



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:44 PM UTC

PDB ID : 8F7V / pdb_00008f7v
Title : Macrocyclic plasmin inhibitor
Authors : Guojie, W.
Deposited on : 2022-11-20
Resolution : 1.65 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

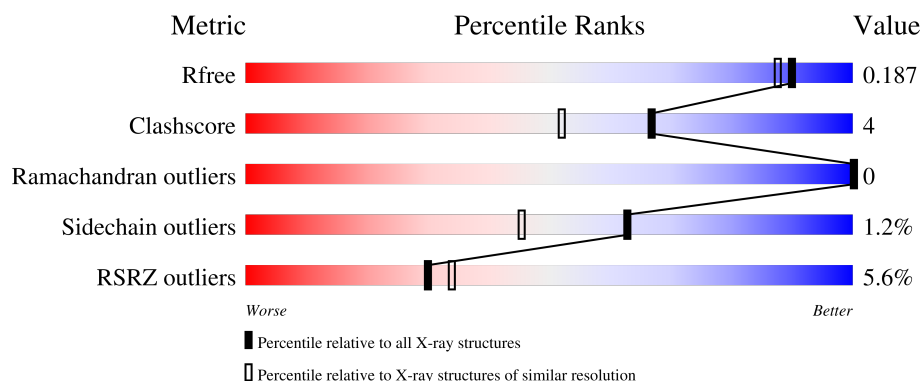
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	250	
1	B	250	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4370 atoms, of which 100 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.

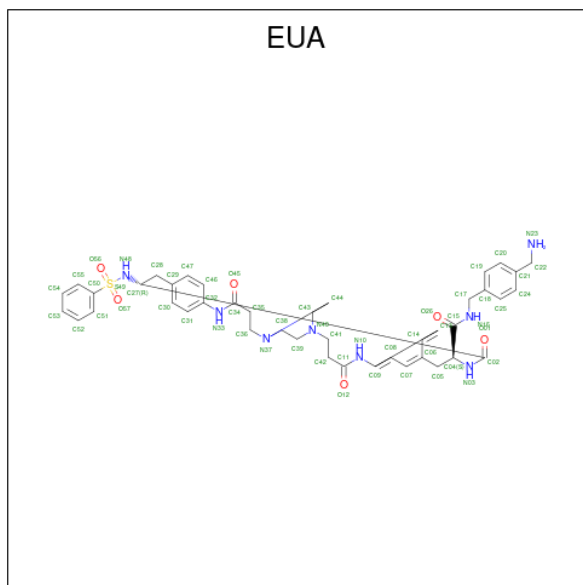
- Molecule 1 is a protein called Plasminogen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	1
			1853	1175	327	337	14			
1	B	242	Total	C	N	O	S	0	3	0
			1875	1193	332	334	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	ALA	SER	engineered mutation	UNP P00747
B	741	ALA	SER	engineered mutation	UNP P00747

- Molecule 2 is (6S,9R,19S,22R)-N-{[4-(aminomethyl)phenyl]methyl}-22-[(benzenesulfonyl)amino]-3,12,21-trioxo-2,6,9,13,20-pentaazatetracyclo[22.2.2.2 6,9 .2 14,17]dotriaconta-1(26), 14,16,24,27,29-hexaene-19-carboxamide (CCD ID: EUA) (formula: C₄₂H₅₀N₈O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			107	42	50	8	6	1		
2	B	1	Total	C	H	N	O	S	0	0
			107	42	50	8	6	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

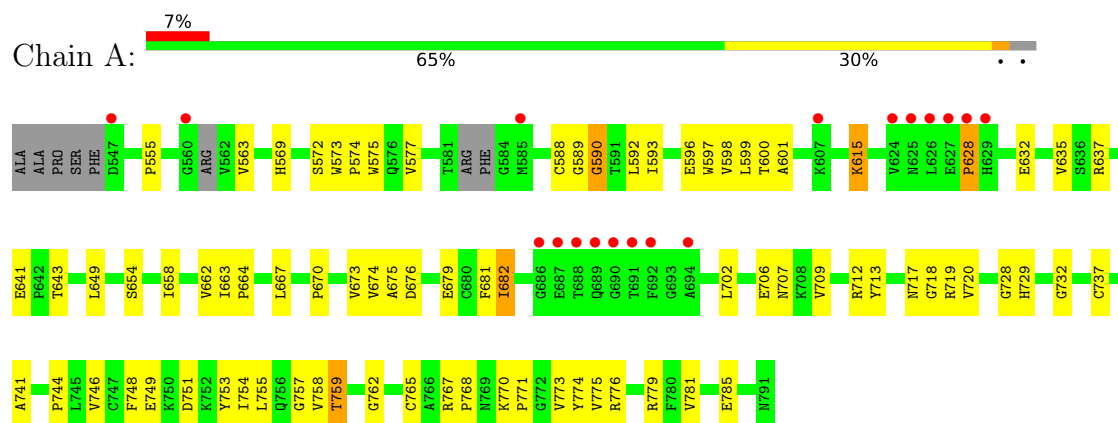
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total	O	0	0
			151	151		
5	B	226	Total	O	0	0
			226	226		

