



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 AM UTC

PDB ID : 4LW2 / pdb_00004lw2
Title : Structural changes during cysteine desulfurase CsdA and sulfur-acceptor CsdE interactions provide insight into the trans-persulfuration
Authors : Kim, S.; Park, S.Y.
Deposited on : 2013-07-26
Resolution : 1.80 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

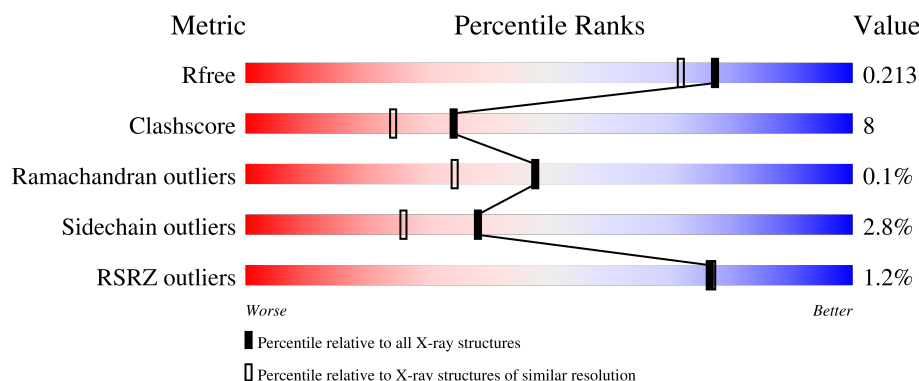
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	404	 84% 13% ...
1	B	404	 2% 81% 16% ..
1	C	404	 % 80% 17% ..

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	GOL	A	502	-	X	X	-
3	GOL	B	502	-	-	X	-
3	GOL	C	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10292 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 Cysteine sulfinate desulfinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	2	0
			3043	1930	531	570	12			
1	B	399	Total	C	N	O	S	0	3	0
			3046	1932	529	573	12			
1	C	398	Total	C	N	O	S	0	2	0
			3033	1925	526	570	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q46925
A	-1	SER	-	expression tag	UNP Q46925
A	0	HIS	-	expression tag	UNP Q46925
B	-2	GLY	-	expression tag	UNP Q46925
B	-1	SER	-	expression tag	UNP Q46925
B	0	HIS	-	expression tag	UNP Q46925
C	-2	GLY	-	expression tag	UNP Q46925
C	-1	SER	-	expression tag	UNP Q46925
C	0	HIS	-	expression tag	UNP Q46925

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

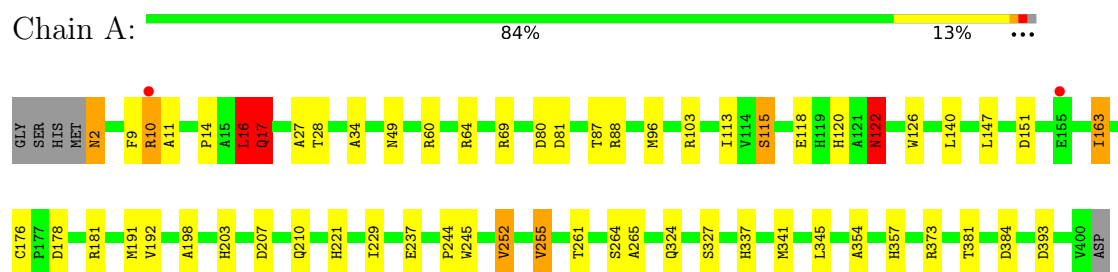
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	386	Total	O	0	0
			386	386		
4	B	363	Total	O	0	0
			363	363		
4	C	358	Total	O	0	0
			358	358		

