



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:42 AM UTC

PDB ID : 5FT8 / pdb_00005ft8
Title : Crystal structure of the complex between the cysteine desulfurase CsdA and the sulfur-acceptor CsdE in the persulfurated state at 2.50 Angstrom resolution
Authors : Fernandez, F.J.; Arda, A.; Lopez-Esteva, M.; Aranda, J.; Playa-Soler, E.; Garces, F.; Round, A.; Campos-Oliva, R.; Bruix, M.; Coll, M.; Tunon, I.; Jimenez-Barbero, J.; Vega, M.C.
Deposited on : 2016-01-11
Resolution : 2.50 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)

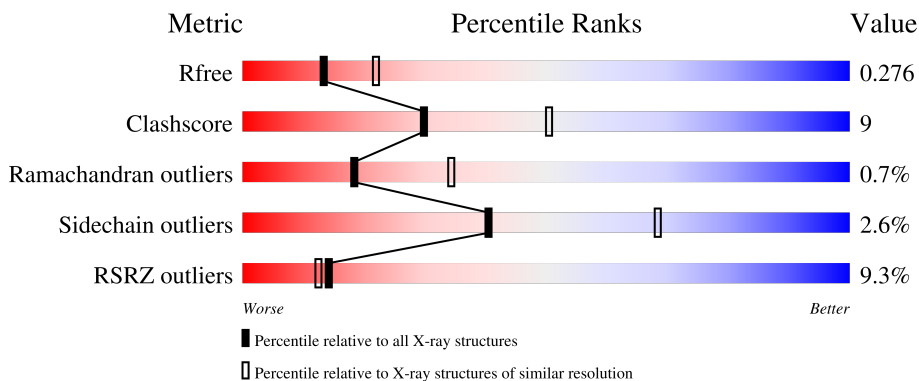
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	403	87% (green), 12% (yellow)
1	C	403	87% (green), 12% (yellow)
1	E	403	89% (green), 10% (yellow), 1% (orange)
1	G	403	88% (green), 11% (yellow)

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Mol	Chain	Length	Quality of chain
1	I	403	% 88% 10% .
1	K	403	6% 85% 12% .
1	M	403	10% 86% 12% ..
1	O	403	24% 88% 11% .
2	Q	154	2% 68% 25% . .
2	S	154	2% 69% 21% . . 6%
2	U	154	29% 58% 27% . . 12%
2	W	154	8% 73% 21% . 6%
2	Y	154	12% 67% 23% . . 8%
2	a	154	24% 60% 27% . . 9%
2	c	154	39% 67% 21% . . 9%
2	e	154	29% 46% 16% . 37%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 34325 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 Cysteine desulfurase CsdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	Total 3058	C 1937	N 532	O 575	S 14	0	2	0
1	C	401	Total 3047	C 1930	N 529	O 574	S 14	0	0	0
1	E	401	Total 3065	C 1940	N 533	O 578	S 14	0	2	0
1	G	401	Total 3059	C 1937	N 530	O 578	S 14	0	2	0
1	I	401	Total 3059	C 1936	N 531	O 578	S 14	0	2	0
1	K	401	Total 3057	C 1936	N 532	O 575	S 14	0	1	0
1	M	399	Total 3034	C 1923	N 526	O 571	S 14	0	1	0
1	O	399	Total 3031	C 1921	N 526	O 571	S 13	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q46925
A	0	ALA	-	expression tag	UNP Q46925
C	-1	GLY	-	expression tag	UNP Q46925
C	0	ALA	-	expression tag	UNP Q46925
E	-1	GLY	-	expression tag	UNP Q46925
E	0	ALA	-	expression tag	UNP Q46925
G	-1	GLY	-	expression tag	UNP Q46925
G	0	ALA	-	expression tag	UNP Q46925
I	-1	GLY	-	expression tag	UNP Q46925
I	0	ALA	-	expression tag	UNP Q46925
K	-1	GLY	-	expression tag	UNP Q46925
K	0	ALA	-	expression tag	UNP Q46925
M	-1	GLY	-	expression tag	UNP Q46925

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	ALA	-	expression tag	UNP Q46925
O	-1	GLY	-	expression tag	UNP Q46925
O	0	ALA	-	expression tag	UNP Q46925

- Molecule 2 is a protein called Sulfur acceptor protein CsdE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	148	Total	C	N	O	S	0	0	0
			1138	721	203	210	4			
2	S	144	Total	C	N	O	S	0	0	0
			1106	699	198	205	4			
2	U	136	Total	C	N	O	S	0	0	0
			1038	657	181	196	4			
2	W	145	Total	C	N	O	S	0	2	0
			1129	715	202	208	4			
2	Y	142	Total	C	N	O	S	0	0	0
			1083	687	189	203	4			
2	a	140	Total	C	N	O	S	0	0	0
			1067	675	187	201	4			
2	c	140	Total	C	N	O	S	0	0	0
			1067	675	187	201	4			
2	e	97	Total	C	N	O	S	0	0	0
			728	458	128	141	1			

There are 56 discrepancies between the modelled and reference sequences:

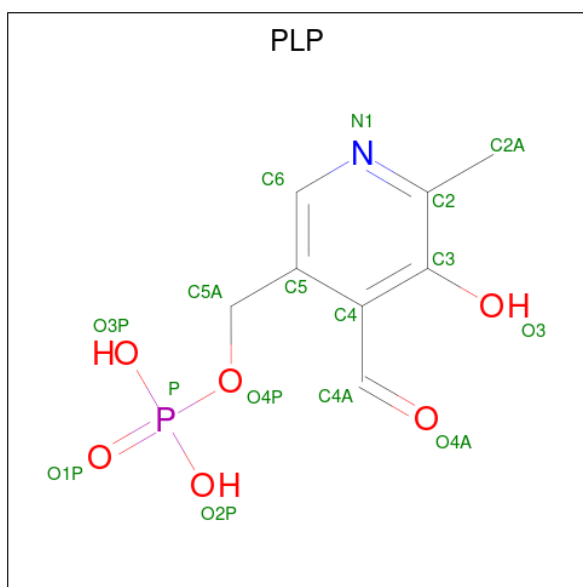
Chain	Residue	Modelled	Actual	Comment	Reference
Q	148	LYS	-	expression tag	UNP P0AGF2
Q	149	HIS	-	expression tag	UNP P0AGF2
Q	150	HIS	-	expression tag	UNP P0AGF2
Q	151	HIS	-	expression tag	UNP P0AGF2
Q	152	HIS	-	expression tag	UNP P0AGF2
Q	153	HIS	-	expression tag	UNP P0AGF2
Q	154	HIS	-	expression tag	UNP P0AGF2
S	148	LYS	-	expression tag	UNP P0AGF2
S	149	HIS	-	expression tag	UNP P0AGF2
S	150	HIS	-	expression tag	UNP P0AGF2
S	151	HIS	-	expression tag	UNP P0AGF2
S	152	HIS	-	expression tag	UNP P0AGF2
S	153	HIS	-	expression tag	UNP P0AGF2
S	154	HIS	-	expression tag	UNP P0AGF2
U	148	LYS	-	expression tag	UNP P0AGF2

