



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:44 PM GMT

PDB ID : 4D9E  
Title : D-Cysteine desulfhydrase from Salmonella typhimurium complexed with L-cycloserine (LCS)  
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.  
Deposited on : 2012-01-11  
Resolution : 2.47 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

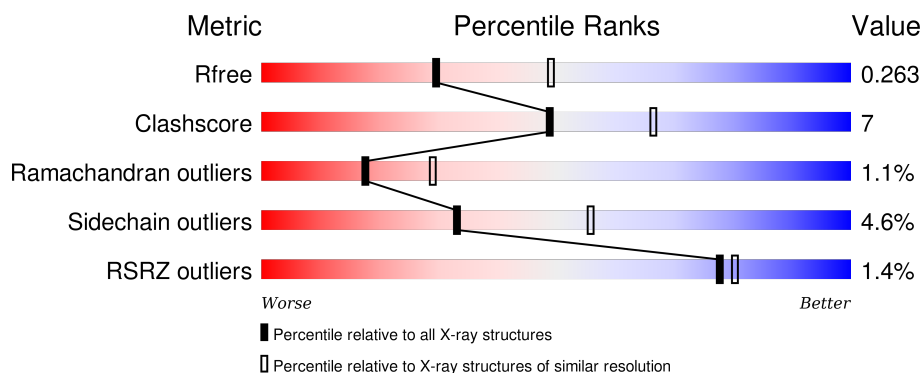
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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>80%</div> <div>14% ..</div> </div>
1	B	342	<div> <div>2%</div> <div>79%</div> <div>13% • 5%</div> </div>
1	C	342	<div> <div>3%</div> <div>79%</div> <div>12% • 6%</div> </div>
1	D	342	<div> <div>85%</div> <div>10% • •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10065 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	4	1	0
			2435	1555	414	457	9			
1	B	325	Total	C	N	O	S	6	1	0
			2414	1537	408	460	9			
1	C	323	Total	C	N	O	S	20	3	0
			2419	1540	412	458	9			
1	D	328	Total	C	N	O	S	10	1	0
			2434	1553	408	464	9			

There are 56 discrepancies between the modelled and reference sequences:

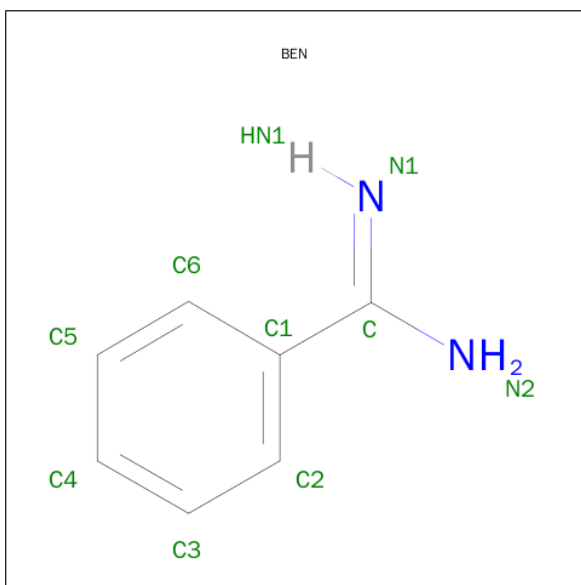
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
A	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-7	HIS	-	EXPRESSION TAG	UNP 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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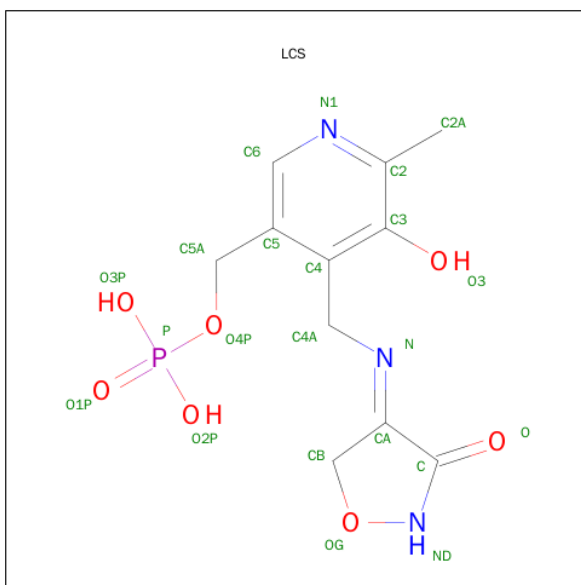
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
B	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
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 [5-HYDROXY-6-METHYL-4-({[(4E)-3-OXO-1,2-OXAZOLIDIN-4-YLIDENE] AMINO}METHYL)PYRIDIN-3-YL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: LCS) (formula: C<sub>11</sub>H<sub>14</sub>N<sub>3</sub>O<sub>7</sub>P).



