



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2016 – 01:59 PM EST

PDB ID : 5FT8  
Title : Structure of a Cysteine Desulfurase-Sulfur Acceptor Complex from Escherichia coli at 2.50 Angstroem resolution  
Authors : Fernandez, F.J.; Arda, A.; Lopez-Esteva, M.; Aranda, J.; Penya-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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

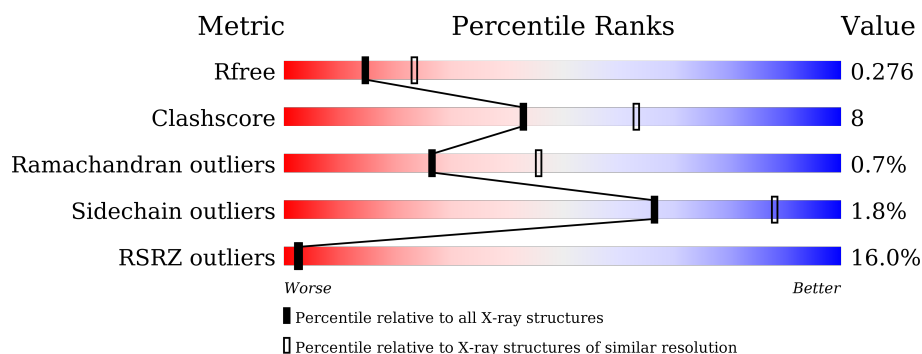
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	88% 11% .
1	C	403	87% 12% .
1	E	403	88% 10% ..
1	G	403	87% 12% .
1	I	403	2% 88% 10% ..
1	K	403	6% 85% 12% ..

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Mol	Chain	Length	Quality of chain
1	M	403	
1	O	403	
2	B	154	
2	D	154	
2	F	154	
2	H	154	
2	J	154	
2	L	154	
2	N	154	
2	P	154	

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
4	CSS	D	1152	-	-	X	-
5	PEG	A	1405	-	-	-	X
5	PEG	I	1404	-	-	-	X
6	GOL	C	1409	-	-	-	X
6	GOL	C	1411	-	-	-	X
6	GOL	G	1406	-	-	-	X
6	GOL	I	1407	-	-	-	X
6	GOL	I	1408	-	-	-	X

## 2 Entry composition

There are 7 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
1	A	400	Total	C	N	O	S	0	2	0
			3051	1934	531	574	12			
1	C	400	Total	C	N	O	S	0	0	0
			3040	1927	528	573	12			
1	E	400	Total	C	N	O	S	0	2	0
			3058	1937	532	577	12			
1	G	400	Total	C	N	O	S	0	2	0
			3052	1934	529	577	12			
1	I	400	Total	C	N	O	S	0	2	0
			3052	1933	530	577	12			
1	K	400	Total	C	N	O	S	0	1	0
			3050	1933	531	574	12			
1	M	398	Total	C	N	O	S	0	1	0
			3027	1920	525	570	12			
1	O	398	Total	C	N	O	S	0	0	0
			3024	1918	525	570	11			

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	B	147	Total	C	N	O	S	0	0	0
			1131	718	202	209	2			
2	D	143	Total	C	N	O	S	0	0	0
			1099	696	197	204	2			
2	F	135	Total	C	N	O	S	0	0	0
			1031	654	180	195	2			
2	H	144	Total	C	N	O	S	0	2	0
			1122	712	201	207	2			
2	J	141	Total	C	N	O	S	0	0	0
			1076	684	188	202	2			
2	L	139	Total	C	N	O	S	0	0	0
			1060	672	186	200	2			
2	N	139	Total	C	N	O	S	0	0	0
			1060	672	186	200	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	458	128	141	1			

There are 56 discrepancies between the modelled and reference sequences:

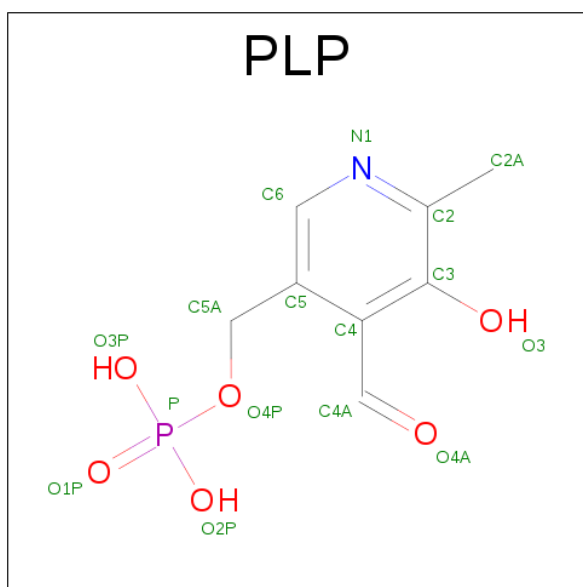
Chain	Residue	Modelled	Actual	Comment	Reference
B	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
B	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
B	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
D	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
D	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	148	LYS	-	EXPRESSION TAG	UNP P0AGF2

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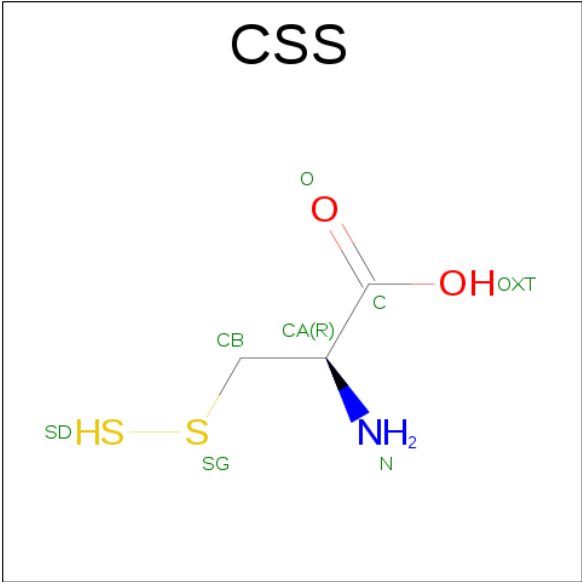
Chain	Residue	Modelled	Actual	Comment	Reference
F	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
F	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
H	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
H	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
J	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
J	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
L	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
L	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
N	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
N	154	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	148	LYS	-	EXPRESSION TAG	UNP P0AGF2
P	149	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	150	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	151	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	152	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	153	HIS	-	EXPRESSION TAG	UNP P0AGF2
P	154	HIS	-	EXPRESSION TAG	UNP P0AGF2

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 S-MERCAPTOCYSTEINE (three-letter code: CSS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	C	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	D	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	E	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	F	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	G	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	H	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	I	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	J	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	K	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	L	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	M	1	Total	C	N	O	S	0	0
			7	3	1	1	2		
4	N	1	Total	C	N	O	S	0	0
			7	3	1	1	2		

