



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:29 PM UTC

PDB ID : 9UOW / pdb_00009uow
Title : Crystal structure of Gossypium hirsutum (Cotton) 5-enol-pyruvyl-shikimate-3-phosphate synthase (EPSPS) in open conformation
Authors : Jangid, K.; Kumar, R.; Sharma, A.K.; Kumar, P.
Deposited on : 2025-04-27
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

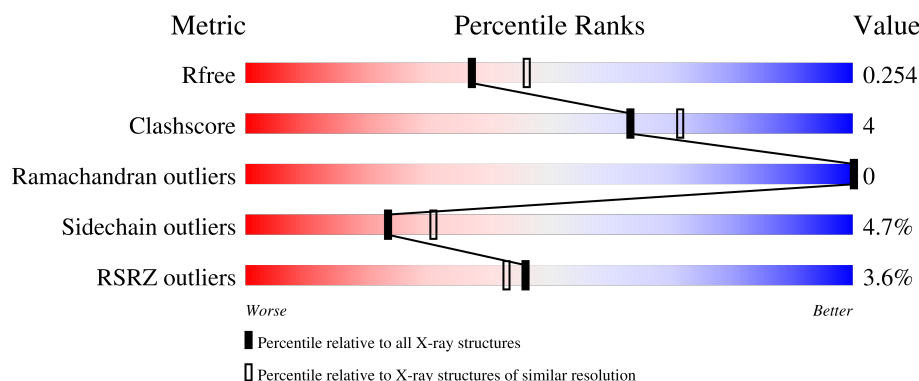
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

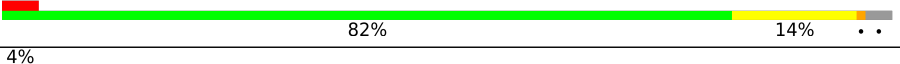
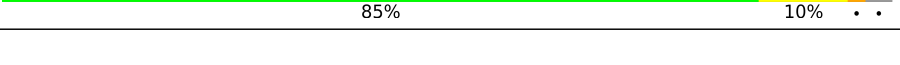
The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	454	
1	B	454	
1	C	454	

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	PEG	A	603	-	-	X	-
3	EDO	A	605	-	-	X	-

2 Entry composition [i](#)

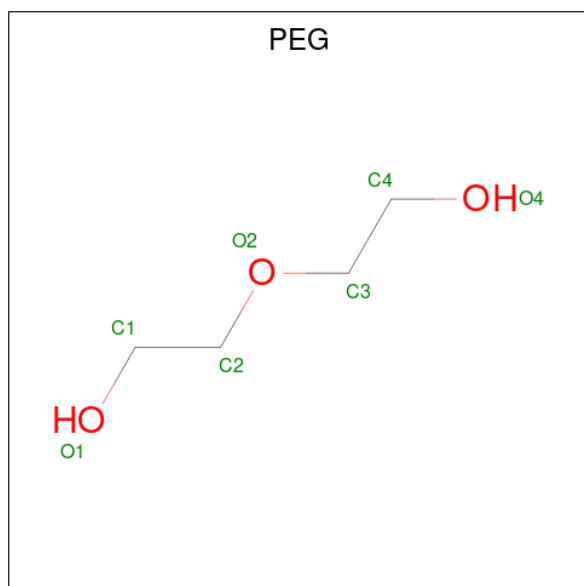
There are 6 unique types of molecules in this entry. The entry contains 10161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-phosphoshikimate 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3298	2078	562	635	23			
1	B	442	Total	C	N	O	S	0	0	0
			3298	2078	562	635	23			
1	C	442	Total	C	N	O	S	0	0	0
			3298	2078	562	635	23			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



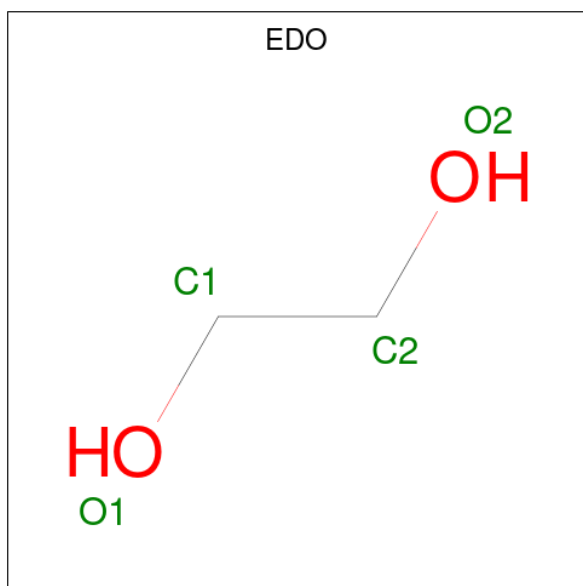
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



