



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:08 AM UTC

PDB ID : 5X2Y / pdb_00005x2y
Title : Crystal structure of Pseudomonas putida methionine gamma-lyase C116H mutant without sulfate ion
Authors : Shiba, T.; Sato, D.; Harada, S.
Deposited on : 2017-02-02
Resolution : 1.79 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

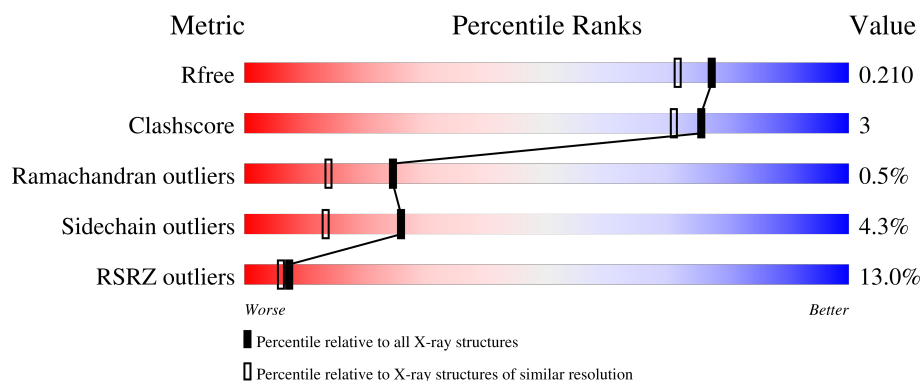
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	398	14% 87% 10% ...
1	B	398	13% 88% 9% ..
1	C	398	10% 87% 9% .
1	D	398	14% 89% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12462 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	P	S	0	0	0
			2970	1874	525	554	1	16			
1	B	392	Total	C	N	O	P	S	0	0	0
			2966	1872	525	552	1	16			
1	C	382	Total	C	N	O	P	S	0	0	0
			2884	1820	510	537	1	16			
1	D	390	Total	C	N	O	P	S	0	0	0
			2946	1858	520	551	1	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	HIS	CYS	engineered mutation	UNP P13254
B	116	HIS	CYS	engineered mutation	UNP P13254
C	116	HIS	CYS	engineered mutation	UNP P13254
D	116	HIS	CYS	engineered mutation	UNP P13254

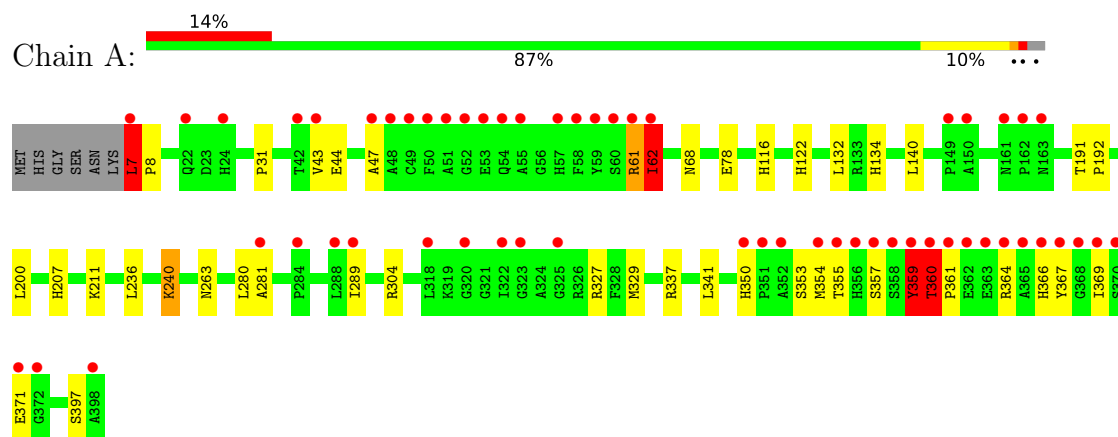
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	129	Total	O	0	0
			129	129		
2	B	196	Total	O	0	0
			196	196		
2	C	176	Total	O	0	0
			176	176		
2	D	195	Total	O	0	0
			195	195		

