



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GPJ
Title : GLUTAMYL-TRNA REDUCTASE FROM METHANOPYRUS KANDLERI
Authors : Moser, J.; Schubert, W.-D.; Beier, V.; Bringemeier, I.; Jahn, D.; Heinz, D.W.
Deposited on : 2001-11-05
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

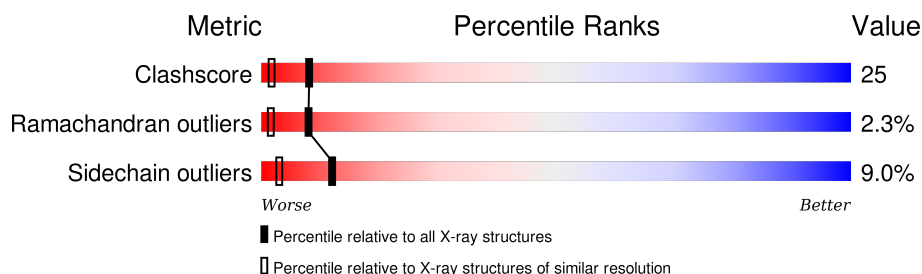
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	404	 69% 22% 5% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3695 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.

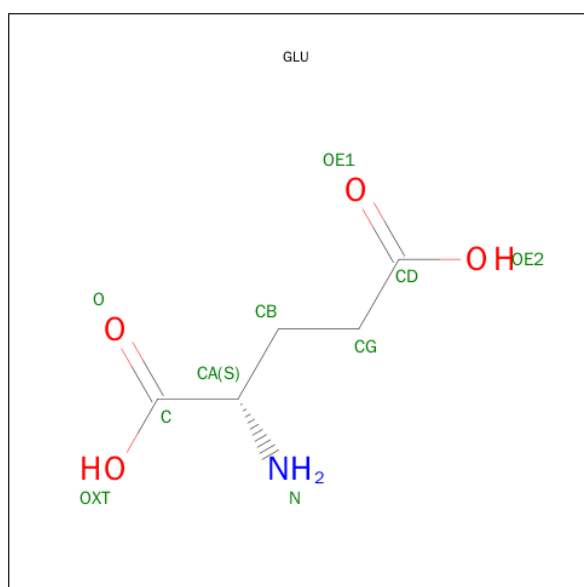
- Molecule 1 is a protein called GLUTAMYL-TRNA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	17	0
			3299	2028	623	643	5			

There are 5 discrepancies between the modelled and reference sequences:

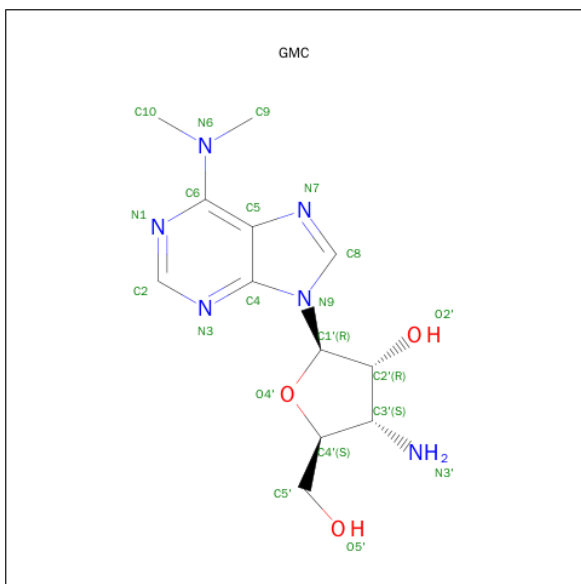
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	SER	CYS	ENGINEERED MUTATION	UNP Q9UXR8
A	42	SER	CYS	ENGINEERED MUTATION	UNP Q9UXR8
A	48	SER	CYS	ENGINEERED MUTATION	UNP Q9UXR8
A	90	SER	CYS	ENGINEERED MUTATION	UNP Q9UXR8
A	393	SER	CYS	ENGINEERED MUTATION	UNP Q9UXR8

