



# Full wwPDB X-ray Structure Validation Report i

Dec 1, 2022 – 12:28 am GMT

PDB ID : 5FT8

Title : Crystal structure of the complex between the cysteine desulfurase CsdA and the sulfur-acceptor CsdE in the persulfurated state at 2.50 Angstroem resolution

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Deposited on : 2016-01-11

Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbitiy : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriaage (Phenix) : 1.13  
EDS : 2.31.3  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

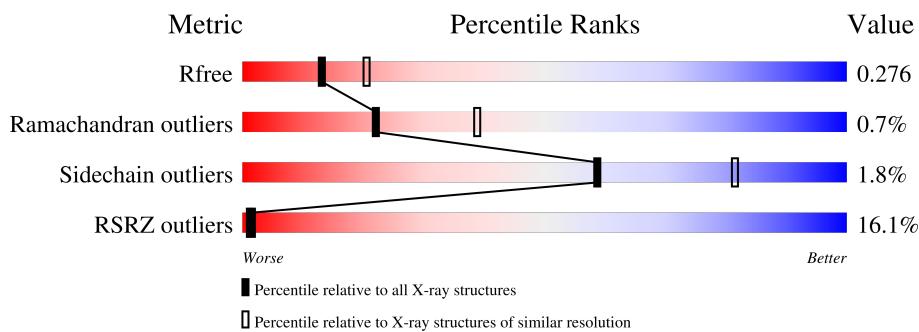
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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.



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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
5	GOL	A	505	-	-	-	X

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

There are 56 discrepancies between the modelled and reference sequences:

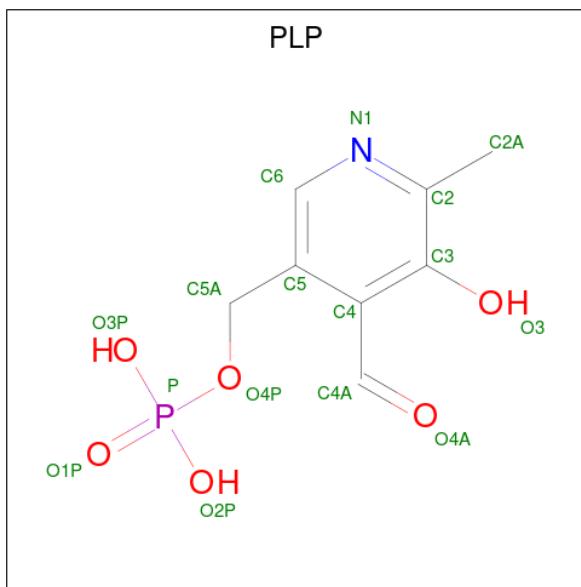
Chain	Residue	Modelled	Actual	Comment	Reference
Q	148	LYS	-	expression tag	UNP P0AGF2
Q	149	HIS	-	expression tag	UNP P0AGF2
Q	150	HIS	-	expression tag	UNP P0AGF2
Q	151	HIS	-	expression tag	UNP P0AGF2
Q	152	HIS	-	expression tag	UNP P0AGF2
Q	153	HIS	-	expression tag	UNP P0AGF2
Q	154	HIS	-	expression tag	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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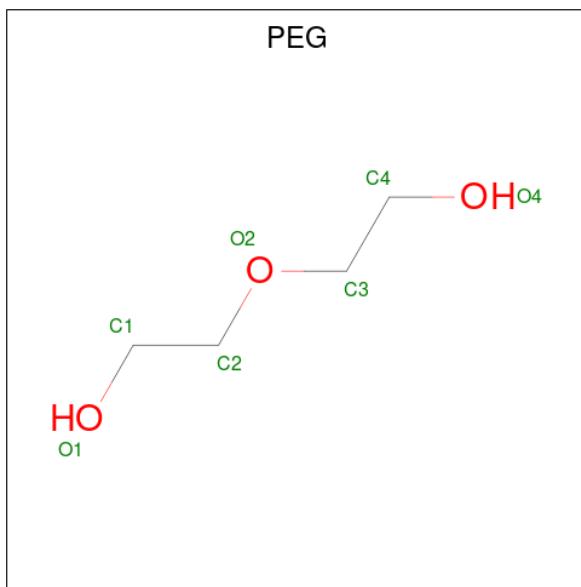
Chain	Residue	Modelled	Actual	Comment	Reference
U	149	HIS	-	expression tag	UNP P0AGF2
U	150	HIS	-	expression tag	UNP P0AGF2
U	151	HIS	-	expression tag	UNP P0AGF2
U	152	HIS	-	expression tag	UNP P0AGF2
U	153	HIS	-	expression tag	UNP P0AGF2
U	154	HIS	-	expression tag	UNP P0AGF2
W	148	LYS	-	expression tag	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 (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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



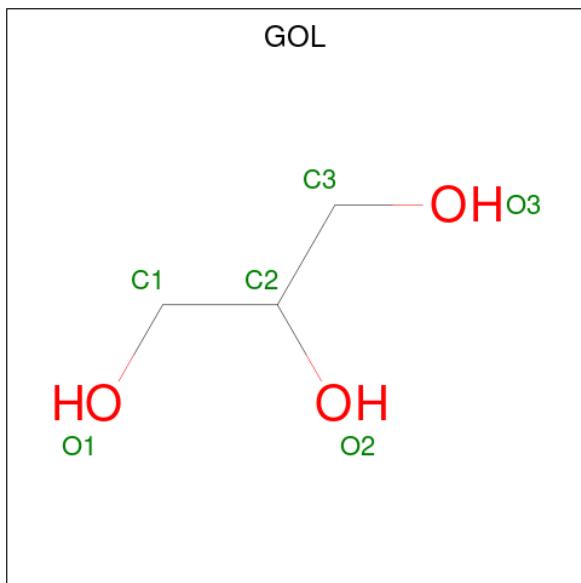
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	Q	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

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

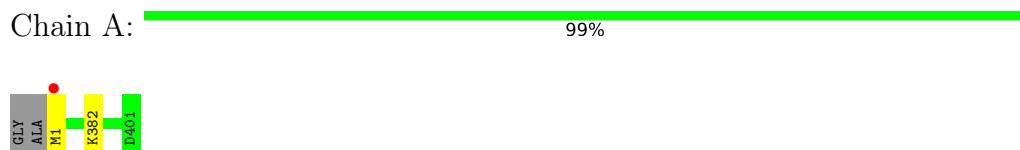
- Molecule 6 is water.

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

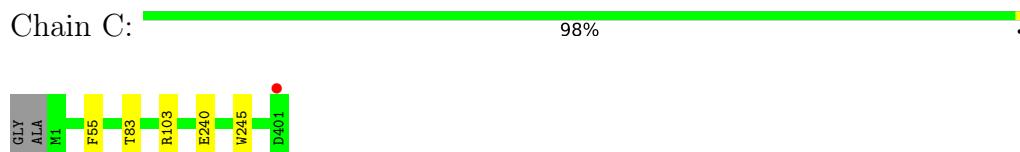
### 3 Residue-property plots [\(i\)](#)

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.

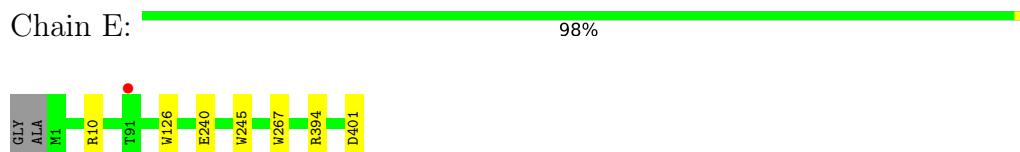
- Molecule 1: Cysteine desulfurase CsdA



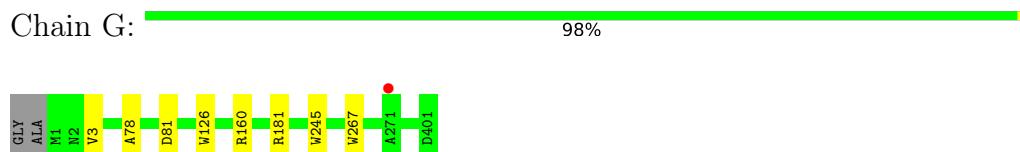
- Molecule 1: Cysteine desulfurase CsdA



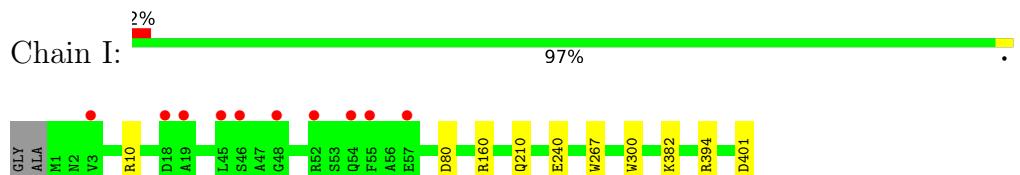
- Molecule 1: Cysteine desulfurase CsdA



- Molecule 1: Cysteine desulfurase CsdA



- Molecule 1: Cysteine desulfurase CsdA



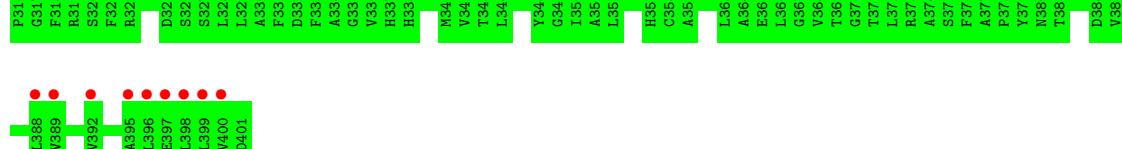
- Molecule 1: Cysteine desulfurase CsdA



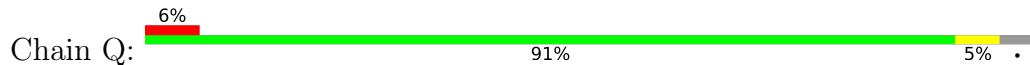
- Molecule 1: Cysteine desulfurase CsdA



- Molecule 1: Cysteine desulfurase CsdA



- Molecule 2: Sulfur acceptor protein CsdE

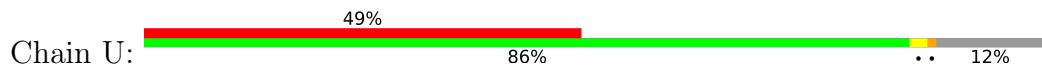


- Molecule 2: Sulfur acceptor protein CsdE





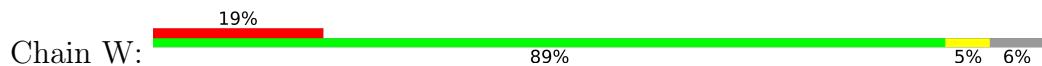
- Molecule 2: Sulfur acceptor protein CsdE



