



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 PM UTC

PDB ID : 9C1C / pdb_00009c1c
Title : Mycobacterium tuberculosis PKS13 acyltransferase serine converted to beta-lactam form by CEC215 via SuFEx reaction
Authors : Tang, S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2024-05-29
Resolution : 2.22 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

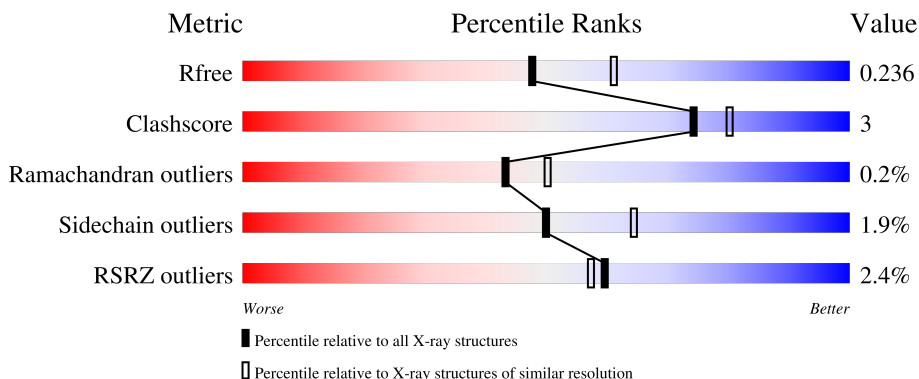
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

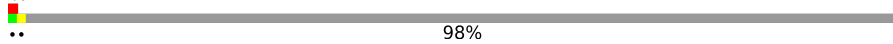
The reported resolution of this entry is 2.22 Å.

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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	491	
2	B	491	
2	D	491	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7669 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 Polyketide synthase Pks13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3536	2240	611	673	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	SER	-	expression tag	UNP I6X8D2
A	574	ASN	-	expression tag	UNP I6X8D2
A	575	ALA	-	expression tag	UNP I6X8D2
A	801	A1ATO	SER	conflict	UNP I6X8D2

- Molecule 2 is a protein called Polyketide synthase Pks13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	469	Total	C	N	O	S	0	0	0
			3545	2244	615	674	12			
2	D	9	Total	C	N	O		0	0	0
			78	51	13	14				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	573	SER	-	expression tag	UNP I6X8D2
B	574	ASN	-	expression tag	UNP I6X8D2
B	575	ALA	-	expression tag	UNP I6X8D2
D	573	SER	-	expression tag	UNP I6X8D2
D	574	ASN	-	expression tag	UNP I6X8D2
D	575	ALA	-	expression tag	UNP I6X8D2

- 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	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	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		

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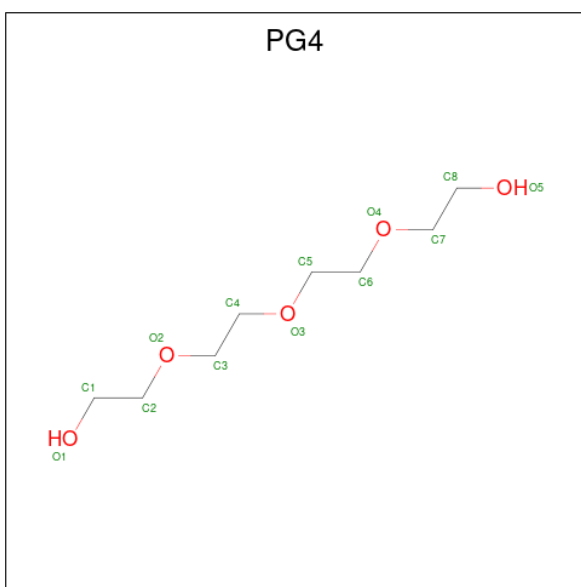
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