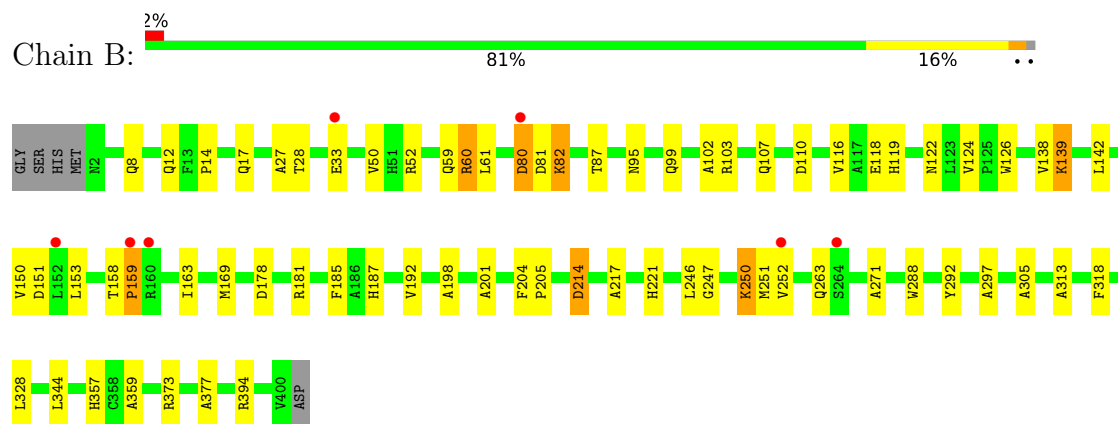
3 Residue-property plots [i](#)

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.

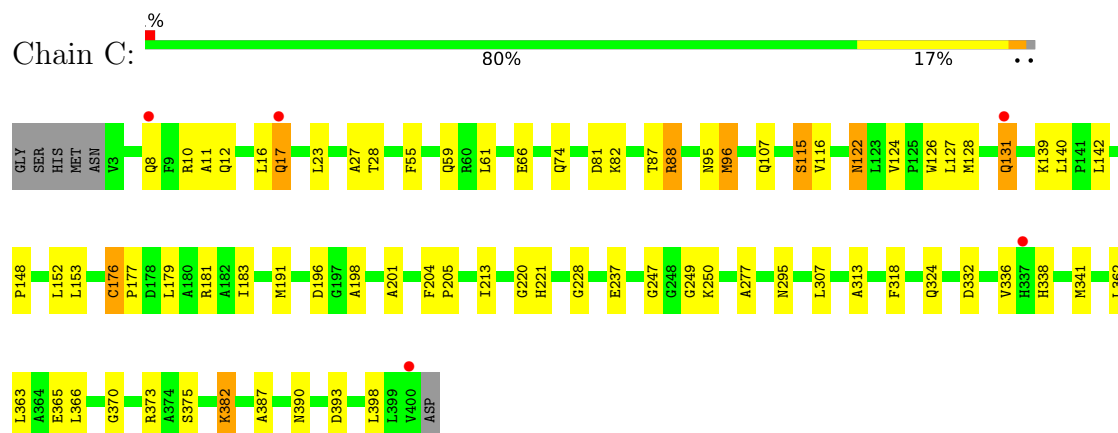
• Molecule 1: Cysteine sulfinic desulfinate



• Molecule 1: Cysteine sulfinic desulfinate



• Molecule 1: Cysteine sulfinic desulfinate



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.30Å 91.44Å 83.89Å 90.00° 97.26° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.80) 99.3 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.165 , 0.212 0.169 , 0.213	Depositor DCC
R_{free} test set	5824 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10292	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: PLP, GOL

