



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:34 AM GMT

PDB ID : 4D97
Title : Salmonella typhimurium D-Cysteine desulphydrase with D-ser bound at active site
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2012-01-11
Resolution : 1.77 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

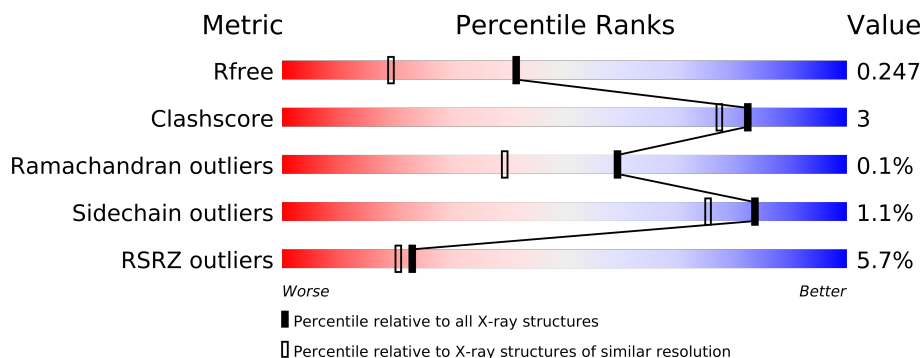
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.77 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}	66092	4987 (1.80-1.76)
Clashscore	79885	6152 (1.80-1.76)
Ramachandran outliers	78287	6074 (1.80-1.76)
Sidechain outliers	78261	6073 (1.80-1.76)
RSRZ outliers	66119	4990 (1.80-1.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	346	
1	B	346	
1	C	346	
1	D	346	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	DSN	A	402	-	X
3	DSN	B	401	-	X
3	DSN	C	402	-	X
3	DSN	D	402	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10536 atoms, of which 0 are hydrogen and 0 are deuterium.

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 desulphydrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	P	S	0	3	0
			2473	1576	416	471	1	9			
1	B	324	Total	C	N	O	P	S	0	3	0
			2438	1552	411	465	1	9			
1	C	322	Total	C	N	O	P	S	0	3	0
			2414	1537	409	458	1	9			
1	D	328	Total	C	N	O	P	S	0	4	0
			2466	1577	411	468	1	9			

There are 72 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
A	329	THR	-	EXPRESSION TAG	UNP Q8ZNT7
A	330	TYR	-	EXPRESSION TAG	UNP Q8ZNT7
A	331	PRO	-	EXPRESSION TAG	UNP Q8ZNT7
A	332	GLU	-	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

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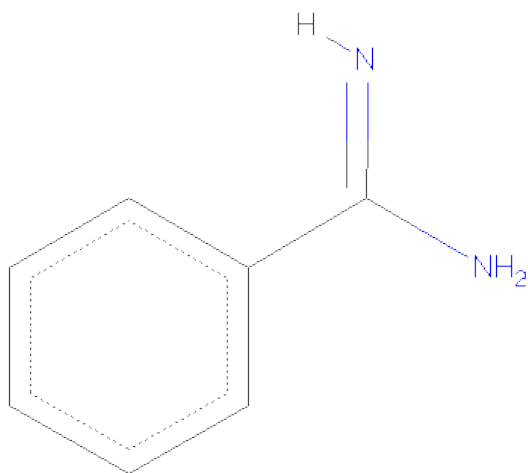
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP 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
B	329	THR	-	EXPRESSION TAG	UNP Q8ZNT7
B	330	TYR	-	EXPRESSION TAG	UNP Q8ZNT7
B	331	PRO	-	EXPRESSION TAG	UNP Q8ZNT7
B	332	GLU	-	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
C	329	THR	-	EXPRESSION TAG	UNP Q8ZNT7
C	330	TYR	-	EXPRESSION TAG	UNP Q8ZNT7
C	331	PRO	-	EXPRESSION TAG	UNP Q8ZNT7
C	332	GLU	-	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