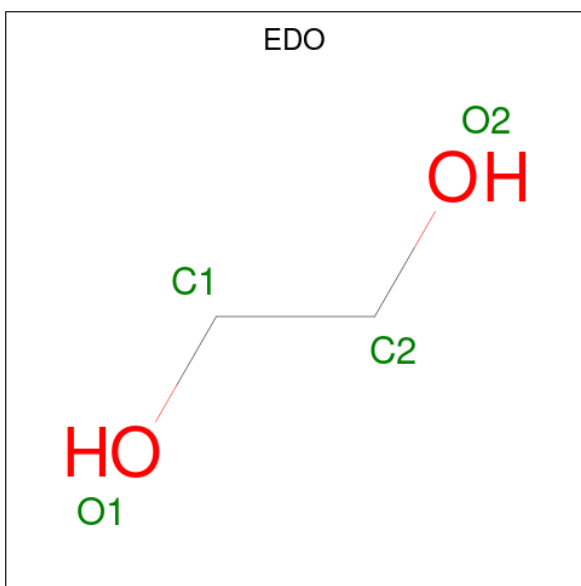
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total Cl 9 9	0	0
4	B	6	Total Cl 6 6	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



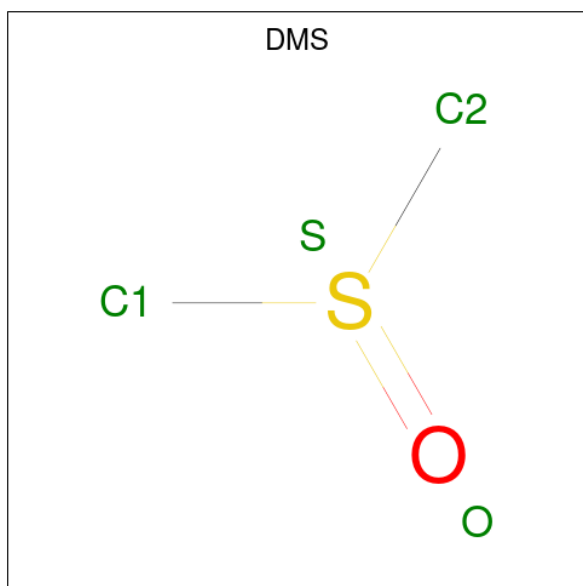
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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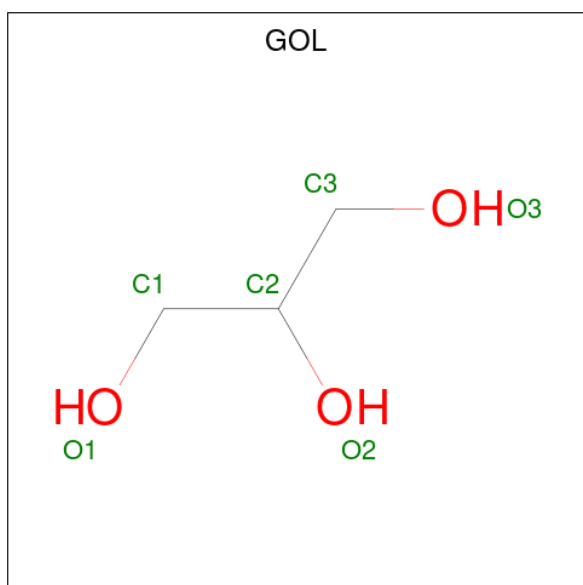
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



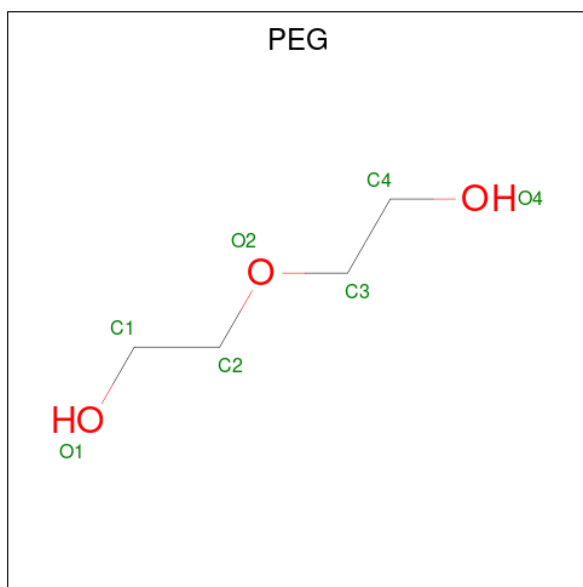
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

