



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:46 AM UTC

PDB ID : 9QBL / pdb_00009qbl
Title : Crystal structure of Xanthobacter autotrophicus SPARDA mutant lacking DREN nuclease domains
Authors : Manakova, E.N.; Grazulis, S.; Zaremba, M.
Deposited on : 2025-03-03
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

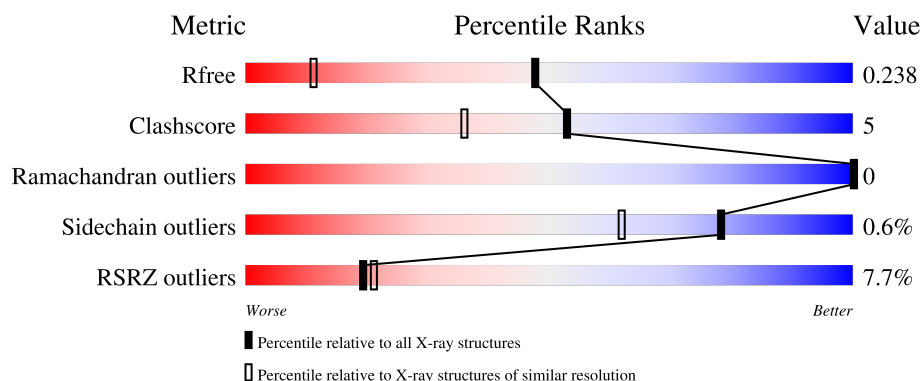
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	321	<div> <div>9%</div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
1	C	321	<div> <div>12%</div> <div>72%</div> <div>10%</div> <div>18%</div> </div>
2	B	482	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
2	D	482	<div> <div>6%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>

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
3	ACY	B	501	-	-	X	-
4	GOL	B	505	-	-	X	-
4	GOL	C	503	-	-	X	-
4	GOL	D	506	-	-	X	-
6	PEG	A	505	-	-	X	-
6	PEG	B	506	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13446 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 DUF4365 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	Se	23	7	0
			2304	1458	425	417	4			
1	C	263	Total	C	N	O	Se	49	11	0
			2243	1416	416	407	4			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MSE	-	initiating methionine	UNP A7ICE8
A	125	ALA	-	expression tag	UNP A7ICE8
A	126	GLY	-	expression tag	UNP A7ICE8
A	127	SER	-	expression tag	UNP A7ICE8
A	128	HIS	-	expression tag	UNP A7ICE8
A	129	HIS	-	expression tag	UNP A7ICE8
A	130	HIS	-	expression tag	UNP A7ICE8
A	131	HIS	-	expression tag	UNP A7ICE8
A	132	HIS	-	expression tag	UNP A7ICE8
A	133	HIS	-	expression tag	UNP A7ICE8
A	134	GLY	-	expression tag	UNP A7ICE8
A	135	MSE	-	expression tag	UNP A7ICE8
A	136	ALA	-	expression tag	UNP A7ICE8
A	137	SER	-	expression tag	UNP A7ICE8
A	138	MSE	-	expression tag	UNP A7ICE8
A	139	THR	-	expression tag	UNP A7ICE8
A	140	GLY	-	expression tag	UNP A7ICE8
A	141	GLY	-	expression tag	UNP A7ICE8
A	142	GLN	-	expression tag	UNP A7ICE8
A	143	GLN	-	expression tag	UNP A7ICE8
A	144	MSE	-	expression tag	UNP A7ICE8
A	145	GLY	-	expression tag	UNP A7ICE8
A	146	ARG	-	expression tag	UNP A7ICE8
A	147	SER	-	expression tag	UNP A7ICE8
A	148	GLY	-	expression tag	UNP A7ICE8