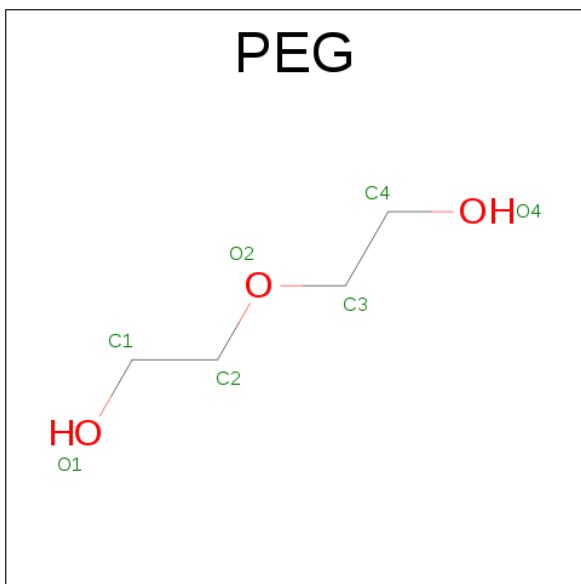
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	O	1	Total	C	N	O	S	0	0
			7	3	1	1	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



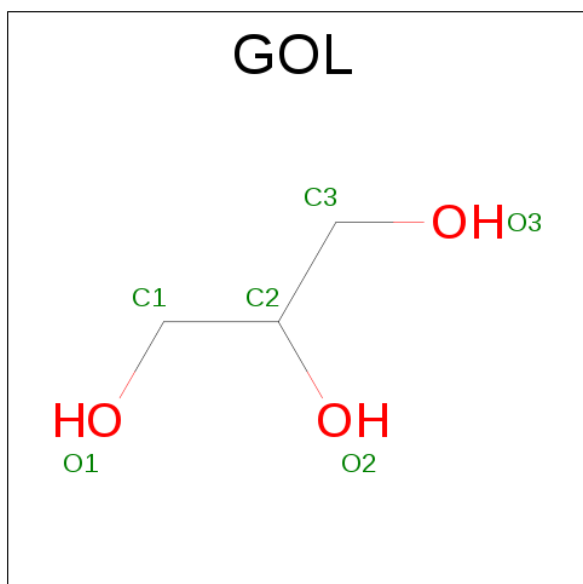
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	M	1	Total	C	O	0	0
			6	3	3		

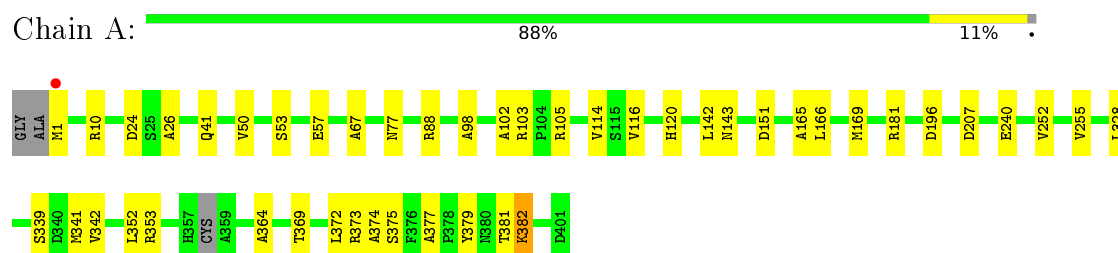
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	197	Total	O	0	0
			197	197		
7	B	57	Total	O	0	0
			57	57		
7	C	132	Total	O	0	0
			132	132		
7	D	34	Total	O	0	0
			34	34		
7	E	180	Total	O	0	0
			180	180		
7	F	15	Total	O	0	0
			15	15		
7	G	169	Total	O	0	0
			169	169		
7	H	38	Total	O	0	0
			38	38		
7	I	127	Total	O	0	0
			127	127		
7	J	14	Total	O	0	0
			14	14		
7	K	38	Total	O	0	0
			38	38		
7	L	3	Total	O	0	0
			3	3		
7	M	13	Total	O	0	0
			13	13		
7	N	2	Total	O	0	0
			2	2		
7	O	2	Total	O	0	0
			2	2		

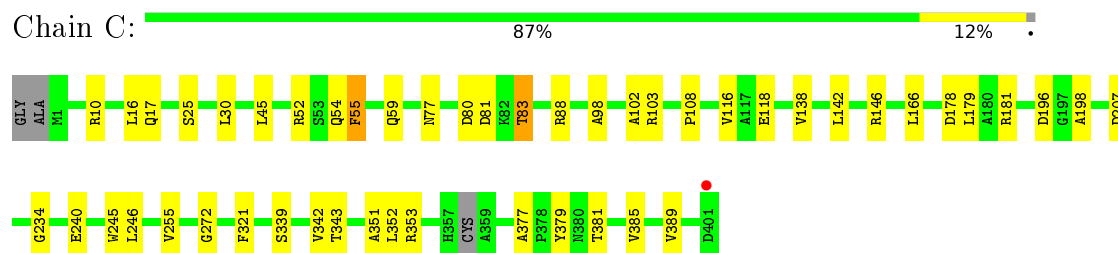
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

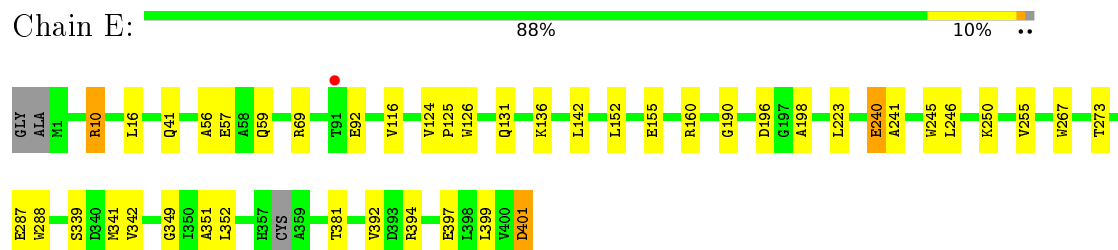
#### • Molecule 1: CYSTEINE DESULFURASE CSDA



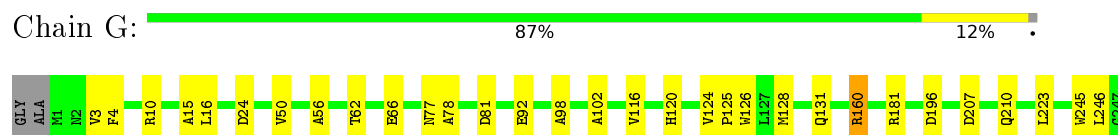
#### • Molecule 1: CYSTEINE DESULFURASE CSDA