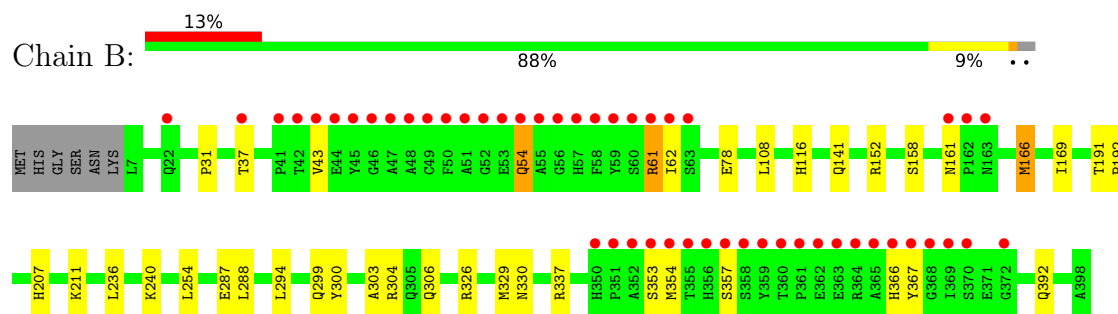
3 Residue-property plots [i](#)

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.

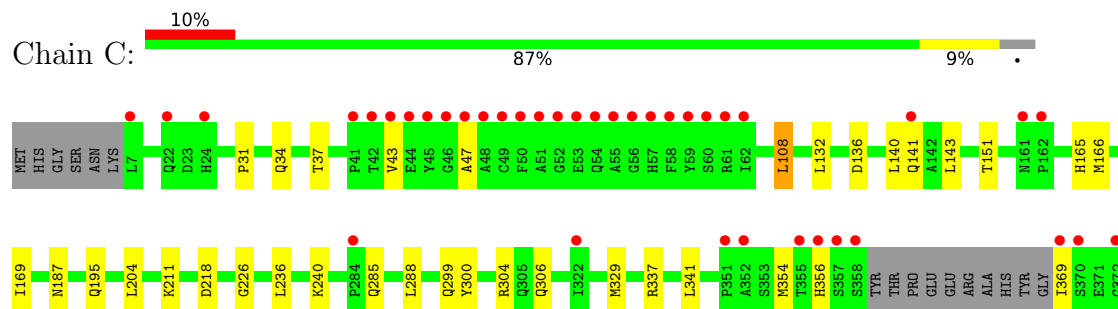
- Molecule 1: L-methionine gamma-lyase

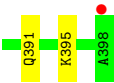


- Molecule 1: L-methionine gamma-lyase

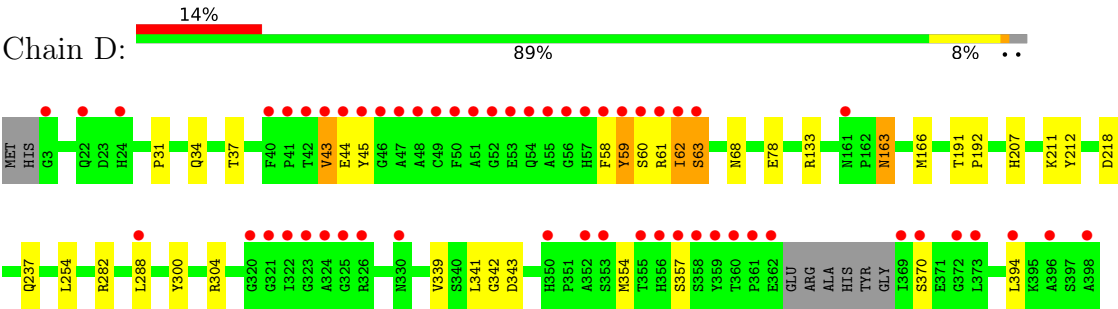


- Molecule 1: L-methionine gamma-lyase





● Molecule 1: L-methionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.79Å 153.38Å 80.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.79 20.00 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-1.79) 97.0 (20.00-1.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.173 , 0.204 0.183 , 0.210	Depositor DCC
R_{free} test set	8763 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12462	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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

