



# Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2017 – 02:27 PM EDT

PDB ID : 4D8W  
Title : Salmonella typhimurium D-Cysteine desulfhydrase soaked with D-cys shows pyruvate bound 4 Å away from active site  
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.  
Deposited on : 2012-01-11  
Resolution : 2.01 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

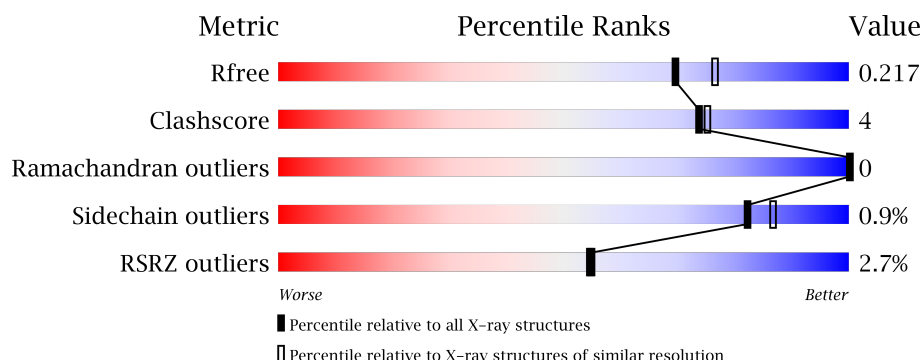
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	
1	B	342	
1	C	342	
1	D	342	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	401	-	-	-	X
3	BEN	A	402	-	-	-	X
4	PYR	A	403	-	-	-	X
4	PYR	C	403	-	-	-	X
4	PYR	D	402	-	-	-	X
5	SO4	A	404	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10615 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 D-Cysteine desulfhydrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	P	S	0	2	0
			2462	1570	414	468	1	9			
1	B	326	Total	C	N	O	P	S	1	4	0
			2450	1562	411	467	1	9			
1	C	322	Total	C	N	O	P	S	0	3	0
			2407	1533	402	462	1	9			
1	D	328	Total	C	N	O	P	S	0	4	0
			2474	1578	415	470	1	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
A	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
A	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
B	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7

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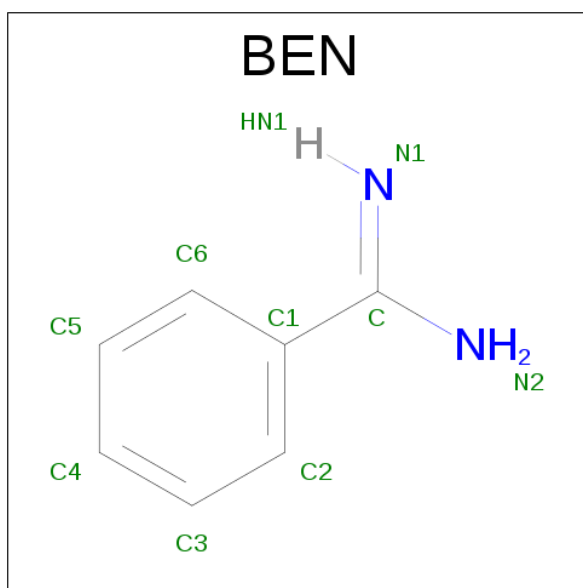
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
B	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
C	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
C	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
C	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
C	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
C	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
C	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
C	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
C	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
D	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
D	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

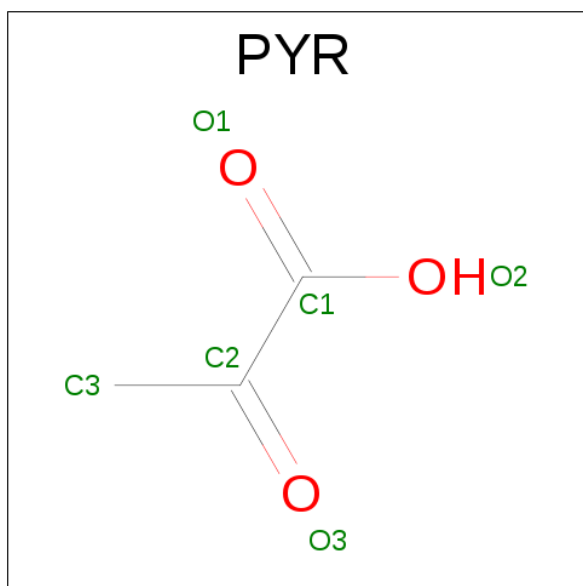
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula:  $C_7H_8N_2$ ).