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Chain	Residue	Modelled	Actual	Comment	Reference
U	149	HIS	-	expression tag	UNP P0AGF2
U	150	HIS	-	expression tag	UNP P0AGF2
U	151	HIS	-	expression tag	UNP P0AGF2
U	152	HIS	-	expression tag	UNP P0AGF2
U	153	HIS	-	expression tag	UNP P0AGF2
U	154	HIS	-	expression tag	UNP P0AGF2
W	148	LYS	-	expression tag	UNP P0AGF2
W	149	HIS	-	expression tag	UNP P0AGF2
W	150	HIS	-	expression tag	UNP P0AGF2
W	151	HIS	-	expression tag	UNP P0AGF2
W	152	HIS	-	expression tag	UNP P0AGF2
W	153	HIS	-	expression tag	UNP P0AGF2
W	154	HIS	-	expression tag	UNP P0AGF2
Y	148	LYS	-	expression tag	UNP P0AGF2
Y	149	HIS	-	expression tag	UNP P0AGF2
Y	150	HIS	-	expression tag	UNP P0AGF2
Y	151	HIS	-	expression tag	UNP P0AGF2
Y	152	HIS	-	expression tag	UNP P0AGF2
Y	153	HIS	-	expression tag	UNP P0AGF2
Y	154	HIS	-	expression tag	UNP P0AGF2
a	148	LYS	-	expression tag	UNP P0AGF2
a	149	HIS	-	expression tag	UNP P0AGF2
a	150	HIS	-	expression tag	UNP P0AGF2
a	151	HIS	-	expression tag	UNP P0AGF2
a	152	HIS	-	expression tag	UNP P0AGF2
a	153	HIS	-	expression tag	UNP P0AGF2
a	154	HIS	-	expression tag	UNP P0AGF2
c	148	LYS	-	expression tag	UNP P0AGF2
c	149	HIS	-	expression tag	UNP P0AGF2
c	150	HIS	-	expression tag	UNP P0AGF2
c	151	HIS	-	expression tag	UNP P0AGF2
c	152	HIS	-	expression tag	UNP P0AGF2
c	153	HIS	-	expression tag	UNP P0AGF2
c	154	HIS	-	expression tag	UNP P0AGF2
e	147	LYS	-	expression tag	UNP P0AGF2
e	148	HIS	-	expression tag	UNP P0AGF2
e	149	HIS	-	expression tag	UNP P0AGF2
e	150	HIS	-	expression tag	UNP P0AGF2
e	151	HIS	-	expression tag	UNP P0AGF2
e	152	HIS	-	expression tag	UNP P0AGF2
e	153	HIS	-	expression tag	UNP P0AGF2

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	M	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	O	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



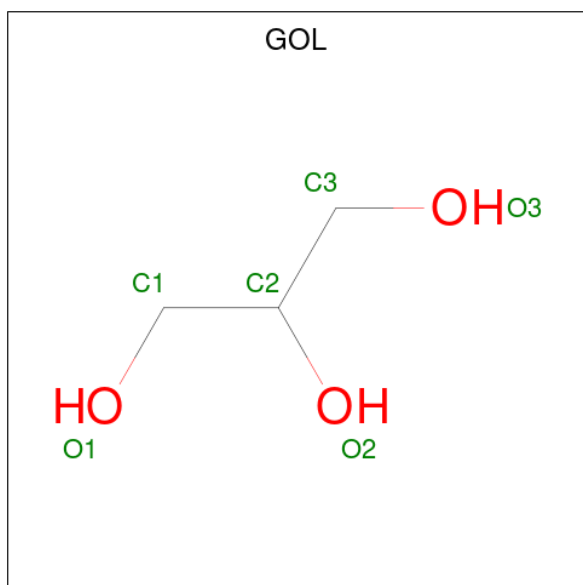
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	Q	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	G	1	Total C O 7 4 3	0	0
4	W	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	Q	1	Total 6	C 3	O 3	0	0
5	Q	1	Total 6	C 3	O 3	0	0
5	Q	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	G	1	Total 6	C 3	O 3	0	0
5	W	1	Total 6	C 3	O 3	0	0
5	I	1	Total 6	C 3	O 3	0	0
5	I	1	Total 6	C 3	O 3	0	0
5	I	1	Total 6	C 3	O 3	0	0
5	I	1	Total 6	C 3	O 3	0	0
5	I	1	Total 6	C 3	O 3	0	0
5	M	1	Total 6	C 3	O 3	0	0

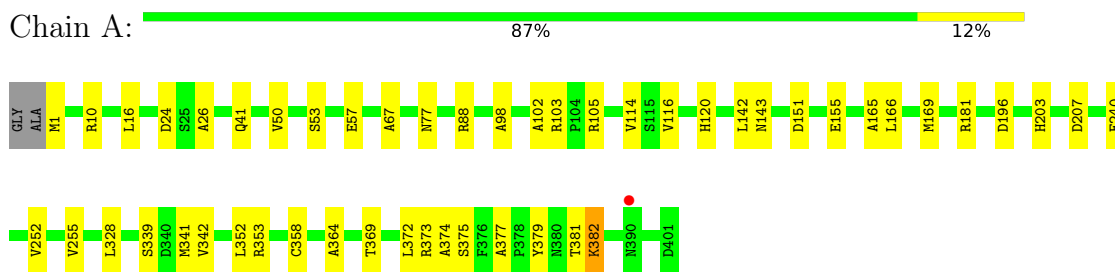
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total 186	O 186	0	0
6	Q	57	Total 57	O 57	0	0
6	C	138	Total 138	O 138	0	0
6	S	36	Total 36	O 36	0	0
6	E	165	Total 165	O 165	0	0
6	U	16	Total 16	O 16	0	0
6	G	182	Total 182	O 182	0	0
6	W	40	Total 40	O 40	0	0
6	I	119	Total 119	O 119	0	0
6	Y	14	Total 14	O 14	0	0
6	K	46	Total 46	O 46	0	0
6	a	5	Total 5	O 5	0	0
6	M	12	Total 12	O 12	0	0
6	c	3	Total 3	O 3	0	0
6	O	2	Total 2	O 2	0	0

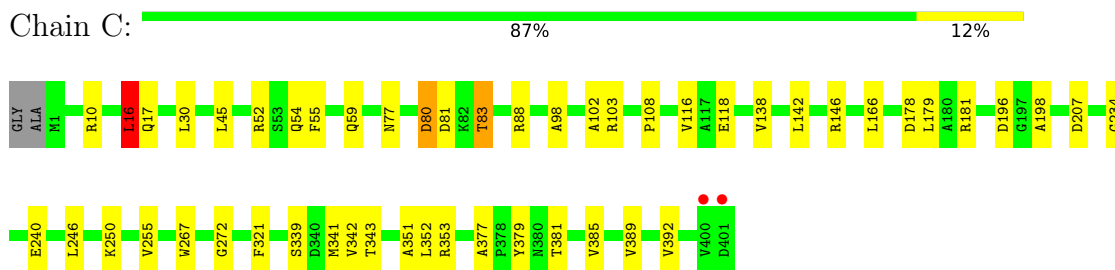
3 Residue-property plots i

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.

