



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:07 PM UTC

PDB ID : 5NSF / pdb_00005nsf
Title : Structure of AzuAla
Authors : Martins, B.M.
Deposited on : 2017-04-26
Resolution : 2.43 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

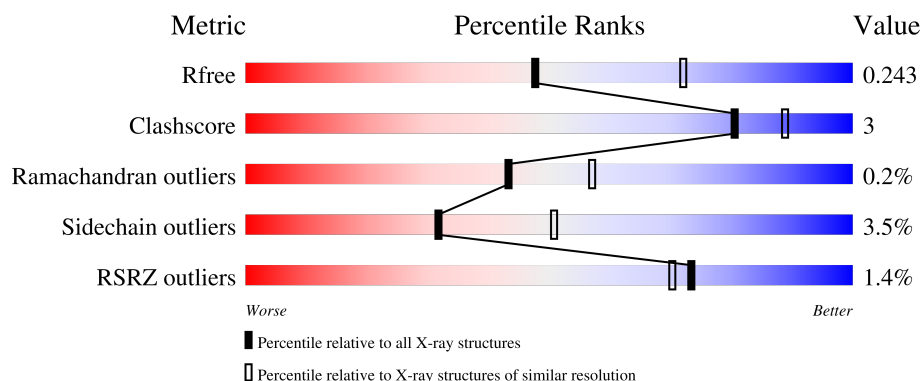
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	318	87% 8% . .
1	B	318	2% 87% 8% . .
1	C	318	% 89% 7% .
1	D	318	2% 86% 8% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20326 atoms, of which 10199 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 Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	306	Total	C	H	N	O	S	0	2	0
			5004	1572	2541	422	456	13			
1	A	305	Total	C	H	N	O	S	0	2	0
			4985	1567	2530	421	455	12			
1	C	306	Total	C	H	N	O	S	0	2	0
			4995	1570	2535	422	456	12			
1	D	305	Total	C	H	N	O	S	0	1	0
			4966	1562	2519	418	455	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q57834
B	-10	ARG	-	expression tag	UNP Q57834
B	-9	GLY	-	expression tag	UNP Q57834
B	-8	SER	-	expression tag	UNP Q57834
B	-7	HIS	-	expression tag	UNP Q57834
B	-6	HIS	-	expression tag	UNP Q57834
B	-5	HIS	-	expression tag	UNP Q57834
B	-4	HIS	-	expression tag	UNP Q57834
B	-3	HIS	-	expression tag	UNP Q57834
B	-2	HIS	-	expression tag	UNP Q57834
B	-1	GLY	-	expression tag	UNP Q57834
B	0	SER	-	expression tag	UNP Q57834
B	32	GLY	TYR	conflict	UNP Q57834
B	65	TRP	LEU	conflict	UNP Q57834
B	70	GLY	HIS	conflict	UNP Q57834
B	108	HIS	PHE	conflict	UNP Q57834
B	109	ASN	GLN	conflict	UNP Q57834
B	158	ALA	ASP	conflict	UNP Q57834
B	162	ASN	LEU	conflict	UNP Q57834
B	286	ARG	ASP	conflict	UNP Q57834
A	-11	MET	-	initiating methionine	UNP Q57834

