



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:39 AM UTC

PDB ID : 8DQP / pdb_00008dqp
Title : Crystal structure of Arabidopsis thaliana COSY in complex with scopoletin
Authors : Kim, C.Y.; Mitchell, A.J.; Gutierrez, M.; Weng, J.K.
Deposited on : 2022-07-19
Resolution : 2.48 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

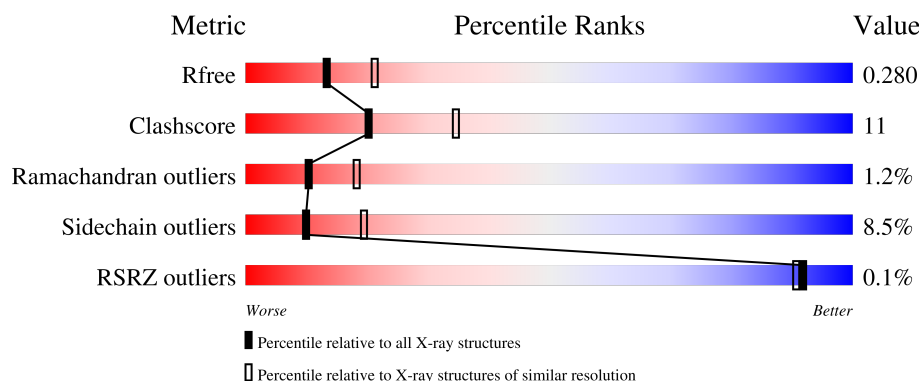
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	A	451	
1	B	451	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	T83	A	501	-	X	-	-
5	PG4	A	505	-	X	X	-

2 Entry composition [i](#)

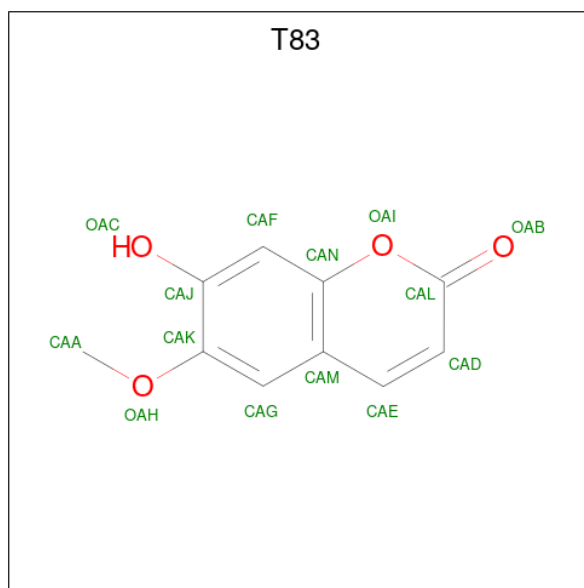
There are 7 unique types of molecules in this entry. The entry contains 6718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coumarin Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	1	0
			3339	2133	568	622	16			
1	B	409	Total	C	N	O	S	0	0	0
			3216	2056	548	597	15			

- Molecule 2 is 7-hydroxy-6-methoxy-2H-1-benzopyran-2-one (CCD ID: T83) (formula: $C_{10}H_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	10	4		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

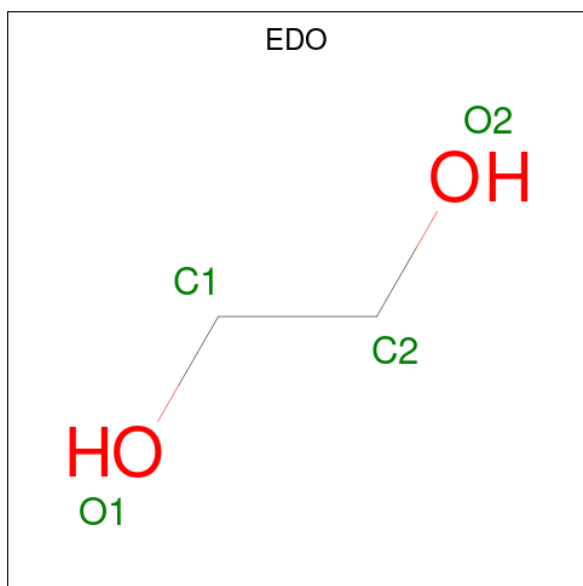
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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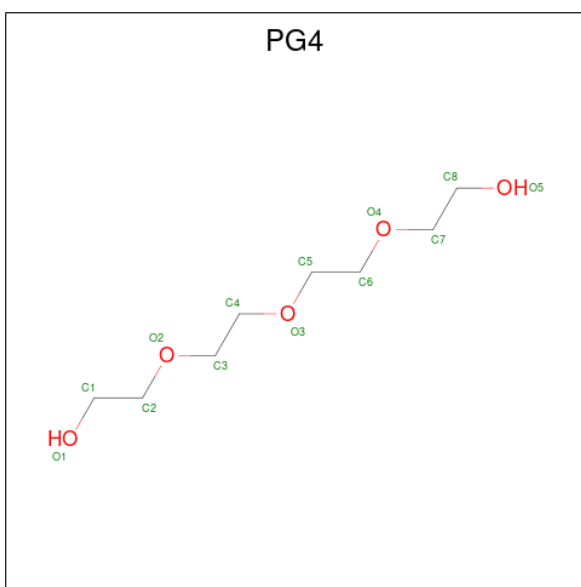
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



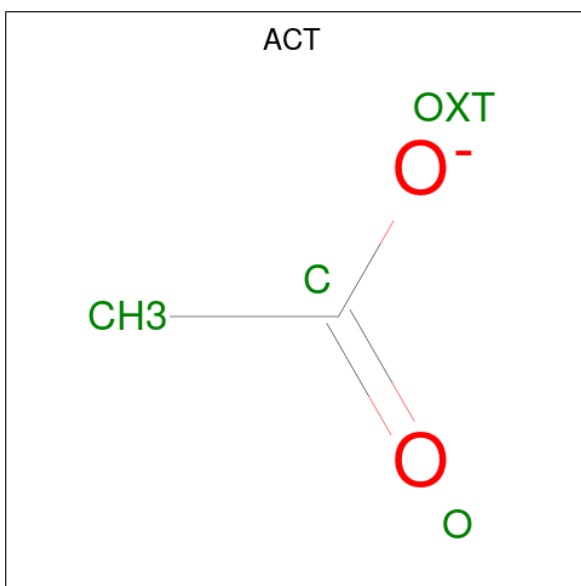
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