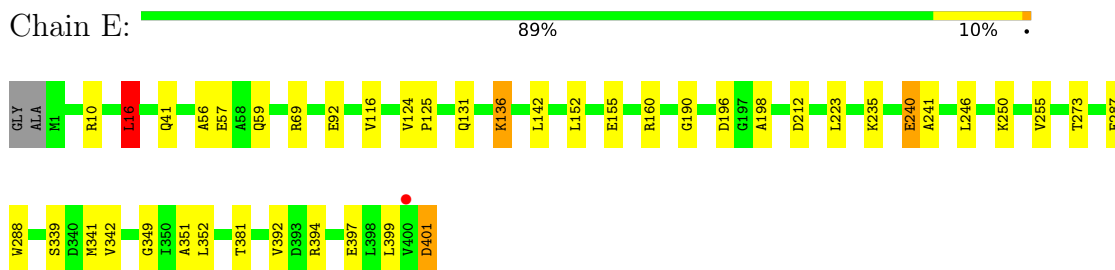
- Molecule 1: Cysteine desulfurase CsdA



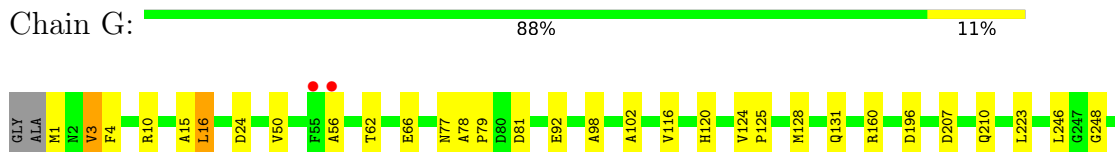
- Molecule 1: Cysteine desulfurase CsdA



- Molecule 1: Cysteine desulfurase CsdA

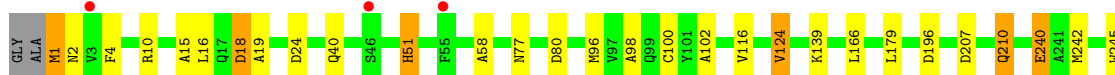
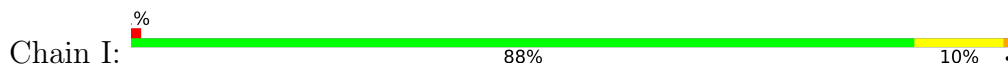


- Molecule 1: Cysteine desulfurase CsdA

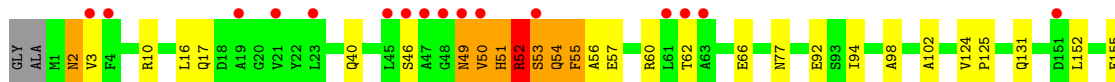
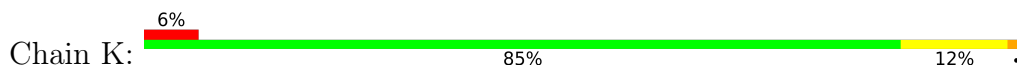




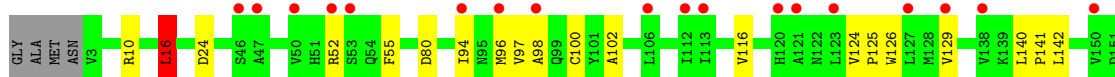
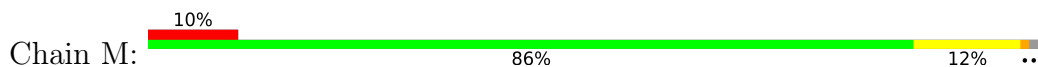
- Molecule 1: Cysteine desulfurase CsdA



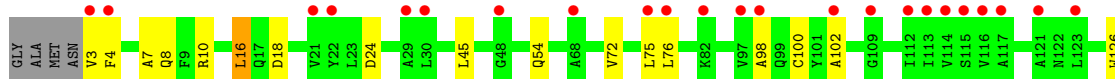
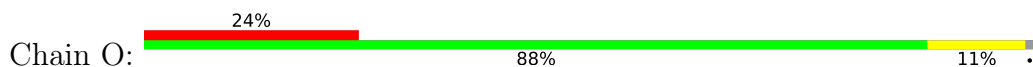
- Molecule 1: Cysteine desulfurase CsdA

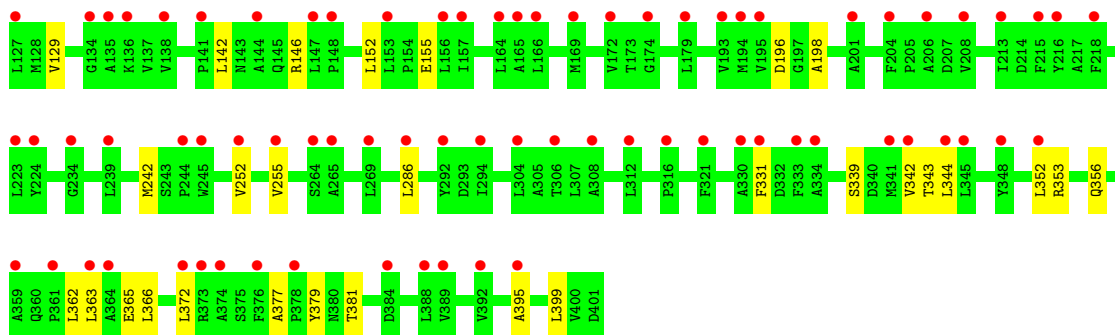


- Molecule 1: Cysteine desulfurase CsdA

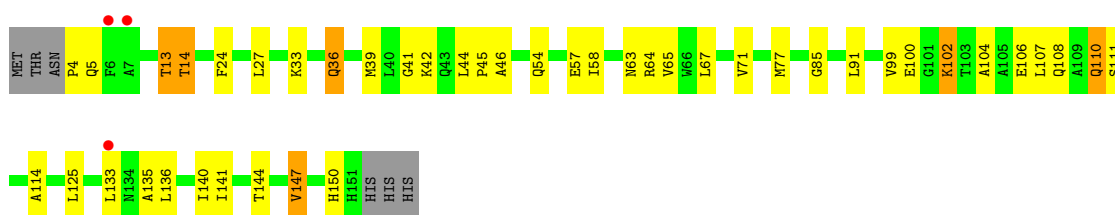


- Molecule 1: Cysteine desulfurase CsdA

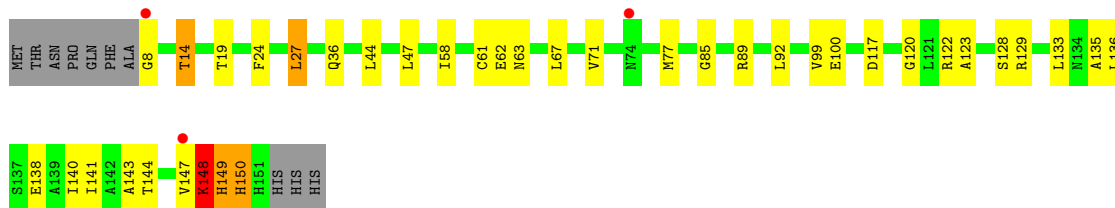




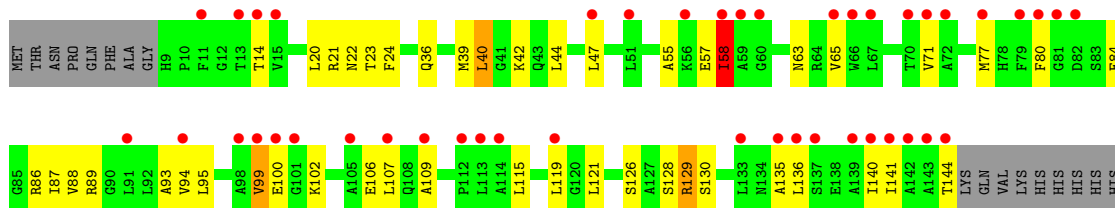
• Molecule 2: Sulfur acceptor protein CsdE



