



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:04 AM UTC

PDB ID : 4D8W / pdb_00004d8w
Title : Salmonella typhimurium D-Cysteine desulfhydrase soaked with D-cys shows pyruvate bound 4 Å away from 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

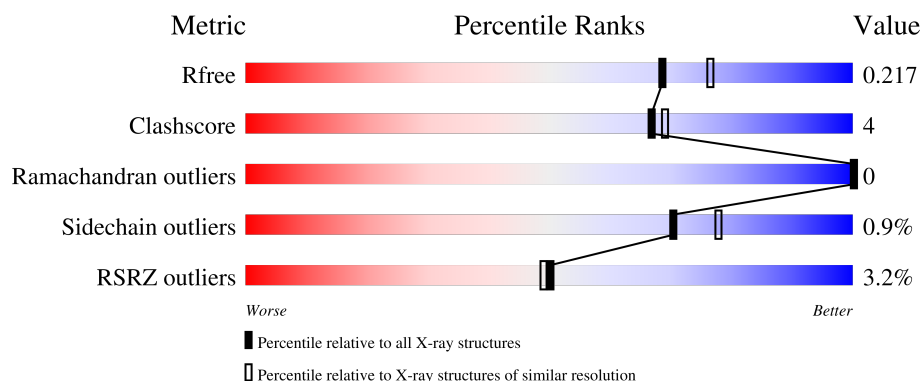
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	0% 89% 6% • •
1	B	342	2% 89% 6% • 5%
1	C	342	9% 87% 6% • 6%
1	D	342	0% 88% 8% •

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
4	PYR	D	402	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10615 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	2	0
			2462	1570	414	468	1	9			
1	B	326	Total	C	N	O	P	S	1	4	0
			2450	1562	411	467	1	9			
1	C	322	Total	C	N	O	P	S	0	3	0
			2407	1533	402	462	1	9			
1	D	328	Total	C	N	O	P	S	0	4	0
			2474	1578	415	470	1	10			

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

Continued on next page...

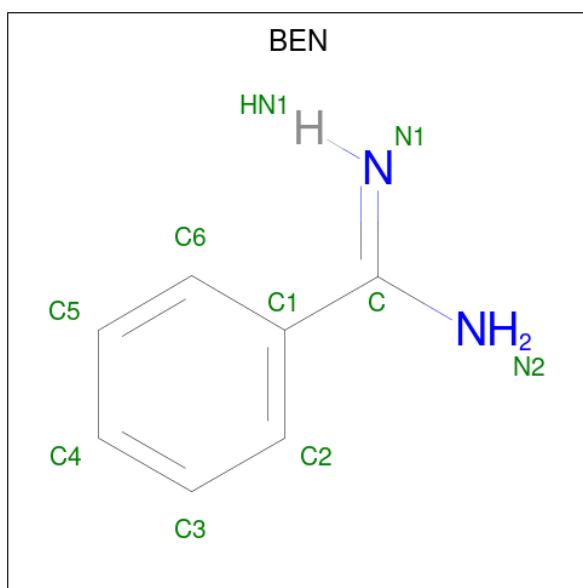
Continued from previous page...

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

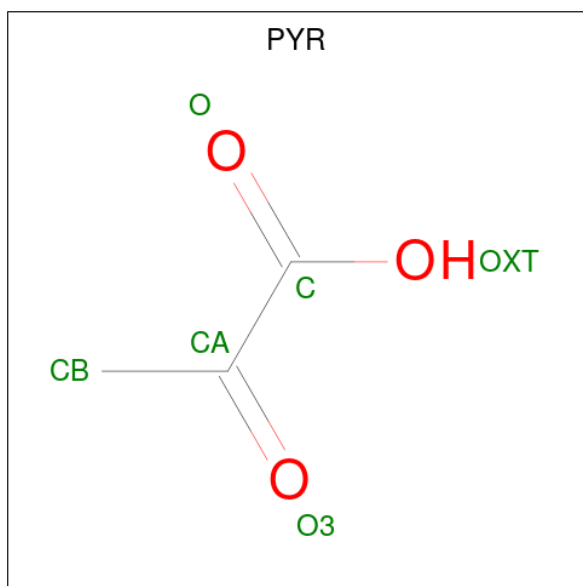
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



