



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 AM UTC

PDB ID : 8BHD / pdb_00008bhd
Title : N-terminal domain of Plasmodium berghei glutamyl-tRNA synthetase (Tbxo4 derivative crystal structure)
Authors : Benas, P.; Jaramillo Ponce, J.R.; Legrand, P.; Frugier, M.; Sauter, C.
Deposited on : 2022-10-31
Resolution : 3.17 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

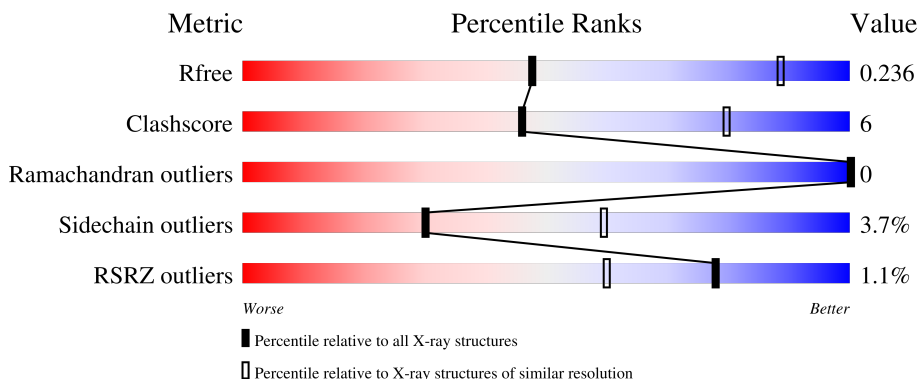
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	249	
1	B	249	
1	C	249	
1	D	249	
1	E	249	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8196 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 Glutamate-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1636	1076	266	290	4			
1	B	196	Total	C	N	O	S	0	0	0
			1670	1095	273	298	4			
1	C	189	Total	C	N	O	S	0	0	0
			1619	1067	263	285	4			
1	D	188	Total	C	N	O	S	0	0	0
			1602	1054	260	284	4			
1	E	187	Total	C	N	O	S	0	0	0
			1598	1051	261	282	4			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A509AR09
A	2	GLY	-	expression tag	UNP A0A509AR09
A	228	ILE	-	expression tag	UNP A0A509AR09
A	229	PHE	-	expression tag	UNP A0A509AR09
A	230	ILE	-	expression tag	UNP A0A509AR09
A	231	ASP	-	expression tag	UNP A0A509AR09
A	232	GLY	-	expression tag	UNP A0A509AR09
A	233	GLY	-	expression tag	UNP A0A509AR09
A	234	SER	-	expression tag	UNP A0A509AR09
A	235	SER	-	expression tag	UNP A0A509AR09
A	236	GLY	-	expression tag	UNP A0A509AR09
A	237	LEU	-	expression tag	UNP A0A509AR09
A	238	VAL	-	expression tag	UNP A0A509AR09
A	239	PRO	-	expression tag	UNP A0A509AR09
A	240	ARG	-	expression tag	UNP A0A509AR09
A	241	GLY	-	expression tag	UNP A0A509AR09
A	242	SER	-	expression tag	UNP A0A509AR09
A	243	SER	-	expression tag	UNP A0A509AR09
A	244	HIS	-	expression tag	UNP A0A509AR09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	245	HIS	-	expression tag	UNP A0A509AR09
A	246	HIS	-	expression tag	UNP A0A509AR09
A	247	HIS	-	expression tag	UNP A0A509AR09
A	248	HIS	-	expression tag	UNP A0A509AR09
A	249	HIS	-	expression tag	UNP A0A509AR09
B	1	MET	-	initiating methionine	UNP A0A509AR09
B	2	GLY	-	expression tag	UNP A0A509AR09
B	228	ILE	-	expression tag	UNP A0A509AR09
B	229	PHE	-	expression tag	UNP A0A509AR09
B	230	ILE	-	expression tag	UNP A0A509AR09
B	231	ASP	-	expression tag	UNP A0A509AR09
B	232	GLY	-	expression tag	UNP A0A509AR09
B	233	GLY	-	expression tag	UNP A0A509AR09
B	234	SER	-	expression tag	UNP A0A509AR09
B	235	SER	-	expression tag	UNP A0A509AR09
B	236	GLY	-	expression tag	UNP A0A509AR09
B	237	LEU	-	expression tag	UNP A0A509AR09
B	238	VAL	-	expression tag	UNP A0A509AR09
B	239	PRO	-	expression tag	UNP A0A509AR09
B	240	ARG	-	expression tag	UNP A0A509AR09
B	241	GLY	-	expression tag	UNP A0A509AR09
B	242	SER	-	expression tag	UNP A0A509AR09
B	243	SER	-	expression tag	UNP A0A509AR09
B	244	HIS	-	expression tag	UNP A0A509AR09
B	245	HIS	-	expression tag	UNP A0A509AR09
B	246	HIS	-	expression tag	UNP A0A509AR09
B	247	HIS	-	expression tag	UNP A0A509AR09
B	248	HIS	-	expression tag	UNP A0A509AR09
B	249	HIS	-	expression tag	UNP A0A509AR09
C	1	MET	-	initiating methionine	UNP A0A509AR09
C	2	GLY	-	expression tag	UNP A0A509AR09
C	228	ILE	-	expression tag	UNP A0A509AR09
C	229	PHE	-	expression tag	UNP A0A509AR09
C	230	ILE	-	expression tag	UNP A0A509AR09
C	231	ASP	-	expression tag	UNP A0A509AR09
C	232	GLY	-	expression tag	UNP A0A509AR09
C	233	GLY	-	expression tag	UNP A0A509AR09
C	234	SER	-	expression tag	UNP A0A509AR09
C	235	SER	-	expression tag	UNP A0A509AR09
C	236	GLY	-	expression tag	UNP A0A509AR09
C	237	LEU	-	expression tag	UNP A0A509AR09
C	238	VAL	-	expression tag	UNP A0A509AR09

