



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:31 AM GMT

PDB ID : 1E8C
Title : STRUCTURE OF MURE THE UDP-N-ACETYLMURAMYL TRIPEPTIDE
SYNTHETASE FROM E. COLI
Authors : Gordon, E.J.; Chantala, L.; Dideberg, O.
Deposited on : 2000-09-19
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

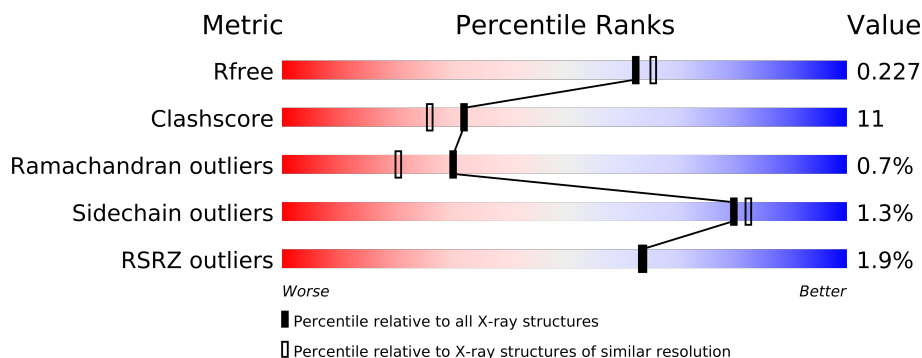
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	498	
1	B	498	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	API	A	1499	-	X
4	API	B	1499	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8093 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMATE-2,6-DIAMINOPIMELATELIGASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	16	5	1
			3772	2355	682	715	8	12			
1	B	497	Total	C	N	O	S	Se	24	5	0
			3787	2363	684	720	8	12			

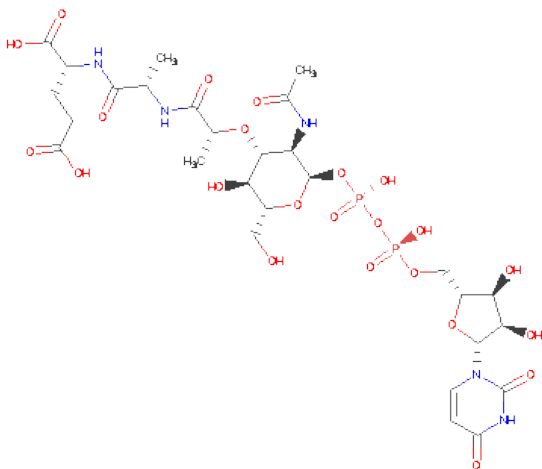
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	-	EXPRESSION TAG	UNP P22188
A	496	SER	-	EXPRESSION TAG	UNP P22188
A	497	HIS	-	EXPRESSION TAG	UNP P22188
A	498	HIS	-	EXPRESSION TAG	UNP P22188
B	495	ARG	-	EXPRESSION TAG	UNP P22188
B	496	SER	-	EXPRESSION TAG	UNP P22188
B	497	HIS	-	EXPRESSION TAG	UNP P22188
B	498	HIS	-	EXPRESSION TAG	UNP P22188

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

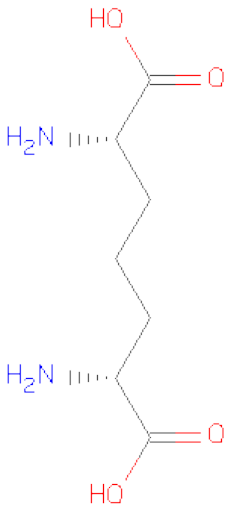
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE-D-GLUTAMATE (three-letter code: UAG) (formula: C₂₈H₄₃N₅O₂₃P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			57	28	5	22	2		
3	B	1	Total	C	N	O	P	0	0
			57	28	5	22	2		

- Molecule 4 is 2,6-DIAMINOPIMELIC ACID (three-letter code: API) (formula: C₇H₁₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	7	2	4		
4	B	1	Total	C	N	O	0	0
			13	7	2	4		

- Molecule 5 is water.