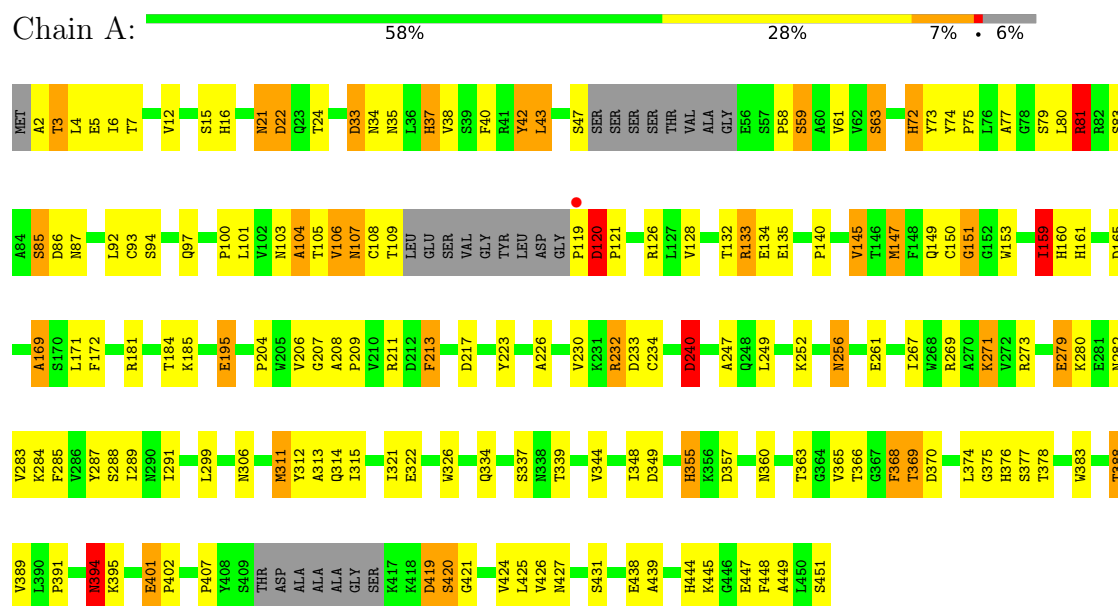
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total 68	O 68	0	0
7	B	54	Total 54	O 54	0	0

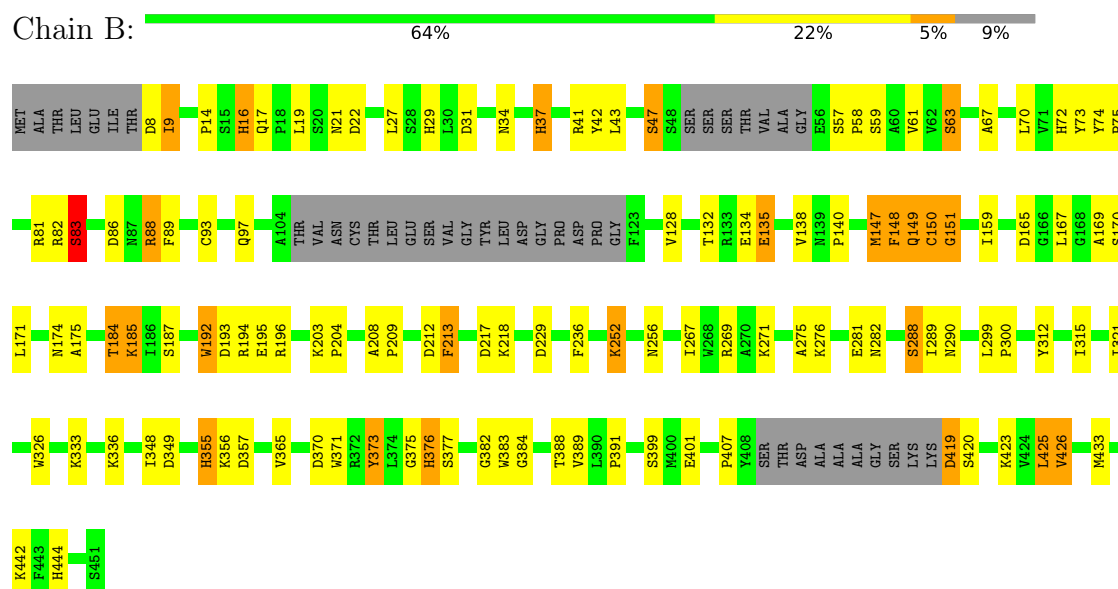
3 Residue-property plots

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: Coumarin Synthase



● Molecule 1: Coumarin Synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.46Å 58.35Å 273.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.32 – 2.48 68.32 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.5 (68.32-2.48) 97.8 (68.32-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.173 , 0.281 0.172 , 0.280	Depositor DCC
R_{free} test set	1563 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6718	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: ACT, T83, PG4, EDO, 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	1.79	92/3421 (2.7%)	1.61	39/4637 (0.8%)
1	B	1.44	32/3296 (1.0%)	1.52	30/4466 (0.7%)
All	All	1.63	124/6717 (1.8%)	1.56	69/9103 (0.8%)