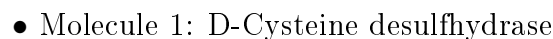
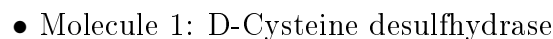
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	C	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	D	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

- Molecule 4 is water.

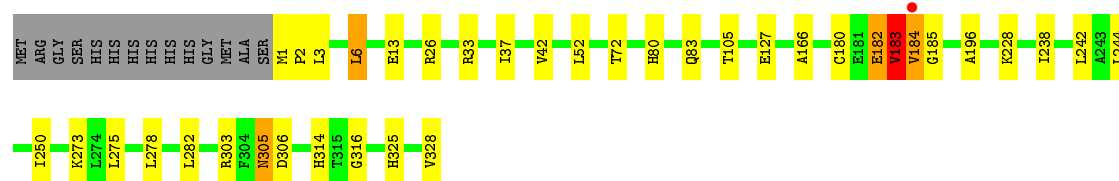
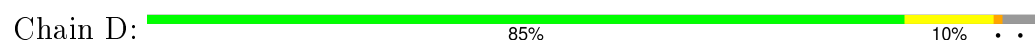
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	53	Total	O	0	0
			53	53		
4	C	54	Total	O	0	0
			54	54		
4	D	73	Total	O	0	0
			73	73		



- Molecule 1: D-Cysteine desulfhydrase



Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.42Å 165.84Å 68.06Å 90.00° 119.03° 90.00°	Depositor
Resolution (Å)	58.08 – 2.47 58.08 – 2.47	Depositor EDS
% Data completeness (in resolution range)	90.1 (58.08-2.47) 90.1 (58.08-2.47)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.213 , 0.263 0.211 , 0.263	Depositor DCC
$R_{free}$ test set	2333 reflections (5.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.1	EDS
Estimated twinning fraction	0.023 for -h-l,k,h 0.023 for l,k,-h-l 0.044 for h,-k,-h-l 0.068 for -h-l,-k,l 0.046 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 41730 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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

### 5.1 Standard geometry

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

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	0.78	1/2482 (0.0%)	0.83	6/3385 (0.2%)
1	B	0.82	2/2460 (0.1%)	0.82	4/3354 (0.1%)
1	C	0.88	4/2474 (0.2%)	0.82	4/3371 (0.1%)
1	D	0.78	2/2484 (0.1%)	0.81	0/3389
All	All	0.82	9/9900 (0.1%)	0.82	14/13499 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	CYS	CB-SG	-8.44	1.67	1.82
1	B	180	CYS	CB-SG	-6.39	1.71	1.82
1	B	90	LYS	CB-CG	-5.94	1.36	1.52
1	C	180	CYS	CB-SG	-5.92	1.72	1.81
1	D	180	CYS	CB-SG	-5.77	1.72	1.81
1	C	132	LEU	CA-CB	5.65	1.66	1.53
1	C	120	ASP	CB-CG	-5.56	1.40	1.51
1	A	230	LYS	CE-NZ	5.12	1.61	1.49
1	D	183	VAL	CA-CB	-5.09	1.44	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	VAL	N-CA-C	-7.78	89.99	111.00
1	A	184	VAL	N-CA-CB	-6.97	96.16	111.50
1	A	183	VAL	CB-CA-C	6.38	123.51	111.40
1	B	275	LEU	CD1-CG-CD2	-5.89	92.83	110.50
1	B	270	GLU	OE1-CD-OE2	-5.78	116.37	123.30
1	A	311	LEU	CD1-CG-CD2	-5.72	93.34	110.50
1	A	120	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	270	GLU	OE1-CD-OE2	-5.40	116.81	123.30
1	B	307	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	C	311	LEU	CD1-CG-CD2	-5.34	94.48	110.50
1	C	26	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	275	LEU	CD1-CG-CD2	-5.28	94.66	110.50
1	B	311	LEU	CD1-CG-CD2	-5.15	95.04	110.50
1	A	186	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	7	THR	Peptide