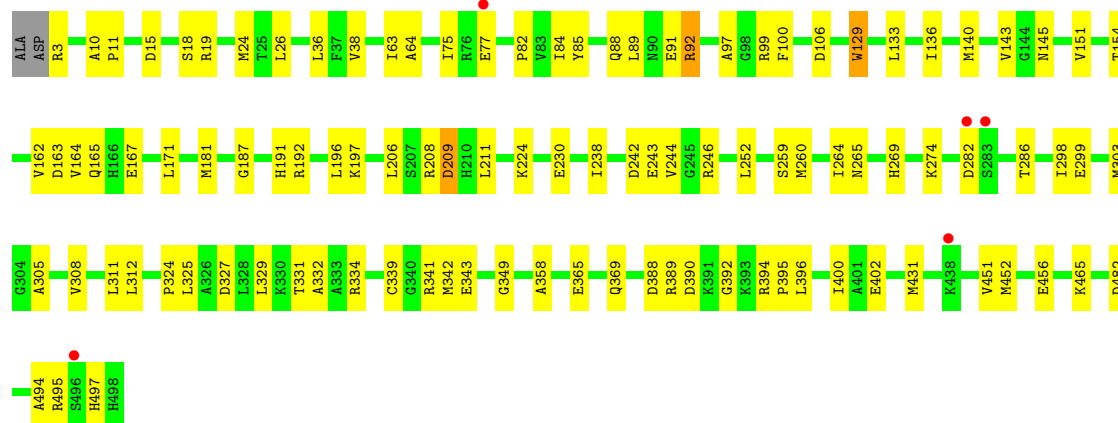
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0
5	B	187	Total 187	O 187	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

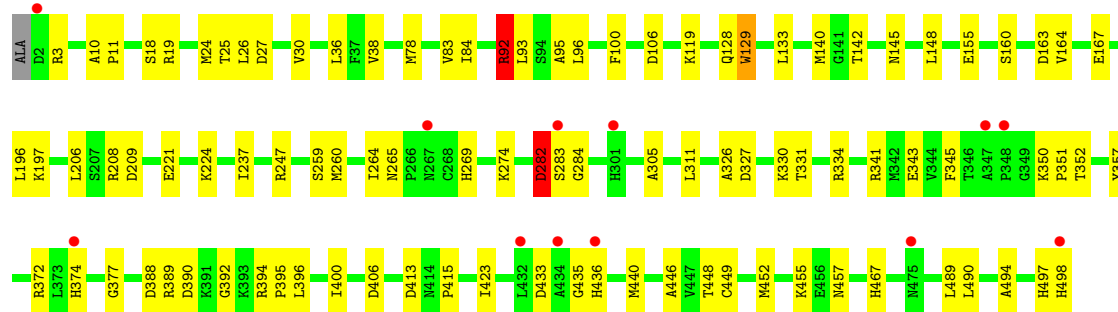
- Molecule 1: UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMATE--2,6-DIAMINOPIME LATELIGASE

Chain A: 



- Molecule 1: UDP-N-ACETYLMURAMOYLALANYL-D-GLUTAMATE--2,6-DIAMINOPIME LATELIGASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	93.47Å 99.69Å 236.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.00 46.73 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.73-2.00) 98.1 (46.73-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.59 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.230 0.199 , 0.227	Depositor DCC
R_{free} test set	7348 reflections (11.25%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 72673 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8093	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: API, KCX, UAG, CL