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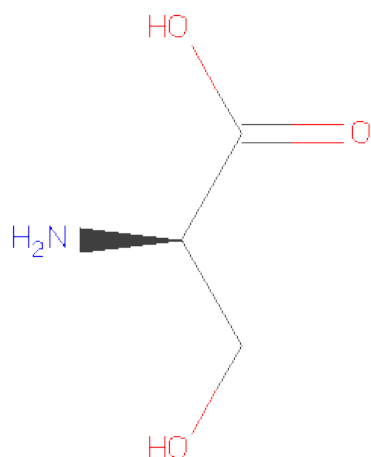
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
D	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	329	THR	-	EXPRESSION TAG	UNP Q8ZNT7
D	330	TYR	-	EXPRESSION TAG	UNP Q8ZNT7
D	331	PRO	-	EXPRESSION TAG	UNP Q8ZNT7
D	332	GLU	-	EXPRESSION TAG	UNP Q8ZNT7

- Molecule 2 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).



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

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



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

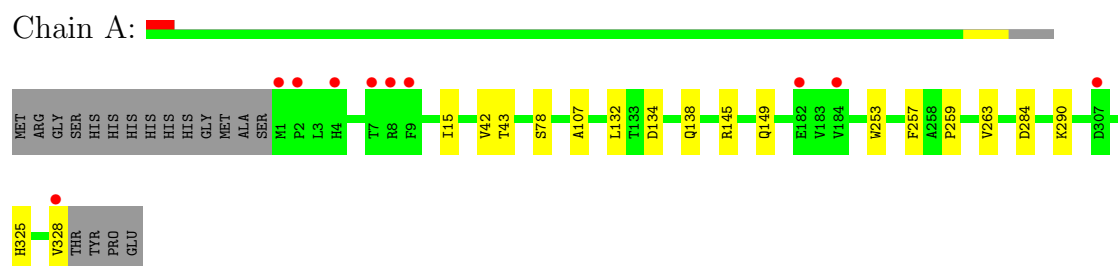
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total	O	0	0
			210	210		
4	B	151	Total	O	0	0
			151	151		
4	C	129	Total	O	0	0
			129	129		
4	D	200	Total	O	0	0
			200	200		

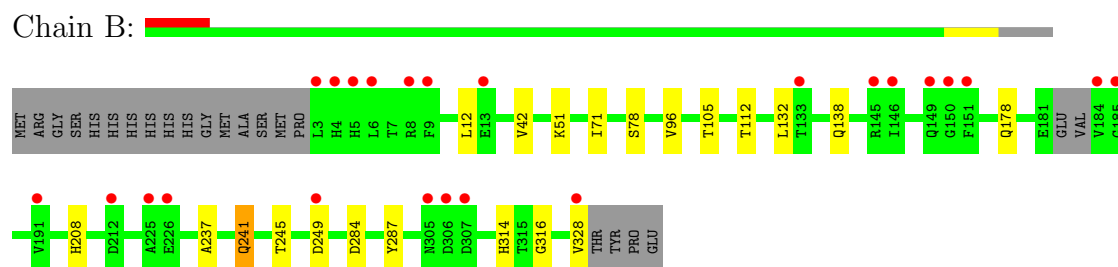
3 Residue-property plots

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.

