



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:47 AM UTC

PDB ID : 1KMK / pdb_00001kmk
Title : E. coli NifS/CsdB protein at 2.20Å with the cysteine perselenide intermediate (residue CSZ).
Authors : Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2001-12-16
Resolution : 2.20 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

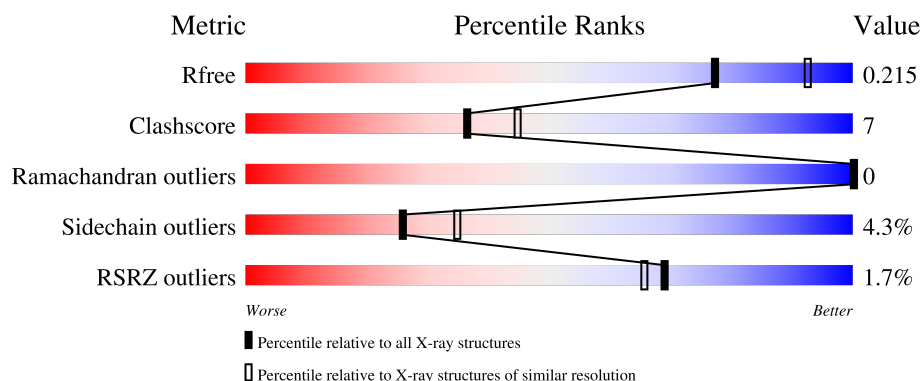
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

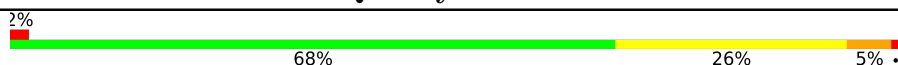
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	406	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3626 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.

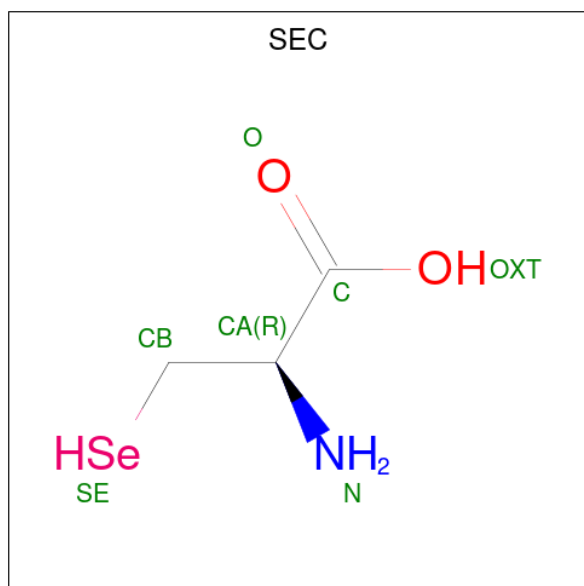
- Molecule 1 is a protein called SELENOCYSTEINE LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	405	3120	1976	548	579	16	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	CSZ	CYS	modified residue	UNP P77444

- Molecule 2 is SELENOCYSTEINE (CCD ID: SEC) (formula: C₃H₇NO₂Se).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

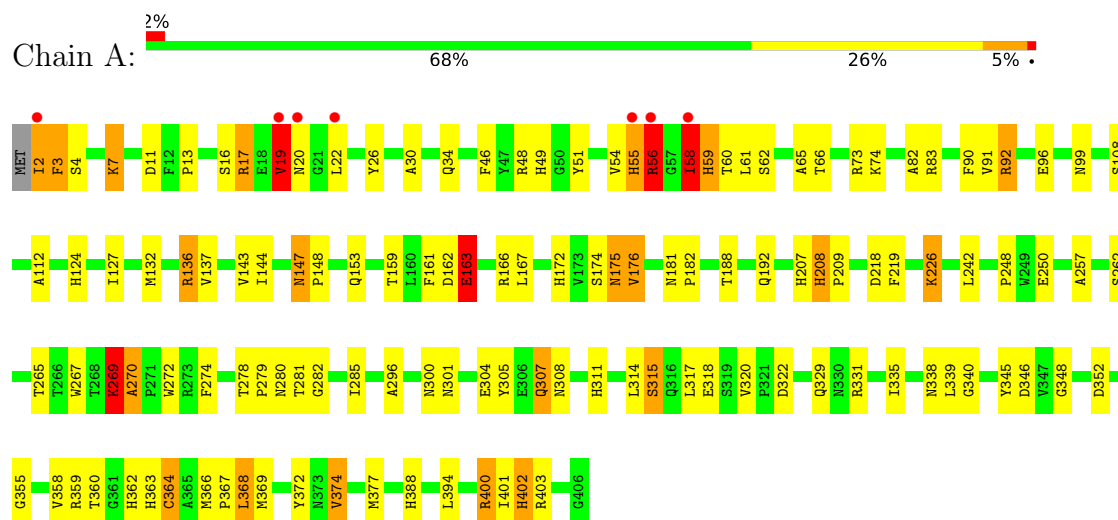
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	485	Total	O	0	0
			485	485		