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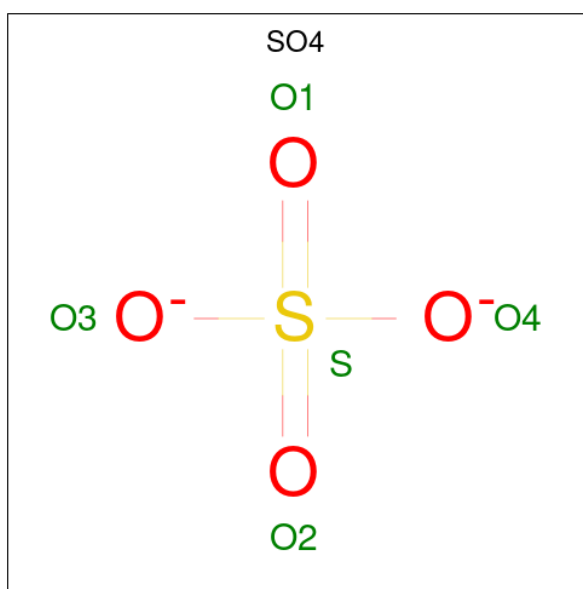
Chain	Residue	Modelled	Actual	Comment	Reference
C	239	PRO	-	expression tag	UNP A0A509AR09
C	240	ARG	-	expression tag	UNP A0A509AR09
C	241	GLY	-	expression tag	UNP A0A509AR09
C	242	SER	-	expression tag	UNP A0A509AR09
C	243	SER	-	expression tag	UNP A0A509AR09
C	244	HIS	-	expression tag	UNP A0A509AR09
C	245	HIS	-	expression tag	UNP A0A509AR09
C	246	HIS	-	expression tag	UNP A0A509AR09
C	247	HIS	-	expression tag	UNP A0A509AR09
C	248	HIS	-	expression tag	UNP A0A509AR09
C	249	HIS	-	expression tag	UNP A0A509AR09
D	1	MET	-	initiating methionine	UNP A0A509AR09
D	2	GLY	-	expression tag	UNP A0A509AR09
D	228	ILE	-	expression tag	UNP A0A509AR09
D	229	PHE	-	expression tag	UNP A0A509AR09
D	230	ILE	-	expression tag	UNP A0A509AR09
D	231	ASP	-	expression tag	UNP A0A509AR09
D	232	GLY	-	expression tag	UNP A0A509AR09
D	233	GLY	-	expression tag	UNP A0A509AR09
D	234	SER	-	expression tag	UNP A0A509AR09
D	235	SER	-	expression tag	UNP A0A509AR09
D	236	GLY	-	expression tag	UNP A0A509AR09
D	237	LEU	-	expression tag	UNP A0A509AR09
D	238	VAL	-	expression tag	UNP A0A509AR09
D	239	PRO	-	expression tag	UNP A0A509AR09
D	240	ARG	-	expression tag	UNP A0A509AR09
D	241	GLY	-	expression tag	UNP A0A509AR09
D	242	SER	-	expression tag	UNP A0A509AR09
D	243	SER	-	expression tag	UNP A0A509AR09
D	244	HIS	-	expression tag	UNP A0A509AR09
D	245	HIS	-	expression tag	UNP A0A509AR09
D	246	HIS	-	expression tag	UNP A0A509AR09
D	247	HIS	-	expression tag	UNP A0A509AR09
D	248	HIS	-	expression tag	UNP A0A509AR09
D	249	HIS	-	expression tag	UNP A0A509AR09
E	1	MET	-	initiating methionine	UNP A0A509AR09
E	2	GLY	-	expression tag	UNP A0A509AR09
E	228	ILE	-	expression tag	UNP A0A509AR09
E	229	PHE	-	expression tag	UNP A0A509AR09
E	230	ILE	-	expression tag	UNP A0A509AR09
E	231	ASP	-	expression tag	UNP A0A509AR09
E	232	GLY	-	expression tag	UNP A0A509AR09