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	0.33	0/3846	0.62	1/5205 (0.0%)
1	B	0.33	0/3863	0.61	1/5227 (0.0%)
All	All	0.33	0/7709	0.61	2/10432 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ARG	O-C-N	5.35	131.25	122.70
1	A	136	ILE	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3711	96	0
1	B	3787	0	3721	76	0
2	A	1	0	0	0	0
3	A	57	0	39	0	0
3	B	57	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	11	1	0
4	B	13	0	10	0	0
5	A	206	0	0	8	0
5	B	187	0	0	3	0
All	All	8093	0	7531	172	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:145:ASN:HB3	1:B:167[B]:GLU:OE2	1.24	1.31
1:A:145:ASN:HB3	1:A:167[B]:GLU:OE2	1.18	1.29
1:A:140:MSE:HE3	1:A:167[B]:GLU:OE1	1.22	1.27
1:A:140:MSE:HE3	1:A:167[B]:GLU:CD	1.53	1.26
1:B:140:MSE:HE3	1:B:167[B]:GLU:OE1	1.47	1.15
1:A:145:ASN:CB	1:A:167[B]:GLU:OE2	2.03	1.06
1:A:402:GLU:HB2	1:A:431:MSE:HE2	1.39	1.02
1:B:78[A]:MSE:HE3	1:B:83:VAL:HG21	1.45	0.99
1:B:25[B]:THR:HG22	1:B:27:ASP:H	1.30	0.97
1:A:260:MSE:HE1	1:A:305:ALA:HB1	1.47	0.92
1:B:145:ASN:CB	1:B:167[B]:GLU:OE2	2.18	0.88
1:B:260:MSE:HE1	1:B:305:ALA:HB1	1.56	0.86
1:A:389:ARG:HH11	1:A:389:ARG:HG3	1.41	0.86
1:B:389:ARG:HH11	1:B:389:ARG:HG3	1.39	0.85
1:A:77:GLU:OE1	1:A:82:PRO:HA	1.76	0.85
1:B:25[B]:THR:HG21	1:B:30:VAL:HG23	1.57	0.85
1:B:440:MSE:HE3	1:B:446:ALA:HA	1.60	0.83
1:A:208:ARG:NE	1:A:211:LEU:HD12	1.93	0.82
1:A:143:VAL:HG22	5:A:2078:HOH:O	1.83	0.79
1:A:75:ILE:HG12	1:A:84:ILE:HD12	1.65	0.77
1:A:341:ARG:HH11	1:A:341:ARG:HG3	1.49	0.77
1:B:265:ASN:H	1:B:269:HIS:HD2	1.34	0.76
1:B:106:ASP:OD1	1:B:197:LYS:HD2	1.86	0.76
1:B:265:ASN:H	1:B:269:HIS:CD2	2.05	0.75
1:A:331:THR:HG22	1:A:334:ARG:HH21	1.49	0.75
1:B:19:ARG:HH11	1:B:19:ARG:HG3	1.52	0.75
1:B:38:VAL:HG11	1:B:93:LEU:HD21	1.69	0.73
1:B:341:ARG:NH2	1:B:357:TYR:CD2	2.56	0.73
1:B:18:SER:O	1:B:19:ARG:HG3	1.89	0.72
1:A:298:ILE:HD11	1:A:329:LEU:HD23	1.71	0.72
1:B:341:ARG:HG3	1:B:341:ARG:HH11	1.59	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:VAL:CG2	5:A:2078:HOH:O	2.40	0.67
1:B:326:ALA:O	1:B:330:LYS:HG3	1.95	0.67
1:A:395:PRO:HG3	5:A:2182:HOH:O	1.96	0.65
1:A:140:MSE:SE	1:A:181:MSE:HE2	2.47	0.64
1:A:19:ARG:HD2	1:A:82:PRO:HG2	1.78	0.64
1:A:77:GLU:CD	5:A:2046:HOH:O	2.35	0.64
1:A:259:SER:HB3	1:A:264:ILE:HG12	1.80	0.63
1:A:208:ARG:NE	1:A:211:LEU:CD1	2.62	0.63
1:A:208:ARG:HE	1:A:211:LEU:HD12	1.62	0.62
1:B:394:ARG:HB2	1:B:395:PRO:HD3	1.80	0.62
1:A:365:GLU:O	1:A:369:GLN:HG3	1.98	0.62
1:A:389:ARG:HG3	1:A:389:ARG:NH1	2.14	0.62
1:B:264:ILE:HG13	1:B:274:LYS:HB3	1.80	0.62
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.65	0.62
1:B:25[B]:THR:HG21	1:B:30:VAL:CG2	2.29	0.61
1:B:395:PRO:HG3	5:B:2163:HOH:O	1.99	0.61
1:B:394:ARG:NH1	1:B:423:ILE:HG23	2.15	0.61
1:A:206:LEU:HD13	1:A:224:KCX:HD3	1.83	0.61
1:A:343:GLU:HA	1:A:497:HIS:CE1	2.35	0.61