3 Residue-property plots

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: SELENOCYSTEINE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.86Å 125.86Å 133.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-2.20) 87.6 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.239 0.186 , 0.215	Depositor DCC
R_{free} test set	4269 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3626	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, CSZ, SEC

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	0.98	0/3183	2.14	114/4330 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	CD-NE-CZ	19.81	152.13	124.40
1	A	403	ARG	CD-NE-CZ	12.98	142.57	124.40
1	A	127	ILE	CA-C-N	12.48	132.42	120.43
1	A	127	ILE	C-N-CA	12.48	132.42	120.43
1	A	270	ALA	CA-C-O	-10.72	105.48	120.16
1	A	402	HIS	CA-CB-CG	-9.92	103.88	113.80
1	A	20	ASN	CA-CB-CG	9.81	122.41	112.60
1	A	83	ARG	CD-NE-CZ	9.69	137.97	124.40
1	A	54	VAL	CA-C-N	-9.24	106.17	122.62
1	A	54	VAL	C-N-CA	-9.24	106.17	122.62
1	A	162	ASP	CA-CB-CG	8.97	121.58	112.60
1	A	136	ARG	CA-C-O	-8.48	111.91	120.82
1	A	55	HIS	CB-CA-C	8.38	122.20	111.40
1	A	49	HIS	N-CA-C	8.18	124.06	113.18
1	A	388	HIS	CA-C-O	8.06	129.09	120.55
1	A	3	PHE	N-CA-C	7.95	121.28	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	PHE	CA-C-O	-7.73	111.87	120.69
1	A	16	SER	CA-C-O	7.69	128.33	119.18
1	A	374	VAL	N-CA-C	-7.68	102.89	109.19
1	A	257	ALA	N-CA-C	-7.46	102.76	112.68
1	A	181	ASN	CA-CB-CG	-7.40	105.20	112.60
1	A	274	PHE	CA-CB-CG	-7.36	106.44	113.80
1	A	49	HIS	CA-CB-CG	-7.34	106.46	113.80
1	A	163	GLU	CB-CG-CD	7.31	125.03	112.60
1	A	73	ARG	CA-C-O	7.20	128.18	120.55
1	A	58	ILE	O-C-N	6.94	129.37	121.94
1	A	192	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	358	VAL	CA-C-O	-6.87	114.66	121.67
1	A	278	THR	CA-C-N	6.78	127.23	120.52
1	A	278	THR	C-N-CA	6.78	127.23	120.52
1	A	300	ASN	CA-C-O	-6.76	112.20	119.97
1	A	161	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	188	THR	CA-C-N	6.62	129.05	120.44
1	A	188	THR	C-N-CA	6.62	129.05	120.44
1	A	3	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	2	ILE	CA-C-O	6.53	131.91	120.80
1	A	262	SER	CA-C-O	-6.52	111.19	120.51
1	A	269	LYS	CA-CB-CG	6.49	127.08	114.10
1	A	352	ASP	CA-C-O	6.47	127.41	120.55
1	A	176	VAL	N-CA-C	-6.47	106.51	111.62
1	A	147	ASN	CA-C-N	6.42	127.87	119.84
1	A	147	ASN	C-N-CA	6.42	127.87	119.84
1	A	279	PRO	CB-CA-C	-6.37	101.32	110.75
1	A	226	LYS	CA-CB-CG	-6.35	101.40	114.10
1	A	51	TYR	CA-CB-CG	-6.29	102.59	113.90
1	A	300	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	136	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	A	59	HIS	CA-C-N	6.22	129.43	120.79
1	A	59	HIS	C-N-CA	6.22	129.43	120.79
1	A	17	ARG	CA-CB-CG	6.21	126.51	114.10
1	A	99	ASN	CB-CG-ND2	6.18	125.67	116.40