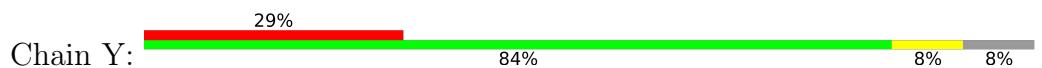
The diagram illustrates the SARS-CoV-2 spike protein's receptor-binding domain (RBD) with various mutations highlighted. The mutations are categorized as follows:

- MET**: MET314I
- THR**: THR147M
- ASN**: ASN142T
- PRO**: PRO152S
- GLN**: GLN143D
- PHE**: PHE145L
- ALA**: ALA146V
- GLY**: GLY147A
- HS**: HS148Q
- P10**: P10F
- F11**: F11L
- G12**: G12A
- T13**: T13V
- T14**: T14P
- V15**: V15I
- L20**: L20G
- Q29**: Q29E
- L44**: L44P
- P45**: P45S
- A46**: A46T
- I47**: I47V
- P48**: P48S
- D49**: D49G
- E50**: E50Q
- L51**: L51I
- Q54**: Q54H
- A55**: A55T
- K56**: K56E
- E57**: E57K
- I58**: I58L
- V65**: V65I
- V66**: V66I
- L67**: L67P
- G68**: G68V
- Y69**: Y69F
- T70**: T70I
- T71**: T71W
- A72**: A72T
- E73**: E73K
- N74**: N74T
- G75**: G75E
- K76**: K76T
- M77**: M77T
- H78**: H78Q
- F79**: F79Q
- F80**: F80Q
- C81**: C81I
- D82**: D82G
- R89**: R89Q
- G90**: G90S
- L91**: L91I
- V94**: V94I
- L95**: L95S

- Molecule 2: Sulfur acceptor protein CsdE



- Molecule 2: Sulfur acceptor protein CsdE



MET  
THR  
ASN  
PRO  
GLN  
F6  
R7  
G12  
T13  
F4  
T14  
A132  
L136  
S137  
E138  
A139  
I140  
I141  
A142  
A143  
T144  
K145  
K146  
V147  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
A55  
W66  
L67  
G68  
Y69  
T70  
W71  
A72  
E73  
W74  
G75  
K76  
H77  
H78  
F79  
F80  
G81  
D82  
E96  
W89  
E100  
G101  
K102  
T103  
A104  
A105  
E106  
L107  
L108  
A109  
Q110

- Molecule 2: Sulfur acceptor protein CsdE

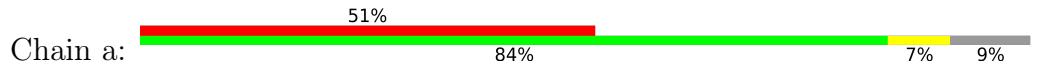
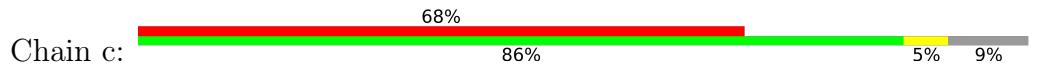
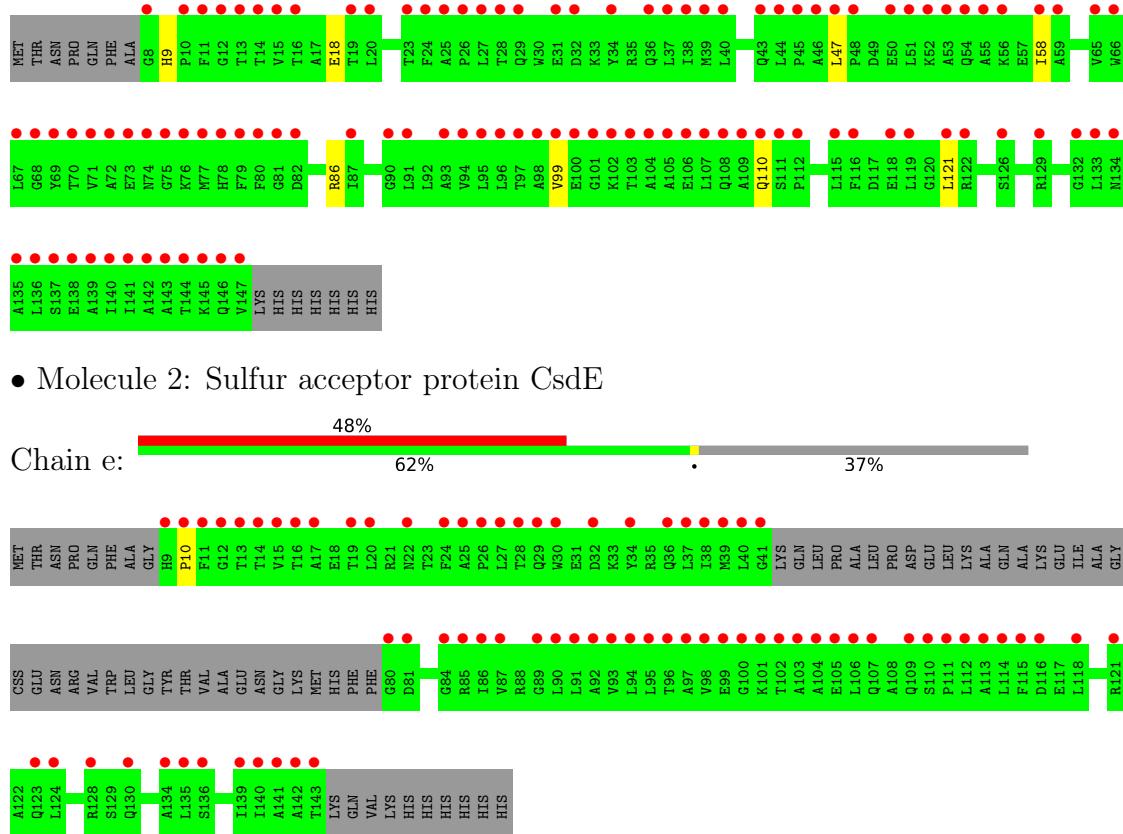


Diagram illustrating the distribution of various HLA loci across chromosomes 6, 11, and 15. Loci are represented by colored boxes:

- Red boxes:** K76, M77, H78, F79, F80, G81.
- Yellow boxes:** R89, L91, A93, V94, L95, L96, T97, A98, V99, E100, G101, K102, T103, E106, L107, Q108, A109, Q110, S111, L115, E118, L119, G120, L121, R122, A123, Q124, L125.
- Green boxes:** L133, L136, S137.
- Blue boxes:** R129.

- Molecule 2: Sulfur acceptor protein CsdE





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.86 Å    115.14 Å    604.97 Å 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
$\langle I/\sigma(I) \rangle^1$	1.75 (at 2.51 Å)	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	2000 reflections (1.12%)	wwPDB-VP
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> )	(Not available) , (Not available)	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	0.90	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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CSS, PEG, PLP, GOL

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	Q	0.57	0/1152	0.66	0/1557
2	S	0.55	0/1118	0.71	2/1511 (0.1%)
2	U	0.55	0/1047	0.69	1/1417 (0.1%)
2	W	0.53	0/1144	0.66	0/1545
2	Y	0.52	0/1093	0.66	0/1478
2	a	0.55	1/1076 (0.1%)	0.67	1/1455 (0.1%)
2	c	0.50	0/1076	0.61	0/1455
2	e	0.41	0/736	0.51	0/997
All	All	0.52	11/33337 (0.0%)	0.64	18/45311 (0.0%)

All (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
1	I	267	TRP	CD2-CE2	5.27	1.47	1.41
1	K	267	TRP	CD2-CE2	5.21	1.47	1.41
2	a	30	TRP	CD2-CE2	5.15	1.47	1.41
1	G	245	TRP	CD2-CE2	5.08	1.47	1.41
1	I	300	TRP	CD2-CE2	5.08	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	245	TRP	CD2-CE2	5.05	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	K	160	ARG	NE-CZ-NH2	-14.29	113.16	120.30
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
1	G	181	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	E	10	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	G	160	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	I	10	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	S	122	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	M	10	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	a	27	LEU	CA-CB-CG	6.60	130.49	115.30
1	C	103	ARG	CB-CG-CD	6.56	128.65	111.60
1	C	103	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	G	78	ALA	C-N-CD	5.66	140.29	128.40
2	S	100	GLU	N-CA-CB	-5.48	100.74	110.60
1	E	10	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	U	89	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	41	61
1	I	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
1	K	399/403 (99%)	386 (97%)	10 (2%)	3 (1%)	19	35
1	M	397/403 (98%)	385 (97%)	11 (3%)	1 (0%)	41	61
1	O	396/403 (98%)	381 (96%)	14 (4%)	1 (0%)	41	61
2	Q	145/154 (94%)	138 (95%)	4 (3%)	3 (2%)	7	11
2	S	141/154 (92%)	137 (97%)	2 (1%)	2 (1%)	11	20
2	U	133/154 (86%)	130 (98%)	1 (1%)	2 (2%)	10	18
2	W	144/154 (94%)	136 (94%)	5 (4%)	3 (2%)	7	11
2	Y	139/154 (90%)	132 (95%)	3 (2%)	4 (3%)	4	6
2	a	137/154 (89%)	129 (94%)	4 (3%)	4 (3%)	4	6
2	c	137/154 (89%)	130 (95%)	3 (2%)	4 (3%)	4	6
2	e	93/154 (60%)	84 (90%)	8 (9%)	1 (1%)	14	26
All	All	4259/4456 (96%)	4102 (96%)	128 (3%)	29 (1%)	22	39

