



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:04 AM UTC

PDB ID : 1S0A / pdb_00001s0a
Title : Crystal Structure of the Y17F Mutant of 7,8-Diaminopelargonic Acid Synthase
Authors : Sandmark, J.; Eliot, A.C.; Famm, K.; Schneider, G.; Kirsch, J.F.
Deposited on : 2003-12-30
Resolution : 1.71 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

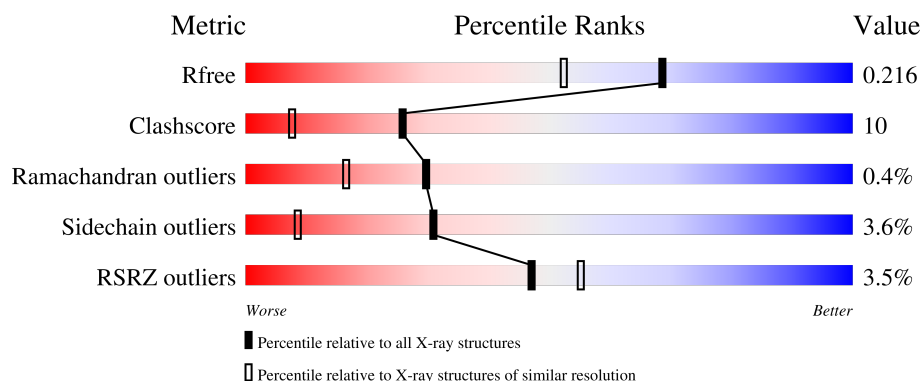
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	429	3% 83% 15% .
1	B	429	4% 82% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7358 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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	P	S	54	6	0
			3340	2118	577	611	1	33			
1	B	428	Total	C	N	O	P	S	42	9	0
			3356	2134	577	612	1	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	LEU	TRP	SEE REMARK 999	UNP P12995
A	17	PHE	TYR	engineered mutation	UNP P12995
A	274	LLP	LYS	modified residue	UNP P12995
B	14	LEU	TRP	SEE REMARK 999	UNP P12995
B	17	PHE	TYR	engineered mutation	UNP P12995
B	274	LLP	LYS	modified residue	UNP P12995

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

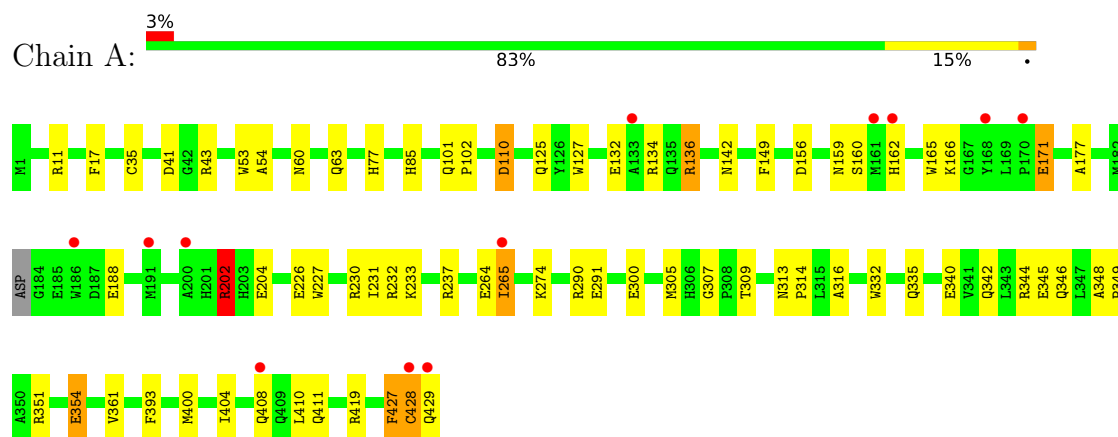
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	334	Total	O	0	0
			334	334		
3	B	326	Total	O	0	0
			326	326		