#### • Molecule 1: CYSTEINE DESULFURASE CSDA

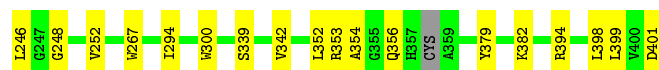
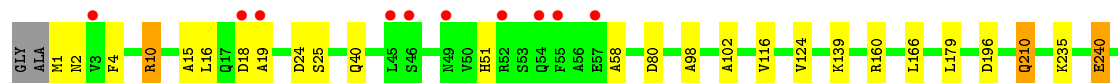
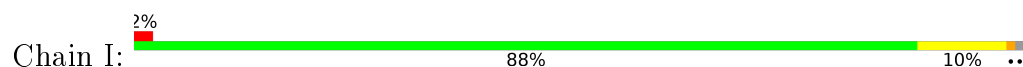


#### • Molecule 1: CYSTEINE DESULFURASE CSDA

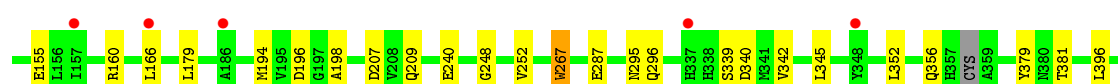
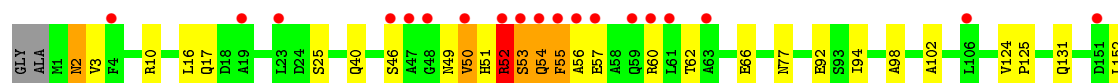
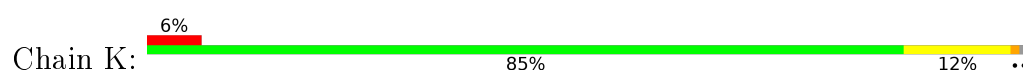




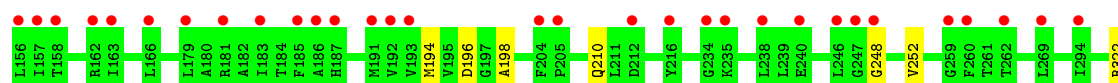
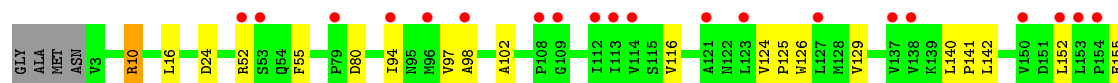
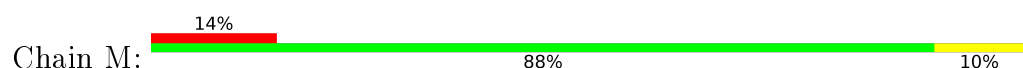
• Molecule 1: CYSTEINE DESULFURASE CSDA



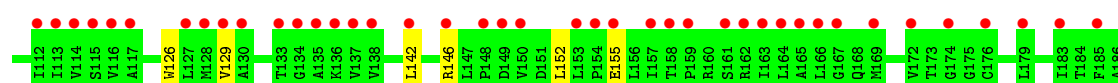
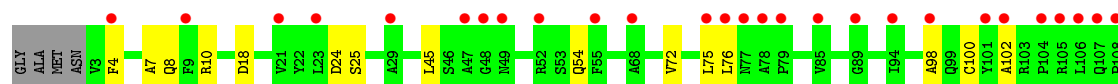
• Molecule 1: CYSTEINE DESULFURASE CSDA

