



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 PM GMT

PDB ID : 4LW2
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

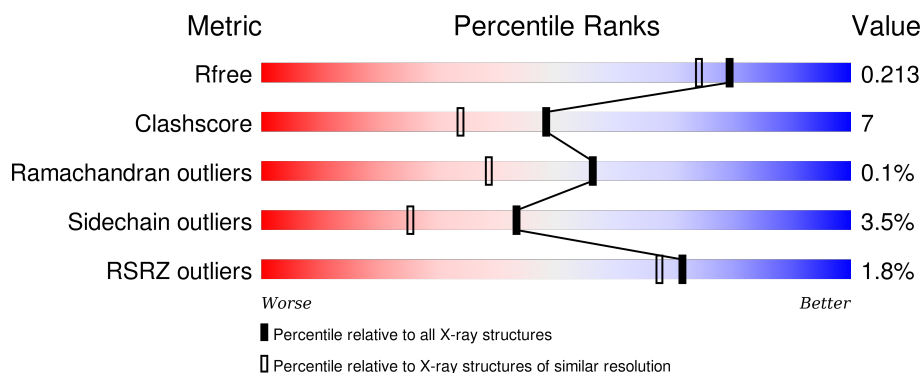
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	404	<div> <div>2%</div> <div>86% 11% ..</div> </div>
1	B	404	<div> <div>2%</div> <div>84% 13% ..</div> </div>
1	C	404	<div> <div>2%</div> <div>83% 14% ..</div> </div>

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	X
3	GOL	C	502	-	-	X	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 sulfinase.

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 (three-letter code: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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		

- Molecule 1: Cysteine sulfinatase desulfinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.30 Å 91.44 Å 83.89 Å 90.00° 97.26° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 37.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.80) 99.2 (37.89-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.79 Å)	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	5817 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 116265 reflections	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, 0.375 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: GOL, PLP

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	1.33	7/3116 (0.2%)	1.01	2/4245 (0.0%)
1	B	1.28	9/3122 (0.3%)	1.03	6/4254 (0.1%)
1	C	1.26	2/3106 (0.1%)	1.02	1/4232 (0.0%)
All	All	1.29	18/9344 (0.2%)	1.02	9/12731 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	TRP	CE3-CZ3	5.96	1.48	1.38
1	B	195	VAL	CB-CG1	-5.89	1.40	1.52
1	B	379	TYR	CD1-CE1	5.80	1.48	1.39
1	B	288	TRP	CB-CG	5.78	1.60	1.50
1	A	204	PHE	CG-CD1	5.78	1.47	1.38
1	B	57	GLU	CG-CD	5.72	1.60	1.51
1	A	42	PHE	CE2-CZ	5.70	1.48	1.37
1	C	277	ALA	CA-CB	5.65	1.64	1.52
1	A	279	VAL	CB-CG1	5.63	1.64	1.52
1	B	9	PHE	CE1-CZ	5.60	1.48	1.37
1	B	327	SER	CB-OG	-5.51	1.35	1.42
1	A	288	TRP	CE3-CZ3	5.50	1.47	1.38
1	B	276	VAL	CB-CG2	5.26	1.64	1.52
1	A	224	TYR	CG-CD2	5.22	1.46	1.39
1	B	42	PHE	CE2-CZ	5.22	1.47	1.37
1	A	204	PHE	CE2-CZ	5.17	1.47	1.37
1	C	42	PHE	CE1-CZ	5.14	1.47	1.37
1	B	71	LYS	CD-CE	5.07	1.64	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	B	246	LEU	CB-CG-CD2	5.60	120.53	111.00
1	C	151	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	322	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	24	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	373	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	322	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	80	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	293	ASP	CB-CG-OD1	5.03	122.82	118.30