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	1.59	19/3116 (0.6%)	1.22	7/4245 (0.2%)
1	B	1.56	16/3122 (0.5%)	1.23	8/4254 (0.2%)
1	C	1.51	15/3106 (0.5%)	1.23	10/4232 (0.2%)
All	All	1.55	50/9344 (0.5%)	1.23	25/12731 (0.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	VAL	CA-CB	11.15	1.60	1.54
1	A	255	VAL	CA-CB	7.64	1.64	1.54
1	A	118	GLU	N-CA	7.25	1.54	1.46
1	C	96	MET	SD-CE	7.15	1.97	1.79
1	C	277	ALA	CA-CB	6.93	1.64	1.53
1	C	213	ILE	CA-CB	6.84	1.62	1.54
1	B	59	GLN	C-O	-6.33	1.16	1.24
1	B	198	ALA	N-CA	6.20	1.53	1.46
1	C	390	ASN	N-CA	6.17	1.53	1.46
1	A	88	ARG	C-N	-6.08	1.25	1.32
1	C	198	ALA	N-CA	6.08	1.53	1.46
1	B	50	VAL	C-O	-6.05	1.18	1.24
1	A	17	GLN	CA-C	6.02	1.60	1.52
1	B	87	THR	C-O	-5.97	1.16	1.24
1	B	118	GLU	N-CA	5.96	1.53	1.46
1	C	387	ALA	CA-CB	5.95	1.62	1.53
1	A	34	ALA	CA-CB	5.91	1.62	1.53
1	C	10	ARG	C-O	-5.89	1.17	1.24
1	A	393	ASP	C-O	-5.87	1.17	1.24
1	A	122	ASN	C-O	-5.80	1.16	1.23
1	A	11	ALA	C-O	-5.79	1.16	1.24
1	C	220	GLY	CA-C	5.71	1.58	1.52
1	C	23	LEU	N-CA	5.66	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	HIS	C-O	5.65	1.31	1.23
1	B	201	ALA	CA-CB	5.64	1.62	1.53
1	C	393	ASP	N-CA	5.62	1.53	1.46
1	B	328	LEU	C-O	-5.61	1.17	1.24
1	B	138	VAL	CA-CB	5.60	1.60	1.54
1	A	87	THR	C-N	5.59	1.41	1.33
1	A	229	ILE	CA-CB	5.58	1.62	1.54
1	B	288	TRP	CA-C	5.48	1.59	1.52
1	A	207	ASP	CA-CB	5.47	1.59	1.52
1	A	9	PHE	C-O	-5.46	1.17	1.24
1	A	384	ASP	N-CA	5.46	1.52	1.46
1	B	305	ALA	CA-C	5.45	1.59	1.52
1	C	61	LEU	N-CA	5.36	1.52	1.46
1	A	16	LEU	CA-C	-5.36	1.45	1.52
1	B	217	ALA	N-CA	5.30	1.52	1.46
1	C	11	ALA	C-O	-5.28	1.17	1.24
1	A	354	ALA	CA-CB	5.25	1.62	1.53
1	A	163	ILE	C-O	5.23	1.29	1.24
1	B	377	ALA	N-CA	-5.23	1.42	1.46
1	A	120	HIS	C-O	-5.22	1.17	1.24
1	B	60	ARG	C-O	-5.18	1.18	1.24
1	B	61	LEU	C-O	-5.16	1.18	1.24
1	C	191	MET	N-CA	5.12	1.52	1.45
1	C	228	GLY	N-CA	5.07	1.52	1.45
1	A	87	THR	C-O	-5.05	1.17	1.23
1	A	265	ALA	C-O	5.04	1.30	1.23
1	B	297	ALA	CA-CB	5.03	1.61	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	VAL	CA-C-N	-7.67	111.06	119.19
1	B	124	VAL	C-N-CA	-7.67	111.06	119.19
1	C	107	GLN	CA-C-N	-7.40	112.14	119.76
1	C	107	GLN	C-N-CA	-7.40	112.14	119.76
1	A	87	THR	CA-C-N	-7.12	110.31	122.56
1	A	87	THR	C-N-CA	-7.12	110.31	122.56
1	B	102	ALA	N-CA-C	6.80	118.35	111.07
1	B	185	PHE	N-CA-C	6.66	118.19	111.07
1	A	244	PRO	CB-CA-C	-6.37	102.91	111.12
1	B	153	LEU	CA-C-N	-6.14	112.53	119.28
1	B	153	LEU	C-N-CA	-6.14	112.53	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	LEU	N-CA-C	6.06	117.89	111.28
1	C	153	LEU	CA-C-N	-5.82	112.71	119.47
1	C	153	LEU	C-N-CA	-5.82	112.71	119.47
1	B	139	LYS	N-CA-C	5.79	118.09	109.59
1	C	398	LEU	N-CA-C	5.64	117.51	111.36
1	B	214	ASP	N-CA-C	5.59	117.18	111.14
1	A	103	ARG	CA-C-N	-5.41	114.25	119.87
1	A	103	ARG	C-N-CA	-5.41	114.25	119.87
1	A	252	VAL	CB-CA-C	-5.33	103.57	111.19
1	C	176	CYS	CA-C-N	-5.19	115.23	120.21
1	C	176	CYS	C-N-CA	-5.19	115.23	120.21
1	C	124	VAL	CA-C-N	-5.18	114.28	119.56
1	C	124	VAL	C-N-CA	-5.18	114.28	119.56
1	C	16	LEU	N-CA-C	5.09	116.83	111.28