1	A	331	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	A	346	ASP	CA-CB-CG	-6.12	106.48	112.60
1	A	82	ALA	N-CA-C	-6.10	102.48	110.53
1	A	20	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	308	ASN	N-CA-CB	-6.07	100.87	110.28
1	A	49	HIS	N-CA-CB	-6.07	96.51	110.83
1	A	338	ASN	OD1-CG-ND2	-6.04	116.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	108	SER	CA-C-O	-5.96	112.69	119.78
1	A	282	GLY	O-C-N	-5.94	116.48	122.19
1	A	175	ASN	CA-C-N	5.92	129.43	123.16
1	A	175	ASN	C-N-CA	5.92	129.43	123.16
1	A	307	GLN	CA-C-O	5.92	126.82	120.55
1	A	60	THR	N-CA-C	5.91	118.23	111.02
1	A	46	PHE	CA-CB-CG	-5.90	107.90	113.80
1	A	345	TYR	CA-CB-CG	-5.88	103.31	113.90
1	A	90	PHE	O-C-N	5.82	129.84	123.04
1	A	358	VAL	N-CA-CB	5.81	120.65	112.52
1	A	335	ILE	CA-C-O	-5.69	114.73	120.31
1	A	174	SER	O-C-N	-5.65	116.00	122.89
1	A	92	ARG	N-CA-C	-5.64	105.12	112.23
1	A	320	VAL	N-CA-C	-5.60	101.44	108.05
1	A	172	HIS	CA-C-O	5.59	126.66	120.90
1	A	270	ALA	CB-CA-C	5.58	121.17	110.17
1	A	74	LYS	O-C-N	5.58	128.11	122.09
1	A	280	ASN	OD1-CG-ND2	5.56	128.16	122.60
1	A	207	HIS	CE1-NE2-CD2	5.55	114.55	109.00
1	A	314	LEU	CA-C-O	5.54	126.42	120.55
1	A	226	LYS	CG-CD-CE	-5.53	98.59	111.30
1	A	394	LEU	CA-C-N	5.53	127.52	120.56
1	A	394	LEU	C-N-CA	5.53	127.52	120.56
1	A	143	VAL	N-CA-C	5.46	115.98	108.12
1	A	296	ALA	CA-C-O	-5.45	113.36	119.79
1	A	317	LEU	CA-C-N	5.39	128.04	120.28
1	A	317	LEU	C-N-CA	5.39	128.04	120.28
1	A	315	SER	CA-C-O	-5.38	115.15	120.70
1	A	26	TYR	CA-C-O	5.37	126.77	120.98
1	A	99	ASN	CA-C-O	-5.35	114.88	120.55
1	A	281	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	372	TYR	O-C-N	5.33	129.72	122.37
1	A	250	GLU	CA-C-O	-5.32	115.35	121.47
1	A	174	SER	CA-C-O	5.32	127.11	121.16
1	A	147	ASN	N-CA-C	-5.31	102.43	110.50
1	A	19	VAL	N-CA-CB	-5.29	104.16	111.99
1	A	112	ALA	CA-C-O	-5.29	115.33	121.15
1	A	166	ARG	N-CA-C	-5.27	107.02	113.50
1	A	144	ILE	CA-C-N	5.25	125.23	120.03
1	A	144	ILE	C-N-CA	5.25	125.23	120.03
1	A	65	ALA	N-CA-C	-5.24	105.65	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ARG	N-CA-CB	5.23	117.59	110.01
1	A	401	ILE	N-CA-C	-5.21	105.46	110.72
1	A	99	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	272	TRP	O-C-N	-5.17	116.17	122.22
1	A	208	HIS	CA-CB-CG	5.14	118.94	113.80
1	A	167	LEU	N-CA-CB	-5.13	101.98	111.52
1	A	322	ASP	CA-CB-CG	-5.11	107.49	112.60
1	A	83	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	305	TYR	CA-C-O	5.10	125.96	120.55
1	A	48	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	A	403	ARG	CB-CA-C	-5.07	102.06	110.68
1	A	91	VAL	O-C-N	-5.06	116.24	122.57
1	A	285	ILE	CA-C-O	5.02	126.17	120.95
1	A	265	THR	CA-CB-CG2	5.01	119.03	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	ALA	Peptide,Mainchain