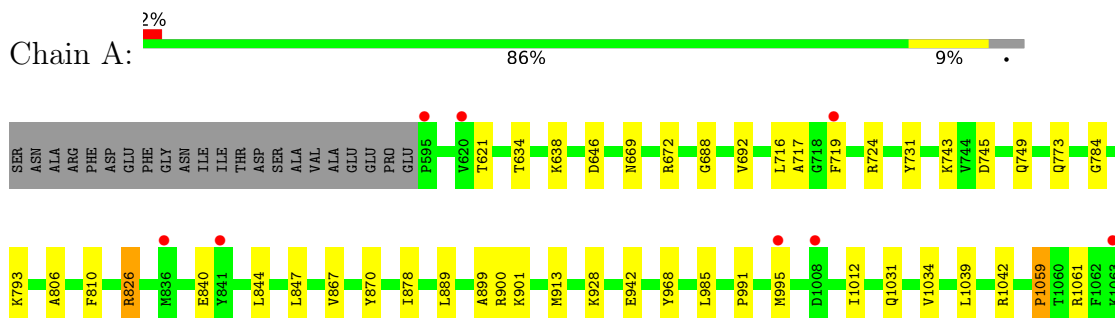
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	156	Total	O	0	0
			156	156		
10	B	158	Total	O	0	0
			158	158		
10	D	2	Total	O	0	0
			2	2		

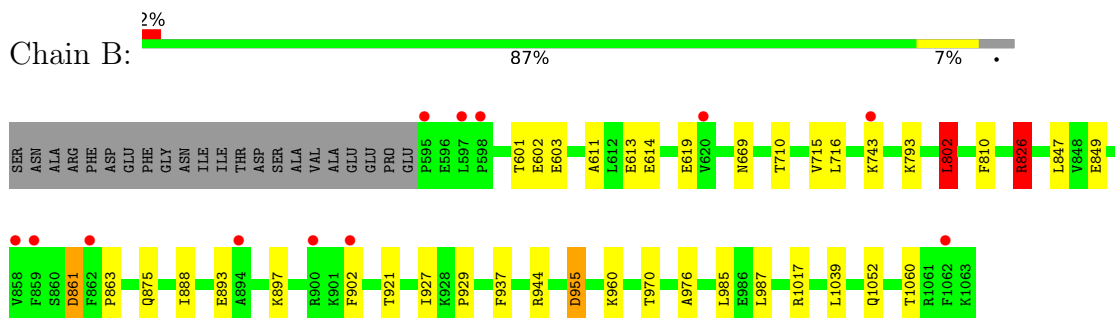
3 Residue-property plots

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.