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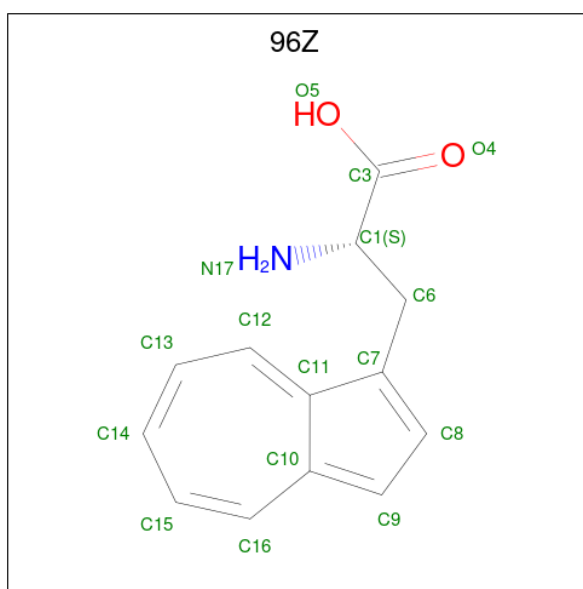
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	ARG	-	expression tag	UNP Q57834
A	-9	GLY	-	expression tag	UNP Q57834
A	-8	SER	-	expression tag	UNP Q57834
A	-7	HIS	-	expression tag	UNP Q57834
A	-6	HIS	-	expression tag	UNP Q57834
A	-5	HIS	-	expression tag	UNP Q57834
A	-4	HIS	-	expression tag	UNP Q57834
A	-3	HIS	-	expression tag	UNP Q57834
A	-2	HIS	-	expression tag	UNP Q57834
A	-1	GLY	-	expression tag	UNP Q57834
A	0	SER	-	expression tag	UNP Q57834
A	32	GLY	TYR	conflict	UNP Q57834
A	65	TRP	LEU	conflict	UNP Q57834
A	70	GLY	HIS	conflict	UNP Q57834
A	108	HIS	PHE	conflict	UNP Q57834
A	109	ASN	GLN	conflict	UNP Q57834
A	158	ALA	ASP	conflict	UNP Q57834
A	162	ASN	LEU	conflict	UNP Q57834
A	286	ARG	ASP	conflict	UNP Q57834
C	-11	MET	-	initiating methionine	UNP Q57834
C	-10	ARG	-	expression tag	UNP Q57834
C	-9	GLY	-	expression tag	UNP Q57834
C	-8	SER	-	expression tag	UNP Q57834
C	-7	HIS	-	expression tag	UNP Q57834
C	-6	HIS	-	expression tag	UNP Q57834
C	-5	HIS	-	expression tag	UNP Q57834
C	-4	HIS	-	expression tag	UNP Q57834
C	-3	HIS	-	expression tag	UNP Q57834
C	-2	HIS	-	expression tag	UNP Q57834
C	-1	GLY	-	expression tag	UNP Q57834
C	0	SER	-	expression tag	UNP Q57834
C	32	GLY	TYR	conflict	UNP Q57834
C	65	TRP	LEU	conflict	UNP Q57834
C	70	GLY	HIS	conflict	UNP Q57834
C	108	HIS	PHE	conflict	UNP Q57834
C	109	ASN	GLN	conflict	UNP Q57834
C	158	ALA	ASP	conflict	UNP Q57834
C	162	ASN	LEU	conflict	UNP Q57834
C	286	ARG	ASP	conflict	UNP Q57834
D	-11	MET	-	initiating methionine	UNP Q57834
D	-10	ARG	-	expression tag	UNP Q57834
D	-9	GLY	-	expression tag	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	SER	-	expression tag	UNP Q57834
D	-7	HIS	-	expression tag	UNP Q57834
D	-6	HIS	-	expression tag	UNP Q57834
D	-5	HIS	-	expression tag	UNP Q57834
D	-4	HIS	-	expression tag	UNP Q57834
D	-3	HIS	-	expression tag	UNP Q57834
D	-2	HIS	-	expression tag	UNP Q57834
D	-1	GLY	-	expression tag	UNP Q57834
D	0	SER	-	expression tag	UNP Q57834
D	32	GLY	TYR	conflict	UNP Q57834
D	65	TRP	LEU	conflict	UNP Q57834
D	70	GLY	HIS	conflict	UNP Q57834
D	108	HIS	PHE	conflict	UNP Q57834
D	109	ASN	GLN	conflict	UNP Q57834
D	158	ALA	ASP	conflict	UNP Q57834
D	162	ASN	LEU	conflict	UNP Q57834
D	286	ARG	ASP	conflict	UNP Q57834

