



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 05:18 pm BST

PDB ID : 6ZEK  
Title : Crystal structure of mouse CSAD  
Authors : Mahootchi, E.; Raasakka, A.; Haavik, J.; Kursula, P.  
Deposited on : 2020-06-16  
Resolution : 2.10 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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

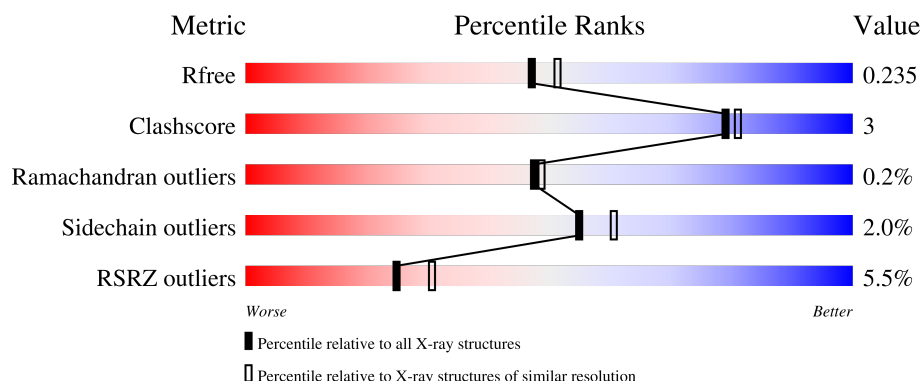
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	<div> <div>4%</div> <div>84%</div> <div>7%</div> <div>9%</div> </div>
1	B	521	<div> <div>5%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	C	521	<div> <div>4%</div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
1	D	521	<div> <div>6%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30749 atoms, of which 15062 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 sulfinic acid decarboxylase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	476	Total	C	H	N	O	P	S		1	0	0
			7545	2398	3775	659	691	1	21				
1	B	470	Total	C	H	N	O	P	S		4	1	0
			7449	2367	3728	649	683	1	21				
1	C	478	Total	C	H	N	O	P	S		6	0	0
			7545	2394	3774	661	694	1	21				
1	D	474	Total	C	H	N	O	P	S		1	0	0
			7499	2380	3754	656	687	1	21				