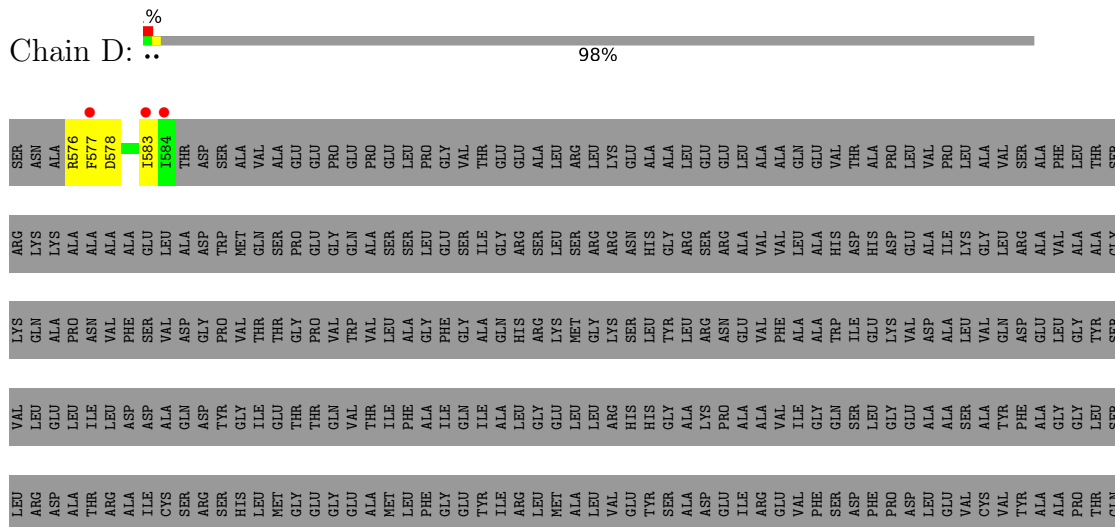
- Molecule 1: Polyketide synthase Pks13



- Molecule 2: Polyketide synthase Pks13



- Molecule 2: Polyketide synthase Pks13



THR	THR
VAL	VAL
ILE	ILE
GLY	GLY
GLY	GLY
PRO	PRO
PRO	PRO
GLU	GLU
GLN	GLN
VAL	VAL
ASP	ASP
ALA	ALA
ILE	ILE
PRO	PRO
ALA	ALA
GLU	GLU
ALA	ALA
GLY	GLY
LYS	LYS
ARG	ARG
LYS	LYS
PHE	PHE
ALA	ALA
THR	THR
LYS	LYS
GLY	GLY
ALA	ALA
SER	SER
VAL	VAL
THR	THR
HIS	HIS
SER	SER
GLN	GLN
MET	MET
ASP	ASP
PRO	PRO
LEU	LEU
GLY	GLY
GLU	GLU
LEU	LEU
THR	THR
ALA	ALA
GLU	GLU
PHE	PHE
LEU	LEU
GLN	GLN
GLY	GLY
ILE	ILE
LYS	LYS
THR	THR
SER	SER
PRO	PRO
VAL	VAL
ALA	ALA
THR	THR
CYS	CYS
GLY	GLY
MET	MET

GLN	GLN
VAL	VAL
ALA	ALA
LEU	LEU
THR	THR
THR	THR
ALA	ALA
ASP	ASP
ALA	ALA
GLY	GLY
LEU	LEU
HIS	HIS
ASP	ASP
ALA	ALA
GLN	GLN
LEU	LEU
ILE	ILE
PRO	PRO
THR	THR
LEU	LEU
ALA	ALA
ARG	ARG
LYS	LYS
GLN	GLN
ASP	ASP
GLU	GLU
VAL	VAL
SER	SER
THR	THR
MET	MET
VAL	VAL
SER	SER
THR	THR
MET	MET
ALA	ALA
GLN	GLN
LEU	LEU
TYR	TYR
VAL	VAL
TYR	TYR
GLY	GLY
HIS	HIS
ASP	ASP
LEU	LEU
ASP	ASP
LEU	LEU
ASP	ASP
ILE	ILE
ARG	ARG
THR	THR
THR	THR
LEU	LEU
PHE	PHE
SER	SER
ARG	ARG
ALA	ALA
SER	SER
GLY	GLY
PRO	PRO
GLN	GLN
ASP	ASP
TYR	TYR
ALA	ALA

ASN
ILE
PRO
PRO
THR
ARG
PHE
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.52Å 106.52Å 258.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.22 49.25 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.25-2.22) 98.7 (49.25-2.22)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.191 , 0.235 0.198 , 0.236	Depositor DCC
R_{free} test set	2770 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.8	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	7669	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, PG4, EDO, PEG, A1ATO, DMS, SO4, CL

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	0.61	0/3604	1.11	8/4896 (0.2%)
2	B	0.62	0/3620	1.17	12/4918 (0.2%)
2	D	0.68	0/79	1.31	1/104 (1.0%)
All	All	0.61	0/7303	1.14	21/9918 (0.2%)