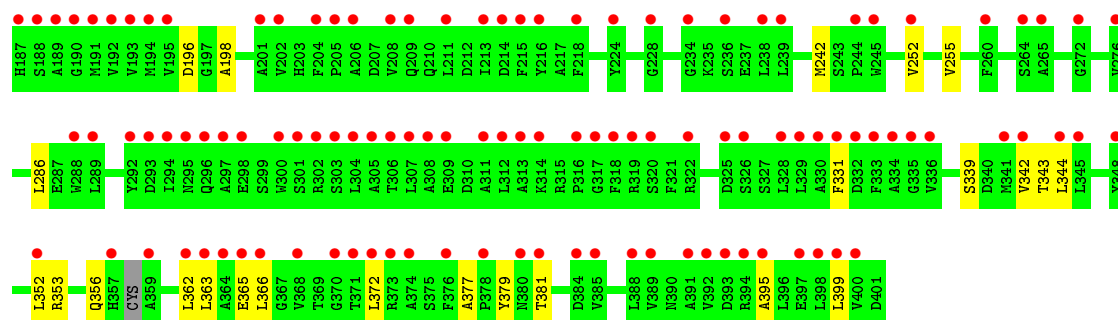


• Molecule 1: CYSTEINE DESULFURASE CSDA

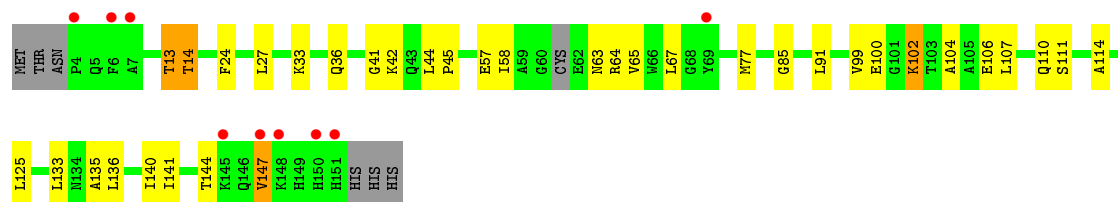


• Molecule 1: CYSTEINE DESULFURASE CSDA

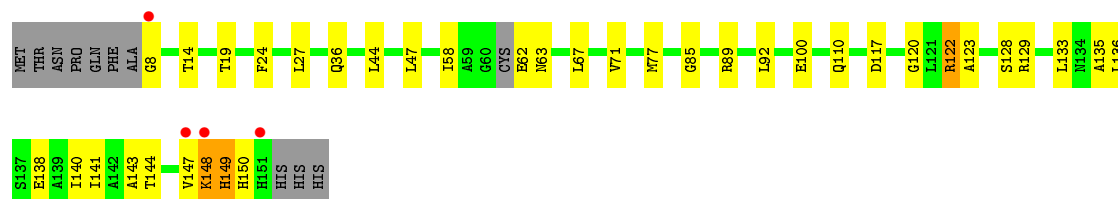




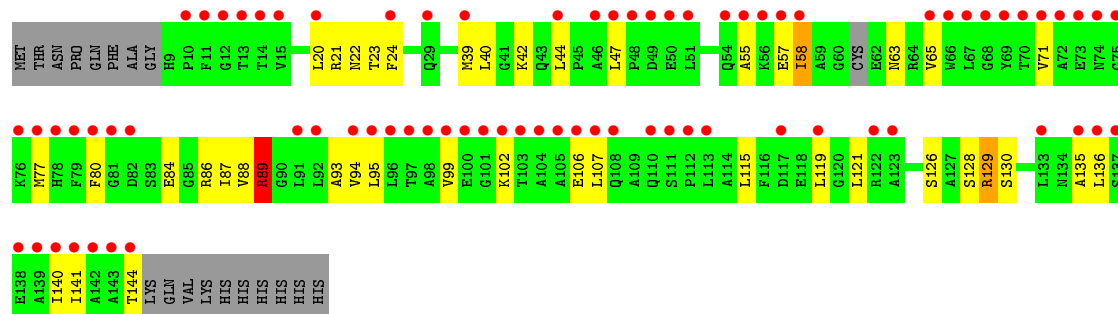
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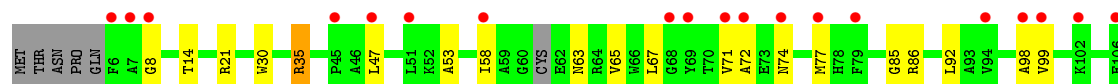
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



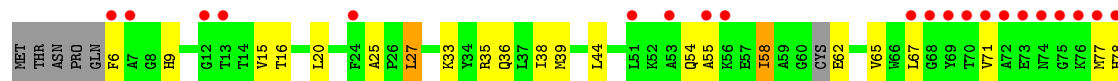
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



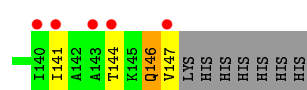
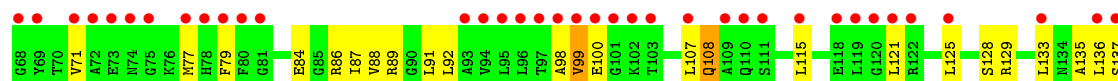
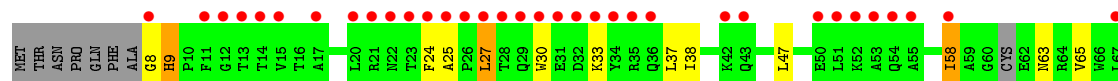




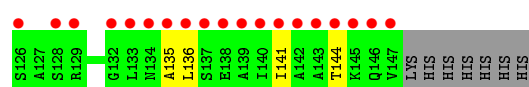
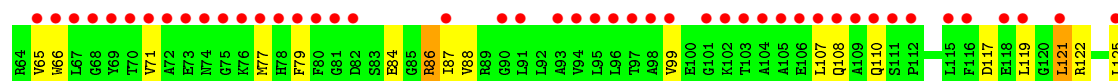
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



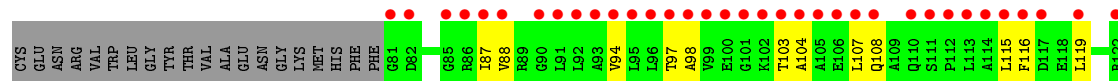
• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE

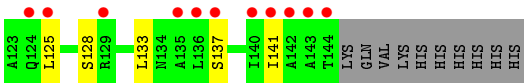


• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE



• Molecule 2: SULFUR ACCEPTOR PROTEIN CSDE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 97.8 (48.30-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.254 , 0.279 0.252 , 0.276	Depositor DCC
$R_{free}$ test set	1999 reflections (1.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	34325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PEG, CSS, PLP

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	0.52	0/3123	0.64	0/4251
1	C	0.52	1/3106 (0.0%)	0.65	3/4229 (0.1%)
1	E	0.54	3/3124 (0.1%)	0.64	2/4253 (0.0%)
1	G	0.55	3/3121 (0.1%)	0.67	3/4249 (0.1%)
1	I	0.53	2/3118 (0.1%)	0.66	2/4245 (0.0%)
1	K	0.50	1/3117 (0.0%)	0.66	2/4244 (0.0%)
1	M	0.48	0/3096	0.58	2/4217 (0.0%)
1	O	0.46	0/3090	0.56	0/4208
2	B	0.57	0/1152	0.66	0/1557
2	D	0.55	0/1118	0.71	2/1511 (0.1%)
2	F	0.55	0/1047	0.69	1/1417 (0.1%)
2	H	0.53	0/1144	0.66	0/1545
2	J	0.52	0/1093	0.66	0/1478
2	L	0.55	1/1076 (0.1%)	0.67	1/1455 (0.1%)
2	N	0.50	0/1076	0.61	0/1455
2	P	0.41	0/736	0.51	0/997
All	All	0.52	11/33337 (0.0%)	0.64	18/45311 (0.0%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	126	TRP	CD2-CE2	5.68	1.48	1.41
1	E	267	TRP	CD2-CE2	5.48	1.48	1.41
1	C	245	TRP	CD2-CE2	5.47	1.48	1.41
1	G	267	TRP	CD2-CE2	5.37	1.47	1.41
1	E	126	TRP	CD2-CE2	5.34	1.47	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	160	ARG	NE-CZ-NH2	-14.29	113.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	160	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	C	103	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	M	10	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	I	160	ARG	NE-CZ-NH1	7.92	124.26	120.30

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	3051	0	3017	41	0
1	C	3040	0	2999	35	0
1	E	3058	0	3013	42	0
1	G	3052	0	3009	40	0
1	I	3052	0	3007	37	0
1	K	3050	0	3005	58	0
1	M	3027	0	2986	42	0
1	O	3024	0	2981	38	0
2	B	1131	0	1141	28	0
2	D	1099	0	1111	31	0
2	F	1031	0	1044	46	0
2	H	1122	0	1138	25	0
2	J	1076	0	1091	33	0
2	L	1060	0	1077	36	0
2	N	1060	0	1077	30	0
2	P	728	0	742	21	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	7	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	5	0	0
4	C	7	0	4	0	0
4	D	7	0	5	5	0
4	E	7	0	4	0	0
4	F	7	0	5	0	0
4	G	7	0	4	0	0
4	H	7	0	5	0	0
4	I	7	0	4	0	0
4	J	7	0	5	1	0
4	K	7	0	4	0	0
4	L	7	0	5	1	0
4	M	7	0	4	0	0
4	N	7	0	5	0	0
4	O	7	0	4	0	0
5	A	21	0	30	3	0
5	B	7	0	10	0	0
5	C	28	0	40	1	0
5	E	28	0	40	0	0
5	G	7	0	10	0	0
5	H	7	0	10	0	0
5	I	7	0	10	0	0
5	K	7	0	10	1	0
6	A	66	0	88	3	0
6	B	18	0	24	0	0
6	C	66	0	88	2	0
6	D	6	0	8	1	0
6	E	66	0	88	1	0
6	G	42	0	56	2	0
6	H	6	0	8	0	0
6	I	30	0	40	3	0
6	M	6	0	8	0	0
7	A	197	0	0	9	0
7	B	57	0	0	5	0
7	C	132	0	0	3	0
7	D	34	0	0	2	0
7	E	180	0	0	5	0
7	F	15	0	0	1	0
7	G	169	0	0	11	0
7	H	38	0	0	1	0
7	I	127	0	0	2	0
7	J	14	0	0	5	0
7	K	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	3	0	0	0	0
7	M	13	0	0	0	0
7	N	2	0	0	0	0
7	O	2	0	0	0	0
All	All	34325	0	33124	542	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 8.