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	4
All	All	0	8

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	VAL	N-CA	-11.40	1.32	1.46
1	B	47	SER	N-CA	11.37	1.58	1.46
1	A	283	VAL	C-O	-10.64	1.10	1.23
1	A	315	ILE	N-CA	-10.19	1.35	1.46
1	A	120	ASP	N-CA	9.94	1.60	1.46
1	A	365	VAL	C-O	-9.82	1.12	1.24
1	A	363	THR	C-O	-9.76	1.10	1.23
1	A	314	GLN	C-O	-9.71	1.11	1.23
1	A	108	CYS	N-CA	9.51	1.58	1.46
1	A	366	THR	N-CA	-9.48	1.34	1.46
1	B	391	PRO	C-O	-9.20	1.14	1.23
1	A	37	HIS	CE1-NE2	9.12	1.41	1.32
1	A	230	VAL	C-O	-9.00	1.14	1.24
1	A	80	LEU	C-O	-8.99	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	LYS	C-O	-8.66	1.12	1.24
1	A	145	VAL	C-O	-7.98	1.15	1.24
1	A	402	PRO	C-O	-7.89	1.14	1.23
1	A	204	PRO	C-O	-7.69	1.14	1.23
1	A	207	GLY	C-O	-7.68	1.12	1.23
1	A	391	PRO	C-O	-7.59	1.16	1.23
1	A	368	PHE	N-CA	-7.54	1.36	1.46
1	A	77	ALA	C-O	7.44	1.33	1.24
1	A	282	ASN	C-O	-7.22	1.15	1.24
1	A	451	SER	C-O	7.11	1.37	1.23
1	A	438	GLU	CD-OE2	7.10	1.38	1.25
1	A	285	PHE	C-O	-7.03	1.16	1.24
1	B	281	GLU	C-O	6.97	1.32	1.23
1	A	133	ARG	N-CA	6.84	1.54	1.46
1	A	326	TRP	C-O	-6.84	1.15	1.24
1	B	376	HIS	CE1-NE2	6.80	1.39	1.32
1	A	105	THR	C-O	6.78	1.32	1.23
1	A	360	ASN	N-CA	-6.75	1.37	1.46
1	A	160	HIS	CE1-NE2	-6.68	1.25	1.32
1	A	161	HIS	CE1-NE2	6.66	1.39	1.32
1	A	313	ALA	N-CA	-6.64	1.37	1.45
1	B	382	GLY	C-O	6.62	1.32	1.23
1	A	438	GLU	CD-OE1	6.60	1.37	1.25
1	B	83	SER	N-CA	6.60	1.54	1.46
1	A	107	ASN	N-CA	6.59	1.54	1.45
1	B	365	VAL	C-O	-6.55	1.16	1.24
1	B	135	GLU	C-O	6.48	1.32	1.24
1	A	344	VAL	N-CA	-6.48	1.38	1.46
1	A	261	GLU	C-O	-6.46	1.16	1.24
1	A	169	ALA	CA-CB	-6.44	1.43	1.53
1	B	147	MET	C-O	6.36	1.31	1.23
1	A	16	HIS	CE1-NE2	6.33	1.38	1.32
1	A	172	PHE	C-O	-6.31	1.16	1.24
1	B	150	CYS	N-CA	6.31	1.54	1.46
1	B	326	TRP	C-O	-6.28	1.16	1.24
1	A	376	HIS	CE1-NE2	6.27	1.38	1.32
1	A	247	ALA	C-O	-6.24	1.16	1.24
1	A	126	ARG	C-O	6.23	1.32	1.24
1	A	226	ALA	N-CA	-6.20	1.38	1.46
1	A	12	VAL	C-O	-6.17	1.17	1.24
1	A	135	GLU	C-O	6.16	1.31	1.24
1	B	41	ARG	C-O	6.08	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	ILE	N-CA	-6.08	1.39	1.46
1	A	7	THR	C-O	-6.08	1.17	1.24
1	A	72	HIS	C-O	6.06	1.31	1.24
1	B	171	LEU	N-CA	6.05	1.53	1.46
1	B	43	LEU	N-CA	-6.04	1.38	1.45
1	A	375	GLY	N-CA	6.01	1.54	1.45
1	B	218	LYS	C-O	-5.99	1.16	1.24
1	A	267	ILE	C-O	-5.96	1.17	1.24
1	A	171	LEU	N-CA	5.92	1.53	1.46
1	A	447	GLU	CD-OE2	5.92	1.36	1.25
1	A	133	ARG	NE-CZ	5.91	1.39	1.33
1	B	213	PHE	N-CA	5.87	1.53	1.46
1	B	204	PRO	C-O	-5.85	1.16	1.23
1	A	401	GLU	N-CA	-5.81	1.40	1.46
1	A	79	SER	N-CA	5.79	1.52	1.46
1	A	105	THR	C-N	5.78	1.39	1.33
1	A	306	ASN	N-CA	-5.78	1.39	1.46
1	A	370	ASP	C-O	-5.77	1.17	1.24
1	A	149	GLN	N-CA	5.71	1.53	1.46
1	B	151	GLY	N-CA	5.70	1.53	1.45
1	A	427	ASN	C-O	-5.66	1.17	1.24
1	B	384	GLY	N-CA	-5.62	1.37	1.45
1	A	217	ASP	CG-OD1	5.61	1.36	1.25
1	A	421	GLY	N-CA	5.60	1.51	1.45
1	A	279	GLU	C-O	-5.56	1.17	1.24
1	A	232	ARG	C-O	-5.54	1.17	1.24
1	A	213	PHE	N-CA	5.53	1.53	1.46
1	B	16	HIS	CE1-NE2	5.52	1.38	1.32
1	B	57	SER	N-CA	5.50	1.53	1.45
1	A	349	ASP	C-O	-5.50	1.17	1.24
1	A	43	LEU	C-O	-5.47	1.17	1.23
1	A	334	GLN	C-O	-5.47	1.17	1.24
1	A	134	GLU	CD-OE2	5.46	1.35	1.25
1	A	3	THR	C-O	5.45	1.30	1.23
1	B	384	GLY	C-O	5.44	1.31	1.23
1	B	37	HIS	CE1-NE2	5.43	1.38	1.32
1	A	106	VAL	CA-C	5.42	1.58	1.52
1	A	444	HIS	CE1-NE2	5.33	1.37	1.32
1	B	355	HIS	CE1-NE2	5.32	1.37	1.32
1	A	355	HIS	CE1-NE2	5.32	1.37	1.32
1	A	431	SER	N-CA	5.32	1.53	1.46
1	A	280	LYS	C-O	5.30	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	ILE	N-CA	-5.27	1.40	1.46
1	A	282	ASN	N-CA	-5.23	1.39	1.46
1	A	206	VAL	C-O	-5.23	1.18	1.24
1	A	159	ILE	C-O	-5.23	1.18	1.24
1	A	322	GLU	CD-OE1	5.22	1.35	1.25
1	A	234	CYS	N-CA	-5.21	1.39	1.46
1	B	267	ILE	C-O	-5.20	1.18	1.24
1	A	104	ALA	N-CA	-5.19	1.39	1.45
1	A	150	CYS	N-CA	5.18	1.53	1.46
1	B	217	ASP	C-O	-5.15	1.17	1.23
1	B	399	SER	C-O	-5.15	1.17	1.23
1	A	337	SER	C-O	-5.07	1.18	1.24
1	A	369	THR	C-O	-5.06	1.18	1.23
1	A	311	MET	N-CA	-5.06	1.39	1.45
1	A	280	LYS	N-CA	5.05	1.52	1.46
1	A	249	LEU	N-CA	-5.05	1.40	1.46
1	A	6	ILE	N-CA	-5.05	1.40	1.46
1	A	389	VAL	C-O	-5.05	1.19	1.24
1	B	175	ALA	C-O	5.04	1.29	1.24
1	A	284	LYS	N-CA	-5.04	1.39	1.45
1	B	282	ASN	C-O	-5.04	1.18	1.24
1	B	170	SER	N-CA	-5.04	1.39	1.46
1	A	374	LEU	C-O	5.03	1.30	1.23
1	A	439	ALA	N-CA	-5.03	1.40	1.46
1	A	223	TYR	C-O	-5.02	1.17	1.24
1	A	40	PHE	N-CA	-5.01	1.40	1.46