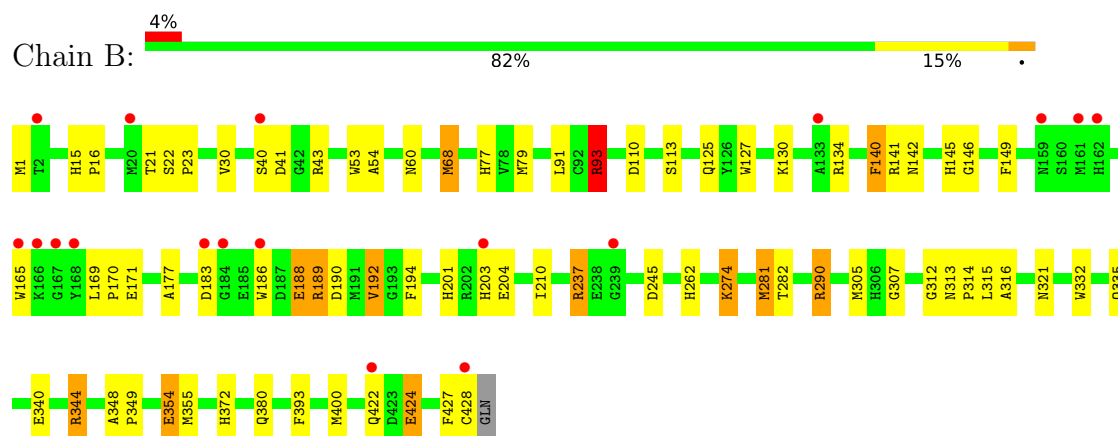
3 Residue-property plots

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: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



- Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.51Å 55.66Å 121.40Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	19.92 – 1.71 19.92 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.92-1.71) 97.0 (19.92-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.186 , 0.206 0.198 , 0.216	Depositor DCC
R_{free} test set	4065 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7358	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 10.52% 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: LLP, NA

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	0.64	5/3417 (0.1%)	1.05	11/4634 (0.2%)
1	B	0.68	5/3450 (0.1%)	0.93	7/4682 (0.1%)
All	All	0.66	10/6867 (0.1%)	0.99	18/9316 (0.2%)

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	1
1	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	MET	SD-CE	-12.25	1.49	1.79
1	B	68	MET	SD-CE	-11.75	1.50	1.79
1	A	202	ARG	CD-NE	-10.64	1.31	1.46
1	A	171	GLU	CB-CG	-9.70	1.23	1.52
1	A	345	GLU	CB-CG	-7.64	1.29	1.52
1	A	345	GLU	CA-C	7.62	1.62	1.52
1	B	79	MET	SD-CE	-6.57	1.63	1.79
1	B	171	GLU	CB-CG	6.33	1.71	1.52
1	B	93	ARG	CD-NE	5.65	1.54	1.46
1	A	171	GLU	CA-CB	-5.25	1.46	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLU	CA-CB-CG	20.56	155.22	114.10
1	A	171	GLU	CB-CG-CD	18.58	144.19	112.60
1	A	354	GLU	CB-CG-CD	16.28	140.27	112.60
1	A	202	ARG	CG-CD-NE	15.88	146.93	112.00
1	B	93	ARG	CG-CD-NE	9.00	131.80	112.00
1	B	54	ALA	N-CA-C	7.68	119.65	111.28
1	A	237	ARG	CG-CD-NE	7.22	127.90	112.00
1	A	54	ALA	N-CA-C	7.17	119.09	111.28
1	A	159	ASN	CA-CB-CG	7.11	119.71	112.60
1	B	93	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	A	427	PHE	N-CA-C	5.27	118.15	109.72
1	A	345	GLU	CB-CA-C	5.21	119.05	110.88
1	A	345	GLU	CA-CB-CG	5.12	124.33	114.10
1	B	140[A]	PHE	CB-CA-C	5.07	119.32	109.33
1	B	140[B]	PHE	CB-CA-C	5.07	119.32	109.33
1	B	354[A]	GLU	CB-CG-CD	5.06	121.20	112.60
1	B	354[B]	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	300	GLU	CA-CB-CG	5.04	124.19	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	ARG	Sidechain
1	B	93	ARG	Sidechain

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	3340	0	3275	61	9
1	B	3356	0	3281	72	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	334	0	0	11	11
3	B	326	0	0	13	3
All	All	7358	0	6556	125	14

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 10.