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



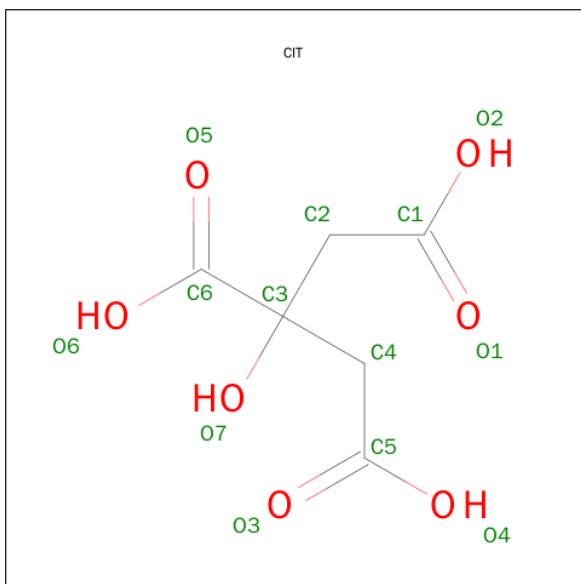
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 3 is (2R,3R,4S,5S)-4-AMINO-2-[6-(DIMETHYLAMINO)-9H-PURIN-9-YL]-5-(HYDROXYMETHYL)TETRAHYDRO-3-FURANOL (three-letter code: GMC) (formula: $C_{12}H_{18}N_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	12	6	3		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

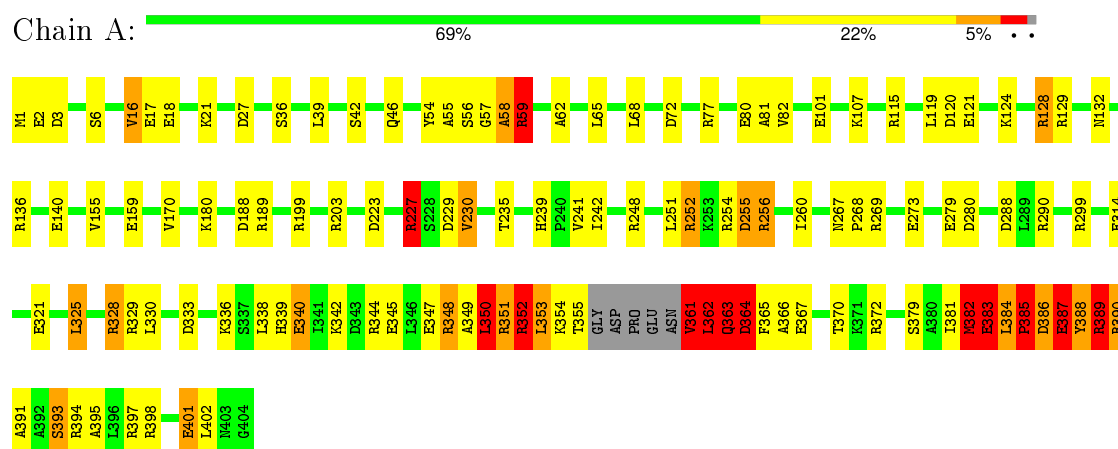
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	353	Total 353	O 353	0	3

3 Residue-property plots [i](#)

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.

Note EDS was not executed.

• Molecule 1: GLUTAMYL-TRNA REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.27Å 98.65Å 68.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.00 – 1.95	Depositor
% Data completeness (in resolution range)	91.1 (69.00-1.95)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3695	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GMC, CIT

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	0.80	1/3324 (0.0%)	1.18	36/4463 (0.8%)