All (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
2	a	9	HIS
2	c	9	HIS
1	O	4	PHE
2	W	8	GLY
2	Y	58	ILE
2	a	58	ILE
2	c	58	ILE
2	e	10	PRO
2	U	58	ILE
2	Y	54	GLN
2	S	47	LEU

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Mol	Chain	Res	Type
2	U	47	LEU
2	W	47	LEU
2	a	47	LEU
1	M	400	VAL
2	c	47	LEU
1	G	3	VAL
2	Q	99	VAL
2	Q	100	GLU
2	W	99	VAL
2	Y	99	VAL
2	a	99	VAL
2	c	99	VAL
2	Q	147	VAL

### 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%)	86 95
1	C	314/314 (100%)	311 (99%)	3 (1%)	76 90
1	E	316/314 (101%)	313 (99%)	3 (1%)	78 92
1	G	316/314 (101%)	315 (100%)	1 (0%)	92 97
1	I	316/314 (101%)	310 (98%)	6 (2%)	57 80
1	K	315/314 (100%)	307 (98%)	8 (2%)	47 73
1	M	313/314 (100%)	309 (99%)	4 (1%)	69 87
1	O	312/314 (99%)	312 (100%)	0	100 100
2	Q	115/121 (95%)	110 (96%)	5 (4%)	29 53
2	S	112/121 (93%)	108 (96%)	4 (4%)	35 61
2	U	105/121 (87%)	103 (98%)	2 (2%)	57 80
2	W	114/121 (94%)	108 (95%)	6 (5%)	22 43
2	Y	109/121 (90%)	101 (93%)	8 (7%)	14 27
2	a	108/121 (89%)	103 (95%)	5 (5%)	27 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	c	108/121 (89%)	104 (96%)	4 (4%)	34 60
2	e	75/121 (62%)	75 (100%)	0	100 100
All	All	3364/3480 (97%)	3303 (98%)	61 (2%)	59 81

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	382	LYS
2	Q	13	THR
2	Q	14	THR
2	Q	36	GLN
2	Q	102	LYS
2	Q	111	SER
1	C	55	PHE
1	C	83	THR
1	C	240	GLU
2	S	19	THR
2	S	36	GLN
2	S	110	GLN
2	S	148	LYS
1	E	240	GLU
1	E	394	ARG
1	E	401	ASP
2	U	89	ARG
2	U	129	ARG
1	G	81	ASP
2	W	14	THR
2	W	21	ARG
2	W	35[A]	ARG
2	W	35[B]	ARG
2	W	110	GLN
2	W	138	GLU
1	I	80	ASP
1	I	210	GLN
1	I	240	GLU
1	I	382	LYS
1	I	394	ARG
1	I	401	ASP
2	Y	6	PHE
2	Y	27	LEU

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Mol	Chain	Res	Type
2	Y	36	GLN
2	Y	110	GLN
2	Y	129	ARG
2	Y	134	ASN
2	Y	138	GLU
2	Y	140	ILE
1	K	2	ASN
1	K	46	SER
1	K	52	ARG
1	K	53	SER
1	K	54	GLN
1	K	55	PHE
1	K	209	GLN
1	K	401	ASP
2	a	89	ARG
2	a	108	GLN
2	a	129	ARG
2	a	137	SER
2	a	146	GLN
1	M	80	ASP
1	M	210	GLN
1	M	352	LEU
1	M	366	LEU
2	c	18	GLU
2	c	86	ARG
2	c	110	GLN
2	c	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	41	GLN
1	A	77	ASN
1	A	275	ASN
2	Q	22	ASN
2	Q	63	ASN
2	Q	124	GLN
1	C	131	GLN
1	C	168	GLN
1	C	203	HIS
2	S	63	ASN

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Mol	Chain	Res	Type
1	E	77	ASN
1	E	107	GLN
1	E	168	GLN
1	E	360	GLN
2	U	63	ASN
1	G	131	GLN
1	G	357	HIS
2	W	63	ASN
2	W	108	GLN
2	W	134	ASN
1	I	17	GLN
1	I	51	HIS
1	I	187	HIS
1	I	203	HIS
1	I	210	GLN
1	I	275	ASN
1	I	390	ASN
2	Y	22	ASN
2	Y	63	ASN
2	Y	134	ASN
1	K	2	ASN
1	K	51	HIS
1	K	74	GLN
1	K	131	GLN
1	K	203	HIS
2	a	22	ASN
2	a	63	ASN
2	a	146	GLN
1	M	12	GLN
1	M	131	GLN
1	M	203	HIS
1	M	210	GLN
1	M	390	ASN
2	c	22	ASN
2	c	63	ASN
2	c	124	GLN
1	O	41	GLN
1	O	131	GLN
1	O	203	HIS
2	e	109	GLN
2	e	133	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	M	358	1	4,6,7	0.78	0	1,6,8	0.56	0
2	CSS	c	61	2	4,6,7	0.87	0	1,6,8	0.24	0
1	CSS	C	358	1	4,6,7	0.87	0	1,6,8	0.45	0
1	CSS	E	358	1	4,6,7	0.76	0	1,6,8	0.37	0
1	CSS	G	358	1	4,6,7	0.76	0	1,6,8	0.44	0
1	CSS	K	358	1	4,6,7	0.97	0	1,6,8	0.57	0
1	CSS	O	358	1	4,6,7	0.82	0	1,6,8	0.51	0
2	CSS	Q	61	2	4,6,7	0.85	0	1,6,8	0.17	0
1	CSS	A	358	1	4,6,7	0.79	0	1,6,8	0.54	0
2	CSS	S	61	2	4,6,7	0.77	0	1,6,8	0.21	0
1	CSS	I	358	1	4,6,7	1.07	0	1,6,8	0.43	0
2	CSS	W	61	2	4,6,7	0.75	0	1,6,8	0.38	0
2	CSS	U	61	2	4,6,7	0.78	0	1,6,8	0.26	0
2	CSS	a	61	2	4,6,7	0.83	0	1,6,8	0.17	0
2	CSS	Y	61	2	4,6,7	0.80	0	1,6,8	0.37	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
1	CSS	M	358	1	-	0/1/5/7	-
2	CSS	c	61	2	-	1/1/5/7	-
1	CSS	C	358	1	-	0/1/5/7	-
1	CSS	E	358	1	-	0/1/5/7	-
1	CSS	G	358	1	-	0/1/5/7	-