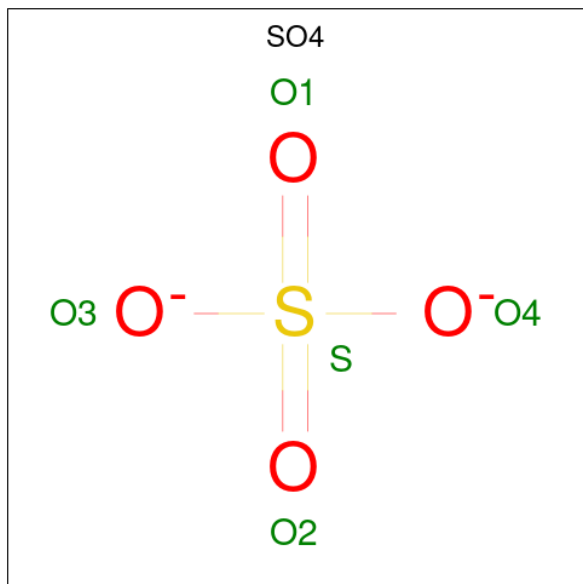
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	D	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



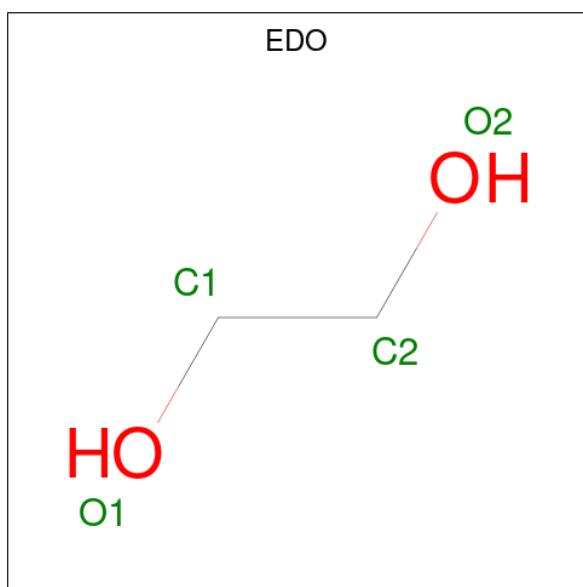
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	216	Total	O	0	0
			216	216		
7	B	175	Total	O	0	0
			175	175		
7	C	141	Total	O	0	0
			141	141		
7	D	216	Total	O	0	0
			216	216		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.29Å 165.19Å 68.06Å 90.00° 118.71° 90.00°	Depositor
Resolution (Å)	48.38 – 2.01 48.38 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-2.01) 99.9 (48.38-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.217 0.183 , 0.217	Depositor DCC
R_{free} test set	4292 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h-l,k,h 0.003 for l,k,-h-l 0.024 for h,-k,-h-l 0.032 for -h-l,-k,l 0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10615	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: EDO, CL, BEN, LLP, PYR, SO4

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	0.61	0/2487	0.78	0/3390
1	B	0.59	0/2483	0.79	0/3385
1	C	0.56	0/2432	0.80	0/3315
1	D	0.60	0/2505	0.79	0/3414
All	All	0.59	0/9907	0.79	0/13504

There are no bond length outliers.