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	3043	0	3010	40	0
1	B	3046	0	3009	48	0
1	C	3033	0	2997	52	0
2	A	15	0	6	2	0
2	B	15	0	7	0	0
2	C	15	0	6	1	0
3	A	6	0	7	5	0
3	B	6	0	8	8	0
3	C	6	0	8	4	0
4	A	386	0	0	6	0
4	B	363	0	0	10	0
4	C	358	0	0	13	0
All	All	10292	0	9058	138	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 8.

All (138) 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:C:8:GLN:HG2	4:C:688:HOH:O	1.52	1.07
1:C:17:GLN:HG3	4:C:854:HOH:O	1.53	1.05
1:B:373:ARG:HH22	3:B:502:GOL:H31	1.22	1.02
1:C:66:GLU:HG2	4:C:791:HOH:O	1.62	0.97
1:A:261:THR:HG23	4:A:756:HOH:O	1.66	0.94
1:C:59:GLN:HG2	4:C:838:HOH:O	1.68	0.93
1:A:373:ARG:HH22	3:A:502:GOL:H31	1.32	0.92
1:C:179:LEU:O	1:C:183:ILE:HD13	1.68	0.91
1:A:176:CYS:H	1:A:324:GLN:HE22	1.10	0.90
1:B:99:GLN:HE22	1:B:103:ARG:HH11	1.16	0.89
1:C:176:CYS:H	1:C:324:GLN:HE22	0.92	0.89
1:B:12:GLN:HG3	4:B:762:HOH:O	1.74	0.88
1:C:176:CYS:H	1:C:324:GLN:NE2	1.72	0.87
1:B:95:ASN:HD21	1:C:247:GLY:H	1.23	0.81
1:C:336:VAL:HG11	1:C:341:MET:HE3	1.61	0.81
1:B:151:ASP:OD1	1:B:181:ARG:NH1	2.14	0.80
1:A:151:ASP:OD1	1:A:181:ARG:NH2	2.15	0.79
1:A:17:GLN:H	1:A:17:GLN:CD	1.89	0.79
1:C:332:ASP:OD1	1:C:338:HIS:HE1	1.65	0.78
1:B:247:GLY:H	1:C:95:ASN:HD21	1.29	0.77
1:A:178:ASP:OD2	1:A:181:ARG:HD3	1.84	0.76
1:C:81:ASP:OD1	1:C:82:LYS:NZ	2.19	0.76
1:C:176:CYS:N	1:C:324:GLN:HE22	1.78	0.75
1:C:336:VAL:HG11	1:C:341:MET:CE	2.17	0.74
1:C:88:ARG:HH21	1:C:88:ARG:HB3	1.50	0.74
1:A:10:ARG:NH2	1:A:381:THR:HG22	2.05	0.72
1:A:176:CYS:H	1:A:324:GLN:NE2	1.86	0.71
1:B:373:ARG:NH2	3:B:502:GOL:H31	2.03	0.71
1:C:295:ASN:ND2	4:C:841:HOH:O	2.25	0.69
1:A:2:ASN:HD22	1:A:2:ASN:N	1.91	0.68
1:B:8:GLN:NE2	1:B:292:TYR:OH	2.28	0.67
1:B:187:HIS:HE1	1:B:214:ASP:OD2	1.76	0.67
1:A:327:SER:HB3	4:A:798:HOH:O	1.93	0.67
1:C:373:ARG:HH22	3:C:502:GOL:H12	1.61	0.66
1:C:128:MET:HA	1:C:131:GLN:OE1	1.96	0.65
1:B:12:GLN:CG	4:B:762:HOH:O	2.36	0.65
1:C:95:ASN:HB2	4:C:737:HOH:O	1.95	0.64
1:B:139:LYS:NZ	4:B:960:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74[B]:GLN:HA	1:C:74[B]:GLN:OE1	1.99	0.62
1:C:183:ILE:HD12	1:C:183:ILE:N	2.14	0.61
1:A:10:ARG:HG2	1:A:16:LEU:CD1	2.30	0.61
1:B:14:PRO:HD3	1:B:33:GLU:HG3	1.81	0.61