## 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	2435	0	2445	39	0
1	B	2414	0	2403	36	0
1	C	2419	0	2434	40	0
1	D	2434	0	2436	29	0
2	A	9	0	7	0	0
2	B	9	0	7	0	0
2	D	9	0	7	0	0
3	A	22	0	11	1	0
3	B	22	0	11	2	0
3	C	22	0	11	5	0
3	D	22	0	11	1	0
4	A	68	0	0	0	0
4	B	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	54	0	0	1	0
4	D	73	0	0	0	0
All	All	10065	0	9783	141	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 7.

All (141) 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:182:GLU:O	1:D:183:VAL:HG23	1.49	1.11
1:B:184:VAL:CB	1:B:185:GLY:HA2	1.90	0.99
1:A:183:VAL:HG12	1:A:184:VAL:HG12	1.42	0.98
1:A:182:GLU:O	1:A:183:VAL:HG23	1.74	0.87
1:D:183:VAL:HG12	1:D:183:VAL:O	1.73	0.87
1:C:183:VAL:HG12	1:C:184:VAL:HG12	1.60	0.83
1:C:183:VAL:HG12	1:C:184:VAL:N	1.93	0.82
1:D:184:VAL:HG12	1:D:184:VAL:O	1.80	0.82
1:B:182:GLU:O	1:B:183:VAL:CB	2.30	0.80
1:A:182:GLU:O	1:A:183:VAL:CG2	2.30	0.79
1:A:182:GLU:O	1:A:183:VAL:CB	2.30	0.77
1:D:182:GLU:O	1:D:183:VAL:CG2	2.30	0.77
1:B:184:VAL:CB	1:B:185:GLY:CA	2.63	0.76
1:A:182:GLU:O	1:A:183:VAL:HB	1.87	0.75
1:B:42:VAL:O	1:B:42:VAL:HG12	1.91	0.70
1:C:314:HIS:HD2	1:C:316:GLY:H	1.38	0.70
1:C:6:LEU:O	1:C:7:THR:C	2.29	0.69
1:D:2:PRO:O	1:D:244:LEU:HD21	1.92	0.68
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.58	0.68
1:B:105:THR:OG1	1:B:328[A]:VAL:HG12	1.93	0.68
1:B:314:HIS:HD2	1:B:316:GLY:H	1.43	0.66
1:A:105:THR:OG1	1:A:328[B]:VAL:HG12	1.94	0.66
1:D:42:VAL:HG12	1:D:42:VAL:O	1.94	0.66
1:C:130:ASP:O	1:C:131:ALA:HB2	1.96	0.66
1:C:7:THR:O	1:C:9:PHE:N	2.29	0.66
1:A:314:HIS:HD2	1:A:316:GLY:H	1.46	0.64
1:A:305:ASN:OD1	1:A:306:ASP:OD1	2.15	0.64
1:D:314:HIS:HD2	1:D:316:GLY:H	1.46	0.63
1:A:181:GLU:O	1:A:182:GLU:O	2.17	0.62
1:C:183:VAL:CG1	1:C:184:VAL:N	2.62	0.62
1:B:183:VAL:C	1:B:184:VAL:O	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:HIS:CD2	1:C:316:GLY:H	2.16	0.61
1:B:134:ASP:H	1:B:138:GLN:NE2	1.98	0.61
1:C:39[A]:ARG:NH1	4:C:508:HOH:O	2.32	0.61
1:C:42:VAL:O	1:C:42:VAL:HG12	2.01	0.61
1:C:305:ASN:OD1	1:C:306:ASP:OD1	2.19	0.61
1:C:180:CYS:O	1:C:182:GLU:N	2.34	0.60
1:B:42:VAL:CG1	1:B:42:VAL:O	2.50	0.60
1:B:51:LYS:CE	3:B:402:LCS:H4A2	2.31	0.60
1:C:51:LYS:CE	3:C:401:LCS:H4A2	2.31	0.60
1:D:184:VAL:O	1:D:184:VAL:CG1	2.50	0.59