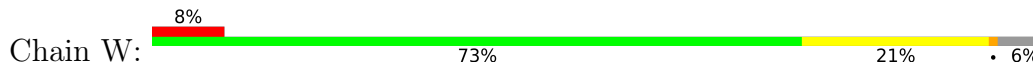
• Molecule 2: Sulfur acceptor protein CsdE

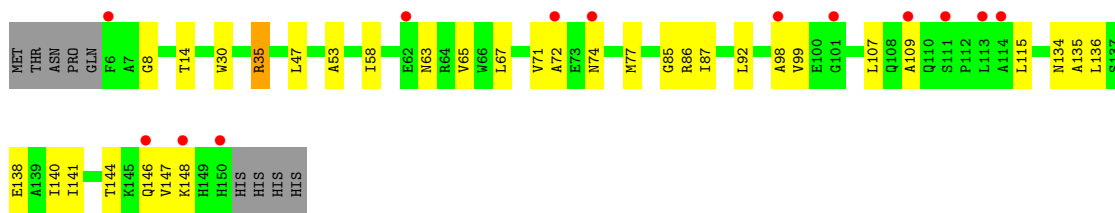


• Molecule 2: Sulfur acceptor protein CsdE

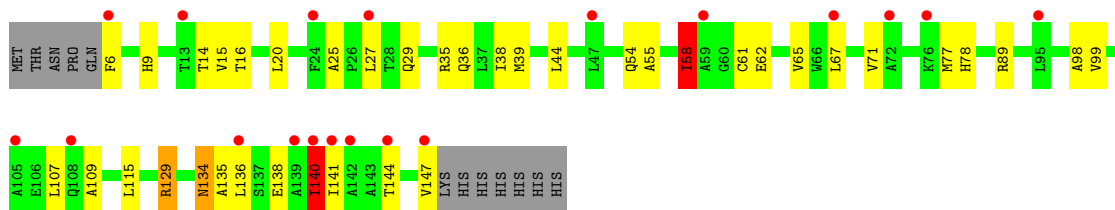


• Molecule 2: Sulfur acceptor protein CsdE

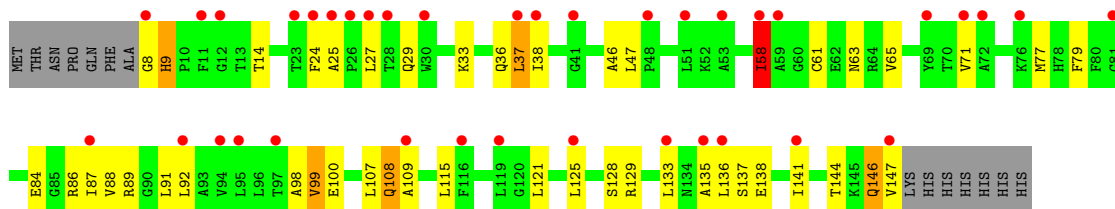




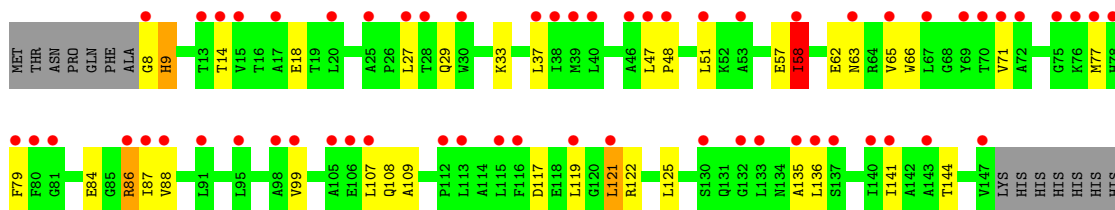
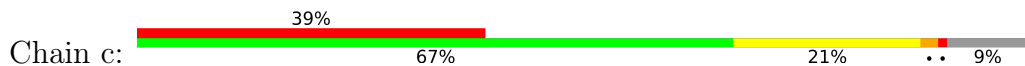
• Molecule 2: Sulfur acceptor protein CsdE



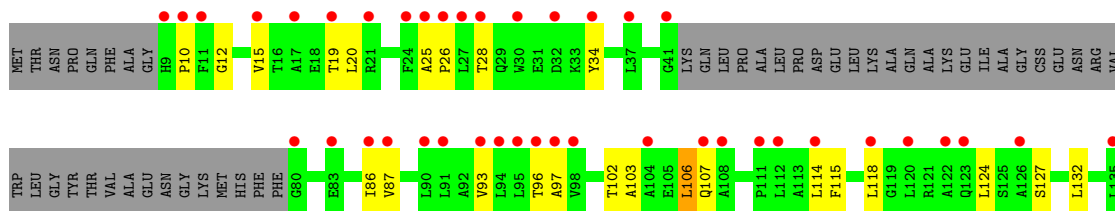
• Molecule 2: Sulfur acceptor protein CsdE



• Molecule 2: Sulfur acceptor protein CsdE



• Molecule 2: Sulfur acceptor protein CsdE



S136		
I139		
I140		
T143		
LYS		
GLN		
VAL		
LYS		
HIS		
HIS		
HIS		
HIS		
HIS		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.86Å 115.14Å 604.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.50 48.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.30-2.50) 97.3 (48.30-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.254 , 0.279 (Not available) , 0.276	Depositor DCC
R_{free} test set	2000 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtrriage
Anisotropy	0.510	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34325	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: GOL, PEG, PLP, CSS

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	0.72	0/3123	0.80	2/4251 (0.0%)
1	C	0.71	0/3106	0.81	2/4229 (0.0%)
1	E	0.72	0/3124	0.80	1/4253 (0.0%)
1	G	0.73	2/3121 (0.1%)	0.82	3/4249 (0.1%)
1	I	0.71	1/3118 (0.0%)	0.80	2/4245 (0.0%)
1	K	0.67	0/3117	0.80	4/4244 (0.1%)
1	M	0.65	1/3096 (0.0%)	0.75	2/4217 (0.0%)
1	O	0.62	0/3090	0.75	1/4208 (0.0%)
2	Q	0.79	0/1152	0.88	1/1557 (0.1%)
2	S	0.78	0/1118	0.93	6/1511 (0.4%)
2	U	0.72	0/1047	0.91	3/1417 (0.2%)
2	W	0.71	0/1144	0.86	2/1545 (0.1%)
2	Y	0.67	1/1093 (0.1%)	0.90	2/1478 (0.1%)
2	a	0.71	0/1076	0.90	3/1455 (0.2%)
2	c	0.64	0/1076	0.85	2/1455 (0.1%)
2	e	0.55	0/736	0.78	0/997
All	All	0.70	5/33337 (0.0%)	0.81	36/45311 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	357	HIS	CG-CD2	5.82	1.42	1.35
1	G	78	ALA	C-N	5.28	1.41	1.34
2	Y	29	GLN	CA-C	5.05	1.58	1.52
1	G	79	PRO	N-CD	5.03	1.54	1.47
1	I	51	HIS	CG-CD2	5.01	1.41	1.35

