



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:44 PM GMT

PDB ID : 4D9F  
Title : D-Cysteine desulfhydrase from Salmonella typhimurium complexed with D-cycloserine (DCS)  
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.  
Deposited on : 2012-01-11  
Resolution : 2.61 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

**i**

## X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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Similar resolution  
(#Entries, resolution range(Å))

## Quality of chain

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
2	BEN	B	401	-	-	-	X
3	DCS	B	402	-	-	X	X
3	DCS	C	401	-	-	X	-
3	DCS	D	402	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9876 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	S	0	0	0
			2437	1553	413	462	9			
1	B	320	Total	C	N	O	S	0	0	0
			2364	1510	396	449	9			
1	C	317	Total	C	N	O	S	0	0	0
			2348	1499	394	446	9			
1	D	328	Total	C	N	O	S	0	0	0
			2437	1553	413	462	9			

There are 56 discrepancies between the modelled and reference sequences:

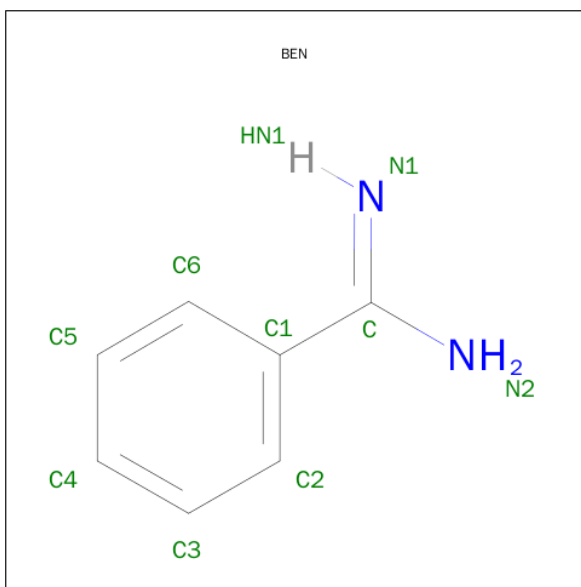
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
A	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-7	HIS	-	EXPRESSION TAG	UNP 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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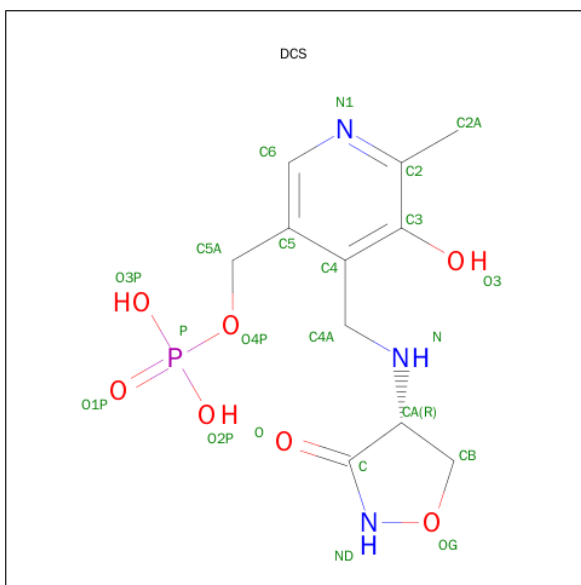
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
B	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
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 D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula:  $C_{11}H_{16}N_3O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	C	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	D	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

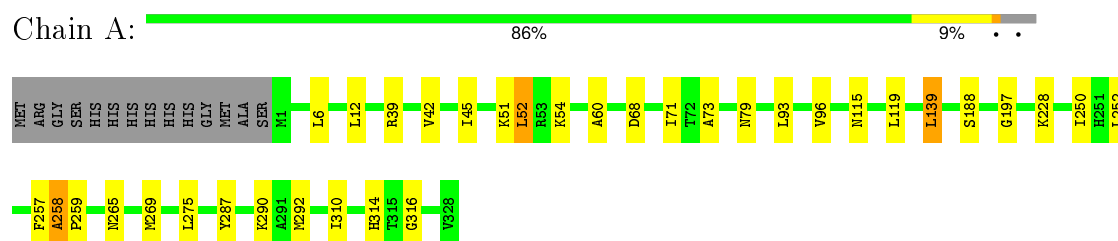
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	39	Total	O	0	0
			39	39		
4	C	29	Total	O	0	0
			29	29		
4	D	54	Total	O	0	0
			54	54		