1:A:365:GLU:HG3	1:A:400:ILE:HD12	1.82	0.60
1:A:77:GLU:OE1	1:A:82:PRO:CA	2.48	0.60
1:B:119:LYS:HG3	5:B:2071:HOH:O	2.03	0.59
1:A:163:ASP:O	1:A:167[A]:GLU:HG3	2.01	0.59
1:A:394:ARG:HB2	1:A:395:PRO:HD3	1.84	0.58
1:B:10:ALA:HB3	1:B:11:PRO:HD3	1.83	0.58
1:A:238:ILE:HD11	1:A:252:LEU:HD12	1.85	0.58
1:A:242:ASP:OD2	1:A:244:VAL:HB	2.04	0.58
1:B:389:ARG:NH1	1:B:389:ARG:HG3	2.14	0.57
1:A:77:GLU:OE2	5:A:2046:HOH:O	2.17	0.57
1:A:341:ARG:HG3	1:A:341:ARG:NH1	2.20	0.57
1:B:374:HIS:CG	1:B:374:HIS:O	2.58	0.57
1:B:343:GLU:HG2	1:B:494:ALA:CB	2.35	0.56
1:B:24:MSE:HE1	1:B:96:LEU:HG	1.88	0.56
1:B:206:LEU:HD13	1:B:224:KCX:HD3	1.88	0.55
1:B:259:SER:HB3	1:B:264:ILE:HG12	1.89	0.55
1:B:140:MSE:HE3	1:B:167[B]:GLU:CD	2.26	0.55
1:B:19:ARG:NH1	1:B:19:ARG:HG3	2.21	0.54
1:B:145:ASN:ND2	1:B:167[B]:GLU:OE1	2.41	0.54
1:A:140:MSE:CE	1:A:167[B]:GLU:CD	2.50	0.53
1:A:388:ASP:O	1:A:389:ARG:HG3	2.09	0.53
1:A:365:GLU:CG	1:A:400:ILE:HD12	2.38	0.53
1:A:331:THR:HG22	1:A:334:ARG:NH2	2.19	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:350:LYS:HE2	1:B:489:LEU:O	2.09	0.53
1:B:3:ARG:HD3	1:B:100:PHE:O	2.08	0.52
1:A:298:ILE:HD11	1:A:329:LEU:CD2	2.38	0.52
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.73	0.52
1:A:264:ILE:HB	1:A:274:LYS:HD3	1.90	0.52
1:A:208:ARG:O	1:A:209:ASP:HB2	2.09	0.52
1:A:24:MSE:HE2	1:A:162:VAL:HG22	1.92	0.52
1:B:331:THR:HG22	1:B:334:ARG:HH21	1.75	0.52
1:A:392:GLY:O	1:A:395:PRO:HD2	2.10	0.51
1:A:264:ILE:HG13	1:A:274:LYS:HB3	1.92	0.51
1:B:396:LEU:O	1:B:400:ILE:HG12	2.10	0.51
1:A:88[A]:GLN:OE1	1:A:91:GLU:OE2	2.29	0.51
1:B:351:PRO:HB3	1:B:455:LYS:O	2.10	0.51
1:A:26:LEU:HD23	1:A:38:VAL:HB	1.93	0.51
1:A:343:GLU:HG2	1:A:494:ALA:HB2	1.94	0.50
1:A:89:LEU:HA	1:A:92:ARG:HG3	1.92	0.50
1:B:389:ARG:CG	1:B:389:ARG:NH1	2.74	0.50
1:B:392:GLY:O	1:B:395:PRO:HD2	2.12	0.50
1:A:265:ASN:H	1:A:269:HIS:CE1	2.29	0.49
1:A:75:ILE:HG12	1:A:84:ILE:CD1	2.39	0.49
1:A:208:ARG:HE	1:A:211:LEU:CD1	2.24	0.49
1:A:396:LEU:O	1:A:400:ILE:HG12	2.12	0.49
1:A:3:ARG:NH1	1:A:3:ARG:HG3	2.26	0.49
1:A:465:LYS:HB2	1:A:482:ASP:OD2	2.12	0.49
1:B:84:ILE:HD12	1:B:84:ILE:N	2.27	0.49
1:A:343:GLU:HG2	1:A:494:ALA:CB	2.44	0.48
1:A:3:ARG:CD	1:A:100:PHE:HA	2.43	0.48
1:B:92:ARG:O	1:B:95:ALA:HB3	2.14	0.48
1:B:341:ARG:CG	1:B:341:ARG:HH11	2.22	0.48
1:B:350:LYS:HD3	1:B:490:LEU:CD2	2.44	0.48
1:A:324:PRO:HG2	1:A:327:ASP:HB2	1.96	0.47
1:B:24:MSE:HE3	1:B:36:LEU:CD2	2.44	0.47
1:B:311:LEU:HD23	1:B:311:LEU:C	2.34	0.47
1:A:308:VAL:O	1:A:312:LEU:HG	2.15	0.47
1:B:237:ILE:N	1:B:237:ILE:HD12	2.29	0.47
1:B:436:HIS:ND1	1:B:436:HIS:O	2.44	0.47
1:B:388:ASP:O	1:B:389:ARG:HG3	2.15	0.46
1:A:97:ALA:HB3	1:A:165:GLN:HG3	1.98	0.46
1:A:91:GLU:HG3	5:A:2056:HOH:O	2.16	0.46
1:A:24:MSE:HE3	1:A:38:VAL:HG21	1.97	0.46
1:A:18:SER:O	1:A:19:ARG:HG3	2.16	0.46