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	39	0
1	B	3046	0	3009	45	0
1	C	3033	0	2997	51	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	8	0
4	C	358	0	0	12	0
All	All	10292	0	9058	133	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 (133) 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: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: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:17:GLN:H	1:A:17:GLN:CD	1.89	0.74
1:C:336:VAL:HG11	1:C:341:MET:HE3	1.70	0.72
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:N	1:A:2:ASN:HD22	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:C:74[B]:GLN:OE1	1:C:74[B]:GLN:HA	1.99	0.62
1:C:183:ILE:N	1:C:183:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:178:ASP:CG	1:B:181:ARG:HG3	2.30	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:C:8:GLN:CG	4:C:688:HOH:O	2.31	0.51
1:A:163:ILE:HD13	1:A:192:VAL:HG23	1.92	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:B:187:HIS:CE1	1:B:214:ASP:OD2	2.62	0.49
1:A:28:THR:OG1	1:A:221:HIS:HD2	1.95	0.49
1:B:81:ASP:OD1	1:B:82:LYS:HD3	2.13	0.49
1:C:116:VAL:CG2	1:C:142:LEU:HG	2.43	0.49
1:A:210:GLN:C	1:A:210:GLN:OE1	2.51	0.48
1:C:373:ARG:NH2	3:C:502:GOL:H31	2.28	0.48
1:B:60:ARG:HD3	4:B:957:HOH:O	2.13	0.48
1:A:27:ALA:HA	3:A:502:GOL:H32	1.95	0.48
1:A:14:PRO:O	1:A:17:GLN:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2:ASN:ND2	1:A:2:ASN:N	2.59	0.46
1:B:82:LYS:HG2	4:B:876:HOH:O	2.15	0.46
1:C:127:LEU:O	1:C:131:GLN:OE1	2.34	0.46
1:A:203:HIS:HE1	4:A:715:HOH:O	1.99	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:373:ARG:NH2	3:B:502:GOL:H12	2.31	0.45
1:B:107:GLN:O	1:B:110:ASP:HB2	2.15	0.45
1:B:52:ARG:HD3	1:B:52:ARG:HA	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:B:357:HIS:HA	3:B:502:GOL:H11	1.98	0.45
1:A:96:MET:HG2	1:A:245:TRP:CD1	2.51	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: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:C:116:VAL:CG1	1:C:139:LYS:HG3	2.49	0.42
1:B:163:ILE:HD13	1:B:192:VAL:HG22	2.01	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
3:B:502:GOL:H2	4:B:913:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLY:O	1:C:250:LYS:HB2	2.19	0.42
1:C:88:ARG:HH21	1:C:88:ARG:CG	2.32	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:A:60:ARG:O	1:A:64:ARG:HG3	2.20	0.41
1:B:263:GLN:HE21	1:B:263:GLN:HB3	1.63	0.41
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
1:C:96:MET:HE2	1:C:96:MET:HB2	1.59	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	399/404 (99%)	388 (97%)	11 (3%)	0	100	100
1	B	400/404 (99%)	386 (96%)	13 (3%)	1 (0%)	46	29
1	C	398/404 (98%)	390 (98%)	8 (2%)	0	100	100
All	All	1197/1212 (99%)	1164 (97%)	32 (3%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	PRO

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	315/317 (99%)	304 (96%)	11 (4%)	43	25
1	B	316/317 (100%)	308 (98%)	8 (2%)	55	39
1	C	314/317 (99%)	300 (96%)	14 (4%)	34	16
All	All	945/951 (99%)	912 (96%)	33 (4%)	43	25

All (33) 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	352	LEU
1	A	379	TYR
1	B	80	ASP
1	B	82	LYS
1	B	122	ASN
1	B	246	LEU
1	B	250	LYS
1	B	252	VAL
1	B	263	GLN
1	B	379	TYR
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
1	C	204	PHE
1	C	236	SER
1	C	237	GLU
1	C	352	LEU
1	C	375	SER

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Mol	Chain	Res	Type
1	C	379	TYR
1	C	382	LYS

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

Mol	Chain	Res	Type
1	A	17	GLN
1	A	49	ASN
1	A	54	GLN
1	A	59	GLN
1	A	122	ASN
1	A	131	GLN
1	A	209	GLN
1	A	221	HIS
1	A	263	GLN
1	A	324	GLN
1	B	2	ASN
1	B	8	GLN
1	B	74	GLN
1	B	77	ASN
1	B	95	ASN
1	B	99	GLN
1	B	122	ASN
1	B	131	GLN
1	B	187	HIS
1	B	221	HIS
1	B	263	GLN
1	C	8	GLN
1	C	59	GLN
1	C	95	ASN
1	C	122	ASN
1	C	221	HIS
1	C	263	GLN
1	C	324	GLN
1	C	338	HIS
1	C	356	GLN