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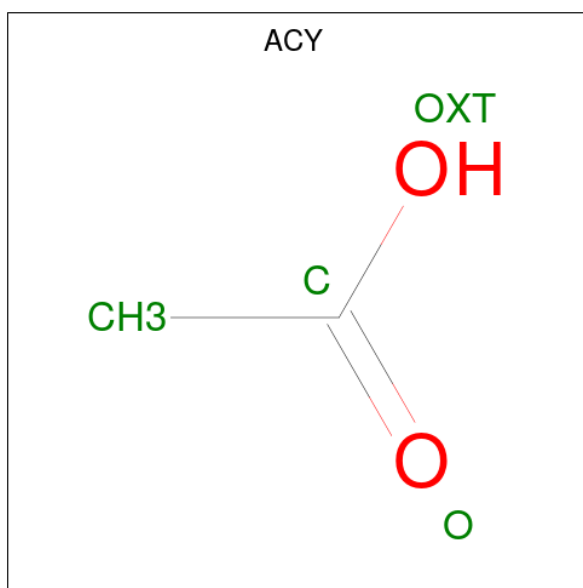
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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	TRP	-	expression tag	UNP A7ICE8
A	150	GLU	-	expression tag	UNP A7ICE8
A	151	LEU	-	expression tag	UNP A7ICE8
A	152	GLN	-	expression tag	UNP A7ICE8
C	124	MSE	-	initiating methionine	UNP A7ICE8
C	125	ALA	-	expression tag	UNP A7ICE8
C	126	GLY	-	expression tag	UNP A7ICE8
C	127	SER	-	expression tag	UNP A7ICE8
C	128	HIS	-	expression tag	UNP A7ICE8
C	129	HIS	-	expression tag	UNP A7ICE8
C	130	HIS	-	expression tag	UNP A7ICE8
C	131	HIS	-	expression tag	UNP A7ICE8
C	132	HIS	-	expression tag	UNP A7ICE8
C	133	HIS	-	expression tag	UNP A7ICE8
C	134	GLY	-	expression tag	UNP A7ICE8
C	135	MSE	-	expression tag	UNP A7ICE8
C	136	ALA	-	expression tag	UNP A7ICE8
C	137	SER	-	expression tag	UNP A7ICE8
C	138	MSE	-	expression tag	UNP A7ICE8
C	139	THR	-	expression tag	UNP A7ICE8
C	140	GLY	-	expression tag	UNP A7ICE8
C	141	GLY	-	expression tag	UNP A7ICE8
C	142	GLN	-	expression tag	UNP A7ICE8
C	143	GLN	-	expression tag	UNP A7ICE8
C	144	MSE	-	expression tag	UNP A7ICE8
C	145	GLY	-	expression tag	UNP A7ICE8
C	146	ARG	-	expression tag	UNP A7ICE8
C	147	SER	-	expression tag	UNP A7ICE8
C	148	GLY	-	expression tag	UNP A7ICE8
C	149	TRP	-	expression tag	UNP A7ICE8
C	150	GLU	-	expression tag	UNP A7ICE8
C	151	LEU	-	expression tag	UNP A7ICE8
C	152	GLN	-	expression tag	UNP A7ICE8

- Molecule 2 is a protein called Protein argonaute.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	463	Total	C	N	O	S	Se	19	17	0
			3783	2395	686	695	3	4			
2	D	459	Total	C	N	O	S	Se	39	16	0
			3742	2371	686	677	3	5			

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



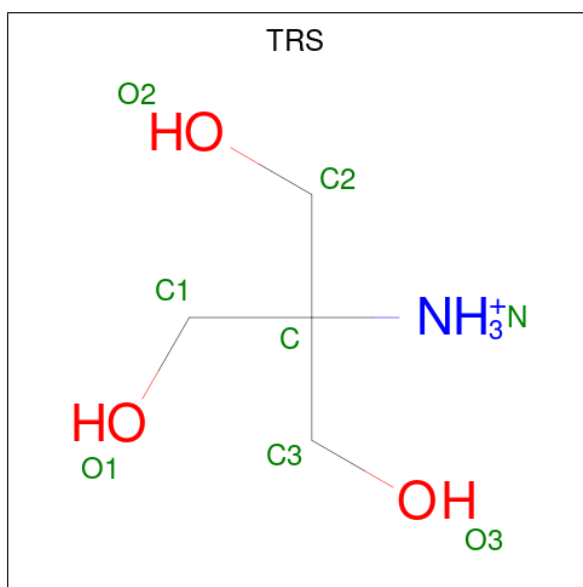
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