The worst 5 of 542 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:J:25:ALA:O	2:J:27:LEU:HD23	1.48	1.14
1:G:62:THR:HG23	7:G:2044:HOH:O	1.50	1.12
2:P:98:ALA:HB2	2:P:115:LEU:HD22	1.22	1.12
1:A:252:VAL:HG21	1:A:255:VAL:HG22	1.38	1.06
1:O:344:LEU:HD12	1:O:399:LEU:HD21	1.43	0.99

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	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	C	396/403 (98%)	385 (97%)	11 (3%)	0	100	100
1	E	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	G	398/403 (99%)	386 (97%)	11 (3%)	1 (0%)	46	68
1	I	398/403 (99%)	386 (97%)	12 (3%)	0	100	100
1	K	397/403 (98%)	385 (97%)	9 (2%)	3 (1%)	24	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	395/403 (98%)	384 (97%)	10 (2%)	1 (0%)	46	68
1	O	394/403 (98%)	380 (96%)	13 (3%)	1 (0%)	46	68
2	B	143/154 (93%)	136 (95%)	4 (3%)	3 (2%)	9	14
2	D	139/154 (90%)	135 (97%)	2 (1%)	2 (1%)	14	24
2	F	131/154 (85%)	128 (98%)	1 (1%)	2 (2%)	13	22
2	H	142/154 (92%)	134 (94%)	5 (4%)	3 (2%)	9	14
2	J	137/154 (89%)	130 (95%)	3 (2%)	4 (3%)	6	8
2	L	135/154 (88%)	127 (94%)	4 (3%)	4 (3%)	5	7
2	N	135/154 (88%)	128 (95%)	3 (2%)	4 (3%)	5	7
2	P	93/154 (60%)	84 (90%)	8 (9%)	1 (1%)	17	31
All	All	4229/4456 (95%)	4080 (96%)	120 (3%)	29 (1%)	26	46

5 of 29 Ramachandran outliers are listed below:

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

### 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	316/315 (100%)	314 (99%)	2 (1%)	90	97
1	C	314/315 (100%)	311 (99%)	3 (1%)	82	95
1	E	316/315 (100%)	313 (99%)	3 (1%)	84	95
1	G	316/315 (100%)	315 (100%)	1 (0%)	94	99
1	I	316/315 (100%)	310 (98%)	6 (2%)	65	87
1	K	315/315 (100%)	307 (98%)	8 (2%)	55	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	313/315 (99%)	309 (99%)	4 (1%)	76	92
1	O	312/315 (99%)	312 (100%)	0	100	100
2	B	115/122 (94%)	110 (96%)	5 (4%)	35	61
2	D	112/122 (92%)	108 (96%)	4 (4%)	42	69
2	F	105/122 (86%)	103 (98%)	2 (2%)	65	87
2	H	114/122 (93%)	108 (95%)	6 (5%)	28	50
2	J	109/122 (89%)	101 (93%)	8 (7%)	17	32
2	L	108/122 (88%)	103 (95%)	5 (5%)	33	57
2	N	108/122 (88%)	104 (96%)	4 (4%)	41	68
2	P	75/122 (62%)	75 (100%)	0	100	100
All	All	3364/3496 (96%)	3303 (98%)	61 (2%)	66	88

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	210	GLN
2	J	36	GLN
1	M	366	LEU
1	I	240	GLU
1	I	394	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	187	HIS
2	J	63	ASN
1	O	131	GLN
1	I	203	HIS
1	I	275	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