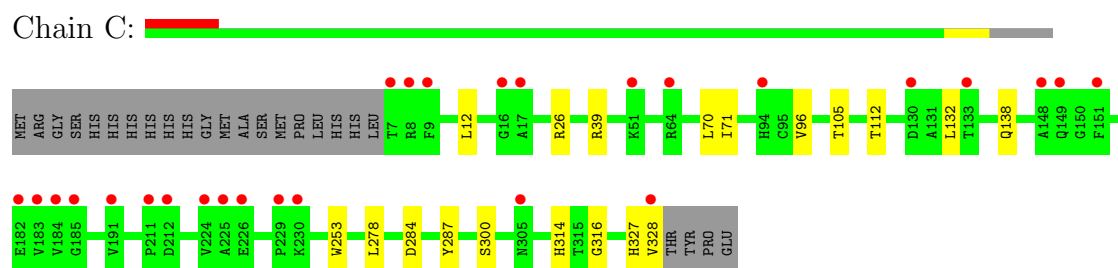
- Molecule 1: D-cysteine desulfhydrase



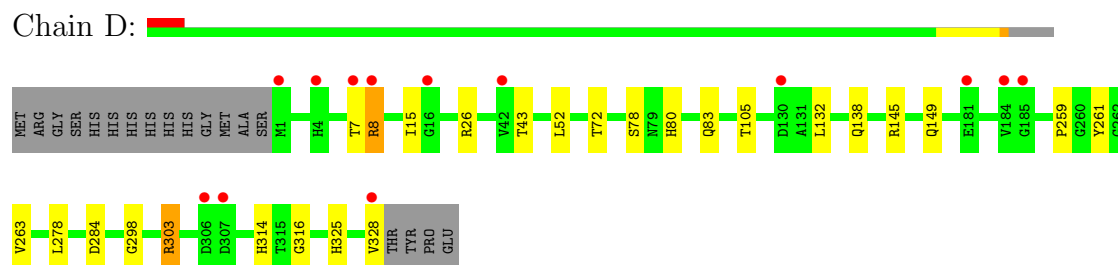
- Molecule 1: D-cysteine desulfhydrase



- 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, α , β , γ	66.44Å 165.29Å 68.71Å 90.00° 118.71° 90.00°	Depositor
Resolution (Å)	29.13 – 1.77 29.13 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.13-1.77) 98.5 (29.13-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.248 0.215 , 0.247	Depositor DCC
R_{free} test set	6203 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.6	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.017 for h,-k,-h-l 0.018 for -h-l,-k,l 0.019 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 123465 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10536	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, 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	0.40	1/2501 (0.0%)	0.52	0/3408
1	B	0.39	0/2464	0.50	0/3356
1	C	0.37	1/2438 (0.0%)	0.52	0/3321
1	D	0.39	0/2497	0.52	0/3404
All	All	0.39	2/9900 (0.0%)	0.52	0/13489