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (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
2	a	61	CSS	N-CA-CB-SG
2	c	61	CSS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides 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
5	GOL	E	513	-	5,5,5	0.54	0	5,5,5	0.52	0
4	PEG	C	502	-	6,6,6	0.54	0	5,5,5	0.20	0
5	GOL	C	511	-	5,5,5	0.51	0	5,5,5	0.34	0
5	GOL	Q	202	-	5,5,5	0.44	0	5,5,5	0.16	0
5	GOL	I	505	-	5,5,5	0.47	0	5,5,5	0.57	0
5	GOL	C	507	-	5,5,5	0.40	0	5,5,5	0.26	0
5	GOL	E	512	-	5,5,5	0.28	0	5,5,5	0.28	0
5	GOL	E	508	-	5,5,5	0.39	0	5,5,5	0.51	0
4	PEG	A	502	-	6,6,6	0.56	0	5,5,5	0.49	0
4	PEG	E	503	-	6,6,6	0.52	0	5,5,5	0.18	0
5	GOL	E	516	-	5,5,5	0.46	0	5,5,5	0.36	0
5	GOL	A	516	-	5,5,5	0.37	0	5,5,5	0.14	0
5	GOL	G	503	-	5,5,5	0.42	0	5,5,5	0.16	0
5	GOL	E	511	-	5,5,5	0.50	0	5,5,5	0.26	0
5	GOL	G	507	-	5,5,5	0.40	0	5,5,5	0.23	0
3	PLP	O	501	1	15,15,16	3.35	3 (20%)	20,22,23	1.34	2 (10%)
5	GOL	A	515	-	5,5,5	0.34	0	5,5,5	0.29	0
4	PEG	Q	201	-	6,6,6	0.53	0	5,5,5	0.26	0
5	GOL	C	514	-	5,5,5	0.42	0	5,5,5	0.25	0
5	GOL	G	505	-	5,5,5	0.48	0	5,5,5	0.19	0
3	PLP	E	501	1	15,15,16	2.91	3 (20%)	20,22,23	1.35	2 (10%)
5	GOL	C	512	-	5,5,5	0.48	0	5,5,5	0.55	0
5	GOL	G	509	-	5,5,5	0.36	0	5,5,5	0.09	0
5	GOL	E	509	-	5,5,5	0.51	0	5,5,5	0.26	0
5	GOL	E	510	-	5,5,5	0.45	0	5,5,5	0.40	0
4	PEG	C	505	-	6,6,6	0.52	0	5,5,5	0.30	0
3	PLP	G	501	1	15,15,16	2.68	3 (20%)	20,22,23	1.98	6 (30%)
5	GOL	A	509	-	5,5,5	0.32	0	5,5,5	0.18	0
3	PLP	I	501	1	15,15,16	3.15	3 (20%)	20,22,23	1.23	2 (10%)
5	GOL	A	511	-	5,5,5	0.47	0	5,5,5	0.32	0
3	PLP	K	501	1	15,15,16	3.09	3 (20%)	20,22,23	1.20	2 (10%)
5	GOL	C	513	-	5,5,5	0.47	0	5,5,5	0.27	0
5	GOL	E	514	-	5,5,5	0.40	0	5,5,5	0.30	0
5	GOL	E	507	-	5,5,5	0.45	0	5,5,5	0.31	0
5	GOL	C	508	-	5,5,5	0.39	0	5,5,5	0.24	0
5	GOL	G	506	-	5,5,5	0.43	0	5,5,5	0.32	0
5	GOL	C	509	-	5,5,5	0.32	0	5,5,5	0.26	0
5	GOL	M	502	-	5,5,5	0.41	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	507	-	5,5,5	0.51	0	5,5,5	0.35	0
4	PEG	E	505	-	6,6,6	0.56	0	5,5,5	0.33	0
5	GOL	C	510	-	5,5,5	0.33	0	5,5,5	0.19	0
5	GOL	A	506	-	5,5,5	0.39	0	5,5,5	0.42	0
5	GOL	S	201	-	5,5,5	0.43	0	5,5,5	0.15	0
5	GOL	A	514	-	5,5,5	0.37	0	5,5,5	0.33	0
3	PLP	M	501	1	15,15,16	3.20	3 (20%)	20,22,23	1.34	3 (15%)
5	GOL	A	513	-	5,5,5	0.53	0	5,5,5	0.31	0
5	GOL	I	506	-	5,5,5	0.34	0	5,5,5	0.18	0
4	PEG	C	504	-	6,6,6	0.56	0	5,5,5	0.29	0
5	GOL	A	510	-	5,5,5	0.30	0	5,5,5	0.39	0
5	GOL	C	515	-	5,5,5	0.40	0	5,5,5	0.37	0
4	PEG	A	503	-	6,6,6	0.61	0	5,5,5	0.32	0
4	PEG	I	502	-	6,6,6	0.57	0	5,5,5	0.17	0
3	PLP	A	501	1	15,15,16	3.46	3 (20%)	20,22,23	1.39	4 (20%)
4	PEG	K	502	-	6,6,6	0.63	0	5,5,5	0.42	0
5	GOL	C	506	-	5,5,5	0.43	0	5,5,5	0.29	0
5	GOL	I	507	-	5,5,5	0.47	0	5,5,5	0.42	0
3	PLP	C	501	1	15,15,16	3.00	3 (20%)	20,22,23	1.42	3 (15%)
5	GOL	G	508	-	5,5,5	0.43	0	5,5,5	0.44	0
4	PEG	E	504	-	6,6,6	0.60	0	5,5,5	0.21	0
4	PEG	C	503	-	6,6,6	0.60	0	5,5,5	0.37	0
4	PEG	A	504	-	6,6,6	0.56	0	5,5,5	0.32	0
4	PEG	G	502	-	6,6,6	0.56	0	5,5,5	0.36	0
5	GOL	A	508	-	5,5,5	0.41	0	5,5,5	0.17	0
5	GOL	Q	203	-	5,5,5	0.49	0	5,5,5	0.32	0
5	GOL	E	506	-	5,5,5	0.46	0	5,5,5	0.34	0
5	GOL	I	504	-	5,5,5	0.37	0	5,5,5	0.14	0
4	PEG	E	502	-	6,6,6	0.58	0	5,5,5	0.33	0
5	GOL	A	512	-	5,5,5	0.35	0	5,5,5	0.17	0
5	GOL	Q	204	-	5,5,5	0.33	0	5,5,5	0.20	0
4	PEG	W	201	-	6,6,6	0.54	0	5,5,5	0.33	0
5	GOL	W	202	-	5,5,5	0.44	0	5,5,5	0.22	0
5	GOL	G	504	-	5,5,5	0.53	0	5,5,5	0.55	0
5	GOL	E	515	-	5,5,5	0.40	0	5,5,5	0.30	0
5	GOL	I	503	-	5,5,5	0.41	0	5,5,5	0.33	0
5	GOL	A	505	-	5,5,5	0.37	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	513	-	-	0/4/4/4	-
4	PEG	C	502	-	-	2/4/4/4	-
5	GOL	C	511	-	-	4/4/4/4	-
5	GOL	Q	202	-	-	4/4/4/4	-
5	GOL	I	505	-	-	2/4/4/4	-
5	GOL	C	507	-	-	2/4/4/4	-
5	GOL	E	512	-	-	2/4/4/4	-
5	GOL	E	508	-	-	2/4/4/4	-
4	PEG	A	502	-	-	3/4/4/4	-
4	PEG	E	503	-	-	2/4/4/4	-
5	GOL	E	516	-	-	2/4/4/4	-
5	GOL	A	516	-	-	4/4/4/4	-
5	GOL	G	503	-	-	4/4/4/4	-
5	GOL	E	511	-	-	2/4/4/4	-
5	GOL	G	507	-	-	0/4/4/4	-
3	PLP	O	501	1	-	0/6/6/8	0/1/1/1
5	GOL	A	515	-	-	2/4/4/4	-
4	PEG	Q	201	-	-	3/4/4/4	-
5	GOL	C	514	-	-	2/4/4/4	-
5	GOL	G	505	-	-	2/4/4/4	-
3	PLP	E	501	1	-	0/6/6/8	0/1/1/1
5	GOL	C	512	-	-	4/4/4/4	-
5	GOL	G	509	-	-	0/4/4/4	-
5	GOL	E	509	-	-	2/4/4/4	-
5	GOL	E	510	-	-	0/4/4/4	-
4	PEG	C	505	-	-	2/4/4/4	-
3	PLP	G	501	1	-	0/6/6/8	0/1/1/1
5	GOL	A	509	-	-	2/4/4/4	-
3	PLP	I	501	1	-	0/6/6/8	0/1/1/1
5	GOL	A	511	-	-	4/4/4/4	-
3	PLP	K	501	1	-	0/6/6/8	0/1/1/1
5	GOL	C	513	-	-	4/4/4/4	-
5	GOL	E	514	-	-	2/4/4/4	-
5	GOL	E	507	-	-	1/4/4/4	-
5	GOL	C	508	-	-	4/4/4/4	-
5	GOL	G	506	-	-	2/4/4/4	-
5	GOL	C	509	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	M	502	-	-	2/4/4/4	-
5	GOL	A	507	-	-	4/4/4/4	-
4	PEG	E	505	-	-	2/4/4/4	-
5	GOL	C	510	-	-	0/4/4/4	-
5	GOL	A	506	-	-	2/4/4/4	-
5	GOL	S	201	-	-	1/4/4/4	-
5	GOL	A	514	-	-	2/4/4/4	-
3	PLP	M	501	1	-	0/6/6/8	0/1/1/1
5	GOL	A	513	-	-	4/4/4/4	-
5	GOL	I	506	-	-	0/4/4/4	-
4	PEG	C	504	-	-	2/4/4/4	-
5	GOL	A	510	-	-	2/4/4/4	-
5	GOL	C	515	-	-	2/4/4/4	-
4	PEG	A	503	-	-	3/4/4/4	-
4	PEG	I	502	-	-	2/4/4/4	-
3	PLP	A	501	1	-	0/6/6/8	0/1/1/1
4	PEG	K	502	-	-	3/4/4/4	-
5	GOL	C	506	-	-	2/4/4/4	-
5	GOL	I	507	-	-	2/4/4/4	-
3	PLP	C	501	1	-	0/6/6/8	0/1/1/1
5	GOL	G	508	-	-	1/4/4/4	-
4	PEG	E	504	-	-	2/4/4/4	-
4	PEG	C	503	-	-	2/4/4/4	-
4	PEG	A	504	-	-	3/4/4/4	-
4	PEG	G	502	-	-	3/4/4/4	-
5	GOL	A	508	-	-	2/4/4/4	-
5	GOL	Q	203	-	-	2/4/4/4	-
5	GOL	E	506	-	-	0/4/4/4	-
5	GOL	I	504	-	-	2/4/4/4	-
4	PEG	E	502	-	-	3/4/4/4	-
5	GOL	A	512	-	-	0/4/4/4	-
5	GOL	Q	204	-	-	2/4/4/4	-
4	PEG	W	201	-	-	2/4/4/4	-
5	GOL	W	202	-	-	2/4/4/4	-
5	GOL	G	504	-	-	4/4/4/4	-
5	GOL	E	515	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	503	-	-	4/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PLP	C5-C4	8.89	1.50	1.40
3	A	501	PLP	C3-C2	8.81	1.49	1.40
3	O	501	PLP	C3-C2	8.48	1.49	1.40
3	O	501	PLP	C5-C4	8.45	1.49	1.40
3	M	501	PLP	C5-C4	8.27	1.49	1.40
3	G	501	PLP	C5-C4	8.19	1.49	1.40
3	I	501	PLP	C3-C2	8.11	1.49	1.40
3	E	501	PLP	C3-C2	7.89	1.48	1.40
3	I	501	PLP	C5-C4	7.82	1.49	1.40
3	M	501	PLP	C3-C2	7.80	1.48	1.40
3	K	501	PLP	C5-C4	7.78	1.49	1.40
3	K	501	PLP	C3-C2	7.76	1.48	1.40
3	C	501	PLP	C5-C4	7.74	1.49	1.40
3	C	501	PLP	C3-C2	7.28	1.48	1.40
3	E	501	PLP	C5-C4	6.51	1.47	1.40
3	G	501	PLP	C3-C2	4.90	1.45	1.40
3	O	501	PLP	C3-C4	4.49	1.49	1.40
3	M	501	PLP	C3-C4	4.29	1.49	1.40
3	E	501	PLP	C3-C4	4.13	1.48	1.40
3	K	501	PLP	C3-C4	4.10	1.48	1.40
3	C	501	PLP	C3-C4	4.03	1.48	1.40
3	A	501	PLP	C3-C4	4.03	1.48	1.40
3	I	501	PLP	C3-C4	3.93	1.48	1.40
3	G	501	PLP	C3-C4	3.58	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	PLP	C2A-C2-C3	-4.48	115.36	120.89
3	G	501	PLP	C2A-C2-N1	3.53	124.57	117.67
3	C	501	PLP	C6-N1-C2	3.29	125.26	119.17
3	G	501	PLP	C6-N1-C2	2.97	124.67	119.17
3	O	501	PLP	C6-N1-C2	2.91	124.55	119.17
3	I	501	PLP	O4P-C5A-C5	2.83	114.74	109.35
3	A	501	PLP	O4P-C5A-C5	2.77	114.62	109.35
3	G	501	PLP	O4P-C5A-C5	2.69	114.48	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	O4P-C5A-C5	2.69	114.47	109.35
3	E	501	PLP	O4P-C5A-C5	2.64	114.38	109.35
3	M	501	PLP	C6-N1-C2	2.56	123.90	119.17
3	K	501	PLP	O4P-C5A-C5	2.55	114.21	109.35
3	O	501	PLP	O4P-C5A-C5	2.47	114.06	109.35
3	M	501	PLP	O4P-C5A-C5	2.45	114.01	109.35
3	A	501	PLP	O3-C3-C2	2.37	122.66	117.49
3	E	501	PLP	C6-N1-C2	2.34	123.50	119.17
3	G	501	PLP	C4A-C4-C5	2.33	123.34	120.94
3	K	501	PLP	C6-N1-C2	2.33	123.49	119.17
3	I	501	PLP	C3-C4-C5	-2.28	116.27	118.74
3	A	501	PLP	C6-N1-C2	2.24	123.31	119.17
3	G	501	PLP	C4-C3-C2	-2.10	116.97	120.07
3	A	501	PLP	C4-C3-C2	-2.05	117.05	120.07
3	C	501	PLP	O3P-P-O2P	2.04	115.44	107.64
3	M	501	PLP	O3P-P-O2P	2.01	115.34	107.64

There are no chirality outliers.