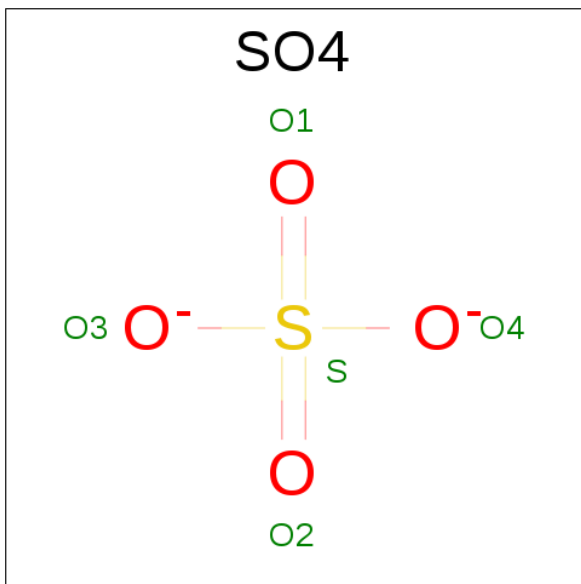
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	D	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



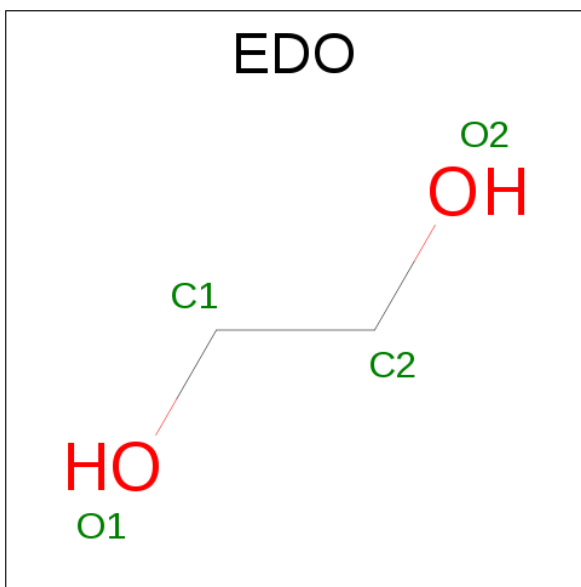
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

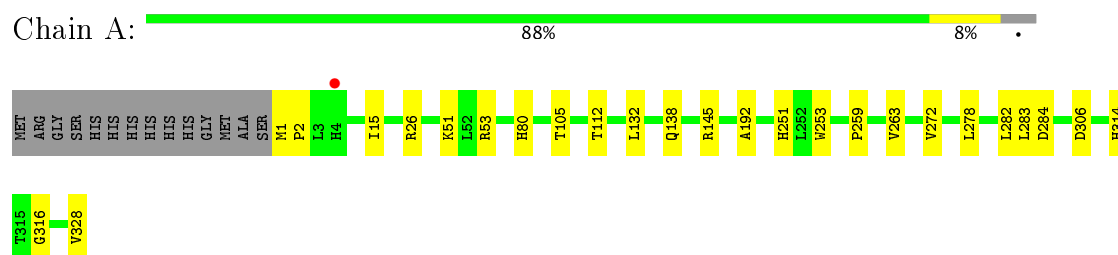
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	216	Total	O	0	0
			216	216		
7	B	175	Total	O	0	0
			175	175		
7	C	141	Total	O	0	0
			141	141		
7	D	216	Total	O	0	0
			216	216		



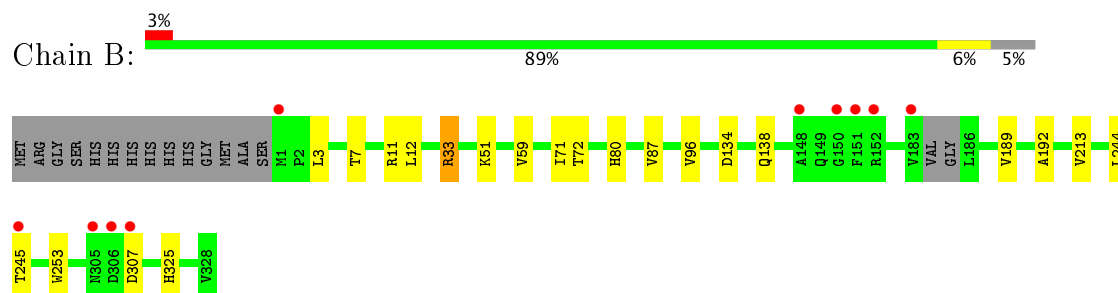
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