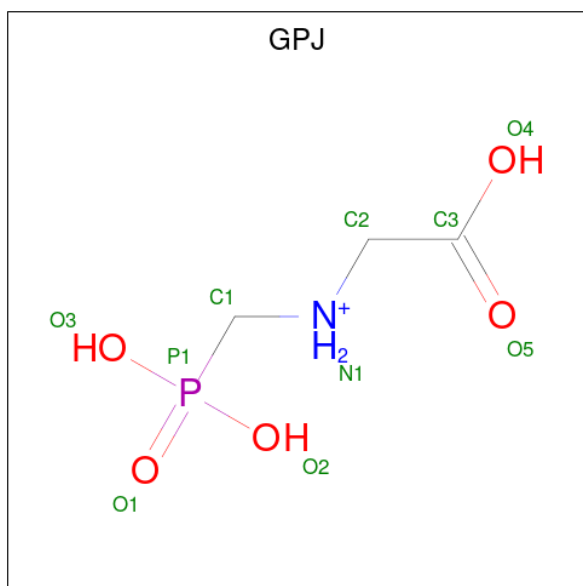
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is GLYPHOSATE (CCD ID: GPJ) (formula: $C_3H_9NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

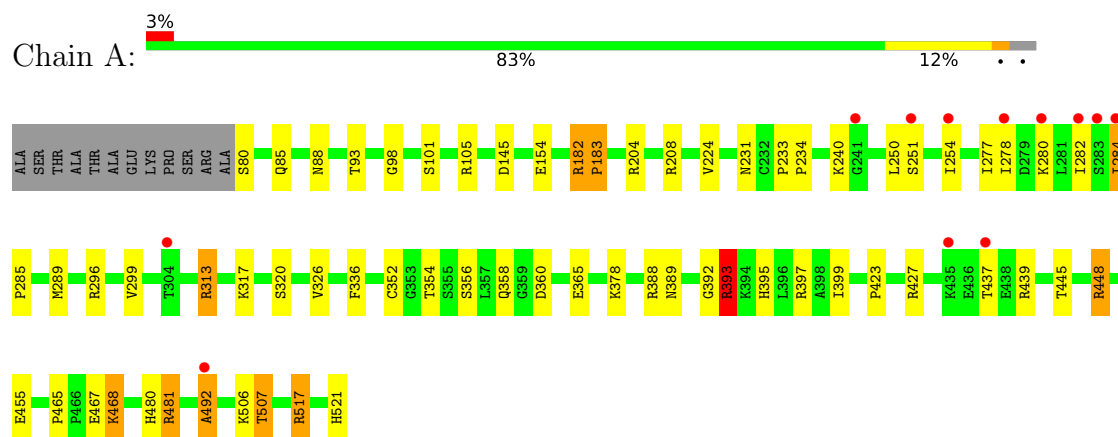
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	87	Total 87	O 87	0	0
6	B	81	Total 81	O 81	0	0
6	C	35	Total 35	O 35	0	0