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	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	955	ASP	CB-CA-C	-10.47	89.58	110.42
2	B	802	LEU	N-CA-CB	-9.40	95.96	110.06
2	B	793	LYS	CB-CA-C	-7.45	97.86	109.55
2	B	861	ASP	CB-CA-C	-6.52	99.92	110.74
2	D	578	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	1059	PRO	N-CA-CB	-5.99	96.02	102.60
2	B	902	PHE	CA-CB-CG	-5.75	108.06	113.80
1	A	995	MET	CG-SD-CE	5.69	113.42	100.90
1	A	719	PHE	N-CA-CB	5.44	117.95	109.85
2	B	893	GLU	N-CA-CB	5.43	118.10	110.12
1	A	826	ARG	N-CA-CB	-5.38	101.92	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1060	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	991	PRO	N-CA-C	5.31	119.65	112.48
2	B	601	THR	OG1-CB-CG2	5.29	119.89	109.30
2	B	613	GLU	CB-CA-C	5.28	120.35	110.70
1	A	743	LYS	N-CA-CB	5.24	117.61	110.01
2	B	810	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	646	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	717	ALA	CA-C-O	5.11	120.91	117.94
2	B	710	THR	CA-CB-OG1	-5.05	102.02	109.60
2	B	826	ARG	CG-CD-NE	-5.04	100.91	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	724	ARG	Sidechain
2	B	826	ARG	Sidechain
2	B	944	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	3536	0	3477	25	0
2	B	3545	0	3502	18	0
2	D	78	0	71	1	0
3	A	80	0	0	3	0
3	B	35	0	0	0	0
3	D	5	0	0	0	0
4	A	9	0	0	0	0
4	B	6	0	0	0	0
5	A	13	0	18	2	0
6	A	8	0	12	0	0
6	B	8	0	12	1	0
7	A	4	0	6	0	0
8	A	6	0	8	0	0
8	B	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	14	0	20	1	0
10	A	156	0	0	2	0
10	B	158	0	0	1	0
10	D	2	0	0	0	0
All	All	7669	0	7134	45	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 3.

All (45) 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:826:ARG:NH2	3:A:1101:SO4:O2	2.04	0.89
2:B:802:LEU:C	2:B:802:LEU:HD23	2.22	0.65
1:A:669:ASN:HB2	10:A:1245:HOH:O	1.98	0.63
1:A:688:GLY:O	1:A:692:VAL:HG23	2.06	0.56
1:A:634:THR:O	1:A:638:LYS:HG3	2.05	0.56
2:D:577:PHE:CE1	2:D:583:ILE:HD13	2.41	0.55