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q9DBE0
A	-26	GLY	-	expression tag	UNP Q9DBE0
A	-25	PRO	-	expression tag	UNP Q9DBE0
A	-24	HIS	-	expression tag	UNP Q9DBE0
A	-23	HIS	-	expression tag	UNP Q9DBE0
A	-22	HIS	-	expression tag	UNP Q9DBE0
A	-21	HIS	-	expression tag	UNP Q9DBE0
A	-20	HIS	-	expression tag	UNP Q9DBE0
A	-19	HIS	-	expression tag	UNP Q9DBE0
A	-18	LEU	-	expression tag	UNP Q9DBE0
A	-17	GLU	-	expression tag	UNP Q9DBE0
A	-16	SER	-	expression tag	UNP Q9DBE0
A	-15	THR	-	expression tag	UNP Q9DBE0
A	-14	SER	-	expression tag	UNP Q9DBE0
A	-13	LEU	-	expression tag	UNP Q9DBE0
A	-12	TYR	-	expression tag	UNP Q9DBE0
A	-11	LYS	-	expression tag	UNP Q9DBE0
A	-10	LYS	-	expression tag	UNP Q9DBE0
A	-9	ALA	-	expression tag	UNP Q9DBE0
A	-8	GLY	-	expression tag	UNP Q9DBE0
A	-7	SER	-	expression tag	UNP Q9DBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLU	-	expression tag	UNP Q9DBE0
A	-5	ASN	-	expression tag	UNP Q9DBE0
A	-4	LEU	-	expression tag	UNP Q9DBE0
A	-3	TYR	-	expression tag	UNP Q9DBE0
A	-2	PHE	-	expression tag	UNP Q9DBE0
A	-1	GLN	-	expression tag	UNP Q9DBE0
A	0	GLY	-	expression tag	UNP Q9DBE0
B	-27	MET	-	initiating methionine	UNP Q9DBE0
B	-26	GLY	-	expression tag	UNP Q9DBE0
B	-25	PRO	-	expression tag	UNP Q9DBE0
B	-24	HIS	-	expression tag	UNP Q9DBE0
B	-23	HIS	-	expression tag	UNP Q9DBE0
B	-22	HIS	-	expression tag	UNP Q9DBE0
B	-21	HIS	-	expression tag	UNP Q9DBE0
B	-20	HIS	-	expression tag	UNP Q9DBE0
B	-19	HIS	-	expression tag	UNP Q9DBE0
B	-18	LEU	-	expression tag	UNP Q9DBE0
B	-17	GLU	-	expression tag	UNP Q9DBE0
B	-16	SER	-	expression tag	UNP Q9DBE0
B	-15	THR	-	expression tag	UNP Q9DBE0
B	-14	SER	-	expression tag	UNP Q9DBE0
B	-13	LEU	-	expression tag	UNP Q9DBE0
B	-12	TYR	-	expression tag	UNP Q9DBE0
B	-11	LYS	-	expression tag	UNP Q9DBE0
B	-10	LYS	-	expression tag	UNP Q9DBE0
B	-9	ALA	-	expression tag	UNP Q9DBE0
B	-8	GLY	-	expression tag	UNP Q9DBE0
B	-7	SER	-	expression tag	UNP Q9DBE0
B	-6	GLU	-	expression tag	UNP Q9DBE0
B	-5	ASN	-	expression tag	UNP Q9DBE0
B	-4	LEU	-	expression tag	UNP Q9DBE0
B	-3	TYR	-	expression tag	UNP Q9DBE0
B	-2	PHE	-	expression tag	UNP Q9DBE0
B	-1	GLN	-	expression tag	UNP Q9DBE0
B	0	GLY	-	expression tag	UNP Q9DBE0
C	-27	MET	-	initiating methionine	UNP Q9DBE0
C	-26	GLY	-	expression tag	UNP Q9DBE0
C	-25	PRO	-	expression tag	UNP Q9DBE0
C	-24	HIS	-	expression tag	UNP Q9DBE0
C	-23	HIS	-	expression tag	UNP Q9DBE0
C	-22	HIS	-	expression tag	UNP Q9DBE0
C	-21	HIS	-	expression tag	UNP Q9DBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q9DBE0
C	-19	HIS	-	expression tag	UNP Q9DBE0
C	-18	LEU	-	expression tag	UNP Q9DBE0
C	-17	GLU	-	expression tag	UNP Q9DBE0
C	-16	SER	-	expression tag	UNP Q9DBE0
C	-15	THR	-	expression tag	UNP Q9DBE0
C	-14	SER	-	expression tag	UNP Q9DBE0
C	-13	LEU	-	expression tag	UNP Q9DBE0
C	-12	TYR	-	expression tag	UNP Q9DBE0
C	-11	LYS	-	expression tag	UNP Q9DBE0
C	-10	LYS	-	expression tag	UNP Q9DBE0
C	-9	ALA	-	expression tag	UNP Q9DBE0
C	-8	GLY	-	expression tag	UNP Q9DBE0
C	-7	SER	-	expression tag	UNP Q9DBE0
C	-6	GLU	-	expression tag	UNP Q9DBE0
C	-5	ASN	-	expression tag	UNP Q9DBE0
C	-4	LEU	-	expression tag	UNP Q9DBE0
C	-3	TYR	-	expression tag	UNP Q9DBE0
C	-2	PHE	-	expression tag	UNP Q9DBE0
C	-1	GLN	-	expression tag	UNP Q9DBE0
C	0	GLY	-	expression tag	UNP Q9DBE0
D	-27	MET	-	initiating methionine	UNP Q9DBE0
D	-26	GLY	-	expression tag	UNP Q9DBE0
D	-25	PRO	-	expression tag	UNP Q9DBE0
D	-24	HIS	-	expression tag	UNP Q9DBE0
D	-23	HIS	-	expression tag	UNP Q9DBE0
D	-22	HIS	-	expression tag	UNP Q9DBE0
D	-21	HIS	-	expression tag	UNP Q9DBE0
D	-20	HIS	-	expression tag	UNP Q9DBE0
D	-19	HIS	-	expression tag	UNP Q9DBE0
D	-18	LEU	-	expression tag	UNP Q9DBE0
D	-17	GLU	-	expression tag	UNP Q9DBE0
D	-16	SER	-	expression tag	UNP Q9DBE0
D	-15	THR	-	expression tag	UNP Q9DBE0
D	-14	SER	-	expression tag	UNP Q9DBE0
D	-13	LEU	-	expression tag	UNP Q9DBE0
D	-12	TYR	-	expression tag	UNP Q9DBE0
D	-11	LYS	-	expression tag	UNP Q9DBE0
D	-10	LYS	-	expression tag	UNP Q9DBE0
D	-9	ALA	-	expression tag	UNP Q9DBE0
D	-8	GLY	-	expression tag	UNP Q9DBE0
D	-7	SER	-	expression tag	UNP Q9DBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLU	-	expression tag	UNP Q9DBE0
D	-5	ASN	-	expression tag	UNP Q9DBE0
D	-4	LEU	-	expression tag	UNP Q9DBE0
D	-3	TYR	-	expression tag	UNP Q9DBE0
D	-2	PHE	-	expression tag	UNP Q9DBE0
D	-1	GLN	-	expression tag	UNP Q9DBE0
D	0	GLY	-	expression tag	UNP Q9DBE0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