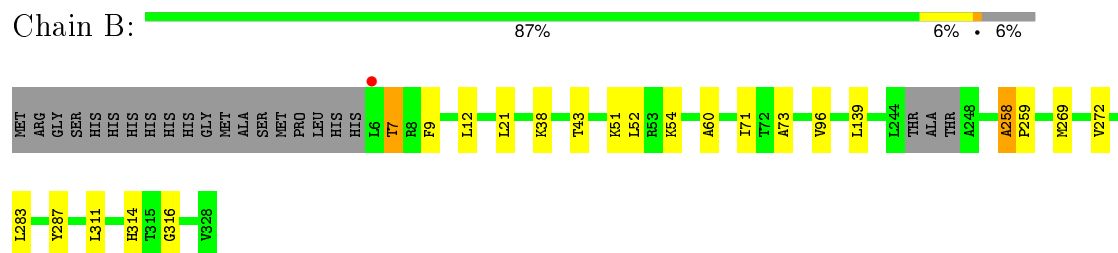
### 3 Residue-property plots [i](#)

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.

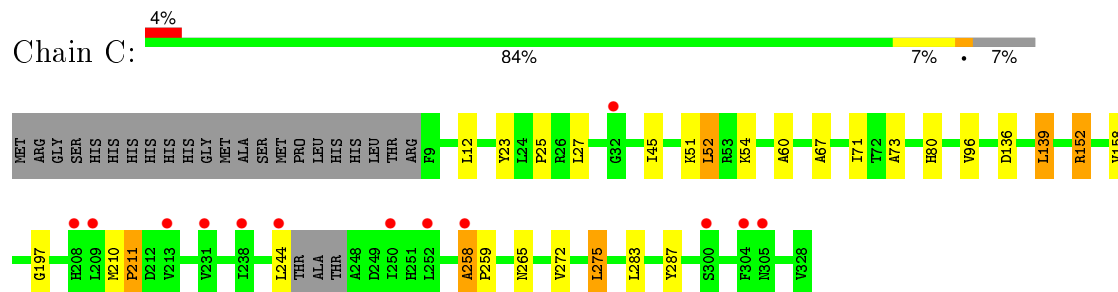
- Molecule 1: D-Cysteine desulphydrase



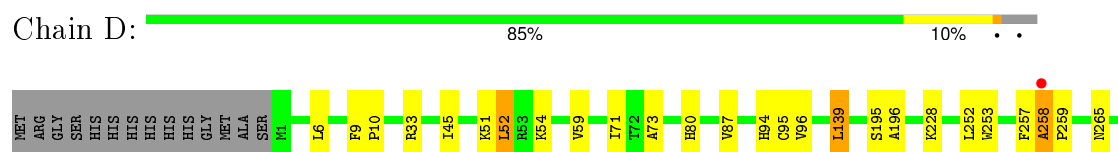
- Molecule 1: D-Cysteine desulphydrase



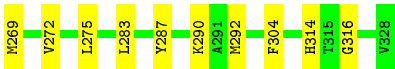
- Molecule 1: D-Cysteine desulphydrase



- Molecule 1: D-Cysteine desulphydrase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.16Å 167.51Å 68.77Å 90.00° 121.28° 90.00°	Depositor
Resolution (Å)	58.74 – 2.61 58.74 – 2.61	Depositor EDS
% Data completeness (in resolution range)	84.8 (58.74-2.61) 84.8 (58.74-2.61)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.228 , 0.283 0.227 , 0.282	Depositor DCC
$R_{free}$ test set	1939 reflections (6.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 7.3	EDS
Estimated twinning fraction	0.037 for l,k,-h-l 0.037 for -h-l,k,h 0.046 for h,-k,-h-l 0.049 for l,-k,h 0.449 for -h-l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32819 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: BEN, DCS

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	0.37	0/2485	0.50	0/3390
1	B	0.36	0/2408	0.48	0/3283
1	C	0.36	0/2392	0.48	0/3260
1	D	0.37	1/2485 (0.0%)	0.50	0/3390
All	All	0.37	1/9770 (0.0%)	0.49	0/13323