1:B:95:ASN:ND2	1:C:247:GLY:H	1.98	0.60
1:B:178:ASP:OD2	1:B:181:ARG:HG3	2.01	0.60
1:B:27:ALA:HA	3:B:502:GOL:H32	1.83	0.60
1:A:176:CYS:N	1:A:324:GLN:HE22	1.93	0.59
1:B:116:VAL:CG2	1:B:142:LEU:HG	2.32	0.59
1:A:337:HIS:HB2	4:A:916:HOH:O	2.02	0.59
1:B:359:ALA:HB2	4:B:955:HOH:O	2.02	0.59
1:B:99:GLN:NE2	1:B:103:ARG:HH11	1.94	0.58
1:B:357:HIS:ND1	3:B:502:GOL:H11	2.19	0.58
1:C:28:THR:OG1	1:C:221:HIS:HD2	1.87	0.58
1:B:80:ASP:OD2	1:B:82:LYS:HB2	2.04	0.57
1:B:178:ASP:CG	1:B:181:ARG:HG3	2.30	0.57
1:A:357:HIS:ND1	3:A:502:GOL:C1	2.68	0.56
1:B:150:VAL:HG21	1:B:178:ASP:HB3	1.88	0.56
1:A:10:ARG:HG2	1:A:16:LEU:HD12	1.87	0.56
1:C:88:ARG:HH21	1:C:88:ARG:CB	2.19	0.55
1:C:122:ASN:ND2	1:C:126:TRP:HE1	2.05	0.54
1:B:17:GLN:HG2	4:C:707:HOH:O	2.08	0.53
1:A:210:GLN:OE1	1:A:210:GLN:C	2.51	0.53
1:C:338:HIS:HD2	4:C:634:HOH:O	1.92	0.53
1:A:122:ASN:ND2	1:A:126:TRP:HE1	2.07	0.53
1:B:28:THR:OG1	1:B:221:HIS:HD2	1.92	0.53
1:B:250:LYS:NZ	4:B:954:HOH:O	2.36	0.52
1:C:12:GLN:HB2	4:C:655:HOH:O	2.08	0.52
1:B:99:GLN:HE22	1:B:103:ARG:NH1	1.96	0.52
1:B:357:HIS:ND1	3:B:502:GOL:C1	2.72	0.52
1:C:115:SER:HA	1:C:140:LEU:HB3	1.90	0.52
1:C:27:ALA:HA	3:C:502:GOL:C1	2.40	0.52
1:B:122:ASN:ND2	1:B:126:TRP:HE1	2.08	0.51
1:C:365:GLU:HG3	4:C:731:HOH:O	2.09	0.51
1:A:163:ILE:HD13	1:A:192:VAL:HG23	1.92	0.51
1:C:8:GLN:CG	4:C:688:HOH:O	2.31	0.51
1:C:27:ALA:HA	3:C:502:GOL:H12	1.92	0.50
1:A:163:ILE:HD13	1:A:192:VAL:CG2	2.42	0.50
1:A:28:THR:OG1	1:A:221:HIS:HD2	1.95	0.49
1:B:187:HIS:CE1	1:B:214:ASP:OD2	2.62	0.49
1:B:81:ASP:OD1	1:B:82:LYS:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:VAL:CG2	1:C:142:LEU:HG	2.43	0.49
1:B:60:ARG:HD3	4:B:957:HOH:O	2.13	0.48
1:C:373:ARG:NH2	3:C:502:GOL:H31	2.28	0.48
1:A:14:PRO:O	1:A:17:GLN:OE1	2.31	0.48
1:A:27:ALA:HA	3:A:502:GOL:H32	1.95	0.48
1:B:116:VAL:HG12	1:B:139:LYS:HG3	1.95	0.48
1:C:148:PRO:HD2	1:C:177:PRO:HB3	1.96	0.48
1:C:313:ALA:HA	1:C:318:PHE:CD2	2.49	0.48
1:A:357:HIS:ND1	3:A:502:GOL:H11	2.29	0.47
1:C:183:ILE:N	1:C:183:ILE:CD1	2.78	0.47
1:C:362:LEU:O	1:C:366:LEU:HG	2.15	0.47
1:C:12:GLN:CG	4:C:655:HOH:O	2.62	0.47
1:A:69:ARG:HB3	1:A:81:ASP:HB2	1.96	0.47
1:A:357:HIS:HA	3:A:502:GOL:H11	1.97	0.46
1:B:169:MET:HE3	4:B:804:HOH:O	2.16	0.46