All (144) 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
5	A	511	GOL	O2-C2-C3-O3
5	A	513	GOL	O1-C1-C2-O2
5	A	513	GOL	O1-C1-C2-C3
5	A	513	GOL	C1-C2-C3-O3
5	A	514	GOL	C1-C2-C3-O3
5	A	515	GOL	C1-C2-C3-O3
5	A	516	GOL	O1-C1-C2-C3
5	A	516	GOL	C1-C2-C3-O3
5	Q	202	GOL	O1-C1-C2-O2
5	Q	203	GOL	C1-C2-C3-O3
5	C	506	GOL	C1-C2-C3-O3
5	C	511	GOL	O1-C1-C2-C3
5	C	511	GOL	C1-C2-C3-O3
5	C	513	GOL	O1-C1-C2-C3
5	C	514	GOL	O1-C1-C2-C3
5	C	515	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	E	508	GOL	C1-C2-C3-O3
5	E	509	GOL	C1-C2-C3-O3
5	E	512	GOL	C1-C2-C3-O3
5	E	514	GOL	C1-C2-C3-O3
5	E	515	GOL	O1-C1-C2-C3
5	G	503	GOL	O1-C1-C2-C3
5	G	504	GOL	O1-C1-C2-O2
5	G	504	GOL	O1-C1-C2-C3
5	W	202	GOL	C1-C2-C3-O3
5	W	202	GOL	O2-C2-C3-O3
5	I	504	GOL	C1-C2-C3-O3
5	I	504	GOL	O2-C2-C3-O3
5	M	502	GOL	O1-C1-C2-O2
5	M	502	GOL	O1-C1-C2-C3
4	C	504	PEG	O1-C1-C2-O2
4	E	505	PEG	O2-C3-C4-O4
4	K	502	PEG	O1-C1-C2-O2
5	A	507	GOL	O2-C2-C3-O3
5	A	510	GOL	O2-C2-C3-O3
5	C	511	GOL	O2-C2-C3-O3
5	G	504	GOL	O2-C2-C3-O3
5	G	505	GOL	O2-C2-C3-O3
4	E	503	PEG	O1-C1-C2-O2
4	E	504	PEG	O1-C1-C2-O2
4	W	201	PEG	O2-C3-C4-O4
4	A	503	PEG	O1-C1-C2-O2
4	E	502	PEG	O2-C3-C4-O4
4	E	505	PEG	O1-C1-C2-O2
4	I	502	PEG	O1-C1-C2-O2
4	I	502	PEG	O2-C3-C4-O4
5	A	505	GOL	C1-C2-C3-O3
5	A	506	GOL	O1-C1-C2-C3
5	A	509	GOL	O1-C1-C2-C3
5	A	510	GOL	C1-C2-C3-O3
5	A	511	GOL	O1-C1-C2-C3
5	Q	202	GOL	O1-C1-C2-C3
5	Q	204	GOL	C1-C2-C3-O3
5	C	507	GOL	C1-C2-C3-O3
5	C	508	GOL	C1-C2-C3-O3
5	C	512	GOL	O1-C1-C2-C3
5	C	512	GOL	C1-C2-C3-O3
5	E	511	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	E	516	GOL	C1-C2-C3-O3
5	G	504	GOL	C1-C2-C3-O3
5	G	505	GOL	C1-C2-C3-O3
5	G	506	GOL	C1-C2-C3-O3
5	I	503	GOL	C1-C2-C3-O3
5	I	505	GOL	C1-C2-C3-O3
5	I	507	GOL	O1-C1-C2-C3
4	A	502	PEG	O2-C3-C4-O4
4	A	503	PEG	O2-C3-C4-O4
4	E	504	PEG	O2-C3-C4-O4
5	A	513	GOL	O2-C2-C3-O3
5	A	514	GOL	O2-C2-C3-O3
5	A	516	GOL	O1-C1-C2-O2
5	Q	203	GOL	O2-C2-C3-O3
5	C	507	GOL	O2-C2-C3-O3
5	C	511	GOL	O1-C1-C2-O2
5	C	514	GOL	O1-C1-C2-O2
5	E	511	GOL	O1-C1-C2-O2
5	E	514	GOL	O2-C2-C3-O3
5	E	515	GOL	O1-C1-C2-O2
5	G	503	GOL	O1-C1-C2-O2
5	G	506	GOL	O2-C2-C3-O3
4	Q	201	PEG	O2-C3-C4-O4
4	C	505	PEG	O2-C3-C4-O4
5	A	508	GOL	O2-C2-C3-O3
5	A	509	GOL	O1-C1-C2-O2
5	A	511	GOL	O1-C1-C2-O2
5	E	509	GOL	O2-C2-C3-O3
5	I	503	GOL	O2-C2-C3-O3
5	I	507	GOL	O1-C1-C2-O2
5	A	505	GOL	O2-C2-C3-O3
5	A	515	GOL	O2-C2-C3-O3
5	Q	202	GOL	O2-C2-C3-O3
5	Q	204	GOL	O2-C2-C3-O3
5	C	506	GOL	O2-C2-C3-O3
5	C	508	GOL	O1-C1-C2-O2
5	C	512	GOL	O2-C2-C3-O3
5	C	513	GOL	O1-C1-C2-O2
5	C	515	GOL	O2-C2-C3-O3
5	I	505	GOL	O2-C2-C3-O3
4	E	503	PEG	O2-C3-C4-O4
4	A	502	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	502	PEG	O1-C1-C2-O2
4	G	502	PEG	O1-C1-C2-O2
4	A	504	PEG	C1-C2-O2-C3
4	C	504	PEG	C4-C3-O2-C2
5	C	513	GOL	O2-C2-C3-O3
5	I	503	GOL	O1-C1-C2-O2
4	G	502	PEG	O2-C3-C4-O4
5	G	503	GOL	C1-C2-C3-O3
4	E	502	PEG	O1-C1-C2-O2
4	Q	201	PEG	C1-C2-O2-C3
4	G	502	PEG	C4-C3-O2-C2
4	E	502	PEG	C4-C3-O2-C2
5	C	508	GOL	O2-C2-C3-O3
5	E	508	GOL	O2-C2-C3-O3
5	E	516	GOL	O2-C2-C3-O3
4	C	503	PEG	O1-C1-C2-O2
4	C	503	PEG	C4-C3-O2-C2
4	A	504	PEG	O2-C3-C4-O4
4	W	201	PEG	O1-C1-C2-O2
4	A	502	PEG	C4-C3-O2-C2
5	E	507	GOL	O1-C1-C2-C3
5	A	506	GOL	O1-C1-C2-O2
5	A	516	GOL	O2-C2-C3-O3
4	K	502	PEG	C1-C2-O2-C3
4	C	505	PEG	C4-C3-O2-C2
5	S	201	GOL	C1-C2-C3-O3
5	C	512	GOL	O1-C1-C2-O2
5	E	512	GOL	O2-C2-C3-O3
5	G	503	GOL	O2-C2-C3-O3
4	K	502	PEG	C4-C3-O2-C2
4	Q	201	PEG	O1-C1-C2-O2
5	Q	202	GOL	C1-C2-C3-O3
5	C	508	GOL	O1-C1-C2-C3
5	C	513	GOL	C1-C2-C3-O3
5	G	508	GOL	O1-C1-C2-C3
5	I	503	GOL	O1-C1-C2-C3
4	A	504	PEG	C4-C3-O2-C2
4	A	503	PEG	C4-C3-O2-C2
4	C	502	PEG	C1-C2-O2-C3

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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%)	0.17	1 (0%)	94	28, 40, 54, 74	0
1	C	400/403 (99%)	0.20	1 (0%)	94	27, 41, 60, 88	0
1	E	400/403 (99%)	0.31	1 (0%)	94	25, 38, 54, 74	0
1	G	400/403 (99%)	0.16	1 (0%)	94	26, 39, 60, 98	0
1	I	400/403 (99%)	0.41	10 (2%)	57	31, 41, 73, 109	0
1	K	400/403 (99%)	0.73	20 (5%)	28	47, 67, 90, 116	0
1	M	398/403 (98%)	0.98	58 (14%)	2	67, 86, 118, 139	0
1	O	398/403 (98%)	2.16	177 (44%)	0	81, 116, 149, 167	0
2	Q	147/154 (95%)	0.52	10 (6%)	17	29, 50, 82, 116	0
2	S	143/154 (92%)	0.39	5 (3%)	44	46, 61, 82, 116	0
2	U	135/154 (87%)	3.13	75 (55%)	0	61, 102, 173, 209	0
2	W	144/154 (93%)	1.13	29 (20%)	1	40, 66, 113, 155	0
2	Y	141/154 (91%)	1.60	45 (31%)	0	49, 87, 145, 171	0
2	a	139/154 (90%)	2.82	78 (56%)	0	100, 116, 142, 148	0
2	c	139/154 (90%)	4.14	105 (75%)	0	122, 142, 161, 178	0
2	e	97/154 (62%)	4.01	74 (76%)	0	147, 158, 166, 172	0
All	All	4281/4456 (96%)	1.01	690 (16%)	1	25, 56, 146, 209	0

All (690) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	72	ALA	12.2
2	c	71	VAL	11.5
2	a	28	THR	11.3
2	a	12	GLY	11.1
1	O	114	VAL	11.1