2:B:716:LEU:HD11	2:B:987:LEU:HD12	1.89	0.54
2:B:921:THR:OG1	2:B:960:LYS:HD2	2.08	0.54
1:A:1031:GLN:O	1:A:1034:VAL:HG12	2.09	0.53
2:B:861:ASP:O	2:B:863:PRO:HD3	2.10	0.51
2:B:611:ALA:HA	2:B:614:GLU:HG3	1.92	0.51
1:A:745:ASP:O	1:A:749:GLN:HG3	2.12	0.49
2:B:802:LEU:C	2:B:802:LEU:CD2	2.86	0.49
1:A:1061:ARG:NH2	3:A:1102:SO4:O4	2.47	0.48
1:A:985:LEU:C	1:A:985:LEU:HD23	2.39	0.47
2:B:602:GLU:N	2:B:602:GLU:CD	2.73	0.47
1:A:784:GLY:HA3	1:A:810:PHE:CZ	2.51	0.46
2:B:1017:ARG:HD2	8:B:1117:GOL:H32	1.97	0.46
1:A:847:LEU:O	1:A:899:ALA:HA	2.16	0.46
1:A:913:MET:HE1	5:A:1126:PG4:H51	1.97	0.46
1:A:621:THR:OG1	3:A:1105:SO4:O4	2.21	0.46
2:B:937:PHE:CZ	2:B:976:ALA:HA	2.51	0.46
1:A:773:GLN:OE1	1:A:826:ARG:NH1	2.49	0.45
2:B:1052:GLN:O	6:B:1118:EDO:H12	2.16	0.45
1:A:840:GLU:CG	1:A:840:GLU:O	2.65	0.45
2:B:715:VAL:C	2:B:716:LEU:HD22	2.43	0.44
1:A:844:LEU:HD13	1:A:901:LYS:HD2	2.00	0.44
2:B:602:GLU:CD	2:B:602:GLU:H	2.26	0.44
2:B:603:GLU:HA	2:B:603:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:THR:HG22	1:A:638:LYS:HE3	2.01	0.43
1:A:716:LEU:HD22	1:A:806:ALA:HB3	2.00	0.42
1:A:1042:ARG:HD2	10:A:1325:HOH:O	2.19	0.42
2:B:849:GLU:HB3	2:B:897:LYS:HB3	2.01	0.42
2:B:927:ILE:O	2:B:929:PRO:HD3	2.18	0.42
2:B:716:LEU:HD22	2:B:716:LEU:N	2.35	0.42
9:B:1114:PEG:H41	10:B:1276:HOH:O	2.19	0.41
2:B:985:LEU:C	2:B:985:LEU:HD23	2.45	0.41
1:A:878:ILE:HD12	1:A:878:ILE:C	2.45	0.41
1:A:1039:LEU:HD13	1:A:1039:LEU:C	2.46	0.41
1:A:731:TYR:CD1	1:A:731:TYR:C	2.99	0.41
2:B:847:LEU:HD11	2:B:875:GLN:HG2	2.03	0.41
1:A:985:LEU:HA	1:A:1012:ILE:O	2.21	0.40
1:A:867:VAL:HG11	1:A:870:TYR:CZ	2.56	0.40
1:A:913:MET:HE1	5:A:1126:PG4:C5	2.52	0.40
1:A:942:GLU:HA	1:A:968:TYR:CG	2.57	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	464/491 (94%)	457 (98%)	7 (2%)	0	100	100
2	B	467/491 (95%)	451 (97%)	14 (3%)	2 (0%)	30	33
2	D	7/491 (1%)	7 (100%)	0	0	100	100
All	All	938/1473 (64%)	915 (98%)	21 (2%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	955	ASP