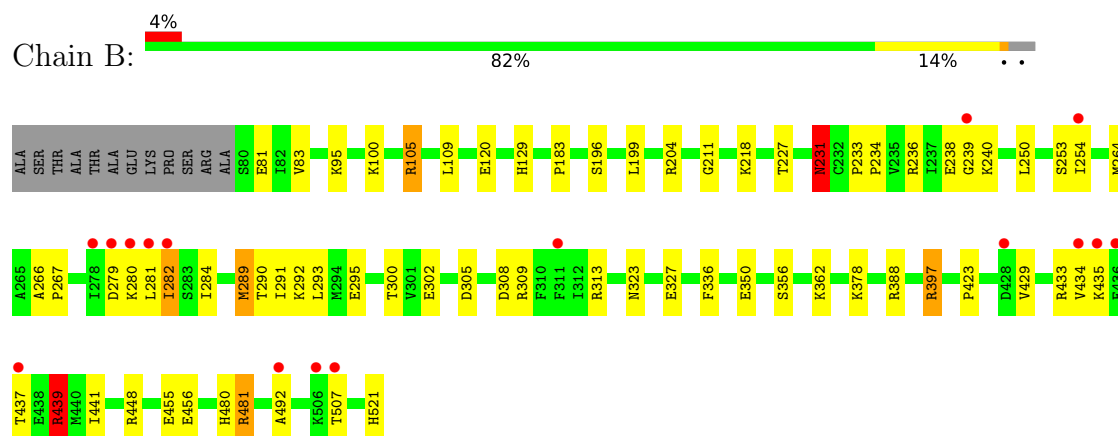
3 Residue-property plots

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.

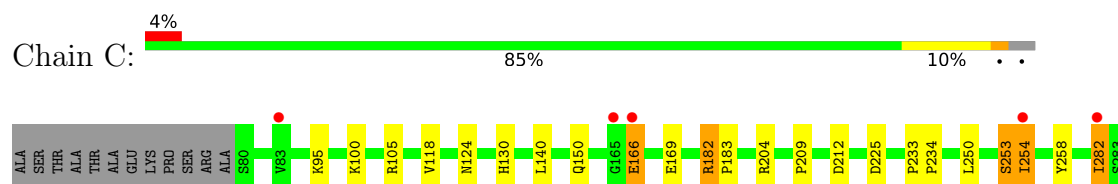
- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase

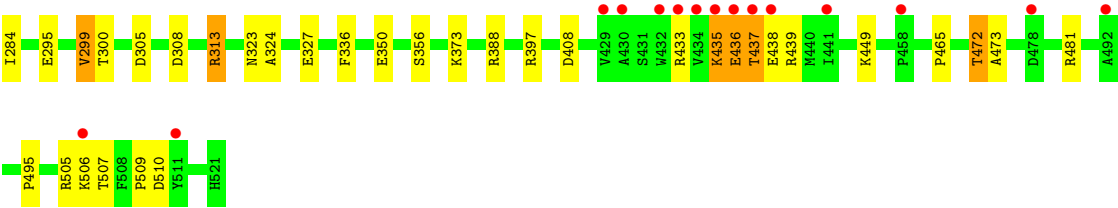


- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase



- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.86Å 89.94Å 116.23Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	24.47 – 2.20 24.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.47-2.20) 99.8 (24.47-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.201 , 0.248 0.211 , 0.254	Depositor DCC
R_{free} test set	3993 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10161	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: GOL, EDO, GPJ, PEG

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	1.15	6/3354 (0.2%)	1.48	24/4547 (0.5%)
1	B	1.05	4/3354 (0.1%)	1.49	32/4547 (0.7%)
1	C	0.94	2/3354 (0.1%)	1.42	24/4547 (0.5%)
All	All	1.05	12/10062 (0.1%)	1.46	80/13641 (0.6%)

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	6
1	B	0	5
1	C	0	6
All	All	0	17

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	THR	C-O	-6.18	1.16	1.24
1	A	389	ASN	C-O	-5.95	1.17	1.23
1	A	465	PRO	C-O	-5.64	1.20	1.24
1	A	204	ARG	NE-CZ	5.62	1.39	1.33
1	B	423	PRO	CA-CB	5.59	1.60	1.53
1	B	455	GLU	CD-OE1	5.52	1.35	1.25
1	B	129	HIS	CG-CD2	5.31	1.41	1.35
1	A	320	SER	C-O	-5.25	1.18	1.24
1	B	356	SER	C-O	-5.20	1.17	1.23
1	C	324	ALA	C-O	-5.15	1.18	1.23
1	A	395	HIS	CD2-NE2	-5.09	1.32	1.37
1	C	130	HIS	CD2-NE2	-5.09	1.32	1.37