1:B:282:ASP:C	1:B:284:GLY:N	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:389:ARG:HE	4:A:1499:API:C1	2.29	0.45
1:A:303:MSE:HE2	1:A:342:MSE:CE	2.46	0.45
1:A:106:ASP:OD1	1:A:197:LYS:HD2	2.17	0.45
1:B:413:ASP:O	1:B:415[B]:PRO:HD3	2.17	0.45
1:A:298:ILE:HD12	1:A:332:ALA:CB	2.46	0.45
1:B:142:THR:HG22	1:B:467:HIS:CE1	2.51	0.45
1:A:99:ARG:HB3	1:A:99:ARG:HH11	1.81	0.45
1:B:497:HIS:O	1:B:498:HIS:OXT	2.35	0.45
1:B:221:GLU:CD	1:B:247:ARG:HH22	2.19	0.45
1:A:495:ARG:HB2	5:A:2204:HOH:O	2.15	0.45
1:B:128:GLN:HA	1:B:148:LEU:HD11	1.98	0.45
1:B:208:ARG:O	1:B:209:ASP:HB2	2.16	0.45
1:B:352:THR:HG21	1:B:374:HIS:NE2	2.32	0.44
1:A:451:VAL:HG12	1:A:452:MSE:HE2	2.00	0.44
1:A:208:ARG:HG3	1:A:209:ASP:N	2.32	0.44
1:A:151:VAL:HG22	5:A:2082:HOH:O	2.17	0.44
1:B:282:ASP:O	1:B:284:GLY:N	2.50	0.44
1:A:389:ARG:NH1	1:A:389:ARG:CG	2.77	0.44
1:A:343:GLU:HG3	1:A:497:HIS:CE1	2.53	0.43
1:A:3:ARG:HD3	1:A:100:PHE:HA	2.00	0.43
1:A:286:THR:HG23	1:A:299:GLU:OE2	2.18	0.43
1:A:10:ALA:HB3	1:A:11:PRO:HD3	1.99	0.43
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.32	0.43
1:A:64:ALA:O	1:A:85:TYR:HA	2.19	0.43
1:A:311:LEU:HD23	1:A:311:LEU:C	2.38	0.43
1:A:187:GLY:HA2	1:A:192:ARG:HD2	2.00	0.43
1:B:26:LEU:HD23	1:B:38:VAL:HB	2.00	0.42
1:A:36:LEU:HD11	1:A:63:ILE:HG13	2.00	0.42
1:B:264:ILE:CG1	1:B:274:LYS:HB3	2.48	0.42
1:A:243:GLU:HG2	1:A:246:ARG:NH1	2.34	0.42
1:B:160:SER:O	1:B:164:VAL:HG23	2.20	0.42
1:A:349:GLY:HA2	1:A:456:GLU:OE1	2.19	0.42
1:B:341:ARG:NH2	1:B:357:TYR:CE2	2.88	0.42
1:A:325:LEU:O	1:A:329:LEU:HG	2.20	0.42
1:B:129:TRP:O	1:B:133:LEU:HD23	2.20	0.41
1:B:433:ASP:C	1:B:435:GLY:H	2.23	0.41
1:B:440:MSE:HE1	1:B:449:CYS:CB	2.51	0.41
1:B:164:VAL:HG11	1:B:196:LEU:HD11	2.01	0.41
1:B:377:GLY:HA3	1:B:457:ASN:ND2	2.35	0.41
1:A:331:THR:HA	1:A:334:ARG:NH2	2.35	0.41
1:B:345:PHE:HB3	1:B:490:LEU:HD12	2.01	0.41
1:A:15:ASP:OD2	1:A:75:ILE:HD12	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:GLU:HG2	1:A:191:HIS:CE1	2.56	0.41
1:B:341:ARG:CG	1:B:341:ARG:NH1	2.80	0.41
1:A:145:ASN:ND2	1:A:154:THR:HG21	2.36	0.41
1:B:448:THR:O	1:B:452:MSE:HG2	2.21	0.41
1:A:208:ARG:CZ	1:A:211:LEU:HD12	2.48	0.41
1:A:164:VAL:HG11	1:A:196:LEU:HD11	2.03	0.41
1:A:129:TRP:O	1:A:133:LEU:HD23	2.21	0.41
1:B:394:ARG:NH1	5:B:2158:HOH:O	2.53	0.41
1:B:24:MSE:HE3	1:B:36:LEU:HD21	2.03	0.40
1:B:440:MSE:HE1	1:B:449:CYS:HB2	2.04	0.40
1:B:343:GLU:HG2	1:B:494:ALA:HB2	2.03	0.40
1:B:372:ARG:HH22	1:B:406:ASP:CG	2.24	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	498/498 (100%)	480 (96%)	14 (3%)	4 (1%)	27	17
1	B	499/498 (100%)	483 (97%)	13 (3%)	3 (1%)	33	24
All	All	997/996 (100%)	963 (97%)	27 (3%)	7 (1%)	30	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASP
1	B	282	ASP
1	B	283	SER
1	B	390	ASP
1	A	390	ASP
1	A	209	ASP
1	A	358	ALA

