



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:45 AM GMT

PDB ID : 3FPH  
Title : Crystal Structure of E81Q mutant of MtNAS in complex with L-Glutamate  
Authors : Dreyfus, C.; Pignol, D.; Arnoux, P.  
Deposited on : 2009-01-05  
Resolution : 1.80 Å(reported)

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

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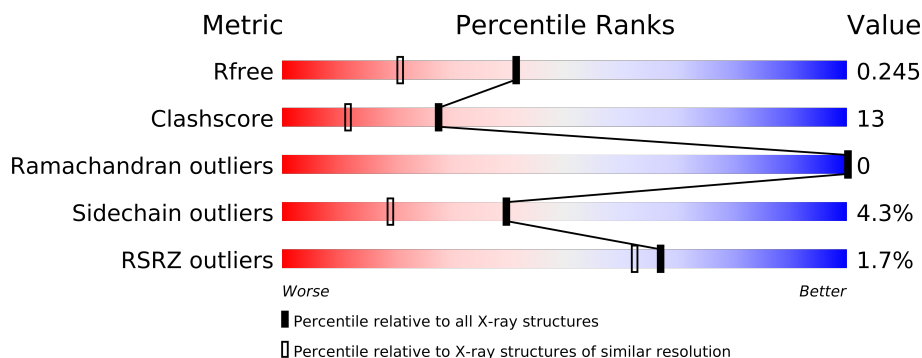
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	298	
1	B	298	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	GLU	B	302[A]	-	X
2	GLU	B	302[B]	-	X
3	NA	B	299	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4977 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2111	1347	360	393	11			
1	B	264	Total	C	N	O	S	0	0	0
			2111	1347	360	393	11			

There are 66 discrepancies between the modelled and reference sequences:

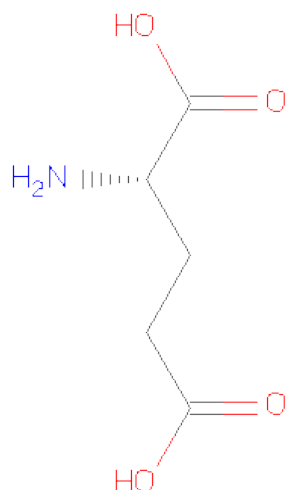
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLN	GLU	ENGINEERED	UNP O26771
A	267	LYS	-	EXPRESSION TAG	UNP O26771
A	268	GLY	-	EXPRESSION TAG	UNP O26771
A	269	GLU	-	EXPRESSION TAG	UNP O26771
A	270	LEU	-	EXPRESSION TAG	UNP O26771
A	271	ASN	-	EXPRESSION TAG	UNP O26771
A	272	SER	-	EXPRESSION TAG	UNP O26771
A	273	LYS	-	EXPRESSION TAG	UNP O26771
A	274	LEU	-	EXPRESSION TAG	UNP O26771
A	275	GLU	-	EXPRESSION TAG	UNP O26771
A	276	GLY	-	EXPRESSION TAG	UNP O26771
A	277	LYS	-	EXPRESSION TAG	UNP O26771
A	278	PRO	-	EXPRESSION TAG	UNP O26771
A	279	ILE	-	EXPRESSION TAG	UNP O26771
A	280	PRO	-	EXPRESSION TAG	UNP O26771
A	281	ASN	-	EXPRESSION TAG	UNP O26771
A	282	PRO	-	EXPRESSION TAG	UNP O26771
A	283	LEU	-	EXPRESSION TAG	UNP O26771
A	284	LEU	-	EXPRESSION TAG	UNP O26771
A	285	GLY	-	EXPRESSION TAG	UNP O26771
A	286	LEU	-	EXPRESSION TAG	UNP O26771
A	287	ASP	-	EXPRESSION TAG	UNP O26771
A	288	SER	-	EXPRESSION TAG	UNP O26771
A	289	THR	-	EXPRESSION TAG	UNP O26771
A	290	ARG	-	EXPRESSION TAG	UNP O26771