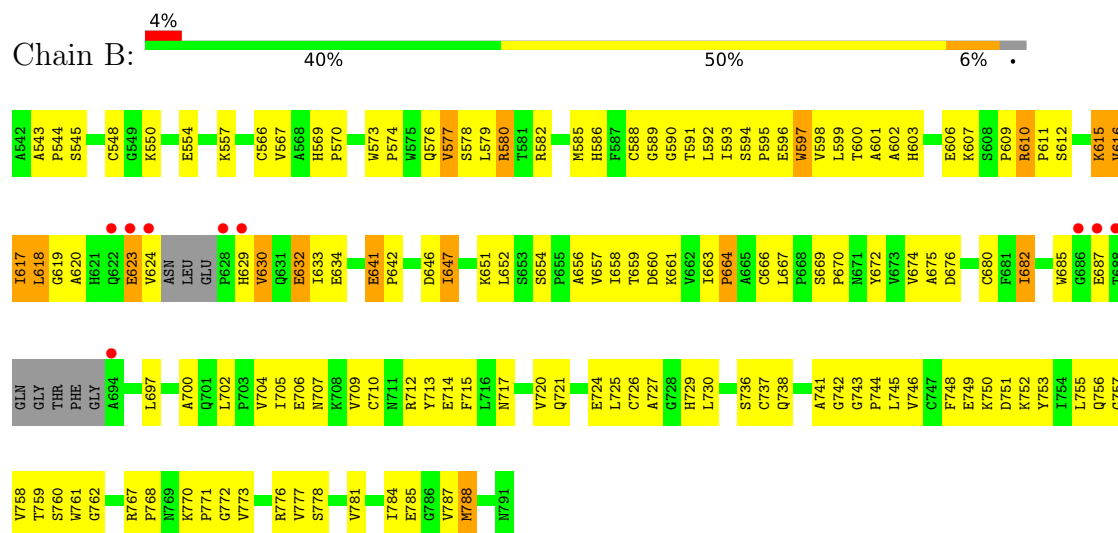
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Plasminogen



• Molecule 1: Plasminogen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.68Å 50.19Å 92.02Å 90.00° 93.31° 90.00°	Depositor
Resolution (Å)	48.60 – 1.65 48.60 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.60-1.65) 99.9 (48.60-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.173 , 0.187 0.173 , 0.187	Depositor DCC
R_{free} test set	2706 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4370	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EUA, SO4, GOL

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	1.98	66/1899 (3.5%)	1.15	4/2579 (0.2%)
1	B	2.33	137/1931 (7.1%)	1.24	15/2618 (0.6%)
All	All	2.16	203/3830 (5.3%)	1.19	19/5197 (0.4%)