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	TRP	CD2-CE2	5.06	1.47	1.41
1	A	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 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2473	0	2475	15	0
1	B	2438	0	2430	16	0
1	C	2414	0	2419	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2466	0	2466	17	0
2	A	9	0	7	0	0
2	C	9	0	7	1	0
2	D	9	0	7	0	0
3	A	7	0	6	3	0
3	B	7	0	6	4	0
3	C	7	0	6	1	0
3	D	7	0	6	4	0
4	A	210	0	0	3	0
4	B	151	0	0	1	0
4	C	129	0	0	1	0
4	D	200	0	0	1	0
All	All	10536	0	9835	60	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (60) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:SER:OG	3:A:402:DSN:HB2	1.71	0.90
1:A:107:ALA:HB2	1:A:328[B]:VAL:HG23	1.55	0.88
1:A:42:VAL:O	1:A:42:VAL:HG23	1.91	0.70
3:D:402:DSN:N	4:D:634:HOH:O	2.25	0.69
1:D:52[B]:LEU:HG	1:D:83:GLN:HE21	1.62	0.63
1:D:78:SER:OG	3:D:402:DSN:N	2.33	0.61
1:B:42:VAL:O	1:B:42:VAL:HG12	2.01	0.61
1:D:7:THR:O	1:D:8:ARG:CB	2.49	0.61
1:B:314:HIS:HD2	1:B:316:GLY:H	1.49	0.61
1:B:105:THR:OG1	1:B:328[A]:VAL:HG12	2.00	0.60
1:D:314:HIS:HD2	1:D:316:GLY:H	1.51	0.58
1:C:314:HIS:HD2	1:C:316:GLY:H	1.50	0.57
1:B:328[A]:VAL:HG11	1:D:145:ARG:HH12	1.69	0.57
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	2.06	0.55
1:B:314:HIS:CD2	1:B:316:GLY:H	2.26	0.54
1:A:145:ARG:HH12	1:C:328[A]:VAL:HG21	1.72	0.53
3:B:401:DSN:HB2	4:B:651:HOH:O	2.06	0.53
1:D:26:ARG:HD3	1:D:278:LEU:O	2.09	0.52
1:C:112:THR:OG1	1:D:325:HIS:HE1	1.92	0.52
1:A:325:HIS:HD2	4:A:673:HOH:O	1.92	0.51
1:D:261:TYR:OH	3:D:402:DSN:HB3	2.10	0.51
1:B:287:TYR:OH	3:B:401:DSN:HA	2.12	0.50
1:A:259:PRO:HG2	1:A:263:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39[A]:ARG:NH1	4:C:620:HOH:O	2.45	0.48
1:D:259:PRO:HG2	1:D:263:VAL:HG11	1.96	0.48
1:C:314:HIS:CD2	1:C:316:GLY:H	2.31	0.47
1:B:237:ALA:O	1:B:241:GLN:HG2	2.14	0.47
1:D:105:THR:OG1	1:D:328[A]:VAL:HG12	2.15	0.47
1:C:132:LEU:HA	1:C:138:GLN:HE22	1.79	0.47
1:D:72:THR:OG1	1:D:80:HIS:HE1	1.98	0.47
1:C:300:SER:OG	2:C:401:BEN:H6	2.15	0.46
1:C:105:THR:CB	1:C:328[A]:VAL:HG12	2.45	0.46
1:D:80:HIS:HB3	3:D:402:DSN:H	1.80	0.45
1:B:71:ILE:HG12	1:B:96:VAL:HB	1.98	0.45
1:A:132:LEU:HA	1:A:138:GLN:HE22	1.81	0.45
1:A:78:SER:HG	3:A:402:DSN:HB2	1.73	0.45
1:A:42:VAL:O	1:A:42:VAL:CG2	2.59	0.45
1:A:325:HIS:HE1	1:B:112:THR:OG1	1.98	0.44
1:A:134:ASP:H	1:A:138:GLN:HE21	1.65	0.44
1:B:132:LEU:HA	1:B:138:GLN:HE22	1.83	0.43
3:A:402:DSN:HB3	4:A:710:HOH:O	2.18	0.43
1:D:314:HIS:CD2	1:D:316:GLY:H	2.34	0.42
1:B:105:THR:CB	1:B:328[A]:VAL:HG12	2.50	0.42
1:B:42:VAL:CG1	1:B:42:VAL:O	2.67	0.42
1:D:132:LEU:HA	1:D:138:GLN:HE22	1.85	0.42
1:B:51:IT1:HEA	3:B:401:DSN:H	1.84	0.42
1:C:71:ILE:HG12	1:C:96:VAL:HB	2.01	0.42
1:D:298:GLY:HA2	1:D:303:ARG:HB2	2.02	0.42
1:B:208:HIS:HE1	1:B:245:THR:O	2.02	0.42
1:A:15:ILE:HG23	1:A:43:THR:HG22	2.02	0.41
1:C:26:ARG:HD3	1:C:278:LEU:O	2.20	0.41
1:A:149:GLN:NE2	1:C:328[A]:VAL:HG13	2.35	0.41
1:B:328[A]:VAL:HG13	1:D:149:GLN:NE2	2.36	0.41
1:C:105:THR:HB	1:C:328[A]:VAL:HG12	2.03	0.41
1:D:15:ILE:HG23	1:D:43:THR:HG22	2.03	0.41
1:B:78:SER:OG	3:B:401:DSN:HB3	2.21	0.40
4:A:634:HOH:O	1:C:327:HIS:HD2	2.05	0.40
1:A:134:ASP:H	1:A:138:GLN:NE2	2.19	0.40
1:A:257:PHE:HA	1:A:290:LYS:HD3	2.02	0.40
1:C:287:TYR:OH	3:C:402:DSN:HA	2.21	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	327/346 (94%)	318 (97%)	9 (3%)	0	100	100
1	B	321/346 (93%)	314 (98%)	7 (2%)	0	100	100
1	C	321/346 (93%)	310 (97%)	11 (3%)	0	100	100
1	D	328/346 (95%)	320 (98%)	7 (2%)	1 (0%)	50	30
All	All	1297/1384 (94%)	1262 (97%)	34 (3%)	1 (0%)	59	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	8	ARG