1:C:112:THR:OG1	1:D:325:HIS:HE1	1.85	0.59
1:A:282:LEU:O	1:A:314:HIS:HE1	1.84	0.59
1:C:183:VAL:HG12	1:C:184:VAL:CG1	2.31	0.59
1:A:325:HIS:ND1	1:A:326:PRO:HA	2.17	0.59
1:C:183:VAL:CG1	1:C:184:VAL:HG12	2.33	0.58
1:B:72:THR:OG1	1:B:80:HIS:HE1	1.87	0.58
1:A:269:MET:CE	1:A:285:PRO:HB3	2.33	0.57
1:D:42:VAL:O	1:D:42:VAL:CG1	2.52	0.57
1:C:42:VAL:O	1:C:42:VAL:CG1	2.52	0.57
1:B:314:HIS:CD2	1:B:316:GLY:H	2.22	0.57
1:A:314:HIS:CD2	1:A:316:GLY:H	2.23	0.57
1:B:90:LYS:O	1:B:90:LYS:HG2	2.06	0.56
1:B:324:TYR:CD1	1:B:328[B]:VAL:HG11	2.41	0.55
1:A:134:ASP:H	1:A:138:GLN:NE2	2.04	0.55
1:A:149:GLN:O	1:C:263:VAL:HG21	2.07	0.55
1:A:184:VAL:O	1:A:184:VAL:HG13	2.08	0.54
1:D:1:MET:N	1:D:2:PRO:HD2	2.22	0.54
1:A:42:VAL:O	1:A:42:VAL:HG23	2.07	0.54
1:C:72:THR:OG1	1:C:80:HIS:HE1	1.91	0.54
1:C:134:ASP:H	1:C:138:GLN:NE2	2.06	0.53
1:C:275:LEU:HG	1:C:283:LEU:HD11	1.90	0.53
1:B:282:LEU:O	1:B:314:HIS:HE1	1.91	0.53
1:C:51:LYS:HE2	3:C:401:LCS:H4A2	1.89	0.53
1:D:305:ASN:OD1	1:D:306:ASP:OD1	2.26	0.53
1:D:282:LEU:O	1:D:314:HIS:HE1	1.91	0.53
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.21	0.53
1:B:59:VAL:HG21	1:B:87:VAL:HG11	1.91	0.53
1:A:37:ILE:HD11	1:A:314:HIS:HB2	1.91	0.52
1:C:166:ALA:CB	1:C:238:ILE:HD11	2.39	0.52
1:B:223:SER:OG	1:B:226:GLU:HG3	2.10	0.51
1:A:52:LEU:HG	1:A:83:GLN:HE21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:HIS:CD2	1:D:127:GLU:OE2	2.64	0.51
1:C:6:LEU:O	1:C:7:THR:O	2.30	0.50
1:B:183:VAL:O	1:B:184:VAL:O	2.30	0.50
1:A:269:MET:HE2	1:A:285:PRO:HB3	1.94	0.50
1:A:1:MET:N	1:A:2:PRO:HD2	2.26	0.49
1:B:324:TYR:CE1	1:B:328[B]:VAL:HG11	2.46	0.49
1:D:228:LYS:HE3	1:D:250:ILE:O	2.13	0.48
1:A:1:MET:N	1:A:2:PRO:CD	2.76	0.48
1:A:59:VAL:HG21	1:A:87:VAL:HG11	1.96	0.48
1:D:72:THR:OG1	1:D:80:HIS:HE1	1.97	0.48
1:D:105:THR:OG1	1:D:328:VAL:HG12	2.14	0.48
1:B:171:GLU:O	1:B:174:LEU:HB2	2.14	0.48
1:D:314:HIS:CD2	1:D:316:GLY:H	2.29	0.47
1:D:182:GLU:O	1:D:183:VAL:CB	2.59	0.47
3:C:401:LCS:H4A1	3:C:401:LCS:HB1	1.71	0.47
1:C:257:PHE:HA	1:C:290:LYS:HD3	1.96	0.47
1:B:6:LEU:HD23	1:B:6:LEU:HA	1.45	0.47
1:D:26:ARG:NH1	1:D:278:LEU:HA	2.30	0.47
1:C:183:VAL:HG12	1:C:184:VAL:CB	2.44	0.47
1:A:282:LEU:O	1:A:314:HIS:CE1	2.67	0.47
1:B:305:ASN:OD1	1:B:306:ASP:OD1	2.32	0.47
1:D:37:ILE:HD11	1:D:314:HIS:HB2	1.97	0.47