All (125) 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:393[B]:PHE:HE2	3:A:1753:HOH:O	1.36	1.07
1:B:140[B]:PHE:CD1	1:B:210:ILE:HG22	1.91	1.04
1:B:140[B]:PHE:CE1	1:B:210:ILE:CG2	2.46	0.98
1:B:1:MET:HE3	1:B:40:SER:OG	1.74	0.88
1:B:203[B]:HIS:HE1	3:B:1816:HOH:O	1.56	0.87
1:A:393[B]:PHE:CE2	3:A:1753:HOH:O	2.18	0.86
1:B:140[B]:PHE:CE1	1:B:210:ILE:HG21	2.12	0.84
1:B:140[B]:PHE:CD1	1:B:210:ILE:CG2	2.62	0.83
1:B:68:MET:HE3	1:B:281:MET:CE	2.09	0.82
1:B:355:MET:SD	1:B:424[B]:GLU:HG2	2.21	0.81
1:B:140[B]:PHE:HD1	1:B:210:ILE:HG22	1.43	0.81
1:B:190:ASP:OD1	3:B:1806:HOH:O	2.00	0.78
1:A:17:PHE:HE2	3:B:1818:HOH:O	1.68	0.76
1:A:160:SER:HB3	3:A:1766:HOH:O	1.85	0.76
1:B:203[B]:HIS:CE1	3:B:1816:HOH:O	2.35	0.76
1:B:125:GLN:HE22	1:B:305:MET:H	1.33	0.75
1:A:340:GLU:HG2	1:A:344:ARG:HH11	1.52	0.75
1:B:380:GLN:NE2	3:B:1761:HOH:O	2.19	0.74
1:A:125:GLN:HE22	1:A:305:MET:H	1.36	0.73
1:A:142:ASN:HD22	1:A:177:ALA:HB2	1.53	0.73
1:A:340:GLU:CG	1:A:344:ARG:NH1	2.52	0.73
1:B:149[B]:PHE:CZ	1:B:170:PRO:HD3	2.23	0.73
1:A:428:CYS:O	1:A:429:GLN:HB2	1.88	0.72
1:A:188:GLU:OE2	1:A:230:ARG:NH2	2.22	0.71
1:B:355:MET:CE	1:B:424[B]:GLU:HG2	2.21	0.69
1:B:140[B]:PHE:HE1	1:B:210:ILE:CG2	2.02	0.69
1:B:186:TRP:HE1	1:B:188:GLU:HG2	1.57	0.69
1:B:201:HIS:HD2	1:B:204:GLU:OE2	1.75	0.68
1:B:340:GLU:O	1:B:344:ARG:HG3	1.93	0.67
1:B:140[B]:PHE:CZ	1:B:194:PHE:CE1	2.85	0.65
1:A:162:HIS:ND1	3:A:1771:HOH:O	2.29	0.65
1:A:53:TRP:CZ2	1:A:400:MET:HE1	2.32	0.64
1:A:346:GLN:HE22	1:A:411[A]:GLN:CG	2.10	0.64
1:A:340:GLU:HG2	1:A:344:ARG:NH1	2.13	0.64
1:B:68:MET:HE3	1:B:281:MET:HE2	1.82	0.61
1:A:346:GLN:NE2	1:A:411[A]:GLN:HG2	2.16	0.61
1:B:140[B]:PHE:CE2	1:B:194:PHE:CD1	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HH11	1:A:136:ARG:HG3	1.65	0.60
1:B:281:MET:HE1	1:B:315:LEU:HG	1.82	0.60
1:A:342:GLN:CD	1:A:410:LEU:HD23	2.28	0.59
1:A:149:PHE:HB3	1:B:149[B]:PHE:CD2	2.37	0.59
1:B:422:GLN:NE2	3:B:1715:HOH:O	2.35	0.58
1:A:313:ASN:ND2	1:A:316:ALA:H	2.02	0.58
1:B:274:LLP:NZ	1:B:274:LLP:O3	2.37	0.58
1:A:226:GLU:OE1	1:A:230:ARG:NH1	2.37	0.57
1:A:53:TRP:CE2	1:A:400:MET:HE1	2.40	0.57
1:A:136:ARG:HG3	1:A:136:ARG:NH1	2.20	0.56
1:B:427:PHE:O	1:B:428:CYS:HB2	2.05	0.56
1:A:41:ASP:OD2	1:A:43:ARG:NE	2.38	0.56
1:A:340:GLU:CD	1:A:344:ARG:HH12	2.14	0.56
1:A:332:TRP:HA	1:A:335:GLN:HE21	1.70	0.56
1:A:110[A]:ASP:OD1	3:A:1541:HOH:O	2.18	0.55
1:A:156:ASP:O	1:A:160:SER:HB2	2.06	0.55
1:B:237:ARG:HG3	3:B:1805:HOH:O	2.06	0.55
1:B:262:HIS:HD2	3:B:1756:HOH:O	1.89	0.54
1:A:149:PHE:HB2	1:B:149[B]:PHE:HD2	1.72	0.54
1:B:68:MET:HE3	1:B:281:MET:HE3	1.87	0.54
1:A:149:PHE:CB	1:B:149[B]:PHE:HD2	2.21	0.53
1:B:145:HIS:HD2	1:B:245:ASP:OD2	1.92	0.53
1:A:136:ARG:HH11	1:A:136:ARG:CG	2.23	0.52
1:B:145:HIS:HE1	3:B:1526:HOH:O	1.91	0.52
