Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2022 – 12:52 PM EDT

PDB ID	:	4LW4
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	:	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 (i) 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 (i)) were used in the production of this report:

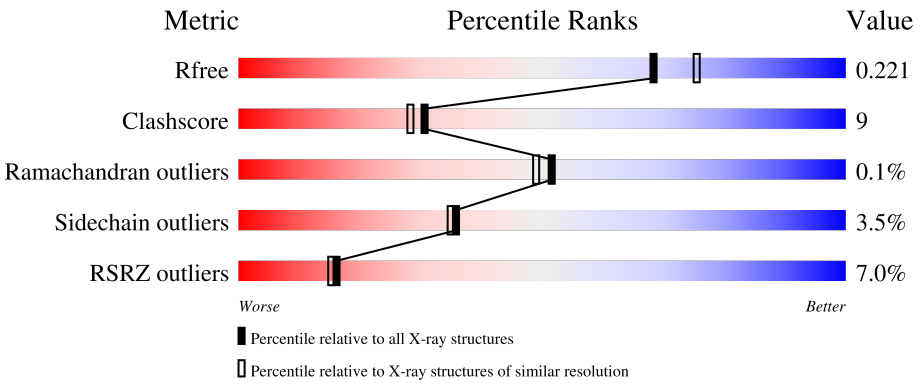
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	404	% 83% 13% • •
1	B	404	% 86% 10% • •
2	C	150	7% 75% 21% • •
2	D	150	38% 64% 25% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8926 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
			Total	C	N	O	S			
1	A	392	2976	1892	512	560	12	0	1	0
1	B	398	3065	1947	530	576	12	0	7	0

There are 6 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

- Molecule 2 is a protein called Cysteine desulfuration protein CsdE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	145	1123	712	198	210	3	0	3	0
2	D	137	1047	665	183	196	3	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP D5CZ88
C	-1	SER	-	expression tag	UNP D5CZ88
C	0	HIS	-	expression tag	UNP D5CZ88
C	49	ASP	GLU	engineered mutation	UNP D5CZ88
D	-2	GLY	-	expression tag	UNP D5CZ88
D	-1	SER	-	expression tag	UNP D5CZ88

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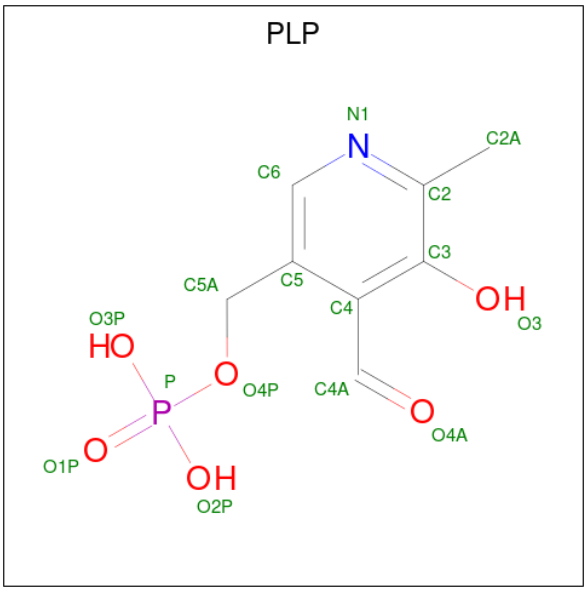
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP D5CZ88
D	49	ASP	GLU	engineered mutation	UNP D5CZ88

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is water.