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Mol	Chain	Res	Type
2	B	1039	LEU

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	358/386 (93%)	352 (98%)	6 (2%)	53	68
2	B	362/387 (94%)	355 (98%)	7 (2%)	50	64
2	D	8/387 (2%)	7 (88%)	1 (12%)	4	3
All	All	728/1160 (63%)	714 (98%)	14 (2%)	50	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	672	ARG
1	A	793	LYS
1	A	889	LEU
1	A	900	ARG
1	A	928	LYS
1	A	1059	PRO
2	B	619	GLU
2	B	669	ASN
2	B	743	LYS
2	B	802	LEU
2	B	826	ARG
2	B	888	ILE
2	B	970	THR
2	D	576	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	649	GLN
1	A	723	HIS

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Mol	Chain	Res	Type
1	A	789	HIS
1	A	800	GLN
1	A	971	HIS
1	A	1010	GLN
2	B	649	GLN
2	B	749	GLN
2	B	780	GLN
2	B	1010	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 15 are monoatomic - leaving 34 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	$\# Z > 2$
3	SO4	B	1101	-	4,4,4	0.39	0	6,6,6	0.11	0
6	EDO	A	1127	-	3,3,3	0.14	0	2,2,2	0.17	0
8	GOL	B	1117	-	5,5,5	0.34	0	5,5,5	0.92	0
9	PEG	B	1114	-	6,6,6	0.21	0	5,5,5	0.12	0
8	GOL	A	1129	-	5,5,5	0.27	0	5,5,5	0.59	0
3	SO4	B	1105	-	4,4,4	0.35	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	A	1126	-	12,12,12	0.26	0	11,11,11	0.20	0
3	SO4	A	1116	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	B	1102	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	A	1111	-	4,4,4	0.30	0	6,6,6	0.12	0
6	EDO	B	1118	-	3,3,3	0.19	0	2,2,2	0.27	0
6	EDO	A	1130	-	3,3,3	0.06	0	2,2,2	0.21	0
3	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	A	1105	-	4,4,4	0.27	0	6,6,6	0.15	0
3	SO4	B	1104	-	4,4,4	0.27	0	6,6,6	0.19	0
3	SO4	A	1113	-	4,4,4	0.35	0	6,6,6	0.14	0
3	SO4	D	1101	-	4,4,4	0.32	0	6,6,6	0.09	0
3	SO4	B	1103	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	A	1107	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	A	1102	-	4,4,4	0.34	0	6,6,6	0.16	0
3	SO4	B	1107	-	4,4,4	0.29	0	6,6,6	0.22	0
3	SO4	A	1108	-	4,4,4	0.34	0	6,6,6	0.17	0
7	DMS	A	1128	-	3,3,3	0.41	0	3,3,3	0.23	0
3	SO4	A	1106	-	4,4,4	0.32	0	6,6,6	0.16	0
3	SO4	A	1115	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	A	1103	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	A	1101	-	4,4,4	0.36	0	6,6,6	0.32	0
3	SO4	B	1106	-	4,4,4	0.58	0	6,6,6	0.26	0
3	SO4	A	1110	-	4,4,4	0.33	0	6,6,6	0.13	0
6	EDO	B	1116	-	3,3,3	0.31	0	2,2,2	0.27	0
9	PEG	B	1115	-	6,6,6	0.85	0	5,5,5	0.51	0
3	SO4	A	1114	-	4,4,4	0.27	0	6,6,6	0.14	0
3	SO4	A	1112	-	4,4,4	0.29	0	6,6,6	0.19	0
3	SO4	A	1109	-	4,4,4	0.32	0	6,6,6	0.11	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
5	PG4	A	1126	-	-	6/10/10/10	-
6	EDO	A	1127	-	-	0/1/1/1	-
8	GOL	B	1117	-	-	2/4/4/4	-
9	PEG	B	1114	-	-	0/4/4/4	-
6	EDO	B	1118	-	-	1/1/1/1	-
6	EDO	B	1116	-	-	1/1/1/1	-
9	PEG	B	1115	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1130	-	-	1/1/1/1	-
8	GOL	A	1129	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1129	GOL	C1-C2-C3-O3
8	B	1117	GOL	C1-C2-C3-O3
5	A	1126	PG4	O2-C3-C4-O3
9	B	1115	PEG	O2-C3-C4-O4
8	A	1129	GOL	O1-C1-C2-C3
8	B	1117	GOL	O1-C1-C2-C3
8	A	1129	GOL	O1-C1-C2-O2
8	A	1129	GOL	O2-C2-C3-O3
5	A	1126	PG4	O1-C1-C2-O2
9	B	1115	PEG	O1-C1-C2-O2
6	A	1130	EDO	O1-C1-C2-O2
6	B	1116	EDO	O1-C1-C2-O2
6	B	1118	EDO	O1-C1-C2-O2
5	A	1126	PG4	O4-C7-C8-O5
5	A	1126	PG4	C1-C2-O2-C3
5	A	1126	PG4	C4-C3-O2-C2
5	A	1126	PG4	O3-C5-C6-O4