- Molecule 2 is beta-(1-azulenyl)-L-alanine (CCD ID: 96Z) (formula: $C_{13}H_{13}NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			28	13	12	1	2		
2	A	1	Total	C	H	N	O	0	0
			28	13	12	1	2		
2	C	1	Total	C	H	N	O	0	0
			28	13	12	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	0	0
			28	13	12	1	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

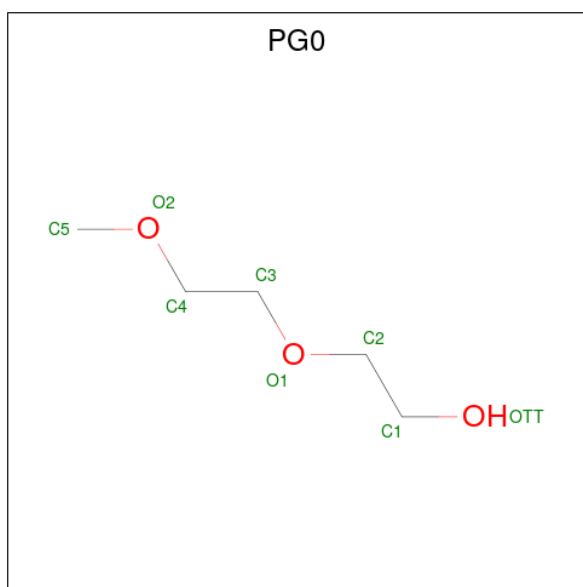


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			18	5	10	3		

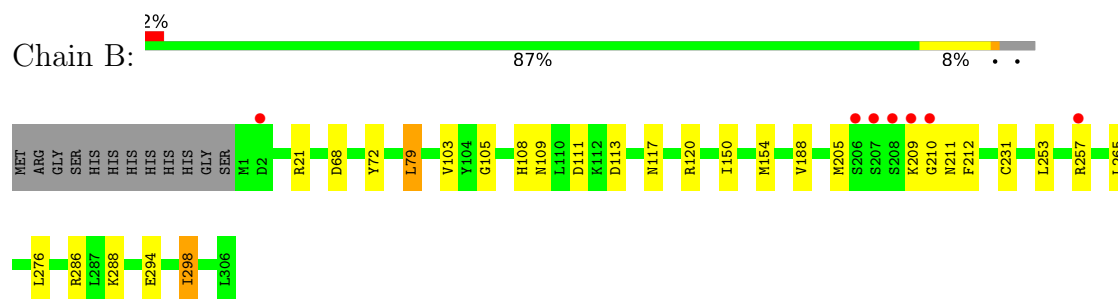
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	61	Total	O	0	0
			61	61		
6	A	55	Total	O	0	0
			55	55		
6	C	67	Total	O	0	0
			67	67		
6	D	32	Total	O	0	0
			32	32		

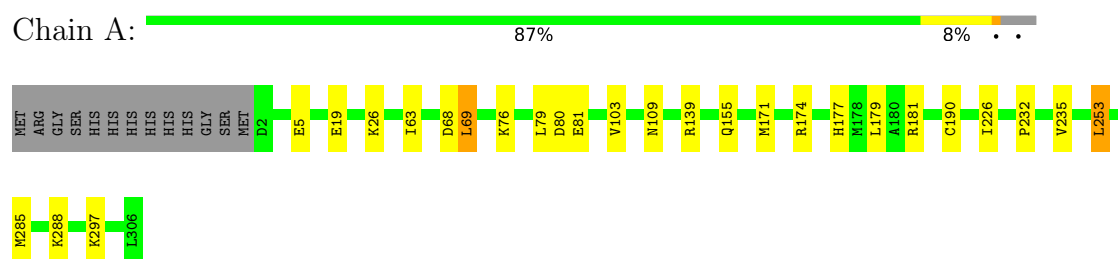
3 Residue-property plots [i](#)

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.