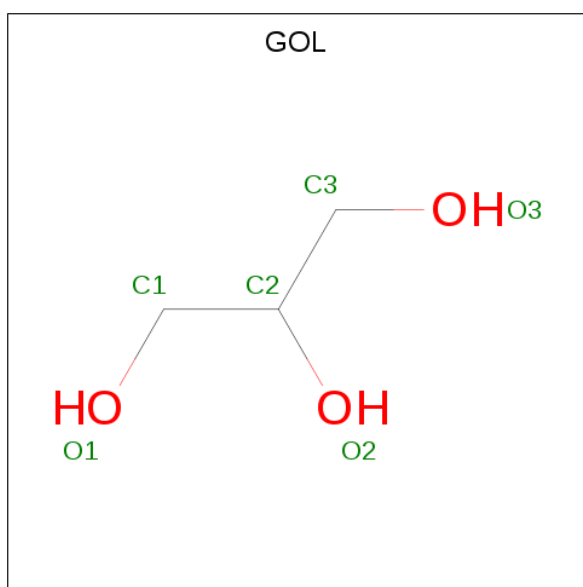
- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Cl 3	0	0
4	B	4	Total 4	Cl 4	0	0
4	C	3	Total 3	Cl 3	0	0
4	D	3	Total 3	Cl 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	B	1	Total 14	C 3	H 8	O 3	0	0
5	C	1	Total 14	C 3	H 8	O 3	0	0
5	C	1	Total 13	C 3	H 7	O 3	0	0
5	D	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	194	Total 194	O 194	0	0

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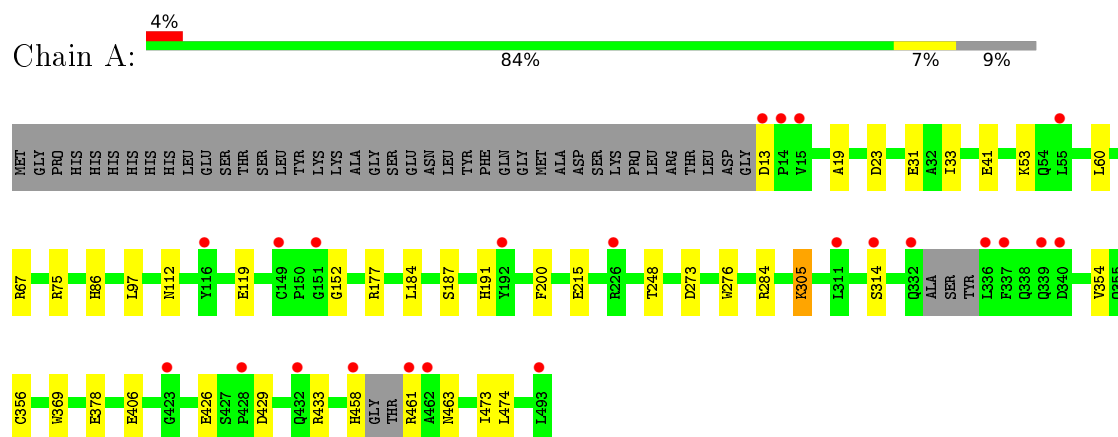
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	123	Total 123	O 123	0	0
6	C	182	Total 182	O 182	0	0
6	D	134	Total 135	O 135	0	1



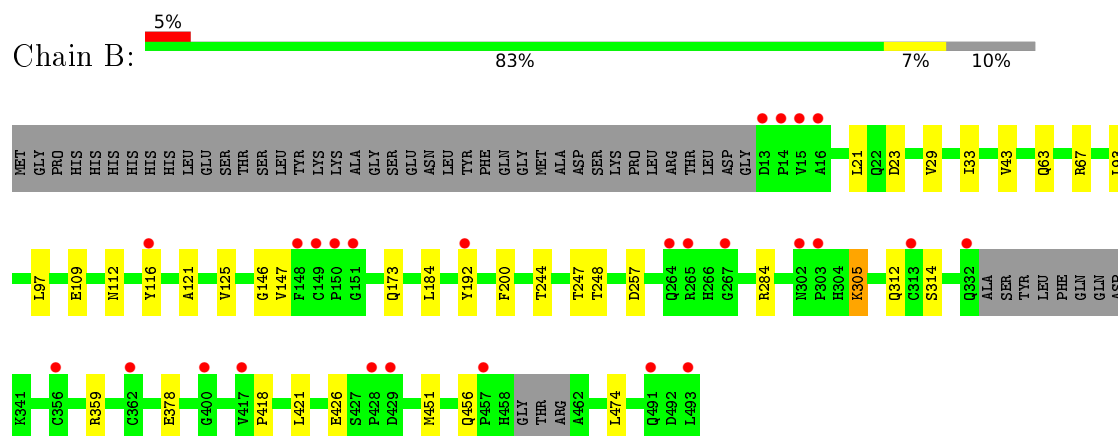
### 3 Residue-property plots [i](#)

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.