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 ⓘ

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$
2	PLP	A	501	1	15,15,16	3.15	5 (33%)	21,22,23	2.46	11 (52%)
3	GOL	A	502	-	5,5,5	1.50	1 (20%)	5,5,5	1.51	1 (20%)
2	PLP	B	501	1	15,15,16	2.19	3 (20%)	21,22,23	2.01	5 (23%)
3	GOL	B	502	-	5,5,5	1.13	0	5,5,5	1.97	1 (20%)
2	PLP	C	501	1	15,15,16	2.62	5 (33%)	21,22,23	1.71	7 (33%)
3	GOL	C	502	-	5,5,5	1.14	0	5,5,5	2.42	2 (40%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C4A-C4	-9.12	1.33	1.51
2	C	501	PLP	C4A-C4	-6.70	1.38	1.51
2	B	501	PLP	C4A-C4	-5.83	1.39	1.51
2	B	501	PLP	C2A-C2	-3.64	1.43	1.50
2	A	501	PLP	O3-C3	-3.01	1.30	1.37
2	A	501	PLP	C5A-C5	-2.85	1.42	1.50
2	C	501	PLP	C2A-C2	-2.77	1.44	1.50
3	A	502	GOL	O3-C3	2.01	1.51	1.42
2	C	501	PLP	C5-C4	2.17	1.43	1.40
2	B	501	PLP	C6-N1	2.42	1.39	1.34
2	A	501	PLP	C3-C2	2.95	1.42	1.40
2	C	501	PLP	C6-N1	3.97	1.43	1.34
2	C	501	PLP	C3-C2	4.56	1.43	1.40
2	A	501	PLP	C6-N1	5.04	1.45	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C5-C6-N1	-4.50	116.04	123.86
2	A	501	PLP	C3-C2-N1	-3.81	115.35	120.61
3	C	502	GOL	O2-C2-C3	-3.61	92.09	108.65
2	C	501	PLP	C3-C2-N1	-2.98	116.50	120.61
2	A	501	PLP	C4A-C4-C5	-2.97	117.78	120.88
2	A	501	PLP	O3P-P-O4P	-2.78	98.56	106.56
2	B	501	PLP	C4A-C4-C5	-2.68	118.09	120.88
2	C	501	PLP	C5-C6-N1	-2.67	119.23	123.86
2	C	501	PLP	C4A-C4-C5	-2.56	118.21	120.88
2	A	501	PLP	C5A-C5-C6	-2.55	114.45	119.28
3	A	502	GOL	O1-C1-C2	-2.26	99.23	110.18
2	B	501	PLP	C6-C5-C4	-2.13	116.34	118.15
2	B	501	PLP	C3-C2-N1	-2.09	117.72	120.61
2	C	501	PLP	C5A-C5-C4	2.08	124.41	121.65
2	A	501	PLP	C3-C4-C5	2.15	121.13	118.78
2	C	501	PLP	C3-C4-C5	2.18	121.16	118.78
2	A	501	PLP	O3P-P-O2P	2.19	115.70	107.38
2	A	501	PLP	C2A-C2-C3	2.21	123.71	121.04
2	C	501	PLP	C6-N1-C2	2.26	123.89	119.28
2	B	501	PLP	C5A-C5-C4	2.95	125.56	121.65
3	C	502	GOL	O1-C1-C2	3.37	126.52	110.18
3	B	502	GOL	O3-C3-C2	3.40	126.67	110.18
2	C	501	PLP	O4P-C5A-C5	3.45	114.70	108.99
2	A	501	PLP	O4P-C5A-C5	3.52	114.82	108.99
2	A	501	PLP	C5A-C5-C4	3.89	126.80	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C6-N1-C2	4.46	128.38	119.28
2	B	501	PLP	O4P-C5A-C5	6.70	120.06	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	2	0
3	A	502	GOL	5	0
3	B	502	GOL	8	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%)	-0.31	4 (1%) 84 82	11, 19, 32, 49	0
1	B	399/404 (98%)	-0.19	8 (2%) 68 64	12, 21, 37, 49	0
1	C	398/404 (98%)	-0.08	10 (2%) 61 56	12, 22, 38, 45	0
All	All	1196/1212 (98%)	-0.19	22 (1%) 71 67	11, 21, 36, 49	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	400	VAL	3.6
1	C	159	PRO	3.4
1	C	160	ARG	3.1
1	A	155	GLU	3.1
1	C	337	HIS	2.7
1	C	17	GLN	2.7
1	C	131	GLN	2.7
1	B	151	ASP	2.6
1	A	159	PRO	2.6
1	B	335	GLY	2.6
1	C	8	GLN	2.5
1	B	400	VAL	2.4
1	B	155	GLU	2.4
1	A	2	ASN	2.4
1	B	154	PRO	2.4
1	B	144	ALA	2.3
1	B	397	GLU	2.3
1	C	158	THR	2.3
1	C	398	LEU	2.2
1	A	160	ARG	2.2
1	C	316	PRO	2.1
1	B	80	ASP	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	C	502	6/6	0.85	0.28	4.65	34,37,39,42	0
3	GOL	A	502	6/6	0.84	0.21	3.85	21,27,35,37	0
3	GOL	B	502	6/6	0.88	0.20	3.35	27,32,33,40	0
2	PLP	A	501	15/16	0.99	0.12	-0.28	12,14,16,17	0
2	PLP	B	501	15/16	0.99	0.09	-1.24	13,15,18,18	0
2	PLP	C	501	15/16	0.98	0.10	-1.59	13,18,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.