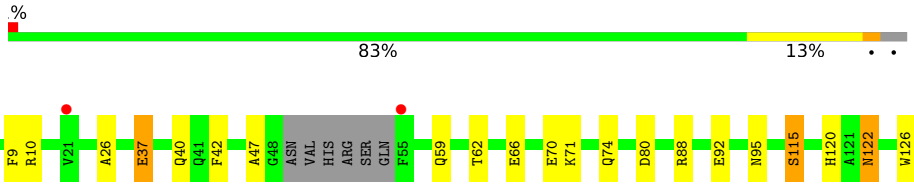
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	289	289	289	0	0
4	B	316	316	316	0	0
4	C	74	74	74	0	0
4	D	6	6	6	0	0

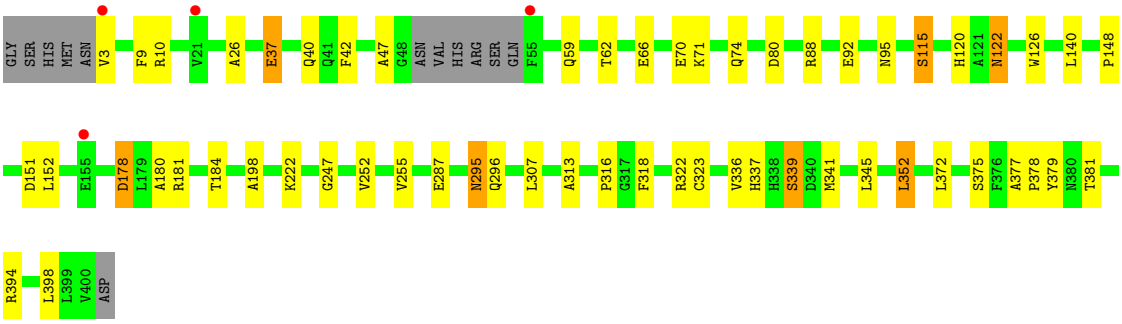
3 Residue-property plots (i)

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

• Molecule 1: Cysteine sulfinate desulfinase

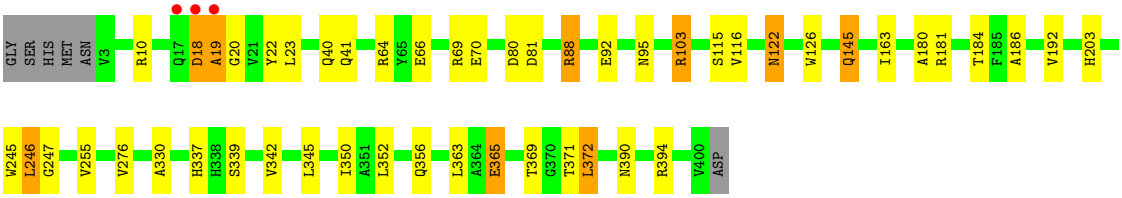
Chain A:





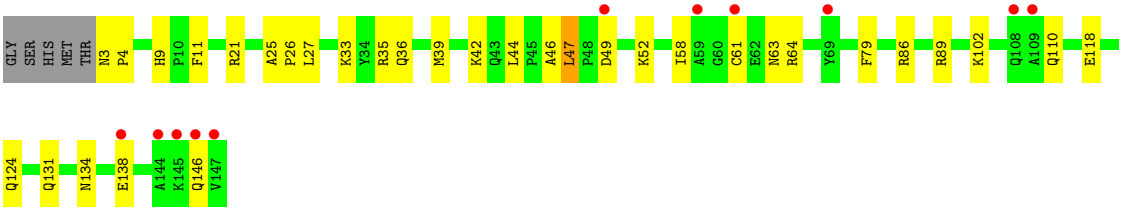
• Molecule 1: Cysteine sulfinate desulfinase

Chain B:



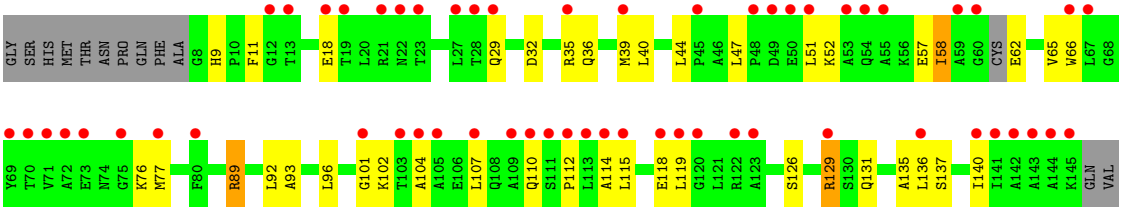
• Molecule 2: Cysteine desulfuration protein CsdE