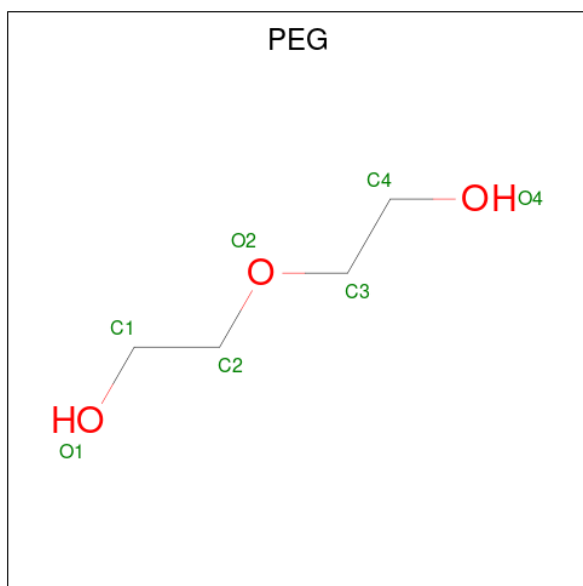
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

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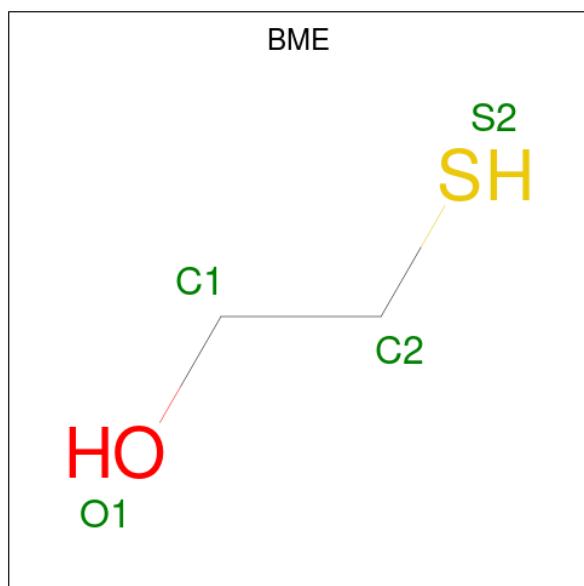
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



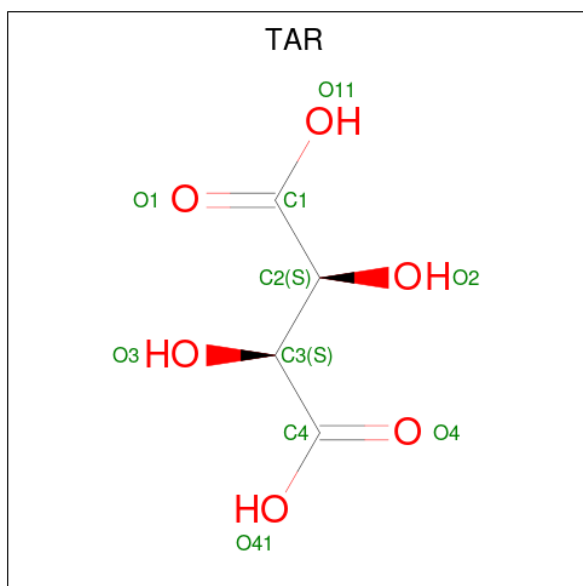
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	D	1	Total	C	O	S	0	0
			4	2	1	1		
8	D	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 9 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).