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	391/376 (104%)	387 (99%)	4 (1%)	85	88
1	B	393/376 (104%)	387 (98%)	6 (2%)	76	79
All	All	784/752 (104%)	774 (99%)	10 (1%)	80	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	129	TRP
1	A	230	GLU
1	A	339	CYS
1	B	92	ARG
1	B	129	TRP
1	B	155	GLU
1	B	163	ASP
1	B	282	ASP
1	B	327	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	90	ASN
1	A	117	ASN
1	A	124	GLN
1	A	156	ASN
1	A	186	HIS
1	A	263	HIS
1	A	336	GLN
1	B	44	GLN
1	B	90	ASN
1	B	124	GLN
1	B	156	ASN
1	B	166	HIS
1	B	219	HIS

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Mol	Chain	Res	Type
1	B	269	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	KCX	A	224	1	11,11,12	6.42	5 (45%)	10,12,14	6.42	5 (50%)
1	KCX	B	224	1	11,11,12	6.21	4 (36%)	10,12,14	6.27	5 (50%)

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	KCX	A	224	1	-	0/8/10/12	0/0/0/0
1	KCX	B	224	1	-	0/8/10/12	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	KCX	O-C	17.93	1.23	1.11
1	B	224	KCX	O-C	17.26	1.23	1.11
1	A	224	KCX	CX-NZ	10.67	1.43	1.32
1	B	224	KCX	CX-NZ	10.49	1.42	1.32
1	A	224	KCX	CA-C	2.63	1.53	1.48
1	A	224	KCX	OQ1-CX	2.50	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	KCX	OQ1-CX	2.32	1.26	1.21
1	B	224	KCX	CA-C	2.29	1.52	1.48
1	A	224	KCX	CE-NZ	2.14	1.51	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	KCX	OQ2-CX-NZ	15.90	136.13	116.33
1	B	224	KCX	OQ2-CX-NZ	15.50	135.63	116.33
1	A	224	KCX	OQ1-CX-NZ	-11.25	106.23	124.94
1	B	224	KCX	OQ1-CX-NZ	-10.78	107.00	124.94
1	B	224	KCX	OQ2-CX-OQ1	-3.90	117.31	122.17
1	A	224	KCX	OQ2-CX-OQ1	-3.66	117.60	122.17
1	A	224	KCX	C-CA-N	-3.56	110.28	113.83
1	B	224	KCX	CE-NZ-CX	-3.29	116.00	121.99
1	B	224	KCX	C-CA-N	-2.99	110.84	113.83
1	A	224	KCX	CE-NZ-CX	-2.39	117.63	121.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	UAG	A	1498	4	59,59,60	3.77	19 (32%)	80,86,88	2.34	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	API	A	1499	3	12,12,12	1.34	1 (8%)	15,15,15	1.20	2 (13%)
3	UAG	B	1498	4	59,59,60	3.77	20 (33%)	80,86,88	2.35	23 (28%)
4	API	B	1499	3	12,12,12	1.33	1 (8%)	15,15,15	1.10	1 (6%)