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Chain	Residue	Modelled	Actual	Comment	Reference
A	291	THR	-	EXPRESSION TAG	UNP O26771
A	292	GLY	-	EXPRESSION TAG	UNP O26771
A	293	HIS	-	EXPRESSION TAG	UNP O26771
A	294	HIS	-	EXPRESSION TAG	UNP O26771
A	295	HIS	-	EXPRESSION TAG	UNP O26771
A	296	HIS	-	EXPRESSION TAG	UNP O26771
A	297	HIS	-	EXPRESSION TAG	UNP O26771
A	298	HIS	-	EXPRESSION TAG	UNP O26771
B	81	GLN	GLU	ENGINEERED	UNP O26771
B	267	LYS	-	EXPRESSION TAG	UNP O26771
B	268	GLY	-	EXPRESSION TAG	UNP O26771
B	269	GLU	-	EXPRESSION TAG	UNP O26771
B	270	LEU	-	EXPRESSION TAG	UNP O26771
B	271	ASN	-	EXPRESSION TAG	UNP O26771
B	272	SER	-	EXPRESSION TAG	UNP O26771
B	273	LYS	-	EXPRESSION TAG	UNP O26771
B	274	LEU	-	EXPRESSION TAG	UNP O26771
B	275	GLU	-	EXPRESSION TAG	UNP O26771
B	276	GLY	-	EXPRESSION TAG	UNP O26771
B	277	LYS	-	EXPRESSION TAG	UNP O26771
B	278	PRO	-	EXPRESSION TAG	UNP O26771
B	279	ILE	-	EXPRESSION TAG	UNP O26771
B	280	PRO	-	EXPRESSION TAG	UNP O26771
B	281	ASN	-	EXPRESSION TAG	UNP O26771
B	282	PRO	-	EXPRESSION TAG	UNP O26771
B	283	LEU	-	EXPRESSION TAG	UNP O26771
B	284	LEU	-	EXPRESSION TAG	UNP O26771
B	285	GLY	-	EXPRESSION TAG	UNP O26771
B	286	LEU	-	EXPRESSION TAG	UNP O26771
B	287	ASP	-	EXPRESSION TAG	UNP O26771
B	288	SER	-	EXPRESSION TAG	UNP O26771
B	289	THR	-	EXPRESSION TAG	UNP O26771
B	290	ARG	-	EXPRESSION TAG	UNP O26771
B	291	THR	-	EXPRESSION TAG	UNP O26771
B	292	GLY	-	EXPRESSION TAG	UNP O26771
B	293	HIS	-	EXPRESSION TAG	UNP O26771
B	294	HIS	-	EXPRESSION TAG	UNP O26771
B	295	HIS	-	EXPRESSION TAG	UNP O26771
B	296	HIS	-	EXPRESSION TAG	UNP O26771
B	297	HIS	-	EXPRESSION TAG	UNP O26771
B	298	HIS	-	EXPRESSION TAG	UNP O26771

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			20	10	2	8		
2	B	1	Total	C	N	O	0	1
			20	10	2	8		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	349	Total	O	0	0
			349	349		
4	B	364	Total	O	0	0
			364	364		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.20Å 69.78Å 146.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.30 – 1.80 60.33 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (60.30-1.80) 96.5 (60.33-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.246 0.190 , 0.245	Depositor DCC
$R_{free}$ test set	3067 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61498 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NA

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	0.85	2/2153 (0.1%)	0.84	5/2912 (0.2%)
1	B	0.90	0/2153	0.95	7/2912 (0.2%)
All	All	0.88	2/4306 (0.0%)	0.90	12/5824 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	GLU	CG-CD	6.14	1.61	1.51
1	A	188	GLU	CD-OE1	5.54	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ARG	NE-CZ-NH2	-15.65	112.48	120.30
1	B	217	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	B	99	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	B	217	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	217	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	217	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	106	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	B	106	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	A	99	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	99	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	217	ARG	CD-NE-CZ	5.54	131.35	123.60
1	B	182	THR	N-CA-CB	-5.27	100.29	110.30

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	2111	0	2108	56	0
1	B	2111	0	2108	51	4
2	A	20	0	10	3	0
2	B	20	0	10	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	349	0	0	20	5
4	B	364	0	0	21	1
All	All	4977	0	4236	109	5

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 13.