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Chain	Residue	Modelled	Actual	Comment	Reference
E	233	GLY	-	expression tag	UNP A0A509AR09
E	234	SER	-	expression tag	UNP A0A509AR09
E	235	SER	-	expression tag	UNP A0A509AR09
E	236	GLY	-	expression tag	UNP A0A509AR09
E	237	LEU	-	expression tag	UNP A0A509AR09
E	238	VAL	-	expression tag	UNP A0A509AR09
E	239	PRO	-	expression tag	UNP A0A509AR09
E	240	ARG	-	expression tag	UNP A0A509AR09
E	241	GLY	-	expression tag	UNP A0A509AR09
E	242	SER	-	expression tag	UNP A0A509AR09
E	243	SER	-	expression tag	UNP A0A509AR09
E	244	HIS	-	expression tag	UNP A0A509AR09
E	245	HIS	-	expression tag	UNP A0A509AR09
E	246	HIS	-	expression tag	UNP A0A509AR09
E	247	HIS	-	expression tag	UNP A0A509AR09
E	248	HIS	-	expression tag	UNP A0A509AR09
E	249	HIS	-	expression tag	UNP A0A509AR09

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is TERBIUM(III) ION (CCD ID: TB) (formula: Tb).

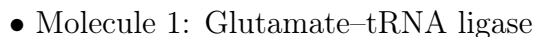
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Tb	0	0
			7	7		
4	B	3	Total	Tb	0	0
			3	3		
4	C	4	Total	Tb	0	0
			4	4		

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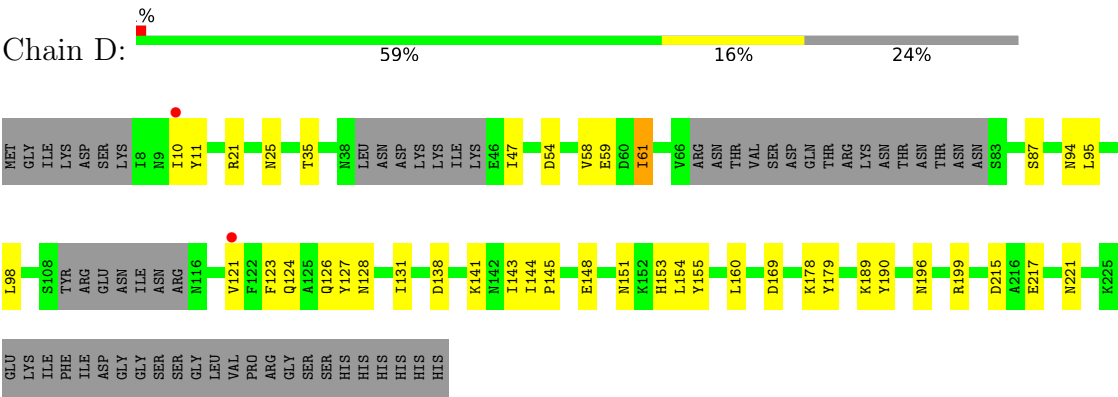
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total 4	Tb 4	0	0
4	E	4	Total 4	Tb 4	0	0