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	UAG	A	1498	4	-	0/52/91/92	0/3/3/3
4	API	A	1499	3	-	0/14/14/14	0/0/0/0
3	UAG	B	1498	4	-	0/52/91/92	0/3/3/3
4	API	B	1499	3	-	0/14/14/14	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1498	UAG	O20-C27	21.96	1.26	1.11
3	B	1498	UAG	O20-C27	21.81	1.26	1.11
3	B	1498	UAG	C2-N1	8.03	1.47	1.38
3	A	1498	UAG	C2-N1	7.72	1.46	1.38
3	A	1498	UAG	C2B-C1B	6.61	1.62	1.53
3	B	1498	UAG	C2B-C1B	6.30	1.62	1.53
3	A	1498	UAG	C21-N4	-6.01	1.33	1.46
3	B	1498	UAG	C21-N4	-5.87	1.33	1.46
3	B	1498	UAG	C6-N1	4.98	1.43	1.35
3	A	1498	UAG	C4-N3	4.95	1.45	1.37
3	B	1498	UAG	C4-N3	4.81	1.45	1.37
3	A	1498	UAG	C6-N1	4.67	1.43	1.35
3	A	1498	UAG	PB-O3A	-4.16	1.52	1.59
3	B	1498	UAG	PB-O3A	-4.11	1.52	1.59
3	A	1498	UAG	C1'-C2'	3.98	1.60	1.53
3	B	1498	UAG	C5-C4	3.95	1.50	1.40
3	B	1498	UAG	C3'-C2'	3.85	1.59	1.53
3	A	1498	UAG	C5-C4	3.81	1.50	1.40
3	A	1498	UAG	C3'-C2'	3.45	1.58	1.53
3	B	1498	UAG	C1'-C2'	3.44	1.59	1.53
4	A	1499	API	O1-C1	3.01	1.32	1.22
4	B	1499	API	O1-C1	2.98	1.32	1.22
3	A	1498	UAG	C2-N3	2.84	1.42	1.37
3	A	1498	UAG	C19-N4	2.80	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1498	UAG	C4'-C5'	2.74	1.59	1.53
3	A	1498	UAG	C4'-C5'	2.73	1.59	1.53
3	B	1498	UAG	C2-N3	2.72	1.42	1.37
3	B	1498	UAG	C6-C5	2.69	1.40	1.36
3	B	1498	UAG	C19-N4	2.69	1.40	1.34
3	B	1498	UAG	O2-C2	2.65	1.29	1.23
3	A	1498	UAG	O2-C2	2.63	1.29	1.23
3	B	1498	UAG	PA-O5B	2.58	1.70	1.59
3	B	1498	UAG	O2'-C2B	-2.45	1.37	1.43
3	B	1498	UAG	PB-O1'	2.40	1.67	1.60
3	A	1498	UAG	PA-O5B	2.33	1.69	1.59
3	A	1498	UAG	O2'-C2B	-2.30	1.37	1.43
3	A	1498	UAG	C6-C5	2.26	1.39	1.36
3	A	1498	UAG	PB-O1'	2.19	1.67	1.60
3	B	1498	UAG	C22-N5	2.07	1.38	1.34
3	B	1498	UAG	C3B-C4B	-2.07	1.47	1.53
3	A	1498	UAG	C3B-C4B	-2.05	1.47	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1498	UAG	C2-N1-C1B	-11.02	111.30	118.21
3	B	1498	UAG	C2-N1-C1B	-10.97	111.33	118.21
3	B	1498	UAG	PB-O3A-PA	8.98	158.02	131.68
3	A	1498	UAG	PB-O3A-PA	8.76	157.36	131.68
3	B	1498	UAG	O4B-C1B-N1	6.91	122.63	108.06
3	A	1498	UAG	O4B-C1B-N1	6.60	121.97	108.06
3	A	1498	UAG	O5'-C1'-O1'	-4.02	106.11	111.36
3	B	1498	UAG	O5'-C1'-O1'	-3.87	106.30	111.36
3	A	1498	UAG	C2B-C3B-C4B	3.76	110.14	102.65
3	B	1498	UAG	C2B-C3B-C4B	3.75	110.12	102.65
3	B	1498	UAG	O5B-C5B-C4B	3.41	121.46	108.94
3	B	1498	UAG	C23-C21-N4	3.03	116.13	110.31
3	A	1498	UAG	O5B-C5B-C4B	3.02	120.03	108.94
3	B	1498	UAG	C6-N1-C1B	3.00	126.76	119.33
3	A	1498	UAG	C6-N1-C1B	2.98	126.71	119.33
3	B	1498	UAG	O4B-C4B-C5B	2.91	119.73	109.36