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	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	VAL	CB-CG1	-5.37	1.41	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	PRO	N-CA-C	11.90	143.03	112.10
1	A	361	VAL	CA-C-N	11.45	142.38	117.20
1	A	361	VAL	O-C-N	-10.05	106.61	122.70
1	A	372	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	363	GLN	N-CA-C	9.12	135.61	111.00
1	A	388	TYR	CB-CA-C	-8.92	92.55	110.40
1	A	350	LEU	CA-CB-CG	8.90	135.78	115.30
1	A	382	MET	C-N-CA	8.55	143.08	121.70
1	A	361	VAL	CA-C-O	-8.32	102.62	120.10
1	A	384[A]	LEU	CA-CB-CG	-8.11	96.65	115.30
1	A	384[B]	LEU	CA-CB-CG	-8.11	96.65	115.30
1	A	383	GLU	N-CA-CB	8.10	125.18	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	361	VAL	CB-CA-C	-6.96	98.17	111.40
1	A	372	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	59	ARG	N-CA-C	6.77	129.28	111.00
1	A	382	MET	CA-C-N	6.54	131.58	117.20
1	A	383	GLU	CB-CA-C	6.49	123.38	110.40
1	A	364	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	188	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	353	LEU	N-CA-C	-6.05	94.66	111.00
1	A	227	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	255	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	229	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	362	LEU	C-N-CA	5.63	135.78	121.70
1	A	350	LEU	CB-CA-C	5.59	120.81	110.20
1	A	389	ARG	N-CA-C	-5.54	96.04	111.00
1	A	364	ASP	N-CA-C	-5.53	96.08	111.00
1	A	382	MET	N-CA-C	5.50	125.86	111.00
1	A	372	ARG	CG-CD-NE	-5.34	100.58	111.80
1	A	364	ASP	N-CA-CB	5.29	120.12	110.60
1	A	333	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	352	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	72	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	27	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	382	MET	O-C-N	-5.04	114.63	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	VAL	Mainchain
1	A	362	LEU	Peptide
1	A	363	GLN	Peptide
1	A	383	GLU	Peptide
1	A	58	ALA	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	3299	0	3355	164	5
2	A	9	0	5	1	0
3	A	21	0	17	1	0
4	A	13	0	5	1	0
5	A	353	0	0	20	0
All	All	3695	0	3382	166	5