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	PHE	CA-CB-CG	13.37	127.17	113.80
1	A	213	PHE	CA-CB-CG	10.93	124.73	113.80
1	A	240	ASP	CA-CB-CG	9.56	122.16	112.60
1	A	151	GLY	CA-C-N	9.36	128.64	122.18
1	A	151	GLY	C-N-CA	9.36	128.64	122.18
1	B	184	THR	CA-CB-OG1	-9.28	95.67	109.60
1	B	165	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	165	ASP	CA-CB-CG	8.52	121.12	112.60
1	A	33	ASP	CA-CB-CG	8.33	120.93	112.60
1	B	357	ASP	CA-CB-CG	8.22	120.82	112.60
1	B	37	HIS	CA-CB-CG	7.65	121.45	113.80
1	B	193	ASP	CA-CB-CG	7.13	119.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	CG-CD-NE	6.80	126.97	112.00
1	B	229	ASP	CA-CB-CG	6.55	119.15	112.60
1	B	149	GLN	CB-CG-CD	6.43	123.53	112.60
1	B	195	GLU	CB-CG-CD	6.37	123.43	112.60
1	B	433	MET	O-C-N	-6.30	114.79	120.71
1	A	100	PRO	N-CA-C	6.22	121.02	110.95
1	A	119	PRO	CA-C-N	6.20	136.94	121.80
1	A	119	PRO	C-N-CA	6.20	136.94	121.80
1	A	378	THR	CA-CB-OG1	-6.09	100.47	109.60
1	A	419	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	21	ASN	CA-CB-CG	6.07	118.67	112.60
1	A	35	ASN	CA-CB-CG	6.05	118.65	112.60
1	B	148	PHE	CB-CA-C	6.03	121.29	109.35
1	B	212	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	384	GLY	O-C-N	5.88	128.97	122.68
1	A	365	VAL	N-CA-CB	-5.87	104.32	110.72
1	A	105	THR	CB-CA-C	5.86	122.96	110.07
1	A	349	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	334	GLN	CB-CG-CD	5.84	122.53	112.60
1	B	174	ASN	CA-C-N	5.83	128.37	120.44
1	B	174	ASN	C-N-CA	5.83	128.37	120.44
1	A	438	GLU	CB-CA-C	5.75	120.33	110.79
1	B	356	LYS	CB-CA-C	5.73	120.95	110.36
1	A	37	HIS	CA-C-N	5.67	128.46	122.11
1	A	37	HIS	C-N-CA	5.67	128.46	122.11
1	A	279	GLU	CB-CG-CD	5.60	122.12	112.60
1	A	195	GLU	CB-CG-CD	5.51	121.97	112.60
1	B	425	LEU	CA-C-N	-5.48	115.96	123.14
1	B	425	LEU	C-N-CA	-5.48	115.96	123.14
1	B	300	PRO	CA-C-N	5.48	128.17	120.28
1	B	300	PRO	C-N-CA	5.48	128.17	120.28
1	B	47	SER	CA-C-N	5.45	131.50	121.70
1	B	47	SER	C-N-CA	5.45	131.50	121.70
1	B	193	ASP	CB-CA-C	-5.44	104.01	111.73
1	A	394	ASN	CB-CG-ND2	5.43	124.54	116.40
1	A	100	PRO	CB-CA-C	-5.41	104.68	111.71
1	B	196	ARG	CB-CG-CD	5.33	123.56	111.30
1	A	407	PRO	CA-C-N	5.30	129.94	122.09
1	A	407	PRO	C-N-CA	5.30	129.94	122.09
1	A	388	THR	CA-CB-OG1	-5.24	101.73	109.60
1	A	134	GLU	CB-CG-CD	5.21	121.45	112.60
1	A	284	LYS	CA-C-N	5.20	130.10	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	LYS	C-N-CA	5.20	130.10	122.77
1	B	349	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	322	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	256	ASN	CA-C-N	-5.13	115.25	122.94
1	A	256	ASN	C-N-CA	-5.13	115.25	122.94
1	A	81	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	339	THR	CB-CA-C	5.12	118.45	110.67
1	B	407	PRO	CA-C-N	5.11	130.90	121.70
1	B	407	PRO	C-N-CA	5.11	130.90	121.70
1	A	357	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	133	ARG	N-CA-CB	5.08	117.51	109.94
1	B	356	LYS	CB-CG-CD	5.03	122.86	111.30
1	A	282	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	B	288	SER	CA-C-N	-5.01	115.98	122.94
1	B	288	SER	C-N-CA	-5.01	115.98	122.94

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	273	ARG	Sidechain
1	A	81	ARG	Sidechain
1	B	269	ARG	Sidechain
1	B	373	TYR	Peptide
1	B	82	ARG	Sidechain
1	B	88	ARG	Sidechain

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	3339	0	3274	70	1
1	B	3216	0	3153	74	0
2	A	14	0	0	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	8	0	12	4	0
5	A	13	0	18	8	0
6	A	4	0	3	1	0
7	A	68	0	0	27	0
7	B	54	0	0	27	0
All	All	6718	0	6460	147	1