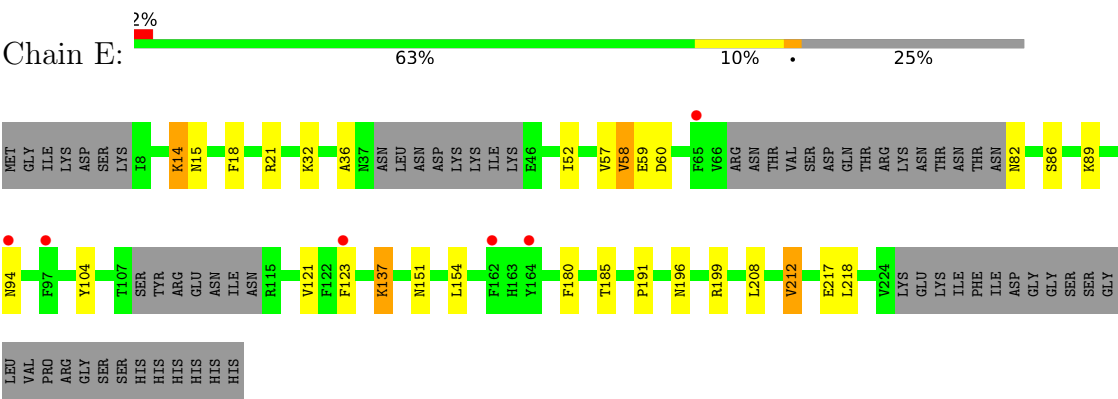
- Molecule 1: Glutamate-tRNA ligase



● Molecule 1: Glutamate–tRNA ligase



● Molecule 1: Glutamate–tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.11Å 88.51Å 168.64Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	47.85 – 3.17 47.85 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.85-3.17) 92.5 (47.85-3.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.19Å)	Xtriage
Refinement program	PHENIX dev_4701	Depositor
R, R_{free}	0.192 , 0.237 0.194 , 0.236	Depositor DCC
R_{free} test set	1578 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	119.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 146.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8196	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: SO4, GOL, TB

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	0.23	0/1674	0.48	0/2260
1	B	0.23	0/1708	0.45	1/2307 (0.0%)
1	C	0.12	0/1657	0.28	0/2237
1	D	0.12	0/1640	0.31	0/2218
1	E	0.14	0/1636	0.35	0/2213
All	All	0.18	0/8315	0.38	1/11235 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	HIS	N-CA-C	-5.40	105.40	111.28

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	1636	0	1641	17	0
1	B	1670	0	1669	24	0
1	C	1619	0	1626	19	0
1	D	1602	0	1597	24	0
1	E	1598	0	1592	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
3	A	12	0	16	1	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
4	A	7	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
All	All	8196	0	8157	94	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 6.