Chain C:



• Molecule 2: Cysteine desulfuration protein CsdE

Chain D:


GLY SER HIS MET THR ASN PRO GLN PHE ALA G8 H9 P10 F11 G12 T13 E18 T19 L20 R21 N22 T23 L27 T28 Q29 D32 R35 Q36 M39 L40 L44 P45 A46 L47 P48 D49 E50 L51 K52 A53 Q54 A55 K56 E57 I58 A59 G60 CYS E62 V65 W66 L67 G68
Y69 T70 V71 A72 E73 N74 G75 K76 M77 F80 R89 L92 A93 L96 G101 K102 T103 A104 A105 E106 L107 Q108 A109 Q110 S111 P112 L113 A114 L115 E118 L119 G120 L121 R122 A123 S126 R129 S130 Q131 A135 L136 S137 I140 I141 A142 A143 A144 K145 GLN VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.14Å 76.87Å 89.36Å 90.00° 104.48° 90.00°	Depositor
Resolution (Å)	50.00 – 2.01 37.06 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.01) 99.4 (37.06-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.08 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.159 , 0.218 0.163 , 0.221	Depositor DCC
R_{free} test set	3411 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8926	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.14	5/3044 (0.2%)	0.91	6/4147 (0.1%)
1	B	1.15	2/3153 (0.1%)	0.91	4/4293 (0.1%)
2	C	1.01	0/1151	0.82	1/1558 (0.1%)
2	D	0.68	0/1066	0.70	0/1440
All	All	1.08	7/8414 (0.1%)	0.88	11/11438 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	VAL	CB-CG2	5.96	1.65	1.52
1	A	323	CYS	CB-SG	-5.59	1.72	1.81
1	A	37	GLU	CG-CD	5.58	1.60	1.51
1	A	377	ALA	CA-CB	5.52	1.64	1.52
1	A	379	TYR	CE2-CZ	5.31	1.45	1.38
1	B	186	ALA	CA-CB	5.13	1.63	1.52
1	A	42	PHE	CE1-CZ	5.12	1.47	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	322	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	C	47	LEU	CA-CB-CG	5.86	128.79	115.30
1	A	394	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	103	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	10	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	178	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	255	VAL	CB-CA-C	-5.18	101.55	111.40
1	A	152	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	88[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88[B]	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	2976	0	2940	56	0
1	B	3065	0	3041	55	0
2	C	1123	0	1141	25	0
2	D	1047	0	1067	40	0
3	A	15	0	7	1	0
3	B	15	0	6	0	0
4	A	289	0	0	3	0
4	B	316	0	0	11	0
4	C	74	0	0	3	0
4	D	6	0	0	0	0
All	All	8926	0	8202	151	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 9.