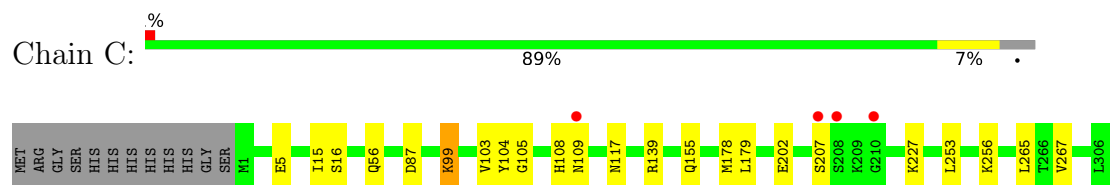
• Molecule 1: Tyrosine-tRNA ligase



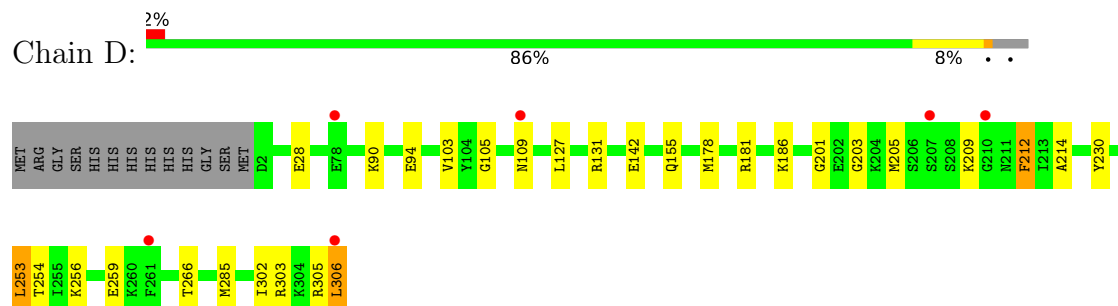
• Molecule 1: Tyrosine-tRNA ligase



• Molecule 1: Tyrosine-tRNA ligase



• Molecule 1: Tyrosine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.14Å 70.63Å 77.62Å 85.70° 89.75° 83.42°	Depositor
Resolution (Å)	46.27 – 2.43 46.27 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.27-2.43) 93.4 (46.27-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1168: ???)	Depositor
R, R_{free}	0.182 , 0.240 0.186 , 0.243	Depositor DCC
R_{free} test set	2089 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20326	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 96Z, GOL, PG0

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	0.14	0/2502	0.38	0/3357
1	B	0.26	0/2510	0.41	0/3367
1	C	0.15	0/2507	0.36	0/3364
1	D	0.45	2/2491 (0.1%)	0.52	2/3343 (0.1%)
All	All	0.28	2/10010 (0.0%)	0.42	2/13431 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	205	MET	CA-CB	6.82	1.65	1.53
1	D	209	LYS	N-CA	5.86	1.52	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	GLY	CA-C-O	-5.27	117.44	122.13
1	D	212	PHE	CA-C-O	-5.22	115.50	121.40

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	2455	2530	2533	11	1
1	B	2463	2541	2545	20	0
1	C	2460	2535	2538	9	0
1	D	2447	2519	2520	12	1
2	A	16	12	0	0	0
2	B	16	12	0	0	0
2	C	16	12	0	1	0
2	D	16	12	0	1	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	8	10	12	1	0
6	A	55	0	0	0	0
6	B	61	0	0	1	0
6	C	67	0	0	3	0
6	D	32	0	0	2	0
All	All	10127	10199	10164	52	1