1:A:2:ASN:N	1:A:2:ASN:ND2	2.59	0.46
1:B:82:LYS:HG2	4:B:876:HOH:O	2.15	0.46
1:C:87:THR:HG22	1:C:96:MET:HE1	1.98	0.46
1:A:203:HIS:HE1	4:A:715:HOH:O	1.99	0.46
1:C:127:LEU:O	1:C:131:GLN:OE1	2.34	0.46
1:A:10:ARG:HH21	1:A:381:THR:HG22	1.78	0.46
1:A:115:SER:HA	1:A:140:LEU:HB3	1.98	0.45
1:C:307:LEU:HD13	1:C:382:LYS:HE3	1.96	0.45
1:B:107:GLN:O	1:B:110:ASP:HB2	2.15	0.45
1:B:373:ARG:NH2	3:B:502:GOL:H12	2.31	0.45
1:B:52:ARG:HA	1:B:52:ARG:HD3	1.73	0.45
1:B:313:ALA:HA	1:B:318:PHE:CD2	2.52	0.45
1:C:55:PHE:CE1	1:C:59:GLN:HG3	2.52	0.45
1:B:116:VAL:HG21	1:B:142:LEU:HG	1.98	0.45
1:C:201:ALA:HA	1:C:205:PRO:HA	1.99	0.45
1:A:96:MET:HG2	1:A:245:TRP:CD1	2.51	0.45
1:B:357:HIS:HA	3:B:502:GOL:H11	1.98	0.45
1:C:179:LEU:O	1:C:183:ILE:CD1	2.54	0.44
1:A:147:LEU:HD12	4:A:867:HOH:O	2.18	0.44
1:A:16:LEU:HD23	1:A:16:LEU:HA	1.84	0.44
1:B:158:THR:HB	1:B:159:PRO:HD2	1.99	0.44
1:C:116:VAL:HG12	1:C:139:LYS:HG3	2.00	0.44
1:A:221:HIS:HE1	2:A:501:PLP:O3P	2.01	0.44
1:C:363:LEU:HD13	1:C:370:GLY:HA2	1.98	0.44
1:A:252:VAL:HG21	1:A:255:VAL:CG2	2.47	0.44
1:C:8:GLN:CD	4:C:688:HOH:O	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:NE2	4:A:737:HOH:O	2.50	0.43
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.81	0.43
1:B:251:MET:HG2	1:B:271:ALA:HB2	2.01	0.43
1:B:163:ILE:HD13	1:B:192:VAL:HG22	2.01	0.42
1:C:116:VAL:CG1	1:C:139:LYS:HG3	2.49	0.42
1:A:96:MET:HG2	1:A:245:TRP:CG	2.53	0.42
1:B:163:ILE:HD13	1:B:192:VAL:CG2	2.49	0.42
1:B:204:PHE:O	1:B:205:PRO:C	2.62	0.42
3:B:502:GOL:H2	4:B:913:HOH:O	2.19	0.42
1:C:88:ARG:HH21	1:C:88:ARG:CG	2.32	0.41
1:A:113:ILE:HD12	1:A:191:MET:HE1	2.01	0.41
1:A:60:ARG:O	1:A:64:ARG:HG3	2.20	0.41
1:A:341:MET:O	1:A:345:LEU:HG	2.21	0.41
1:C:196:ASP:OD2	2:C:501:PLP:N1	2.53	0.41
1:B:263:GLN:HE21	1:B:263:GLN:HB3	1.63	0.41
1:C:249:GLY:O	1:C:250:LYS:HB2	2.19	0.40
1:A:198:ALA:HB3	2:A:501:PLP:C2	2.51	0.40
1:B:394:ARG:HD3	4:B:958:HOH:O	2.22	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	399/404 (99%)	388 (97%)	11 (3%)	0	100	100
1	B	400/404 (99%)	386 (96%)	13 (3%)	1 (0%)	36	25
1	C	398/404 (98%)	390 (98%)	8 (2%)	0	100	100
All	All	1197/1212 (99%)	1164 (97%)	32 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	PRO