1:A:344:ARG:NH2	1:A:361:VAL:O	2.44	0.51
1:A:149:PHE:CB	1:B:149[B]:PHE:CD2	2.94	0.50
1:B:149[B]:PHE:CE1	1:B:170:PRO:HD3	2.46	0.50
1:A:340:GLU:CD	1:A:344:ARG:NH1	2.69	0.50
1:A:264:GLU:HG2	3:A:1829:HOH:O	2.11	0.50
1:B:53:TRP:CE2	1:B:400:MET:HE1	2.47	0.50
1:A:127:TRP:CD2	1:A:134:ARG:HD2	2.48	0.49
1:A:354:GLU:O	1:A:354:GLU:HG3	2.09	0.49
1:A:291:GLU:HG2	3:A:1745:HOH:O	2.11	0.49
1:B:372:HIS:CD2	1:B:424[B]:GLU:OE2	2.65	0.49
1:B:186:TRP:NE1	1:B:188:GLU:HG2	2.27	0.49
1:B:91:LEU:HA	1:B:321:ASN:OD1	2.13	0.48
1:A:11:ARG:O	1:B:290:ARG:NH2	2.35	0.48
1:A:393[A]:PHE:CE1	3:A:1794:HOH:O	2.55	0.48
1:B:127:TRP:CD2	1:B:134:ARG:HD2	2.48	0.48
1:A:309:THR:OG1	1:B:274:LLP:HE2	2.12	0.48
1:B:355:MET:HG2	3:B:1803:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLN:HE22	1:A:411[A]:GLN:HG2	1.74	0.47
1:B:22:SER:N	1:B:23:PRO:HD3	2.29	0.47
1:B:313:ASN:ND2	1:B:316:ALA:H	2.13	0.47
1:B:140[B]:PHE:HE2	1:B:194:PHE:CD1	2.31	0.47
1:A:53:TRP:CH2	1:A:400:MET:HE1	2.49	0.46
1:A:165:TRP:CH2	1:B:125:GLN:HG3	2.50	0.46
1:B:372:HIS:HD2	1:B:424[B]:GLU:OE2	1.99	0.46
1:A:340:GLU:CG	1:A:344:ARG:HH12	2.27	0.46
1:B:21:THR:C	1:B:23:PRO:HD3	2.41	0.46
1:B:140[B]:PHE:HZ	1:B:194:PHE:CE1	2.33	0.45
1:A:227:TRP:O	1:A:231:ILE:HG13	2.17	0.45
1:B:332:TRP:HA	1:B:335:GLN:HE21	1.81	0.45
1:B:142:ASN:HD22	1:B:177:ALA:HB2	1.81	0.45
1:A:85:HIS:HE1	3:A:1503:HOH:O	1.99	0.45
1:B:30:VAL:HG13	1:B:40:SER:OG	2.17	0.45
1:A:348:ALA:N	1:A:349:PRO:CD	2.80	0.44
1:B:312:GLY:O	1:B:313:ASN:C	2.60	0.44
1:A:232:ARG:HG2	1:A:265:ILE:HG13	1.99	0.44
1:A:354:GLU:HG2	3:A:1811:HOH:O	2.18	0.44
1:B:149[B]:PHE:CD1	1:B:169:LEU:HD23	2.53	0.44
1:B:77:HIS:HA	1:B:314:PRO:HD2	1.99	0.44
1:A:226:GLU:O	1:A:230:ARG:HG2	2.17	0.44
1:A:346:GLN:HE22	1:A:411[A]:GLN:HG3	1.80	0.44
1:B:189:ARG:O	1:B:192:VAL:HG13	2.18	0.43
1:B:53:TRP:CZ2	1:B:400:MET:HE1	2.53	0.43
1:A:346:GLN:NE2	1:A:411[A]:GLN:CG	2.76	0.43
1:B:237:ARG:CG	3:B:1814:HOH:O	2.67	0.42
1:B:141:ARG:O	1:B:142:ASN:HB2	2.19	0.42
1:A:136:ARG:NH1	1:A:204:GLU:OE2	2.53	0.42
1:B:41:ASP:OD2	1:B:43:ARG:NE	2.52	0.42
1:B:140[B]:PHE:CZ	1:B:194:PHE:HE1	2.33	0.42
1:B:30:VAL:CG1	1:B:40:SER:HA	2.50	0.42
1:A:77:HIS:HA	1:A:314:PRO:HD2	2.01	0.41
1:B:15:HIS:HB3	1:B:16:PRO:HD2	2.03	0.41
1:A:11:ARG:HG3	3:A:1525:HOH:O	2.19	0.41
1:A:110[A]:ASP:HB3	1:B:282:THR:HG21	2.02	0.41
1:A:101:GLN:HB3	1:A:102:PRO:HD3	2.01	0.41
1:B:348:ALA:N	1:B:349:PRO:CD	2.83	0.41
1:A:427:PHE:O	1:A:428:CYS:HB2	2.20	0.41
1:B:113[A]:SER:OG	1:B:146:GLY:HA3	2.21	0.41
1:B:140[B]:PHE:CE2	1:B:194:PHE:HD1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149[B]:PHE:CZ	1:B:170:PRO:CD	3.01	0.41
1:A:400:MET:HE2	1:A:400:MET:HB3	1.83	0.41
1:A:17:PHE:CE2	3:B:1818:HOH:O	2.56	0.40
1:A:35[A]:CYS:SG	1:A:404:ILE:HG13	2.61	0.40
1:B:237:ARG:HG2	3:B:1814:HOH:O	2.21	0.40

