



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:44 PM GMT

PDB ID : 4D99  
Title : Salmonella typhimurium D-Cysteine desulphydrase with L-ser bound non-covalently at the 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

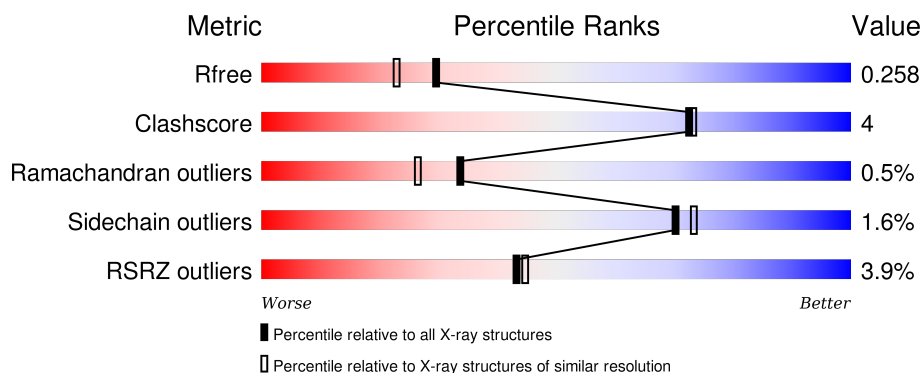
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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	<div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	342	<div> <div>8%</div> <div>88%</div> <div>6%</div> <div>5%</div> </div>
1	C	342	<div> <div>5%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	D	342	<div> <div>%</div> <div>85%</div> <div>9%</div> <div>..</div> </div>

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
3	SER	A	402	-	-	-	X
3	SER	B	402	-	-	-	X
3	SER	C	402	-	-	-	X
3	SER	D	402	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10364 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	1	0
			2463	1568	414	471	1	9			
1	B	324	Total	C	N	O	P	S	0	1	0
			2393	1523	402	458	1	9			
1	C	323	Total	C	N	O	P	S	0	3	0
			2412	1534	406	462	1	9			
1	D	328	Total	C	N	O	P	S	0	0	0
			2446	1561	411	464	1	9			

There are 56 discrepancies between the modelled and reference sequences:

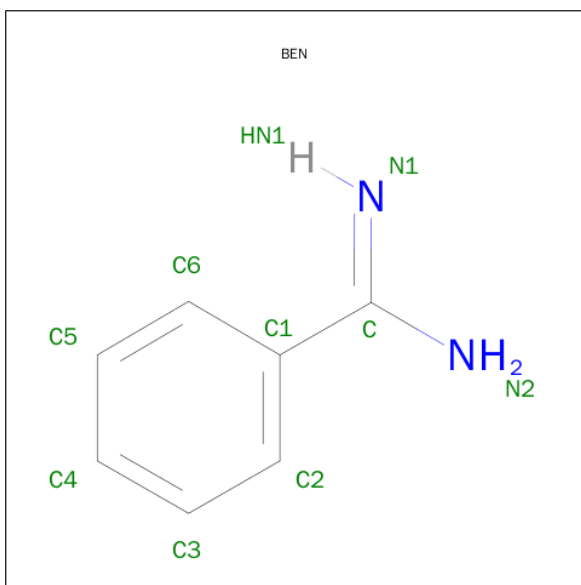
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
A	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-7	HIS	-	EXPRESSION TAG	UNP 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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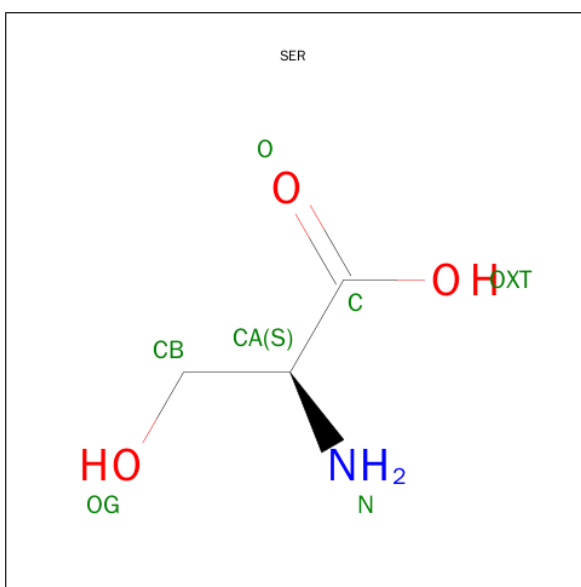
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
B	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
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 BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