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 (52) 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:186:LYS:NZ	6:D:501:HOH:O	2.00	0.93
1:D:90:LYS:NZ	1:D:94:GLU:OE2	2.16	0.79
1:C:87:ASP:OD1	1:C:104:TYR:OH	2.08	0.71
1:C:155:GLN:OE1	2:C:401:96Z:N17	2.28	0.67
1:A:19:GLU:OE2	1:A:181:ARG:NH2	2.34	0.61
1:C:56:GLN:NE2	1:C:99:LYS:O	2.37	0.57
1:C:253:LEU:HD23	1:C:267:VAL:HB	1.88	0.56
1:D:212:PHE:HE1	1:D:214:ALA:HB2	1.71	0.55
1:D:181:ARG:NH1	6:D:502:HOH:O	2.34	0.55
1:A:80:ASP:OD1	1:A:81:GLU:N	2.41	0.54
1:B:209:LYS:O	1:B:211:ASN:N	2.42	0.53
1:A:253:LEU:HD23	1:A:253:LEU:C	2.34	0.52
1:B:265:LEU:HD13	1:B:276:LEU:HD13	1.94	0.50
1:B:257:ARG:NH1	6:B:504:HOH:O	2.45	0.50
1:A:155:GLN:HE21	5:A:405:PG0:H21	1.77	0.49
1:C:105:GLY:O	1:C:109:ASN:N	2.44	0.49
1:B:205:MET:HE2	1:B:212:PHE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:TYR:HB2	1:B:79:LEU:CD1	2.43	0.48
1:D:201:GLY:HA3	1:D:230:TYR:CD2	2.49	0.48
1:C:5:GLU:OE1	6:C:501:HOH:O	2.20	0.47
1:B:105:GLY:O	1:B:109:ASN:N	2.41	0.47
1:B:257:ARG:HD2	1:B:286:ARG:CD	2.44	0.47
1:C:109:ASN:ND2	6:C:505:HOH:O	2.46	0.47
1:B:21[B]:ARG:NH2	6:C:504:HOH:O	2.48	0.46
1:B:103:VAL:HG23	1:B:108:HIS:CE1	2.50	0.46
1:A:69:LEU:HB3	1:A:109:ASN:HD21	1.80	0.46
1:D:105:GLY:O	1:D:109:ASN:N	2.41	0.45
1:D:155:GLN:OE1	2:D:401:96Z:N17	2.50	0.44
1:B:72:TYR:HB2	1:B:79:LEU:HD13	2.00	0.44
1:B:257:ARG:CD	1:B:286:ARG:HD3	2.48	0.44
1:A:226:ILE:O	1:A:288:LYS:HD3	2.18	0.44
1:B:294:GLU:O	1:B:298:ILE:HD12	2.18	0.44
1:B:257:ARG:NH2	1:B:265:LEU:HG	2.33	0.43
1:D:253:LEU:O	1:D:253:LEU:HD23	2.18	0.43
1:B:150:ILE:O	1:B:154:MET:HG3	2.19	0.42
1:B:205:MET:HG3	1:B:212:PHE:HB3	2.02	0.42
1:D:302:ILE:H	1:D:302:ILE:HD12	1.84	0.42
1:B:68:ASP:OD1	1:B:68:ASP:N	2.53	0.42
1:A:232:PRO:HG2	1:A:235:VAL:HB	2.02	0.41
1:C:15:ILE:HA	1:C:16:SER:HA	1.86	0.41
1:B:117:ASN:OD1	1:B:120:ARG:NH1	2.53	0.41
1:D:302:ILE:HD12	1:D:302:ILE:N	2.35	0.41
1:A:177:HIS:HB3	1:A:190:CYS:SG	2.60	0.41
1:B:205:MET:HG3	1:B:212:PHE:CB	2.51	0.41
1:D:127:LEU:O	1:D:131:ARG:HG3	2.20	0.41
1:B:231:CYS:HB3	1:B:288:LYS:HE3	2.02	0.41
1:A:177:HIS:O	1:A:181:ARG:HG3	2.21	0.41
1:D:305:ARG:O	1:D:306:LEU:C	2.63	0.41
1:A:171:MET:O	1:A:174:ARG:HB2	2.20	0.41
1:B:257:ARG:HD2	1:B:286:ARG:HD2	2.03	0.41
1:C:103:VAL:HG13	1:C:108:HIS:CD2	2.56	0.40
1:A:68:ASP:OD1	1:A:68:ASP:N	2.55	0.40