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	788[A]	MET	N-CA	16.38	1.66	1.46
1	B	788[B]	MET	N-CA	16.38	1.66	1.46
1	B	712[A]	ARG	C-N	-14.81	1.14	1.33
1	B	712[B]	ARG	C-N	-14.81	1.14	1.33
1	B	788[A]	MET	CA-C	12.68	1.69	1.52
1	B	788[B]	MET	CA-C	12.68	1.69	1.52
1	A	771	PRO	C-O	-8.52	1.14	1.23
1	B	616	VAL	C-O	-8.28	1.15	1.24
1	B	741	ALA	C-O	-8.14	1.14	1.23
1	B	598	VAL	C-O	-8.06	1.15	1.24
1	B	657	VAL	C-O	-8.04	1.15	1.24
1	A	598	VAL	C-O	-7.83	1.16	1.24
1	A	601	ALA	C-O	-7.70	1.14	1.23
1	B	590	GLY	C-O	-7.64	1.16	1.23
1	B	712[A]	ARG	C-O	7.57	1.34	1.23
1	B	712[B]	ARG	C-O	7.57	1.34	1.23
1	B	588	CYS	C-O	-7.57	1.15	1.23
1	B	550	LYS	C-O	-7.50	1.17	1.24
1	A	682	ILE	C-O	-7.50	1.16	1.24
1	B	591	THR	C-O	-7.49	1.15	1.24
1	B	594	SER	C-O	-7.40	1.14	1.24
1	B	610	ARG	C-O	-7.36	1.15	1.24
1	B	700	ALA	C-O	-7.36	1.15	1.23
1	A	770	LYS	C-O	-7.31	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	706	GLU	C-O	-7.27	1.15	1.23
1	B	745	LEU	C-O	-7.24	1.15	1.24
1	A	737	CYS	C-O	-7.23	1.16	1.23
1	B	772	GLY	C-O	-7.22	1.14	1.23
1	B	586	HIS	C-O	-7.22	1.15	1.23
1	B	674	VAL	C-O	-7.21	1.16	1.24
1	A	706	GLU	C-O	-7.20	1.15	1.23
1	B	641	GLU	C-O	-7.17	1.15	1.24
1	A	781	VAL	C-O	-7.10	1.15	1.24
1	B	788[A]	MET	C-O	-7.09	1.15	1.24
1	B	788[B]	MET	C-O	-7.09	1.15	1.24
1	B	724	GLU	C-O	-7.06	1.15	1.23
1	B	600	THR	C-O	-6.85	1.16	1.23
1	B	755	LEU	C-O	-6.85	1.15	1.24
1	A	762	GLY	C-O	-6.81	1.17	1.23
1	B	593	ILE	C-O	-6.79	1.16	1.24
1	B	654	SER	C-O	-6.78	1.17	1.24
1	B	770	LYS	C-O	-6.75	1.16	1.24
1	B	776	ARG	C-O	-6.75	1.15	1.23
1	B	573	TRP	C-O	-6.73	1.16	1.24
1	B	709	VAL	C-O	-6.73	1.16	1.24
1	A	675	ALA	C-O	-6.71	1.15	1.23
1	A	702	LEU	C-O	-6.71	1.15	1.24
1	B	570	PRO	C-O	-6.69	1.14	1.23
1	A	741	ALA	C-O	-6.68	1.16	1.23
1	A	768	PRO	C-O	-6.66	1.16	1.23
1	A	597	TRP	C-O	-6.64	1.16	1.24
1	B	615	LYS	C-O	-6.61	1.15	1.23
1	B	617	ILE	C-O	-6.59	1.17	1.24
1	B	666	CYS	C-O	-6.59	1.15	1.23
1	A	748	PHE	C-O	-6.56	1.16	1.24
1	B	611	PRO	C-O	-6.55	1.16	1.24
1	B	777	VAL	C-O	-6.50	1.16	1.24
1	B	618	LEU	C-O	-6.50	1.15	1.23
1	B	787	VAL	C-O	-6.46	1.16	1.24
1	A	674	VAL	C-O	-6.45	1.17	1.24
1	B	771	PRO	C-O	-6.38	1.16	1.23
1	A	641	GLU	C-O	-6.36	1.16	1.24
1	B	634	GLU	C-O	-6.36	1.15	1.23
1	B	702	LEU	C-O	-6.36	1.15	1.24
1	B	712[A]	ARG	CA-C	-6.36	1.45	1.52
1	B	712[B]	ARG	CA-C	-6.36	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	710	CYS	C-O	-6.35	1.16	1.24
1	B	545	SER	C-O	-6.34	1.14	1.24
1	B	746	VAL	C-O	-6.34	1.17	1.24
1	B	599	LEU	C-O	-6.34	1.16	1.24
1	A	593	ILE	C-O	-6.34	1.16	1.24
1	B	744	PRO	C-O	-6.29	1.16	1.23
1	B	663	ILE	C-O	-6.28	1.16	1.24
1	B	781	VAL	C-O	-6.28	1.16	1.24
1	A	635	VAL	C-O	-6.27	1.17	1.24
1	B	659	THR	C-O	-6.27	1.16	1.23
1	B	749	GLU	C-O	-6.26	1.16	1.23
1	A	775	VAL	C-O	-6.26	1.17	1.24
1	A	712	ARG	C-O	-6.25	1.15	1.23
1	B	680	CYS	C-O	-6.22	1.15	1.23
1	B	664	PRO	C-O	-6.22	1.16	1.23
1	B	762	GLY	C-O	-6.21	1.17	1.23
1	B	632	GLU	C-O	-6.20	1.16	1.24
1	B	785	GLU	C-O	-6.19	1.16	1.24
1	B	619	GLY	C-O	-6.17	1.16	1.24
1	B	589	GLY	C-O	-6.14	1.16	1.23
1	B	748	PHE	C-O	-6.12	1.16	1.23
1	A	757	GLY	C-O	-6.10	1.15	1.23
1	B	675	ALA	C-O	-6.09	1.16	1.23
1	A	785	GLU	C-O	-6.08	1.17	1.24
1	B	705	ILE	C-O	-6.07	1.17	1.24
1	B	720	VAL	C-O	-6.06	1.16	1.24
1	A	592	LEU	C-O	-6.06	1.16	1.24
1	A	755	LEU	C-O	-6.05	1.16	1.24
1	B	620	ALA	C-O	-6.04	1.16	1.23
1	A	573	TRP	C-O	-6.03	1.17	1.24
1	A	670	PRO	C-O	-5.98	1.16	1.23
1	B	697	LEU	C-O	-5.96	1.16	1.23
1	B	548	CYS	C-O	-5.89	1.16	1.23
1	A	765	CYS	C-O	-5.88	1.17	1.24
1	B	737	CYS	C-O	-5.88	1.17	1.23
1	A	759	THR	C-O	-5.87	1.17	1.24
1	A	746	VAL	C-O	-5.87	1.17	1.24
1	A	707	ASN	C-O	-5.86	1.17	1.24
1	B	602	ALA	C-O	-5.86	1.17	1.24
1	A	749	GLU	C-O	-5.85	1.17	1.24
1	B	585[A]	MET	C-N	-5.84	1.25	1.33
1	B	585[B]	MET	C-N	-5.84	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	753	TYR	C-O	-5.83	1.17	1.24
1	B	651	LYS	C-O	-5.82	1.17	1.24
1	B	715	PHE	C-O	-5.82	1.15	1.25
1	B	676	ASP	C-O	-5.82	1.17	1.23