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

- Molecule 3 is SERINE (three-letter code: SER) (formula:  $C_3H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	3	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	3	1	3		
3	C	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

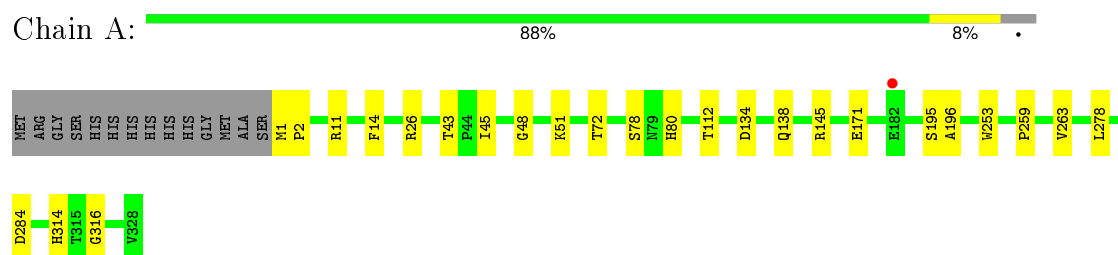
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		
5	B	120	Total	O	0	0
			120	120		
5	C	104	Total	O	0	0
			104	104		
5	D	183	Total	O	0	0
			183	183		

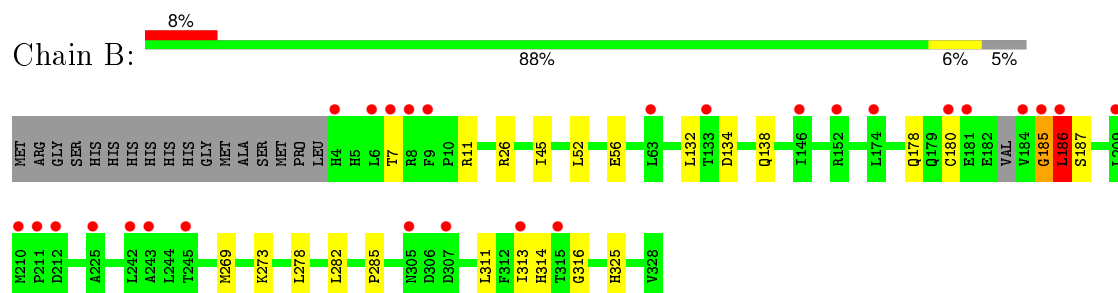
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