90 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	A	1402	1	15,15,16	4.06	3 (20%)	21,22,23	1.32	2 (9%)
4	CSS	A	1403	1	3,6,7	0.81	0	3,6,8	1.31	0
5	PEG	A	1404	-	6,6,6	0.58	0	5,5,5	0.50	0
5	PEG	A	1405	-	6,6,6	0.63	0	5,5,5	0.32	0
5	PEG	A	1406	-	6,6,6	0.58	0	5,5,5	0.33	0
6	GOL	A	1407	-	5,5,5	0.33	0	5,5,5	0.35	0
6	GOL	A	1408	-	5,5,5	0.34	0	5,5,5	0.39	0
6	GOL	A	1409	-	5,5,5	0.47	0	5,5,5	0.37	0
6	GOL	A	1410	-	5,5,5	0.37	0	5,5,5	0.22	0
6	GOL	A	1411	-	5,5,5	0.27	0	5,5,5	0.20	0
6	GOL	A	1412	-	5,5,5	0.25	0	5,5,5	0.35	0
6	GOL	A	1413	-	5,5,5	0.42	0	5,5,5	0.37	0
6	GOL	A	1414	-	5,5,5	0.32	0	5,5,5	0.17	0
6	GOL	A	1415	-	5,5,5	0.48	0	5,5,5	0.37	0
6	GOL	A	1416	-	5,5,5	0.32	0	5,5,5	0.34	0
6	GOL	A	2401	-	5,5,5	0.29	0	5,5,5	0.28	0
4	CSS	B	1152	2	3,6,7	0.85	0	3,6,8	1.91	1 (33%)
5	PEG	B	1153	-	6,6,6	0.55	0	5,5,5	0.29	0
6	GOL	B	1154	-	5,5,5	0.40	0	5,5,5	0.23	0
6	GOL	B	1155	-	5,5,5	0.44	0	5,5,5	0.38	0
6	GOL	B	2401	-	5,5,5	0.30	0	5,5,5	0.18	0
3	PLP	C	1402	1	15,15,16	3.48	3 (20%)	21,22,23	1.28	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CSS	C	1403	1	3,6,7	0.90	0	3,6,8	1.14	0
5	PEG	C	1404	-	6,6,6	0.56	0	5,5,5	0.21	0
5	PEG	C	1405	-	6,6,6	0.62	0	5,5,5	0.38	0
5	PEG	C	1406	-	6,6,6	0.58	0	5,5,5	0.30	0
5	PEG	C	1407	-	6,6,6	0.55	0	5,5,5	0.31	0
6	GOL	C	1408	-	5,5,5	0.38	0	5,5,5	0.30	0
6	GOL	C	1409	-	5,5,5	0.35	0	5,5,5	0.28	0
6	GOL	C	1410	-	5,5,5	0.34	0	5,5,5	0.27	0
6	GOL	C	1411	-	5,5,5	0.29	0	5,5,5	0.25	0
6	GOL	C	1412	-	5,5,5	0.29	0	5,5,5	0.19	0
6	GOL	C	1413	-	5,5,5	0.46	0	5,5,5	0.38	0
6	GOL	C	1414	-	5,5,5	0.44	0	5,5,5	0.56	0
6	GOL	C	1415	-	5,5,5	0.42	0	5,5,5	0.31	0
6	GOL	C	1416	-	5,5,5	0.37	0	5,5,5	0.30	0
6	GOL	C	1417	-	5,5,5	0.36	0	5,5,5	0.36	0
6	GOL	C	1418	-	5,5,5	0.32	0	5,5,5	0.19	0
4	CSS	D	1152	2	3,6,7	0.77	0	3,6,8	1.52	0
6	GOL	D	1153	-	5,5,5	0.39	0	5,5,5	0.21	0
3	PLP	E	1402	1	15,15,16	3.51	3 (20%)	21,22,23	1.20	2 (9%)
4	CSS	E	1403	1	3,6,7	0.75	0	3,6,8	1.36	0
5	PEG	E	1404	-	6,6,6	0.60	0	5,5,5	0.34	0
5	PEG	E	1405	-	6,6,6	0.54	0	5,5,5	0.21	0
5	PEG	E	1406	-	6,6,6	0.62	0	5,5,5	0.19	0
5	PEG	E	1407	-	6,6,6	0.57	0	5,5,5	0.34	0
6	GOL	E	1408	-	5,5,5	0.41	0	5,5,5	0.36	0
6	GOL	E	1409	-	5,5,5	0.40	0	5,5,5	0.33	0
6	GOL	E	1410	-	5,5,5	0.34	0	5,5,5	0.50	0
6	GOL	E	1411	-	5,5,5	0.46	0	5,5,5	0.30	0
6	GOL	E	1412	-	5,5,5	0.40	0	5,5,5	0.43	0
6	GOL	E	1413	-	5,5,5	0.45	0	5,5,5	0.31	0
6	GOL	E	1414	-	5,5,5	0.24	0	5,5,5	0.28	0
6	GOL	E	1415	-	5,5,5	0.49	0	5,5,5	0.51	0
6	GOL	E	1416	-	5,5,5	0.36	0	5,5,5	0.30	0
6	GOL	E	1417	-	5,5,5	0.36	0	5,5,5	0.31	0
6	GOL	E	2401	-	5,5,5	0.41	0	5,5,5	0.38	0
4	CSS	F	1145	2	3,6,7	0.79	0	3,6,8	1.39	0
3	PLP	G	1402	1	15,15,16	2.88	3 (20%)	21,22,23	1.92	4 (19%)
4	CSS	G	1403	1	3,6,7	0.78	0	3,6,8	1.27	1 (33%)
5	PEG	G	1404	-	6,6,6	0.58	0	5,5,5	0.37	0
6	GOL	G	1405	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	G	1406	-	5,5,5	0.48	0	5,5,5	0.55	0
6	GOL	G	1407	-	5,5,5	0.44	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	G	1408	-	5,5,5	0.38	0	5,5,5	0.35	0
6	GOL	G	1409	-	5,5,5	0.35	0	5,5,5	0.25	0
6	GOL	G	1410	-	5,5,5	0.39	0	5,5,5	0.43	0
6	GOL	G	1411	-	5,5,5	0.31	0	5,5,5	0.12	0
4	CSS	H	1151	2	3,6,7	0.77	0	3,6,8	1.52	0
5	PEG	H	1152	-	6,6,6	0.56	0	5,5,5	0.35	0
6	GOL	H	1153	-	5,5,5	0.39	0	5,5,5	0.27	0
3	PLP	I	1402	1	15,15,16	3.73	3 (20%)	21,22,23	1.13	2 (9%)
4	CSS	I	1403	1	3,6,7	1.05	0	3,6,8	1.21	1 (33%)
5	PEG	I	1404	-	6,6,6	0.59	0	5,5,5	0.17	0
6	GOL	I	1405	-	5,5,5	0.36	0	5,5,5	0.37	0
6	GOL	I	1406	-	5,5,5	0.32	0	5,5,5	0.16	0
6	GOL	I	1407	-	5,5,5	0.43	0	5,5,5	0.58	0
6	GOL	I	1408	-	5,5,5	0.30	0	5,5,5	0.22	0
6	GOL	I	2401	-	5,5,5	0.43	0	5,5,5	0.45	0
4	CSS	J	1148	2	3,6,7	0.82	0	3,6,8	1.68	1 (33%)
3	PLP	K	1402	1	15,15,16	3.62	3 (20%)	21,22,23	1.09	2 (9%)
4	CSS	K	1403	1	3,6,7	0.95	0	3,6,8	1.36	1 (33%)
5	PEG	K	1404	-	6,6,6	0.64	0	5,5,5	0.42	0
4	CSS	L	1148	2	3,6,7	0.85	0	3,6,8	1.73	1 (33%)
3	PLP	M	1402	1	15,15,16	3.71	3 (20%)	21,22,23	1.22	2 (9%)
4	CSS	M	1403	1	3,6,7	0.77	0	3,6,8	1.24	0
6	GOL	M	1404	-	5,5,5	0.36	0	5,5,5	0.27	0
4	CSS	N	1148	2	3,6,7	0.89	0	3,6,8	1.87	1 (33%)
3	PLP	O	1402	1	15,15,16	3.94	3 (20%)	21,22,23	1.27	2 (9%)
4	CSS	O	1403	1	3,6,7	0.83	0	3,6,8	1.17	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	A	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	A	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	A	1404	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1405	-	-	0/4/4/4	0/0/0/0
5	PEG	A	1406	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1409	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1411	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1413	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1414	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1415	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1416	-	-	0/4/4/4	0/0/0/0
6	GOL	A	2401	-	-	0/4/4/4	0/0/0/0
4	CSS	B	1152	2	-	0/1/5/7	0/0/0/0