1	B	567	VAL	C-O	-5.78	1.17	1.24
1	B	713	TYR	C-O	-5.78	1.17	1.24
1	B	612	SER	C-O	-5.77	1.16	1.24
1	B	576	GLN	C-O	-5.77	1.17	1.23
1	A	720	VAL	C-O	-5.76	1.17	1.24
1	B	574	PRO	C-O	-5.76	1.16	1.24
1	B	773	VAL	C-O	-5.75	1.18	1.24
1	B	730	LEU	C-O	-5.74	1.16	1.24
1	A	776	ARG	C-O	-5.72	1.16	1.23
1	B	609	PRO	C-O	-5.72	1.17	1.24
1	B	725	LEU	C-O	-5.71	1.16	1.23
1	B	656	ALA	C-O	-5.70	1.16	1.23
1	A	643	THR	C-O	-5.70	1.16	1.23
1	B	582	ARG	C-O	-5.67	1.17	1.24
1	B	566	CYS	C-O	-5.66	1.17	1.23
1	B	595	PRO	C-O	-5.66	1.17	1.24
1	B	729	HIS	C-O	-5.65	1.17	1.23
1	A	663	ILE	C-O	-5.64	1.17	1.24
1	B	652	LEU	C-O	-5.61	1.16	1.23
1	A	758	VAL	C-O	-5.60	1.18	1.24
1	B	603	HIS	C-O	-5.60	1.17	1.24
1	A	729	HIS	C-O	-5.58	1.17	1.24
1	B	743	GLY	C-O	-5.58	1.15	1.24
1	B	667	LEU	C-O	-5.57	1.16	1.23
1	A	767	ARG	C-O	-5.56	1.16	1.24
1	A	709	VAL	C-O	-5.52	1.17	1.24
1	B	577	VAL	C-O	-5.52	1.18	1.24
1	A	673	VAL	C-O	-5.51	1.18	1.24
1	A	563	VAL	C-O	-5.50	1.17	1.24
1	B	557	LYS	C-O	-5.49	1.16	1.23
1	A	773	VAL	C-O	-5.49	1.18	1.24
1	A	590	GLY	C-O	-5.44	1.18	1.23
1	B	601	ALA	C-O	-5.41	1.17	1.23
1	A	649	LEU	C-O	-5.41	1.17	1.24
1	A	744	PRO	C-O	-5.41	1.17	1.23
1	B	753	TYR	C-O	-5.41	1.17	1.23
1	B	721	GLN	C-O	-5.40	1.16	1.23
1	B	592	LEU	C-O	-5.39	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	757	GLY	C-O	-5.39	1.16	1.23
1	B	670	PRO	C-O	-5.38	1.17	1.23
1	B	767	ARG	C-O	-5.38	1.17	1.23
1	A	637	ARG	C-O	-5.36	1.17	1.23
1	B	761	TRP	C-O	-5.36	1.17	1.23
1	A	662	VAL	C-O	-5.36	1.18	1.24
1	B	707	ASN	C-O	-5.36	1.17	1.24
1	B	726	CYS	C-O	-5.35	1.17	1.23
1	B	554	GLU	C-O	-5.34	1.16	1.24
1	A	667	LEU	C-O	-5.34	1.16	1.23
1	A	589	GLY	C-O	-5.33	1.17	1.23
1	A	679	GLU	C-O	-5.33	1.17	1.24
1	B	579	LEU	C-O	-5.33	1.17	1.24
1	A	728	GLY	C-O	-5.32	1.15	1.23
1	B	736	SER	C-O	-5.32	1.16	1.23
1	B	752	LYS	C-O	-5.32	1.17	1.23
1	B	758	VAL	C-O	-5.32	1.18	1.24
1	B	784	ILE	C-O	-5.30	1.18	1.24
1	A	713	TYR	C-O	-5.29	1.18	1.24
1	B	768	PRO	C-O	-5.29	1.17	1.23
1	A	681	PHE	C-O	-5.26	1.17	1.24
1	B	760	SER	C-O	-5.26	1.17	1.24
1	A	779	ARG	C-O	-5.26	1.17	1.24
1	B	751	ASP	C-O	-5.25	1.17	1.24
1	B	742	GLY	C-O	-5.25	1.16	1.24
1	A	654	SER	N-CA	-5.24	1.41	1.45
1	B	661	LYS	C-O	-5.24	1.17	1.24
1	B	596	GLU	C-O	-5.23	1.16	1.23
1	B	633	ILE	C-O	-5.22	1.18	1.24
1	B	682	ILE	C-O	-5.21	1.18	1.24
1	B	647	ILE	C-O	-5.19	1.17	1.23
1	B	714	GLU	C-O	-5.18	1.17	1.24
1	B	669	SER	C-O	-5.17	1.17	1.23
1	B	727	ALA	C-O	-5.17	1.17	1.23
1	B	543	ALA	C-O	-5.15	1.17	1.23
1	A	575	TRP	C-O	-5.14	1.17	1.24
1	B	704	VAL	C-O	-5.13	1.18	1.24
1	A	719	ARG	C-O	-5.12	1.17	1.24
1	B	756	GLN	C-O	-5.09	1.17	1.24
1	A	600	THR	C-O	-5.08	1.18	1.23
1	B	580	ARG	C-O	-5.08	1.17	1.23
1	B	759	THR	C-O	-5.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	778	SER	C-O	-5.08	1.17	1.24
1	A	676	ASP	C-O	-5.07	1.17	1.23
1	A	751	ASP	N-CA	-5.07	1.41	1.46
1	A	588	CYS	C-O	-5.06	1.17	1.23
1	A	599	LEU	C-O	-5.06	1.17	1.24
1	B	544	PRO	C-O	-5.06	1.18	1.23
1	B	660	ASP	C-O	-5.06	1.17	1.24
1	B	672	TYR	C-O	-5.05	1.17	1.23
1	A	754	ILE	C-O	-5.04	1.18	1.24
1	A	718	GLY	C-O	-5.03	1.17	1.24
1	B	646	ASP	C-O	-5.01	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	712[A]	ARG	O-C-N	-11.24	109.59	122.75
1	B	712[B]	ARG	O-C-N	-11.24	109.59	122.75
1	B	712[A]	ARG	CA-C-N	8.31	131.76	120.38
1	B	712[A]	ARG	C-N-CA	8.31	131.76	120.38
1	B	712[B]	ARG	CA-C-N	8.31	131.76	120.38
1	B	712[B]	ARG	C-N-CA	8.31	131.76	120.38
1	B	569	HIS	N-CA-C	-7.14	99.00	109.50
1	A	717	ASN	N-CA-C	6.42	120.11	111.24
1	B	629	HIS	N-CA-C	-6.26	105.50	113.01
1	A	628	PRO	CB-CA-C	-6.02	101.63	111.56
1	B	642	PRO	N-CA-C	5.46	120.75	114.03
1	B	744	PRO	N-CA-C	5.45	120.77	111.68
1	B	717	ASN	N-CA-C	5.43	118.88	111.39
1	A	569	HIS	N-CA-C	-5.43	101.52	109.50
1	B	597	TRP	N-CA-C	5.32	117.75	108.76
1	B	720	VAL	N-CA-C	5.21	116.09	108.58
1	B	745	LEU	N-CA-C	-5.21	98.90	108.02
1	A	720	VAL	N-CA-C	5.12	115.96	108.58
1	B	736	SER	N-CA-C	-5.11	103.65	110.55