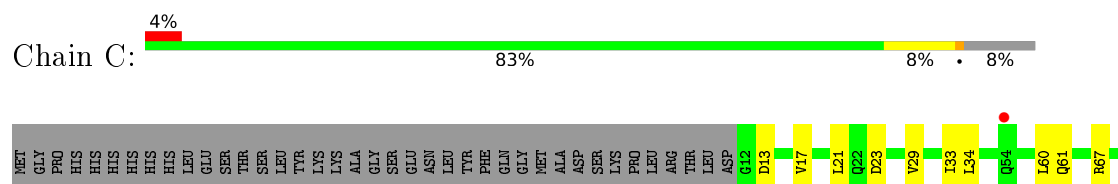
- Molecule 1: Cysteine sulfinic acid decarboxylase

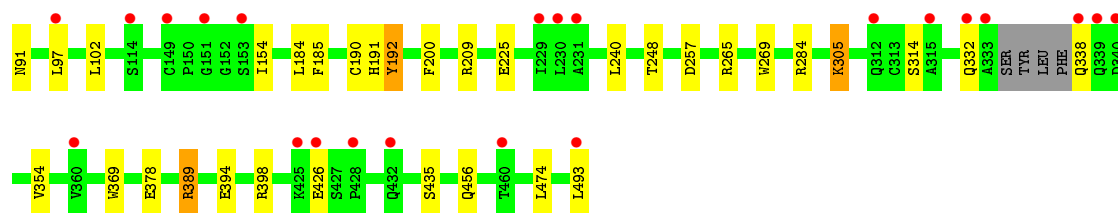


- Molecule 1: Cysteine sulfinic acid decarboxylase

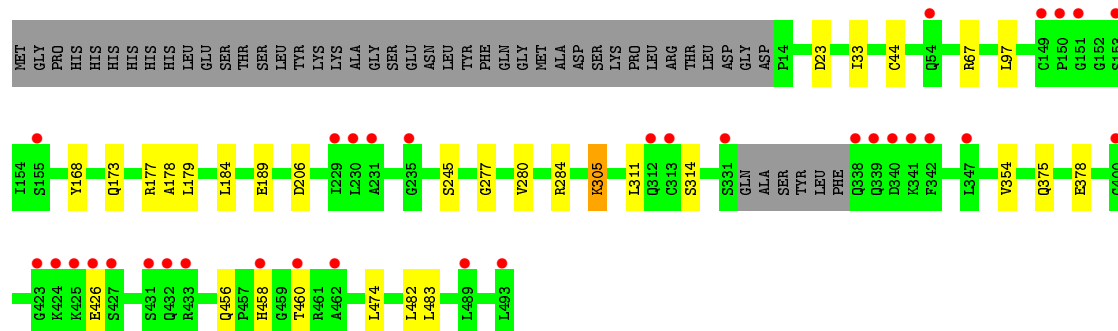
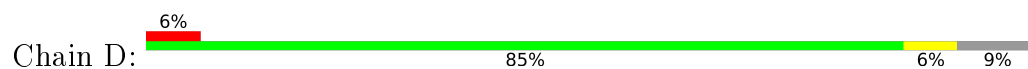


- Molecule 1: Cysteine sulfinic acid decarboxylase





● Molecule 1: Cysteine sulfinic acid decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.94Å 113.26Å 113.37Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	46.89 – 2.10 46.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.7 (46.89-2.10) 90.7 (46.89-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.179 , 0.235 0.180 , 0.235	Depositor DCC
$R_{free}$ test set	2000 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	30749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: GOL, CO, SO4, CL, LLP

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	0.40	0/3821	0.59	0/5162
1	B	0.37	0/3771	0.54	0/5096
1	C	0.39	0/3822	0.57	0/5165
1	D	0.39	0/3796	0.55	0/5129
All	All	0.39	0/15210	0.56	0/20552