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	2462	0	2460	16	0
1	B	2450	0	2448	19	0
1	C	2407	0	2393	23	0
1	D	2474	0	2477	17	0
2	A	1	0	0	1	0
3	A	9	0	7	1	0
3	B	9	0	7	0	0
3	D	9	0	7	0	0
4	A	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	0	0	0
4	D	6	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
7	A	216	0	0	2	0
7	B	175	0	0	0	0
7	C	141	0	0	1	0
7	D	216	0	0	3	0
All	All	10615	0	9811	73	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 (73) 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:B:11[B]:ARG:HG2	1:B:11[B]:ARG:HH11	0.98	1.11
1:B:11[B]:ARG:HG2	1:B:11[B]:ARG:NH1	1.74	0.94
1:B:11[B]:ARG:HH11	1:B:11[B]:ARG:CG	1.88	0.76
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	1.85	0.76
1:C:43:THR:CG2	1:C:52:LEU:HD22	2.16	0.74
1:C:167:MET:HE1	1:C:242:LEU:HD11	1.71	0.70
1:C:43:THR:HG21	1:C:52:LEU:HD22	1.79	0.64
1:B:33:ARG:HH11	1:B:33:ARG:CG	2.10	0.64
1:A:251:HIS:HE1	7:A:631:HOH:O	1.83	0.61
1:C:325:HIS:HD2	7:C:614:HOH:O	1.82	0.61
1:D:314:HIS:HD2	1:D:316:GLY:H	1.48	0.61
1:B:11[B]:ARG:NH1	1:B:11[B]:ARG:CG	2.54	0.60
1:A:314:HIS:HD2	1:A:316:GLY:H	1.49	0.60
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.68	0.58
1:C:157:PRO:HG3	1:C:162:SER:HB3	1.85	0.58
1:B:33:ARG:HG3	1:B:33:ARG:NH1	2.19	0.57
1:A:105:THR:OG1	1:A:328[A]:VAL:HG12	2.06	0.56
7:A:625:HOH:O	1:C:327:HIS:HD2	1.90	0.55
1:D:52:LEU:HD22	7:D:715:HOH:O	2.05	0.54
1:C:314:HIS:HD2	1:C:316:GLY:H	1.55	0.54
1:B:134:ASP:H	1:B:138:GLN:HE21	1.55	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:THR:CG2	1:C:52:LEU:CD2	2.87	0.52
1:B:134:ASP:H	1:B:138:GLN:NE2	2.08	0.52
1:C:71:ILE:HG12	1:C:96:VAL:HB	1.93	0.51
1:B:3:LEU:HD23	1:B:244:LEU:HD11	1.92	0.51
1:B:33:ARG:CG	1:B:33:ARG:NH1	2.73	0.51
1:A:306:ASP:OD2	1:A:306:ASP:C	2.53	0.51
1:D:51:LLP:HE3	1:D:80:HIS:HB2	1.93	0.50
1:D:251:HIS:HE1	7:D:691:HOH:O	1.95	0.50
1:A:51:LLP:HE3	1:A:80:HIS:HB2	1.94	0.49
1:B:7:THR:HA	1:B:11[B]:ARG:HH22	1.78	0.49
1:D:26:ARG:HD3	1:D:278:LEU:O	2.13	0.49
2:A:401:CL:CL	3:A:402:BEN:N2	2.84	0.48
1:B:51:LLP:HE3	1:B:80:HIS:HB2	1.96	0.48
1:C:43:THR:HG23	1:C:52:LEU:CD2	2.43	0.48
1:C:112:THR:OG1	1:D:325:HIS:HE1	1.97	0.48
1:A:314:HIS:CD2	1:A:316:GLY:H	2.31	0.47
1:D:259:PRO:HG2	1:D:263:VAL:HG11	1.97	0.47
1:A:132:LEU:HA	1:A:138:GLN:HE22	1.80	0.46
1:C:134:ASP:H	1:C:138:GLN:HE21	1.62	0.46
1:C:43:THR:HG23	1:C:52:LEU:HD22	1.92	0.46
1:B:189:VAL:HG23	1:B:213:VAL:HG11	1.98	0.46
1:D:51:LLP:H6	1:D:192:ALA:HB3	1.98	0.46
1:C:51:LLP:H6	1:C:192:ALA:HB3	1.96	0.46
1:B:72:THR:OG1	1:B:80:HIS:HE1	1.99	0.46
1:D:94:HIS:HD2	7:D:501:HOH:O	2.00	0.45
1:C:314:HIS:CD2	1:C:316:GLY:H	2.35	0.44
1:A:1:MET:N	1:A:2:PRO:HD2	2.33	0.44
1:A:259:PRO:HG2	1:A:263:VAL:HG11	2.00	0.43
1:C:134:ASP:H	1:C:138:GLN:NE2	2.16	0.43
1:A:15:ILE:CD1	1:A:53:ARG:HG2	2.49	0.43
1:A:282:LEU:O	1:A:314:HIS:HE1	2.02	0.43
1:C:105:THR:CB	1:C:328[A]:VAL:HG12	2.48	0.43
1:D:94:HIS:HE1	1:D:125:GLN:NE2	2.16	0.43
1:D:33:ARG:NH1	1:D:307[A]:ASP:OD1	2.52	0.43
1:A:272:VAL:HG22	1:A:283:LEU:HB2	2.01	0.43
1:A:51:LLP:H6	1:A:192:ALA:HB3	2.01	0.43
1:B:59:VAL:HG21	1:B:87:VAL:HG11	2.01	0.43
1:B:71:ILE:HG12	1:B:96:VAL:HB	2.00	0.43
1:D:185:GLY:O	1:D:309:PRO:HD2	2.19	0.42
1:C:325:HIS:HE1	1:D:112:THR:OG1	2.03	0.42
1:C:51:LLP:HE3	1:C:80:HIS:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:O	1:C:42:VAL:HG22	2.19	0.42
1:A:26:ARG:HD3	1:A:278:LEU:O	2.20	0.42
1:C:43:THR:HG21	1:C:52:LEU:CD2	2.49	0.41
1:D:134:ASP:H	1:D:138:GLN:NE2	2.18	0.41
1:A:15:ILE:HD11	1:A:53:ARG:HG2	2.02	0.41
1:A:112:THR:OG1	1:B:325:HIS:HE1	2.04	0.41
1:B:51:LLP:H6	1:B:192:ALA:HB3	2.03	0.41
1:C:26:ARG:HD3	1:C:278:LEU:O	2.20	0.41
1:D:2:PRO:HB2	1:D:3:LEU:HD22	2.03	0.41
1:D:199:HIS:CE1	1:D:217:GLY:HA3	2.56	0.41
1:D:301:GLN:HB2	1:D:303:ARG:HG3	2.03	0.41