All (14) 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)
1:A:171:GLU:CD	3:A:1777:HOH:O[1_545]	0.54	1.66
1:A:171:GLU:OE1	3:A:1777:HOH:O[1_545]	0.98	1.22
1:A:419:ARG:CZ	3:A:1795:HOH:O[2_655]	1.03	1.17
1:A:419:ARG:NE	3:A:1795:HOH:O[2_655]	1.13	1.07
1:A:171:GLU:OE2	3:A:1777:HOH:O[1_545]	1.25	0.95
1:A:419:ARG:NH2	3:A:1795:HOH:O[2_655]	1.28	0.92
3:A:1703:HOH:O	3:A:1817:HOH:O[1_565]	1.29	0.91
3:B:1666:HOH:O	3:B:1807:HOH:O[2_656]	1.72	0.48
3:B:1740:HOH:O	3:B:1814:HOH:O[2_656]	1.86	0.34
1:A:171:GLU:CG	3:A:1777:HOH:O[1_545]	2.03	0.17
3:A:1685:HOH:O	3:A:1756:HOH:O[1_655]	2.03	0.17
3:A:1730:HOH:O	3:B:1636:HOH:O[1_655]	2.04	0.16
1:A:351:ARG:O	1:A:408:GLN:NE2[2_645]	2.05	0.15
1:A:408:GLN:CD	3:A:1792:HOH:O[2_655]	2.17	0.03