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3770	3775	3773	26	0
1	B	3721	3728	3726	21	0
1	C	3771	3774	3772	30	0
1	D	3745	3754	3752	21	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	B	6	8	8	0	0
5	C	12	15	16	0	0
5	D	6	8	8	0	0
6	A	194	0	0	5	0
6	B	123	0	0	1	0
6	C	182	0	0	7	0
6	D	135	0	0	3	0
All	All	15687	15062	15055	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASP:OD2	1:B:67:ARG:NH2	2.07	0.87
1:A:461:ARG:NH1	6:A:601:HOH:O	2.09	0.86
1:C:13:ASP:O	1:C:17:VAL:HG23	1.87	0.74
1:D:23:ASP:OD2	1:D:67:ARG:NH2	2.19	0.74
1:A:23:ASP:OD2	1:A:67:ARG:NH2	2.27	0.68
1:C:97:LEU:HD23	1:C:97:LEU:O	1.94	0.68
1:A:248:THR:HG22	1:A:305:LLP:O3	1.96	0.66
1:D:314:SER:OG	6:D:601:HOH:O	2.00	0.65
1:C:190:CYS:SG	6:C:768:HOH:O	2.55	0.64
1:B:359:ARG:NH1	1:D:311:LEU:O	2.35	0.59
1:A:215:GLU:O	6:A:602:HOH:O	2.17	0.59
1:A:461:ARG:CZ	6:A:601:HOH:O	2.49	0.58
1:A:458:HIS:O	1:A:458:HIS:ND1	2.37	0.57
1:D:305:LLP:O3	1:D:305:LLP:NZ	2.29	0.57
1:C:191:HIS:HD2	1:C:248:THR:HG21	1.71	0.56
1:D:97:LEU:HD23	1:D:97:LEU:O	2.07	0.55
1:B:244:THR:HG21	1:B:247:THR:HG22	1.87	0.55
1:C:225:GLU:OE2	1:C:265:ARG:NH2	2.33	0.54
1:D:189:GLU:OE1	1:D:458:HIS:NE2	2.39	0.54
1:B:109:GLU:OE2	1:B:359:ARG:NH2	2.39	0.54
1:C:248:THR:HG22	1:C:305:LLP:O3	2.07	0.53
1:D:305:LLP:OP1	6:D:602[A]:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:OE1	6:A:603:HOH:O	2.19	0.52
1:B:284:ARG:HD3	1:B:378:GLU:OE2	2.09	0.52
1:B:29:VAL:HA	1:B:33:ILE:HD12	1.92	0.52
1:C:61:GLN:NE2	6:C:613:HOH:O	2.42	0.52
1:D:44:CYS:O	6:D:603:HOH:O	2.18	0.52
1:A:191:HIS:HD2	1:A:248:THR:HG21	1.75	0.52
1:C:209:ARG:NE	6:C:603:HOH:O	2.26	0.51
1:A:356:CYS:SG	1:C:192:TYR:OH	2.67	0.51
1:B:97:LEU:O	1:B:97:LEU:HD23	2.11	0.51
1:C:23:ASP:OD2	1:C:67:ARG:NH2	2.45	0.50
1:A:60:LEU:HD22	1:C:369:TRP:CG	2.45	0.50
1:A:200:PHE:CD1	1:C:354:VAL:HG11	2.47	0.50
1:D:482:LEU:HD12	1:D:483:LEU:N	2.27	0.50
1:B:43:VAL:HG21	1:B:451:MET:HA	1.94	0.49
1:D:284:ARG:HD3	1:D:378:GLU:OE2	2.13	0.48
1:A:31:GLU:HG3	1:A:75:ARG:HG3	1.96	0.48
1:A:473:ILE:C	1:A:473:ILE:HD12	2.34	0.48
1:A:97:LEU:O	1:A:97:LEU:HD23	2.14	0.48
1:A:33:ILE:HD13	1:C:21:LEU:HD13	1.95	0.48
1:C:338:GLN:N	6:C:621:HOH:O	2.47	0.48
1:C:265:ARG:NH1	1:D:173:GLN:OE1	2.42	0.47
1:A:19:ALA:HB1	1:A:67:ARG:HH22	1.79	0.47
1:B:305:LLP:OP4	1:B:305:LLP:H4'1	2.15	0.47
1:A:41:GLU:O	1:A:86:HIS:NE2	2.46	0.46
1:C:240:LEU:HD12	1:C:269:TRP:CD1	2.49	0.46
1:A:273:ASP:OD2	1:A:305:LLP:N1	2.49	0.46
1:C:389:ARG:HD3	6:C:606:HOH:O	2.16	0.46
1:B:146:GLY:O	1:B:147:VAL:HG13	2.16	0.45
1:A:187:SER:HB3	6:A:663:HOH:O	2.16	0.45
1:C:305:LLP:H4'1	1:C:305:LLP:OP4	2.17	0.45
1:D:482:LEU:HD12	1:D:482:LEU:C	2.38	0.44
1:A:429:ASP:OD1	1:A:433:ARG:NH2	2.46	0.44
1:C:394:GLU:O	1:C:398:ARG:HG3	2.18	0.44
1:D:280:VAL:HG12	1:D:280:VAL:O	2.17	0.44
1:B:93:LEU:HD11	1:B:248[B]:THR:HG23	1.99	0.43
1:A:369:TRP:HB3	1:C:60:LEU:HD22	2.00	0.43
1:D:245:SER:O	1:D:277:GLY:HA3	2.18	0.43
1:A:284:ARG:CD	1:A:378:GLU:OE2	2.66	0.43
1:A:354:VAL:HG11	1:C:200:PHE:CD1	2.54	0.43
1:C:154:ILE:HG12	6:C:670:HOH:O	2.19	0.43
1:B:284:ARG:CD	1:B:378:GLU:OE2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LLP:OP4	1:B:305:LLP:C4'	2.66	0.42
1:B:305:LLP:NZ	1:B:305:LLP:O3	2.48	0.42
1:D:168:TYR:CB	1:D:179:LEU:HD21	2.49	0.42
1:C:33:ILE:HD11	1:C:102:LEU:HD21	2.00	0.42
1:B:418:PRO:HD2	1:B:421:LEU:HD12	2.00	0.42
1:C:29:VAL:O	1:C:34:LEU:HG	2.19	0.42
1:C:305:LLP:O3	1:C:305:LLP:NZ	2.40	0.42
1:C:305:LLP:OP4	1:C:305:LLP:C4'	2.68	0.42
1:A:119:GLU:OE2	1:C:91:ASN:ND2	2.48	0.42
1:C:185:PHE:CD1	1:C:209:ARG:HB2	2.54	0.42
1:C:284:ARG:CD	1:C:378:GLU:OE2	2.69	0.41
1:B:121:ALA:O	1:B:125:VAL:HG23	2.21	0.41
1:B:173:GLN:HG3	1:D:206:ASP:OD1	2.20	0.41
1:B:21:LEU:HD13	1:D:33:ILE:HD13	2.02	0.41
6:B:627:HOH:O	1:D:177:ARG:HD2	2.20	0.41
1:D:178:ALA:C	1:D:179:LEU:HD12	2.41	0.41
1:B:146:GLY:O	1:B:147:VAL:CG1	2.69	0.40
1:A:177:ARG:HD2	6:C:688:HOH:O	2.20	0.40
1:B:63:GLN:OE1	1:D:375:GLN:NE2	2.53	0.40
1:C:284:ARG:HD2	1:C:378:GLU:OE2	2.21	0.40
1:A:152:GLY:HA3	1:A:305:LLP:H5'2	2.04	0.40
1:B:200:PHE:CD1	1:D:354:VAL:HG11	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/521 (90%)	451 (96%)	16 (3%)	2 (0%)	34	32
1	B	464/521 (89%)	447 (96%)	16 (3%)	1 (0%)	47	49
1	C	473/521 (91%)	456 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	469/521 (90%)	452 (96%)	17 (4%)	0	100	100
All	All	1875/2084 (90%)	1806 (96%)	66 (4%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	A	112	ASN
1	B	112	ASN