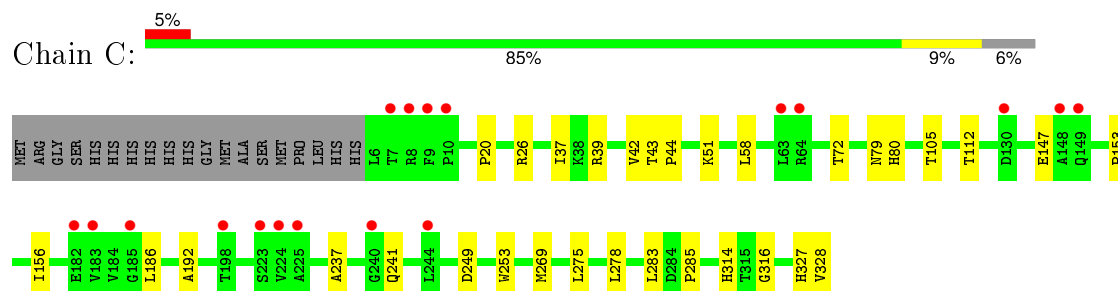
- Molecule 1: D-cysteine desulfhydrase



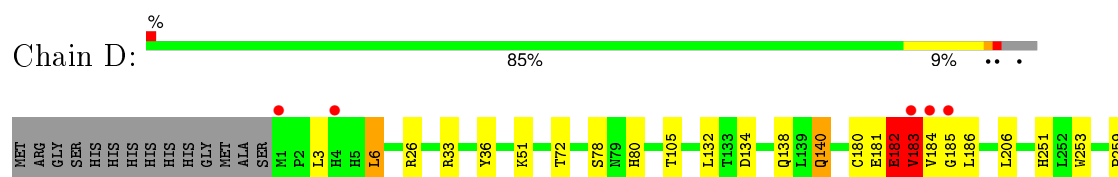
- Molecule 1: D-cysteine desulfhydrase



- Molecule 1: D-cysteine desulfhydrase



- Molecule 1: D-cysteine desulfhydrase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.56Å 165.49Å 68.88Å 90.00° 119.34° 90.00°	Depositor
Resolution (Å)	32.63 – 2.01 32.63 – 2.01	Depositor EDS
% Data completeness (in resolution range)	90.5 (32.63-2.01) 90.6 (32.63-2.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.13 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.212 , 0.259 0.211 , 0.258	Depositor DCC
$R_{free}$ test set	4301 reflections (5.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.8	EDS
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.020 for h,-k,-h-l 0.022 for l,-k,h 0.026 for -h-l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78287 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, BEN, IT1

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	0.42	1/2489 (0.0%)	0.57	0/3394
1	B	0.40	0/2415	0.54	0/3295
1	C	0.39	1/2436 (0.0%)	0.53	0/3321
1	D	0.42	1/2469 (0.0%)	0.57	0/3367
All	All	0.41	3/9809 (0.0%)	0.55	0/13377

