Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 01:10 PM EDT

PDB ID	:	4D99
Title	:	Salmonella typhimurium D-Cysteine desulfhydrase 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

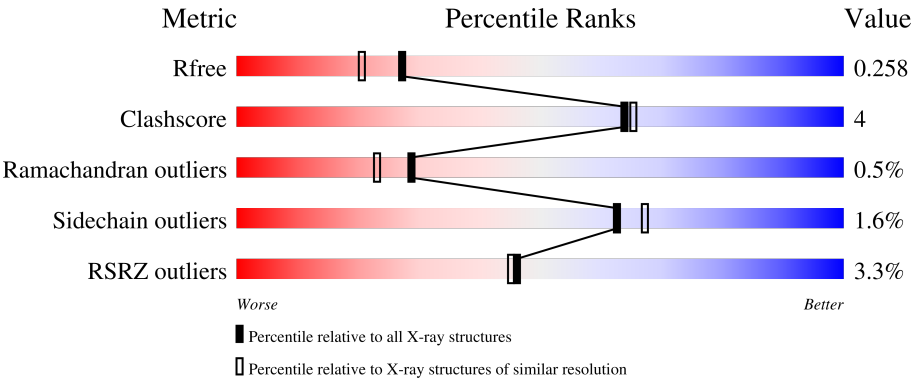
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	88% 7% .
1	B	342	7% 87% 7% 5%
1	C	342	4% 85% 9% 6%
1	D	342	% 85% 9% .. .

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	B	402	-	X	-	-

2 Entry composition (i)

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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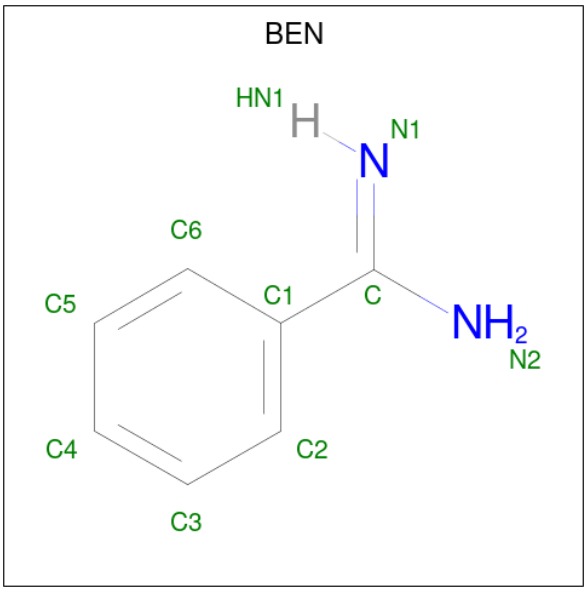
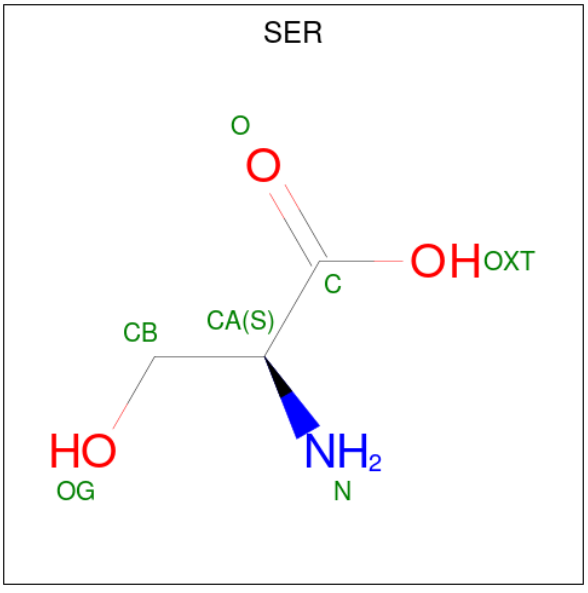
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q8ZNT7
B	-5	HIS	-	expression tag	UNP Q8ZNT7
B	-4	HIS	-	expression tag	UNP Q8ZNT7
B	-3	GLY	-	expression tag	UNP Q8ZNT7
B	-2	MET	-	expression tag	UNP Q8ZNT7
B	-1	ALA	-	expression tag	UNP Q8ZNT7
B	0	SER	-	expression tag	UNP Q8ZNT7
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: $C_7H_8N_2$).



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

- 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 7 3 1 3	0	0

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

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

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

- Molecule 5 is water.