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 11.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ALA:HB2	2:A:501:T83:CAA	1.32	1.54
1:A:169:ALA:CB	2:A:501:T83:CAA	1.95	1.44
4:A:504:EDO:H12	7:A:649:HOH:O	1.10	1.22
5:A:505:PG4:H72	7:A:632:HOH:O	1.39	1.19
1:A:355:HIS:HB3	7:A:617:HOH:O	1.43	1.18
1:B:192:TRP:CZ2	7:B:605:HOH:O	1.98	1.17
1:A:92:LEU:HB2	7:A:620:HOH:O	1.44	1.14
1:A:271:LYS:HD2	7:A:642:HOH:O	1.53	1.07
1:A:369:THR:HA	5:A:505:PG4:H52	1.36	1.06
4:A:504:EDO:C1	7:A:649:HOH:O	1.76	1.01
1:A:72:HIS:CD2	7:A:657:HOH:O	2.16	0.98
1:B:59:SER:H	1:B:147:MET:HE1	1.24	0.98
1:A:72:HIS:HD2	7:A:657:HOH:O	1.46	0.98
1:A:377:SER:HB2	7:A:648:HOH:O	1.66	0.93
1:A:38:VAL:HG23	7:A:645:HOH:O	1.70	0.92
1:B:132:THR:OG1	1:B:135:GLU:OE1	1.88	0.91
1:A:369:THR:HG23	5:A:505:PG4:H41	1.58	0.86
1:A:59:SER:OG	1:A:103:ASN:OD1	1.93	0.85
1:B:58:PRO:CD	1:B:147:MET:HE2	2.09	0.82
1:A:109:THR:CB	7:A:614:HOH:O	2.27	0.82
1:B:169:ALA:HA	7:B:651:HOH:O	1.78	0.81
1:B:9:ILE:HG13	7:B:609:HOH:O	1.80	0.81
1:A:169:ALA:HB3	2:A:501:T83:CAA	2.07	0.80
1:B:185:LYS:HE3	7:B:629:HOH:O	1.81	0.80
1:B:194:ARG:HD2	7:B:605:HOH:O	1.84	0.78
1:A:240:ASP:HB2	7:A:666:HOH:O	1.85	0.75
1:B:59:SER:N	1:B:147:MET:HE1	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:CE1	7:B:612:HOH:O	2.42	0.72
1:B:58:PRO:CG	1:B:147:MET:HE2	2.19	0.72
1:A:401:GLU:OE1	6:A:506:ACT:H2	1.91	0.71
1:B:58:PRO:HD2	1:B:147:MET:HE2	1.71	0.71
1:B:59:SER:H	1:B:147:MET:CE	2.02	0.71
1:A:369:THR:HA	5:A:505:PG4:C5	2.20	0.70
1:A:132:THR:C	7:A:603:HOH:O	2.35	0.70
1:B:192:TRP:CH2	7:B:605:HOH:O	2.29	0.70
1:A:377:SER:CB	7:A:648:HOH:O	2.32	0.69
1:A:34:ASN:HB2	7:A:618:HOH:O	1.93	0.67
1:B:167:LEU:CD1	1:B:290:ASN:ND2	2.59	0.66
1:B:72:HIS:CD2	7:B:633:HOH:O	2.49	0.65
1:B:59:SER:N	1:B:147:MET:CE	2.60	0.65
1:B:83:SER:O	1:B:86:ASP:O	2.15	0.65
1:A:107:ASN:CB	7:A:604:HOH:O	2.44	0.64
1:B:185:LYS:HE2	7:B:636:HOH:O	1.97	0.64
1:A:74:TYR:N	1:A:75:PRO:CD	2.61	0.63
1:B:147:MET:O	1:B:148:PHE:HD1	1.82	0.63
1:A:73:TYR:C	1:A:75:PRO:HD2	2.24	0.62
1:B:27:LEU:HD23	7:B:605:HOH:O	1.99	0.62
1:B:58:PRO:CB	1:B:147:MET:HE2	2.31	0.59
1:A:133:ARG:HA	7:A:603:HOH:O	2.01	0.59
1:A:232:ARG:HD3	1:A:425:LEU:HD21	1.84	0.59
1:B:74:TYR:N	1:B:75:PRO:CD	2.66	0.59
1:B:236:PHE:HB3	7:B:618:HOH:O	2.03	0.59
1:B:8:ASP:OD1	1:B:8:ASP:C	2.45	0.58
1:B:16:HIS:CE1	7:B:643:HOH:O	2.55	0.58
1:B:442:LYS:HD2	7:B:650:HOH:O	2.03	0.58
1:B:58:PRO:HB2	1:B:147:MET:CE	2.34	0.57
1:B:134:GLU:O	1:B:138:VAL:HG23	2.04	0.57
1:A:287:TYR:HB2	5:A:505:PG4:H51	1.84	0.57
1:A:3:THR:CG2	7:A:668:HOH:O	2.52	0.57
1:A:147:MET:HE3	1:A:153:TRP:HB3	1.86	0.57
1:A:3:THR:HG21	7:A:668:HOH:O	2.04	0.56
1:B:425:LEU:C	1:B:425:LEU:HD23	2.29	0.56
1:B:29:HIS:HB2	1:B:348:ILE:HG23	1.88	0.56
1:B:17:GLN:HB2	7:B:649:HOH:O	2.06	0.56
1:B:88:ARG:HH21	1:B:355:HIS:HB3	1.73	0.54
1:A:420:SER:CB	7:A:602:HOH:O	2.56	0.53
1:B:375:GLY:C	1:B:377:SER:H	2.17	0.53
1:B:419:ASP:N	1:B:419:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:HG2	7:B:636:HOH:O	2.10	0.52
1:B:58:PRO:CB	1:B:147:MET:CE	2.88	0.52
1:A:106:VAL:HG22	1:A:107:ASN:O	2.09	0.52
1:B:147:MET:O	1:B:148:PHE:CD1	2.61	0.52
1:A:240:ASP:CB	7:A:666:HOH:O	2.52	0.52
1:A:93:CYS:HA	1:A:97:GLN:OE1	2.10	0.51
1:B:373:TYR:HB2	7:B:654:HOH:O	2.09	0.51
1:B:93:CYS:HA	1:B:97:GLN:OE1	2.09	0.51
1:B:167:LEU:HD11	1:B:290:ASN:ND2	2.26	0.51
1:A:271:LYS:CD	7:A:642:HOH:O	2.30	0.51
1:A:22:ASP:OD1	1:A:94:SER:HB3	2.11	0.50