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	TRP	CD2-CE2	5.37	1.47	1.41
1	D	253	TRP	CD2-CE2	5.07	1.47	1.41
1	A	253	TRP	CD2-CE2	5.00	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	2463	0	2458	20	0
1	B	2393	0	2358	14	0
1	C	2412	0	2393	22	0
1	D	2446	0	2440	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	7	0	0
2	B	9	0	7	0	0
2	D	9	0	7	0	0
3	A	7	0	4	2	0
3	B	7	0	4	0	0
3	C	7	0	4	1	0
3	D	7	0	4	3	0
4	C	1	0	0	0	0
5	A	187	0	0	1	0
5	B	120	0	0	0	0
5	C	104	0	0	0	0
5	D	183	0	0	4	0
All	All	10364	0	9686	82	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 (82) 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:D:184:VAL:CG1	1:D:185:GLY:HA2	1.68	1.23
1:D:184:VAL:HG13	1:D:185:GLY:HA2	1.03	1.00
1:D:184:VAL:HG13	1:D:185:GLY:CA	1.95	0.94
1:B:185:GLY:O	1:B:186:LEU:HB2	1.68	0.93
1:D:105:THR:OG1	1:D:328:VAL:HG12	1.71	0.91
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	1.75	0.86
1:D:251:HIS:HD2	5:D:665:HOH:O	1.60	0.84
1:D:181:GLU:O	1:D:182:GLU:HB2	1.80	0.80
1:D:182:GLU:O	1:D:183:VAL:HB	1.84	0.77
1:D:287:TYR:HH	3:D:402:SER:N	1.87	0.72
1:A:145:ARG:HH12	1:C:328[A]:VAL:HG11	1.54	0.71
1:D:269:MET:HG2	5:D:679:HOH:O	1.90	0.71
1:D:314:HIS:HD2	1:D:316:GLY:H	1.41	0.68
1:D:184:VAL:HG12	1:D:185:GLY:HA2	1.75	0.66
1:A:43:THR:OG1	1:A:48:GLY:HA2	1.98	0.64
1:D:184:VAL:CG1	1:D:185:GLY:CA	2.61	0.64
1:C:26:ARG:HD3	1:C:278:LEU:O	1.97	0.63
3:D:402:SER:HB3	5:D:683:HOH:O	1.98	0.62
1:C:79:ASN:N	3:C:402:SER:OXT	2.34	0.61
1:D:183:VAL:O	1:D:183:VAL:HG13	2.03	0.59
1:A:1:MET:N	1:A:2:PRO:HD2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HG23	1:C:39[A]:ARG:HD3	1.85	0.59
1:A:145:ARG:NH1	1:C:328[A]:VAL:HG11	2.18	0.59
1:D:78:SER:OG	3:D:402:SER:HB2	2.02	0.58
1:D:185:GLY:O	1:D:309:PRO:HD2	2.04	0.57
1:A:314:HIS:HD2	1:A:316:GLY:H	1.52	0.57
1:C:147:GLU:HG3	1:C:153:PRO:HD2	1.89	0.55
1:B:26:ARG:HD3	1:B:278:LEU:O	2.07	0.54
1:C:314:HIS:HD2	1:C:316:GLY:H	1.53	0.54
1:D:72:THR:OG1	1:D:80:HIS:HE1	1.91	0.53
1:D:140:GLN:HA	1:D:140:GLN:HE21	1.73	0.53
1:A:259:PRO:HG2	1:A:263:VAL:HG11	1.91	0.52
1:B:314:HIS:HD2	1:B:316:GLY:H	1.58	0.52
1:D:180:CYS:HA	1:D:183:VAL:HG12	1.93	0.51
1:A:78:SER:OG	3:A:402:SER:HA	2.11	0.50
1:A:145:ARG:HH22	1:C:328[A]:VAL:HG21	1.75	0.50
1:C:72:THR:OG1	1:C:80:HIS:HE1	1.95	0.49
1:A:1:MET:H2	1:A:2:PRO:HD2	1.78	0.49
1:C:42:VAL:O	1:C:42:VAL:HG12	2.11	0.49
1:D:26:ARG:HD3	1:D:278:LEU:O	2.12	0.49
1:A:78:SER:CB	3:A:402:SER:HA	2.42	0.48
1:A:26:ARG:HD3	1:A:278:LEU:O	2.13	0.48
1:B:45:ILE:HD12	1:B:52:LEU:HD11	1.95	0.48
1:B:180:CYS:HB3	1:B:186:LEU:HD21	1.96	0.48
5:A:629:HOH:O	1:C:327:HIS:HD2	1.95	0.47
1:A:134:ASP:H	1:A:138:GLN:NE2	2.12	0.47
1:C:269:MET:SD	1:C:285:PRO:HB3	2.54	0.47
1:D:251:HIS:HE1	5:D:666:HOH:O	1.96	0.47
1:A:72:THR:OG1	1:A:80:HIS:HE1	1.97	0.47
1:A:314:HIS:CD2	1:A:316:GLY:H	2.31	0.46
1:D:132:LEU:HA	1:D:138:GLN:HE22	1.80	0.46
1:A:1:MET:N	1:A:2:PRO:CD	2.79	0.45
1:A:112:THR:OG1	1:B:325:HIS:HE1	1.98	0.45
1:C:43:THR:HB	1:C:44:PRO:HD2	1.99	0.45
1:C:237:ALA:O	1:C:241:GLN:HG2	2.17	0.45
1:D:36:TYR:CE2	1:D:183:VAL:HG22	2.52	0.45
1:C:20:PRO:HD2	1:C:39[A]:ARG:HB2	1.99	0.45
1:C:51:IT1:H6	1:C:192:ALA:HB3	1.99	0.45
1:D:51:IT1:HEA	1:D:80:HIS:HB2	1.99	0.44
1:B:282:LEU:O	1:B:314:HIS:HE1	2.01	0.44
1:C:112:THR:OG1	1:D:325:HIS:HE1	2.01	0.44
1:A:195:SER:O	1:A:196:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASP:C	1:B:138:GLN:HE21	2.21	0.44
1:D:259:PRO:HG2	1:D:263:VAL:HG11	2.00	0.43
1:D:3:LEU:O	1:D:6:LEU:HB2	2.20	0.42
1:C:58:LEU:HD13	1:C:156:ILE:HG23	2.01	0.42
1:C:275:LEU:HG	1:C:283:LEU:HD11	2.02	0.42
1:C:37:ILE:HD11	1:C:314:HIS:HB2	2.00	0.42
1:C:314:HIS:CD2	1:C:316:GLY:H	2.35	0.42
1:B:11:ARG:NH2	1:B:56:GLU:OE1	2.53	0.42
1:B:282:LEU:O	1:B:314:HIS:CE1	2.72	0.41
1:B:311:LEU:CD1	1:B:313:ILE:HD13	2.50	0.41
1:B:269:MET:SD	1:B:285:PRO:HB3	2.60	0.41
1:A:51:IT1:HEA	1:A:80:HIS:HB2	2.02	0.41
1:D:283:LEU:HD23	1:D:314:HIS:CE1	2.54	0.41
1:A:11:ARG:HH12	1:A:171:GLU:HG2	1.86	0.41
1:D:184:VAL:HG22	1:D:186:LEU:HB2	2.03	0.41
1:B:132:LEU:HA	1:B:138:GLN:HE22	1.86	0.40
1:D:314:HIS:CD2	1:D:316:GLY:H	2.29	0.40
1:B:273:LYS:HD2	1:B:273:LYS:HA	1.96	0.40
1:D:134:ASP:H	1:D:138:GLN:NE2	2.19	0.40
1:A:14:PHE:HB3	1:A:45:ILE:HD12	2.04	0.40