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	100	GLU	N-CA-C	7.81	120.78	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	29	GLN	N-CA-C	7.56	120.06	108.42
1	C	103	ARG	CB-CG-CD	7.54	128.65	111.30
2	S	148	LYS	N-CA-C	-7.54	103.14	111.36
2	Y	109	ALA	N-CA-C	-7.44	104.00	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3058	0	3022	44	0
1	C	3047	0	3004	39	0
1	E	3065	0	3018	47	0
1	G	3059	0	3014	41	0
1	I	3059	0	3012	40	0
1	K	3057	0	3010	59	0
1	M	3034	0	2991	47	0
1	O	3031	0	2986	38	0
2	Q	1138	0	1147	30	0
2	S	1106	0	1117	31	0
2	U	1038	0	1050	48	0
2	W	1129	0	1144	26	0
2	Y	1083	0	1097	32	0
2	a	1067	0	1083	37	0
2	c	1067	0	1083	30	0
2	e	728	0	742	22	0
3	A	15	0	7	1	0
3	C	15	0	6	2	0
3	E	15	0	6	2	0
3	G	15	0	7	1	0
3	I	15	0	6	1	0
3	K	15	0	6	2	0
3	M	15	0	6	2	0
3	O	15	0	7	2	0
4	A	21	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	40	1	0
4	E	28	0	40	0	0
4	G	7	0	10	0	0
4	I	7	0	10	0	0
4	K	7	0	10	1	0
4	Q	7	0	10	0	0
4	W	7	0	10	0	0
5	A	72	0	96	3	0
5	C	60	0	80	2	0
5	E	66	0	88	1	0
5	G	42	0	56	2	0
5	I	30	0	40	2	0
5	M	6	0	8	0	0
5	Q	18	0	24	0	0
5	S	6	0	8	1	0
5	W	6	0	8	0	0
6	A	186	0	0	8	0
6	C	138	0	0	4	0
6	E	165	0	0	5	0
6	G	182	0	0	11	0
6	I	119	0	0	2	0
6	K	46	0	0	1	0
6	M	12	0	0	0	0
6	O	2	0	0	0	0
6	Q	57	0	0	5	0
6	S	36	0	0	2	0
6	U	16	0	0	1	0
6	W	40	0	0	1	0
6	Y	14	0	0	4	0
6	a	5	0	0	0	0
6	c	3	0	0	0	0
All	All	34325	0	33139	566	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 9.

The worst 5 of 566 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:Y:25:ALA:O	2:Y:27:LEU:HD23	1.48	1.14
1:G:62:THR:HG23	6:G:665:HOH:O	1.50	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:97:ALA:HB2	2:e:114:LEU:HD22	1.22	1.12
2:Q:77:MET:HE3	2:Q:107:LEU:HD12	1.35	1.08
1:A:252:VAL:HG21	1:A:255:VAL:HG22	1.38	1.06

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	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
1	C	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	E	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
1	G	400/403 (99%)	387 (97%)	12 (3%)	1 (0%)	36	55
1	I	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
1	K	399/403 (99%)	386 (97%)	10 (2%)	3 (1%)	16	31
1	M	397/403 (98%)	385 (97%)	11 (3%)	1 (0%)	36	55
1	O	396/403 (98%)	381 (96%)	14 (4%)	1 (0%)	36	55
2	Q	145/154 (94%)	138 (95%)	4 (3%)	3 (2%)	5	9
2	S	141/154 (92%)	137 (97%)	2 (1%)	2 (1%)	9	17
2	U	133/154 (86%)	130 (98%)	1 (1%)	2 (2%)	8	16
2	W	144/154 (94%)	136 (94%)	5 (4%)	3 (2%)	5	9
2	Y	139/154 (90%)	132 (95%)	3 (2%)	4 (3%)	3	5
2	a	137/154 (89%)	129 (94%)	4 (3%)	4 (3%)	3	5
2	c	137/154 (89%)	130 (95%)	3 (2%)	4 (3%)	3	5
2	e	93/154 (60%)	84 (90%)	8 (9%)	1 (1%)	11	22
All	All	4259/4456 (96%)	4102 (96%)	128 (3%)	29 (1%)	18	34

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	149	HIS
2	Y	55	ALA
1	K	17	GLN
1	K	50	VAL
1	K	52	ARG

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	316/314 (101%)	314 (99%)	2 (1%)	78 91
1	C	314/314 (100%)	310 (99%)	4 (1%)	61 82
1	E	316/314 (101%)	311 (98%)	5 (2%)	55 79
1	G	316/314 (101%)	313 (99%)	3 (1%)	70 87
1	I	316/314 (101%)	309 (98%)	7 (2%)	45 73
1	K	315/314 (100%)	307 (98%)	8 (2%)	42 69
1	M	313/314 (100%)	307 (98%)	6 (2%)	50 76
1	O	312/314 (99%)	310 (99%)	2 (1%)	78 91
2	Q	115/121 (95%)	105 (91%)	10 (9%)	9 21
2	S	112/121 (93%)	107 (96%)	5 (4%)	24 49
2	U	105/121 (87%)	100 (95%)	5 (5%)	23 46
2	W	114/121 (94%)	109 (96%)	5 (4%)	25 50
2	Y	109/121 (90%)	101 (93%)	8 (7%)	13 27
2	a	108/121 (89%)	98 (91%)	10 (9%)	8 18
2	c	108/121 (89%)	102 (94%)	6 (6%)	19 39
2	e	75/121 (62%)	74 (99%)	1 (1%)	61 82
All	All	3364/3480 (97%)	3277 (97%)	87 (3%)	40 68

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	53	SER
2	a	146	GLN
1	K	55	PHE
2	a	58	ILE
1	M	352	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
2	c	54	GLN
2	c	124	GLN
1	O	357	HIS
1	G	8	GLN
1	G	2	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

15 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	$\# Z > 2$
1	CSS	A	358	1	4,6,7	0.80	0	2,6,8	0.38	0
2	CSS	a	61	2	4,6,7	0.83	0	2,6,8	0.13	0
2	CSS	S	61	2	4,6,7	0.78	0	2,6,8	0.17	0
1	CSS	O	358	1	4,6,7	0.83	0	2,6,8	0.38	0
1	CSS	K	358	1	4,6,7	0.98	0	2,6,8	0.40	0
2	CSS	W	61	2	4,6,7	0.76	0	2,6,8	0.33	0
2	CSS	Y	61	2	4,6,7	0.81	0	2,6,8	0.32	0
2	CSS	c	61	2	4,6,7	0.87	0	2,6,8	0.19	0
1	CSS	C	358	1	4,6,7	0.87	0	2,6,8	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSS	G	358	1	4,6,7	0.77	0	2,6,8	0.33	0
2	CSS	Q	61	2	4,6,7	0.86	0	2,6,8	0.11	0
1	CSS	I	358	1	4,6,7	1.07	0	2,6,8	0.30	0
1	CSS	E	358	1	4,6,7	0.78	0	2,6,8	0.30	0
1	CSS	M	358	1	4,6,7	0.79	0	2,6,8	0.40	0
2	CSS	U	61	2	4,6,7	0.79	0	2,6,8	0.20	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	A	358	1	-	0/1/5/7	-
2	CSS	a	61	2	-	1/1/5/7	-
2	CSS	S	61	2	-	1/1/5/7	-
1	CSS	O	358	1	-	0/1/5/7	-
1	CSS	K	358	1	-	0/1/5/7	-
2	CSS	W	61	2	-	1/1/5/7	-
2	CSS	Y	61	2	-	1/1/5/7	-
2	CSS	c	61	2	-	1/1/5/7	-
1	CSS	C	358	1	-	0/1/5/7	-
1	CSS	G	358	1	-	0/1/5/7	-
2	CSS	Q	61	2	-	1/1/5/7	-
1	CSS	I	358	1	-	0/1/5/7	-
1	CSS	E	358	1	-	0/1/5/7	-
1	CSS	M	358	1	-	0/1/5/7	-
2	CSS	U	61	2	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	61	CSS	N-CA-CB-SG
2	S	61	CSS	N-CA-CB-SG
2	U	61	CSS	N-CA-CB-SG
2	W	61	CSS	N-CA-CB-SG
2	Y	61	CSS	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	358	CSS	1	0
2	a	61	CSS	1	0
2	S	61	CSS	3	0
2	Y	61	CSS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