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	315/317 (99%)	305 (97%)	10 (3%)	34	22
1	B	316/317 (100%)	311 (98%)	5 (2%)	55	47
1	C	314/317 (99%)	303 (96%)	11 (4%)	32	19
All	All	945/951 (99%)	919 (97%)	26 (3%)	38	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	10	ARG
1	A	16	LEU
1	A	17	GLN
1	A	49	ASN
1	A	80	ASP
1	A	115	SER
1	A	122	ASN
1	A	237	GLU
1	A	264	SER
1	B	80	ASP
1	B	82	LYS
1	B	246	LEU
1	B	250	LYS
1	B	252	VAL
1	C	17	GLN
1	C	88	ARG
1	C	115	SER
1	C	122	ASN
1	C	131	GLN
1	C	152	LEU
1	C	181	ARG

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Mol	Chain	Res	Type
1	C	204	PHE
1	C	237	GLU
1	C	375	SER
1	C	382	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	49	ASN
1	A	59	GLN
1	A	122	ASN
1	A	131	GLN
1	A	221	HIS
1	A	263	GLN
1	A	324	GLN
1	B	2	ASN
1	B	8	GLN
1	B	77	ASN
1	B	95	ASN
1	B	99	GLN
1	B	122	ASN
1	B	187	HIS
1	B	221	HIS
1	B	263	GLN
1	B	295	ASN
1	B	337	HIS
1	C	41	GLN
1	C	95	ASN
1	C	107	GLN
1	C	122	ASN
1	C	221	HIS
1	C	263	GLN
1	C	324	GLN
1	C	338	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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$
3	GOL	A	502	-	5,5,5	1.47	1 (20%)	5,5,5	1.67	2 (40%)
3	GOL	B	502	-	5,5,5	1.15	0	5,5,5	2.09	1 (20%)
2	PLP	A	501	1	15,15,16	3.23	6 (40%)	21,22,23	2.51	11 (52%)
2	PLP	C	501	1	15,15,16	2.61	6 (40%)	21,22,23	1.74	6 (28%)
2	PLP	B	501	1	15,15,16	2.35	4 (26%)	21,22,23	1.84	4 (19%)
3	GOL	C	502	-	5,5,5	1.14	0	5,5,5	2.67	3 (60%)