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	254/270 (94%)	253 (100%)	1 (0%)	95	93
1	B	250/270 (93%)	245 (98%)	5 (2%)	68	50
1	C	246/270 (91%)	243 (99%)	3 (1%)	82	72
1	D	251/270 (93%)	249 (99%)	2 (1%)	89	84
All	All	1001/1080 (93%)	990 (99%)	11 (1%)	84	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	ASP
1	B	12	LEU

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Mol	Chain	Res	Type
1	B	178	GLN
1	B	241	GLN
1	B	249	ASP
1	B	284	ASP
1	C	12	LEU
1	C	70	LEU
1	C	284	ASP
1	D	284	ASP
1	D	303	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	125	GLN
1	A	138	GLN
1	A	149	GLN
1	A	325	HIS
1	B	125	GLN
1	B	138	GLN
1	B	208	HIS
1	B	314	HIS
1	C	80	HIS
1	C	83	GLN
1	C	125	GLN
1	C	138	GLN
1	C	314	HIS
1	C	327	HIS
1	D	80	HIS
1	D	83	GLN
1	D	125	GLN
1	D	138	GLN
1	D	149	GLN
1	D	241	GLN
1	D	314	HIS
1	D	325	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	24,24,25	3.73	1 (4%)	30,32,34	1.10	1 (3%)
1	IT1	B	51	1	24,24,25	3.73	2 (8%)	30,32,34	1.24	1 (3%)
1	IT1	C	51	1	24,24,25	3.74	2 (8%)	30,32,34	1.16	2 (6%)
1	IT1	D	51	1	24,24,25	3.68	2 (8%)	30,32,34	1.10	1 (3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	IT1	O-C	17.83	1.23	1.11
1	A	51	IT1	O-C	17.82	1.23	1.11
1	B	51	IT1	O-C	17.75	1.23	1.11
1	D	51	IT1	O-C	17.57	1.23	1.11
1	B	51	IT1	C3-C2	-2.56	1.38	1.40
1	C	51	IT1	C3-C2	-2.48	1.39	1.40
1	D	51	IT1	C3-C2	-2.33	1.39	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	IT1	C-CA-N	-3.30	110.53	113.83
1	A	51	IT1	C-CA-N	-2.74	111.09	113.83
1	D	51	IT1	C-CA-N	-2.56	111.28	113.83
1	C	51	IT1	C-CA-N	-2.13	111.70	113.83
1	C	51	IT1	CD-CE-NZ	-2.11	107.41	110.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	0.89	1 (11%)	11,11,11	0.80	0
3	DSN	A	402	-	6,6,6	1.00	1 (16%)	7,7,7	1.60	2 (28%)
3	DSN	B	401	-	6,6,6	0.88	0	7,7,7	1.49	1 (14%)
2	BEN	C	401	-	9,9,9	0.76	0	11,11,11	0.69	0
3	DSN	C	402	-	6,6,6	0.97	1 (16%)	7,7,7	1.63	2 (28%)
2	BEN	D	401	-	9,9,9	0.78	0	11,11,11	0.59	0
3	DSN	D	402	-	6,6,6	0.86	0	7,7,7	1.68	2 (28%)