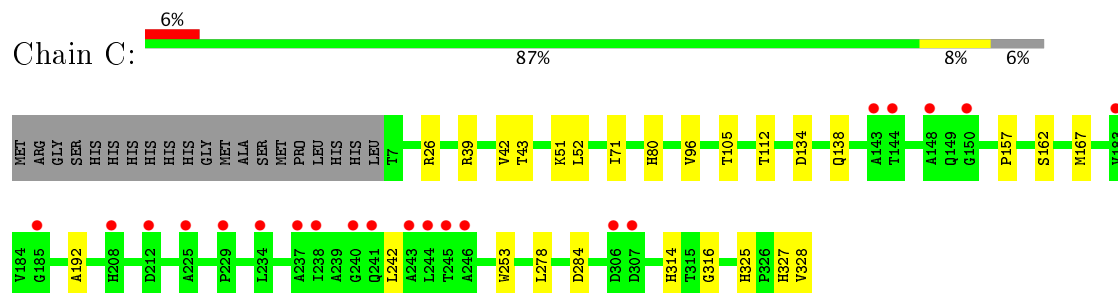
- Molecule 1: D-Cysteine desulphydrase



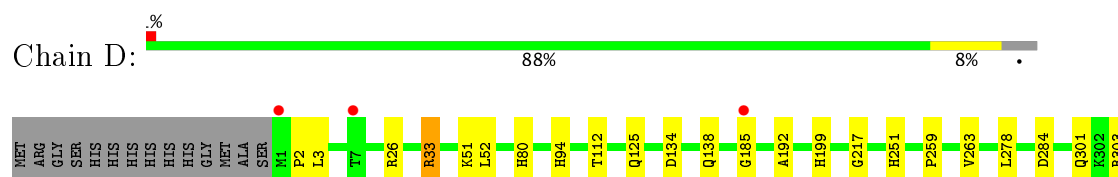
- Molecule 1: D-Cysteine desulphydrase



- Molecule 1: D-Cysteine desulphydrase



- Molecule 1: D-Cysteine desulphydrase



D307	H308	P309	H314	H315	H316	H325	V328
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.29Å 165.19Å 68.06Å 90.00° 118.71° 90.00°	Depositor
Resolution (Å)	48.38 – 2.01 48.38 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-2.01) 99.4 (48.38-2.01)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.183 , 0.217 0.183 , 0.217	Depositor DCC
$R_{free}$ test set	4263 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h-l,k,h 0.003 for l,k,-h-l 0.024 for h,-k,-h-l 0.032 for -h-l,-k,l 0.023 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: BEN, CL, PYR, LLP, EDO, SO4

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	1/2487 (0.0%)	0.53	0/3390
1	B	0.39	1/2483 (0.0%)	0.51	0/3385
1	C	0.38	1/2432 (0.0%)	0.51	0/3315
1	D	0.39	0/2505	0.53	0/3414
All	All	0.39	3/9907 (0.0%)	0.52	0/13504

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	TRP	CD2-CE2	5.19	1.47	1.41
1	B	253	TRP	CD2-CE2	5.16	1.47	1.41
1	C	253	TRP	CD2-CE2	5.13	1.47	1.41

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	2462	0	2460	16	0
1	B	2450	0	2448	19	0
1	C	2407	0	2393	24	0
1	D	2474	0	2477	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	1	0
3	A	9	0	7	1	0
3	B	9	0	7	0	0
3	D	9	0	7	0	0
4	A	6	0	3	0	0
4	C	6	0	3	0	0
4	D	6	0	3	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
7	A	216	0	0	2	0
7	B	175	0	0	0	0
7	C	141	0	0	1	0
7	D	216	0	0	3	0
All	All	10615	0	9820	74	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 4.