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	320/342 (94%)	308 (96%)	8 (2%)	4 (1%)	15	7
1	C	322/342 (94%)	312 (97%)	10 (3%)	0	100	100
1	D	325/342 (95%)	315 (97%)	8 (2%)	2 (1%)	30	22
All	All	1293/1368 (94%)	1253 (97%)	34 (3%)	6 (0%)	34	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	SER
1	D	182	GLU
1	D	183	VAL
1	B	186	LEU
1	B	7	THR
1	B	185	GLY

### 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	253/266 (95%)	252 (100%)	1 (0%)	93	95
1	B	240/266 (90%)	238 (99%)	2 (1%)	86	89
1	C	244/266 (92%)	242 (99%)	2 (1%)	86	89
1	D	248/266 (93%)	240 (97%)	8 (3%)	46	44
All	All	985/1064 (93%)	972 (99%)	13 (1%)	70	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	ASP
1	B	178	GLN
1	B	186	LEU
1	C	186	LEU
1	C	249	ASP
1	D	6	LEU
1	D	33	ARG
1	D	140	GLN
1	D	182	GLU
1	D	183	VAL
1	D	206	LEU
1	D	269	MET
1	D	284	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	GLN
1	A	125	GLN
1	A	138	GLN
1	A	314	HIS
1	B	138	GLN
1	B	178	GLN
1	B	208	HIS
1	B	314	HIS
1	B	325	HIS
1	C	80	HIS
1	C	83	GLN
1	C	138	GLN
1	C	314	HIS
1	D	80	HIS
1	D	83	GLN
1	D	125	GLN
1	D	138	GLN
1	D	140	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	IT1	A	51	1	23,24,25	0.82	1 (4%)	28,32,34	1.17	2 (7%)
1	IT1	B	51	1	23,24,25	0.88	1 (4%)	28,32,34	1.25	1 (3%)
1	IT1	C	51	1	23,24,25	0.83	1 (4%)	28,32,34	1.22	3 (10%)
1	IT1	D	51	1	23,24,25	0.86	1 (4%)	28,32,34	1.12	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	IT1	A	51	1	-	0/15/17/19	0/1/1/1
1	IT1	B	51	1	-	0/15/17/19	0/1/1/1
1	IT1	C	51	1	-	0/15/17/19	0/1/1/1
1	IT1	D	51	1	-	0/15/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	IT1	C3-C2	-2.80	1.38	1.40
1	B	51	IT1	C3-C2	-2.73	1.38	1.40
1	C	51	IT1	C3-C2	-2.10	1.39	1.40
1	A	51	IT1	C3-C2	-2.01	1.39	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	IT1	OP4-P-OP1	-2.27	101.37	107.14
1	A	51	IT1	C5-C6-N1	-2.04	120.32	123.86
1	C	51	IT1	CE-NZ-C4A	2.08	124.98	118.97
1	A	51	IT1	OP4-C5A-C5	2.37	112.91	108.99
1	C	51	IT1	OP4-C5A-C5	2.42	113.00	108.99
1	B	51	IT1	OP4-C5A-C5	2.93	113.84	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	51	IT1	1	0
1	C	51	IT1	1	0
1	D	51	IT1	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	BEN	A	401	-	9,9,9	0.98	1 (11%)	9,11,11	0.54	0
3	SER	A	402	-	3,6,6	0.34	0	1,7,7	0.08	0
2	BEN	B	401	-	9,9,9	1.00	1 (11%)	9,11,11	0.61	0
3	SER	B	402	-	3,6,6	0.37	0	1,7,7	0.53	0
3	SER	C	402	-	3,6,6	0.33	0	1,7,7	0.82	0
2	BEN	D	401	-	9,9,9	0.90	1 (11%)	9,11,11	0.62	0
3	SER	D	402	-	3,6,6	0.40	0	1,7,7	0.96	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