1:A:251:HIS:ND1	1:A:251:HIS:N	2.63	0.47
1:A:42:VAL:O	1:A:42:VAL:CG2	2.63	0.46
1:B:257:PHE:HA	1:B:290:LYS:HD3	1.97	0.46
1:A:175:GLU:O	1:A:179:GLN:HG3	2.14	0.46
1:C:282:LEU:O	1:C:314:HIS:HE1	1.97	0.46
1:D:52:LEU:HG	1:D:83:GLN:HE21	1.81	0.46
1:B:183:VAL:O	1:B:184:VAL:C	2.54	0.46
1:A:195:SER:HB3	3:A:402:LCS:HB2	1.98	0.45
1:B:45:ILE:HB	1:B:52:LEU:HD21	1.99	0.45
1:B:324:TYR:CD1	1:B:328[B]:VAL:CG1	3.00	0.44
1:A:305:ASN:OD1	1:A:305:ASN:C	2.55	0.44
1:A:259:PRO:HG2	1:A:263:VAL:HG11	1.99	0.44
1:C:195:SER:O	1:C:196:ALA:HB3	2.18	0.44
1:A:166:ALA:CB	1:A:238:ILE:HD11	2.48	0.44
1:B:298:GLY:HA2	1:B:303:ARG:HB2	1.99	0.43
1:C:112:THR:OG1	1:D:325:HIS:CE1	2.68	0.43
1:D:166:ALA:CB	1:D:238:ILE:HD11	2.49	0.43
1:D:1:MET:N	1:D:2:PRO:CD	2.82	0.43
1:A:305:ASN:OD1	1:A:306:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:MET:SD	1:B:285:PRO:HB3	2.59	0.43
1:C:37:ILE:HD11	1:C:314:HIS:HB2	2.00	0.43
1:D:6:LEU:HD13	1:D:242:LEU:HD21	2.00	0.43
1:C:26:ARG:HD3	1:C:278:LEU:O	2.18	0.42
1:C:305:ASN:OD1	1:C:306:ASP:N	2.52	0.42
1:C:79:ASN:ND2	3:C:401:LCS:H2A1	2.33	0.42
3:D:402:LCS:H4A1	3:D:402:LCS:HB1	1.13	0.42
1:C:166:ALA:HB3	1:C:238:ILE:HD11	2.01	0.42
1:C:6:LEU:C	1:C:7:THR:O	2.57	0.42
1:A:151:PHE:CE2	1:C:259:PRO:HG3	2.55	0.42
1:A:72:THR:OG1	1:A:80:HIS:HE1	2.01	0.42
1:D:6:LEU:HD12	1:D:6:LEU:HA	1.83	0.42
1:D:3:LEU:HD23	1:D:244:LEU:HD11	2.02	0.41
1:B:98:LEU:HG	1:B:132:LEU:HD21	2.02	0.41
1:C:298:GLY:HA2	1:C:303:ARG:HB2	2.01	0.41
1:D:275:LEU:HA	1:D:275:LEU:HD13	1.79	0.41
1:B:275:LEU:HA	1:B:275:LEU:HD13	1.84	0.41
1:C:273:LYS:HD2	1:C:273:LYS:HA	1.82	0.41
1:C:51:LYS:NZ	3:C:401:LCS:O3P	2.53	0.41
1:B:253:TRP:CZ2	1:B:303:ARG:HB3	2.56	0.41
1:A:217:GLY:O	1:A:252:LEU:HA	2.21	0.41
1:A:3:LEU:O	1:A:6:LEU:HB2	2.21	0.41
1:B:51:LYS:HE2	3:B:402:LCS:H4A2	2.01	0.41
1:B:273:LYS:HD2	1:B:273:LYS:HA	1.87	0.40
1:B:305:ASN:OD1	1:B:306:ASP:N	2.54	0.40
1:B:228:LYS:HB3	1:B:229:PRO:HD3	2.02	0.40
1:A:1:MET:H2	1:A:2:PRO:HD2	1.85	0.40
1:C:305:ASN:C	1:C:305:ASN:OD1	2.60	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%)	314 (96%)	9 (3%)	3 (1%)	21	36
1	B	323/342 (94%)	314 (97%)	7 (2%)	2 (1%)	30	48
1	C	324/342 (95%)	307 (95%)	13 (4%)	4 (1%)	16	27
1	D	327/342 (96%)	312 (95%)	10 (3%)	5 (2%)	13	21
All	All	1300/1368 (95%)	1247 (96%)	39 (3%)	14 (1%)	17	29