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	THR	CA-CB-OG1	-14.76	87.46	109.60
1	B	240	LYS	CB-CA-C	-11.86	93.04	111.66
1	A	204	ARG	CD-NE-CZ	8.56	136.39	124.40
1	A	481	ARG	NE-CZ-NH2	-7.67	112.30	119.20
1	C	166	GLU	N-CA-C	-7.67	102.92	111.28
1	C	465	PRO	N-CA-CB	7.59	107.17	103.22
1	C	509	PRO	CA-C-N	7.57	135.06	120.99
1	C	509	PRO	C-N-CA	7.57	135.06	120.99
1	B	455	GLU	CG-CD-OE2	-7.48	101.20	118.40
1	C	204	ARG	CD-NE-CZ	7.30	134.62	124.40
1	C	510	ASP	N-CA-CB	-7.29	97.06	110.32
1	A	296	ARG	CB-CA-C	-7.25	97.22	110.63
1	C	436	GLU	N-CA-C	-7.22	95.88	108.08
1	B	481	ARG	NE-CZ-NH2	-7.12	112.79	119.20
1	C	308	ASP	CA-CB-CG	7.04	119.64	112.60
1	C	327	GLU	CB-CA-C	-6.93	98.55	109.70
1	B	81	GLU	N-CA-CB	-6.92	100.40	111.62
1	B	455	GLU	CG-CD-OE1	6.84	134.12	118.40
1	A	88	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	C	295	GLU	CB-CG-CD	6.63	123.88	112.60
1	B	120	GLU	CG-CD-OE2	-6.60	103.22	118.40
1	B	240	LYS	CA-CB-CG	6.59	127.29	114.10
1	C	507	THR	CA-CB-OG1	-6.58	99.73	109.60
1	A	240	LYS	CB-CA-C	-6.54	101.39	111.66
1	C	408	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	492	ALA	CA-C-N	6.50	129.88	120.38
1	B	492	ALA	C-N-CA	6.50	129.88	120.38
1	B	231	ASN	CA-CB-CG	-6.49	106.11	112.60
1	B	327	GLU	CB-CA-C	-6.47	98.18	109.64
1	C	100	LYS	N-CA-CB	-6.38	100.83	110.07
1	A	336	PHE	CA-CB-CG	-6.36	107.44	113.80
1	A	481	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	B	282	ILE	N-CA-CB	6.33	117.53	110.51
1	A	360	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	397	ARG	CB-CG-CD	6.29	125.78	111.30
1	B	183	PRO	N-CA-CB	6.17	110.12	103.33
1	C	472	THR	CA-CB-OG1	-6.16	100.36	109.60
1	C	313	ARG	N-CA-CB	6.10	118.94	109.97
1	B	100	LYS	N-CA-CB	-6.03	101.32	110.07
1	B	300	THR	OG1-CB-CG2	-6.02	97.27	109.30
1	B	323	ASN	CB-CA-C	-6.01	97.48	109.33
1	A	465	PRO	N-CA-CB	5.99	106.33	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	ARG	CD-NE-CZ	5.98	132.77	124.40
1	B	456	GLU	CB-CA-C	-5.96	98.98	109.71
1	B	439	ARG	CA-CB-CG	5.87	125.84	114.10
1	C	505	ARG	CA-C-N	5.84	128.38	120.38
1	C	505	ARG	C-N-CA	5.84	128.38	120.38
1	B	313	ARG	N-CA-CB	5.80	118.49	109.97
1	B	289	MET	CG-SD-CE	5.79	113.65	100.90
1	C	495	PRO	N-CA-C	-5.76	102.81	111.57
1	B	83	VAL	N-CA-CB	-5.75	104.44	111.00
1	A	448	ARG	N-CA-CB	5.67	118.55	110.16
1	B	336	PHE	CA-CB-CG	-5.62	108.17	113.80
1	C	336	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	218	LYS	CG-CD-CE	5.58	124.13	111.30
1	A	354	THR	CA-CB-OG1	-5.52	101.32	109.60
1	B	218	LYS	CB-CG-CD	5.49	123.94	111.30
1	A	492	ALA	CB-CA-C	-5.47	102.59	113.80
1	C	299	VAL	N-CA-CB	-5.45	100.64	111.91
1	A	313	ARG	N-CA-CB	5.41	117.93	109.97
1	B	309	ARG	N-CA-CB	5.33	120.79	111.13