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Mol	Chain	Res	Type	RSRZ
2	c	28	THR	10.6
2	U	140	ILE	10.4
2	a	24	PHE	10.3
2	e	9	HIS	10.3
2	e	34	TYR	9.8
2	c	142	ALA	9.7
2	e	98	VAL	9.7
2	c	73	GLU	9.6
2	Y	72	ALA	9.5
2	U	79	PHE	9.3
2	c	72	ALA	9.2
2	c	13	THR	9.1
2	c	67	LEU	9.1
2	e	24	PHE	9.1
2	e	95	LEU	9.1
2	e	91	LEU	9.0
2	U	67	LEU	9.0
2	U	136	LEU	8.9
2	c	14	THR	8.9
2	c	136	LEU	8.8
2	a	27	LEU	8.8
2	c	140	ILE	8.8
2	U	70	THR	8.6
2	c	143	ALA	8.5
1	K	48	GLY	8.5
1	K	46	SER	8.4
2	U	98	ALA	8.4
1	O	234	GLY	8.3
2	c	103	THR	8.3
1	K	47	ALA	8.2
2	U	69	TYR	8.0
1	O	135	ALA	8.0
2	c	137	SER	8.0
2	c	78	HIS	8.0
2	a	80	PHE	7.9
1	M	150	VAL	7.9
2	c	69	TYR	7.9
2	e	115	PHE	7.9
2	e	80	GLY	7.8
2	U	101	GLY	7.7
2	e	140	ILE	7.7
1	K	53	SER	7.7