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	DSN	A	402	-	-	0/6/6/6	0/0/0/0
3	DSN	B	401	-	-	0/6/6/6	0/0/0/0
2	BEN	C	401	-	-	0/4/4/4	0/1/1/1
3	DSN	C	402	-	-	0/6/6/6	0/0/0/0
2	BEN	D	401	-	-	0/4/4/4	0/1/1/1
3	DSN	D	402	-	-	0/6/6/6	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	DSN	OXT-C	-2.19	1.22	1.30
3	A	402	DSN	OXT-C	-2.16	1.22	1.30
2	A	401	BEN	C1-C	2.03	1.51	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	DSN	OXT-C-O	-3.39	116.41	124.07
3	B	401	DSN	OXT-C-O	-3.15	116.94	124.07
3	A	402	DSN	OXT-C-O	-3.12	117.02	124.07
3	D	402	DSN	OXT-C-CA	3.07	123.76	116.88
3	D	402	DSN	OXT-C-O	-2.60	118.19	124.07
3	A	402	DSN	OXT-C-CA	2.13	121.66	116.88
3	C	402	DSN	OXT-C-CA	2.06	121.51	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	328/346 (94%)	0.19	10 (3%) 48 45	14, 20, 35, 45	0
1	B	324/346 (93%)	0.47	24 (7%) 14 13	18, 26, 43, 63	0
1	C	322/346 (93%)	0.67	27 (8%) 11 10	18, 28, 45, 52	0
1	D	328/346 (94%)	0.21	13 (3%) 36 33	13, 20, 35, 44	0
All	All	1302/1384 (94%)	0.38	74 (5%) 23 20	13, 24, 41, 63	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	THR	5.3
1	B	305	ASN	4.4
1	D	1	MET	4.3
1	B	4	HIS	4.3
1	A	1	MET	4.2
1	D	7	THR	4.2
1	C	8	ARG	4.0
1	D	16	GLY	3.8
1	D	185	GLY	3.7
1	B	185	GLY	3.7
1	C	225	ALA	3.7
1	B	307	ASP	3.5
1	A	328[A]	VAL	3.5
1	D	8	ARG	3.4
1	C	183	VAL	3.4
1	C	185	GLY	3.3
1	B	184	VAL	3.2
1	C	148	ALA	3.2
1	D	4	HIS	3.1
1	B	146	ILE	3.1
1	A	182	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	305	ASN	3.0
1	B	225	ALA	3.0
1	C	212	ASP	2.9
1	C	130	ASP	2.9
1	C	7	THR	2.9
1	B	8	ARG	2.9
1	C	16	GLY	2.8
1	B	149	GLN	2.8
1	C	64	ARG	2.8
1	D	307	ASP	2.8
1	B	306	ASP	2.8
1	D	184	VAL	2.8
1	D	328[A]	VAL	2.8
1	A	4	HIS	2.7
1	C	149	GLN	2.7
1	B	3	LEU	2.7
1	B	5	HIS	2.7
1	C	184	VAL	2.7
1	B	249	ASP	2.7
1	B	151	PHE	2.7
1	B	226	GLU	2.7
1	C	224	VAL	2.6
1	D	181	GLU	2.6
1	C	151	PHE	2.6
1	C	51	IT1	2.6
1	B	133	THR	2.6
1	D	42	VAL	2.6
1	C	17	ALA	2.5
1	C	226	GLU	2.5
1	A	2	PRO	2.4
1	B	212	ASP	2.4
1	C	133	THR	2.4
1	B	9	PHE	2.4
1	B	328[A]	VAL	2.4
1	D	130	ASP	2.3
1	C	229	PRO	2.3
1	B	191	VAL	2.3
1	C	328[A]	VAL	2.3
1	B	150	GLY	2.3
1	A	307	ASP	2.3
1	A	8	ARG	2.3
1	C	182	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	191	VAL	2.2
1	C	9	PHE	2.2
1	A	184	VAL	2.1
1	C	211	PRO	2.1
1	B	13	GLU	2.1
1	C	230	LYS	2.1
1	A	9	PHE	2.0
1	B	145	ARG	2.0
1	C	94	HIS	2.0
1	B	6	LEU	2.0
1	D	306	ASP	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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	IT1	B	51	24/25	0.12	1.14	21,23,25,26	0
1	IT1	C	51	24/25	0.15	1.13	23,24,28,29	0
1	IT1	A	51	24/25	0.12	0.46	17,18,20,20	0
1	IT1	D	51	24/25	0.12	0.45	16,18,19,19	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DSN	C	402	7/7	0.28	9.85	36,38,40,40	0
3	DSN	A	402	7/7	0.26	9.21	28,28,30,31	0
3	DSN	D	402	7/7	0.20	6.56	27,28,28,28	0
3	DSN	B	401	7/7	0.20	5.95	33,34,35,36	0
2	BEN	C	401	9/9	0.11	-0.26	35,36,36,37	0
2	BEN	D	401	9/9	0.07	-1.17	15,15,16,16	0
2	BEN	A	401	9/9	0.07	-1.20	16,16,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.