All (74) 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:11[B]:ARG:HG2	1:B:11[B]:ARG:HH11	0.98	1.11
1:B:11[B]:ARG:HG2	1:B:11[B]:ARG:NH1	1.74	0.94
1:B:11[B]:ARG:CG	1:B:11[B]:ARG:HH11	1.88	0.76
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	1.85	0.76
1:C:43:THR:CG2	1:C:52:LEU:HD22	2.16	0.74
1:C:43:THR:HG21	1:C:52:LEU:HD22	1.79	0.64
1:B:33:ARG:HH11	1:B:33:ARG:CG	2.10	0.64
1:A:251:HIS:HE1	7:A:631:HOH:O	1.83	0.61
1:C:325:HIS:HD2	7:C:614:HOH:O	1.82	0.61
1:D:314:HIS:HD2	1:D:316:GLY:H	1.48	0.61
1:B:11[B]:ARG:CG	1:B:11[B]:ARG:NH1	2.54	0.60
1:A:314:HIS:HD2	1:A:316:GLY:H	1.49	0.60
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.68	0.58
1:C:157:PRO:HG3	1:C:162:SER:HB3	1.85	0.58
1:B:33:ARG:HG3	1:B:33:ARG:NH1	2.19	0.57
1:A:105:THR:OG1	1:A:328[A]:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:625:HOH:O	1:C:327:HIS:HD2	1.90	0.55
1:D:52:LEU:HD22	7:D:715:HOH:O	2.05	0.54
1:C:314:HIS:HD2	1:C:316:GLY:H	1.55	0.54
1:B:134:ASP:H	1:B:138:GLN:HE21	1.55	0.53
1:C:43:THR:CG2	1:C:52:LEU:CD2	2.87	0.52
1:B:134:ASP:H	1:B:138:GLN:NE2	2.08	0.52
1:C:71:ILE:HG12	1:C:96:VAL:HB	1.93	0.51
1:B:3:LEU:HD23	1:B:244:LEU:HD11	1.92	0.51
1:B:33:ARG:NH1	1:B:33:ARG:CG	2.73	0.51
1:D:251:HIS:HE1	7:D:691:HOH:O	1.95	0.50
1:D:51:LLP:HE3	1:D:80:HIS:HB2	1.93	0.50
1:A:51:LLP:HE3	1:A:80:HIS:HB2	1.94	0.49
1:B:7:THR:HA	1:B:11[B]:ARG:HH22	1.78	0.49
1:C:167:MET:HE1	1:C:242:LEU:HD21	1.93	0.49
1:D:26:ARG:HD3	1:D:278:LEU:O	2.13	0.49
2:A:401:CL:CL	3:A:402:BEN:N2	2.84	0.48
1:B:51:LLP:HE3	1:B:80:HIS:HB2	1.96	0.48
1:C:43:THR:HG23	1:C:52:LEU:CD2	2.43	0.48
1:C:112:THR:OG1	1:D:325:HIS:HE1	1.97	0.48
1:A:306:ASP:OD2	1:A:306:ASP:C	2.53	0.47
1:A:314:HIS:CD2	1:A:316:GLY:H	2.31	0.47
1:D:259:PRO:HG2	1:D:263:VAL:HG11	1.97	0.47
1:A:132:LEU:HA	1:A:138:GLN:HE22	1.80	0.46
1:C:134:ASP:H	1:C:138:GLN:HE21	1.62	0.46
1:C:43:THR:HG23	1:C:52:LEU:HD22	1.92	0.46
1:B:189:VAL:HG23	1:B:213:VAL:HG11	1.98	0.46
1:D:51:LLP:H6	1:D:192:ALA:HB3	1.98	0.46
1:C:51:LLP:H6	1:C:192:ALA:HB3	1.96	0.46
1:B:72:THR:OG1	1:B:80:HIS:HE1	1.99	0.46