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	0.83	0/3010	0.92	3/4086 (0.1%)
1	B	0.87	0/3006	0.91	1/4081 (0.0%)
1	C	0.83	0/2919	0.92	1/3960 (0.0%)
1	D	0.86	0/2983	0.92	3/4047 (0.1%)
All	All	0.85	0/11918	0.92	8/16174 (0.0%)

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	3
1	B	0	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	TYR	N-CA-C	-8.32	99.43	110.24
1	A	359	TYR	CB-CA-C	5.61	121.05	111.68
1	D	163	ASN	N-CA-C	5.55	119.90	113.18
1	D	282	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	366	HIS	N-CA-C	5.45	116.90	111.07
1	A	7	LEU	CA-C-N	-5.15	114.41	119.92
1	A	7	LEU	C-N-CA	-5.15	114.41	119.92
1	C	356	HIS	N-CA-C	5.13	115.78	108.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	TYR	Peptide
1	A	360	THR	Peptide
1	A	62	ILE	Peptide
1	B	367	TYR	Peptide
1	B	61	ARG	Peptide
1	D	58	PHE	Peptide

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	2970	0	2927	29	0
1	B	2966	0	2922	21	0
1	C	2884	0	2854	18	0
1	D	2946	0	2910	19	0
2	A	129	0	0	0	0
2	B	196	0	0	0	0
2	C	176	0	0	0	0
2	D	195	0	0	2	0
All	All	12462	0	11613	69	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 3.