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1117	GOL	1	0
9	B	1114	PEG	1	0
5	A	1126	PG4	2	0
6	B	1118	EDO	1	0
3	A	1105	SO4	1	0
3	A	1102	SO4	1	0
3	A	1101	SO4	1	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	468/491 (95%)	-0.19	8 (1%) 69 67	34, 47, 71, 124	0
2	B	469/491 (95%)	-0.13	12 (2%) 57 55	30, 45, 79, 126	0
2	D	9/491 (1%)	1.25	3 (33%) 1 0	59, 69, 88, 90	0
All	All	946/1473 (64%)	-0.15	23 (2%) 59 57	30, 46, 75, 126	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	858	VAL	4.5
1	A	595	PRO	3.8
2	B	595	PRO	3.6
1	A	719	PHE	3.1
2	D	584	ILE	2.9
2	B	902	PHE	2.8
1	A	841	TYR	2.8
2	B	859	PHE	2.7
2	B	597	LEU	2.7
2	B	862	PHE	2.7
2	B	620	VAL	2.5
1	A	995	MET	2.5
1	A	1008	ASP	2.4
2	B	1062	PHE	2.4
2	B	900	ARG	2.3
2	D	577	PHE	2.2
1	A	620	VAL	2.2
1	A	836	MET	2.2
1	A	1063	LYS	2.2
2	D	583	ILE	2.1
2	B	598	PRO	2.1
2	B	743	LYS	2.0
2	B	894	ALA	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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1115	5/5	0.72	0.12	72,72,76,88	5
4	CL	A	1117	1/1	0.73	0.17	97,97,97,97	0
3	SO4	A	1107	5/5	0.77	0.09	64,70,78,79	5
3	SO4	B	1103	5/5	0.77	0.12	66,75,77,82	5
3	SO4	A	1108	5/5	0.77	0.11	70,75,78,81	5
8	GOL	B	1117	6/6	0.77	0.19	68,79,83,83	0
3	SO4	B	1104	5/5	0.78	0.14	65,68,82,87	5
7	DMS	A	1128	4/4	0.80	0.26	86,93,107,111	0
3	SO4	A	1114	5/5	0.80	0.16	74,76,77,88	5
3	SO4	A	1116	5/5	0.85	0.09	68,71,82,83	5
3	SO4	A	1110	5/5	0.85	0.14	61,67,79,88	5
9	PEG	B	1114	7/7	0.85	0.19	66,72,81,86	0
3	SO4	B	1107	5/5	0.86	0.14	61,66,69,76	5
6	EDO	A	1127	4/4	0.86	0.14	70,71,75,81	0
6	EDO	B	1116	4/4	0.86	0.17	59,63,69,73	0
3	SO4	A	1105	5/5	0.87	0.19	52,59,66,69	5
3	SO4	B	1105	5/5	0.87	0.07	66,74,77,77	5
3	SO4	A	1112	5/5	0.87	0.18	54,77,84,91	5
3	SO4	D	1101	5/5	0.88	0.08	57,57,68,71	5
6	EDO	A	1130	4/4	0.88	0.20	75,75,76,77	0
3	SO4	A	1113	5/5	0.88	0.18	57,59,63,71	5
4	CL	A	1119	1/1	0.89	0.11	88,88,88,88	0
4	CL	A	1125	1/1	0.90	0.10	85,85,85,85	0
6	EDO	B	1118	4/4	0.90	0.14	56,60,65,66	0
4	CL	B	1113	1/1	0.90	0.08	81,81,81,81	0
3	SO4	B	1102	5/5	0.90	0.12	60,63,68,70	5
4	CL	A	1123	1/1	0.90	0.19	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	1129	6/6	0.91	0.12	56,73,77,82	0
3	SO4	A	1109	5/5	0.91	0.13	63,69,73,76	5
4	CL	B	1112	1/1	0.91	0.10	80,80,80,80	0
3	SO4	A	1111	5/5	0.92	0.10	60,65,70,73	5
3	SO4	A	1104	5/5	0.92	0.11	53,55,72,82	5
4	CL	B	1111	1/1	0.93	0.15	76,76,76,76	0
3	SO4	A	1102	5/5	0.93	0.08	51,53,61,62	5
4	CL	A	1122	1/1	0.93	0.12	83,83,83,83	0
5	PG4	A	1126	13/13	0.93	0.15	66,72,83,83	0
9	PEG	B	1115	7/7	0.93	0.14	52,68,75,76	0
4	CL	A	1121	1/1	0.94	0.09	68,68,68,68	0
3	SO4	A	1103	5/5	0.94	0.12	60,61,72,76	5
3	SO4	A	1106	5/5	0.94	0.09	53,68,71,72	5
3	SO4	A	1101	5/5	0.94	0.11	38,39,46,48	5
4	CL	B	1110	1/1	0.94	0.09	72,72,72,72	0
3	SO4	B	1101	5/5	0.94	0.07	53,58,63,63	5
4	CL	B	1108	1/1	0.95	0.12	71,71,71,71	0
4	CL	B	1109	1/1	0.95	0.11	77,77,77,77	0
4	CL	A	1124	1/1	0.97	0.06	70,70,70,70	0
4	CL	A	1120	1/1	0.97	0.15	69,69,69,69	0
3	SO4	B	1106	5/5	0.97	0.15	47,49,60,63	5
4	CL	A	1118	1/1	0.98	0.04	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.