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 25.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384[B]:LEU:HD23	1:A:385:PRO:CD	1.33	1.51
1:A:384[B]:LEU:CD2	1:A:385:PRO:CD	2.23	1.17
1:A:384[B]:LEU:HD23	1:A:385:PRO:HD3	1.18	1.13
1:A:254:ARG:HB2	1:A:256[B]:ARG:HH21	1.02	1.11
1:A:384[B]:LEU:HD23	1:A:385:PRO:HD2	1.28	1.07
1:A:329[A]:ARG:NH2	5:A:2312:HOH:O	1.87	1.04
1:A:384[B]:LEU:CD2	1:A:385:PRO:HD2	1.87	1.02
1:A:347:GLU:O	1:A:350:LEU:HG	1.61	0.99
1:A:254:ARG:HB2	1:A:256[B]:ARG:NH2	1.79	0.98
1:A:223[B]:ASP:OD1	5:A:2210:HOH:O	1.84	0.94
1:A:379:SER:O	1:A:383:GLU:HB2	1.68	0.94
1:A:388:TYR:O	1:A:389:ARG:C	2.05	0.93
1:A:254:ARG:CB	1:A:256[B]:ARG:HH21	1.83	0.92
1:A:384[B]:LEU:CD2	1:A:385:PRO:HD3	1.96	0.91
1:A:385:PRO:O	1:A:388:TYR:HB2	1.72	0.89
1:A:18:GLU:OE1	1:A:21:LYS:NZ	2.08	0.86
1:A:362:LEU:C	1:A:364:ASP:HB2	1.97	0.85
1:A:394:ARG:HD3	5:A:2337:HOH:O	1.75	0.84
1:A:124[B]:LYS:NZ	5:A:2132:HOH:O	2.11	0.84
1:A:362:LEU:C	1:A:364:ASP:CB	2.46	0.83
1:A:388:TYR:O	1:A:389:ARG:O	1.96	0.83
1:A:384[A]:LEU:HG	1:A:385:PRO:CD	2.07	0.82
1:A:363:GLN:N	1:A:364:ASP:HB2	1.93	0.82
1:A:386:ASP:HA	1:A:389:ARG:HB2	1.61	0.82
1:A:132[B]:ASN:HD22	1:A:132[B]:ASN:C	1.83	0.82
1:A:336:LYS:NZ	1:A:340[A]:GLU:OE2	2.13	0.81
1:A:388:TYR:C	1:A:389:ARG:O	2.17	0.80
1:A:390:ARG:N	1:A:393[A]:SER:OG	2.15	0.79
1:A:362:LEU:HD12	1:A:364:ASP:OD2	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:O	1:A:361:VAL:HG23	1.80	0.79
1:A:391:ALA:HA	1:A:394:ARG:HB2	1.66	0.77
1:A:339:HIS:HD2	1:A:342:LYS:NZ	1.83	0.76
1:A:384[B]:LEU:HD23	1:A:385:PRO:N	2.00	0.75
1:A:347:GLU:O	1:A:350:LEU:CG	2.34	0.74
1:A:339:HIS:CD2	1:A:342:LYS:NZ	2.57	0.73
1:A:18:GLU:OE1	1:A:21:LYS:CE	2.38	0.72
1:A:390:ARG:HB3	1:A:390:ARG:HH11	1.55	0.72
1:A:391:ALA:O	1:A:395:ALA:N	2.19	0.72
1:A:390:ARG:HB3	1:A:390:ARG:NH1	2.03	0.72
1:A:159:GLU:OE2	1:A:189[B]:ARG:NE	2.23	0.71
1:A:394:ARG:HG2	1:A:394:ARG:HH11	1.56	0.70
1:A:336:LYS:CG	1:A:397:ARG:HH22	2.05	0.70
1:A:362:LEU:C	1:A:364:ASP:HB3	2.11	0.68
1:A:381:ILE:O	1:A:389:ARG:HG2	1.93	0.68
1:A:386:ASP:C	1:A:388:TYR:N	2.48	0.67
1:A:107[B]:LYS:NZ	5:A:2119:HOH:O	2.28	0.67
1:A:402:LEU:O	5:A:2343:HOH:O	2.13	0.67
1:A:344:ARG:NH1	1:A:401:GLU:O	2.28	0.66
1:A:362:LEU:HA	1:A:364:ASP:CB	2.25	0.66
1:A:132[B]:ASN:C	1:A:132[B]:ASN:ND2	2.49	0.66
1:A:381:ILE:O	1:A:389:ARG:CG	2.43	0.65
1:A:389:ARG:O	1:A:390:ARG:CB	2.45	0.65
1:A:330:LEU:HD11	1:A:381:ILE:HG21	1.80	0.64