75 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	PLP	C	501	1	15,15,16	2.96	3 (20%)	21,22,23	1.41	3 (14%)
5	GOL	E	511	-	5,5,5	0.52	0	5,5,5	0.26	0
5	GOL	A	515	-	5,5,5	0.35	0	5,5,5	0.31	0
5	GOL	E	515	-	5,5,5	0.41	0	5,5,5	0.31	0
4	PEG	E	505	-	6,6,6	0.56	0	5,5,5	0.32	0
5	GOL	G	507	-	5,5,5	0.41	0	5,5,5	0.24	0
4	PEG	E	504	-	6,6,6	0.61	0	5,5,5	0.21	0
5	GOL	Q	202	-	5,5,5	0.45	0	5,5,5	0.15	0
5	GOL	E	507	-	5,5,5	0.46	0	5,5,5	0.31	0
3	PLP	A	501	1	15,15,16	3.39	3 (20%)	21,22,23	1.35	3 (14%)
5	GOL	A	509	-	5,5,5	0.33	0	5,5,5	0.19	0
5	GOL	E	509	-	5,5,5	0.52	0	5,5,5	0.27	0
5	GOL	E	516	-	5,5,5	0.47	0	5,5,5	0.36	0
3	PLP	K	501	1	15,15,16	3.04	3 (20%)	21,22,23	1.17	2 (9%)
4	PEG	I	502	-	6,6,6	0.58	0	5,5,5	0.16	0
5	GOL	Q	204	-	5,5,5	0.34	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	505	-	5,5,5	0.38	0	5,5,5	0.37	0
5	GOL	E	506	-	5,5,5	0.47	0	5,5,5	0.36	0
5	GOL	C	510	-	5,5,5	0.34	0	5,5,5	0.22	0
5	GOL	G	508	-	5,5,5	0.44	0	5,5,5	0.46	0
5	GOL	I	505	-	5,5,5	0.49	0	5,5,5	0.58	0
4	PEG	C	504	-	6,6,6	0.56	0	5,5,5	0.28	0
4	PEG	C	505	-	6,6,6	0.53	0	5,5,5	0.29	0
5	GOL	A	506	-	5,5,5	0.40	0	5,5,5	0.45	0
4	PEG	E	503	-	6,6,6	0.53	0	5,5,5	0.18	0
4	PEG	K	502	-	6,6,6	0.63	0	5,5,5	0.42	0
5	GOL	A	512	-	5,5,5	0.35	0	5,5,5	0.17	0
5	GOL	G	506	-	5,5,5	0.45	0	5,5,5	0.33	0
5	GOL	I	504	-	5,5,5	0.38	0	5,5,5	0.14	0
3	PLP	G	501	1	15,15,16	2.65	3 (20%)	21,22,23	1.97	5 (23%)
5	GOL	C	507	-	5,5,5	0.41	0	5,5,5	0.27	0
3	PLP	M	501	1	15,15,16	3.15	3 (20%)	21,22,23	1.31	3 (14%)
5	GOL	A	516	-	5,5,5	0.37	0	5,5,5	0.15	0
5	GOL	E	514	-	5,5,5	0.40	0	5,5,5	0.32	0
4	PEG	C	503	-	6,6,6	0.61	0	5,5,5	0.36	0
5	GOL	G	503	-	5,5,5	0.43	0	5,5,5	0.18	0
5	GOL	A	510	-	5,5,5	0.30	0	5,5,5	0.41	0
5	GOL	I	507	-	5,5,5	0.49	0	5,5,5	0.44	0
5	GOL	C	509	-	5,5,5	0.32	0	5,5,5	0.28	0
5	GOL	E	512	-	5,5,5	0.28	0	5,5,5	0.31	0
5	GOL	E	510	-	5,5,5	0.46	0	5,5,5	0.42	0
4	PEG	W	201	-	6,6,6	0.54	0	5,5,5	0.32	0
5	GOL	E	508	-	5,5,5	0.40	0	5,5,5	0.56	0
5	GOL	G	509	-	5,5,5	0.37	0	5,5,5	0.12	0
5	GOL	A	514	-	5,5,5	0.38	0	5,5,5	0.34	0
4	PEG	G	502	-	6,6,6	0.57	0	5,5,5	0.36	0
5	GOL	C	512	-	5,5,5	0.50	0	5,5,5	0.57	0
5	GOL	C	514	-	5,5,5	0.43	0	5,5,5	0.24	0
4	PEG	E	502	-	6,6,6	0.59	0	5,5,5	0.33	0
4	PEG	A	503	-	6,6,6	0.61	0	5,5,5	0.31	0
5	GOL	C	511	-	5,5,5	0.52	0	5,5,5	0.35	0
3	PLP	I	501	1	15,15,16	3.09	3 (20%)	21,22,23	1.18	1 (4%)
5	GOL	S	201	-	5,5,5	0.44	0	5,5,5	0.15	0
5	GOL	G	505	-	5,5,5	0.50	0	5,5,5	0.20	0
5	GOL	I	506	-	5,5,5	0.35	0	5,5,5	0.19	0
5	GOL	G	504	-	5,5,5	0.54	0	5,5,5	0.56	0
5	GOL	Q	203	-	5,5,5	0.50	0	5,5,5	0.31	0
3	PLP	O	501	1	15,15,16	3.30	3 (20%)	21,22,23	1.31	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	508	-	5,5,5	0.40	0	5,5,5	0.25	0
5	GOL	M	502	-	5,5,5	0.42	0	5,5,5	0.24	0
4	PEG	Q	201	-	6,6,6	0.53	0	5,5,5	0.26	0
3	PLP	E	501	1	15,15,16	2.86	3 (20%)	21,22,23	1.31	2 (9%)
4	PEG	A	504	-	6,6,6	0.57	0	5,5,5	0.32	0
5	GOL	A	507	-	5,5,5	0.53	0	5,5,5	0.35	0
4	PEG	A	502	-	6,6,6	0.57	0	5,5,5	0.48	0
5	GOL	C	513	-	5,5,5	0.49	0	5,5,5	0.27	0
5	GOL	W	202	-	5,5,5	0.45	0	5,5,5	0.21	0
4	PEG	C	502	-	6,6,6	0.54	0	5,5,5	0.19	0
5	GOL	A	508	-	5,5,5	0.42	0	5,5,5	0.18	0
5	GOL	I	503	-	5,5,5	0.43	0	5,5,5	0.33	0
5	GOL	C	506	-	5,5,5	0.45	0	5,5,5	0.31	0
5	GOL	A	513	-	5,5,5	0.55	0	5,5,5	0.31	0
5	GOL	C	515	-	5,5,5	0.41	0	5,5,5	0.40	0
5	GOL	A	511	-	5,5,5	0.49	0	5,5,5	0.31	0
5	GOL	E	513	-	5,5,5	0.55	0	5,5,5	0.54	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	PLP	C	501	1	-	0/6/6/8	0/1/1/1
5	GOL	E	511	-	-	2/4/4/4	-
5	GOL	A	515	-	-	2/4/4/4	-
5	GOL	E	515	-	-	2/4/4/4	-
4	PEG	E	505	-	-	2/4/4/4	-
5	GOL	G	507	-	-	0/4/4/4	-
4	PEG	E	504	-	-	2/4/4/4	-
5	GOL	Q	202	-	-	3/4/4/4	-
5	GOL	E	507	-	-	1/4/4/4	-
3	PLP	A	501	1	-	0/6/6/8	0/1/1/1
5	GOL	A	509	-	-	2/4/4/4	-
5	GOL	E	509	-	-	2/4/4/4	-
5	GOL	E	516	-	-	2/4/4/4	-
3	PLP	K	501	1	-	0/6/6/8	0/1/1/1
4	PEG	I	502	-	-	2/4/4/4	-
5	GOL	Q	204	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	E	506	-	-	0/4/4/4	-
5	GOL	C	510	-	-	0/4/4/4	-
5	GOL	G	508	-	-	1/4/4/4	-
5	GOL	I	505	-	-	2/4/4/4	-
4	PEG	C	504	-	-	2/4/4/4	-
4	PEG	C	505	-	-	2/4/4/4	-
5	GOL	A	506	-	-	2/4/4/4	-
4	PEG	E	503	-	-	2/4/4/4	-
4	PEG	K	502	-	-	3/4/4/4	-
5	GOL	A	512	-	-	0/4/4/4	-
5	GOL	G	506	-	-	2/4/4/4	-
5	GOL	I	504	-	-	2/4/4/4	-
3	PLP	G	501	1	-	0/6/6/8	0/1/1/1
5	GOL	C	507	-	-	2/4/4/4	-
3	PLP	M	501	1	-	0/6/6/8	0/1/1/1
5	GOL	A	516	-	-	4/4/4/4	-
5	GOL	E	514	-	-	2/4/4/4	-
4	PEG	C	503	-	-	2/4/4/4	-
5	GOL	G	503	-	-	4/4/4/4	-
5	GOL	A	510	-	-	2/4/4/4	-
5	GOL	I	507	-	-	2/4/4/4	-
5	GOL	C	509	-	-	0/4/4/4	-
5	GOL	E	512	-	-	2/4/4/4	-
5	GOL	E	510	-	-	0/4/4/4	-
4	PEG	W	201	-	-	2/4/4/4	-
5	GOL	E	508	-	-	2/4/4/4	-
5	GOL	G	509	-	-	0/4/4/4	-
5	GOL	A	514	-	-	2/4/4/4	-
4	PEG	G	502	-	-	3/4/4/4	-
5	GOL	C	512	-	-	4/4/4/4	-
5	GOL	C	514	-	-	2/4/4/4	-
4	PEG	E	502	-	-	3/4/4/4	-
4	PEG	A	503	-	-	3/4/4/4	-
5	GOL	C	511	-	-	4/4/4/4	-
3	PLP	I	501	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	S	201	-	-	1/4/4/4	-
5	GOL	G	505	-	-	2/4/4/4	-
5	GOL	I	506	-	-	0/4/4/4	-
5	GOL	G	504	-	-	4/4/4/4	-
5	GOL	Q	203	-	-	2/4/4/4	-
3	PLP	O	501	1	-	0/6/6/8	0/1/1/1
5	GOL	C	508	-	-	3/4/4/4	-
5	GOL	M	502	-	-	2/4/4/4	-
4	PEG	Q	201	-	-	3/4/4/4	-
3	PLP	E	501	1	-	0/6/6/8	0/1/1/1
4	PEG	A	504	-	-	3/4/4/4	-
5	GOL	A	507	-	-	4/4/4/4	-
4	PEG	A	502	-	-	3/4/4/4	-
5	GOL	C	513	-	-	3/4/4/4	-
5	GOL	W	202	-	-	2/4/4/4	-
4	PEG	C	502	-	-	2/4/4/4	-
5	GOL	A	508	-	-	2/4/4/4	-
5	GOL	I	503	-	-	3/4/4/4	-
5	GOL	C	506	-	-	2/4/4/4	-
5	GOL	A	513	-	-	4/4/4/4	-
5	GOL	C	515	-	-	2/4/4/4	-
5	GOL	A	511	-	-	4/4/4/4	-
5	GOL	E	513	-	-	0/4/4/4	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PLP	C5-C4	8.69	1.50	1.40
3	A	501	PLP	C3-C2	8.43	1.49	1.41
3	O	501	PLP	C5-C4	8.26	1.49	1.40
3	O	501	PLP	C3-C2	8.11	1.49	1.41
3	M	501	PLP	C5-C4	8.08	1.49	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	PLP	C2A-C2-C3	-4.65	115.36	120.80
3	G	501	PLP	C2A-C2-N1	3.68	124.57	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	C6-N1-C2	3.34	125.26	119.20
3	G	501	PLP	C6-N1-C2	3.01	124.67	119.20
3	O	501	PLP	C6-N1-C2	2.95	124.55	119.20