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	253	TRP	CD2-CE2	5.04	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	2437	0	2442	26	0
1	B	2364	0	2355	18	0
1	C	2348	0	2347	21	0
1	D	2437	0	2442	25	0
2	A	9	0	7	0	0
2	B	9	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	9	0	7	0	0
3	A	22	0	13	6	0
3	B	22	0	13	7	0
3	C	22	0	13	7	0
3	D	22	0	13	6	0
4	A	53	0	0	0	0
4	B	39	0	0	0	0
4	C	29	0	0	0	0
4	D	54	0	0	0	0
All	All	9876	0	9659	98	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 5.

All (98) 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:A:258:ALA:HB3	1:A:259:PRO:HD3	1.42	1.02
1:C:258:ALA:HB3	1:C:259:PRO:HD3	1.49	0.94
1:B:258:ALA:HB3	1:B:259:PRO:HD3	1.49	0.93
1:D:258:ALA:CB	1:D:259:PRO:HD3	1.97	0.91
1:D:258:ALA:HB3	1:D:259:PRO:HD3	1.50	0.90
1:D:51:LYS:HE3	3:D:402:DCS:H4A1	1.61	0.81
1:A:51:LYS:HE3	3:A:402:DCS:H4A1	1.64	0.80
1:A:258:ALA:CB	1:A:259:PRO:HD3	2.12	0.78
1:B:51:LYS:CE	3:B:402:DCS:H4A1	2.15	0.77
1:D:258:ALA:HB3	1:D:259:PRO:CD	2.15	0.75
1:D:258:ALA:CB	1:D:259:PRO:CD	2.68	0.71
3:A:402:DCS:H5A1	3:A:402:DCS:N	2.08	0.69
1:B:73:ALA:HB2	1:B:139:LEU:HD11	1.77	0.67
1:C:51:LYS:CE	3:C:401:DCS:H4A1	2.24	0.66
1:B:314:HIS:HD2	1:B:316:GLY:H	1.43	0.65
1:D:73:ALA:HB2	1:D:139:LEU:HD11	1.78	0.63
1:D:51:LYS:CE	3:D:402:DCS:H4A1	2.30	0.62
1:A:45:ILE:HB	1:A:52:LEU:HD21	1.81	0.62
1:A:51:LYS:CE	3:A:402:DCS:H4A1	2.30	0.62
3:D:402:DCS:HN	3:D:402:DCS:H5A1	1.66	0.61
1:C:51:LYS:HE2	3:C:401:DCS:H4A1	1.83	0.61
1:D:258:ALA:HB1	1:D:259:PRO:HD3	1.83	0.59
1:D:258:ALA:HB2	1:D:265:ASN:HB3	1.83	0.59
1:C:258:ALA:CB	1:C:259:PRO:HD3	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:TYR:OH	3:D:402:DCS:HA	2.02	0.58
1:A:258:ALA:HB3	1:A:265:ASN:HB3	1.86	0.58
1:B:51:LYS:HE3	3:B:402:DCS:H4A1	1.85	0.58
3:A:402:DCS:H5A1	3:A:402:DCS:HN	1.67	0.58
1:A:258:ALA:HB3	1:A:259:PRO:CD	2.26	0.57
1:C:54:LYS:NZ	3:C:401:DCS:O2P	2.35	0.57
1:C:73:ALA:HB2	1:C:139:LEU:HD11	1.85	0.57
1:C:67:ALA:HA	1:C:152:ARG:HB3	1.87	0.57
1:A:258:ALA:CB	1:A:265:ASN:HB3	2.36	0.56
1:B:258:ALA:CB	1:B:259:PRO:HD3	2.29	0.56
1:C:12:LEU:HG	1:C:60:ALA:HB2	1.88	0.56
1:A:73:ALA:HB2	1:A:139:LEU:HD11	1.88	0.56
1:B:71:ILE:HG12	1:B:96:VAL:HB	1.88	0.56
1:A:314:HIS:HD2	1:A:316:GLY:H	1.52	0.55
1:A:228:LYS:HE2	1:A:250:ILE:O	2.07	0.54
1:D:71:ILE:HG12	1:D:96:VAL:HB	1.89	0.54
3:D:402:DCS:N	3:D:402:DCS:H5A1	2.23	0.54
1:A:258:ALA:CB	1:A:259:PRO:CD	2.85	0.54
1:D:45:ILE:HB	1:D:52:LEU:HD21	1.90	0.53
1:B:287:TYR:OH	3:B:402:DCS:HA	2.09	0.53
1:C:71:ILE:HG12	1:C:96:VAL:HB	1.91	0.52
3:C:401:DCS:H5A1	3:C:401:DCS:HN	1.73	0.52
1:A:287:TYR:OH	3:A:402:DCS:HA	2.10	0.52