2	BEN	A	401	-	-	0/4/4/4	0/1/1/1
3	SER	A	402	-	-	0/2/6/6	0/0/0/0
2	BEN	B	401	-	-	0/4/4/4	0/1/1/1
3	SER	B	402	-	-	0/2/6/6	0/0/0/0
3	SER	C	402	-	-	0/2/6/6	0/0/0/0
2	BEN	D	401	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SER	D	402	-	-	0/2/6/6	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	BEN	C1-C	2.05	1.50	1.47
2	A	401	BEN	C1-C	2.18	1.51	1.47
2	B	401	BEN	C1-C	2.43	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SER	2	0
3	C	402	SER	1	0
3	D	402	SER	3	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%)	-0.11	1 (0%) 94 94	18, 26, 42, 54	0
1	B	323/342 (94%)	0.45	27 (8%) 14 14	22, 35, 54, 79	0
1	C	322/342 (94%)	0.39	18 (5%) 28 29	22, 35, 51, 69	0
1	D	327/342 (95%)	-0.13	5 (1%) 76 77	17, 25, 44, 62	0
All	All	1299/1368 (94%)	0.15	51 (3%) 43 45	17, 30, 50, 79	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	7.6
1	C	7	THR	7.2
1	B	6	LEU	5.7
1	B	185	GLY	4.8
1	C	183	VAL	4.0
1	B	305	ASN	3.9
1	C	8	ARG	3.9
1	B	243	ALA	3.8
1	D	183	VAL	3.7
1	C	225	ALA	3.3
1	B	4	HIS	3.2
1	C	148	ALA	3.1
1	B	210	MET	3.1
1	B	242	LEU	3.0
1	B	7	THR	2.9
1	B	9	PHE	2.9
1	B	212	ASP	2.8
1	C	240	GLY	2.7
1	C	64	ARG	2.7
1	C	185	GLY	2.7
1	B	313	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	133	THR	2.6
1	B	180	CYS	2.6
1	B	8	ARG	2.6
1	D	4	HIS	2.5
1	B	152	ARG	2.5
1	C	182	GLU	2.5
1	C	130	ASP	2.4
1	B	211	PRO	2.4
1	B	174	LEU	2.4
1	D	185	GLY	2.3
1	B	315	THR	2.3
1	C	223	SER	2.3
1	C	63	LEU	2.3
1	B	184	VAL	2.3
1	B	146	ILE	2.3
1	B	181	GLU	2.2
1	C	198	THR	2.2
1	B	307	ASP	2.2
1	B	209	LEU	2.2
1	A	182	GLU	2.2
1	B	63	LEU	2.1
1	C	224	VAL	2.1
1	B	225	ALA	2.1
1	C	10	PRO	2.1
1	C	149	GLN	2.0
1	C	244	LEU	2.0
1	C	9	PHE	2.0
1	B	245	THR	2.0
1	D	184	VAL	2.0
1	D	1	MET	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. 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	IT1	A	51	24/25	0.97	0.15	-	23,24,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	IT1	C	51	24/25	0.94	0.18	-	30,32,35,37	0
1	IT1	B	51	24/25	0.94	0.21	-	30,34,36,37	0
1	IT1	D	51	24/25	0.97	0.12	-	24,25,26,27	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
3	SER	B	402	7/7	0.75	0.34	6.20	47,48,50,54	0
3	SER	D	402	7/7	0.82	0.20	5.00	40,42,43,43	0
3	SER	A	402	7/7	0.79	0.21	4.34	35,38,40,41	0
3	SER	C	402	7/7	0.86	0.21	2.56	41,44,47,47	0
2	BEN	B	401	9/9	0.87	0.14	0.38	45,46,47,47	0
4	NA	C	401	1/1	0.95	0.10	-0.89	38,38,38,38	0
2	BEN	D	401	9/9	0.97	0.08	-1.40	19,19,19,19	0
2	BEN	A	401	9/9	0.95	0.09	-1.43	20,21,21,21	0

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

There are no such residues in this entry.