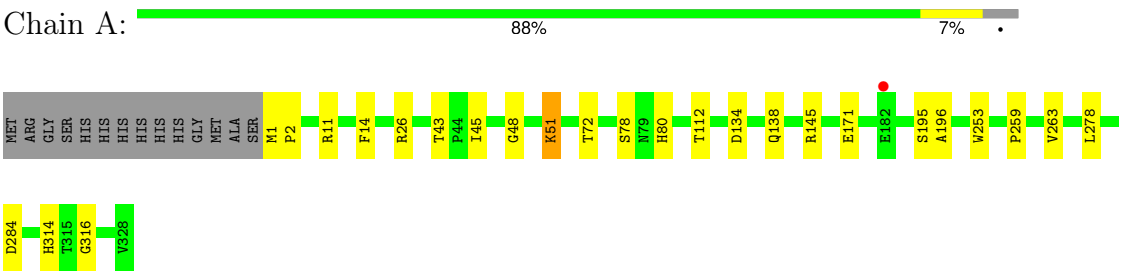
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	187	Total O 187 187	0	0
5	B	120	Total O 120 120	0	0
5	C	104	Total O 104 104	0	0
5	D	183	Total O 183 183	0	0

3 Residue-property plots (i)

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

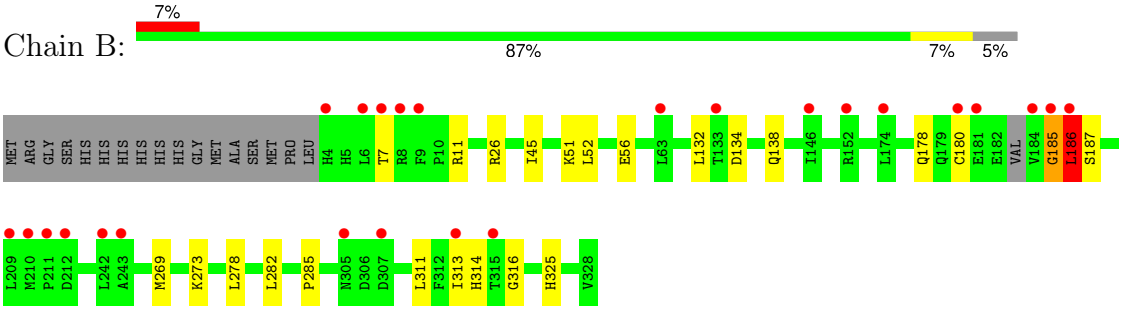
• Molecule 1: D-cysteine desulfhydrase

Chain A:



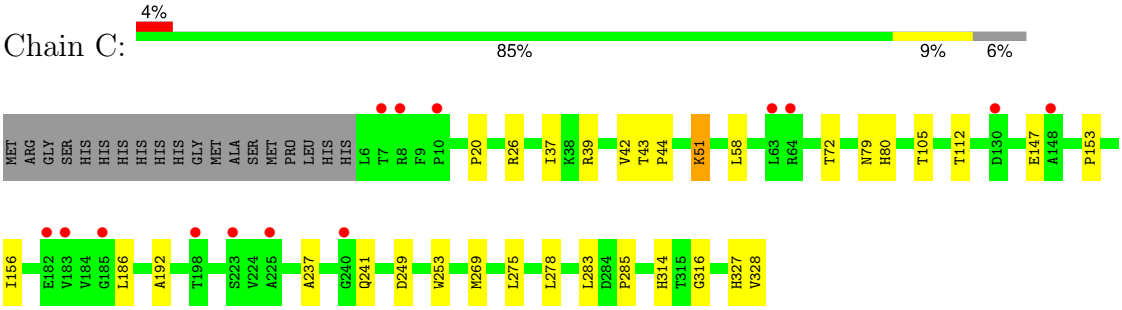
• Molecule 1: D-cysteine desulfhydrase

Chain B:



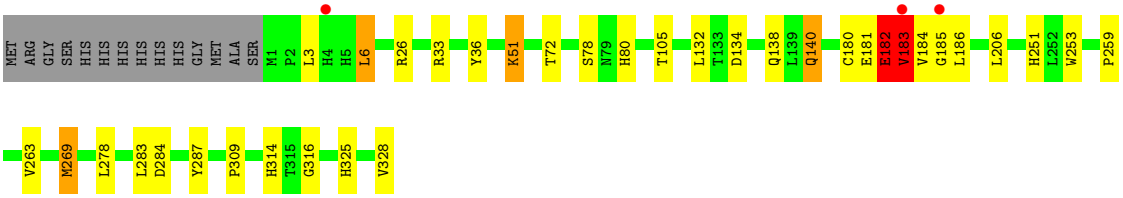
• Molecule 1: D-cysteine desulfhydrase

Chain C:



• Molecule 1: D-cysteine desulfhydrase

Chain D:


MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
HIS
GLY
MET
ALA
SER
M1
P2
L3
H4
H5
L6
R26
R33
Y36
K51
T72
S78
N79
H80
T105
L132
T133
D134
Q138
L139
Q140
C180
E181
E182
V183
V184
G185
L186
L206
H251
L252
W253
P259
V263
M269
L278
L283
D284
Y287
P309
H314
T315
G316
H325
V328

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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	3920 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
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
F_o,F_c correlation	0.94	EDS
Total number of atoms	10364	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEN, NA, LLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	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

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	2459	20	0
1	B	2393	0	2359	14	0
1	C	2412	0	2394	22	0
1	D	2446	0	2441	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	9690	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:O	2.34	0.61
1:A:1:MET:N	1:A:2:PRO:HD2	2.18	0.59
1:D:183:VAL:HG13	1:D:183:VAL:O	2.03	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:HE21	1:D:140:GLN:HA	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:LLP:H6	1:C:192:ALA:HB3	1.99	0.45
1:D:51:LLP:HE3	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:C:58:LEU:HD13	1:C:156:ILE:HG23	2.01	0.42
1:D:3:LEU:O	1:D:6:LEU:HB2	2.20	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:B:11:ARG:NH2	1:B:56:GLU:OE1	2.53	0.42
1:C:314:HIS:CD2	1:C:316:GLY:H	2.35	0.42
1:B:269:MET:SD	1:B:285:PRO:HB3	2.60	0.41
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:A:51:LLP:HE3	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:HA	1:B:273:LYS:HD2	1.96	0.40
1:A:14:PHE:HB3	1:A:45:ILE:HD12	2.04	0.40
1:D:134:ASP:H	1:D:138:GLN:NE2	2.19	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%)	8 (2%)	0	100 100
1	B	320/342 (94%)	308 (96%)	8 (2%)	4 (1%)	12 6
1	C	322/342 (94%)	312 (97%)	10 (3%)	0	100 100
1	D	325/342 (95%)	315 (97%)	8 (2%)	2 (1%)	25 19
All	All	1293/1368 (94%)	1253 (97%)	34 (3%)	6 (0%)	29 23

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 (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	253/266 (95%)	252 (100%)	1 (0%)	91	93
1	B	240/266 (90%)	238 (99%)	2 (1%)	81	86
1	C	244/266 (92%)	242 (99%)	2 (1%)	81	86
1	D	248/266 (93%)	240 (97%)	8 (3%)	39	38
All	All	985/1064 (93%)	972 (99%)	13 (1%)	62	74

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	23,24,25	0.78	0	25,32,34	1.13	1 (4%)
1	LLP	B	51	1	23,24,25	0.80	1 (4%)	25,32,34	1.15	1 (4%)
1	LLP	D	51	1	23,24,25	0.76	1 (4%)	25,32,34	1.03	0
1	LLP	C	51	1	23,24,25	0.78	0	25,32,34	1.15	1 (4%)