1:B:88:ARG:HH21	1:B:355:HIS:CB	2.25	0.49
1:A:394:ASN:HD22	1:A:395:LYS:HG3	1.77	0.49
1:B:213:PHE:CD1	1:B:312:TYR:CB	2.95	0.49
1:B:420:SER:HB3	7:B:601:HOH:O	2.13	0.49
1:B:89:PHE:HE1	7:B:612:HOH:O	1.89	0.48
1:B:375:GLY:C	1:B:377:SER:N	2.72	0.48
1:B:140:PRO:O	1:B:159:ILE:HA	2.14	0.47
1:A:33:ASP:O	4:A:503:EDO:H21	2.15	0.47
1:A:213:PHE:HB2	1:A:312:TYR:CZ	2.49	0.47
1:B:194:ARG:CD	7:B:605:HOH:O	2.53	0.47
1:B:370:ASP:O	1:B:371:TRP:HD1	1.97	0.47
1:B:58:PRO:HB2	1:B:147:MET:HE3	1.95	0.47
1:B:208:ALA:N	1:B:209:PRO:CD	2.77	0.47
1:A:73:TYR:C	1:A:75:PRO:CD	2.88	0.47
1:B:444:HIS:CE1	7:B:618:HOH:O	2.67	0.47
1:B:425:LEU:HD23	1:B:426:VAL:N	2.29	0.47
1:A:368:PHE:O	5:A:505:PG4:H52	2.15	0.47
1:A:140:PRO:O	1:A:159:ILE:HA	2.15	0.47
1:B:72:HIS:HD2	7:B:633:HOH:O	1.92	0.46
1:A:42:TYR:CD1	1:A:42:TYR:N	2.84	0.46
1:A:271:LYS:HZ2	1:A:401:GLU:HB3	1.80	0.46
1:B:58:PRO:HG3	1:B:383:TRP:CE2	2.51	0.45
1:B:419:ASP:CG	7:B:622:HOH:O	2.59	0.45
1:A:291:ILE:C	1:A:291:ILE:HD12	2.41	0.45
1:B:73:TYR:C	1:B:75:PRO:HD2	2.41	0.45
1:B:37:HIS:HB3	7:B:634:HOH:O	2.16	0.45
1:B:213:PHE:CE1	1:B:312:TYR:HB3	2.52	0.44
1:B:58:PRO:CD	1:B:147:MET:CE	2.90	0.44
1:B:271:LYS:NZ	1:B:401:GLU:OE1	2.42	0.44
1:A:37:HIS:HB2	4:A:503:EDO:H22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD11	1:A:145:VAL:HG23	2.00	0.44
1:A:420:SER:HB3	7:A:602:HOH:O	2.17	0.44
1:A:85:SER:OG	1:A:86:ASP:N	2.50	0.44
1:B:27:LEU:HB3	1:B:31:ASP:CB	2.48	0.44
1:B:58:PRO:HG3	1:B:383:TRP:CZ2	2.52	0.44
1:B:63:SER:CB	7:B:603:HOH:O	2.66	0.44
1:B:194:ARG:CZ	7:B:605:HOH:O	2.66	0.43
1:A:208:ALA:N	1:A:209:PRO:CD	2.81	0.43
1:B:58:PRO:HD2	1:B:147:MET:CE	2.44	0.43
1:A:195:GLU:HB2	7:A:609:HOH:O	2.19	0.43
1:A:311:MET:HE3	1:A:311:MET:HA	2.01	0.43
1:A:3:THR:HG23	1:A:3:THR:O	2.19	0.43
1:A:448:PHE:O	1:A:449:ALA:C	2.63	0.42
1:B:19:LEU:HD11	1:B:93:CYS:HB3	2.01	0.42
1:A:133:ARG:N	7:A:603:HOH:O	2.48	0.42
1:A:425:LEU:C	1:A:425:LEU:HD23	2.43	0.42
1:B:185:LYS:CE	7:B:636:HOH:O	2.59	0.42
1:A:2:ALA:O	1:A:3:THR:HG22	2.18	0.42
1:A:5:GLU:O	1:A:104:ALA:HB1	2.19	0.42
1:A:213:PHE:CE1	1:A:312:TYR:HB3	2.54	0.42
1:B:275:ALA:O	1:B:276:LYS:C	2.61	0.42
1:A:58:PRO:HG3	1:A:383:TRP:CZ2	2.54	0.42
1:A:59:SER:O	1:A:63:SER:OG	2.37	0.42
1:A:74:TYR:CG	1:A:75:PRO:HD3	2.55	0.41
1:A:169:ALA:HB1	2:A:501:T83:CAA	2.26	0.41
1:B:194:ARG:NH1	7:B:605:HOH:O	2.52	0.41
1:A:107:ASN:CA	7:A:604:HOH:O	2.68	0.41
1:A:120:ASP:O	1:A:121:PRO:C	2.62	0.41
1:A:15:SER:HA	7:A:619:HOH:O	2.21	0.41
1:A:369:THR:CG2	5:A:505:PG4:H41	2.41	0.41
1:A:394:ASN:ND2	1:A:395:LYS:HG3	2.35	0.41
1:B:70:LEU:HD23	1:B:70:LEU:HA	1.91	0.41
1:A:86:ASP:OD1	1:A:86:ASP:C	2.64	0.41
1:B:27:LEU:HB3	1:B:31:ASP:HB2	2.02	0.41
1:A:21:ASN:O	1:A:22:ASP:O	2.39	0.40
1:A:368:PHE:O	5:A:505:PG4:C5	2.69	0.40
1:B:14:PRO:HA	1:B:67:ALA:O	2.22	0.40
1:B:29:HIS:CB	1:B:348:ILE:HG23	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH2	1:A:279:GLU:OE2[4_465]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/451 (93%)	393 (94%)	23 (6%)	3 (1%)	18	32
1	B	401/451 (89%)	382 (95%)	12 (3%)	7 (2%)	7	12
All	All	820/902 (91%)	775 (94%)	35 (4%)	10 (1%)	10	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	B	22	ASP
1	B	149	GLN
1	B	150	CYS
1	B	151	GLY
1	B	376	HIS
1	B	83	SER
1	A	120	ASP
1	A	151	GLY
1	B	192	TRP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/380 (95%)	327 (91%)	34 (9%)	8	16
1	B	348/380 (92%)	322 (92%)	26 (8%)	12	24
All	All	709/760 (93%)	649 (92%)	60 (8%)	10	19