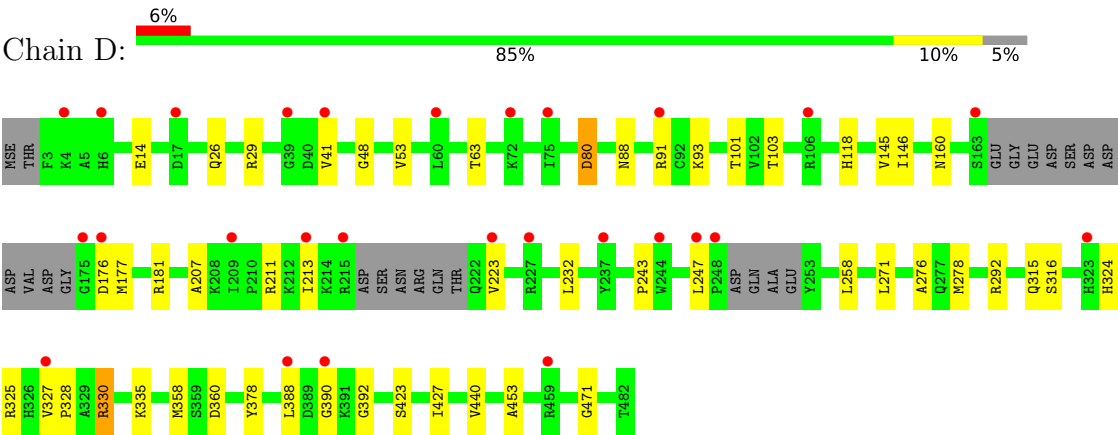


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O		0	0
			10	4	6			
9	D	1	Total	C	O		0	0
			10	4	6			

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	212	Total	O	0	0
			212	212		
10	B	498	Total	O	0	0
			498	498		
10	C	139	Total	O	0	0
			139	139		
10	D	379	Total	O	0	0
			379	379		

● Molecule 2: Protein argonaute



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.71Å 155.40Å 161.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.67 – 1.50 80.67 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.4 (80.67-1.50) 92.3 (80.67-1.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.237 0.203 , 0.238	Depositor DCC
R_{free} test set	27155 reflections (9.38%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13446	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: CME, PEG, TAR, CL, TRS, BME, GOL, ACY

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	0.62	0/2351	1.01	2/3169 (0.1%)
1	C	0.58	1/2285 (0.0%)	1.05	3/3077 (0.1%)
2	B	0.66	0/3853	1.05	1/5214 (0.0%)
2	D	0.63	1/3817 (0.0%)	1.06	9/5159 (0.2%)
All	All	0.63	2/12306 (0.0%)	1.05	15/16619 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	HIS	CB-CG	-5.61	1.42	1.50
2	D	118	HIS	CE1-NE2	5.12	1.37	1.32

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	388	LEU	N-CA-C	-8.22	99.45	110.55
1	C	356	PRO	N-CA-C	6.18	121.11	114.68
1	A	213	PHE	CA-C-O	-5.76	114.47	120.98
2	B	315	GLN	CB-CG-CD	5.45	121.86	112.60
2	D	330	ARG	CB-CG-CD	5.33	123.57	111.30

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	2304	0	2276	13	0
1	C	2243	0	2215	23	0
2	B	3783	0	3785	52	0
2	D	3742	0	3768	36	0
3	A	4	0	3	0	0
3	B	4	0	3	4	0
3	C	4	0	3	0	0
3	D	8	0	6	0	0
4	A	12	0	16	2	0
4	B	18	0	24	6	0
4	C	6	0	8	5	0
4	D	6	0	8	4	0
5	A	8	0	12	0	0
6	A	7	0	10	5	0
6	B	21	0	30	8	0
6	D	5	0	5	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	4	0	6	0	0
8	C	4	0	6	1	0
8	D	12	0	18	2	0
9	B	10	0	4	3	0
9	D	10	0	4	0	0
10	A	212	0	0	1	0
10	B	498	0	0	4	0
10	C	139	0	0	1	0
10	D	379	0	0	2	0
All	All	13446	0	12210	122	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 5.

The worst 5 of 122 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)
2:B:444[B]:THR:HG22	2:B:446:GLN:H	1.11	1.07
1:C:236:VAL:HG22	1:C:240:LEU:HD12	1.40	1.02
2:D:292:ARG:HE	4:D:506:GOL:H11	1.31	0.95
2:D:63:THR:HG21	2:D:232:LEU:HD11	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:VAL:CG2	1:C:240:LEU:HD12	2.03	0.89