5	PEG	B	1153	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1154	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1155	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2401	-	-	0/4/4/4	0/0/0/0
3	PLP	C	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	C	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	C	1404	-	-	0/4/4/4	0/0/0/0
5	PEG	C	1405	-	-	0/4/4/4	0/0/0/0
5	PEG	C	1406	-	-	0/4/4/4	0/0/0/0
5	PEG	C	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1411	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1413	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1414	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1415	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1416	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1417	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1418	-	-	0/4/4/4	0/0/0/0
4	CSS	D	1152	2	-	0/1/5/7	0/0/0/0
6	GOL	D	1153	-	-	0/4/4/4	0/0/0/0
3	PLP	E	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	E	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	E	1404	-	-	0/4/4/4	0/0/0/0
5	PEG	E	1405	-	-	0/4/4/4	0/0/0/0
5	PEG	E	1406	-	-	0/4/4/4	0/0/0/0
5	PEG	E	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1411	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	E	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1413	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1414	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1415	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1416	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1417	-	-	0/4/4/4	0/0/0/0
6	GOL	E	2401	-	-	0/4/4/4	0/0/0/0
4	CSS	F	1145	2	-	0/1/5/7	0/0/0/0
3	PLP	G	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	G	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	G	1404	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1405	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1406	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1409	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1410	-	-	0/4/4/4	0/0/0/0
6	GOL	G	1411	-	-	0/4/4/4	0/0/0/0
4	CSS	H	1151	2	-	0/1/5/7	0/0/0/0
5	PEG	H	1152	-	-	0/4/4/4	0/0/0/0
6	GOL	H	1153	-	-	0/4/4/4	0/0/0/0
3	PLP	I	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	I	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	I	1404	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1405	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1406	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1407	-	-	0/4/4/4	0/0/0/0
6	GOL	I	1408	-	-	0/4/4/4	0/0/0/0
6	GOL	I	2401	-	-	0/4/4/4	0/0/0/0
4	CSS	J	1148	2	-	0/1/5/7	0/0/0/0
3	PLP	K	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	K	1403	1	-	0/1/5/7	0/0/0/0
5	PEG	K	1404	-	-	0/4/4/4	0/0/0/0
4	CSS	L	1148	2	-	0/1/5/7	0/0/0/0
3	PLP	M	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	M	1403	1	-	0/1/5/7	0/0/0/0
6	GOL	M	1404	-	-	0/4/4/4	0/0/0/0
4	CSS	N	1148	2	-	0/1/5/7	0/0/0/0
3	PLP	O	1402	1	-	0/6/6/8	0/1/1/1
4	CSS	O	1403	1	-	0/1/5/7	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1402	PLP	C3-C4	3.31	1.47	1.40
3	I	1402	PLP	C3-C4	3.62	1.48	1.40
3	A	1402	PLP	C3-C4	3.72	1.48	1.40
3	C	1402	PLP	C3-C4	3.72	1.48	1.40
3	K	1402	PLP	C3-C4	3.78	1.48	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1402	PLP	C2A-C2-C3	-5.48	115.36	120.90
4	B	1152	CSS	CB-SG-SD	-2.76	98.55	103.94
4	N	1148	CSS	CB-SG-SD	-2.67	98.72	103.94
4	L	1148	CSS	CB-SG-SD	-2.44	99.16	103.94
4	K	1403	CSS	O-C-CA	-2.18	119.88	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	PLP	1	0
4	A	1403	CSS	1	0
5	A	1404	PEG	1	0
5	A	1405	PEG	2	0
6	A	1409	GOL	2	0
6	A	1411	GOL	1	0
3	C	1402	PLP	2	0
5	C	1405	PEG	1	0
6	C	1414	GOL	1	0
6	C	1416	GOL	1	0
4	D	1152	CSS	5	0
6	D	1153	GOL	1	0
3	E	1402	PLP	2	0
6	E	1409	GOL	1	0
3	G	1402	PLP	1	0
6	G	1406	GOL	1	0
6	G	1408	GOL	1	0
3	I	1402	PLP	1	0
6	I	1405	GOL	2	0
6	I	1408	GOL	1	0
4	J	1148	CSS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1402	PLP	2	0
5	K	1404	PEG	1	0
4	L	1148	CSS	1	0
3	M	1402	PLP	2	0
3	O	1402	PLP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/403 (99%)	-0.03	1 (0%) 94 95	28, 40, 54, 74	0
1	C	400/403 (99%)	-0.01	1 (0%) 94 95	27, 41, 60, 88	0
1	E	400/403 (99%)	0.08	1 (0%) 94 95	25, 38, 54, 74	0
1	G	400/403 (99%)	-0.04	1 (0%) 94 95	26, 39, 60, 98	0
1	I	400/403 (99%)	0.16	10 (2%) 61 65	31, 41, 73, 109	0
1	K	400/403 (99%)	0.61	24 (6%) 25 28	47, 67, 90, 116	0
1	M	398/403 (98%)	0.94	57 (14%) 4 3	67, 86, 118, 139	0
1	O	398/403 (98%)	2.14	180 (45%) 0 0	81, 116, 149, 167	0
2	B	147/154 (95%)	0.35	9 (6%) 25 27	29, 50, 82, 116	0
2	D	143/154 (92%)	0.30	4 (2%) 56 61	46, 61, 82, 116	0
2	F	135/154 (87%)	2.99	76 (56%) 0 0	61, 102, 173, 209	0
2	H	144/154 (93%)	0.99	28 (19%) 1 1	40, 66, 113, 155	0
2	J	141/154 (91%)	1.48	36 (25%) 1 1	49, 87, 145, 171	0
2	L	139/154 (90%)	2.74	76 (54%) 0 0	100, 116, 142, 148	0
2	N	139/154 (90%)	4.08	107 (76%) 0 0	122, 142, 161, 178	0
2	P	97/154 (62%)	3.85	72 (74%) 0 0	147, 158, 166, 172	0
All	All	4281/4456 (96%)	0.87	683 (15%) 3 2	25, 56, 146, 209	0