There are no chirality outliers.

There are no planarity outliers.

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	1853	0	1828	10	0
1	B	1875	0	1868	18	0
2	A	57	50	0	0	0
2	B	57	50	0	0	0
3	A	15	0	0	0	0
3	B	30	0	0	0	0
4	B	6	0	8	0	0
5	A	151	0	0	2	0
5	B	226	0	0	2	0
All	All	4270	100	3704	28	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 4.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:VAL:HG13	1:B:616:VAL:HG13	1.53	0.91
1:B:606:GLU:OE1	1:B:607:LYS:HE2	1.84	0.77
1:B:577:VAL:CG1	1:B:616:VAL:HG13	2.16	0.75
1:B:597:TRP:CD1	1:B:788[B]:MET:HE3	2.26	0.70
1:A:577:VAL:HG22	1:A:590:GLY:C	2.29	0.58
1:B:623:GLU:HG2	1:B:685:TRP:CD1	2.38	0.57
1:A:682:ILE:HD12	1:A:682:ILE:C	2.36	0.50
1:A:596:GLU:HG2	5:A:1023:HOH:O	2.12	0.49
1:A:615:LYS:HE2	1:A:632:GLU:OE1	2.11	0.49
1:B:682:ILE:C	1:B:682:ILE:HD12	2.40	0.47
1:B:641:GLU:HB2	1:B:647:ILE:HG23	1.97	0.46
1:B:578:SER:HB3	1:B:617:ILE:HB	1.96	0.46
1:B:617:ILE:HG23	1:B:630:VAL:HG13	1.97	0.46
1:B:687:GLU:HG2	1:B:738:GLN:HB2	1.98	0.46
1:B:615:LYS:NZ	1:B:632:GLU:OE2	2.46	0.45
1:A:658:ILE:HD12	1:A:664:PRO:HD3	1.98	0.44
1:B:606:GLU:CD	1:B:607:LYS:HE2	2.41	0.43
1:B:750:LYS:HE2	5:B:1086:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:ARG:NH1	5:B:906:HOH:O	2.47	0.43
1:B:577:VAL:HG22	1:B:618:LEU:CD2	2.48	0.43
1:A:732:GLY:HA2	5:A:953:HOH:O	2.19	0.42
1:A:555:PRO:CA	1:A:572:SER:HB2	2.50	0.42
1:B:617:ILE:HG23	1:B:630:VAL:CG1	2.50	0.41
1:A:572:SER:C	1:A:574:PRO:HD3	2.46	0.41
1:A:682:ILE:HD12	1:A:682:ILE:O	2.21	0.40
1:A:759:THR:HA	1:A:774:TYR:CD2	2.56	0.40
1:B:658:ILE:HD12	1:B:664:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/250 (95%)	226 (95%)	11 (5%)	0	100	100
1	B	237/250 (95%)	231 (98%)	6 (2%)	0	100	100
All	All	474/500 (95%)	457 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	203/209 (97%)	201 (99%)	2 (1%)	68	52
1	B	206/209 (99%)	203 (98%)	3 (2%)	57	37
All	All	409/418 (98%)	404 (99%)	5 (1%)	63	45

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	615	LYS
1	A	628	PRO
1	B	623	GLU
1	B	624	VAL
1	B	630	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	HIS
1	A	625	ASN
1	A	769	ASN
1	B	769	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 ⓘ

12 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
3	SO4	A	804	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	B	803	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	B	804	-	4,4,4	0.21	0	6,6,6	0.16	0
3	SO4	B	806	-	4,4,4	0.80	0	6,6,6	0.89	0
2	EUA	A	801	-	62,62,62	3.32	28 (45%)	85,85,85	1.77	18 (21%)
3	SO4	B	805	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	B	807	-	4,4,4	0.49	0	6,6,6	0.34	0
3	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.09	0
2	EUA	B	801	-	62,62,62	2.70	23 (37%)	85,85,85	1.90	17 (20%)
4	GOL	B	808	-	5,5,5	0.88	0	5,5,5	1.18	1 (20%)
3	SO4	A	803	-	4,4,4	0.22	0	6,6,6	0.12	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	EUA	A	801	-	-	10/56/66/66	0/5/6/6
2	EUA	B	801	-	-	12/56/66/66	0/5/6/6
4	GOL	B	808	-	-	0/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	EUA	O56-S49	-11.27	1.30	1.43
2	A	801	EUA	C41-N40	-8.33	1.28	1.47
2	B	801	EUA	C41-N40	-7.93	1.29	1.47
2	A	801	EUA	C36-N37	-7.27	1.30	1.47
2	A	801	EUA	O26-C15	-6.66	1.10	1.23
2	B	801	EUA	C36-N37	-6.05	1.33	1.47
2	B	801	EUA	C34-N33	5.91	1.48	1.35
2	A	801	EUA	C43-N40	-5.87	1.31	1.46
2	B	801	EUA	C15-N16	5.84	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	EUA	O01-C02	-4.94	1.13	1.23
2	A	801	EUA	C51-C50	-4.93	1.31	1.38
2	B	801	EUA	C02-N03	4.84	1.44	1.34
2	B	801	EUA	C50-S49	4.80	1.83	1.76
2	A	801	EUA	C15-N16	4.78	1.44	1.33
2	B	801	EUA	C11-N10	4.77	1.45	1.35
2	A	801	EUA	O57-S49	-4.77	1.38	1.43
2	A	801	EUA	C02-N03	4.71	1.44	1.34
2	A	801	EUA	O45-C34	-4.58	1.14	1.23
2	B	801	EUA	O57-S49	4.49	1.48	1.43
2	A	801	EUA	C38-N37	-4.26	1.35	1.46
2	B	801	EUA	C36-C35	4.23	1.60	1.52
2	A	801	EUA	C39-N40	-4.09	1.35	1.46
2	A	801	EUA	O12-C11	-4.02	1.15	1.23
2	B	801	EUA	S49-N48	4.01	1.68	1.61
2	A	801	EUA	C27-N48	-3.96	1.39	1.46
2	B	801	EUA	C43-N40	-3.95	1.36	1.46
2	B	801	EUA	C17-C18	3.86	1.60	1.51
2	A	801	EUA	C34-N33	3.73	1.43	1.35
2	B	801	EUA	C09-N10	3.56	1.48	1.41
2	A	801	EUA	C17-C18	3.50	1.59	1.51
2	A	801	EUA	C36-C35	3.46	1.59	1.52
2	A	801	EUA	C44-N37	-3.43	1.37	1.46
2	A	801	EUA	C24-C21	-3.30	1.32	1.38
2	A	801	EUA	C09-N10	3.29	1.48	1.41
2	B	801	EUA	C38-N37	-3.23	1.38	1.46
2	A	801	EUA	C19-C18	-3.16	1.32	1.38
2	B	801	EUA	C44-N37	-3.07	1.38	1.46
2	B	801	EUA	C39-N40	-3.04	1.38	1.46
2	A	801	EUA	C52-C51	-3.02	1.33	1.38
2	B	801	EUA	O56-S49	3.01	1.47	1.43
2	A	801	EUA	C11-N10	2.98	1.42	1.35
2	A	801	EUA	C28-C29	2.69	1.57	1.51
2	B	801	EUA	C05-C06	2.56	1.57	1.51
2	B	801	EUA	C32-N33	2.38	1.46	1.41
2	B	801	EUA	O26-C15	-2.38	1.18	1.23
2	B	801	EUA	C28-C29	2.32	1.56	1.51
2	A	801	EUA	C55-C50	-2.27	1.35	1.38
2	B	801	EUA	O12-C11	-2.25	1.18	1.23
2	A	801	EUA	C08-C07	-2.17	1.35	1.38
2	B	801	EUA	C25-C24	2.16	1.42	1.38
2	A	801	EUA	S49-N48	2.06	1.65	1.61