All (69) 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:D:63:SER:HB3	1:D:68:ASN:HD21	1.43	0.82
1:B:166:MET:H	1:B:299:GLN:HE22	1.33	0.75
1:C:169:ILE:H	1:C:306:GLN:HE22	1.41	0.69
1:C:166:MET:H	1:C:299:GLN:HE22	1.41	0.68
1:B:166:MET:HE1	1:B:303:ALA:HB2	1.76	0.67
1:D:60:SER:O	1:D:63:SER:HB2	1.99	0.62
1:A:47:ALA:HB1	1:B:357:SER:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:TYR:CZ	1:D:304:ARG:HD2	2.41	0.56
1:C:236:LEU:O	1:C:240:LYS:HE3	2.05	0.55
1:C:43:VAL:HG12	1:D:354:MET:SD	2.47	0.55
1:A:350:HIS:ND1	1:A:353:SER:OG	2.37	0.54
1:B:78:GLU:OE2	1:B:207:HIS:HE1	1.91	0.53
1:D:339:VAL:O	1:D:339:VAL:HG23	2.08	0.53
1:B:31:PRO:HB2	1:C:31:PRO:HB2	1.91	0.53
1:B:329:MET:HE3	1:B:337:ARG:HG2	1.91	0.52
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.93	0.52
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.45	0.50
1:C:108:LEU:HD22	1:C:151:THR:HG21	1.92	0.50
1:D:78:GLU:OE1	1:D:207:HIS:HE1	1.94	0.50
1:A:31:PRO:HB2	1:D:31:PRO:HB2	1.94	0.49
1:A:240:LYS:HE3	1:B:116:HIS:CE1	2.47	0.49
1:A:43:VAL:HG12	1:B:354:MET:HE2	1.94	0.49
1:C:187:ASN:ND2	1:C:195:GLN:HE21	2.11	0.49
1:B:300:TYR:CZ	1:B:304:ARG:HD2	2.47	0.49
1:A:329:MET:HE3	1:A:337:ARG:HG2	1.95	0.49
1:A:360:THR:HG22	1:A:361:PRO:HD3	1.95	0.48
1:B:169:ILE:H	1:B:306:GLN:HE22	1.61	0.48
1:D:191:THR:HB	1:D:192:PRO:HD2	1.95	0.48
1:B:158:SER:OG	1:B:166:MET:HG3	2.14	0.48
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.67	0.48
1:B:78:GLU:OE2	1:B:207:HIS:CE1	2.67	0.48
1:A:47:ALA:HA	1:B:354:MET:O	2.14	0.47
1:D:343:ASP:HB3	2:D:546:HOH:O	2.14	0.47
1:A:44:GLU:OE1	1:B:326:ARG:HD3	2.14	0.47
1:D:78:GLU:OE1	1:D:207:HIS:CE1	2.68	0.47
1:B:191:THR:HB	1:B:192:PRO:HD2	1.96	0.46
1:A:327:ARG:NH2	1:A:397:SER:O	2.49	0.46
1:A:366:HIS:HB3	1:A:369:ILE:HD12	1.98	0.46
1:A:7:LEU:HB3	1:A:8:PRO:HD3	1.97	0.45
1:D:59:TYR:O	1:D:61:ARG:HB2	2.16	0.45
1:A:236:LEU:O	1:A:240:LYS:HE2	2.16	0.45
1:A:360:THR:HB	1:A:361:PRO:HD3	1.98	0.45
1:C:354:MET:HG3	1:D:43:VAL:HG22	1.98	0.45
1:A:47:ALA:HB1	1:B:357:SER:HB2	1.99	0.45
1:B:254:LEU:HD21	1:D:254:LEU:HD21	1.99	0.45
1:A:364:ARG:NH1	1:A:371:GLU:OE2	2.50	0.45
1:C:166:MET:H	1:C:299:GLN:NE2	2.11	0.45
1:A:7:LEU:HB3	1:A:8:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:H	1:B:330:ASN:HD21	1.64	0.44
1:C:204:LEU:HD23	1:C:226:GLY:HA3	1.99	0.44
1:A:281:ALA:HA	1:A:289:ILE:HD11	2.00	0.44
1:A:337:ARG:HB3	1:A:354:MET:CE	2.47	0.44
1:A:122:HIS:NE2	1:A:134:HIS:HE1	2.16	0.44
1:A:360:THR:CG2	1:A:361:PRO:HD3	2.47	0.44
1:D:59:TYR:O	1:D:60:SER:C	2.59	0.44
1:C:37:THR:HG22	2:D:405:HOH:O	2.18	0.43
1:A:61:ARG:NH1	1:A:68:ASN:HD22	2.16	0.42
1:C:369:ILE:O	1:C:369:ILE:HG22	2.19	0.42
1:C:136:ASP:OD1	1:C:165:HIS:HE1	2.01	0.42
1:C:329:MET:HE3	1:C:337:ARG:HG2	2.00	0.42
1:C:34:GLN:HG3	1:D:218:ASP:O	2.20	0.41
1:D:62:ILE:O	1:D:62:ILE:HG23	2.20	0.41
1:A:116:HIS:CE1	1:B:240:LYS:HE3	2.55	0.41
1:D:212:TYR:CE1	1:D:342:GLY:HA2	2.56	0.41
1:A:47:ALA:HB1	1:B:357:SER:HB3	2.01	0.40
1:A:191:THR:HB	1:A:192:PRO:HD2	2.03	0.40
1:C:218:ASP:O	1:D:34:GLN:HG3	2.21	0.40
1:A:47:ALA:HB2	1:B:353:SER:O	2.21	0.40
1:C:47:ALA:HB1	1:D:357:SER:HB3	2.02	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	389/398 (98%)	379 (97%)	6 (2%)	4 (1%)	12	4
1	B	389/398 (98%)	378 (97%)	9 (2%)	2 (0%)	24	14
1	C	377/398 (95%)	368 (98%)	9 (2%)	0	100	100
1	D	385/398 (97%)	374 (97%)	10 (3%)	1 (0%)	36	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1540/1592 (97%)	1499 (97%)	34 (2%)	7 (0%)	24	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	B	62	ILE
1	A	367	TYR
1	A	61	ARG
1	D	45	TYR
1	B	54	GLN
1	A	360	THR