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Mol	Chain	Res	Type	RSRZ
2	c	75	GLY	7.6
2	Y	140	ILE	7.6
2	e	99	GLU	7.6
2	U	144	THR	7.6
2	c	115	LEU	7.5
2	e	94	LEU	7.5
2	e	11	PHE	7.5
2	e	10	PRO	7.4
2	U	133	LEU	7.3
1	O	193	VAL	7.3
2	U	99	VAL	7.3
2	a	81	GLY	7.3
2	U	102	LYS	7.3
2	a	69	TYR	7.2
2	e	93	VAL	7.2
2	c	133	LEU	7.2
2	a	79	PHE	7.1
2	Y	70	THR	7.1
1	O	224	TYR	7.1
1	O	342	VAL	7.1
2	e	106	LEU	7.1
2	c	51	LEU	7.0
2	c	53	ALA	7.0
2	U	77	MET	7.0
2	U	68	GLY	6.9
1	O	206	ALA	6.9
2	U	76	LYS	6.8
2	U	143	ALA	6.8
2	Y	76	LYS	6.7
2	c	145	LYS	6.7
1	K	52	ARG	6.7
2	c	76	LYS	6.7
2	c	47	LEU	6.7
2	c	107	LEU	6.7
2	c	112	PRO	6.7
2	a	95	LEU	6.6
2	e	81	ASP	6.6
2	c	45	PRO	6.6
2	U	139	ALA	6.6
1	O	348	TYR	6.6
2	c	70	THR	6.5
2	c	48	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
2	c	27	LEU	6.5
2	e	102	THR	6.5
1	O	157	ILE	6.5
2	e	96	THR	6.5
2	U	142	ALA	6.5
2	Y	71	VAL	6.5
1	M	157	ILE	6.4
1	O	312	LEU	6.4
2	a	25	ALA	6.4
2	U	56	LYS	6.4
2	Y	136	LEU	6.3
2	c	91	LEU	6.3
2	a	53	ALA	6.3
2	c	80	PHE	6.3
2	U	80	PHE	6.3
1	I	55	PHE	6.2
2	e	90	LEU	6.2
2	U	100	GLU	6.2
2	U	95	LEU	6.2
2	e	139	ILE	6.2
2	U	137	SER	6.2
2	c	139	ALA	6.2
1	O	216	TYR	6.2
2	e	143	THR	6.2
1	O	179	LEU	6.0
1	O	165	ALA	6.0
2	U	71	VAL	6.0
1	O	185	PHE	6.0
2	a	121	LEU	6.0
2	e	118	LEU	6.0
1	O	153	LEU	5.9
1	O	317	GLY	5.9
2	e	13	THR	5.9
2	U	111	SER	5.9
1	O	322	ARG	5.9
2	c	79	PHE	5.8
2	e	15	VAL	5.8
1	O	334	ALA	5.8
2	a	23	THR	5.8
2	Y	73	GLU	5.8
2	Y	147	VAL	5.8
2	U	65	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	c	119	LEU	5.7
1	O	204	PHE	5.7
1	O	331	PHE	5.7
2	c	24	PHE	5.7
2	a	50	GLU	5.7
2	U	81	GLY	5.7
2	a	29	GLN	5.7
2	a	103	THR	5.7
2	U	103	THR	5.7
2	e	16	THR	5.7
2	a	115	LEU	5.7
2	Y	144	THR	5.7
2	c	81	GLY	5.7
2	c	111	SER	5.6
1	O	208	VAL	5.6
1	O	311	ALA	5.6
2	c	74	ASN	5.6
2	U	75	GLY	5.6
2	a	13	THR	5.6
2	W	74	ASN	5.6
2	a	119	LEU	5.6
2	c	105	ALA	5.6
1	O	195	VAL	5.6
2	U	108	GLN	5.5
2	e	36	GLN	5.5
2	e	103	ALA	5.5
2	a	26	PRO	5.5
2	a	133	LEU	5.5
2	a	110	GLN	5.4
2	U	12	GLY	5.4
2	c	101	GLY	5.4
1	O	333	PHE	5.4
2	c	29	GLN	5.4
1	M	192	VAL	5.4
1	O	304	LEU	5.4
1	O	308	ALA	5.4
2	W	7	ALA	5.4
2	a	22	ASN	5.4
1	O	328	LEU	5.3
2	c	82	ASP	5.3
2	a	14	THR	5.3
2	U	78	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
1	O	388	LEU	5.3
1	O	306	THR	5.3
2	c	116	PHE	5.3
2	c	146	GLN	5.3
1	O	108	PRO	5.3
2	W	6	PHE	5.3
2	c	23	THR	5.2
2	c	108	GLN	5.2
2	U	48	PRO	5.2
2	e	114	LEU	5.2
2	c	144	THR	5.2
2	e	97	ALA	5.1
2	U	112	PRO	5.1
1	O	102	ALA	5.1
1	O	305	ALA	5.1
1	O	400	VAL	5.1
2	W	98	ALA	5.0
1	O	313	ALA	5.0
2	c	50	GLU	5.0
2	U	94	VAL	5.0
2	a	74	ASN	5.0
1	O	188	SER	5.0
2	c	68	GLY	5.0
1	O	297	ALA	4.9
1	M	294	ILE	4.9
1	O	395	ALA	4.9
2	U	107	LEU	4.9
2	U	73	GLU	4.9
2	U	110	GLN	4.9
1	O	384	ASP	4.9
1	M	152	LEU	4.8
2	c	15	VAL	4.8
2	c	102	LYS	4.8
2	Y	75	GLY	4.8
2	e	101	LYS	4.8
1	O	137	VAL	4.8
2	a	58	ILE	4.8
2	Y	69	TYR	4.8
1	O	378	PRO	4.8
1	O	385	VAL	4.8
2	Q	4	PRO	4.8
2	a	78	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	61	LEU	4.7
1	O	164	LEU	4.7
1	O	9	PHE	4.7
1	M	179	LEU	4.7
1	O	150	VAL	4.7
2	e	32	ASP	4.7
2	Y	7	ALA	4.7
2	c	121	LEU	4.7
2	Y	77	MET	4.7
2	c	98	ALA	4.7
1	O	372	LEU	4.7
2	e	100	GLY	4.7
2	c	110	GLN	4.7
2	Q	147	VAL	4.6
2	Y	80	PHE	4.6
2	e	41	GLY	4.6
1	O	300	TRP	4.6
2	U	74	ASN	4.6
2	e	40	LEU	4.6
2	c	99	VAL	4.5
2	a	77	MET	4.5
2	e	14	THR	4.5
2	Y	107	LEU	4.5
2	c	138	GLU	4.5
2	e	142	ALA	4.5
1	O	399	LEU	4.5
2	U	51	LEU	4.5
2	e	111	PRO	4.5
1	O	192	VAL	4.5
1	O	292	TYR	4.5
1	O	134	GLY	4.5
1	O	294	ILE	4.5
2	c	104	ALA	4.5
2	U	11	PHE	4.5
1	O	309	GLU	4.5
2	U	138	GLU	4.4
2	W	150	HIS	4.4
1	O	75	LEU	4.4
2	c	16	THR	4.4
2	e	89	GLY	4.4
2	a	20	LEU	4.4
2	e	37	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	O	136	LYS	4.4
2	a	97	THR	4.4
2	c	26	PRO	4.3
1	O	293	ASP	4.3
2	W	114	ALA	4.3
2	c	46	ALA	4.3
2	U	66	TRP	4.3
2	c	11	PHE	4.3
2	c	36	GLN	4.3
1	O	189	ALA	4.3
2	U	141	ILE	4.3
2	c	141	ILE	4.3
2	Y	68	GLY	4.3
2	a	120	GLY	4.3
2	a	21	ARG	4.3
2	a	111	SER	4.3
1	O	215	PHE	4.3
2	e	104	ALA	4.3
1	C	401	ASP	4.2
2	a	32	ASP	4.2
1	O	376	PHE	4.2
2	c	55	ALA	4.2
1	M	183	ILE	4.2
1	O	166	LEU	4.2
1	O	363	LEU	4.2
2	c	135	ALA	4.2
2	e	112	LEU	4.2
1	O	205	PRO	4.2
2	a	98	ALA	4.2
2	Y	79	PHE	4.2
1	O	183	ILE	4.2
2	c	95	LEU	4.2
2	Y	139	ALA	4.2
1	M	112	ILE	4.2
2	c	58	ILE	4.2
1	M	127	LEU	4.2
2	e	105	GLU	4.1
2	c	94	VAL	4.1
1	O	142	LEU	4.1
2	a	54	GLN	4.1
1	O	112	ILE	4.1
2	U	91	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	O	158	THR	4.1
2	c	87	ILE	4.1
1	M	185	PHE	4.1
1	O	301	SER	4.0
1	O	303	SER	4.0
1	O	194	MET	4.0
1	O	116	VAL	4.0
2	U	44	LEU	4.0
2	c	77	MET	4.0
2	a	71	VAL	4.0
1	O	148	PRO	4.0
1	O	329	LEU	4.0
2	W	149	HIS	4.0
2	c	38	ILE	4.0
2	c	52	LYS	4.0
2	a	118	GLU	4.0
2	e	28	THR	4.0
1	K	50	VAL	4.0
2	c	147	VAL	4.0
1	K	348	TYR	3.9
1	O	163	ILE	3.9
1	O	307	LEU	3.9
2	c	25	ALA	3.9
2	e	141	ALA	3.9
1	I	54	GLN	3.9
2	a	11	PHE	3.8
2	c	66	TRP	3.9
1	O	371	THR	3.8
1	O	78	ALA	3.8
2	U	135	ALA	3.8
2	e	113	ALA	3.8
1	O	129	VAL	3.8
1	O	169	MET	3.8
1	K	54	GLN	3.8
1	M	137	VAL	3.8
2	a	100	GLU	3.8
1	O	318	PHE	3.8
2	U	46	ALA	3.8
2	e	39	MET	3.8
2	U	50	GLU	3.8
2	e	135	LEU	3.8
1	M	401	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	Y	101	GLY	3.8
2	a	68	GLY	3.8
2	c	118	GLU	3.8
2	a	141	ILE	3.8
2	a	96	LEU	3.8
2	U	55	ALA	3.7
2	e	17	ALA	3.7
2	c	96	LEU	3.7
2	Y	13	THR	3.7
2	a	30	TRP	3.7
2	c	54	GLN	3.7
2	c	43	GLN	3.7
1	O	104	PRO	3.7
2	S	147	VAL	3.7
2	a	99	VAL	3.7
1	O	146	ARG	3.7
2	c	129	ARG	3.7
2	Y	51	LEU	3.6
2	e	20	LEU	3.6
2	c	40	LEU	3.6
2	Y	105	ALA	3.6
1	O	218	PHE	3.6
2	Y	74	ASN	3.6
1	O	23	LEU	3.6
2	e	27	LEU	3.6
2	c	56	LYS	3.6
1	I	18	ASP	3.6
1	O	115	SER	3.6
1	M	216	TYR	3.6
2	Y	12	GLY	3.5
1	O	365	GLU	3.5
2	a	52	LYS	3.5
2	Y	109	ALA	3.5
2	U	58	ILE	3.5
1	O	344	LEU	3.5
2	a	125	LEU	3.5
2	Y	78	HIS	3.5
1	O	272	GLY	3.5
1	O	295	ASN	3.5
1	O	113	ILE	3.5
2	U	96	LEU	3.5
2	a	143	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	W	47	LEU	3.4
2	e	123	GLN	3.4
2	e	12	GLY	3.4
1	O	392	VAL	3.4
1	M	113	ILE	3.4
1	O	47	ALA	3.4
2	c	134	ASN	3.4
2	U	104	ALA	3.4
1	M	109	GLY	3.4
2	e	107	GLN	3.4
2	a	31	GLU	3.4
2	W	109	ALA	3.4
1	O	209	GLN	3.4
1	O	4	PHE	3.4
1	M	234	GLY	3.4
2	W	106	GLU	3.4
2	c	106	GLU	3.4
2	c	65	VAL	3.4
1	I	46	SER	3.4
2	a	136	LEU	3.4
1	O	98	ALA	3.4
2	a	33	LYS	3.4
2	a	122	ARG	3.4
1	O	79	PRO	3.3
1	O	264	SER	3.3
1	O	352	LEU	3.3
1	O	101	TYR	3.3
1	O	49	ASN	3.3
2	U	15	VAL	3.3
2	a	72	ALA	3.3
2	e	116	ASP	3.3
1	M	52	ARG	3.3
1	O	159	PRO	3.3
2	Y	108	GLN	3.3
1	O	319	ARG	3.3
2	W	107	LEU	3.3
2	W	72	ALA	3.3
2	e	128	ARG	3.3
2	a	51	LEU	3.2
1	K	337[A]	HIS	3.2
2	S	151	HIS	3.2
2	c	12	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	176	CYS	3.2
1	M	138	VAL	3.2
2	a	15	VAL	3.2
1	O	238	LEU	3.2
1	O	288	TRP	3.2
2	e	134	ALA	3.2
2	a	101	GLY	3.2
1	O	133	THR	3.2
2	Y	53	ALA	3.2
2	U	20	LEU	3.2
1	A	1	MET	3.2
2	a	107	LEU	3.2
2	Q	6	PHE	3.2
1	O	161	SER	3.2
1	O	368	VAL	3.2
2	U	119	LEU	3.2
2	U	106	GLU	3.1
2	U	117	ASP	3.1
2	Y	6	PHE	3.1
1	O	374	ALA	3.1
2	c	37	LEU	3.1
2	W	102	LYS	3.1
2	c	19	THR	3.1
2	a	42	LYS	3.1
1	I	52	ARG	3.1
1	O	239	LEU	3.1
2	U	13	THR	3.1
1	O	332	ASP	3.1
2	a	75	GLY	3.1
2	e	92	ALA	3.1
2	W	99	VAL	3.1
2	e	121	ARG	3.0
1	O	373	ARG	3.0
1	M	191	MET	3.0
2	U	14	THR	3.0
2	a	67	LEU	3.0
2	c	97	THR	3.0
1	M	79	PRO	3.0
2	U	47	LEU	3.0
2	a	93	ALA	3.0
1	O	191	MET	3.0
2	a	140	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	W	69	TYR	3.0
1	M	246	LEU	3.0
2	U	105	ALA	3.0
2	e	84	GLY	3.0
1	O	106	LEU	3.0
1	O	330	ALA	3.0
2	a	17	ALA	3.0
2	a	144	THR	3.0
1	M	205	PRO	3.0
2	Q	145	LYS	3.0
2	W	79	PHE	3.0
1	O	68	ALA	3.0
1	K	63	ALA	2.9
2	W	113	LEU	2.9
1	O	48	GLY	2.9
2	c	32	ASP	2.9
2	a	35	ARG	2.9
1	O	366	LEU	2.9
1	O	149	ASP	2.9
1	O	398	LEU	2.9
2	e	109	GLN	2.9
2	c	39	MET	2.9
1	K	23	LEU	2.9
2	e	25	ALA	2.9
2	e	22	ASN	2.9
1	O	381	THR	2.9
1	O	357	HIS	2.9
1	O	341	MET	2.8
1	M	187	HIS	2.8
2	Y	67	LEU	2.8
1	O	302	ARG	2.8
1	O	55	PHE	2.8
1	O	316	PRO	2.8
2	c	93	ALA	2.8
2	a	73	GLU	2.8
1	M	153	LEU	2.8
2	U	29	GLN	2.8
1	M	163	ILE	2.8
1	O	380	ASN	2.8
2	W	45	PRO	2.8
2	U	54	GLN	2.8
2	a	43	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	48	GLY	2.8
2	Q	7	ALA	2.8
2	Q	109	ALA	2.8
1	O	320	SER	2.8
1	I	3	VAL	2.7
1	O	370	GLY	2.7
2	U	97	THR	2.7
1	O	201	ALA	2.7
2	W	111	SER	2.7
1	O	296	GLN	2.7
1	O	127	LEU	2.7
2	Q	69	TYR	2.7
2	Y	49	ASP	2.7
1	M	260	PHE	2.7
2	Q	150	HIS	2.7
2	W	8	GLY	2.7
1	M	96	MET	2.7
2	W	76	LYS	2.7
1	O	214	ASP	2.7
1	M	193	VAL	2.7
1	M	186	ALA	2.7
1	O	117	ALA	2.7
1	M	94	ILE	2.7
2	U	113	LEU	2.7
1	O	325	ASP	2.7
1	O	389	VAL	2.6
1	O	147	LEU	2.6
2	e	110	SER	2.6
2	a	109	ALA	2.6
2	e	86	ILE	2.6
2	W	77	MET	2.6
2	c	8	GLY	2.6
2	U	122	ARG	2.6
1	O	364	ALA	2.6
1	M	108	PRO	2.6
1	O	109	GLY	2.6
1	O	326	SER	2.6
1	O	245	TRP	2.5
1	O	337	HIS	2.5
1	M	156	LEU	2.5
2	e	124	LEU	2.5
1	M	162	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	197	GLY	2.5
1	M	247	GLY	2.5
1	O	89	GLY	2.5
1	I	19	ALA	2.5
2	c	109	ALA	2.5
1	O	138	VAL	2.5
1	O	162	ARG	2.5
1	O	174	GLY	2.5
1	E	91	THR	2.5
2	U	45	PRO	2.5
1	M	269	LEU	2.5
2	U	49	ASP	2.5
1	M	134	GLY	2.5
1	M	259	GLY	2.5
1	O	3	VAL	2.5
2	U	57	GLU	2.5
2	Y	81	GLY	2.5
1	K	166	LEU	2.5
2	Q	151	HIS	2.5
1	O	52	ARG	2.5
2	c	10	PRO	2.5
1	M	262	THR	2.5
1	O	298	GLU	2.5
1	M	114	VAL	2.4
1	O	228	GLY	2.4
2	W	144	THR	2.4
1	O	397	GLU	2.4
2	Y	138	GLU	2.4
1	M	238	LEU	2.4
2	c	122	ARG	2.4
1	M	181	ARG	2.4
1	O	107	GLN	2.4
2	Y	54	GLN	2.4
1	K	157	ILE	2.4
2	c	34	TYR	2.4
1	O	29	ALA	2.4
1	K	60	ARG	2.4
1	M	240	GLU	2.4
1	O	187	HIS	2.4
2	U	82	ASP	2.4
1	M	166	LEU	2.4
1	O	202	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	336	VAL	2.4
1	O	244	PRO	2.4
2	U	10	PRO	2.4
1	O	396	LEU	2.4
2	a	91	LEU	2.4
2	W	71	VAL	2.3
2	W	108	GLN	2.3
2	e	29	GLN	2.3
1	M	359	ALA	2.3
2	W	68	GLY	2.3
2	e	30	TRP	2.3
2	Y	82	ASP	2.3
1	O	213	ILE	2.3
1	O	359	ALA	2.3
1	O	379	TYR	2.3
2	W	51	LEU	2.3
2	W	67	LEU	2.3
1	K	186	ALA	2.3
1	M	384	ASP	2.3
1	M	158	THR	2.3
1	O	167	GLY	2.3
1	O	211	LEU	2.3
2	S	145	LYS	2.3
2	c	20	LEU	2.3
1	O	21	VAL	2.3
1	M	245	TRP	2.3
1	O	190	GLY	2.3
1	O	338	HIS	2.3
2	W	73	GLU	2.3
2	e	85	ARG	2.3
2	e	87	VAL	2.3
1	M	76	LEU	2.3
1	M	366	LEU	2.3
1	O	155	GLU	2.3
2	a	36	GLN	2.2
1	M	391	ALA	2.2
2	Q	148	LYS	2.2
2	Y	66	TRP	2.2
1	K	109	GLY	2.2
1	O	314	LYS	2.2
2	U	109	ALA	2.2
2	e	136	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	a	39	MET	2.2
2	a	147	VAL	2.2
2	Y	142	ALA	2.2
2	c	59	ALA	2.2
2	S	8	GLY	2.2
2	c	132	GLY	2.2
1	M	204	PHE	2.2
1	O	278	GLY	2.2
2	U	121	LEU	2.2
2	c	44	LEU	2.2
2	e	26	PRO	2.2
1	O	181	ARG	2.2
2	c	126	SER	2.2
2	a	16	THR	2.2
1	O	154	PRO	2.2
1	O	299	SER	2.2
1	M	248	GLY	2.1
2	Y	50	GLU	2.1
2	Y	56	LYS	2.1
2	Y	145	LYS	2.1
1	G	271	ALA	2.1
2	a	94	VAL	2.1
2	c	90	GLY	2.1
2	Y	103	THR	2.1
2	e	19	THR	2.1
2	a	102	LYS	2.1
1	O	152	LEU	2.1
1	O	77	ASN	2.1
2	Y	55	ALA	2.1
1	M	344	LEU	2.1
1	M	228	GLY	2.1
2	Y	146	GLN	2.1
1	M	98	ALA	2.1
1	I	57	GLU	2.1
1	O	85	VAL	2.1
1	O	265	ALA	2.1
2	c	100	GLU	2.1
1	M	398	LEU	2.1
2	a	137	SER	2.1
2	S	112	PRO	2.1
1	O	94	ILE	2.1
2	c	31	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	22	TYR	2.0
2	e	38	ILE	2.0
2	Y	24	PHE	2.0
1	M	160	ARG	2.0
1	I	45	LEU	2.0
1	K	328	LEU	2.0
1	K	58	ALA	2.0
1	M	53	SER	2.0
1	O	350	ILE	2.0
2	Y	95	LEU	2.0
2	a	106	GLU	2.0
2	a	124	GLN	2.0
2	e	130	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSS	c	61	7/8	0.64	0.23	141,146,147,148	0
2	CSS	W	61	7/8	0.75	0.21	94,97,107,114	0
2	CSS	U	61	7/8	0.77	0.21	97,104,108,115	0
1	CSS	M	358	7/8	0.80	0.15	85,87,88,92	0
1	CSS	O	358	7/8	0.80	0.16	113,114,116,116	0
2	CSS	S	61	7/8	0.82	0.16	86,87,98,101	0
2	CSS	a	61	7/8	0.84	0.15	105,106,109,110	0
2	CSS	Y	61	7/8	0.84	0.15	87,91,97,104	0
1	CSS	C	358	7/8	0.86	0.16	36,39,42,51	0
2	CSS	Q	61	7/8	0.89	0.14	71,73,83,95	0
1	CSS	G	358	7/8	0.92	0.15	33,34,35,42	0
1	CSS	K	358	7/8	0.92	0.13	59,61,62,64	0
1	CSS	E	358	7/8	0.93	0.17	30,32,34,48	0
1	CSS	A	358	7/8	0.93	0.15	35,35,38,46	0
1	CSS	I	358	7/8	0.93	0.14	35,38,41,49	0