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	EUA	O57-S49-O56	-9.97	107.42	119.52
2	A	801	EUA	O57-S49-O56	-6.62	111.48	119.52
2	B	801	EUA	C18-C17-N16	-5.63	101.20	113.07
2	A	801	EUA	C43-N40-C39	4.59	118.72	108.84
2	B	801	EUA	C27-N48-S49	-4.22	112.03	121.30
2	A	801	EUA	C27-N48-S49	-4.16	112.16	121.30
2	A	801	EUA	C18-C17-N16	-4.13	104.37	113.07
2	B	801	EUA	C43-N40-C39	3.34	116.03	108.84
2	B	801	EUA	C32-N33-C34	-3.33	121.62	127.52
2	A	801	EUA	O57-S49-C50	3.31	112.15	107.98
2	A	801	EUA	C54-C55-C50	-3.06	115.82	118.95
2	A	801	EUA	C51-C50-S49	-2.96	116.50	119.76
2	B	801	EUA	C50-S49-N48	2.92	111.80	107.79
2	A	801	EUA	C50-S49-N48	2.75	111.57	107.79
2	B	801	EUA	C28-C27-N48	2.67	113.88	110.64
2	B	801	EUA	C43-C44-N37	2.67	116.03	110.65
2	A	801	EUA	O56-S49-C50	-2.63	104.66	107.98
2	B	801	EUA	C15-C04-N03	-2.52	104.29	111.11
2	B	801	EUA	O57-S49-C50	2.50	111.13	107.98
2	B	801	EUA	C02-C27-N48	-2.46	104.90	111.28
2	A	801	EUA	O12-C11-N10	-2.43	119.29	123.64
2	B	801	EUA	C39-C38-N37	2.34	115.37	110.65
2	A	801	EUA	O45-C34-N33	-2.33	119.46	123.64
2	A	801	EUA	C32-N33-C34	-2.30	123.45	127.52
4	B	808	GOL	C3-C2-C1	-2.27	103.46	111.80
2	B	801	EUA	C24-C21-C20	2.26	121.59	118.23
2	A	801	EUA	C30-C31-C32	2.25	122.89	120.30
2	A	801	EUA	O57-S49-N48	2.25	110.96	106.88
2	B	801	EUA	O57-S49-N48	2.18	110.83	106.88
2	A	801	EUA	C41-N40-C39	2.14	116.95	111.24
2	A	801	EUA	C31-C30-C29	-2.10	118.24	121.00
2	B	801	EUA	C05-C04-N03	-2.08	106.52	110.83
2	A	801	EUA	O26-C15-C04	2.08	124.83	120.48
2	A	801	EUA	C52-C51-C50	2.06	121.05	118.95
2	B	801	EUA	C44-C43-N40	2.05	114.78	110.65
2	B	801	EUA	C25-C18-C19	2.03	121.25	118.23

There are no chirality outliers.

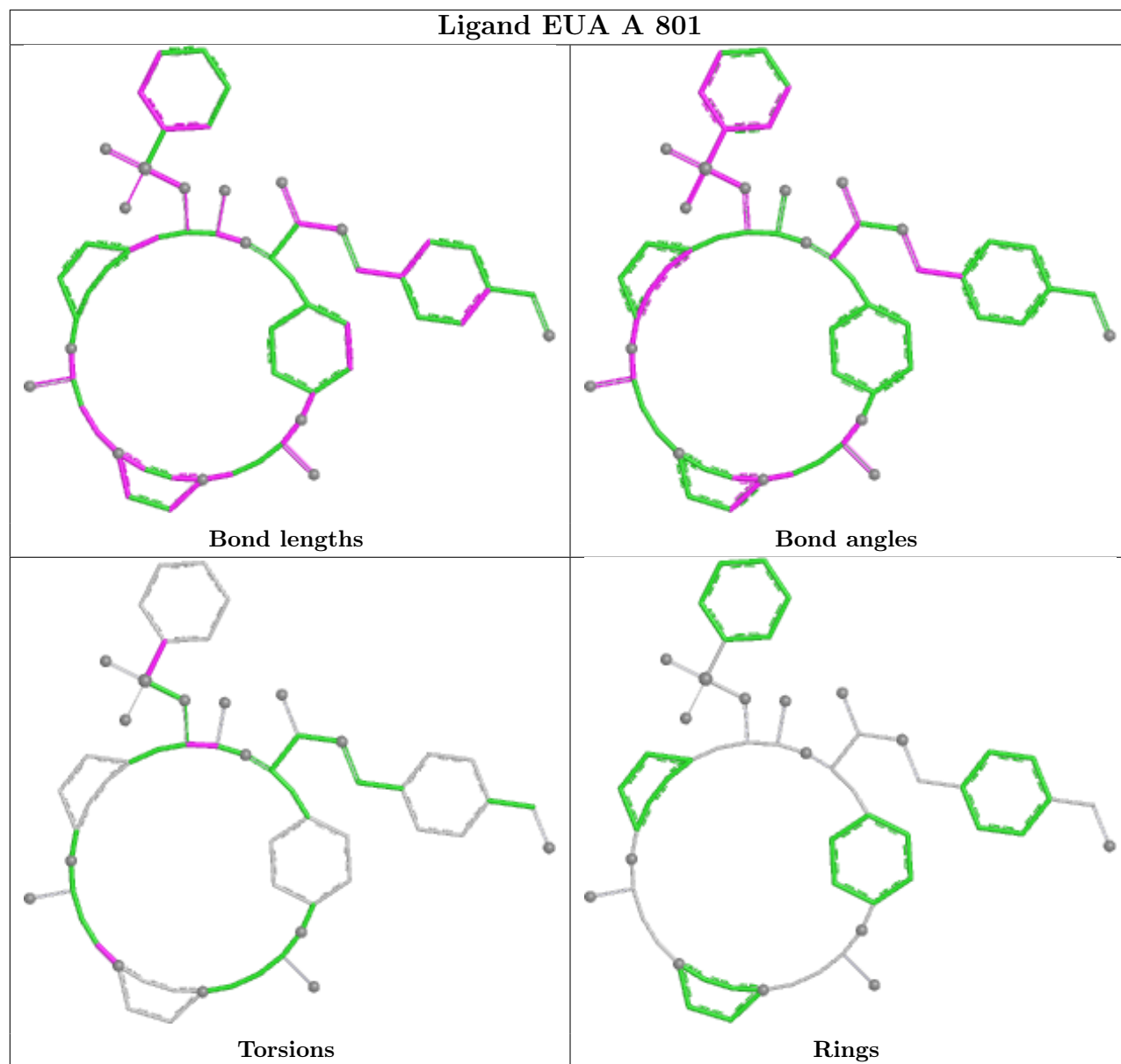
All (22) torsion outliers are listed below:

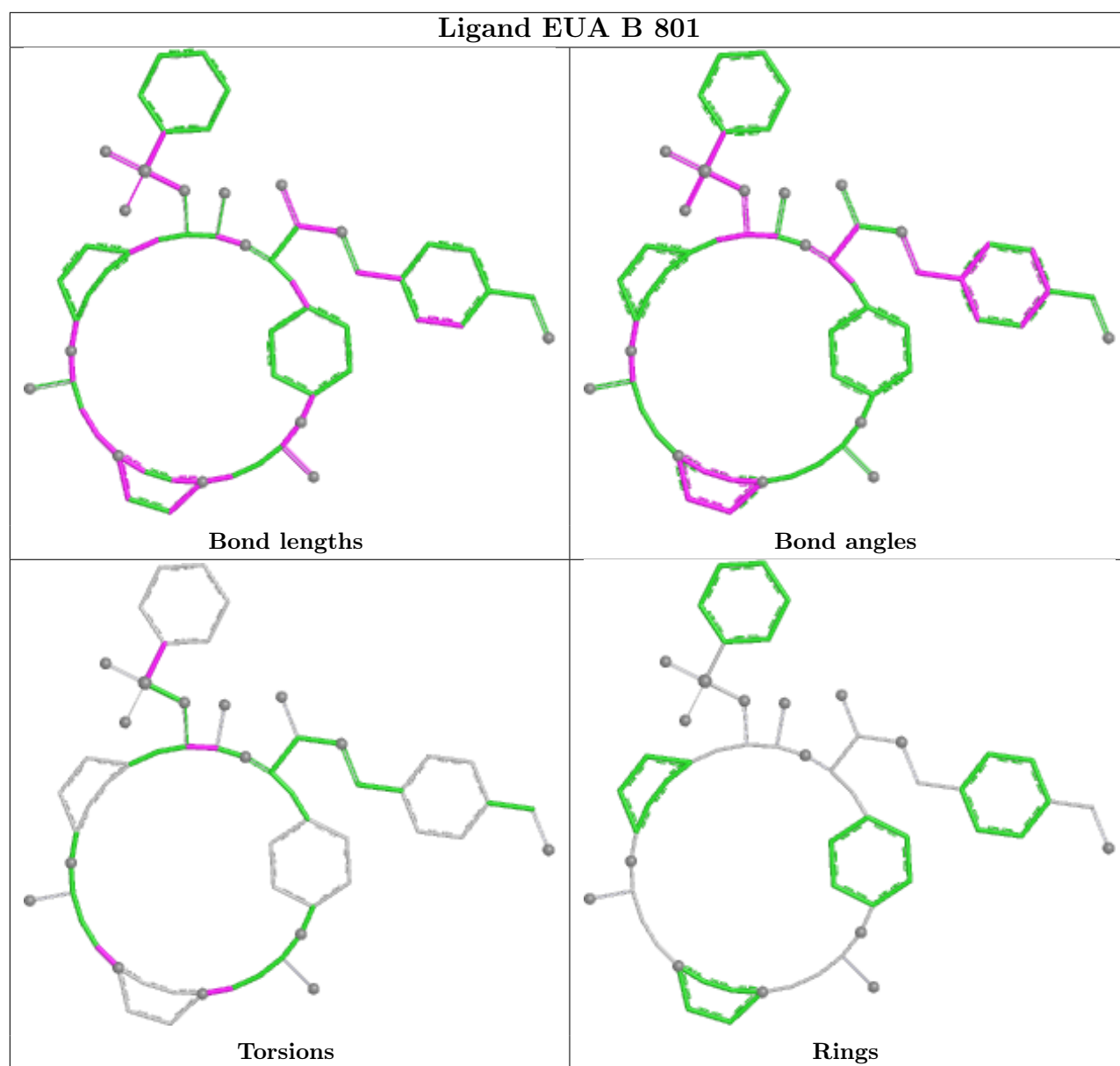
Mol	Chain	Res	Type	Atoms
2	A	801	EUA	N03-C02-C27-N48
2	B	801	EUA	N03-C02-C27-N48
2	B	801	EUA	C42-C41-N40-C39
2	B	801	EUA	C42-C41-N40-C43
2	A	801	EUA	C51-C50-S49-O56
2	A	801	EUA	C51-C50-S49-N48
2	A	801	EUA	C55-C50-S49-N48
2	A	801	EUA	C55-C50-S49-O56
2	B	801	EUA	C51-C50-S49-O56
2	B	801	EUA	C55-C50-S49-O56
2	B	801	EUA	C35-C36-N37-C44
2	B	801	EUA	O01-C02-C27-N48
2	A	801	EUA	O01-C02-C27-N48
2	B	801	EUA	O01-C02-C27-C28
2	A	801	EUA	O01-C02-C27-C28
2	B	801	EUA	N03-C02-C27-C28
2	B	801	EUA	C35-C36-N37-C38
2	B	801	EUA	C55-C50-S49-N48
2	B	801	EUA	C51-C50-S49-N48
2	A	801	EUA	N03-C02-C27-C28
2	A	801	EUA	C35-C36-N37-C44
2	A	801	EUA	C35-C36-N37-C38