All (151) 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:A:10:ARG:NH1	1:A:381:THR:HG21	1.28	1.45
1:A:10:ARG:NH1	1:A:381:THR:CG2	1.91	1.33
1:B:66:GLU:HG2	4:B:790:HOH:O	1.42	1.16
2:D:126:SER:O	2:D:129:ARG:HG2	1.62	1.00
1:B:70:GLU:HG3	4:B:908:HOH:O	1.67	0.94
1:A:88:ARG:HH21	1:B:88[A]:ARG:CD	1.82	0.93
1:A:10:ARG:HH12	1:A:381:THR:HG21	1.12	0.91
1:A:10:ARG:HH11	1:A:381:THR:HG21	1.17	0.90
1:A:151:ASP:OD1	1:A:181:ARG:NH1	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:NH1	1:A:381:THR:HG23	1.86	0.88
1:A:10:ARG:HH11	1:A:381:THR:CG2	1.74	0.87
1:B:342:VAL:HG11	2:D:62:GLU:OE2	1.77	0.85
1:A:95:ASN:HD21	1:B:247:GLY:H	1.22	0.84
1:A:88:ARG:HH21	1:B:88[A]:ARG:HD2	1.42	0.84
1:A:337:HIS:HD2	1:A:339:SER:HB2	1.40	0.84
1:A:337:HIS:CD2	1:A:339:SER:HB2	2.13	0.83
1:B:88[B]:ARG:CZ	4:B:792:HOH:O	2.26	0.83
2:C:58:ILE:O	2:C:58:ILE:HG22	1.77	0.82
2:D:126:SER:O	2:D:129:ARG:CG	2.29	0.81
1:A:247:GLY:H	1:B:95:ASN:HD21	1.28	0.80
1:B:369:THR:HG22	4:B:839:HOH:O	1.81	0.79
2:D:40:LEU:HD22	2:D:93:ALA:CB	2.14	0.78
2:C:9:HIS:HD2	2:C:11:PHE:H	1.31	0.77
2:D:40:LEU:HD21	2:D:93:ALA:HB1	1.65	0.77
2:C:21:ARG:HD3	2:C:118:GLU:OE2	1.87	0.74
2:D:44:LEU:HD23	2:D:89:ARG:HD2	1.68	0.74
2:D:40:LEU:CD2	2:D:93:ALA:CB	2.66	0.73
1:B:88[B]:ARG:NH1	4:B:792:HOH:O	2.21	0.73
1:A:62:THR:O	1:A:66[A]:GLU:HG2	1.88	0.72
1:A:88:ARG:HH21	1:B:88[A]:ARG:HD3	1.55	0.71
1:B:356:GLN:OE1	1:B:363:LEU:HD12	1.90	0.71
1:A:180:ALA:O	1:A:184:THR:HG23	1.92	0.70
1:A:316:PRO:HD2	4:A:738:HOH:O	1.92	0.69
1:B:371:THR:HG22	1:B:372:LEU:O	1.92	0.69
2:D:35:ARG:O	2:D:39[A]:MET:HG2	1.92	0.69
2:D:40:LEU:CD2	2:D:93:ALA:HB1	2.23	0.68
2:C:44:LEU:O	2:C:89[B]:ARG:NH1	2.17	0.67
1:A:37:GLU:HB3	4:A:775:HOH:O	1.96	0.65
1:A:339:SER:OG	2:C:63:ASN:HB2	1.95	0.65
1:B:163:ILE:HD13	1:B:192:VAL:HG22	1.79	0.65
2:D:40:LEU:HD22	2:D:93:ALA:HB3	1.79	0.64
1:A:10:ARG:HH12	1:A:381:THR:CG2	1.82	0.64
1:B:40[B]:GLN:HE21	1:B:41:GLN:HE21	1.45	0.63
1:B:337:HIS:CD2	1:B:339:SER:H	2.15	0.63
1:B:339:SER:HB2	2:D:131:GLN:NE2	2.13	0.63
2:C:47:LEU:O	2:C:52:LYS:HE2	1.98	0.63
2:D:36:GLN:HA	2:D:39[A]:MET:HG3	1.82	0.62
2:C:42:LYS:HZ3	2:C:86:ARG:HH21	1.48	0.62
1:A:95:ASN:ND2	1:B:247:GLY:H	1.95	0.61
1:A:47:ALA:O	1:B:20:GLY:HA3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:ALA:HA	2:C:89[B]:ARG:NH2	2.16	0.61