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	-	4/16/17/19	0/1/1/1
1	LLP	B	51	1	-	4/16/17/19	0/1/1/1
1	LLP	D	51	1	-	3/16/17/19	0/1/1/1
1	LLP	C	51	1	-	2/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	LLP	C3-C2	-2.06	1.38	1.41
1	B	51	LLP	C3-C2	-2.01	1.38	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	51	LLP	OP4-C5'-C5	2.39	113.84	109.36
1	A	51	LLP	C5-C6-N1	-2.16	120.32	123.83
1	C	51	LLP	C5-C6-N1	-2.04	120.51	123.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	51	LLP	O-C-CA-CB
1	A	51	LLP	C4-C4'-NZ-CE
1	C	51	LLP	C4-C4'-NZ-CE
1	D	51	LLP	C4-C4'-NZ-CE
1	B	51	LLP	C4-C4'-NZ-CE
1	B	51	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	A	51	LLP	C3-C4-C4'-NZ
1	C	51	LLP	C3-C4-C4'-NZ
1	D	51	LLP	C3-C4-C4'-NZ
1	B	51	LLP	C5-C4-C4'-NZ
1	B	51	LLP	CE-CD-CG-CB
1	A	51	LLP	C5-C4-C4'-NZ
1	D	51	LLP	CE-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	B	401	-	9,9,9	1.44	2 (22%)	7,11,11	0.61	0
2	BEN	A	401	-	9,9,9	0.98	1 (11%)	7,11,11	0.66	0
2	BEN	D	401	-	9,9,9	1.32	1 (11%)	7,11,11	0.68	0
3	SER	B	402	-	4,6,6	1.16	1 (25%)	2,7,7	2.35	1 (50%)
3	SER	C	402	-	4,6,6	1.22	1 (25%)	2,7,7	2.70	1 (50%)
3	SER	D	402	-	4,6,6	1.29	1 (25%)	2,7,7	2.48	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SER	A	402	-	4,6,6	1.03	0	2,7,7	1.98	1 (50%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	BEN	C-N2	-2.84	1.26	1.33
2	D	401	BEN	C-N2	-2.64	1.27	1.33
3	D	402	SER	OXT-C	-2.53	1.22	1.30
3	C	402	SER	OXT-C	-2.42	1.22	1.30
3	B	402	SER	OXT-C	-2.25	1.23	1.30
2	B	401	BEN	C1-C	2.23	1.51	1.47
2	A	401	BEN	C1-C	2.01	1.51	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	SER	OXT-C-O	-3.75	115.57	124.08
3	D	402	SER	OXT-C-O	-3.44	116.28	124.08
3	B	402	SER	OXT-C-O	-3.26	116.68	124.08
3	A	402	SER	OXT-C-O	-2.76	117.82	124.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	SER	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
3	A	402	SER	C-CA-CB-OG
3	B	402	SER	O-C-CA-N
3	B	402	SER	O-C-CA-CB
3	B	402	SER	OXT-C-CA-CB
3	B	402	SER	N-CA-CB-OG
3	B	402	SER	C-CA-CB-OG
3	C	402	SER	N-CA-CB-OG
3	A	402	SER	OXT-C-CA-N
3	B	402	SER	OXT-C-CA-N
3	D	402	SER	OXT-C-CA-N
3	C	402	SER	C-CA-CB-OG
3	A	402	SER	O-C-CA-N
3	D	402	SER	O-C-CA-N
3	C	402	SER	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	SER	1	0
3	D	402	SER	3	0
3	A	402	SER	2	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^{th} 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	327/342 (95%)	-0.16	1 (0%)	94	93	18, 26, 42, 54	0
1	B	323/342 (94%)	0.38	25 (7%)	13	12	22, 35, 54, 79	0
1	C	322/342 (94%)	0.32	14 (4%)	35	34	22, 35, 51, 69	0
1	D	327/342 (95%)	-0.17	3 (0%)	84	83	17, 25, 44, 62	0
All	All	1299/1368 (94%)	0.09	43 (3%)	46	45	17, 30, 50, 79	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	7.3
1	C	7	THR	7.0
1	B	6	LEU	5.4
1	B	185	GLY	4.6
1	B	305	ASN	3.8
1	C	8	ARG	3.8
1	C	183	VAL	3.7
1	B	243	ALA	3.7
1	D	183	VAL	3.5
1	C	225	ALA	3.1
1	B	4	HIS	3.1
1	B	210	MET	3.0
1	C	148	ALA	3.0
1	B	242	LEU	2.8
1	B	7	THR	2.8
1	B	9	PHE	2.7
1	B	212	ASP	2.7
1	C	64	ARG	2.6
1	C	240	GLY	2.6
1	C	185	GLY	2.5
1	B	133	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	8	ARG	2.5
1	B	313	ILE	2.4
1	D	4	HIS	2.4
1	B	180	CYS	2.4
1	B	152	ARG	2.4
1	C	182	GLU	2.4
1	B	211	PRO	2.3
1	C	130	ASP	2.3
1	B	174	LEU	2.2
1	C	223	SER	2.2
1	D	185	GLY	2.2
1	B	315	THR	2.2
1	B	181	GLU	2.2
1	C	63	LEU	2.1
1	B	146	ILE	2.1
1	B	184	VAL	2.1
1	C	198	THR	2.1
1	B	307	ASP	2.1
1	A	182	GLU	2.1
1	B	63	LEU	2.0
1	B	209	LEU	2.0
1	C	10	PRO	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	B	51	24/25	0.94	0.21	30,34,36,37	0
1	LLP	C	51	24/25	0.94	0.18	30,32,35,37	0
1	LLP	A	51	24/25	0.97	0.15	23,24,26,27	0
1	LLP	D	51	24/25	0.97	0.12	24,25,26,27	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SER	B	402	7/7	0.75	0.34	47,48,50,54	0
3	SER	A	402	7/7	0.79	0.22	35,38,40,41	0
3	SER	D	402	7/7	0.82	0.20	40,42,43,43	0
3	SER	C	402	7/7	0.86	0.21	41,44,47,47	0
2	BEN	B	401	9/9	0.87	0.14	45,46,47,47	0
2	BEN	A	401	9/9	0.95	0.09	20,21,21,21	0
4	NA	C	401	1/1	0.95	0.10	38,38,38,38	0
2	BEN	D	401	9/9	0.97	0.08	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.