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	301/306 (98%)	287 (95%)	14 (5%)	23	11
1	B	300/306 (98%)	286 (95%)	14 (5%)	23	11
1	C	293/306 (96%)	283 (97%)	10 (3%)	32	20
1	D	300/306 (98%)	287 (96%)	13 (4%)	26	13
All	All	1194/1224 (98%)	1143 (96%)	51 (4%)	26	13

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	62	ILE
1	A	132	LEU
1	A	140	LEU
1	A	200	LEU
1	A	240	LYS
1	A	263	ASN
1	A	280	LEU

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Mol	Chain	Res	Type
1	A	304	ARG
1	A	341	LEU
1	A	355	THR
1	A	357	SER
1	A	359	TYR
1	A	360	THR
1	B	37	THR
1	B	43	VAL
1	B	54	GLN
1	B	61	ARG
1	B	108	LEU
1	B	141	GLN
1	B	152	ARG
1	B	161	ASN
1	B	166	MET
1	B	236	LEU
1	B	287	GLU
1	B	288	LEU
1	B	294	LEU
1	B	392	GLN
1	C	108	LEU
1	C	132	LEU
1	C	140	LEU
1	C	141	GLN
1	C	143	LEU
1	C	285	GLN
1	C	288	LEU
1	C	341	LEU
1	C	391	GLN
1	C	395	LYS
1	D	37	THR
1	D	43	VAL
1	D	44	GLU
1	D	62	ILE
1	D	63	SER
1	D	133	ARG
1	D	163	ASN
1	D	166	MET
1	D	237	GLN
1	D	288	LEU
1	D	341	LEU
1	D	370	SER

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Mol	Chain	Res	Type
1	D	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	111	ASN
1	A	116	HIS
1	A	134	HIS
1	A	207	HIS
1	A	250	HIS
1	A	263	ASN
1	A	391	GLN
1	B	64	ASN
1	B	68	ASN
1	B	111	ASN
1	B	116	HIS
1	B	161	ASN
1	B	207	HIS
1	B	274	GLN
1	B	290	HIS
1	B	299	GLN
1	B	306	GLN
1	B	330	ASN
1	B	392	GLN
1	C	22	GLN
1	C	34	GLN
1	C	54	GLN
1	C	116	HIS
1	C	141	GLN
1	C	163	ASN
1	C	165	HIS
1	C	187	ASN
1	C	250	HIS
1	C	290	HIS
1	C	299	GLN
1	C	305	GLN
1	C	306	GLN
1	C	349	GLN
1	C	356	HIS
1	D	34	GLN
1	D	68	ASN

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Mol	Chain	Res	Type
1	D	116	HIS
1	D	207	HIS
1	D	274	GLN
1	D	285	GLN
1	D	305	GLN
1	D	330	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	C	211	1	23,24,25	2.24	5 (21%)	25,32,34	1.47	7 (28%)
1	LLP	D	211	1	23,24,25	2.49	5 (21%)	25,32,34	1.50	6 (24%)
1	LLP	A	211	1	23,24,25	2.33	5 (21%)	25,32,34	1.48	4 (16%)
1	LLP	B	211	1	23,24,25	2.68	5 (21%)	25,32,34	1.64	6 (24%)