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	325/342 (95%)	319 (98%)	6 (2%)	0	100	100
1	C	321/342 (94%)	312 (97%)	9 (3%)	0	100	100
1	D	328/342 (96%)	321 (98%)	7 (2%)	0	100	100
All	All	1300/1368 (95%)	1270 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	251/266 (94%)	248 (99%)	3 (1%)	63	70
1	B	251/266 (94%)	247 (98%)	4 (2%)	55	62
1	C	245/266 (92%)	244 (100%)	1 (0%)	84	89
1	D	254/266 (96%)	251 (99%)	3 (1%)	63	70
All	All	1001/1064 (94%)	990 (99%)	11 (1%)	70	73

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

Mol	Chain	Res	Type
1	A	145	ARG
1	A	328[A]	VAL
1	A	328[B]	VAL
1	B	12	LEU
1	B	33	ARG
1	B	245	THR
1	B	307	ASP
1	C	43	THR
1	D	33	ARG
1	D	328[A]	VAL
1	D	328[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	94	HIS
1	A	125	GLN
1	A	138	GLN
1	A	149	GLN
1	A	208	HIS
1	A	251	HIS
1	A	314	HIS
1	A	325	HIS
1	B	80	HIS
1	B	125	GLN
1	B	138	GLN
1	B	149	GLN
1	B	251	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	325	HIS
1	C	138	GLN
1	C	149	GLN
1	C	208	HIS
1	C	241	GLN
1	C	301	GLN
1	C	314	HIS
1	C	325	HIS
1	D	94	HIS
1	D	125	GLN
1	D	138	GLN
1	D	149	GLN
1	D	251	HIS
1	D	301	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 ⓘ