### 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	402/439 (92%)	395 (98%)	7 (2%)	60	67
1	B	397/439 (90%)	388 (98%)	9 (2%)	50	55
1	C	401/439 (91%)	390 (97%)	11 (3%)	44	48
1	D	399/439 (91%)	394 (99%)	5 (1%)	69	75
All	All	1599/1756 (91%)	1567 (98%)	32 (2%)	55	60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	53	LYS
1	A	184	LEU
1	A	276	TRP
1	A	314	SER
1	A	426	GLU
1	A	474	LEU
1	B	116	TYR
1	B	184	LEU
1	B	192	TYR
1	B	257	ASP

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Mol	Chain	Res	Type
1	B	312	GLN
1	B	314	SER
1	B	426	GLU
1	B	456	GLN
1	B	474	LEU
1	C	184	LEU
1	C	192	TYR
1	C	257	ASP
1	C	314	SER
1	C	332	GLN
1	C	389	ARG
1	C	426	GLU
1	C	435	SER
1	C	456	GLN
1	C	474	LEU
1	C	493	LEU
1	D	184	LEU
1	D	426	GLU
1	D	456	GLN
1	D	460	THR
1	D	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	191	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	LLP	D	305	1	23,24,25	2.81	8 (34%)	25,32,34	1.67	5 (20%)
1	LLP	B	305	1	23,24,25	2.66	6 (26%)	25,32,34	1.30	3 (12%)
1	LLP	C	305	1	23,24,25	2.65	7 (30%)	25,32,34	1.36	3 (12%)
1	LLP	A	305	1	23,24,25	2.49	5 (21%)	25,32,34	1.36	4 (16%)