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	24	THR
1	A	42	TYR
1	A	43	LEU
1	A	47	SER
1	A	59	SER
1	A	61	VAL
1	A	63	SER
1	A	81	ARG
1	A	83	SER
1	A	85	SER
1	A	87	ASN
1	A	120	ASP
1	A	128	VAL
1	A	147	MET
1	A	159	ILE
1	A	184	THR
1	A	185	LYS
1	A	233	ASP
1	A	240	ASP
1	A	252	LYS
1	A	256	ASN
1	A	271	LYS
1	A	288	SER
1	A	289	ILE
1	A	299	LEU
1	A	321	ILE
1	A	388	THR
1	A	394	ASN
1	A	419	ASP
1	A	420	SER
1	A	424	VAL
1	A	426	VAL
1	A	445	LYS
1	B	9	ILE

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Mol	Chain	Res	Type
1	B	21	ASN
1	B	34	ASN
1	B	42	TYR
1	B	47	SER
1	B	61	VAL
1	B	63	SER
1	B	81	ARG
1	B	128	VAL
1	B	184	THR
1	B	185	LYS
1	B	187	SER
1	B	203	LYS
1	B	252	LYS
1	B	256	ASN
1	B	288	SER
1	B	289	ILE
1	B	299	LEU
1	B	321	ILE
1	B	333	LYS
1	B	336	LYS
1	B	388	THR
1	B	389	VAL
1	B	419	ASP
1	B	423	LYS
1	B	426	VAL

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

Mol	Chain	Res	Type
1	A	13	GLN
1	A	35	ASN
1	A	149	GLN
1	A	161	HIS
1	A	256	ASN
1	A	282	ASN
1	A	306	ASN
1	A	376	HIS
1	A	394	ASN
1	B	13	GLN
1	B	37	HIS
1	B	256	ASN
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	306	ASN

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
4	EDO	A	504	-	3,3,3	0.96	0	2,2,2	1.02	0
5	PG4	A	505	-	12,12,12	1.99	7 (58%)	11,11,11	2.37	5 (45%)
6	ACT	A	506	-	3,3,3	2.90	2 (66%)	3,3,3	1.29	0
4	EDO	A	503	-	3,3,3	1.47	0	2,2,2	1.49	1 (50%)
2	T83	A	501	-	15,15,15	2.15	4 (26%)	21,21,21	4.20	14 (66%)

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
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
5	PG4	A	505	-	-	8/10/10/10	-
2	T83	A	501	-	-	2/2/2/2	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	T83	CAD-CAE	5.43	1.43	1.34
6	A	506	ACT	O-C	3.63	1.38	1.22
2	A	501	T83	CAF-CAN	3.62	1.45	1.38
6	A	506	ACT	CH3-C	2.92	1.60	1.49
2	A	501	T83	OAC-CAJ	2.89	1.42	1.36
2	A	501	T83	CAG-CAK	2.71	1.43	1.38
5	A	505	PG4	O3-C4	2.47	1.52	1.42
5	A	505	PG4	O4-C7	2.40	1.52	1.42
5	A	505	PG4	C6-C5	2.35	1.60	1.49
5	A	505	PG4	O4-C6	2.26	1.51	1.42
5	A	505	PG4	C7-C8	2.25	1.61	1.49
5	A	505	PG4	O2-C3	2.13	1.51	1.42
5	A	505	PG4	C4-C3	2.10	1.59	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	T83	CAA-OAH-CAK	-12.78	98.76	117.51
2	A	501	T83	CAG-CAK-CAJ	7.86	127.98	120.04
2	A	501	T83	OAI-CAL-CAD	5.73	125.09	117.14
5	A	505	PG4	O3-C5-C6	5.09	133.56	110.35
2	A	501	T83	OAB-CAL-CAD	-4.02	118.84	126.00
2	A	501	T83	CAE-CAD-CAL	-3.82	116.73	121.39
2	A	501	T83	CAF-CAJ-CAK	-3.58	116.34	119.81
2	A	501	T83	CAN-CAM-CAE	3.45	122.31	117.87
2	A	501	T83	CAM-CAG-CAK	-3.11	115.78	120.74
2	A	501	T83	CAM-CAE-CAD	-3.11	117.20	121.52
5	A	505	PG4	C7-O4-C6	3.02	126.48	113.26
5	A	505	PG4	O3-C4-C3	3.02	124.11	110.35
2	A	501	T83	CAG-CAM-CAN	-2.65	116.23	119.42
2	A	501	T83	CAF-CAN-CAM	2.61	125.65	120.15
5	A	505	PG4	C3-O2-C2	2.45	123.99	113.26
2	A	501	T83	CAN-OAI-CAL	-2.37	118.71	121.67
5	A	505	PG4	O4-C7-C8	2.35	120.48	110.11
2	A	501	T83	OAH-CAK-CAG	-2.33	120.07	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	T83	OAI-CAN-CAM	-2.31	117.91	120.51
4	A	503	EDO	O2-C2-C1	2.11	128.42	112.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