1	B	308	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	204	ARG	N-CA-CB	5.30	117.84	109.94
1	A	399	ILE	O-C-N	5.29	129.00	123.02
1	A	204	ARG	N-CA-CB	5.24	117.82	110.12
1	C	253	SER	CA-C-N	5.23	127.50	120.50
1	C	253	SER	C-N-CA	5.23	127.50	120.50
1	C	282	ILE	N-CA-CB	5.21	116.30	110.62
1	C	510	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	224	VAL	CA-C-O	-5.12	115.16	120.64
1	A	154	GLU	N-CA-CB	-5.11	102.09	110.21
1	B	105	ARG	N-CA-CB	5.09	117.70	110.16
1	B	227	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	427	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	183	PRO	N-CA-CB	5.07	108.91	103.33
1	A	468	LYS	CG-CD-CE	5.04	122.89	111.30
1	A	145	ASP	CA-CB-CG	5.03	117.62	112.60
1	B	293	LEU	N-CA-CB	-5.02	102.73	110.01
1	A	313	ARG	CD-NE-CZ	5.01	131.42	124.40
1	B	448	ARG	CG-CD-NE	-5.01	100.98	112.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	388	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	397	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	388	ARG	Sidechain
1	B	397	ARG	Sidechain
1	B	439	ARG	Sidechain
1	C	105	ARG	Sidechain
1	C	182	ARG	Sidechain
1	C	313	ARG	Sidechain
1	C	388	ARG	Sidechain
1	C	397	ARG	Sidechain
1	C	433	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	3298	0	3352	35	0
1	B	3298	0	3352	23	0
1	C	3298	0	3352	18	0
2	A	28	0	40	11	0
3	A	16	0	24	9	0
3	B	4	0	6	2	0
4	A	6	0	8	2	0
5	B	10	0	6	1	0
6	A	87	0	0	7	0
6	B	81	0	0	5	0
6	C	35	0	0	0	0
All	All	10161	0	10140	80	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 (80) 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:378:LYS:HD2	6:B:779:HOH:O	1.70	0.91
1:B:239:GLY:HA2	6:B:754:HOH:O	1.74	0.85
1:A:445:THR:HG23	3:A:605:EDO:H22	1.62	0.79
1:A:105:ARG:HG3	2:A:601:PEG:H11	1.64	0.79
1:A:521:HIS:HE1	6:A:759:HOH:O	1.69	0.74
3:A:605:EDO:H12	6:A:772:HOH:O	1.90	0.71
1:A:378:LYS:HE3	6:A:706:HOH:O	1.90	0.71
1:A:455:GLU:HA	2:A:602:PEG:H41	1.75	0.68
1:B:211:GLY:HA3	1:B:231:ASN:ND2	2.11	0.64
1:B:239:GLY:CA	6:B:754:HOH:O	2.41	0.61
1:A:521:HIS:HB3	2:A:603:PEG:H41	1.83	0.61
1:A:365:GLU:OE2	3:A:607:EDO:O2	2.20	0.60
1:C:284:ILE:HD12	1:C:284:ILE:H	1.67	0.59
1:A:101:SER:HB2	2:A:601:PEG:H12	1.84	0.59
1:A:392:GLY:HA3	3:A:606:EDO:H11	1.86	0.58
1:C:472:THR:HG22	1:C:473:ALA:N	2.18	0.58
1:A:85:GLN:HB3	2:A:603:PEG:H31	1.86	0.57
1:A:289:MET:HE1	1:A:358:GLN:CG	2.33	0.57
1:A:480:HIS:CD2	1:A:507:THR:HG21	2.39	0.57
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.70	0.56
1:B:253:SER:HA	1:B:282:ILE:HG23	1.87	0.56
1:A:251:SER:O	1:A:254:ILE:HG12	2.05	0.56
1:A:423:PRO:O	3:A:608:EDO:H22	2.06	0.56
2:A:602:PEG:H42	6:A:761:HOH:O	2.08	0.53
1:A:445:THR:HA	3:A:605:EDO:H21	1.90	0.53
1:A:521:HIS:CG	2:A:603:PEG:H21	2.42	0.53
1:B:233:PRO:HA	1:B:234:PRO:C	2.35	0.52
