	MLA	4-A	901	7/7	-	-	17,20,25,28	7
2	MLA	5-A	901	7/7	-	-	22,25,25,28	7
2	MLA	6-A	901	7/7	-	-	19,24,24,28	7
2	MLA	7-A	901	7/7	-	-	20,23,25,26	7
2	MLA	8-A	901	7/7	-	-	22,24,25,27	7
2	MLA	9-A	901	7/7	-	-	23,26,27,28	7
2	MLA	10-A	901	7/7	-	-	0,11,25,28	7
2	MLA	11-A	901	7/7	-	-	2,10,19,22	7
2	MLA	12-A	901	7/7	-	-	0,11,29,31	7
2	MLA	13-A	901	7/7	-	-	17,21,22,24	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLA	14-A	901	7/7	-	-	8,15,24,27	7
2	MLA	15-A	901	7/7	-	-	20,21,25,25	7
2	MLA	16-A	901	7/7	-	-	12,18,24,26	7

6.5 Other polymers [i](#)

There are no such residues in this entry.