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	276/321 (86%)	269 (98%)	7 (2%)	0	100	100
1	C	266/321 (83%)	259 (97%)	7 (3%)	0	100	100
2	B	473/482 (98%)	464 (98%)	9 (2%)	0	100	100
2	D	466/482 (97%)	454 (97%)	12 (3%)	0	100	100
All	All	1481/1606 (92%)	1446 (98%)	35 (2%)	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	248/266 (93%)	248 (100%)	0	100	100
1	C	241/266 (91%)	241 (100%)	0	100	100
2	B	403/398 (101%)	401 (100%)	2 (0%)	81	66
2	D	399/398 (100%)	393 (98%)	6 (2%)	57	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1291/1328 (97%)	1283 (99%)	8 (1%)	78 62

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	335	LYS
2	D	325	ARG
2	D	176	ASP
2	D	26[B]	GLN
2	D	223	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	443	ASN
1	C	344	HIS
2	D	443	ASN
1	C	369	ASN
1	A	415	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CME	D	22	2	8,9,10	0.44	0	6,9,11	0.43	0
2	CME	B	22	2	8,9,10	0.48	0	6,9,11	0.60	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	CME	D	22	2	-	1/5/8/10	-
2	CME	B	22	2	-	3/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	22	CME	SD-CE-CZ-OH
2	B	22	CME	CZ-CE-SD-SG
2	B	22	CME	CA-CB-SG-SD
2	D	22	CME	CA-CB-SG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 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	$\# Z > 2$
6	PEG	B	508	-	6,6,6	0.41	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	TAR	D	508	-	9,9,9	1.02	0	12,12,12	0.93	0
3	ACY	C	501	-	3,3,3	1.02	0	3,3,3	0.73	0
4	GOL	B	505	-	5,5,5	0.19	0	5,5,5	0.64	0
5	TRS	A	504	-	7,7,7	0.28	0	9,9,9	0.27	0
4	GOL	B	503	-	5,5,5	0.10	0	5,5,5	0.37	0
8	BME	D	504	-	3,3,3	0.14	0	2,2,2	0.14	0
3	ACY	D	502	-	3,3,3	1.21	0	3,3,3	0.90	0
6	PEG	A	505	-	6,6,6	0.12	0	5,5,5	0.09	0
6	PEG	B	507	-	6,6,6	0.17	0	5,5,5	0.28	0
4	GOL	B	504	-	5,5,5	0.18	0	5,5,5	0.87	0
4	GOL	A	502	-	5,5,5	0.07	0	5,5,5	0.35	0
4	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.22	0
3	ACY	B	501	-	3,3,3	1.45	0	3,3,3	0.84	0
3	ACY	A	501	-	3,3,3	1.09	0	3,3,3	0.73	0
8	BME	C	502	-	3,3,3	0.12	0	2,2,2	0.62	0
4	GOL	D	506	-	5,5,5	0.09	0	5,5,5	0.31	0
3	ACY	D	501	-	3,3,3	1.14	0	3,3,3	0.65	0
8	BME	D	503	-	3,3,3	0.18	0	2,2,2	0.58	0
9	TAR	B	509	-	9,9,9	1.09	1 (11%)	12,12,12	0.92	0
8	BME	D	505	-	3,3,3	0.22	0	2,2,2	0.45	0
6	PEG	B	506	-	6,6,6	0.39	0	5,5,5	0.22	0
6	PEG	D	507	-	4,4,6	0.19	0	3,3,5	0.20	0
8	BME	B	502	-	3,3,3	0.43	0	2,2,2	1.47	0
4	GOL	C	503	-	5,5,5	0.17	0	5,5,5	0.32	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
6	PEG	B	508	-	-	1/4/4/4	-
9	TAR	D	508	-	-	6/12/12/12	-
8	BME	B	502	-	-	0/1/1/1	-
4	GOL	B	505	-	-	1/4/4/4	-
5	TRS	A	504	-	-	0/9/9/9	-
4	GOL	B	503	-	-	2/4/4/4	-
6	PEG	A	505	-	-	1/4/4/4	-
6	PEG	B	507	-	-	4/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	503	-	-	0/4/4/4	-
8	BME	C	502	-	-	1/1/1/1	-
4	GOL	D	506	-	-	0/4/4/4	-
9	TAR	B	509	-	-	6/12/12/12	-
8	BME	D	503	-	-	1/1/1/1	-
8	BME	D	505	-	-	1/1/1/1	-
6	PEG	B	506	-	-	2/4/4/4	-
6	PEG	D	507	-	-	0/2/2/4	-
8	BME	D	504	-	-	1/1/1/1	-
4	GOL	C	503	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	509	TAR	O41-C4	-2.11	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	GOL	C1-C2-C3-O3
4	B	504	GOL	O1-C1-C2-O2
8	C	502	BME	O1-C1-C2-S2
8	D	504	BME	O1-C1-C2-S2
8	D	505	BME	O1-C1-C2-S2

There are no ring outliers.