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	3120	0	3074	45	0
2	A	6	0	1	2	0
3	A	15	0	6	0	0
4	A	485	0	0	10	4
All	All	3626	0	3081	45	4

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 (45) 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:364:CSZ:SG	1:A:364:CSZ:SE	2.46	1.23
1:A:55:HIS:CD2	4:A:978:HOH:O	2.35	0.79
1:A:2:ILE:HG12	1:A:3:PHE:H	1.50	0.75
1:A:2:ILE:HD11	1:A:304:GLU:OE1	1.98	0.62
1:A:359:ARG:HD3	1:A:363:HIS:ND1	2.15	0.60
1:A:96:GLU:OE2	4:A:950:HOH:O	2.17	0.59
1:A:307:GLN:HB2	4:A:975:HOH:O	2.04	0.56
1:A:315:SER:O	1:A:318:GLU:HB2	2.06	0.55
1:A:59:HIS:CE1	1:A:62:SER:HB2	2.42	0.54
1:A:362:HIS:HD2	1:A:364:CSZ:N	2.06	0.53
1:A:56:ARG:HG2	1:A:66:THR:HG21	1.90	0.53
1:A:147:ASN:ND2	1:A:153:GLN:HG2	2.24	0.53
1:A:311:HIS:HB3	4:A:736:HOH:O	2.09	0.51
1:A:4:SER:HB3	1:A:7:LYS:HD2	1.94	0.50
1:A:2:ILE:HG13	1:A:301:ASN:ND2	2.27	0.49
1:A:58:ILE:HB	4:A:725:HOH:O	2.11	0.49
1:A:369:MET:SD	1:A:377:MET:HG3	2.52	0.49
1:A:163:GLU:H	1:A:163:GLU:CD	2.21	0.49
1:A:348:GLY:HA3	1:A:360:THR:HG21	1.95	0.49
1:A:30:ALA:O	1:A:226:LYS:HE2	2.12	0.48
1:A:269:LYS:NZ	4:A:812:HOH:O	2.47	0.48
1:A:124:HIS:HD1	1:A:364:CSZ:SE	2.46	0.48
1:A:248:PRO:HG3	1:A:267:TRP:CE2	2.49	0.48
1:A:339:LEU:O	1:A:340:GLY:C	2.57	0.47
1:A:359:ARG:HH12	2:A:502:SEC:SE	2.48	0.46
1:A:132:MET:O	1:A:136:ARG:HG3	2.15	0.46
1:A:55:HIS:HB2	4:A:636:HOH:O	2.16	0.45
1:A:17:ARG:HH11	1:A:17:ARG:HD3	1.58	0.44
1:A:218:ASP:HB3	1:A:242:LEU:CD1	2.47	0.44
1:A:11:ASP:O	1:A:13:PRO:HD3	2.18	0.43
1:A:19:VAL:HG12	1:A:355:GLY:HA2	2.00	0.43
1:A:4:SER:CB	1:A:7:LYS:HD2	2.48	0.43
1:A:92:ARG:N	1:A:96:GLU:OE1	2.48	0.43
1:A:176:VAL:HB	1:A:368:LEU:HD21	2.01	0.43
1:A:34:GLN:HA	1:A:34:GLN:OE1	2.18	0.42
1:A:92:ARG:HH21	1:A:92:ARG:HD3	1.58	0.42
1:A:56:ARG:NH1	4:A:834:HOH:O	2.43	0.42
1:A:22:LEU:HD11	4:A:770:HOH:O	2.19	0.42
1:A:208:HIS:HB2	1:A:209:PRO:CD	2.50	0.42
1:A:402:HIS:HB3	4:A:730:HOH:O	2.20	0.42
1:A:248:PRO:HG3	1:A:267:TRP:CD2	2.54	0.41
1:A:369:MET:HB3	1:A:374:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HD22	2:A:502:SEC:C	2.35	0.40
1:A:366:MET:N	1:A:367:PRO:CD	2.84	0.40
1:A:400:ARG:HH11	1:A:400:ARG:HD3	1.76	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:950:HOH:O	4:A:950:HOH:O[7_555]	1.42	0.78
4:A:519:HOH:O	4:A:519:HOH:O[7_555]	1.98	0.22
4:A:541:HOH:O	4:A:676:HOH:O[7_555]	1.99	0.21
4:A:536:HOH:O	4:A:536:HOH:O[7_555]	2.03	0.17