The worst 5 of 683 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	72	ALA	12.5
2	L	12	GLY	11.9
2	L	24	PHE	11.7
2	N	28	THR	11.4
1	O	114	VAL	11.4

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	I	1407	6/6	0.90	0.39	7.84	42,53,56,69	0
6	GOL	I	1408	6/6	0.72	0.24	4.97	62,71,73,76	0
6	GOL	C	1411	6/6	0.92	0.25	4.23	49,58,74,77	0
6	GOL	C	1409	6/6	0.91	0.24	3.86	55,67,72,73	0
5	PEG	A	1405	7/7	0.86	0.24	3.26	43,51,55,57	0
6	GOL	G	1406	6/6	0.91	0.22	2.61	35,49,53,56	0
5	PEG	I	1404	7/7	0.93	0.16	2.36	36,47,53,55	0
6	GOL	A	1408	6/6	0.89	0.27	1.82	47,62,64,65	0
5	PEG	A	1404	7/7	0.90	0.18	1.80	48,55,57,60	0
6	GOL	E	1413	6/6	0.82	0.20	1.75	50,59,64,64	0
6	GOL	G	1410	6/6	0.84	0.19	1.22	48,52,53,54	0
6	GOL	D	1153	6/6	0.87	0.23	1.18	44,60,64,64	0
6	GOL	C	1417	6/6	0.88	0.20	1.01	43,46,48,52	0
5	PEG	B	1153	7/7	0.84	0.19	0.85	50,58,67,68	0
5	PEG	A	1406	7/7	0.94	0.20	0.82	45,51,56,56	0
4	CSS	H	1151	7/8	0.72	0.24	0.80	94,97,107,114	0
3	PLP	C	1402	15/16	0.97	0.18	0.75	29,31,32,33	0
6	GOL	G	1405	6/6	0.88	0.18	0.46	54,60,64,66	0
6	GOL	A	1412	6/6	0.91	0.17	0.34	48,58,59,60	0
4	CSS	D	1152	7/8	0.86	0.15	0.19	86,87,98,101	0
5	PEG	E	1407	7/7	0.91	0.14	-0.08	50,54,59,61	0
3	PLP	E	1402	15/16	0.97	0.18	-0.16	28,29,31,31	0
4	CSS	F	1145	7/8	0.83	0.18	-0.21	97,104,108,115	0
3	PLP	A	1402	15/16	0.98	0.14	-0.23	28,29,30,31	0
3	PLP	O	1402	15/16	0.84	0.22	-0.29	98,103,109,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PLP	G	1402	15/16	0.97	0.14	-0.29	28,30,32,37	0
3	PLP	K	1402	15/16	0.96	0.18	-0.34	51,53,55,56	0
4	CSS	G	1403	7/8	0.92	0.15	-0.52	33,34,35,42	0
4	CSS	L	1148	7/8	0.86	0.14	-0.63	105,106,109,110	0
3	PLP	I	1402	15/16	0.97	0.17	-0.71	31,33,38,39	0
4	CSS	I	1403	7/8	0.92	0.14	-0.76	35,38,41,49	0
4	CSS	N	1148	7/8	0.71	0.19	-0.92	141,146,147,148	0
6	GOL	H	1153	6/6	0.85	0.19	-0.97	64,74,75,76	0
6	GOL	C	1418	6/6	0.86	0.15	-1.00	55,56,58,62	0
6	GOL	I	1405	6/6	0.94	0.11	-1.10	37,48,51,53	0
4	CSS	B	1152	7/8	0.89	0.14	-1.12	71,73,83,95	0
4	CSS	E	1403	7/8	0.93	0.15	-1.16	30,32,34,48	0
4	CSS	J	1148	7/8	0.89	0.12	-1.16	87,91,97,104	0
3	PLP	M	1402	15/16	0.93	0.14	-1.18	79,82,85,86	0
4	CSS	C	1403	7/8	0.90	0.13	-1.20	36,39,42,51	0
4	CSS	O	1403	7/8	0.75	0.17	-1.41	113,114,116,116	0
4	CSS	M	1403	7/8	0.79	0.15	-1.55	85,87,88,92	0
4	CSS	K	1403	7/8	0.89	0.14	-1.81	59,61,62,64	0
4	CSS	A	1403	7/8	0.94	0.12	-1.92	35,35,38,46	0
5	PEG	C	1404	7/7	0.91	0.14	-	55,59,72,73	0
5	PEG	C	1407	7/7	0.92	0.24	-	40,57,74,75	0
5	PEG	E	1404	7/7	0.81	0.15	-	50,55,60,64	0
5	PEG	E	1405	7/7	0.90	0.14	-	54,60,65,65	0
6	GOL	A	1409	6/6	0.75	0.25	-	54,59,60,61	0
6	GOL	B	2401	6/6	0.90	0.36	-	54,62,67,71	0
6	GOL	E	1417	6/6	0.90	0.20	-	52,54,56,57	0
6	GOL	A	1410	6/6	0.89	0.17	-	48,57,60,65	0
5	PEG	K	1404	7/7	0.85	0.20	-	57,58,64,65	0
6	GOL	G	1411	6/6	0.86	0.18	-	54,57,67,70	0
6	GOL	C	1416	6/6	0.89	0.19	-	66,71,76,77	0
5	PEG	G	1404	7/7	0.87	0.14	-	54,61,68,70	0
6	GOL	C	1408	6/6	0.81	0.26	-	55,61,67,67	0
6	GOL	I	1406	6/6	0.89	0.21	-	59,65,70,73	0
6	GOL	E	1414	6/6	0.92	0.26	-	58,64,68,71	0
6	GOL	A	1407	6/6	0.82	0.37	-	55,58,60,69	0
6	GOL	M	1404	6/6	0.85	0.21	-	57,62,69,70	0
5	PEG	E	1406	7/7	0.83	0.20	-	45,53,56,57	0
6	GOL	C	1410	6/6	0.92	0.17	-	53,57,58,72	0
6	GOL	E	1412	6/6	0.85	0.29	-	50,59,65,80	0
6	GOL	E	2401	6/6	0.80	0.33	-	44,52,58,62	0
6	GOL	A	1414	6/6	0.88	0.20	-	49,51,53,54	0
6	GOL	E	1410	6/6	0.80	0.16	-	40,43,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	1154	6/6	0.91	0.29	-	47,53,57,58	0
6	GOL	A	1413	6/6	0.86	0.27	-	49,61,64,65	0
6	GOL	C	1414	6/6	0.93	0.45	-	43,45,55,68	0
6	GOL	E	1409	6/6	0.80	0.27	-	50,56,60,60	0
6	GOL	A	1415	6/6	0.83	0.24	-	50,52,55,56	0
5	PEG	C	1405	7/7	0.81	0.26	-	56,64,70,81	0
6	GOL	E	1411	6/6	0.87	0.26	-	46,54,62,63	0
6	GOL	C	1415	6/6	0.84	0.26	-	57,66,69,75	0
6	GOL	A	1411	6/6	0.90	0.12	-	61,63,68,68	0
6	GOL	G	1408	6/6	0.89	0.19	-	51,62,64,67	0
6	GOL	E	1408	6/6	0.90	0.21	-	42,51,53,54	0
5	PEG	H	1152	7/7	0.83	0.27	-	57,58,64,66	0
5	PEG	C	1406	7/7	0.84	0.15	-	48,55,69,69	0
6	GOL	E	1416	6/6	0.81	0.50	-	59,65,72,78	0
6	GOL	B	1155	6/6	0.90	0.14	-	44,52,52,56	0
6	GOL	C	1413	6/6	0.71	0.21	-	52,55,59,66	0
6	GOL	A	2401	6/6	0.90	0.22	-	48,54,63,64	0
6	GOL	G	1409	6/6	0.85	0.20	-	57,61,66,67	0
6	GOL	G	1407	6/6	0.71	0.20	-	57,71,75,75	0
6	GOL	E	1415	6/6	0.81	0.24	-	52,54,59,64	0
6	GOL	A	1416	6/6	0.88	0.24	-	63,70,72,73	0
6	GOL	C	1412	6/6	0.89	0.21	-	48,65,70,73	0
6	GOL	I	2401	6/6	0.73	0.29	-	53,64,68,69	0

## 6.5 Other polymers

There are no such residues in this entry.