1:A:289:MET:HE1	1:A:358:GLN:HG3	1.92	0.52
1:C:254:ILE:HG12	1:C:258:TYR:HD2	1.75	0.51
1:C:233:PRO:HA	1:C:234:PRO:C	2.36	0.51
2:A:602:PEG:C4	6:A:761:HOH:O	2.59	0.51
1:A:233:PRO:HA	1:A:234:PRO:C	2.35	0.51
3:A:605:EDO:C1	6:A:772:HOH:O	2.57	0.50
1:B:480:HIS:CD2	1:B:507:THR:HG21	2.48	0.49
1:A:289:MET:HE1	1:A:358:GLN:HG2	1.93	0.49
5:B:602:GPJ:P1	6:B:722:HOH:O	2.71	0.48
1:B:253:SER:HA	1:B:282:ILE:CG2	2.43	0.48
1:A:517:ARG:HD2	1:C:118:VAL:HG21	1.96	0.47
1:B:521:HIS:HE1	6:B:756:HOH:O	1.98	0.47
1:B:95:LYS:HE2	1:B:350:GLU:OE1	2.15	0.47
1:A:445:THR:HA	3:A:605:EDO:C2	2.44	0.47
1:A:467:GLU:OE2	2:A:604:PEG:H42	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:H	4:A:609:GOL:H32	1.80	0.47
1:C:284:ILE:HD12	1:C:284:ILE:N	2.28	0.47
1:A:393:ARG:HD2	1:A:492:ALA:HB1	1.97	0.46
1:A:467:GLU:H	4:A:609:GOL:C3	2.28	0.46
1:C:95:LYS:HE3	1:C:350:GLU:OE1	2.16	0.45
1:B:362:LYS:HD3	3:B:601:EDO:H22	1.99	0.45
1:C:449:LYS:HE2	1:C:472:THR:HG21	1.99	0.45
1:C:437:THR:C	1:C:439:ARG:N	2.75	0.45
1:C:182:ARG:HB2	1:C:183:PRO:HD3	1.99	0.44
1:A:480:HIS:HD2	1:A:507:THR:HG21	1.79	0.44
1:B:109:LEU:HD21	1:B:264:MET:CE	2.48	0.44
1:B:291:ILE:O	1:B:295:GLU:HG3	2.18	0.44
1:A:182:ARG:NE	6:A:708:HOH:O	2.49	0.43
1:C:472:THR:CG2	1:C:473:ALA:N	2.81	0.43
1:B:199:LEU:HD12	1:B:199:LEU:N	2.33	0.43
1:A:85:GLN:HG3	2:A:603:PEG:H12	2.00	0.43
1:A:467:GLU:OE2	2:A:604:PEG:C4	2.67	0.43
1:A:445:THR:CG2	3:A:605:EDO:H22	2.39	0.43
1:C:435:LYS:O	1:C:436:GLU:C	2.60	0.43
1:B:362:LYS:NZ	3:B:601:EDO:H21	2.34	0.43
1:B:481:ARG:HH11	1:B:481:ARG:HG2	1.83	0.43
1:C:449:LYS:HB3	1:C:472:THR:HG21	2.00	0.43
1:B:266:ALA:N	1:B:267:PRO:CD	2.83	0.42
1:B:211:GLY:HA3	1:B:231:ASN:HD22	1.83	0.41
1:B:196:SER:OG	1:B:238:GLU:OE1	2.38	0.41
1:C:212:ASP:HB3	1:C:254:ILE:HD11	2.02	0.41
1:A:481:ARG:HG2	1:A:481:ARG:HH11	1.84	0.41
1:C:437:THR:O	1:C:438:GLU:C	2.63	0.41
1:B:109:LEU:HD21	1:B:264:MET:HE3	2.02	0.41
1:C:472:THR:HG22	1:C:473:ALA:H	1.85	0.41
1:A:98:GLY:HA3	1:A:326:VAL:HG12	2.03	0.41
1:A:284:ILE:N	1:A:285:PRO:CD	2.84	0.41
1:A:448:ARG:HH11	1:A:448:ARG:HD2	1.76	0.41
1:B:281:LEU:HD23	1:B:284:ILE:HG12	2.02	0.41
1:C:253:SER:HA	1:C:282:ILE:HG23	2.02	0.41
1:C:481:ARG:HG2	1:C:481:ARG:HH11	1.86	0.40
1:A:182:ARG:HB2	1:A:183:PRO:HD3	2.03	0.40
1:B:292:LYS:HA	1:B:292:LYS:HD3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/454 (97%)	427 (97%)	13 (3%)	0	100	100
1	B	440/454 (97%)	425 (97%)	15 (3%)	0	100	100
1	C	440/454 (97%)	424 (96%)	16 (4%)	0	100	100
All	All	1320/1362 (97%)	1276 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	358/366 (98%)	341 (95%)	17 (5%)	23	31
1	B	358/366 (98%)	343 (96%)	15 (4%)	26	36
1	C	358/366 (98%)	340 (95%)	18 (5%)	22	28
All	All	1074/1098 (98%)	1024 (95%)	50 (5%)	23	31