All (94) 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:B:89:LYS:HG3	1:B:90:ILE:HG12	1.80	0.63
1:C:123:PHE:HB2	1:C:162:PHE:CE2	2.39	0.57
1:B:212:VAL:HG13	1:B:218:LEU:HD22	1.86	0.56
1:B:104:TYR:HA	1:B:123:PHE:HE2	1.71	0.55
1:A:6:SER:HB2	1:A:47:ILE:HG12	1.87	0.55
1:D:10:ILE:HG23	1:D:61:ILE:HD12	1.87	0.54
1:D:25:ASN:ND2	1:D:215:ASP:OD2	2.33	0.54
1:A:89:LYS:HG2	2:A:301:SO4:O2	2.08	0.54
1:B:151:ASN:OD1	1:B:197:ILE:HG13	2.08	0.54
1:D:178:LYS:HE3	1:D:179:TYR:CZ	2.43	0.53
1:D:127:TYR:CE2	1:D:131:ILE:HD11	2.43	0.53
1:B:184:ILE:HG22	1:B:186:THR:HG22	1.91	0.53
1:E:154:LEU:HB3	1:E:199:ARG:HH22	1.75	0.52
1:E:212:VAL:HG12	1:E:218:LEU:HD13	1.90	0.52
1:E:208:LEU:O	1:E:212:VAL:HG22	2.09	0.52
1:B:121:VAL:HG13	1:C:94:ASN:HB3	1.91	0.52
1:C:104:TYR:HA	1:C:123:PHE:HE2	1.74	0.52
1:B:160:LEU:HD12	1:B:169:ASP:HA	1.91	0.51
1:C:97:PHE:HB2	1:C:105:TYR:CE2	2.45	0.51
1:A:102:ASN:OD1	1:A:106:PHE:HA	2.11	0.51
1:B:136:ASN:H	3:B:303:GOL:H12	1.76	0.51
1:E:21:ARG:HH12	1:E:217:GLU:CD	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LYS:HE3	1:B:179:TYR:CZ	2.46	0.51
1:A:104:TYR:HA	1:A:123:PHE:HE2	1.75	0.50
1:B:94:ASN:HB3	1:C:121:VAL:HG13	1.92	0.50
1:D:121:VAL:HG13	1:E:94:ASN:HB3	1.92	0.50
1:E:60:ASP:HB2	1:E:86:SER:O	2.12	0.49
1:A:107:THR:O	1:A:108:SER:C	2.54	0.49
1:D:123:PHE:O	1:D:126:GLN:N	2.45	0.49
1:D:124:GLN:O	1:D:128:ASN:ND2	2.45	0.49
1:E:154:LEU:O	1:E:199:ARG:NH2	2.46	0.49
1:E:180:PHE:HA	1:E:191:PRO:HG3	1.96	0.48
1:B:96:ASP:OD1	1:B:101:THR:OG1	2.24	0.47
1:E:104:TYR:HA	1:E:123:PHE:HE2	1.79	0.47
1:E:32:LYS:O	1:E:36:ALA:HB3	2.15	0.47
1:C:144:ILE:HB	1:C:145:PRO:HD3	1.96	0.47
1:D:153:HIS:NE2	1:D:160:LEU:O	2.33	0.47
1:E:137:LYS:HB2	1:E:137:LYS:HE2	1.49	0.46
1:E:14:LYS:HG2	1:E:15:ASN:N	2.30	0.46
1:C:9:ASN:HB2	1:C:64:GLU:HB3	1.97	0.46
1:D:151:ASN:OD1	1:D:196:ASN:HB2	2.15	0.46
1:E:58:VAL:HG13	1:E:59:GLU:H	1.80	0.46
1:A:97:PHE:HB2	1:A:105:TYR:CE2	2.50	0.46
1:D:47:ILE:HD13	1:D:98:LEU:HG	1.98	0.45
1:D:143:ILE:HD13	1:D:190:TYR:CE1	2.51	0.45
1:A:35:THR:O	1:A:35:THR:OG1	2.26	0.45
1:A:129:GLU:HB3	1:B:55:LYS:HE2	1.99	0.45
1:C:138:ASP:HB3	1:C:141:LYS:HB3	1.99	0.45
1:B:118:ILE:H	1:B:118:ILE:HD12	1.82	0.44
1:B:123:PHE:HB2	1:B:162:PHE:CE2	2.53	0.44
1:B:215:ASP:O	1:B:216:ALA:HB3	2.18	0.44
1:D:144:ILE:HB	1:D:145:PRO:HD3	1.97	0.44
1:A:138:ASP:HB3	1:A:141:LYS:HB3	1.99	0.44
1:B:13:GLY:C	1:B:15:ASN:H	2.25	0.44
1:E:196:ASN:HB3	1:E:199:ARG:HH21	1.82	0.44
1:A:151:ASN:OD1	1:A:196:ASN:HB2	2.17	0.44
1:B:227:LYS:HB2	1:B:227:LYS:HE2	1.49	0.44
1:D:58:VAL:HG12	1:D:59:GLU:HG3	1.99	0.44
1:C:17:PRO:HB2	1:C:20:CYS:HB2	2.00	0.44
1:C:195:LYS:HD3	1:D:155:TYR:CE1	2.53	0.44
1:B:226:GLU:O	1:B:227:LYS:C	2.61	0.44
1:C:123:PHE:HB2	1:C:162:PHE:HE2	1.81	0.43
1:D:11:TYR:HB3	1:D:54:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:NH1	3:A:304:GOL:O3	2.49	0.43
1:B:154:LEU:O	1:B:199:ARG:NH2	2.52	0.43
1:A:208:LEU:O	1:A:212:VAL:HG22	2.18	0.43
1:C:63:VAL:HG11	1:C:91:PHE:CZ	2.54	0.43
1:A:63:VAL:HG11	1:A:91:PHE:CZ	2.54	0.43
1:C:195:LYS:HD3	1:D:155:TYR:OH	2.19	0.43
1:B:63:VAL:HG11	1:B:91:PHE:CZ	2.54	0.43
1:B:97:PHE:HB2	1:B:105:TYR:CE2	2.53	0.43
1:E:151:ASN:OD1	1:E:196:ASN:HB2	2.19	0.43
1:C:208:LEU:O	1:C:212:VAL:HG22	2.19	0.42
1:D:61:ILE:HG23	1:D:87:SER:HA	2.00	0.42
1:A:96:ASP:OD1	1:A:101:THR:OG1	2.30	0.42
1:D:21:ARG:NH2	1:D:217:GLU:OE1	2.51	0.42
1:D:94:ASN:HB3	1:E:121:VAL:HG13	2.00	0.42
1:A:144:ILE:HB	1:A:145:PRO:HD3	2.01	0.42
1:C:150:ILE:HG22	1:C:197:ILE:HG12	2.01	0.42
1:C:154:LEU:O	1:C:199:ARG:NH2	2.52	0.42
1:D:138:ASP:HB3	1:D:141:LYS:HB3	2.02	0.42
1:D:154:LEU:O	1:D:199:ARG:NH2	2.53	0.42
1:C:215:ASP:C	1:C:217:GLU:H	2.28	0.41
1:D:215:ASP:C	1:D:217:GLU:H	2.28	0.41
1:C:59:GLU:N	1:C:59:GLU:OE1	2.53	0.41
1:B:154:LEU:HD13	1:B:200:TRP:HB3	2.02	0.41
1:A:189:LYS:HA	1:A:192:LYS:HE2	2.01	0.41
1:D:95:LEU:HD23	1:D:95:LEU:HA	1.96	0.41
1:E:18:PHE:HD1	1:E:218:LEU:HG	1.86	0.41
1:D:160:LEU:HD12	1:D:169:ASP:HA	2.02	0.41
1:A:192:LYS:HE2	1:A:192:LYS:HB3	1.88	0.41
1:B:178:LYS:HA	1:B:226:GLU:OE2	2.21	0.40
1:B:27:TYR:CD1	1:B:99:LEU:HB3	2.57	0.40
1:C:120:ASN:O	1:C:124:GLN:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	184/249 (74%)	177 (96%)	7 (4%)	0	100	100
1	B	188/249 (76%)	179 (95%)	9 (5%)	0	100	100
1	C	181/249 (73%)	175 (97%)	6 (3%)	0	100	100
1	D	180/249 (72%)	174 (97%)	6 (3%)	0	100	100
1	E	179/249 (72%)	170 (95%)	9 (5%)	0	100	100
All	All	912/1245 (73%)	875 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	184/236 (78%)	174 (95%)	10 (5%)	20	50
1	B	188/236 (80%)	183 (97%)	5 (3%)	39	65
1	C	182/236 (77%)	177 (97%)	5 (3%)	39	65
1	D	180/236 (76%)	175 (97%)	5 (3%)	38	64
1	E	179/236 (76%)	170 (95%)	9 (5%)	22	52
All	All	913/1180 (77%)	879 (96%)	34 (4%)	30	59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	35	THR
1	A	45	LYS
1	A	47	ILE
1	A	61	ILE
1	A	66	VAL
1	A	89	LYS