1:C:167:MET:HE1	1:C:242:LEU:HD11	1.99	0.45
1:D:94:HIS:HD2	7:D:501:HOH:O	2.00	0.45
1:C:314:HIS:CD2	1:C:316:GLY:H	2.35	0.44
1:A:1:MET:N	1:A:2:PRO:HD2	2.33	0.44
1:A:259:PRO:HG2	1:A:263:VAL:HG11	2.00	0.43
1:C:134:ASP:H	1:C:138:GLN:NE2	2.16	0.43
1:A:282:LEU:O	1:A:314:HIS:HE1	2.02	0.43
1:A:15:ILE:CD1	1:A:53:ARG:HG2	2.49	0.43
1:C:105:THR:CB	1:C:328[A]:VAL:HG12	2.48	0.43
1:D:94:HIS:HE1	1:D:125:GLN:NE2	2.16	0.43
1:D:33:ARG:NH1	1:D:307[A]:ASP:OD1	2.52	0.43
1:A:272:VAL:HG22	1:A:283:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LLP:H6	1:A:192:ALA:HB3	2.01	0.43
1:B:59:VAL:HG21	1:B:87:VAL:HG11	2.01	0.43
1:B:71:ILE:HG12	1:B:96:VAL:HB	2.00	0.43
1:D:185:GLY:O	1:D:309:PRO:HD2	2.19	0.42
1:C:325:HIS:HE1	1:D:112:THR:OG1	2.03	0.42
1:C:51:LLP:HE3	1:C:80:HIS:HB2	2.02	0.42
1:C:39:ARG:O	1:C:42:VAL:HG22	2.19	0.42
1:A:26:ARG:HD3	1:A:278:LEU:O	2.20	0.42
1:C:43:THR:HG21	1:C:52:LEU:CD2	2.49	0.41
1:D:134:ASP:H	1:D:138:GLN:NE2	2.18	0.41
1:A:15:ILE:HD11	1:A:53:ARG:HG2	2.02	0.41
1:A:112:THR:OG1	1:B:325:HIS:HE1	2.04	0.41
1:B:51:LLP:H6	1:B:192:ALA:HB3	2.03	0.41
1:D:301:GLN:HB2	1:D:303:ARG:HG3	2.03	0.41
1:C:26:ARG:HD3	1:C:278:LEU:O	2.20	0.41
1:D:199:HIS:CE1	1:D:217:GLY:HA3	2.56	0.41
1:D:2:PRO:HB2	1:D:3:LEU:HD22	2.03	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
1	B	325/342 (95%)	319 (98%)	6 (2%)	0	100	100
1	C	321/342 (94%)	312 (97%)	9 (3%)	0	100	100
1	D	328/342 (96%)	321 (98%)	7 (2%)	0	100	100
All	All	1300/1368 (95%)	1270 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	251/266 (94%)	249 (99%)	2 (1%)	85	88
1	B	251/266 (94%)	247 (98%)	4 (2%)	68	72
1	C	245/266 (92%)	244 (100%)	1 (0%)	93	95
1	D	254/266 (96%)	252 (99%)	2 (1%)	85	88
All	All	1001/1064 (94%)	992 (99%)	9 (1%)	82	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ARG
1	A	284	ASP
1	B	12	LEU
1	B	33	ARG
1	B	245	THR
1	B	307	ASP
1	C	284	ASP
1	D	33	ARG
1	D	284	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	94	HIS
1	A	125	GLN
1	A	138	GLN
1	A	149	GLN
1	A	208	HIS
1	A	251	HIS
1	A	314	HIS
1	A	325	HIS
1	B	80	HIS