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
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
3	GOL	C	502	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C4A-C4	-9.31	1.33	1.51
2	C	501	PLP	C4A-C4	-6.83	1.38	1.51
2	B	501	PLP	C4A-C4	-5.94	1.39	1.51
2	A	501	PLP	C6-N1	5.32	1.45	1.34
2	B	501	PLP	C2A-C2	-4.63	1.43	1.50
2	C	501	PLP	C6-N1	4.20	1.43	1.34
2	C	501	PLP	C2A-C2	-3.53	1.44	1.50
2	A	501	PLP	C5A-C5	-3.15	1.42	1.50
2	A	501	PLP	O3-C3	-3.02	1.30	1.36
2	C	501	PLP	C3-C2	2.84	1.43	1.41
2	B	501	PLP	C6-N1	2.56	1.39	1.34
2	A	501	PLP	C2A-C2	-2.45	1.46	1.50
2	C	501	PLP	C5-C4	2.22	1.43	1.40
2	A	501	PLP	C3-C4	2.11	1.44	1.40
2	B	501	PLP	C2-N1	-2.10	1.30	1.33
3	A	502	GOL	O3-C3	2.05	1.51	1.42
2	C	501	PLP	C5A-C5	-2.00	1.45	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLP	O4P-C5A-C5	5.71	120.06	109.36
2	A	501	PLP	C6-N1-C2	5.06	128.38	119.20
2	A	501	PLP	C5-C6-N1	-4.79	116.04	123.83
2	A	501	PLP	C3-C2-N1	-4.45	115.35	120.96
3	C	502	GOL	O2-C2-C3	-4.13	92.09	109.18
3	B	502	GOL	O3-C3-C2	3.62	126.67	110.38
3	C	502	GOL	O1-C1-C2	3.58	126.52	110.38
2	C	501	PLP	C3-C2-N1	-3.54	116.50	120.96
2	A	501	PLP	O3P-P-O4P	-3.11	98.56	106.67
2	A	501	PLP	C4A-C4-C5	-3.06	117.78	120.94
2	A	501	PLP	C5A-C5-C6	-3.01	114.45	119.36
2	A	501	PLP	O4P-C5A-C5	2.91	114.82	109.36
2	C	501	PLP	O4P-C5A-C5	2.85	114.70	109.36
2	C	501	PLP	C5-C6-N1	-2.83	119.23	123.83
2	B	501	PLP	C4A-C4-C5	-2.76	118.09	120.94
2	C	501	PLP	C4A-C4-C5	-2.65	118.21	120.94
2	C	501	PLP	C6-N1-C2	2.59	123.89	119.20
2	B	501	PLP	C3-C2-N1	-2.56	117.72	120.96
2	A	501	PLP	C2A-C2-C3	2.49	123.71	120.80
3	A	502	GOL	O1-C1-C2	-2.48	99.23	110.38
2	C	501	PLP	C3-C4-C5	2.14	121.16	118.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLP	C6-C5-C4	-2.14	116.34	118.10
2	A	501	PLP	C3-C4-C5	2.11	121.13	118.59
2	A	501	PLP	C5A-C5-C4	2.11	126.80	122.64
2	A	501	PLP	O3P-P-O2P	2.11	115.70	107.80
3	A	502	GOL	O2-C2-C1	-2.06	100.65	109.18
3	C	502	GOL	O3-C3-C2	-2.01	101.32	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	B	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	5	0
3	B	502	GOL	8	0
2	A	501	PLP	2	0
2	C	501	PLP	1	0
3	C	502	GOL	4	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, 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	399/404 (98%)	-0.35	2 (0%) 87 88	11, 19, 32, 49	2 (0%)
1	B	399/404 (98%)	-0.16	7 (1%) 67 68	11, 21, 37, 49	3 (0%)
1	C	398/404 (98%)	-0.14	5 (1%) 75 75	12, 22, 38, 45	2 (0%)
All	All	1196/1212 (98%)	-0.22	14 (1%) 76 77	11, 21, 36, 49	7 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	GLN	4.2
1	A	155	GLU	2.8
1	B	160	ARG	2.7
1	C	337	HIS	2.5
1	B	80	ASP	2.5
1	B	33	GLU	2.4
1	C	8	GLN	2.4
1	A	10	ARG	2.3
1	B	159	PRO	2.2
1	B	252	VAL	2.2
1	B	264	SER	2.1
1	C	400	VAL	2.0
1	B	152	LEU	2.0
1	C	17	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
3	GOL	A	502	6/6	0.78	0.17	21,27,35,37	0
3	GOL	C	502	6/6	0.82	0.16	34,37,39,42	0
3	GOL	B	502	6/6	0.87	0.15	27,32,33,40	0
2	PLP	C	501	15/16	0.98	0.05	13,18,21,21	0
2	PLP	A	501	15/16	0.98	0.04	12,14,16,17	0
2	PLP	B	501	15/16	0.99	0.03	13,15,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.