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	511	6/6	0.64	0.23	52,55,59,66	0
5	GOL	C	506	6/6	0.68	0.31	55,61,67,67	0
5	GOL	A	507	6/6	0.72	0.28	54,59,60,61	0
5	GOL	A	511	6/6	0.72	0.27	49,61,64,65	0
5	GOL	I	506	6/6	0.72	0.25	62,71,73,76	0
5	GOL	I	507	6/6	0.72	0.28	53,64,68,69	0
5	GOL	E	507	6/6	0.74	0.25	50,56,60,60	0
5	GOL	G	505	6/6	0.74	0.19	57,71,75,75	0
5	GOL	A	505	6/6	0.76	0.41	55,58,60,69	0
4	PEG	E	504	7/7	0.77	0.23	45,53,56,57	0
4	PEG	Q	201	7/7	0.77	0.24	50,58,67,68	0
5	GOL	E	509	6/6	0.79	0.32	46,54,62,63	0
5	GOL	E	516	6/6	0.79	0.36	44,52,58,62	0
4	PEG	E	502	7/7	0.79	0.16	50,55,60,64	0
5	GOL	G	509	6/6	0.79	0.23	54,57,67,70	0
5	GOL	I	504	6/6	0.79	0.24	59,65,70,73	0
4	PEG	A	503	7/7	0.79	0.28	43,51,55,57	0
4	PEG	G	502	7/7	0.79	0.20	54,61,68,70	0
5	GOL	W	202	6/6	0.80	0.21	64,74,75,76	0
5	GOL	E	511	6/6	0.80	0.20	50,59,64,64	0
5	GOL	A	513	6/6	0.81	0.21	50,52,55,56	0
5	GOL	A	506	6/6	0.81	0.34	47,62,64,65	0
5	GOL	E	513	6/6	0.81	0.22	52,54,59,64	0
4	PEG	K	502	7/7	0.81	0.26	57,58,64,65	0
4	PEG	C	503	7/7	0.81	0.28	56,64,70,81	0
5	GOL	M	502	6/6	0.81	0.23	57,62,69,70	0
5	GOL	C	513	6/6	0.82	0.24	57,66,69,75	0
4	PEG	C	505	7/7	0.82	0.27	40,57,74,75	0
5	GOL	G	507	6/6	0.82	0.22	57,61,66,67	0
5	GOL	G	508	6/6	0.82	0.19	48,52,53,54	0
5	GOL	E	508	6/6	0.82	0.16	40,43,54,54	0
5	GOL	Q	203	6/6	0.83	0.19	44,52,52,56	0
5	GOL	E	514	6/6	0.83	0.48	59,65,72,78	0
4	PEG	W	201	7/7	0.83	0.27	57,58,64,66	0
5	GOL	A	516	6/6	0.84	0.15	55,56,58,62	0
5	GOL	C	515	6/6	0.84	0.25	43,46,48,52	0
5	GOL	A	510	6/6	0.85	0.20	48,58,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	E	515	6/6	0.85	0.26	52,54,56,57	0
5	GOL	A	514	6/6	0.85	0.32	63,70,72,73	0
5	GOL	E	510	6/6	0.85	0.25	50,59,65,80	0
5	GOL	E	506	6/6	0.85	0.24	42,51,53,54	0
3	PLP	O	501	15/16	0.85	0.23	98,103,109,111	0
5	GOL	A	509	6/6	0.86	0.14	61,63,68,68	0
5	GOL	G	506	6/6	0.86	0.17	51,62,64,67	0
5	GOL	S	201	6/6	0.86	0.21	44,60,64,64	0
5	GOL	A	512	6/6	0.86	0.20	49,51,53,54	0
4	PEG	C	504	7/7	0.86	0.16	48,55,69,69	0
4	PEG	E	505	7/7	0.87	0.16	50,54,59,61	0
5	GOL	A	508	6/6	0.87	0.15	48,57,60,65	0
5	GOL	I	505	6/6	0.87	0.31	42,53,56,69	0
5	GOL	A	515	6/6	0.87	0.27	48,54,63,64	0
4	PEG	A	502	7/7	0.87	0.22	48,55,57,60	0
5	GOL	G	503	6/6	0.87	0.19	54,60,64,66	0
5	GOL	G	504	6/6	0.88	0.24	35,49,53,56	0
4	PEG	C	502	7/7	0.88	0.17	55,59,72,73	0
5	GOL	Q	204	6/6	0.88	0.37	54,62,67,71	0
5	GOL	C	507	6/6	0.89	0.26	55,67,72,73	0
4	PEG	E	503	7/7	0.89	0.18	54,60,65,65	0
5	GOL	C	510	6/6	0.90	0.24	48,65,70,73	0
5	GOL	C	514	6/6	0.90	0.20	66,71,76,77	0
5	GOL	Q	202	6/6	0.90	0.33	47,53,57,58	0
5	GOL	I	503	6/6	0.91	0.13	37,48,51,53	0
5	GOL	C	508	6/6	0.91	0.25	53,57,58,72	0
5	GOL	C	509	6/6	0.91	0.25	49,58,74,77	0
3	PLP	M	501	15/16	0.93	0.16	79,82,85,86	0
4	PEG	I	502	7/7	0.93	0.18	36,47,53,55	0
5	GOL	E	512	6/6	0.93	0.28	58,64,68,71	0
5	GOL	C	512	6/6	0.94	0.52	43,45,55,68	0
4	PEG	A	504	7/7	0.94	0.17	45,51,56,56	0
3	PLP	K	501	15/16	0.95	0.19	51,53,55,56	0
3	PLP	G	501	15/16	0.95	0.17	28,30,32,37	0
3	PLP	A	501	15/16	0.96	0.16	28,29,30,31	0
3	PLP	I	501	15/16	0.96	0.19	31,33,38,39	0
3	PLP	C	501	15/16	0.96	0.19	29,31,32,33	0
3	PLP	E	501	15/16	0.97	0.20	28,29,31,31	0

## 6.5 Other polymers (i)

There are no such residues in this entry.