14 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	508	PEG	1	0
4	B	505	GOL	4	0
6	A	505	PEG	5	0
6	B	507	PEG	1	0
4	B	504	GOL	2	0
4	A	502	GOL	2	0
3	B	501	ACY	4	0
8	C	502	BME	1	0
4	D	506	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	503	BME	1	0
9	B	509	TAR	3	0
8	D	505	BME	1	0
6	B	506	PEG	6	0
4	C	503	GOL	5	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 [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	271/321 (84%)	0.65	28 (10%)	12 12	14, 37, 70, 117	14 (5%)
1	C	259/321 (80%)	1.06	37 (14%)	6 6	18, 45, 79, 98	21 (8%)
2	B	458/482 (95%)	0.18	19 (4%)	41 45	12, 30, 53, 119	21 (4%)
2	D	454/482 (94%)	0.44	27 (5%)	28 30	15, 37, 61, 94	27 (5%)
All	All	1442/1606 (89%)	0.51	111 (7%)	19 21	12, 36, 69, 119	83 (5%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	LEU	6.9
1	C	392	GLY	6.2
2	B	253	TYR	5.2
1	C	393	LEU	5.0
2	D	106	ARG	5.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	CME	D	22	10/11	0.92	0.12	35,42,72,74	0
2	CME	B	22	10/11	0.94	0.12	25,32,64,66	0

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
3	ACY	A	501	4/4	0.68	0.21	78,81,86,86	0
9	TAR	B	509	10/10	0.69	0.15	45,59,65,69	0
9	TAR	D	508	10/10	0.74	0.18	73,79,89,95	0
6	PEG	B	507	7/7	0.76	0.17	43,47,62,64	0
3	ACY	B	501	4/4	0.78	0.17	38,45,50,59	0
6	PEG	D	507	5/7	0.78	0.19	41,51,68,74	0
8	BME	D	505	4/4	0.78	0.24	78,81,82,95	0
4	GOL	A	502	6/6	0.78	0.15	40,54,59,61	0
4	GOL	B	503	6/6	0.78	0.18	42,52,56,59	0
4	GOL	C	503	6/6	0.79	0.15	41,56,58,60	0
6	PEG	A	505	7/7	0.79	0.18	39,58,64,69	0
6	PEG	B	506	7/7	0.79	0.17	51,62,70,71	0
3	ACY	D	502	4/4	0.79	0.17	51,56,62,66	0
3	ACY	C	501	4/4	0.80	0.16	67,72,79,80	0
8	BME	D	503	4/4	0.81	0.15	46,48,49,70	0
6	PEG	B	508	7/7	0.83	0.18	58,71,79,86	0
4	GOL	B	504	6/6	0.83	0.19	56,59,64,73	0
4	GOL	B	505	6/6	0.83	0.16	44,59,69,69	0
5	TRS	A	504	8/8	0.86	0.11	44,51,56,59	0
4	GOL	D	506	6/6	0.86	0.12	33,37,43,59	0
8	BME	B	502	4/4	0.88	0.15	39,48,54,93	0
7	CL	B	510	1/1	0.89	0.12	65,65,65,65	0
3	ACY	D	501	4/4	0.90	0.13	43,59,61,66	0
8	BME	C	502	4/4	0.90	0.16	50,50,50,77	0
4	GOL	A	503	6/6	0.90	0.16	37,49,54,69	0
8	BME	D	504	4/4	0.91	0.13	60,61,71,84	0
7	CL	C	504	1/1	0.92	0.16	68,68,68,68	0
7	CL	A	506	1/1	0.95	0.25	65,65,65,65	0

6.5 Other polymers

There are no such residues in this entry.