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	231	ASN
1	A	250	LEU
1	A	277	ILE
1	A	278	ILE

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Mol	Chain	Res	Type
1	A	280	LYS
1	A	282	ILE
1	A	284	ILE
1	A	299	VAL
1	A	317	LYS
1	A	352	CYS
1	A	356	SER
1	A	393	ARG
1	A	437	THR
1	A	439	ARG
1	A	468	LYS
1	A	506	LYS
1	B	231	ASN
1	B	250	LEU
1	B	254	ILE
1	B	279	ASP
1	B	280	LYS
1	B	289	MET
1	B	290	THR
1	B	302	GLU
1	B	305	ASP
1	B	429	VAL
1	B	434	VAL
1	B	435	LYS
1	B	437	THR
1	B	439	ARG
1	B	441	ILE
1	C	124	ASN
1	C	140	LEU
1	C	150	GLN
1	C	166	GLU
1	C	169	GLU
1	C	209	PRO
1	C	225	ASP
1	C	250	LEU
1	C	254	ILE
1	C	299	VAL
1	C	300	THR
1	C	305	ASP
1	C	323	ASN
1	C	356	SER
1	C	373	LYS

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Mol	Chain	Res	Type
1	C	435	LYS
1	C	437	THR
1	C	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	130	HIS
1	A	480	HIS
1	A	521	HIS
1	B	85	GLN
1	B	159	GLN
1	B	231	ASN
1	B	480	HIS
1	C	144	HIS
1	C	323	ASN
1	C	480	HIS

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](#)

11 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	EDO	A	606	-	3,3,3	0.97	0	2,2,2	1.98	1 (50%)
2	PEG	A	603	-	6,6,6	0.12	0	5,5,5	0.07	0
3	EDO	A	608	-	3,3,3	0.46	0	2,2,2	0.84	0
3	EDO	B	601	-	3,3,3	0.54	0	2,2,2	0.56	0
3	EDO	A	607	-	3,3,3	0.59	0	2,2,2	0.52	0
2	PEG	A	602	-	6,6,6	0.50	0	5,5,5	0.54	0
3	EDO	A	605	-	3,3,3	0.39	0	2,2,2	0.90	0
2	PEG	A	604	-	6,6,6	0.74	0	5,5,5	0.63	0
2	PEG	A	601	-	6,6,6	0.66	0	5,5,5	0.54	0
5	GPJ	B	602	-	9,9,9	3.95	6 (66%)	9,12,12	1.30	1 (11%)
4	GOL	A	609	-	5,5,5	0.55	0	5,5,5	0.64	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
3	EDO	A	606	-	-	1/1/1/1	-
2	PEG	A	603	-	-	3/4/4/4	-
3	EDO	A	608	-	-	1/1/1/1	-
3	EDO	B	601	-	-	0/1/1/1	-
3	EDO	A	607	-	-	1/1/1/1	-
2	PEG	A	602	-	-	2/4/4/4	-
3	EDO	A	605	-	-	1/1/1/1	-
2	PEG	A	604	-	-	3/4/4/4	-
2	PEG	A	601	-	-	4/4/4/4	-
5	GPJ	B	602	-	-	2/7/7/7	-
4	GOL	A	609	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	GPJ	P1-C1	7.72	1.98	1.81
5	B	602	GPJ	P1-O3	6.81	1.70	1.55
5	B	602	GPJ	P1-O2	3.58	1.63	1.55
5	B	602	GPJ	C2-N1	2.65	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	GPJ	O4-C3	-2.17	1.23	1.30
5	B	602	GPJ	C1-N1	2.07	1.53	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	606	EDO	O1-C1-C2	2.74	133.23	112.39
5	B	602	GPJ	O3-P1-O2	2.68	115.59	107.96