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	561:ARG	C	562:VAL	N	19.20
1	B	712:ARG	C	713:TYR	N	1.14

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	A	242/250 (96%)	0.32	18 (7%) 20 23	8, 25, 55, 83	1 (0%)
1	B	242/250 (96%)	-0.09	9 (3%) 45 49	11, 16, 35, 56	3 (1%)
All	All	484/500 (96%)	0.11	27 (5%) 30 34	8, 20, 50, 83	4 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	686	GLY	6.2
1	A	688	THR	4.7
1	A	560	GLY	4.7
1	A	692	PHE	4.4
1	B	688	THR	4.0
1	B	624	VAL	3.8
1	A	691	THR	3.6
1	B	687	GLU	3.4
1	B	623	GLU	3.2
1	B	628	PRO	3.0
1	A	629	HIS	3.0
1	A	690	GLY	3.0
1	A	628	PRO	2.9
1	A	624	VAL	2.9
1	A	694	ALA	2.9
1	B	629	HIS	2.8
1	A	585	MET	2.8
1	B	694	ALA	2.7
1	A	626	LEU	2.5
1	A	625	ASN	2.4
1	A	607	LYS	2.4
1	A	686	GLY	2.3
1	A	547	ASP	2.3
1	A	627	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	687	GLU	2.0
1	A	689	GLN	2.0
1	B	622	GLN	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](#)

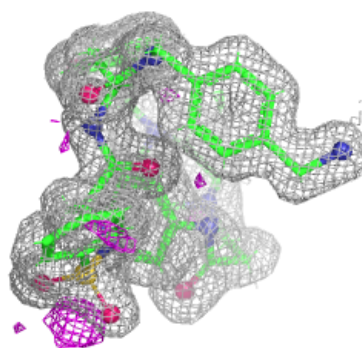
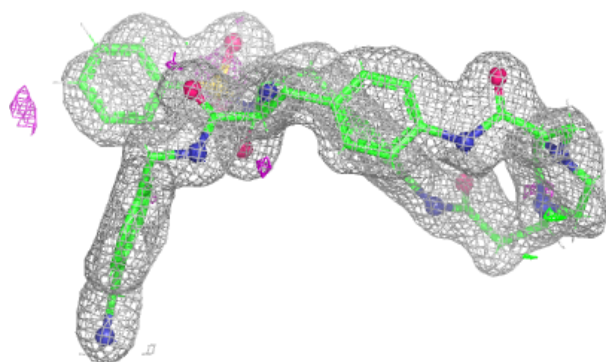
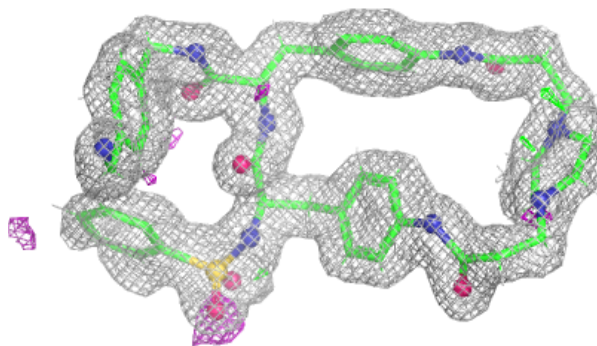
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	804	5/5	0.82	0.11	37,53,60,65	0
3	SO4	A	802	5/5	0.84	0.12	50,56,67,69	0
3	SO4	B	805	5/5	0.85	0.10	40,48,66,73	0
3	SO4	B	806	5/5	0.86	0.11	49,53,55,67	0
3	SO4	B	807	5/5	0.87	0.10	38,41,48,48	0
3	SO4	A	804	5/5	0.88	0.10	30,40,41,41	0
4	GOL	B	808	6/6	0.91	0.10	22,27,33,35	0
3	SO4	A	803	5/5	0.92	0.08	42,48,58,60	0
2	EUA	B	801	57/57	0.94	0.08	14,23,43,62	0
2	EUA	A	801	57/57	0.96	0.07	13,22,33,35	0
3	SO4	B	803	5/5	0.97	0.06	29,31,36,37	0
3	SO4	B	802	5/5	0.98	0.06	29,32,38,42	0

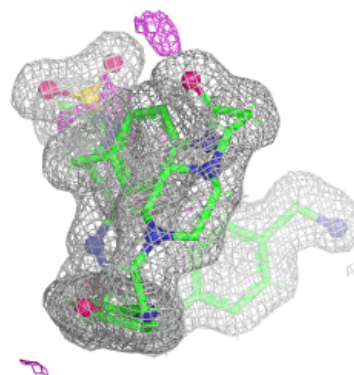
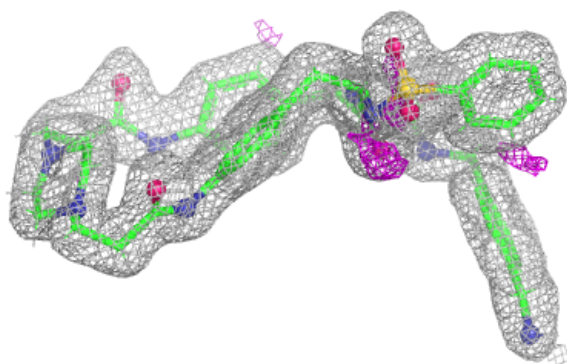
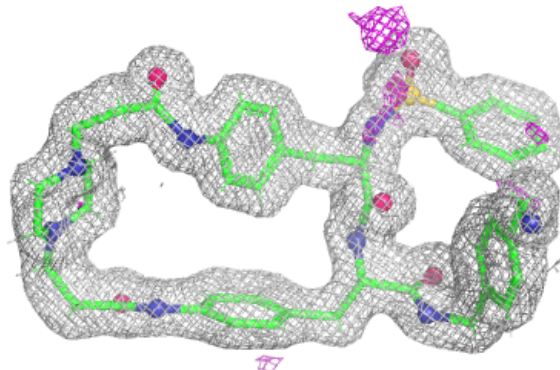
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EUA B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around EUA A 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.