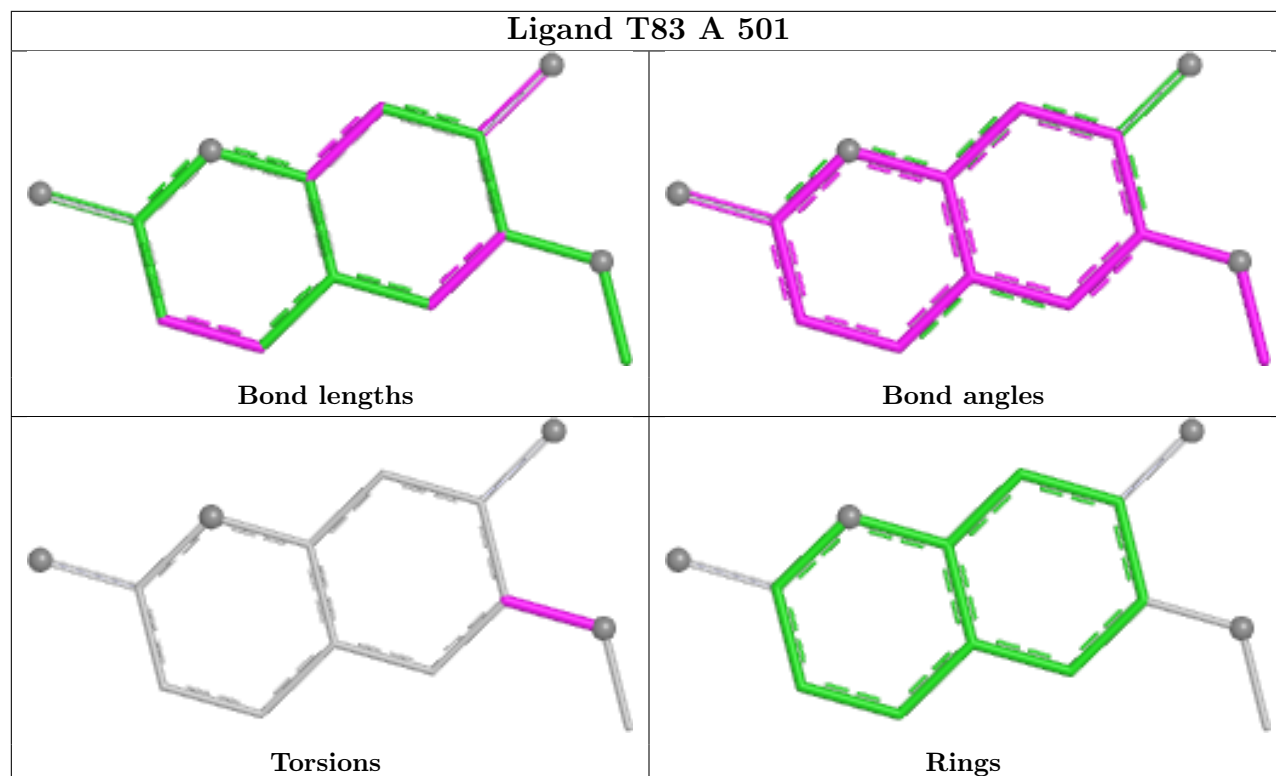
Mol	Chain	Res	Type	Atoms
5	A	505	PG4	C6-C5-O3-C4
2	A	501	T83	CAJ-CAK-OAH-CAA
2	A	501	T83	CAG-CAK-OAH-CAA
5	A	505	PG4	O4-C7-C8-O5
5	A	505	PG4	O1-C1-C2-O2
5	A	505	PG4	O2-C3-C4-O3
5	A	505	PG4	C5-C6-O4-C7
5	A	505	PG4	C8-C7-O4-C6
4	A	504	EDO	O1-C1-C2-O2
5	A	505	PG4	C1-C2-O2-C3
5	A	505	PG4	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	EDO	2	0
5	A	505	PG4	8	0
6	A	506	ACT	1	0
4	A	503	EDO	2	0
2	A	501	T83	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	A	426/451 (94%)	-0.53	1 (0%) 91 90	26, 68, 104, 133	1 (0%)
1	B	409/451 (90%)	-0.48	0 100 100	65, 86, 111, 132	0
All	All	835/902 (92%)	-0.50	1 (0%) 92 91	26, 79, 108, 133	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	PRO	2.5

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.

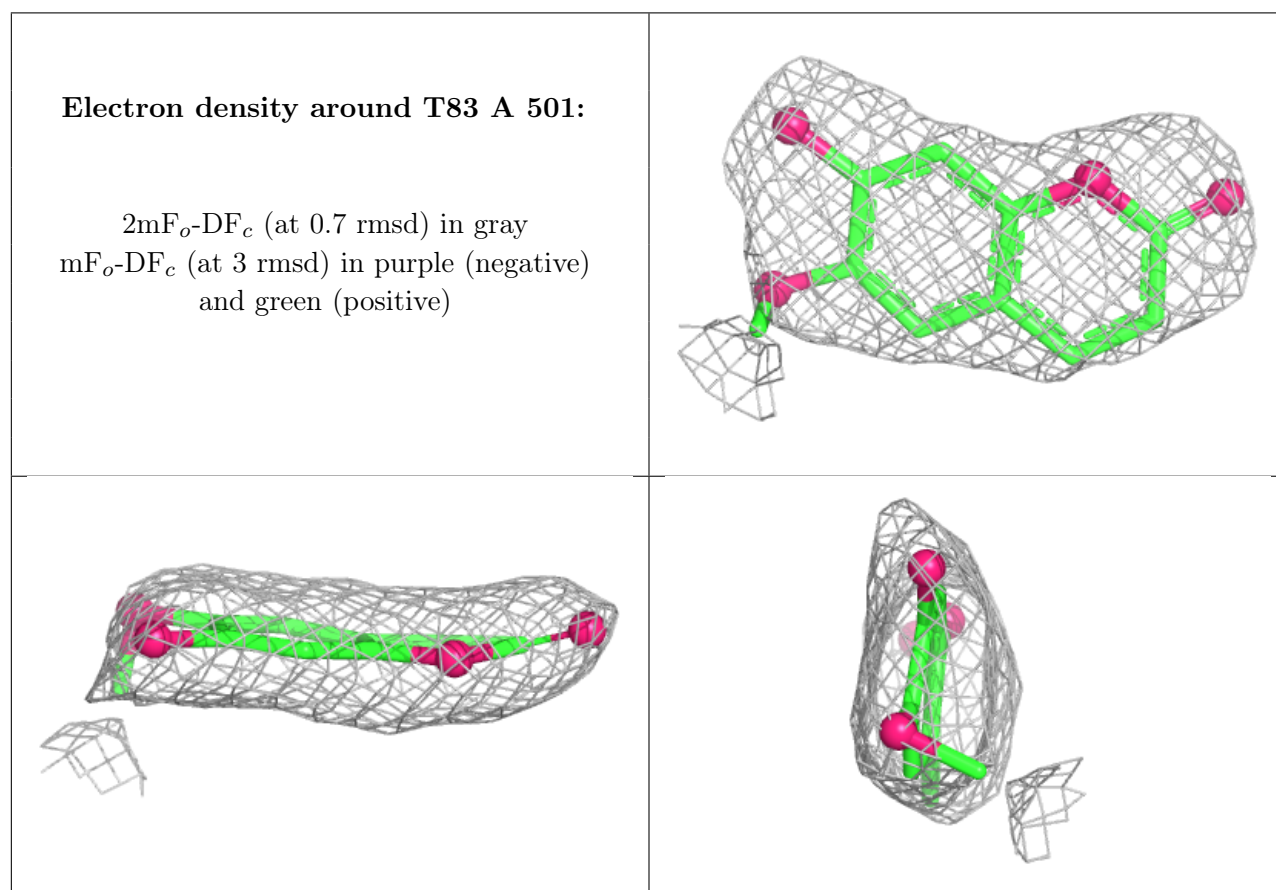
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	A	505	13/13	0.87	0.12	67,76,87,87	0
4	EDO	A	504	4/4	0.95	0.09	71,72,76,79	0
2	T83	A	501	14/14	0.95	0.08	62,68,83,105	0
3	CA	A	502	1/1	0.97	0.05	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	501	1/1	0.98	0.03	80,80,80,80	0
4	EDO	A	503	4/4	0.98	0.07	65,66,78,80	0
6	ACT	A	506	4/4	0.98	0.08	56,63,65,78	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 ⓘ

There are no such residues in this entry.