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Mol	Chain	Res	Type
1	A	155	TYR
1	A	186	THR
1	A	226	GLU
1	B	152	LYS
1	B	156	LEU
1	B	161	SER
1	B	217	GLU
1	B	227	LYS
1	C	47	ILE
1	C	57	VAL
1	C	66	VAL
1	C	155	TYR
1	C	186	THR
1	D	35	THR
1	D	61	ILE
1	D	148	GLU
1	D	189	LYS
1	D	221	ASN
1	E	14	LYS
1	E	52	ILE
1	E	57	VAL
1	E	58	VAL
1	E	82	ASN
1	E	89	LYS
1	E	137	LYS
1	E	185	THR
1	E	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	142	ASN
1	A	220	GLN
1	B	50	ASN
1	B	136	ASN
1	B	142	ASN
1	C	142	ASN
1	C	163	HIS
1	E	142	ASN
1	E	198	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 31 ligands modelled in this entry, 22 are monoatomic - leaving 9 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	A	304	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	C	302	-	5,5,5	0.32	0	5,5,5	0.42	0
2	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	302	-	4,4,4	0.25	0	6,6,6	0.08	0
3	GOL	B	303	-	5,5,5	0.34	0	5,5,5	0.40	0
2	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	301	-	4,4,4	0.24	0	6,6,6	0.16	0
3	GOL	A	303	-	5,5,5	0.08	0	5,5,5	0.30	0
2	SO4	B	301	-	4,4,4	0.40	0	6,6,6	0.08	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	A	303	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	303	-	-	2/4/4/4	-
3	GOL	A	304	-	-	0/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	GOL	C1-C2-C3-O3
3	B	303	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	GOL	1	0
2	A	301	SO4	1	0
3	B	303	GOL	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	192/249 (77%)	0.03	0 100 100	91, 118, 174, 265	0
1	B	196/249 (78%)	-0.04	1 (0%) 87 75	96, 129, 190, 293	0
1	C	189/249 (75%)	0.02	1 (0%) 87 75	115, 156, 208, 246	0
1	D	188/249 (75%)	-0.19	2 (1%) 78 60	150, 202, 248, 279	0
1	E	187/249 (75%)	-0.11	6 (3%) 50 30	171, 223, 281, 322	0
All	All	952/1245 (76%)	-0.06	10 (1%) 78 60	91, 165, 254, 322	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	162	PHE	3.9
1	D	121	VAL	2.9
1	E	123	PHE	2.7
1	E	94	ASN	2.6
1	E	97	PHE	2.5
1	C	164	TYR	2.4
1	B	182	GLY	2.1
1	E	164	TYR	2.1
1	D	10	ILE	2.1
1	E	65	PHE	2.1