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	402/406 (99%)	387 (96%)	15 (4%)	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	327/328 (100%)	313 (96%)	14 (4%)	26	35

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	19	VAL
1	A	56	ARG
1	A	58	ILE
1	A	61	LEU
1	A	137	VAL
1	A	148	PRO
1	A	159	THR
1	A	163	GLU
1	A	182	PRO
1	A	269	LYS
1	A	329	GLN
1	A	368	LEU
1	A	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	147	ASN
1	A	193	HIS
1	A	244	GLN
1	A	300	ASN
1	A	301	ASN
1	A	316	GLN
1	A	362	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSZ	A	364	1	3,6,7	1.03	0	1,6,8	2.15	1 (100%)

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	CSZ	A	364	1	-	0/0/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	364	CSZ	CB-CA-C	2.15	116.64	110.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	364	CSZ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1,2	15,15,16	1.83	4 (26%)	21,22,23	3.44	13 (61%)
2	SEC	A	502	3	2,5,6	2.09	1 (50%)	0,5,7	-	-

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	1,2	-	0/6/6/8	0/1/1/1
2	SEC	A	502	3	-	0/0/4/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	C3-C2	-5.08	1.35	1.41
2	A	502	SEC	CA-N	2.53	1.55	1.48
3	A	500	PLP	C4A-C4	2.52	1.56	1.51
3	A	500	PLP	C2A-C2	2.42	1.54	1.50
3	A	500	PLP	P-O1P	-2.08	1.44	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLP	C4A-C4-C3	-6.75	109.27	120.52
3	A	500	PLP	C6-N1-C2	5.60	129.35	119.20
3	A	500	PLP	C3-C4-C5	5.58	125.29	118.59
3	A	500	PLP	C2A-C2-N1	4.52	126.17	117.64
3	A	500	PLP	O2P-P-O4P	-4.42	95.14	106.67
3	A	500	PLP	C5-C6-N1	-4.40	116.67	123.83
3	A	500	PLP	C4A-C4-C5	4.37	125.44	120.94
3	A	500	PLP	C2A-C2-C3	-3.46	116.75	120.80
3	A	500	PLP	C3-C2-N1	-3.07	117.09	120.96
3	A	500	PLP	C6-C5-C4	-2.84	115.77	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLP	C4-C3-C2	-2.74	115.78	119.89
3	A	500	PLP	C5A-C5-C4	2.36	127.30	122.64
3	A	500	PLP	O3-C3-C4	2.35	124.22	118.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	SEC	2	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	404/406 (99%)	-0.50	7 (1%) 69 66	23, 34, 50, 78	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	6.3
1	A	20	ASN	5.8
1	A	56	ARG	3.4
1	A	58	ILE	3.0
1	A	19	VAL	3.0
1	A	55	HIS	2.6
1	A	22	LEU	2.3

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	CSZ	A	364	7/8	0.90	0.17	29,32,34,38	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($\text{\AA}^2$)	Q<0.9
2	SEC	A	502	6/7	0.83	0.26	41,42,43,45	0
3	PLP	A	500	15/16	0.99	0.05	27,31,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.