1:A:328:ARG:HH11	1:A:328:ARG:HG3	1.63	0.63
1:A:129:ARG:NH2	1:A:321:GLU:OE2	2.29	0.63
1:A:251:LEU:HD21	1:A:260:ILE:HD12	1.80	0.62
1:A:339:HIS:CD2	1:A:342:LYS:HZ1	2.18	0.61
1:A:59:ARG:HG2	1:A:59:ARG:O	2.00	0.61
1:A:119:LEU:HD13	1:A:124[B]:LYS:HG2	1.82	0.61
1:A:361:VAL:O	1:A:363:GLN:N	2.33	0.60
1:A:397:ARG:NH1	5:A:2339:HOH:O	2.33	0.60
1:A:119:LEU:HD13	1:A:124[A]:LYS:HG2	1.84	0.60
1:A:251:LEU:HD21	1:A:260:ILE:CD1	2.32	0.59
1:A:339:HIS:HE1	5:A:2314:HOH:O	1.84	0.59
1:A:386:ASP:C	1:A:388:TYR:H	2.05	0.59
1:A:384[A]:LEU:HG	1:A:385:PRO:HD3	1.83	0.58
1:A:115:ARG:HD2	5:A:2127[A]:HOH:O	2.03	0.58
1:A:390:ARG:H	1:A:393[A]:SER:HG	1.48	0.57
1:A:252:ARG:NH2	5:A:2233:HOH:O	2.36	0.57
1:A:398:ARG:NH2	5:A:2342:HOH:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16[B]:VAL:HG23	5:A:2020:HOH:O	2.05	0.56
1:A:136:ARG:HD2	1:A:140:GLU:OE2	2.04	0.56
1:A:325:LEU:HD21	1:A:329[B]:ARG:HD2	1.87	0.56
1:A:279[A]:GLU:O	1:A:280:ASP:HB2	2.06	0.56
1:A:39:LEU:HD13	1:A:55:ALA:HB1	1.88	0.56
1:A:299:ARG:HD2	5:A:2274:HOH:O	2.07	0.55
1:A:115:ARG:HG2	1:A:115:ARG:O	2.04	0.55
1:A:345[B]:GLU:OE1	5:A:2320:HOH:O	2.18	0.55
1:A:339:HIS:CD2	1:A:342:LYS:HZ3	2.25	0.55
1:A:352:ARG:C	1:A:354:LYS:H	2.07	0.55
1:A:336:LYS:HG3	1:A:397:ARG:HH22	1.71	0.54
1:A:59:ARG:HD2	5:A:2007:HOH:O	2.07	0.54
1:A:339:HIS:HD2	1:A:342:LYS:HZ3	1.53	0.54
1:A:362:LEU:HA	1:A:364:ASP:HB2	1.89	0.54
1:A:6:SER:HB2	1:A:81:ALA:HB1	1.90	0.53
1:A:267:ASN:HA	1:A:268:PRO:C	2.29	0.53
1:A:390:ARG:CA	1:A:393[A]:SER:OG	2.57	0.53
1:A:385:PRO:O	1:A:388:TYR:CB	2.49	0.53
1:A:279[B]:GLU:O	1:A:280:ASP:HB2	2.09	0.53
1:A:199:ARG:HH12	1:A:239:HIS:HD2	1.58	0.52
1:A:248:ARG:O	1:A:252:ARG:HG2	2.09	0.52
1:A:391:ALA:O	1:A:394:ARG:HB2	2.09	0.52
1:A:390:ARG:O	1:A:394:ARG:N	2.43	0.52
1:A:362:LEU:CD1	1:A:364:ASP:OD2	2.58	0.51
1:A:386:ASP:O	1:A:388:TYR:N	2.43	0.51
1:A:386:ASP:O	1:A:387:GLU:C	2.49	0.51
1:A:279[A]:GLU:CD	1:A:279[A]:GLU:H	2.15	0.51
1:A:361:VAL:CG2	1:A:363:GLN:HB2	2.41	0.50
1:A:394:ARG:HG2	1:A:394:ARG:NH1	2.25	0.50
1:A:349:ALA:HA	5:A:2322:HOH:O	2.11	0.50
1:A:199:ARG:HH22	1:A:239:HIS:HB2	1.76	0.50
1:A:391:ALA:CA	1:A:394:ARG:HB2	2.39	0.50
1:A:136:ARG:NH1	1:A:140:GLU:OE1	2.45	0.50
1:A:325:LEU:CD2	1:A:329[B]:ARG:HD2	2.42	0.50
1:A:180:LYS:NZ	5:A:2173:HOH:O	2.40	0.50
1:A:39:LEU:CD2	1:A:58:ALA:HA	2.42	0.49
1:A:361:VAL:O	1:A:361:VAL:CG2	2.35	0.49
3:A:1405:GMC:HC1	3:A:1405:GMC:N7	2.27	0.49
1:A:383:GLU:HB2	5:A:2333:HOH:O	2.12	0.49