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	VAL
1	B	183	VAL
1	B	184	VAL
1	C	8	ARG
1	C	181	GLU
1	D	182	GLU
1	D	183	VAL
1	A	182	GLU
1	C	131	ALA
1	D	185	GLY
1	A	196	ALA
1	C	196	ALA
1	D	184	VAL
1	D	196	ALA

### 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	250/267 (94%)	240 (96%)	10 (4%)	38	63
1	B	248/267 (93%)	233 (94%)	15 (6%)	24	41
1	C	251/267 (94%)	236 (94%)	15 (6%)	24	41
1	D	251/267 (94%)	245 (98%)	6 (2%)	57	81
All	All	1000/1068 (94%)	954 (95%)	46 (5%)	33	56



All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	35	ILE
1	A	64	ARG
1	A	130	ASP
1	A	178	GLN
1	A	184	VAL
1	A	251	HIS
1	A	273	LYS
1	A	284	ASP
1	A	305	ASN
1	B	6	LEU
1	B	7	THR
1	B	33	ARG
1	B	52	LEU
1	B	90	LYS
1	B	120	ASP
1	B	127	GLU
1	B	129	CYS
1	B	178	GLN
1	B	181	GLU
1	B	234	LEU
1	B	273	LYS
1	B	300	SER
1	B	305	ASN
1	B	327	HIS
1	C	7	THR
1	C	33	ARG
1	C	52	LEU
1	C	64	ARG
1	C	65	GLU
1	C	120	ASP
1	C	127	GLU
1	C	142	LEU
1	C	174	LEU
1	C	182	GLU
1	C	183	VAL
1	C	273	LYS
1	C	303	ARG
1	C	305	ASN
1	C	307	ASP
1	D	6	LEU
1	D	13	GLU

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Mol	Chain	Res	Type
1	D	33	ARG
1	D	273	LYS
1	D	303	ARG
1	D	305	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	GLN
1	A	138	GLN
1	A	140	GLN
1	A	208	HIS
1	A	314	HIS
1	B	80	HIS
1	B	83	GLN
1	B	125	GLN
1	B	138	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	178	GLN
1	C	314	HIS
1	C	325	HIS
1	D	80	HIS
1	D	83	GLN
1	D	138	GLN
1	D	140	GLN
1	D	149	GLN
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	1.56	1 (11%)	9,11,11	0.70	0
3	LCS	A	402	-	22,23,23	3.62	14 (63%)	24,33,33	3.41	10 (41%)
2	BEN	B	401	-	9,9,9	1.21	1 (11%)	9,11,11	1.05	1 (11%)
3	LCS	B	402	-	22,23,23	3.32	11 (50%)	24,33,33	2.82	13 (54%)
3	LCS	C	401	-	22,23,23	4.05	8 (36%)	24,33,33	2.84	14 (58%)
2	BEN	D	401	-	9,9,9	1.22	1 (11%)	9,11,11	1.58	1 (11%)
3	LCS	D	402	-	22,23,23	3.31	11 (50%)	24,33,33	2.55	10 (41%)