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	C	211	1	-	5/16/17/19	0/1/1/1
1	LLP	D	211	1	-	6/16/17/19	0/1/1/1
1	LLP	A	211	1	-	5/16/17/19	0/1/1/1
1	LLP	B	211	1	-	6/16/17/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LLP	C3-C2	7.50	1.48	1.41
1	D	211	LLP	C3-C2	6.69	1.47	1.41
1	B	211	LLP	C4'-NZ	6.30	1.48	1.27
1	A	211	LLP	C3-C2	5.86	1.47	1.41
1	C	211	LLP	C4'-NZ	5.84	1.46	1.27
1	D	211	LLP	C4'-NZ	5.70	1.46	1.27
1	A	211	LLP	C4'-NZ	5.61	1.45	1.27
1	B	211	LLP	C4-C5	5.53	1.49	1.42
1	D	211	LLP	C4-C5	5.05	1.49	1.42
1	C	211	LLP	C3-C2	4.92	1.46	1.41
1	C	211	LLP	C4-C5	4.80	1.48	1.42
1	A	211	LLP	C4-C5	4.61	1.48	1.42
1	D	211	LLP	C4-C3	4.57	1.48	1.41
1	C	211	LLP	C4-C3	4.34	1.48	1.41
1	A	211	LLP	C4-C3	4.30	1.48	1.41
1	B	211	LLP	C4-C3	3.76	1.47	1.41
1	B	211	LLP	C4-C4'	3.59	1.54	1.46
1	D	211	LLP	C4-C4'	2.94	1.52	1.46
1	A	211	LLP	C4-C4'	2.70	1.52	1.46
1	C	211	LLP	C4-C4'	2.18	1.51	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LLP	C4-C3-C2	-3.66	118.08	120.14
1	A	211	LLP	OP3-P-OP4	-3.16	98.42	106.67
1	B	211	LLP	O3-C3-C2	2.89	123.58	117.58
1	A	211	LLP	C4-C3-C2	-2.76	118.59	120.14
1	D	211	LLP	C3-C4-C5	-2.74	116.08	118.28
1	A	211	LLP	C6-N1-C2	2.71	124.12	119.20
1	B	211	LLP	OP4-P-OP1	-2.70	99.13	106.44
1	C	211	LLP	OP4-P-OP1	-2.70	99.15	106.44
1	C	211	LLP	C2'-C2-N1	2.67	122.67	117.64
1	D	211	LLP	OP3-P-OP2	2.66	117.79	107.80
1	A	211	LLP	O3-C3-C2	2.64	123.05	117.58
1	C	211	LLP	C6-N1-C2	2.55	123.83	119.20
1	D	211	LLP	C3-C2-N1	-2.45	117.87	120.96
1	D	211	LLP	O3-C3-C2	2.43	122.62	117.58
1	B	211	LLP	CD-CE-NZ	2.27	116.84	110.83
1	B	211	LLP	C6-N1-C2	2.23	123.25	119.20
1	D	211	LLP	CD-CE-NZ	2.22	116.69	110.83
1	C	211	LLP	C3-C2-N1	-2.19	118.20	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	LLP	C6-N1-C2	2.14	123.07	119.20
1	C	211	LLP	C4-C4'-NZ	-2.09	114.40	124.04
1	C	211	LLP	O3-C3-C2	2.08	121.89	117.58
1	B	211	LLP	C4-C4'-NZ	-2.04	114.64	124.04
1	C	211	LLP	OP3-P-OP1	2.03	118.73	110.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	O-C-CA-CB
1	C	211	LLP	O-C-CA-CB
1	D	211	LLP	O-C-CA-CB
1	B	211	LLP	C4-C4'-NZ-CE
1	D	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	C4-C4'-NZ-CE
1	C	211	LLP	C4-C4'-NZ-CE
1	A	211	LLP	CG-CD-CE-NZ