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	C	51	1	23,24,25	0.75	0	25,32,34	1.09	1 (4%)
1	LLP	A	51	1	23,24,25	0.71	0	25,32,34	1.18	2 (8%)
1	LLP	D	51	1	23,24,25	0.76	0	25,32,34	1.03	0
1	LLP	B	51	1	23,24,25	0.75	0	25,32,34	1.17	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	C	51	1	-	2/16/17/19	0/1/1/1
1	LLP	A	51	1	-	3/16/17/19	0/1/1/1
1	LLP	D	51	1	-	2/16/17/19	0/1/1/1
1	LLP	B	51	1	-	3/16/17/19	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LLP	C5-C6-N1	-2.42	119.89	123.83
1	C	51	LLP	C5-C6-N1	-2.09	120.44	123.83
1	B	51	LLP	OP3-P-OP2	2.06	115.53	107.80
1	A	51	LLP	C4-C3-C2	-2.03	119.00	120.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	51	LLP	2	0
1	A	51	LLP	2	0
1	D	51	LLP	2	0
1	B	51	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
6	EDO	C	401	-	3,3,3	0.42	0	2,2,2	0.45	0
4	PYR	A	403	-	5,5,5	1.59	2 (40%)	3,6,6	0.79	0
5	SO4	D	403	-	4,4,4	0.42	0	6,6,6	0.42	0
3	BEN	A	402	-	9,9,9	0.99	1 (11%)	7,11,11	0.73	0
5	SO4	A	404	-	4,4,4	0.42	0	6,6,6	0.25	0
5	SO4	B	403	-	4,4,4	0.37	0	6,6,6	0.13	0
3	BEN	B	401	-	9,9,9	0.81	0	7,11,11	0.64	0
5	SO4	C	402	-	4,4,4	0.42	0	6,6,6	0.22	0
4	PYR	D	402	-	5,5,5	1.50	1 (20%)	3,6,6	1.49	1 (33%)
3	BEN	D	401	-	9,9,9	1.35	1 (11%)	7,11,11	0.76	0
6	EDO	B	402	-	3,3,3	0.43	0	2,2,2	0.35	0
4	PYR	C	403	-	5,5,5	1.42	1 (20%)	3,6,6	1.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	401	-	-	0/1/1/1	-
4	PYR	A	403	-	-	2/4/4/4	-
3	BEN	A	402	-	-	0/4/4/4	0/1/1/1
3	BEN	B	401	-	-	0/4/4/4	0/1/1/1
4	PYR	D	402	-	-	4/4/4/4	-
3	BEN	D	401	-	-	0/4/4/4	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	402	-	-	0/1/1/1	-
4	PYR	C	403	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	BEN	C-N2	-2.77	1.26	1.33
4	D	402	PYR	CA-C	-2.53	1.46	1.54
4	A	403	PYR	CA-C	-2.38	1.46	1.54
4	C	403	PYR	CA-C	-2.30	1.46	1.54
3	A	402	BEN	C1-C	2.14	1.51	1.47
4	A	403	PYR	OXT-C	-2.02	1.25	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	PYR	OXT-C-CA	2.20	119.70	113.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	PYR	OXT-C-CA-CB
4	D	402	PYR	O-C-CA-O3
4	D	402	PYR	OXT-C-CA-O3
4	D	402	PYR	OXT-C-CA-CB
4	A	403	PYR	O-C-CA-CB
4	D	402	PYR	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	BEN	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, 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	327/342 (95%)	-0.36	2 (0%) 85 85	11, 16, 30, 39	2 (0%)
1	B	325/342 (95%)	-0.02	6 (1%) 67 67	12, 21, 40, 53	5 (1%)
1	C	321/342 (93%)	0.46	30 (9%) 14 13	9, 26, 45, 61	3 (0%)
1	D	327/342 (95%)	-0.35	4 (1%) 76 76	8, 17, 32, 49	4 (1%)
All	All	1300/1368 (95%)	-0.07	42 (3%) 50 49	8, 19, 39, 61	14 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LEU	4.1
1	B	183	VAL	3.8
1	B	1	MET	3.8
1	C	7	THR	3.7
1	B	245	THR	3.5
1	C	150	GLY	3.4
1	D	185	GLY	3.2
1	B	2	PRO	3.2
1	C	243	ALA	3.1
1	C	208	HIS	3.1
1	C	211	PRO	3.1
1	D	16	GLY	3.0
1	B	182	GLU	3.0
1	C	146	ILE	3.0
1	C	148	ALA	2.9
1	B	148	ALA	2.9
1	A	328[A]	VAL	2.9
1	C	242	LEU	2.8
1	C	143	ALA	2.8
1	C	328[A]	VAL	2.8
1	D	328[A]	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	145	ARG	2.7
1	D	1	MET	2.7
1	C	239	ALA	2.6
1	C	144	THR	2.6
1	C	212	ASP	2.5
1	C	225	ALA	2.5
1	C	151	PHE	2.3
1	C	135	PRO	2.3
1	C	246	ALA	2.3
1	C	240	GLY	2.3
1	C	244	LEU	2.2
1	C	153	PRO	2.2
1	C	238	ILE	2.2
1	C	305	ASN	2.2
1	C	241	GLN	2.1
1	C	16	GLY	2.1
1	C	248	ALA	2.1
1	C	149	GLN	2.1
1	C	8	ARG	2.0
1	C	133	THR	2.0
1	A	16	GLY	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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	C	51	24/25	0.94	0.08	19,21,23,24	0
1	LLP	B	51	24/25	0.95	0.07	16,17,19,20	0
1	LLP	D	51	24/25	0.97	0.06	12,13,14,15	0
1	LLP	A	51	24/25	0.98	0.05	11,12,13,14	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PYR	C	403	6/6	0.65	0.21	36,37,37,38	6
4	PYR	A	403	6/6	0.67	0.20	29,30,30,32	6
4	PYR	D	402	6/6	0.86	0.13	28,29,29,29	6
6	EDO	B	402	4/4	0.88	0.15	34,34,34,35	0
3	BEN	B	401	9/9	0.91	0.08	29,30,30,31	0
6	EDO	C	401	4/4	0.91	0.10	29,30,31,32	0
3	BEN	A	402	9/9	0.94	0.07	14,14,15,15	0
3	BEN	D	401	9/9	0.95	0.06	13,13,14,14	0
5	SO4	C	402	5/5	0.95	0.09	23,24,24,25	5
5	SO4	A	404	5/5	0.97	0.06	16,16,16,16	5
5	SO4	D	403	5/5	0.97	0.06	15,15,15,16	5
5	SO4	B	403	5/5	0.98	0.05	22,22,22,22	5
2	CL	A	401	1/1	0.99	0.22	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.