All (1) 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:5:GLU:OE2	1:D:254:THR:OG1[1_556]	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	305/318 (96%)	302 (99%)	3 (1%)	0	100	100
1	B	306/318 (96%)	302 (99%)	3 (1%)	1 (0%)	36	49
1	C	306/318 (96%)	304 (99%)	2 (1%)	0	100	100
1	D	304/318 (96%)	298 (98%)	5 (2%)	1 (0%)	36	49
All	All	1221/1272 (96%)	1206 (99%)	13 (1%)	2 (0%)	43	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	GLY
1	D	259	GLU

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	266/275 (97%)	255 (96%)	11 (4%)	27	44
1	B	267/275 (97%)	261 (98%)	6 (2%)	45	66
1	C	266/275 (97%)	256 (96%)	10 (4%)	29	47
1	D	265/275 (96%)	255 (96%)	10 (4%)	29	47
All	All	1064/1100 (97%)	1027 (96%)	37 (4%)	32	51

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	LEU
1	B	111	ASP
1	B	113	ASP
1	B	188	VAL
1	B	253	LEU
1	B	298	ILE
1	A	26	LYS
1	A	63	ILE
1	A	69	LEU
1	A	76	LYS
1	A	79	LEU
1	A	103	VAL
1	A	139	ARG
1	A	179	LEU
1	A	253	LEU
1	A	285	MET
1	A	297	LYS
1	C	99	LYS
1	C	117	ASN
1	C	139	ARG
1	C	178	MET
1	C	179	LEU
1	C	202	GLU
1	C	207	SER
1	C	227	LYS
1	C	256	LYS
1	C	265	LEU
1	D	28	GLU
1	D	103	VAL
1	D	142	GLU
1	D	178	MET
1	D	253	LEU
1	D	256	LYS
1	D	266	THR
1	D	285	MET
1	D	303	ARG
1	D	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	GLN
1	B	108	HIS

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Mol	Chain	Res	Type
1	C	268	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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	GOL	B	402	-	5,5,5	0.38	0	5,5,5	0.20	0
2	96Z	C	401	-	15,17,17	1.74	5 (33%)	10,23,23	1.83	2 (20%)
2	96Z	A	401	-	15,17,17	1.74	5 (33%)	10,23,23	1.75	2 (20%)
2	96Z	D	401	-	15,17,17	1.80	5 (33%)	10,23,23	1.87	2 (20%)
2	96Z	B	401	-	15,17,17	1.78	5 (33%)	10,23,23	1.89	2 (20%)
5	PG0	A	405	-	7,7,7	0.52	0	6,6,6	0.18	0
3	GOL	A	402	-	5,5,5	0.38	0	5,5,5	0.22	0