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Mol	Chain	Res	Type
1	B	125	GLN
1	B	138	GLN
1	B	251	HIS
1	B	325	HIS
1	C	138	GLN
1	C	149	GLN
1	C	208	HIS
1	C	314	HIS
1	C	325	HIS
1	D	94	HIS
1	D	125	GLN
1	D	138	GLN
1	D	251	HIS
1	D	314	HIS
1	D	325	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	A	51	1	24,24,25	0.73	0	28,32,34	1.15	1 (3%)
1	LLP	B	51	1	24,24,25	0.81	1 (4%)	28,32,34	1.17	0
1	LLP	C	51	1	24,24,25	0.83	1 (4%)	28,32,34	1.10	1 (3%)
1	LLP	D	51	1	24,24,25	0.83	1 (4%)	28,32,34	1.06	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	LLP	A	51	1	-	0/15/17/19	0/1/1/1
1	LLP	B	51	1	-	0/15/17/19	0/1/1/1
1	LLP	C	51	1	-	0/15/17/19	0/1/1/1
1	LLP	D	51	1	-	0/15/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	LLP	C3-C2	-2.36	1.39	1.40
1	C	51	LLP	C3-C2	-2.29	1.39	1.40
1	D	51	LLP	C3-C2	-2.29	1.39	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LLP	C5-C6-N1	-2.35	119.89	123.87
1	C	51	LLP	C5-C6-N1	-2.03	120.44	123.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	51	LLP	2	0
1	B	51	LLP	2	0
1	C	51	LLP	2	0
1	D	51	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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$
3	BEN	A	402	-	9,9,9	1.05	1 (11%)	9,11,11	0.61	0
4	PYR	A	403	-	2,5,5	0.20	0	2,6,6	0.49	0
5	SO4	A	404	-	4,4,4	0.39	0	6,6,6	0.31	0
3	BEN	B	401	-	9,9,9	0.87	0	9,11,11	0.55	0
6	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.33	0
5	SO4	B	403	-	4,4,4	0.34	0	6,6,6	0.18	0
6	EDO	C	401	-	3,3,3	0.45	0	2,2,2	0.44	0
5	SO4	C	402	-	4,4,4	0.39	0	6,6,6	0.19	0
4	PYR	C	403	-	2,5,5	0.19	0	2,6,6	0.34	0
3	BEN	D	401	-	9,9,9	1.44	2 (22%)	9,11,11	0.65	0
4	PYR	D	402	-	2,5,5	0.22	0	2,6,6	0.68	0
5	SO4	D	403	-	4,4,4	0.38	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	A	402	-	-	0/4/4/4	0/1/1/1
4	PYR	A	403	-	-	0/0/4/4	0/0/0/0
5	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	BEN	B	401	-	-	0/4/4/4	0/1/1/1
6	EDO	B	402	-	-	0/1/1/1	0/0/0/0
5	SO4	B	403	-	-	0/0/0/0	0/0/0/0
6	EDO	C	401	-	-	0/1/1/1	0/0/0/0
5	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	PYR	C	403	-	-	0/0/4/4	0/0/0/0
3	BEN	D	401	-	-	0/4/4/4	0/1/1/1
4	PYR	D	402	-	-	0/0/4/4	0/0/0/0
5	SO4	D	403	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	BEN	C-N2	-3.04	1.26	1.33
3	D	401	BEN	C1-C	2.08	1.50	1.47
3	A	402	BEN	C1-C	2.37	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	BEN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	327/342 (95%)	-0.33	1 (0%) 93 93	11, 16, 30, 39	0
1	B	325/342 (95%)	-0.09	10 (3%) 49 49	12, 21, 41, 53	1 (0%)
1	C	321/342 (93%)	0.31	21 (6%) 20 20	14, 26, 45, 61	0
1	D	327/342 (95%)	-0.31	3 (0%) 84 83	12, 17, 32, 49	0
All	All	1300/1368 (95%)	-0.11	35 (2%) 55 54	11, 19, 40, 61	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	GLY	5.3
1	B	148	ALA	4.2
1	C	148	ALA	3.9
1	D	1	MET	3.6
1	C	241	GLN	3.4
1	C	237	ALA	3.4
1	B	245	THR	3.2
1	C	144	THR	3.1
1	C	183	VAL	3.1
1	A	4	HIS	2.9
1	B	305	ASN	2.9
1	C	240	GLY	2.9
1	C	229	PRO	2.8
1	C	244	LEU	2.7
1	C	246	ALA	2.7
1	B	1	MET	2.6
1	D	185	GLY	2.6
1	C	212	ASP	2.5
1	B	306	ASP	2.5
1	C	243	ALA	2.5
1	C	143	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	7	THR	2.5
1	B	151	PHE	2.4
1	C	208	HIS	2.4
1	C	225	ALA	2.3
1	C	306	ASP	2.3
1	C	307	ASP	2.3
1	B	307	ASP	2.2
1	B	150	GLY	2.2
1	C	245	THR	2.2
1	C	185	GLY	2.1
1	C	234	LEU	2.1
1	B	152	ARG	2.1
1	B	183	VAL	2.0
1	C	238	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	C	51	24/25	0.94	0.11	-	19,21,23,24	0
1	LLP	D	51	24/25	0.97	0.10	-	12,13,14,15	0
1	LLP	A	51	24/25	0.97	0.10	-	11,12,13,14	0
1	LLP	B	51	24/25	0.95	0.10	-	16,17,19,20	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	401	1/1	0.99	0.22	22.16	35,35,35,35	0
4	PYR	A	403	6/6	0.66	0.26	8.67	29,30,30,32	6
4	PYR	D	402	6/6	0.92	0.16	3.23	28,29,29,29	6
3	BEN	A	402	9/9	0.93	0.12	2.63	14,14,15,15	0
4	PYR	C	403	6/6	0.59	0.24	2.40	36,37,37,38	6
5	SO4	A	404	5/5	0.97	0.13	2.07	16,16,16,16	5
5	SO4	D	403	5/5	0.98	0.12	1.59	15,15,15,16	5
5	SO4	B	403	5/5	0.98	0.11	1.01	22,22,22,22	5
5	SO4	C	402	5/5	0.96	0.12	0.85	23,24,24,25	5
3	BEN	D	401	9/9	0.96	0.10	0.75	13,13,14,14	0
3	BEN	B	401	9/9	0.92	0.15	0.32	29,30,30,31	0
6	EDO	C	401	4/4	0.94	0.14	0.01	29,30,31,32	0
6	EDO	B	402	4/4	0.75	0.35	-	34,34,34,35	0

## 6.5 Other polymers

There are no such residues in this entry.