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	GOL	O1-C1-C2-O2
4	A	609	GOL	O1-C1-C2-C3
4	A	609	GOL	C1-C2-C3-O3
5	B	602	GPJ	N1-C2-C3-O4
5	B	602	GPJ	N1-C2-C3-O5
2	A	604	PEG	O1-C1-C2-O2
2	A	603	PEG	O1-C1-C2-O2
2	A	602	PEG	O2-C3-C4-O4
2	A	601	PEG	O1-C1-C2-O2
4	A	609	GOL	O2-C2-C3-O3
3	A	608	EDO	O1-C1-C2-O2
2	A	601	PEG	O2-C3-C4-O4
2	A	602	PEG	C4-C3-O2-C2
2	A	603	PEG	C4-C3-O2-C2
2	A	604	PEG	C1-C2-O2-C3
2	A	601	PEG	C1-C2-O2-C3
3	A	606	EDO	O1-C1-C2-O2
3	A	607	EDO	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2
2	A	603	PEG	C1-C2-O2-C3
2	A	601	PEG	C4-C3-O2-C2
2	A	604	PEG	C4-C3-O2-C2

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	606	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	PEG	4	0
3	A	608	EDO	1	0
3	B	601	EDO	2	0
3	A	607	EDO	1	0
2	A	602	PEG	3	0
3	A	605	EDO	6	0
2	A	604	PEG	2	0
2	A	601	PEG	2	0
5	B	602	GPJ	1	0
4	A	609	GOL	2	0

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

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	442/454 (97%)	-0.19	12 (2%) 56 53	13, 28, 56, 93	0
1	B	442/454 (97%)	-0.01	16 (3%) 46 43	16, 33, 66, 115	0
1	C	442/454 (97%)	0.27	20 (4%) 38 35	19, 39, 75, 135	0
All	All	1326/1362 (97%)	0.02	48 (3%) 46 43	13, 33, 68, 135	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	437	THR	7.3
1	C	434	VAL	6.8
1	C	438	GLU	5.5
1	C	436	GLU	5.3
1	B	279	ASP	5.2
1	C	435	LYS	4.7
1	B	280	LYS	4.4
1	A	282	ILE	4.4
1	C	492	ALA	4.3
1	B	282	ILE	3.9
1	B	281	LEU	3.9
1	A	437	THR	3.8
1	B	254	ILE	3.7
1	B	434	VAL	3.5
1	C	254	ILE	3.5
1	C	458	PRO	3.4
1	B	435	LYS	3.4
1	B	437	THR	3.3
1	A	284	ILE	3.1
1	C	165	GLY	3.1
1	C	441	ILE	3.1
1	A	283	SER	3.0
1	B	278	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	430	ALA	2.9
1	C	433	ARG	2.8
1	A	304	THR	2.7
1	A	435	LYS	2.7
1	A	280	LYS	2.6
1	B	506	LYS	2.6
1	A	278	ILE	2.6
1	A	492	ALA	2.5
1	A	241	GLY	2.5
1	B	436	GLU	2.4
1	B	507	THR	2.4
1	A	254	ILE	2.4
1	B	239	GLY	2.3
1	B	311	PHE	2.3
1	C	166	GLU	2.3
1	C	83	VAL	2.3
1	A	251	SER	2.2
1	B	428	ASP	2.2
1	C	506	LYS	2.2
1	C	432	TRP	2.1
1	C	478	ASP	2.1
1	C	511	TYR	2.0
1	C	429	VAL	2.0
1	B	492	ALA	2.0
1	C	282	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
5	GPJ	B	602	10/10	0.74	0.15	44,48,57,67	0
2	PEG	A	603	7/7	0.75	0.20	43,57,76,88	0
4	GOL	A	609	6/6	0.80	0.17	42,46,50,53	0
2	PEG	A	604	7/7	0.83	0.25	37,48,63,63	0
3	EDO	B	601	4/4	0.85	0.12	33,33,33,42	0
2	PEG	A	601	7/7	0.87	0.16	30,60,71,75	0
3	EDO	A	606	4/4	0.89	0.15	19,31,32,45	0
3	EDO	A	608	4/4	0.90	0.10	40,46,48,49	0
3	EDO	A	607	4/4	0.92	0.09	32,36,38,41	0
2	PEG	A	602	7/7	0.93	0.13	34,41,53,55	0
3	EDO	A	605	4/4	0.96	0.22	33,37,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.