1	B	211	LLP	CG-CD-CE-NZ
1	D	211	LLP	CG-CD-CE-NZ
1	D	211	LLP	CA-CB-CG-CD
1	A	211	LLP	CA-CB-CG-CD
1	C	211	LLP	CG-CD-CE-NZ
1	B	211	LLP	CA-CB-CG-CD
1	B	211	LLP	C3-C4-C4'-NZ
1	D	211	LLP	C3-C4-C4'-NZ
1	A	211	LLP	C3-C4-C4'-NZ
1	C	211	LLP	C3-C4-C4'-NZ
1	B	211	LLP	CD-CE-NZ-C4'
1	D	211	LLP	CD-CE-NZ-C4'
1	C	211	LLP	CD-CE-NZ-C4'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	391/398 (98%)	0.59	57 (14%) 6 5	12, 25, 73, 128	0
1	B	391/398 (98%)	0.24	50 (12%) 7 6	10, 18, 79, 98	0
1	C	381/398 (95%)	0.29	40 (10%) 11 10	10, 20, 70, 114	0
1	D	389/398 (97%)	0.34	55 (14%) 6 5	10, 18, 79, 119	0
All	All	1552/1592 (97%)	0.37	202 (13%) 7 6	10, 20, 77, 128	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	10.2
1	A	367	TYR	9.5
1	B	365	ALA	9.2
1	C	58	PHE	7.6
1	B	369	ILE	7.1
1	D	62	ILE	7.0
1	D	59	TYR	6.9
1	D	55	ALA	6.8
1	D	58	PHE	6.7
1	A	369	ILE	6.5
1	B	359	TYR	6.5
1	D	57	HIS	6.4
1	A	360	THR	6.3
1	C	62	ILE	6.3
1	A	62	ILE	6.2
1	C	59	TYR	6.1
1	C	57	HIS	6.1
1	C	369	ILE	6.1
1	A	55	ALA	5.9
1	B	368	GLY	5.8
1	B	59	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLY	5.7
1	B	50	PHE	5.7
1	C	45	TYR	5.7
1	B	62	ILE	5.6
1	D	360	THR	5.6
1	D	48	ALA	5.6
1	D	60	SER	5.5
1	A	365	ALA	5.5
1	A	361	PRO	5.5
1	A	359	TYR	5.5
1	C	43	VAL	5.4
1	B	367	TYR	5.4
1	C	50	PHE	5.3
1	D	369	ILE	5.2
1	D	50	PHE	5.2
1	C	47	ALA	5.2
1	C	52	GLY	5.1
1	D	51	ALA	5.1
1	B	58	PHE	5.1
1	D	43	VAL	5.1
1	A	366	HIS	5.0
1	C	46	GLY	4.9
1	D	52	GLY	4.9
1	B	57	HIS	4.8
1	B	360	THR	4.8
1	C	42	THR	4.7
1	B	356	HIS	4.7
1	A	368	GLY	4.6
1	B	52	GLY	4.6
1	C	60	SER	4.6
1	D	361	PRO	4.6
1	D	47	ALA	4.6
1	D	53	GLU	4.5
1	B	48	ALA	4.5
1	A	58	PHE	4.4
1	B	43	VAL	4.4
1	A	355	THR	4.4
1	B	46	GLY	4.4
1	D	161	ASN	4.4
1	B	42	THR	4.4
1	D	61	ARG	4.4
1	C	51	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	60	SER	4.3
1	A	61	ARG	4.3
1	B	44	GLU	4.3
1	B	51	ALA	4.3
1	A	372	GLY	4.3
1	D	45	TYR	4.2
1	B	358	SER	4.2
1	D	322	ILE	4.2
1	B	56	GLY	4.2
1	D	56	GLY	4.2
1	D	324	ALA	4.1
1	B	351	PRO	4.1
1	B	355	THR	4.1
1	A	48	ALA	4.0
1	B	47	ALA	4.0
1	A	352	ALA	4.0
1	C	48	ALA	4.0
1	D	320	GLY	4.0
1	A	288	LEU	3.9
1	C	358	SER	3.9
1	D	49	CYS	3.9
1	D	321	GLY	3.9
1	D	352	ALA	3.9
1	B	45	TYR	3.9
1	B	366	HIS	3.9
1	D	46	GLY	3.8
1	A	362	GLU	3.8