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	LLP	D	305	1	-	6/16/17/19	0/1/1/1
1	LLP	B	305	1	-	3/16/17/19	0/1/1/1
1	LLP	C	305	1	-	3/16/17/19	0/1/1/1
1	LLP	A	305	1	-	4/16/17/19	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	LLP	C4-C4'	8.53	1.62	1.46
1	C	305	LLP	C4-C4'	8.17	1.62	1.46
1	A	305	LLP	C4-C4'	8.05	1.61	1.46
1	D	305	LLP	C4-C4'	7.86	1.61	1.46
1	D	305	LLP	C4'-NZ	5.01	1.44	1.27
1	B	305	LLP	C4'-NZ	4.99	1.44	1.27
1	A	305	LLP	C4'-NZ	4.96	1.43	1.27
1	C	305	LLP	C4'-NZ	4.91	1.43	1.27
1	D	305	LLP	C4-C5	-4.44	1.36	1.42
1	A	305	LLP	C4-C5	-4.37	1.36	1.42
1	D	305	LLP	C3-C2	4.00	1.44	1.40
1	C	305	LLP	C2'-C2	3.88	1.57	1.50
1	D	305	LLP	C2'-C2	3.85	1.56	1.50
1	B	305	LLP	C4-C5	-3.79	1.37	1.42
1	C	305	LLP	C4-C5	-3.71	1.37	1.42
1	D	305	LLP	C6-N1	3.34	1.41	1.34
1	C	305	LLP	C6-N1	3.23	1.41	1.34
1	B	305	LLP	C2'-C2	3.14	1.55	1.50
1	B	305	LLP	C6-N1	3.13	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	305	LLP	C3-C2	2.68	1.43	1.40
1	C	305	LLP	C3-C2	2.58	1.43	1.40
1	A	305	LLP	C6-N1	2.47	1.39	1.34
1	D	305	LLP	CB-CA	-2.36	1.50	1.53
1	C	305	LLP	C5'-C5	2.12	1.56	1.50
1	A	305	LLP	C2'-C2	2.09	1.53	1.50
1	D	305	LLP	C5'-C5	2.04	1.56	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	LLP	C4-C4'-NZ	-4.00	105.96	124.31
1	C	305	LLP	C4-C4'-NZ	-3.73	107.17	124.31
1	D	305	LLP	C4-C4'-NZ	-3.56	107.96	124.31
1	D	305	LLP	O3-C3-C2	3.17	124.40	117.49
1	B	305	LLP	C4-C4'-NZ	-3.16	109.81	124.31
1	D	305	LLP	CE-NZ-C4'	-2.97	109.80	118.90
1	D	305	LLP	C3-C4-C5	2.71	120.34	118.26
1	B	305	LLP	C5-C6-N1	-2.46	119.73	123.82
1	B	305	LLP	OP4-P-OP1	2.23	112.73	106.47
1	A	305	LLP	OP4-P-OP1	2.22	112.69	106.47
1	A	305	LLP	CE-NZ-C4'	-2.20	112.15	118.90
1	A	305	LLP	C5-C6-N1	-2.19	120.17	123.82
1	D	305	LLP	C2'-C2-C3	2.17	123.56	120.89
1	C	305	LLP	CE-NZ-C4'	-2.06	112.57	118.90
1	C	305	LLP	OP3-P-OP4	2.00	112.07	106.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	305	LLP	C4-C5-C5'-OP4
1	A	305	LLP	C6-C5-C5'-OP4
1	B	305	LLP	C4-C5-C5'-OP4
1	B	305	LLP	C6-C5-C5'-OP4
1	C	305	LLP	C4-C5-C5'-OP4
1	C	305	LLP	C6-C5-C5'-OP4
1	D	305	LLP	C4-C5-C5'-OP4
1	D	305	LLP	C6-C5-C5'-OP4
1	D	305	LLP	O-C-CA-CB
1	A	305	LLP	C4-C4'-NZ-CE
1	B	305	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	D	305	LLP	C4-C4'-NZ-CE
1	D	305	LLP	CD-CE-NZ-C4'
1	A	305	LLP	C3-C4-C4'-NZ
1	D	305	LLP	C-CA-CB-CG
1	C	305	LLP	C4-C4'-NZ-CE

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	305	LLP	2	0
1	B	305	LLP	3	0
1	C	305	LLP	4	0
1	A	305	LLP	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 17 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.33	0
5	GOL	B	501	-	5,5,5	1.02	0	5,5,5	0.80	0
5	GOL	C	502	-	5,5,5	0.96	0	5,5,5	0.76	0
5	GOL	C	501	-	5,5,5	0.82	0	5,5,5	0.91	0
5	GOL	D	501	-	5,5,5	1.09	0	5,5,5	0.87	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	B	501	-	-	2/4/4/4	-
5	GOL	C	502	-	-	2/4/4/4	-
5	GOL	C	501	-	-	2/4/4/4	-
5	GOL	D	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GOL	C1-C2-C3-O3
5	C	502	GOL	O1-C1-C2-C3
5	B	501	GOL	O2-C2-C3-O3
5	C	502	GOL	O1-C1-C2-O2
5	C	501	GOL	C1-C2-C3-O3
5	C	501	GOL	O2-C2-C3-O3