2:C:42:LYS:HZ3	2:C:86:ARG:NH2	1.98	0.60
2:D:40:LEU:O	2:D:40:LEU:HD23	2.02	0.60
1:A:337:HIS:CD2	1:A:339:SER:H	2.19	0.59
2:D:47:LEU:HD23	2:D:52:LYS:HG2	1.84	0.59
1:B:181:ARG:HG3	4:B:815:HOH:O	2.01	0.59
2:C:42:LYS:NZ	2:C:86:ARG:NH2	2.51	0.59
2:C:58:ILE:O	2:C:58:ILE:CG2	2.47	0.59
2:D:40:LEU:HD23	2:D:40:LEU:C	2.23	0.58
1:B:339:SER:HB2	2:D:131:GLN:HE21	1.68	0.58
1:A:122:ASN:ND2	1:A:126:TRP:HE1	2.00	0.58
1:A:88:ARG:NH2	1:B:88[A]:ARG:CD	2.62	0.58
1:A:47:ALA:HB1	1:B:22:TYR:HB2	1.86	0.57
2:D:77:MET:CE	2:D:107:LEU:HD12	2.34	0.57
1:A:88:ARG:NH2	1:B:88[A]:ARG:HD2	2.17	0.57
1:B:337:HIS:HD2	1:B:339:SER:H	1.52	0.57
2:C:9:HIS:HD2	2:C:11:PHE:N	2.03	0.57
2:D:76:LYS:HG2	2:D:101:GLY:O	2.05	0.57
2:C:9:HIS:HE1	2:C:79:PHE:O	1.87	0.56
2:D:57:GLU:HG3	2:D:66:TRP:NE1	2.20	0.56
2:D:9:HIS:HD2	2:D:11:PHE:H	1.52	0.56
1:A:88:ARG:NH1	1:B:246:LEU:CD2	2.69	0.55
1:A:337:HIS:HD2	1:A:339:SER:H	1.55	0.53
2:D:114:ALA:O	2:D:118:GLU:HG3	2.08	0.53
1:B:245:TRP:CD1	1:B:246:LEU:HD13	2.43	0.53
1:A:88:ARG:NH1	1:B:246:LEU:HD21	2.23	0.53
1:A:247:GLY:H	1:B:95:ASN:ND2	2.01	0.53
1:B:163:ILE:HD13	1:B:192:VAL:CG2	2.39	0.53
1:B:64:ARG:HG2	4:B:672:HOH:O	2.08	0.52
1:B:23:LEU:HB2	1:B:352:LEU:HD12	1.91	0.52
2:D:77:MET:HE1	2:D:107:LEU:HD12	1.90	0.52
2:D:110:GLN:OE1	2:D:112:PRO:HA	2.10	0.52
1:A:295:ASN:HD22	1:A:295:ASN:H	1.58	0.51
1:B:116:VAL:HG21	1:B:365:GLU:HG3	1.92	0.51
1:A:295:ASN:H	1:A:295:ASN:ND2	2.09	0.51
2:D:129:ARG:HB2	2:D:129:ARG:NH1	2.27	0.50
1:A:88:ARG:NH1	1:B:92:GLU:OE2	2.45	0.50
1:B:18:ASP:O	1:B:19:ALA:O	2.30	0.49
2:D:40:LEU:CD2	2:D:40:LEU:C	2.81	0.49
2:C:9:HIS:CE1	2:C:79:PHE:O	2.66	0.49
2:C:131:GLN:O	2:C:134[B]:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:HG22	1:B:352:LEU:HD13	1.95	0.49
2:C:3:ASN:N	2:C:4:PRO:HD2	2.27	0.49
2:C:35:ARG:NH2	4:C:236:HOH:O	2.46	0.49
1:B:122:ASN:ND2	1:B:126:TRP:HE1	2.10	0.49
2:D:58:ILE:HD12	2:D:135:ALA:HB1	1.95	0.49
2:C:27:LEU:HD11	2:C:36:GLN:HG3	1.94	0.48
2:D:77:MET:HG3	2:D:102:LYS:O	2.12	0.48
2:D:92:LEU:HD13	2:D:136:LEU:HD13	1.95	0.48
1:A:88:ARG:CZ	1:B:92:GLU:OE2	2.61	0.47
2:D:115:LEU:O	2:D:119:LEU:HG	2.14	0.47
2:D:29:GLN:HB2	2:D:32:ASP:OD2	2.14	0.47
1:A:88:ARG:HE	1:B:88[A]:ARG:CG	2.28	0.47
1:A:115:SER:HA	1:A:140:LEU:HB3	1.96	0.47
2:D:129:ARG:HB2	2:D:129:ARG:HH11	1.79	0.47