1	A	59	TYR	3.8
1	A	357	SER	3.8
1	D	359	TYR	3.7
1	C	162	PRO	3.7
1	C	355	THR	3.6
1	D	323	GLY	3.6
1	B	363	GLU	3.6
1	A	364	ARG	3.6
1	D	54	GLN	3.6
1	A	7	LEU	3.6
1	B	370	SER	3.5
1	B	55	ALA	3.5
1	C	61	ARG	3.5
1	D	42	THR	3.5
1	C	7	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	350	HIS	3.4
1	A	358	SER	3.4
1	B	353	SER	3.4
1	D	288	LEU	3.4
1	C	357	SER	3.3
1	D	325	GLY	3.3
1	D	373	LEU	3.3
1	D	63	SER	3.3
1	C	44	GLU	3.3
1	D	44	GLU	3.3
1	C	49	CYS	3.3
1	D	370	SER	3.3
1	A	322	ILE	3.2
1	D	398	ALA	3.2
1	B	162	PRO	3.2
1	A	356	HIS	3.1
1	B	352	ALA	3.1
1	A	398	ALA	3.0
1	D	22	GLN	3.0
1	D	372	GLY	3.0
1	A	161	ASN	3.0
1	C	53	GLU	3.0
1	D	24	HIS	2.9
1	A	47	ALA	2.9
1	B	354	MET	2.9
1	D	330	ASN	2.9
1	A	371	GLU	2.9
1	D	40	PHE	2.8
1	A	325	GLY	2.8
1	B	61	ARG	2.8
1	D	326	ARG	2.8
1	A	50	PHE	2.8
1	B	364	ARG	2.8
1	C	356	HIS	2.8
1	C	398	ALA	2.8
1	A	162	PRO	2.7
1	C	284	PRO	2.7
1	A	370	SER	2.7
1	A	351	PRO	2.7
1	A	57	HIS	2.7
1	D	355	THR	2.7
1	A	51	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	352	ALA	2.7
1	D	362	GLU	2.6
1	B	49	CYS	2.6
1	A	24	HIS	2.6
1	A	60	SER	2.6
1	C	370	SER	2.6
1	D	357	SER	2.6
1	B	362	GLU	2.6
1	C	141	GLN	2.6
1	D	396	ALA	2.6
1	C	54	GLN	2.5
1	D	394	LEU	2.5
1	A	281	ALA	2.5
1	A	318	LEU	2.5
1	A	323	GLY	2.5
1	D	41	PRO	2.5
1	A	354	MET	2.5
1	D	353	SER	2.5
1	A	54	GLN	2.4
1	C	24	HIS	2.4
1	A	320	GLY	2.4
1	B	357	SER	2.4
1	C	372	GLY	2.4
1	C	41	PRO	2.4
1	A	163	ASN	2.4
1	B	54	GLN	2.4
1	A	350	HIS	2.4
1	C	22	GLN	2.4
1	B	163	ASN	2.3
1	A	149	PRO	2.3
1	B	53	GLU	2.3
1	A	52	GLY	2.3
1	A	49	CYS	2.3
1	B	161	ASN	2.3
1	C	161	ASN	2.3
1	A	284	PRO	2.2
1	D	356	HIS	2.2
1	A	22	GLN	2.2
1	B	350	HIS	2.2
1	A	43	VAL	2.2
1	D	358	SER	2.2
1	A	363	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	63	SER	2.1
1	A	42	THR	2.1
1	A	289	ILE	2.1
1	B	372	GLY	2.1
1	B	22	GLN	2.1
1	B	41	PRO	2.1
1	C	322	ILE	2.1
1	A	150	ALA	2.1
1	A	53	GLU	2.1
1	B	361	PRO	2.1
1	C	351	PRO	2.1
1	D	3	GLY	2.0
1	B	37	THR	2.0

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	LLP	D	211	24/25	0.97	0.07	10,19,23,24	0
1	LLP	B	211	24/25	0.98	0.06	11,19,24,27	0
1	LLP	C	211	24/25	0.98	0.05	12,16,21,22	0
1	LLP	A	211	24/25	0.98	0.05	13,20,22,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.