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 ⓘ

### 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	475/521 (91%)	0.19	23 (4%)	30	36	21, 31, 49, 69	0
1	B	469/521 (90%)	0.32	26 (5%)	25	31	25, 36, 55, 73	1 (0%)
1	C	477/521 (91%)	0.15	23 (4%)	30	36	22, 31, 50, 75	1 (0%)
1	D	473/521 (90%)	0.33	33 (6%)	16	20	23, 35, 53, 75	0
All	All	1894/2084 (90%)	0.25	105 (5%)	25	31	21, 34, 52, 75	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	339	GLN	6.6
1	B	15	VAL	5.3
1	D	340	ASP	5.2
1	D	342	PHE	4.5
1	D	493	LEU	4.4
1	A	337	PHE	4.2
1	A	336	LEU	4.1
1	D	338	GLN	4.0
1	C	230	LEU	4.0
1	A	461	ARG	3.9
1	D	423	GLY	3.9
1	B	493	LEU	3.9
1	B	428	PRO	3.9
1	B	14	PRO	3.8
1	C	340	ASP	3.8
1	A	15	VAL	3.7
1	D	426	GLU	3.6
1	A	13	ASP	3.6
1	A	14	PRO	3.6
1	B	149	CYS	3.5
1	D	230	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	432	GLN	3.5
1	B	429	ASP	3.4
1	D	400	GLY	3.2
1	B	16	ALA	3.2
1	D	229	ILE	3.2
1	A	339	GLN	3.1
1	B	192	TYR	3.1
1	B	303	PRO	3.0
1	D	460	THR	2.9
1	D	432	GLN	2.9
1	D	331	SER	2.9
1	C	426	GLU	2.9
1	C	339	GLN	2.9
1	D	313	CYS	2.8
1	A	116	TYR	2.8
1	A	192	TYR	2.8
1	D	424	LYS	2.8
1	A	311	LEU	2.7
1	C	338	GLN	2.7
1	D	235	GLY	2.7
1	B	491	GLN	2.6
1	D	433	ARG	2.6
1	A	340	ASP	2.6
1	B	356	CYS	2.6
1	B	417	VAL	2.5
1	D	231	ALA	2.5
1	B	313	CYS	2.5
1	C	333	ALA	2.5
1	C	97	LEU	2.5
1	A	151	GLY	2.5
1	C	332	GLN	2.5
1	C	460	THR	2.5
1	A	493	LEU	2.4
1	A	226	ARG	2.4
1	A	428	PRO	2.4
1	A	432	GLN	2.4
1	B	267	GLY	2.4
1	A	462	ALA	2.4
1	D	431	SER	2.4
1	D	489	LEU	2.4
1	B	332	GLN	2.4
1	C	153	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	302	ASN	2.4
1	D	341	LYS	2.3
1	D	347	LEU	2.3
1	B	362	CYS	2.3
1	B	150	PRO	2.3
1	B	265	ARG	2.3
1	C	54	GLN	2.3
1	D	149	CYS	2.3
1	C	229	ILE	2.3
1	C	151	GLY	2.3
1	D	427	SER	2.3
1	D	54	GLN	2.2
1	D	151	GLY	2.2
1	A	458	HIS	2.2
1	A	55	LEU	2.2
1	D	425	LYS	2.2
1	B	148	PHE	2.2
1	D	312	GLN	2.2
1	A	423	GLY	2.2
1	B	151	GLY	2.2
1	D	153	SER	2.2
1	D	150	PRO	2.2
1	C	312	GLN	2.1
1	B	116	TYR	2.1
1	C	315	ALA	2.1
1	B	400	GLY	2.1
1	C	231	ALA	2.1
1	A	332	GLN	2.1
1	C	425	LYS	2.1
1	D	462	ALA	2.1
1	A	149	CYS	2.1
1	C	114	SER	2.1
1	B	457	PRO	2.1
1	C	360	VAL	2.1
1	C	428	PRO	2.1
1	D	458	HIS	2.1
1	B	13	ASP	2.0
1	B	264	GLN	2.0
1	A	314	SER	2.0
1	D	155	SER	2.0
1	C	493	LEU	2.0
1	C	149	CYS	2.0



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

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
1	LLP	B	305	24/25	0.93	0.18	29,39,47,51	0
1	LLP	C	305	24/25	0.95	0.16	27,35,41,43	0
1	LLP	D	305	24/25	0.95	0.20	29,38,45,48	0
1	LLP	A	305	24/25	0.96	0.18	24,32,40,41	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B	501	6/6	0.75	0.25	42,53,59,64	0
4	CL	B	503	1/1	0.81	0.12	67,67,67,67	0
2	SO4	A	501	5/5	0.91	0.17	50,52,56,68	0
5	GOL	C	502	6/6	0.91	0.13	35,42,49,49	0
5	GOL	D	501	6/6	0.93	0.12	35,42,52,52	0
5	GOL	C	501	6/6	0.94	0.14	32,44,53,54	0
3	CO	B	502	1/1	0.97	0.07	39,39,39,39	1
4	CL	D	504	1/1	0.98	0.14	39,39,39,39	0
3	CO	C	503	1/1	0.98	0.10	30,30,30,30	1
3	CO	A	502	1/1	0.98	0.04	48,48,48,48	0
4	CL	C	504	1/1	0.98	0.22	20,20,20,20	0
4	CL	C	505	1/1	0.98	0.12	40,40,40,40	0
4	CL	A	505	1/1	0.99	0.25	22,22,22,22	0
4	CL	C	506	1/1	0.99	0.27	23,23,23,23	0
4	CL	D	503	1/1	0.99	0.29	24,24,24,24	0
3	CO	D	502	1/1	0.99	0.06	41,41,41,41	1
4	CL	D	505	1/1	0.99	0.27	26,26,26,26	0
4	CL	B	504	1/1	0.99	0.32	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	505	1/1	0.99	0.14	42,42,42,42	0
4	CL	B	506	1/1	0.99	0.22	27,27,27,27	0
4	CL	A	504	1/1	0.99	0.16	33,33,33,33	0
4	CL	A	503	1/1	1.00	0.27	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.