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	GOL	B	402	-	-	3/4/4/4	-
2	96Z	C	401	-	-	0/7/12/12	0/2/2/2
2	96Z	A	401	-	-	0/7/12/12	0/2/2/2
2	96Z	D	401	-	-	2/7/12/12	0/2/2/2
2	96Z	B	401	-	-	2/7/12/12	0/2/2/2
5	PG0	A	405	-	-	1/5/5/5	-
3	GOL	A	402	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	96Z	C12-C11	3.71	1.49	1.40
2	B	401	96Z	C12-C11	3.63	1.49	1.40
2	A	401	96Z	C12-C11	3.60	1.49	1.40
2	C	401	96Z	C12-C11	3.58	1.49	1.40
2	A	401	96Z	C16-C10	3.19	1.47	1.40
2	B	401	96Z	C16-C10	3.15	1.47	1.40
2	C	401	96Z	C16-C10	3.15	1.47	1.40
2	D	401	96Z	C16-C10	3.11	1.47	1.40
2	C	401	96Z	C13-C12	-2.57	1.33	1.38
2	A	401	96Z	C13-C12	-2.56	1.33	1.38
2	D	401	96Z	C13-C12	-2.51	1.33	1.38
2	B	401	96Z	C13-C12	-2.47	1.33	1.38
2	B	401	96Z	C15-C16	-2.37	1.34	1.38
2	C	401	96Z	C15-C16	-2.30	1.34	1.38
2	D	401	96Z	C15-C16	-2.30	1.34	1.38
2	A	401	96Z	C15-C16	-2.23	1.34	1.38
2	C	401	96Z	C9-C10	-2.21	1.39	1.42
2	B	401	96Z	C9-C10	-2.20	1.39	1.42
2	A	401	96Z	C9-C10	-2.18	1.39	1.42
2	D	401	96Z	C9-C10	-2.17	1.39	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	96Z	C16-C10-C9	-4.35	121.11	126.09
2	D	401	96Z	C16-C10-C9	-4.30	121.16	126.09
2	C	401	96Z	C16-C10-C9	-4.17	121.31	126.09
2	A	401	96Z	C16-C10-C9	-3.99	121.52	126.09
2	D	401	96Z	C15-C14-C13	3.20	134.13	128.50
2	B	401	96Z	C15-C14-C13	3.19	134.11	128.50
2	C	401	96Z	C15-C14-C13	3.16	134.06	128.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	96Z	C15-C14-C13	3.10	133.95	128.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GOL	O1-C1-C2-O2
2	B	401	96Z	C6-C1-C3-O5
2	B	401	96Z	C6-C1-C3-O4
3	B	402	GOL	O1-C1-C2-C3
3	B	402	GOL	O2-C2-C3-O3
2	D	401	96Z	C6-C1-C3-O5
2	D	401	96Z	C6-C1-C3-O4
5	A	405	PG0	C3-C4-O2-C5

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	96Z	1	0
2	D	401	96Z	1	0
5	A	405	PG0	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	305/318 (95%)	-0.16	0 100 100	21, 41, 70, 110	2 (0%)
1	B	306/318 (96%)	-0.08	7 (2%) 61 57	23, 43, 74, 163	2 (0%)
1	C	306/318 (96%)	-0.16	4 (1%) 75 72	23, 43, 72, 104	2 (0%)
1	D	305/318 (95%)	0.17	6 (1%) 65 61	26, 52, 90, 119	1 (0%)
All	All	1222/1272 (96%)	-0.06	17 (1%) 73 70	21, 44, 80, 163	7 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	SER	4.1
1	B	257	ARG	3.8
1	D	261	PHE	3.6
1	B	207	SER	3.2
1	D	207	SER	3.2
1	C	208	SER	3.1
1	D	306	LEU	2.9
1	C	207	SER	2.9
1	D	109	ASN	2.6
1	C	109	ASN	2.5
1	B	206	SER	2.3
1	D	210	GLY	2.2
1	B	2	ASP	2.2
1	B	209	LYS	2.2
1	B	210	GLY	2.1
1	C	210	GLY	2.0
1	D	78	GLU	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 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
3	GOL	A	402	6/6	0.67	0.17	60,73,87,91	0
3	GOL	B	402	6/6	0.82	0.10	55,66,77,79	0
5	PG0	A	405	8/8	0.86	0.22	27,37,62,62	0
4	CA	A	404	1/1	0.88	0.11	78,78,78,78	0
2	96Z	A	401	16/16	0.93	0.09	23,38,48,53	0
2	96Z	D	401	16/16	0.93	0.09	32,44,55,59	0
2	96Z	B	401	16/16	0.93	0.08	24,36,46,56	0
4	CA	A	403	1/1	0.94	0.09	54,54,54,54	0
4	CA	B	403	1/1	0.96	0.06	94,94,94,94	0
2	96Z	C	401	16/16	0.96	0.06	24,39,51,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.