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	LCS	A	402	-	-	0/9/21/21	0/1/2/2
2	BEN	B	401	-	-	0/4/4/4	0/1/1/1
3	LCS	B	402	-	-	0/9/21/21	0/1/2/2
3	LCS	C	401	-	-	0/9/21/21	0/1/2/2
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	LCS	D	402	-	-	2/9/21/21	0/1/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	LCS	OG-ND	-7.49	1.29	1.45
3	A	402	LCS	OG-ND	-7.19	1.29	1.45
3	B	402	LCS	OG-ND	-6.68	1.30	1.45
3	C	401	LCS	OG-ND	-5.35	1.33	1.45
3	A	402	LCS	P-O2P	-4.61	1.38	1.54
3	D	402	LCS	P-O2P	-4.47	1.38	1.54
3	A	402	LCS	P-O3P	-4.28	1.39	1.54
3	B	402	LCS	C4A-N	-4.23	1.40	1.46
3	A	402	LCS	P-O1P	-4.16	1.37	1.51
2	A	401	BEN	C1-C	-3.74	1.41	1.47
3	B	402	LCS	P-O3P	-3.45	1.42	1.54
3	D	402	LCS	P-O1P	-3.36	1.40	1.51
2	B	401	BEN	C1-C	-3.36	1.41	1.47
3	B	402	LCS	P-O2P	-3.24	1.43	1.54
3	D	402	LCS	P-O3P	-3.14	1.43	1.54
3	B	402	LCS	P-O1P	-3.14	1.40	1.51
3	C	401	LCS	P-O2P	-3.14	1.43	1.54
3	A	402	LCS	OG-CB	-3.06	1.39	1.44
3	D	402	LCS	P-O4P	-2.92	1.50	1.60
3	D	402	LCS	C4A-N	-2.85	1.42	1.46
3	A	402	LCS	CB-CA	-2.81	1.46	1.50
3	A	402	LCS	C-ND	-2.75	1.31	1.35
3	B	402	LCS	O3-C3	-2.74	1.30	1.37
3	C	401	LCS	P-O3P	-2.66	1.45	1.54
3	D	402	LCS	OG-CB	-2.60	1.39	1.44
3	B	402	LCS	C6-N1	-2.46	1.29	1.34
3	D	402	LCS	O3-C3	-2.44	1.31	1.37
3	C	401	LCS	P-O1P	-2.40	1.43	1.51
3	A	402	LCS	C6-N1	-2.38	1.29	1.34
3	A	402	LCS	P-O4P	-2.31	1.52	1.60
3	A	402	LCS	O3-C3	-2.29	1.31	1.37
2	D	401	BEN	C1-C	-2.21	1.43	1.47
3	B	402	LCS	C-ND	-2.18	1.32	1.35
3	A	402	LCS	C2-N1	-2.04	1.29	1.34
3	C	401	LCS	CB-CA	2.43	1.53	1.50
3	A	402	LCS	C3-C4	3.62	1.45	1.40
3	B	402	LCS	C3-C4	3.74	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	LCS	C3-C4	4.78	1.47	1.40
3	D	402	LCS	C5-C4	5.28	1.47	1.40
3	B	402	LCS	C5-C4	5.31	1.48	1.40
3	D	402	LCS	C3-C4	5.37	1.48	1.40
3	A	402	LCS	C5-C4	6.47	1.49	1.40
3	D	402	LCS	C3-C2	6.55	1.45	1.40
3	C	401	LCS	C5-C4	7.94	1.51	1.40
3	B	402	LCS	C3-C2	8.60	1.46	1.40
3	A	402	LCS	C3-C2	8.62	1.46	1.40
3	C	401	LCS	C3-C2	14.29	1.50	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	LCS	CB-CA-N	-10.99	94.94	128.98
3	D	402	LCS	CB-CA-N	-8.69	102.08	128.98
3	A	402	LCS	C3-C4-C5	-7.36	111.07	118.82
3	B	402	LCS	C4A-C4-C5	-6.32	110.00	119.56
3	C	401	LCS	CB-CA-N	-5.94	110.59	128.98
3	B	402	LCS	CB-CA-N	-5.67	111.43	128.98
3	D	402	LCS	O2P-P-O4P	-3.58	96.25	106.56
3	B	402	LCS	C3-C4-C5	-3.29	115.35	118.82
3	B	402	LCS	O4P-P-O1P	-3.00	99.49	107.14
3	A	402	LCS	O2P-P-O4P	-2.88	98.26	106.56
3	B	402	LCS	O2P-P-O4P	-2.85	98.36	106.56
3	C	401	LCS	O3P-P-O1P	-2.74	101.78	110.58
3	C	401	LCS	C3-C4-C5	-2.59	116.09	118.82
3	C	401	LCS	O4P-C5A-C5	-2.56	104.76	108.99
3	D	402	LCS	C3-C4-C5	-2.54	116.14	118.82
3	C	401	LCS	C5-C6-N1	-2.54	119.45	123.86
3	C	401	LCS	O2P-P-O1P	-2.53	102.44	110.58
3	A	402	LCS	C5A-C5-C6	-2.52	114.52	119.28
3	D	402	LCS	O4P-P-O1P	-2.49	100.80	107.14
3	C	401	LCS	O4P-P-O1P	-2.41	101.00	107.14
3	D	402	LCS	C4A-C4-C5	-2.33	116.03	119.56
3	C	401	LCS	C4-C3-C2	-2.30	115.89	120.03
3	B	402	LCS	C4-C3-C2	-2.08	116.29	120.03
3	B	402	LCS	C6-N1-C2	2.24	123.84	119.28
3	B	402	LCS	O4P-C5A-C5	2.25	112.71	108.99
3	D	402	LCS	C4-C4A-N	2.26	122.97	113.97
3	D	402	LCS	O2P-P-O1P	2.29	117.94	110.58
3	C	401	LCS	C6-N1-C2	2.34	124.06	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	LCS	O3-C3-C4	2.37	125.19	118.11
3	D	402	LCS	C6-N1-C2	2.43	124.24	119.28
3	B	402	LCS	O3P-P-O2P	2.43	116.65	107.38
3	A	402	LCS	O3P-P-O4P	2.51	113.79	106.56
3	B	402	LCS	C2A-C2-C3	2.62	124.19	121.04
3	A	402	LCS	C4-C4A-N	2.67	124.62	113.97
3	A	402	LCS	O3P-P-O2P	2.70	117.66	107.38
3	B	402	LCS	O2P-P-O1P	2.80	119.59	110.58
2	B	401	BEN	C1-C-N2	2.93	122.79	118.11
3	A	402	LCS	C6-C5-C4	3.32	120.57	118.09
2	D	401	BEN	C1-C-N2	3.39	123.53	118.11
3	C	401	LCS	O3P-P-O2P	3.44	120.46	107.38
3	D	402	LCS	O4P-C5A-C5	3.44	114.68	108.99
3	B	402	LCS	C6-C5-C4	3.80	120.93	118.09
3	C	401	LCS	C4-C4A-N	3.90	129.52	113.97
3	C	401	LCS	O3-C3-C2	4.19	124.94	117.66
3	C	401	LCS	O3P-P-O4P	4.27	118.87	106.56
3	A	402	LCS	O4P-C5A-C5	4.39	116.25	108.99
3	A	402	LCS	C4A-C4-C5	4.92	127.00	119.56
3	B	402	LCS	C4-C4A-N	5.01	133.97	113.97
3	C	401	LCS	C6-C5-C4	6.30	122.79	118.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	LCS	C3-C4-C4A-N
3	D	402	LCS	C5-C4-C4A-N