1:A:336:VAL:HG11	1:A:341:MET:HE3	1.97	0.47
2:D:77:MET:CE	2:D:104:ALA:HA	2.45	0.47
2:C:25:ALA:N	2:C:26:PRO:CD	2.78	0.47
1:A:70:GLU:O	1:A:74:GLN:HG3	2.14	0.47
2:D:52:LYS:HD2	2:D:66:TRP:CE2	2.49	0.47
2:D:77:MET:HE2	2:D:104:ALA:HB2	1.97	0.46
1:A:88:ARG:NH2	1:A:92:GLU:OE2	2.48	0.46
1:B:390:ASN:HD21	1:B:394:ARG:CZ	2.29	0.46
1:A:120:HIS:CD2	1:B:255:VAL:HG11	2.51	0.45
2:D:126:SER:O	2:D:129:ARG:HG3	2.16	0.45
1:A:3:VAL:HA	1:A:296:GLN:OE1	2.17	0.44
1:B:180:ALA:O	1:B:184:THR:HG23	2.18	0.44
1:B:64:ARG:NH2	4:B:696:HOH:O	2.51	0.44
1:B:345:LEU:HD13	1:B:352:LEU:HD22	1.99	0.44
1:A:88:ARG:NH1	1:B:246:LEU:HD22	2.33	0.44
1:A:40:GLN:OE1	1:B:40[A]:GLN:NE2	2.51	0.44
2:D:77:MET:HE2	2:D:104:ALA:CA	2.48	0.44
1:B:103:ARG:HD2	4:B:747:HOH:O	2.17	0.43
2:D:137:SER:O	2:D:140:ILE:HB	2.18	0.43
1:B:69:ARG:HB3	1:B:81:ASP:HB2	1.99	0.43
2:D:9:HIS:HD2	2:D:11:PHE:N	2.13	0.43
2:C:33:LYS:HE3	2:C:124:GLN:NE2	2.33	0.43
1:A:88:ARG:NH2	1:B:92:GLU:OE2	2.53	0.42
1:A:88:ARG:NH2	1:B:88[A]:ARG:HD3	2.30	0.42
1:A:313:ALA:HA	1:A:318:PHE:CD2	2.54	0.42
2:D:65:VAL:CG1	2:D:136:LEU:HD21	2.49	0.42
2:C:39:MET:CE	2:C:42:LYS:HE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:HIS:HE1	4:B:734:HOH:O	2.03	0.41
1:B:145:GLN:H	1:B:145:GLN:HG3	1.52	0.41
2:C:64:ARG:HD3	4:C:217:HOH:O	2.20	0.41
1:A:71:LYS:HE3	1:A:287:GLU:HB2	2.02	0.41
1:A:352:LEU:C	1:A:352:LEU:HD12	2.40	0.41
1:B:88[B]:ARG:HG2	4:B:761:HOH:O	2.21	0.41
1:A:178:ASP:C	1:A:178:ASP:OD1	2.59	0.41
2:C:110:GLN:HG3	4:C:247:HOH:O	2.20	0.41
1:A:26:ALA:O	1:A:222:LYS:HE2	2.20	0.41
1:A:375:SER:HB2	4:A:702:HOH:O	2.21	0.41
2:C:49:ASP:HA	2:C:52:LYS:HD2	2.03	0.41
1:A:122:ASN:HD22	1:A:122:ASN:HA	1.71	0.40
2:D:77:MET:HE3	2:D:107:LEU:HD12	2.02	0.40
1:A:9:PHE:CE1	1:A:378:PRO:HB2	2.56	0.40
1:A:341:MET:HG2	1:A:372:LEU:HD21	2.03	0.40
1:B:371:THR:HG22	1:B:372:LEU:N	2.35	0.40
1:A:198:ALA:HB3	3:A:500:PLP:C2	2.51	0.40
1:B:330:ALA:HB1	1:B:371:THR:HG21	2.03	0.40
2:C:138:GLU:OE1	2:C:138:GLU:HA	2.20	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	389/404 (96%)	379 (97%)	10 (3%)	0	100	100
1	B	403/404 (100%)	389 (96%)	13 (3%)	1 (0%)	47	44
2	C	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
2	D	134/150 (89%)	131 (98%)	3 (2%)	0	100	100
All	All	1072/1108 (97%)	1041 (97%)	30 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ALA