1:A:170:VAL:HG22	1:A:230:VAL:CG1	2.42	0.49
1:A:363:GLN:CA	1:A:364:ASP:HB2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HH21	1:A:241:VAL:HG12	1.79	0.48
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.25	0.48
1:A:364:ASP:HB3	1:A:365:PHE:H	1.48	0.47
1:A:362:LEU:HA	1:A:364:ASP:OD2	2.16	0.47
1:A:121:GLU:OE2	1:A:328:ARG:NH2	2.43	0.47
1:A:290:ARG:HG2	1:A:290:ARG:HH11	1.81	0.46
1:A:389:ARG:O	1:A:390:ARG:HB2	2.15	0.46
1:A:256[A]:ARG:NH1	1:A:256[A]:ARG:HB3	2.31	0.46
1:A:362:LEU:CA	1:A:364:ASP:HB2	2.45	0.46
1:A:223[A]:ASP:O	1:A:227:ARG:HG2	2.16	0.45
1:A:362:LEU:CA	1:A:364:ASP:CB	2.92	0.45
1:A:155:VAL:HG11	1:A:189[B]:ARG:HD3	1.97	0.45
1:A:354:LYS:HA	1:A:355:THR:C	2.37	0.45
1:A:189[A]:ARG:NH2	5:A:2181:HOH:O	2.49	0.45
1:A:256[B]:ARG:H	1:A:256[B]:ARG:CZ	2.29	0.45
1:A:254:ARG:CA	1:A:256[B]:ARG:HH21	2.29	0.45
1:A:361:VAL:HG23	1:A:363:GLN:HB2	1.97	0.45
1:A:18:GLU:OE1	1:A:21:LYS:HE3	2.16	0.45
1:A:235:THR:HG21	1:A:241:VAL:HG11	1.98	0.45
4:A:1407:CIT:C5	4:A:1407:CIT:C1	2.95	0.44
1:A:347:GLU:C	1:A:350:LEU:HG	2.32	0.44
1:A:330:LEU:HD21	1:A:381:ILE:HB	2.00	0.44
1:A:101:GLU:OE1	2:A:1406:GLU:N	2.50	0.44
1:A:223[B]:ASP:O	1:A:227:ARG:HG2	2.18	0.44
1:A:124[B]:LYS:O	1:A:128:ARG:HB2	2.17	0.43
1:A:385:PRO:HB2	1:A:386:ASP:H	1.24	0.43
1:A:364:ASP:H	1:A:367:GLU:H	1.66	0.43
1:A:42:SER:HA	1:A:54:TYR:O	2.18	0.43
1:A:391:ALA:O	1:A:394:ARG:N	2.51	0.43
1:A:255:ASP:N	1:A:256[B]:ARG:NH2	2.67	0.43
1:A:124[A]:LYS:O	1:A:128:ARG:HB2	2.18	0.43
1:A:170:VAL:HG22	1:A:230:VAL:HG13	2.00	0.43
1:A:256[A]:ARG:HH11	1:A:256[A]:ARG:HB3	1.83	0.42
1:A:348:ARG:C	1:A:350:LEU:N	2.71	0.42
1:A:362:LEU:HA	1:A:364:ASP:CG	2.39	0.42
1:A:366:ALA:O	1:A:370:THR:CB	2.68	0.42
1:A:203:ARG:HA	1:A:203:ARG:NE	2.35	0.42
1:A:241:VAL:HG23	1:A:242:ILE:HG12	2.02	0.42
1:A:394:ARG:HB3	5:A:2338:HOH:O	2.20	0.42
1:A:56:SER:OG	1:A:120:ASP:OD2	2.22	0.42
1:A:384[A]:LEU:HG	1:A:385:PRO:N	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:HB3	1:A:342:LYS:HE2	1.64	0.41
1:A:62:ALA:HB3	1:A:77:ARG:HH22	1.84	0.41
1:A:18:GLU:HA	1:A:18:GLU:OE1	2.19	0.41
1:A:3:ASP:OD1	1:A:57:GLY:N	2.53	0.41
1:A:379:SER:O	1:A:383:GLU:CB	2.53	0.41
1:A:330:LEU:HD23	1:A:382:MET:HG2	2.03	0.41
1:A:361:VAL:O	1:A:363:GLN:HB2	2.21	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.74	0.41
1:A:1:MET:SD	1:A:82:VAL:HG21	2.61	0.41
1:A:388:TYR:HB2	1:A:389:ARG:H	1.14	0.40
1:A:129:ARG:CG	1:A:314:GLU:OE2	2.69	0.40
1:A:279[B]:GLU:HG3	1:A:279[B]:GLU:H	1.53	0.40