There are no chirality outliers.

5 of 140 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	GOL	O1-C1-C2-O2
5	A	507	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	508	GOL	C1-C2-C3-O3
5	A	511	GOL	C1-C2-C3-O3

There are no ring outliers.

21 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	PLP	2	0
5	E	507	GOL	1	0
3	A	501	PLP	1	0
5	A	509	GOL	1	0
3	K	501	PLP	2	0
4	K	502	PEG	1	0
5	G	506	GOL	1	0
3	G	501	PLP	1	0
3	M	501	PLP	2	0
4	C	503	PEG	1	0
5	C	512	GOL	1	0
5	C	514	GOL	1	0
4	A	503	PEG	2	0
3	I	501	PLP	1	0
5	S	201	GOL	1	0
5	G	504	GOL	1	0
3	O	501	PLP	2	0
3	E	501	PLP	2	0
5	A	507	GOL	2	0
4	A	502	PEG	1	0
5	I	503	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 [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	400/403 (99%)	-0.02	1 (0%) 90 87	28, 40, 54, 74	2 (0%)
1	C	400/403 (99%)	-0.03	2 (0%) 87 85	27, 41, 60, 88	0
1	E	400/403 (99%)	-0.02	1 (0%) 90 87	17, 38, 54, 74	2 (0%)
1	G	400/403 (99%)	-0.01	2 (0%) 87 85	26, 39, 60, 98	2 (0%)
1	I	400/403 (99%)	0.11	4 (1%) 79 76	17, 41, 73, 109	2 (0%)
1	K	400/403 (99%)	0.75	26 (6%) 25 22	40, 67, 90, 116	1 (0%)
1	M	398/403 (98%)	1.08	42 (10%) 11 9	53, 86, 118, 139	1 (0%)
1	O	398/403 (98%)	1.53	97 (24%) 2 1	81, 116, 149, 167	0
2	Q	147/154 (95%)	0.34	3 (2%) 65 61	29, 50, 82, 116	0
2	S	143/154 (92%)	0.65	3 (2%) 63 59	46, 61, 82, 116	0
2	U	135/154 (87%)	1.66	44 (32%) 1 1	61, 102, 173, 209	0
2	W	144/154 (93%)	0.80	13 (9%) 15 13	24, 66, 112, 155	2 (1%)
2	Y	141/154 (91%)	1.13	19 (13%) 7 5	49, 87, 145, 171	0
2	a	139/154 (90%)	1.64	37 (26%) 1 1	100, 116, 142, 148	0
2	c	139/154 (90%)	1.96	60 (43%) 0 0	122, 142, 161, 178	0
2	e	97/154 (62%)	1.97	44 (45%) 0 0	147, 158, 166, 172	0
All	All	4281/4456 (96%)	0.63	398 (9%) 14 12	17, 56, 146, 209	12 (0%)