1:D:258:ALA:CB	1:D:265:ASN:HB3	2.39	0.51
1:D:275:LEU:HD13	1:D:292:MET:HG2	1.92	0.51
1:B:51:LYS:HE2	3:B:402:DCS:H4A1	1.90	0.51
3:B:402:DCS:N	3:B:402:DCS:H5A1	2.27	0.50
1:A:275:LEU:HD13	1:A:292:MET:HG2	1.93	0.50
1:D:314:HIS:HD2	1:D:316:GLY:H	1.58	0.49
1:D:51:LYS:HG3	1:D:80:HIS:HA	1.95	0.49
1:A:71:ILE:HG12	1:A:96:VAL:HB	1.95	0.48
1:D:54:LYS:NZ	3:D:402:DCS:O2P	2.45	0.48
1:C:51:LYS:HG3	1:C:80:HIS:HA	1.93	0.48
1:A:68:ASP:HA	1:A:93:LEU:HD22	1.96	0.48
1:A:54:LYS:HZ3	1:A:197:GLY:HA3	1.77	0.48
1:D:228:LYS:HG2	1:D:252:LEU:HD12	1.95	0.48
1:A:258:ALA:H	1:A:265:ASN:HD22	1.61	0.48
1:B:7:THR:C	1:B:9:PHE:H	2.17	0.47
1:C:287:TYR:OH	3:C:401:DCS:HA	2.15	0.47
3:B:402:DCS:HN	3:B:402:DCS:H5A1	1.80	0.47
1:B:73:ALA:CB	1:B:139:LEU:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ALA:HB3	1:B:259:PRO:CD	2.34	0.46
1:B:54:LYS:NZ	3:B:402:DCS:O2P	2.48	0.46
1:B:43:THR:HB	1:B:52:LEU:HD22	1.98	0.46
1:A:79:ASN:HB2	3:A:402:DCS:O3	2.16	0.46
1:C:51:LYS:HE3	1:C:80:HIS:HB2	1.98	0.45
1:C:258:ALA:H	1:C:265:ASN:HD22	1.64	0.45
1:C:158:VAL:HG12	3:C:401:DCS:HND	1.81	0.45
1:A:257:PHE:CG	1:A:257:PHE:O	2.69	0.45
1:C:258:ALA:HB3	1:C:259:PRO:CD	2.34	0.45
1:B:272:VAL:HG22	1:B:283:LEU:HB2	1.98	0.44
1:A:39:ARG:O	1:A:42:VAL:HG22	2.16	0.44
1:D:33:ARG:HH22	1:D:304:PHE:HB2	1.81	0.44
1:A:12:LEU:HG	1:A:60:ALA:HB2	2.00	0.44
1:D:59:VAL:HG21	1:D:87:VAL:HG11	2.00	0.44
1:A:188:SER:HB2	1:A:310:ILE:HG12	1.99	0.44
1:D:94:HIS:ND1	1:D:95:CYS:N	2.65	0.44
3:C:401:DCS:H5A1	3:C:401:DCS:N	2.32	0.43
1:D:272:VAL:HG22	1:D:283:LEU:HB2	2.01	0.43
1:B:12:LEU:HG	1:B:60:ALA:HB2	2.00	0.42
1:C:23:TYR:O	1:C:25:PRO:HD3	2.19	0.42
1:C:54:LYS:HZ3	1:C:197:GLY:HA3	1.84	0.42
1:C:210:MET:HA	1:C:211:PRO:HD3	1.76	0.42
1:D:195:SER:O	1:D:196:ALA:HB3	2.19	0.41
1:C:272:VAL:HG22	1:C:283:LEU:HB2	2.02	0.41
1:D:257:PHE:HA	1:D:290:LYS:HD3	2.01	0.41
1:A:228:LYS:HG2	1:A:252:LEU:HD12	2.02	0.41
1:B:38:LYS:HB2	1:B:311:LEU:HD21	2.02	0.41
1:C:27:LEU:HD22	1:C:275:LEU:HD21	2.01	0.41
1:B:314:HIS:CD2	1:B:316:GLY:H	2.32	0.41
1:D:9:PHE:HA	1:D:10:PRO:HD2	1.95	0.41
1:A:257:PHE:HA	1:A:290:LYS:HD3	2.02	0.41
1:A:115:ASN:O	1:A:119:LEU:HD13	2.21	0.41
1:C:45:ILE:HB	1:C:52:LEU:HD21	2.02	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	326/342 (95%)	318 (98%)	7 (2%)	1 (0%)	46	70
1	B	316/342 (92%)	300 (95%)	14 (4%)	2 (1%)	30	54
1	C	313/342 (92%)	296 (95%)	15 (5%)	2 (1%)	30	54
1	D	326/342 (95%)	317 (97%)	8 (2%)	1 (0%)	46	70
All	All	1281/1368 (94%)	1231 (96%)	44 (3%)	6 (0%)	34	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	THR
1	D	258	ALA
1	A	258	ALA
1	B	258	ALA
1	C	258	ALA
1	C	211	PRO