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	307/317 (97%)	295 (96%)	12 (4%)	32	30
1	B	319/317 (101%)	311 (98%)	8 (2%)	47	49
2	C	115/116 (99%)	112 (97%)	3 (3%)	46	48
2	D	106/116 (91%)	100 (94%)	6 (6%)	20	16
All	All	847/866 (98%)	818 (97%)	29 (3%)	36	36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	80	ASP
1	A	115	SER
1	A	122	ASN
1	A	148	PRO
1	A	252	VAL
1	A	295	ASN
1	A	307	LEU
1	A	339	SER
1	A	345	LEU
1	A	352	LEU
1	A	398	LEU
1	B	18	ASP
1	B	80	ASP
1	B	115	SER
1	B	122	ASN
1	B	145	GLN
1	B	246	LEU
1	B	365	GLU

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Mol	Chain	Res	Type
1	B	372	LEU
2	C	61	CYS
2	C	102	LYS
2	C	146	GLN
2	D	18	GLU
2	D	51	LEU
2	D	58	ILE
2	D	89	ARG
2	D	96	LEU
2	D	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	77	ASN
1	A	95	ASN
1	A	122	ASN
1	A	253	HIS
1	A	295	ASN
1	A	337	HIS
1	A	338	HIS
1	B	41	GLN
1	B	95	ASN
1	B	122	ASN
1	B	253	HIS
1	B	337	HIS
1	B	357	HIS
1	B	390	ASN
2	C	9	HIS
2	D	9	HIS
2	D	78	HIS
2	D	131	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	PLP	A	500	1	15,15,16	2.01	3 (20%)	20,22,23	2.19	9 (45%)
3	PLP	B	500	1	15,15,16	1.96	4 (26%)	20,22,23	1.76	6 (30%)