All (5) 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:352:ARG:NH2	1:A:362:LEU:CD2[2_665]	1.55	0.65
1:A:352:ARG:NH2	1:A:362:LEU:CG[2_665]	1.63	0.57
1:A:352:ARG:NH2	1:A:362:LEU:CD1[2_665]	1.95	0.25
1:A:352:ARG:CZ	1:A:362:LEU:CD2[2_665]	2.09	0.11
1:A:352:ARG:NH1	1:A:362:LEU:CD2[2_665]	2.16	0.04

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	412/404 (102%)	388 (94%)	14 (3%)	10 (2%)	7 1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	363	GLN
1	A	364	ASP
1	A	387	GLU
1	A	389	ARG
1	A	390	ARG
1	A	383	GLU
1	A	351	ARG
1	A	16[A]	VAL
1	A	16[B]	VAL

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	350/339 (103%)	316 (90%)	34 (10%)	10 2

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

Mol	Chain	Res	Type
1	A	17	GLU
1	A	36	SER
1	A	46	GLN
1	A	59	ARG
1	A	65	LEU
1	A	68	LEU
1	A	80[A]	GLU
1	A	80[B]	GLU
1	A	128	ARG
1	A	227	ARG
1	A	252	ARG
1	A	256[A]	ARG
1	A	256[B]	ARG
1	A	269	ARG
1	A	273	GLU
1	A	325	LEU
1	A	328	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	338	LEU
1	A	340[A]	GLU
1	A	340[B]	GLU
1	A	348	ARG
1	A	350	LEU
1	A	351	ARG
1	A	352	ARG
1	A	353	LEU
1	A	363	GLN
1	A	382	MET
1	A	383	GLU
1	A	385	PRO
1	A	386	ASP
1	A	387	GLU
1	A	393[A]	SER
1	A	393[B]	SER
1	A	401	GLU

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

Mol	Chain	Res	Type
1	A	100	GLN
1	A	239	HIS
1	A	339	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands 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	$\# Z > 2$
3	GMC	A	1405	2	17,23,23	1.39	2 (11%)	15,34,34	4.53	8 (53%)
2	GLU	A	1406	3	4,8,9	0.94	0	3,9,11	1.39	1 (33%)
4	CIT	A	1407	-	3,12,12	2.78	1 (33%)	3,17,17	3.31	1 (33%)

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	GMC	A	1405	2	-	0/6/26/26	0/3/3/3
2	GLU	A	1406	3	-	0/3/7/9	0/0/0/0
4	CIT	A	1407	-	-	0/6/16/16	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1407	CIT	C2-C3	-4.64	1.47	1.54
3	A	1405	GMC	C5-C4	2.86	1.46	1.40
3	A	1405	GMC	O4'-C1'	4.13	1.46	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1405	GMC	N3-C2-N1	-8.26	122.57	128.89
4	A	1407	CIT	C3-C2-C1	-5.56	106.06	114.96
3	A	1405	GMC	O4'-C1'-N9	-4.99	97.66	108.10
3	A	1405	GMC	C4-C5-N7	-3.17	106.56	109.48
2	A	1406	GLU	O-C-CA	-2.26	119.59	125.49
3	A	1405	GMC	O4'-C4'-C3'	-2.23	100.75	104.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1405	GMC	O4'-C4'-C5'	2.55	114.69	109.17
3	A	1405	GMC	C1'-N9-C4	2.61	130.88	126.94
3	A	1405	GMC	C2-N1-C6	5.12	122.33	111.43
3	A	1405	GMC	C2'-C1'-N9	12.40	133.24	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1405	GMC	1	0
2	A	1406	GLU	1	0
4	A	1407	CIT	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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.