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	LCS	1	0
3	B	402	LCS	2	0
3	C	401	LCS	5	0
3	D	402	LCS	1	0

## 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, 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%)	-0.19	0 100 100	11, 20, 40, 47	3 (0%)
1	B	325/342 (95%)	-0.03	8 (2%) 61 64	11, 20, 37, 47	2 (0%)
1	C	323/342 (94%)	-0.02	9 (2%) 56 60	11, 20, 38, 45	5 (1%)
1	D	328/342 (95%)	-0.17	1 (0%) 94 95	11, 20, 40, 47	2 (0%)
All	All	1304/1368 (95%)	-0.10	18 (1%) 78 80	11, 20, 40, 47	12 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ALA	4.7
1	D	184	VAL	3.4
1	B	183	VAL	3.1
1	B	305	ASN	3.0
1	C	240	GLY	3.0
1	C	183	VAL	2.6
1	C	150	GLY	2.5
1	C	184	VAL	2.5
1	C	208	HIS	2.5
1	C	158	VAL	2.4
1	B	6	LEU	2.4
1	C	144	THR	2.4
1	C	243	ALA	2.3
1	B	149	GLN	2.3
1	B	211	PRO	2.3
1	B	242	LEU	2.2
1	B	245	THR	2.2
1	C	146	ILE	2.2



## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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	LCS	D	402	22/22	0.94	0.16	1.85	18,21,21,23	6
2	BEN	B	401	9/9	0.95	0.19	1.79	19,20,21,21	0
3	LCS	B	402	22/22	0.92	0.16	1.18	19,21,21,24	6
3	LCS	C	401	22/22	0.93	0.18	1.08	18,21,22,23	6
3	LCS	A	402	22/22	0.94	0.15	0.73	19,21,22,23	0
2	BEN	A	401	9/9	0.92	0.17	0.71	10,14,18,19	0
2	BEN	D	401	9/9	0.97	0.13	-1.14	10,11,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.