### 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	252/267 (94%)	248 (98%)	4 (2%)	70	88
1	B	241/267 (90%)	239 (99%)	2 (1%)	86	95
1	C	241/267 (90%)	235 (98%)	6 (2%)	55	80
1	D	252/267 (94%)	248 (98%)	4 (2%)	70	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	986/1068 (92%)	970 (98%)	16 (2%)	70	88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	52	LEU
1	A	139	LEU
1	A	269	MET
1	B	21	LEU
1	B	269	MET
1	C	52	LEU
1	C	136	ASP
1	C	139	LEU
1	C	152	ARG
1	C	244	LEU
1	C	275	LEU
1	D	6	LEU
1	D	52	LEU
1	D	139	LEU
1	D	269	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	HIS
1	A	325	HIS
1	B	241	GLN
1	B	314	HIS
1	B	325	HIS
1	C	199	HIS
1	C	208	HIS
1	C	325	HIS
1	D	305	ASN
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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$
2	BEN	A	401	-	9,9,9	0.84	0	9,11,11	0.73	0
3	DCS	A	402	-	23,23,23	3.42	5 (21%)	24,33,33	2.17	5 (20%)
2	BEN	B	401	-	9,9,9	0.85	1 (11%)	9,11,11	0.56	0
3	DCS	B	402	-	23,23,23	3.40	5 (21%)	24,33,33	2.03	4 (16%)
3	DCS	C	401	-	23,23,23	3.32	5 (21%)	24,33,33	2.05	5 (20%)
2	BEN	D	401	-	9,9,9	0.90	1 (11%)	9,11,11	0.54	0
3	DCS	D	402	-	23,23,23	3.41	5 (21%)	24,33,33	2.19	5 (20%)