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	429/429 (100%)	417 (97%)	10 (2%)	2 (0%)	24 11
1	B	434/429 (101%)	420 (97%)	13 (3%)	1 (0%)	43 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	863/858 (101%)	837 (97%)	23 (3%)	3 (0%)	30	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	CYS
1	A	307	GLY
1	B	307	GLY

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	349/344 (102%)	338 (97%)	11 (3%)	34	11
1	B	351/344 (102%)	332 (95%)	19 (5%)	20	3
All	All	700/688 (102%)	670 (96%)	30 (4%)	31	6

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	GLN
1	A	110[A]	ASP
1	A	110[B]	ASP
1	A	132	GLU
1	A	136	ARG
1	A	166	LYS
1	A	202	ARG
1	A	233	LYS
1	A	265	ILE
1	A	290	ARG
1	B	60	ASN
1	B	93	ARG
1	B	110[A]	ASP
1	B	110[B]	ASP

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Mol	Chain	Res	Type
1	B	130	LYS
1	B	165	TRP
1	B	183	ASP
1	B	188	GLU
1	B	189	ARG
1	B	192	VAL
1	B	237	ARG
1	B	290	ARG
1	B	344	ARG
1	B	354[A]	GLU
1	B	354[B]	GLU
1	B	393[A]	PHE
1	B	393[B]	PHE
1	B	424[A]	GLU
1	B	424[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	125	GLN
1	A	135	GLN
1	A	142	ASN
1	A	313	ASN
1	A	333	GLN
1	A	334	GLN
1	A	335	GLN
1	A	346	GLN
1	A	386	GLN
1	A	418	ASN
1	B	63	GLN
1	B	125	GLN
1	B	142	ASN
1	B	145	HIS
1	B	201	HIS
1	B	262	HIS
1	B	313	ASN
1	B	334	GLN
1	B	335	GLN
1	B	342	GLN
1	B	346	GLN
1	B	411	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	B	274	1	23,24,25	1.66	2 (8%)	25,32,34	1.88	4 (16%)
1	LLP	A	274	1	23,24,25	1.70	4 (17%)	25,32,34	1.82	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	274	1	-	1/16/17/19	0/1/1/1
1	LLP	A	274	1	-	5/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	LLP	O3-C3	-5.65	1.24	1.36
1	B	274	LLP	O3-C3	-5.35	1.24	1.36
1	A	274	LLP	C2-N1	2.38	1.38	1.33
1	B	274	LLP	C2-N1	2.35	1.38	1.33
1	A	274	LLP	C6-N1	2.24	1.39	1.34
1	A	274	LLP	P-OP3	-2.11	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	LLP	OP4-C5'-C5	6.85	122.19	109.36
1	B	274	LLP	OP4-C5'-C5	6.19	120.95	109.36
1	B	274	LLP	C4-C4'-NZ	-4.38	103.81	124.04
1	A	274	LLP	C4-C4'-NZ	-3.53	107.77	124.04
1	B	274	LLP	OP3-P-OP4	-2.58	99.94	106.67
1	B	274	LLP	C5-C6-N1	-2.35	120.02	123.83
1	A	274	LLP	C5-C6-N1	-2.10	120.42	123.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	274	LLP	C4-C4'-NZ-CE
1	A	274	LLP	C3-C4-C4'-NZ
1	A	274	LLP	C5-C4-C4'-NZ
1	A	274	LLP	CD-CE-NZ-C4'
1	A	274	LLP	CG-CD-CE-NZ
1	B	274	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	274	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	427/429 (99%)	0.24	12 (2%)	55 63	10, 22, 37, 44	19 (4%)
1	B	427/429 (99%)	0.29	18 (4%)	40 48	12, 22, 36, 44	21 (4%)
All	All	854/858 (99%)	0.27	30 (3%)	47 55	10, 22, 36, 44	40 (4%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	CYS	4.8
1	A	429	GLN	4.2
1	B	183	ASP	3.3
1	A	428	CYS	3.2
1	B	161	MET	3.1
1	B	203[A]	HIS	3.0
1	A	161	MET	3.0
1	B	162	HIS	2.9
1	A	168	TYR	2.7
1	A	170	PRO	2.6
1	A	133	ALA	2.5
1	B	239	GLY	2.4
1	A	408	GLN	2.4
1	B	20	MET	2.3
1	B	40	SER	2.3
1	B	166	LYS	2.3
1	B	184	GLY	2.3
1	B	2	THR	2.2
1	A	191	MET	2.2
1	B	159	ASN	2.2
1	A	162	HIS	2.2
1	B	133	ALA	2.2
1	A	265	ILE	2.2
1	B	165	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	186	TRP	2.1
1	B	186	TRP	2.1
1	B	422	GLN	2.1
1	B	168	TYR	2.1
1	A	200	ALA	2.1
1	B	167	GLY	2.1

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($\text{\AA}^2$)	Q<0.9
1	LLP	A	274	24/25	0.96	0.07	11,15,21,22	0
1	LLP	B	274	24/25	0.97	0.05	12,15,17,18	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	NA	A	1501	1/1	0.96	0.20	10,10,10,10	0
2	NA	B	1502	1/1	0.98	0.17	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.