3	A	1498	UAG	C3'-O3'-C18	2.79	120.88	115.45
3	A	1498	UAG	C23-C21-N4	2.79	115.67	110.31
3	B	1498	UAG	O2'-C2B-C3B	2.72	120.67	111.83
3	A	1498	UAG	C22-C21-N4	-2.71	105.28	111.76
3	B	1498	UAG	C3'-O3'-C18	2.66	120.62	115.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1498	UAG	O2'-C2B-C3B	2.65	120.47	111.83
4	A	1499	API	C1-C2-N2	2.65	113.76	109.36
3	A	1498	UAG	C21-N4-C19	2.64	127.19	121.22
3	A	1498	UAG	O4B-C4B-C5B	2.49	118.26	109.36
3	B	1498	UAG	C1'-C2'-N2'	-2.48	106.33	111.02
3	A	1498	UAG	O3'-C18-C19	-2.43	106.29	111.37
3	A	1498	UAG	O3A-PA-O5B	2.42	114.24	103.41
3	B	1498	UAG	C4'-C3'-C2'	-2.41	106.78	110.47
3	B	1498	UAG	O3A-PA-O5B	2.41	114.17	103.41
3	A	1498	UAG	C4'-C3'-C2'	-2.37	106.84	110.47
3	B	1498	UAG	C22-C21-N4	-2.37	106.09	111.76
3	A	1498	UAG	O1'-C1'-C2'	2.36	111.66	107.91
3	B	1498	UAG	O3'-C18-C19	-2.35	106.46	111.37
3	B	1498	UAG	C21-N4-C19	2.32	126.47	121.22
3	B	1498	UAG	O1'-C1'-C2'	2.29	111.55	107.91
3	A	1498	UAG	C5B-C4B-C3B	-2.26	106.16	115.21
3	A	1498	UAG	O3A-PA-O1A	-2.26	95.06	111.28
3	B	1498	UAG	O3A-PA-O1A	-2.22	95.32	111.28
3	A	1498	UAG	C26-C25-C24	2.20	115.84	112.24
3	A	1498	UAG	O2A-PA-O1A	2.16	124.26	112.21
3	B	1498	UAG	O2A-PA-O1A	2.15	124.21	112.21
4	A	1499	API	C5-C6-C7	-2.11	105.97	110.98
3	B	1498	UAG	C25-C24-C28	-2.08	106.23	110.71
3	A	1498	UAG	O4B-C4B-C3B	2.08	109.38	105.17
3	B	1498	UAG	C5B-C4B-C3B	-2.07	106.90	115.21
3	B	1498	UAG	C23-C21-C22	-2.07	106.04	110.22
4	B	1499	API	C1-C2-N2	2.05	112.76	109.36
3	A	1498	UAG	O5B-PA-O1A	-2.04	101.39	109.37
3	A	1498	UAG	C1'-C2'-N2'	-2.04	107.17	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	496/498 (99%)	-0.05	5 (1%) 79 80	17, 32, 50, 62	19 (3%)
1	B	497/498 (99%)	0.02	12 (2%) 56 56	18, 33, 52, 65	19 (3%)
All	All	993/996 (99%)	-0.02	17 (1%) 64 67	17, 32, 51, 65	38 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	6.1
1	B	374	HIS	4.5
1	B	283	SER	3.6
1	B	498	HIS	3.3
1	B	434	ALA	3.0
1	B	432	LEU	2.7
1	B	436	HIS	2.6
1	B	2	ASP	2.5
1	A	282	ASP	2.4
1	B	301	HIS	2.3
1	A	496	SER	2.3
1	B	475	ASN	2.3
1	B	267	ASN	2.2
1	A	77	GLU	2.2
1	B	347	ALA	2.2
1	B	348	PRO	2.1
1	A	438	LYS	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	KCX	B	224	12/13	0.11	-0.11	17,20,25,27	0
1	KCX	A	224	12/13	0.10	-0.43	19,21,28,28	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	API	A	1499	13/13	0.30	6.22	60,66,74,75	0
4	API	B	1499	13/13	0.27	4.76	52,63,69,75	0
3	UAG	B	1498	57/58	0.13	0.48	22,32,45,52	0
3	UAG	A	1498	57/58	0.12	0.34	21,30,46,55	0
2	CL	A	1001	1/1	0.74	-	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.