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	DCS	A	402	-	-	0/10/21/21	0/2/2/2
2	BEN	B	401	-	-	0/4/4/4	0/1/1/1
3	DCS	B	402	-	-	0/10/21/21	0/2/2/2
3	DCS	C	401	-	-	0/10/21/21	0/2/2/2
2	BEN	D	401	-	-	0/4/4/4	0/1/1/1
3	DCS	D	402	-	-	0/10/21/21	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	DCS	OG-ND	-5.14	1.34	1.45
3	B	402	DCS	OG-ND	-5.02	1.34	1.45
3	D	402	DCS	OG-ND	-4.73	1.35	1.45
3	C	401	DCS	OG-ND	-3.48	1.37	1.45
3	B	402	DCS	CA-C	-3.31	1.50	1.52
3	A	402	DCS	CA-C	-3.29	1.50	1.52
3	C	401	DCS	CA-C	-3.16	1.50	1.52
3	D	402	DCS	CA-C	-3.02	1.50	1.52
2	B	401	BEN	C1-C	2.00	1.50	1.47
2	D	401	BEN	C1-C	2.09	1.51	1.47
3	D	402	DCS	C3-C4	5.81	1.49	1.40
3	A	402	DCS	C3-C4	5.89	1.49	1.40
3	C	401	DCS	C3-C4	5.91	1.49	1.40
3	B	402	DCS	C3-C4	5.93	1.49	1.40
3	D	402	DCS	C5-C4	6.91	1.50	1.40
3	A	402	DCS	C5-C4	6.99	1.50	1.40
3	C	401	DCS	C5-C4	7.02	1.50	1.40
3	B	402	DCS	C5-C4	7.11	1.50	1.40
3	B	402	DCS	C3-C2	11.71	1.48	1.40
3	C	401	DCS	C3-C2	11.78	1.48	1.40
3	A	402	DCS	C3-C2	11.90	1.49	1.40
3	D	402	DCS	C3-C2	12.17	1.49	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	DCS	C3-C4-C5	-3.02	115.63	118.82
3	D	402	DCS	C3-C4-C5	-3.02	115.64	118.82
3	B	402	DCS	C3-C4-C5	-2.61	116.07	118.82
3	C	401	DCS	C3-C4-C5	-2.39	116.30	118.82
3	C	401	DCS	C6-N1-C2	2.05	123.45	119.28
3	D	402	DCS	C6-C5-C4	2.05	119.62	118.09
3	A	402	DCS	C6-C5-C4	2.16	119.70	118.09
3	B	402	DCS	CA-C-ND	2.76	109.29	107.45
3	A	402	DCS	CA-C-ND	3.16	109.55	107.45
3	B	402	DCS	C4A-N-CA	3.16	118.64	113.81
3	D	402	DCS	CA-C-ND	3.49	109.78	107.45
3	C	401	DCS	CA-C-ND	3.67	109.89	107.45
3	A	402	DCS	C4A-N-CA	3.84	119.67	113.81
3	C	401	DCS	C4A-N-CA	3.88	119.74	113.81
3	D	402	DCS	C4A-N-CA	4.19	120.22	113.81
3	C	401	DCS	C4A-C4-C5	6.47	125.48	119.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	DCS	C4A-C4-C5	6.97	125.92	119.71
3	D	402	DCS	C4A-C4-C5	7.06	126.00	119.71
3	A	402	DCS	C4A-C4-C5	7.10	126.04	119.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	DCS	6	0
3	B	402	DCS	7	0
3	C	401	DCS	7	0
3	D	402	DCS	6	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	328/342 (95%)	-0.48	0 100 100	18, 25, 41, 46	0
1	B	320/342 (93%)	-0.19	1 (0%) 94 93	23, 38, 54, 59	0
1	C	317/342 (92%)	0.15	13 (4%) 41 34	26, 43, 57, 68	0
1	D	328/342 (95%)	-0.49	1 (0%) 94 93	18, 25, 38, 44	0
All	All	1293/1368 (94%)	-0.26	15 (1%) 81 77	18, 31, 52, 68	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	4.1
1	C	208	HIS	3.2
1	C	305	ASN	2.9
1	C	244	LEU	2.8
1	C	32	GLY	2.7
1	C	300	SER	2.6
1	C	304	PHE	2.5
1	B	6	LEU	2.4
1	C	209	LEU	2.3
1	C	258	ALA	2.3
1	C	213	VAL	2.2
1	C	238	ILE	2.1
1	C	250	ILE	2.1
1	D	258	ALA	2.0
1	C	231	VAL	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DCS	D	402	22/22	0.94	0.19	3.17	22,24,26,26	6
3	DCS	B	402	22/22	0.89	0.22	2.23	32,36,38,38	6
2	BEN	B	401	9/9	0.78	0.33	2.12	52,53,55,55	0
3	DCS	C	401	22/22	0.87	0.24	1.96	41,45,47,48	6
3	DCS	A	402	22/22	0.95	0.17	1.26	23,25,28,28	6
2	BEN	D	401	9/9	0.95	0.14	0.52	24,25,25,25	0
2	BEN	A	401	9/9	0.98	0.12	-1.49	20,20,21,21	0

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

There are no such residues in this entry.