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 ⓘ

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
2	SO4	C	301	5/5	0.57	0.08	184,206,224,225	0
2	SO4	A	302	5/5	0.70	0.07	200,234,242,257	0
4	TB	B	306	1/1	0.71	0.08	227,227,227,227	1
4	TB	E	304	1/1	0.71	0.06	280,280,280,280	1
4	TB	E	303	1/1	0.78	0.06	253,253,253,253	1
4	TB	A	310	1/1	0.78	0.10	252,252,252,252	1
4	TB	A	307	1/1	0.80	0.07	324,324,324,324	0
3	GOL	A	303	6/6	0.82	0.20	145,167,191,191	0
2	SO4	B	301	5/5	0.82	0.05	170,171,197,199	0
2	SO4	A	301	5/5	0.82	0.09	160,190,197,224	0
3	GOL	A	304	6/6	0.83	0.09	126,157,162,187	0
4	TB	E	302	1/1	0.83	0.05	248,248,248,248	1
3	GOL	C	302	6/6	0.84	0.10	154,155,177,181	0
4	TB	B	305	1/1	0.84	0.09	217,217,217,217	1
4	TB	C	306	1/1	0.87	0.06	271,271,271,271	1
4	TB	D	304	1/1	0.88	0.05	258,258,258,258	1
3	GOL	B	303	6/6	0.89	0.07	140,159,179,182	0
4	TB	A	311	1/1	0.89	0.05	224,224,224,224	1
4	TB	A	309	1/1	0.89	0.07	220,220,220,220	1
4	TB	C	305	1/1	0.90	0.06	248,248,248,248	1
2	SO4	B	302	5/5	0.91	0.14	160,171,181,209	0
4	TB	D	303	1/1	0.91	0.07	328,328,328,328	0
4	TB	C	304	1/1	0.92	0.08	211,211,211,211	1
4	TB	A	308	1/1	0.93	0.05	278,278,278,278	1
4	TB	E	301	1/1	0.94	0.05	271,271,271,271	1
4	TB	D	301	1/1	0.94	0.06	290,290,290,290	0
4	TB	B	304	1/1	0.94	0.07	230,230,230,230	0
4	TB	A	306	1/1	0.94	0.05	259,259,259,259	0
4	TB	C	303	1/1	0.95	0.10	240,240,240,240	0
4	TB	A	305	1/1	0.96	0.12	227,227,227,227	1
4	TB	D	302	1/1	0.96	0.08	278,278,278,278	0

6.5 Other polymers ⓘ

There are no such residues in this entry.