The worst 5 of 398 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	46	SER	7.3
2	U	136	LEU	6.4
1	O	224	TYR	5.9
2	c	136	LEU	5.6
2	a	24	PHE	5.1

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	CSS	c	61	7/8	0.54	0.13	141,146,147,148	0
2	CSS	U	61	7/8	0.64	0.16	97,104,108,115	0
2	CSS	W	61	7/8	0.73	0.15	94,97,107,114	0
2	CSS	S	61	7/8	0.75	0.13	86,87,98,101	0
1	CSS	M	358	7/8	0.76	0.15	85,87,88,92	0
2	CSS	a	61	7/8	0.79	0.11	105,106,109,110	0
1	CSS	O	358	7/8	0.80	0.11	113,114,116,116	0
2	CSS	Q	61	7/8	0.83	0.12	71,73,83,95	0
2	CSS	Y	61	7/8	0.86	0.11	87,91,97,104	0
1	CSS	K	358	7/8	0.87	0.13	59,61,62,64	0
1	CSS	G	358	7/8	0.90	0.15	33,34,35,42	0
1	CSS	C	358	7/8	0.90	0.14	36,39,42,51	0
1	CSS	E	358	7/8	0.91	0.10	30,32,34,48	0
1	CSS	I	358	7/8	0.92	0.10	35,38,41,49	0
1	CSS	A	358	7/8	0.93	0.11	35,35,38,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	509	6/6	0.69	0.13	61,63,68,68	0
5	GOL	G	505	6/6	0.76	0.11	57,71,75,75	0
4	PEG	C	503	7/7	0.77	0.16	56,64,70,81	0
5	GOL	G	509	6/6	0.79	0.11	54,57,67,70	0
5	GOL	A	511	6/6	0.80	0.12	49,61,64,65	0
5	GOL	C	511	6/6	0.80	0.11	52,55,59,66	0
4	PEG	K	502	7/7	0.81	0.13	57,58,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	E	508	6/6	0.81	0.11	40,43,54,54	0
5	GOL	E	510	6/6	0.82	0.12	50,59,65,80	0
5	GOL	C	514	6/6	0.82	0.10	66,71,76,77	0
4	PEG	E	502	7/7	0.82	0.13	50,55,60,64	0
5	GOL	W	202	6/6	0.82	0.11	64,74,75,76	0
4	PEG	C	502	7/7	0.83	0.13	55,59,72,73	0
5	GOL	E	514	6/6	0.83	0.12	59,65,72,78	0
5	GOL	C	513	6/6	0.83	0.11	57,66,69,75	0
5	GOL	G	507	6/6	0.83	0.11	57,61,66,67	0
5	GOL	A	505	6/6	0.83	0.17	55,58,60,69	0
5	GOL	Q	204	6/6	0.83	0.15	54,62,67,71	0
5	GOL	I	507	6/6	0.83	0.12	53,64,68,69	0
5	GOL	S	201	6/6	0.84	0.10	44,60,64,64	0
5	GOL	A	513	6/6	0.84	0.12	50,52,55,56	0
5	GOL	I	504	6/6	0.84	0.09	59,65,70,73	0
5	GOL	G	508	6/6	0.84	0.09	48,52,53,54	0
4	PEG	E	503	7/7	0.85	0.10	54,60,65,65	0
4	PEG	W	201	7/7	0.85	0.09	57,58,64,66	0
5	GOL	E	509	6/6	0.85	0.14	46,54,62,63	0
5	GOL	C	506	6/6	0.85	0.12	55,61,67,67	0
5	GOL	E	512	6/6	0.86	0.11	58,64,68,71	0
5	GOL	A	507	6/6	0.86	0.14	54,59,60,61	0
5	GOL	A	514	6/6	0.86	0.10	63,70,72,73	0
5	GOL	A	516	6/6	0.86	0.09	55,56,58,62	0
4	PEG	A	503	7/7	0.86	0.14	43,51,55,57	0
4	PEG	A	502	7/7	0.86	0.16	48,55,57,60	0
5	GOL	C	507	6/6	0.86	0.14	55,67,72,73	0
5	GOL	C	510	6/6	0.86	0.10	48,65,70,73	0
5	GOL	E	511	6/6	0.86	0.11	50,59,64,64	0
4	PEG	C	504	7/7	0.87	0.14	48,55,69,69	0
5	GOL	G	503	6/6	0.87	0.10	54,60,64,66	0
5	GOL	I	506	6/6	0.87	0.10	62,71,73,76	0
4	PEG	E	504	7/7	0.87	0.11	45,53,56,57	0
4	PEG	G	502	7/7	0.88	0.11	54,61,68,70	0
5	GOL	A	515	6/6	0.88	0.11	48,54,63,64	0
5	GOL	A	512	6/6	0.88	0.10	49,51,53,54	0
5	GOL	E	506	6/6	0.88	0.12	42,51,53,54	0
5	GOL	E	513	6/6	0.88	0.10	52,54,59,64	0
5	GOL	E	507	6/6	0.88	0.16	50,56,60,60	0
5	GOL	E	516	6/6	0.88	0.11	44,52,58,62	0
3	PLP	O	501	15/16	0.88	0.12	98,103,109,111	0
5	GOL	M	502	6/6	0.88	0.08	57,62,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	508	6/6	0.89	0.11	48,57,60,65	0
4	PEG	Q	201	7/7	0.89	0.11	50,58,67,68	0
5	GOL	Q	202	6/6	0.89	0.09	47,53,57,58	0
5	GOL	G	506	6/6	0.89	0.11	51,62,64,67	0
5	GOL	C	508	6/6	0.89	0.12	53,57,58,72	0
5	GOL	C	515	6/6	0.89	0.10	43,46,48,52	0
4	PEG	E	505	7/7	0.90	0.12	50,54,59,61	0
3	PLP	M	501	15/16	0.90	0.10	79,82,85,86	0
5	GOL	C	512	6/6	0.91	0.16	43,45,55,68	0
4	PEG	A	504	7/7	0.91	0.11	45,51,56,56	0
5	GOL	E	515	6/6	0.91	0.11	52,54,56,57	0
4	PEG	C	505	7/7	0.91	0.10	40,57,74,75	0
5	GOL	C	509	6/6	0.91	0.08	49,58,74,77	0
5	GOL	I	505	6/6	0.91	0.14	42,53,56,69	0
5	GOL	G	504	6/6	0.91	0.09	35,49,53,56	0
5	GOL	A	510	6/6	0.91	0.12	48,58,59,60	0
4	PEG	I	502	7/7	0.91	0.09	36,47,53,55	0
5	GOL	A	506	6/6	0.92	0.12	47,62,64,65	0
5	GOL	Q	203	6/6	0.92	0.07	44,52,52,56	0
5	GOL	I	503	6/6	0.95	0.06	37,48,51,53	0
3	PLP	K	501	15/16	0.95	0.08	51,53,55,56	0
3	PLP	C	501	15/16	0.96	0.07	29,31,32,33	0
3	PLP	I	501	15/16	0.96	0.07	31,33,38,39	0
3	PLP	G	501	15/16	0.97	0.07	28,30,32,37	0
3	PLP	E	501	15/16	0.97	0.06	28,29,31,31	0
3	PLP	A	501	15/16	0.98	0.05	28,29,30,31	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.