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	PLP	A	500	1	-	0/6/6/8	0/1/1/1
3	PLP	B	500	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	C4A-C4	-5.19	1.40	1.51
3	B	500	PLP	C4A-C4	-4.91	1.41	1.51
3	B	500	PLP	C2A-C2	-3.81	1.43	1.50
3	A	500	PLP	C2A-C2	-3.67	1.44	1.50
3	B	500	PLP	C6-N1	2.64	1.40	1.34
3	A	500	PLP	C2-N1	2.64	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	PLP	C5A-C5	-2.60	1.43	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	PLP	O4P-C5A-C5	4.20	117.35	109.35
3	A	500	PLP	C4A-C4-C5	-3.70	117.13	120.94
3	A	500	PLP	C2A-C2-C3	3.60	125.33	120.89
3	A	500	PLP	C3-C2-N1	-3.44	116.32	120.77
3	B	500	PLP	O4P-C5A-C5	3.18	115.42	109.35
3	B	500	PLP	O4P-P-O1P	3.07	115.08	106.47
3	B	500	PLP	C3-C2-N1	-2.96	116.94	120.77
3	A	500	PLP	C3-C4-C5	2.92	121.90	118.74
3	B	500	PLP	C4A-C4-C5	-2.62	118.24	120.94
3	B	500	PLP	O2P-P-O4P	-2.46	100.20	106.73
3	A	500	PLP	O3-C3-C2	2.45	122.83	117.49
3	B	500	PLP	O3P-P-O1P	2.44	120.24	110.68
3	A	500	PLP	O3P-P-O1P	2.30	119.67	110.68
3	A	500	PLP	C6-N1-C2	2.23	123.30	119.17
3	A	500	PLP	O4P-P-O1P	2.17	112.57	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PLP	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	392/404 (97%)	-0.45	4 (1%)	82	81	10, 18, 31, 65	0
1	B	398/404 (98%)	-0.55	3 (0%)	86	85	8, 15, 29, 48	0
2	C	145/150 (96%)	0.12	11 (7%)	13	13	13, 28, 50, 62	0
2	D	137/150 (91%)	1.81	57 (41%)	0	0	35, 55, 75, 81	0
All	All	1072/1108 (96%)	-0.12	75 (6%)	16	15	8, 19, 59, 81	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	111	SER	7.5
2	D	141	ILE	7.1
2	C	61	CYS	6.8
2	D	69	TYR	5.2
1	A	55	PHE	5.0
2	D	51	LEU	5.0
2	D	144	ALA	4.8
2	D	71	VAL	4.7
2	D	72	ALA	4.6
2	D	110	GLN	4.5
1	B	19	ALA	4.4
2	D	109	ALA	4.0
2	C	147	VAL	4.0
2	D	105	ALA	4.0
2	D	28	THR	3.9
2	D	67	LEU	3.9
2	D	50	GLU	3.7
2	D	140	ILE	3.7
2	D	143	ALA	3.7
2	C	69	TYR	3.7
2	D	53	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	80	PHE	3.6
2	D	145	LYS	3.6
2	D	54	GLN	3.5
2	D	136	LEU	3.4
2	D	59	ALA	3.3
2	D	104	ALA	3.3
2	D	19	THR	3.3
2	D	18	GLU	3.2
2	D	120	GLY	3.2
2	D	39[A]	MET	3.2
2	D	115	LEU	3.1
2	D	123	ALA	3.1
2	D	27	LEU	3.1
2	D	114	ALA	3.1
2	D	107	LEU	3.0
2	C	59	ALA	2.9
2	D	49	ASP	2.9
2	D	119	LEU	2.9
2	C	146	GLN	2.8
2	D	73	GLU	2.8
2	D	23	THR	2.8
2	D	21	ARG	2.8
2	D	142	ALA	2.8
2	D	60	GLY	2.7
2	C	144	ALA	2.7
2	D	45	PRO	2.7
2	D	12	GLY	2.7
2	D	66	TRP	2.7
2	D	122	ARG	2.7
2	D	29	GLN	2.7
2	D	48	PRO	2.6
2	D	112	PRO	2.6
2	D	101	GLY	2.6
1	A	3	VAL	2.6
2	D	70	THR	2.6
2	C	138	GLU	2.6
2	D	118	GLU	2.6
2	D	77	MET	2.5
2	C	145	LYS	2.5
2	D	13	THR	2.4
1	A	21	VAL	2.3
1	A	155	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	75	GLY	2.3
1	B	18	ASP	2.3
1	B	17	GLN	2.3
2	D	113	LEU	2.2
2	C	109	ALA	2.2
2	D	55	ALA	2.2
2	D	129	ARG	2.1
2	D	22	ASN	2.1
2	D	35	ARG	2.1
2	C	108	GLN	2.1
2	D	103	THR	2.0
2	C	49	ASP	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	PLP	A	500	15/16	0.99	0.10	11,15,18,21	0
3	PLP	B	500	15/16	0.99	0.12	8,12,14,15	0

6.5 Other polymers (i)

There are no such residues in this entry.