All (109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:LYS:HZ3	1:A:112:LYS:CB	1.01	1.44
1:A:175:ASN:HB2	4:A:709:HOH:O	1.15	1.25
1:A:147:MET:SD	4:A:721:HOH:O	1.93	1.23
1:A:157:ASP:HB2	4:A:522:HOH:O	1.49	1.11
1:B:217:ARG:HD3	4:B:343:HOH:O	1.53	1.09
1:A:112:LYS:HB3	1:A:112:LYS:NZ	1.09	1.08
1:A:236:ASP:HB3	4:A:387:HOH:O	1.52	1.06
1:B:36:LEU:HD11	1:B:73:TYR:HE1	1.16	1.05
1:A:237:ASP:O	1:A:240:THR:HG23	1.62	0.99
1:A:90:GLU:HG3	4:A:442:HOH:O	1.62	0.99
1:B:26:GLU:HG3	4:B:696:HOH:O	1.65	0.95
1:B:106:ARG:HG3	4:B:303:HOH:O	1.66	0.94
1:A:141:LEU:HD22	1:A:147:MET:HE3	1.48	0.93
1:B:36:LEU:HD11	1:B:73:TYR:CE1	2.05	0.91
1:B:2:SER:HA	4:B:509:HOH:O	1.76	0.86
1:B:36:LEU:CD1	1:B:73:TYR:HE1	1.90	0.83
1:B:29:THR:HG23	4:B:601:HOH:O	1.81	0.81
1:B:207:ASN:ND2	1:B:210:ARG:CZ	2.42	0.80
1:A:112:LYS:HB3	1:A:112:LYS:HZ1	1.46	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:210:ARG:HD3	4:B:719:HOH:O	1.81	0.80
1:A:141:LEU:HD22	1:A:147:MET:CE	2.12	0.79
1:A:141:LEU:CD2	1:A:147:MET:HE3	2.12	0.79
1:A:18:GLU:HG2	1:A:68:LEU:HD11	1.66	0.77
1:B:29:THR:HG21	1:B:83:GLU:OE1	1.85	0.76
1:B:210:ARG:NH1	4:B:371:HOH:O	2.19	0.76
1:B:36:LEU:CD1	1:B:73:TYR:CE1	2.69	0.75
1:A:112:LYS:HB3	1:A:112:LYS:HZ2	1.51	0.72
1:B:207:ASN:ND2	1:B:210:ARG:NE	2.37	0.72
1:A:217:ARG:HD3	4:A:400:HOH:O	1.88	0.71
1:B:2:SER:CA	4:B:509:HOH:O	2.38	0.69
1:A:29:THR:HG21	1:A:83:GLU:OE1	1.92	0.69
1:B:206:ARG:O	1:B:210:ARG:HG3	1.92	0.68
1:A:73:TYR:HE1	4:A:365:HOH:O	1.76	0.68
1:B:27:MET:HG2	4:B:470:HOH:O	1.93	0.68
1:B:119:ARG:HD3	4:B:494:HOH:O	1.93	0.68
1:A:2:SER:N	4:A:487:HOH:O	2.28	0.67
1:B:10:ILE:HD12	1:B:56:ILE:HD11	1.75	0.67
1:B:207:ASN:HD21	1:B:210:ARG:CZ	2.07	0.67
1:B:180:ASP:OD1	1:B:182:THR:HB	1.94	0.67
1:A:145:TYR:HB2	1:A:147:MET:HE2	1.75	0.67
1:A:172:ASP:OD2	4:A:605:HOH:O	2.12	0.67
1:B:29:THR:CG2	4:B:601:HOH:O	2.40	0.67
1:B:207:ASN:HD22	1:B:210:ARG:NE	1.94	0.65
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.62	0.64
1:A:112:LYS:CB	1:A:112:LYS:NZ	1.87	0.64
1:A:112:LYS:HZ3	1:A:112:LYS:HB3	0.46	0.62
1:A:119:ARG:NH2	1:A:121:ARG:HD3	2.16	0.60
1:B:237:ASP:O	1:B:240:THR:HG22	2.02	0.59
1:A:2:SER:HB2	4:A:487:HOH:O	2.01	0.59
1:A:51:GLU:HG3	4:A:508:HOH:O	2.02	0.59
1:B:6:TYR:CE1	1:B:42:ILE:HG12	2.38	0.59
1:B:210:ARG:HB3	4:B:719:HOH:O	2.03	0.58
1:B:27:MET:HE3	4:B:470:HOH:O	2.04	0.57
1:B:107:TYR:CZ	2:B:302[A]:GLU:HB2	2.37	0.57
1:B:123:GLY:O	1:B:148:ARG:CZ	2.52	0.56
1:A:141:LEU:CD2	1:A:147:MET:CE	2.80	0.56
1:B:123:GLY:O	1:B:148:ARG:NH2	2.38	0.56
1:B:207:ASN:HD22	1:B:210:ARG:CD	2.20	0.55
1:B:24:PHE:HA	4:B:470:HOH:O	2.06	0.55
1:A:154:ILE:HD13	1:A:180:ASP:HB3	1.89	0.54
1:B:237:ASP:O	1:B:240:THR:CG2	2.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:SER:CA	4:A:487:HOH:O	2.56	0.54
1:A:207:ASN:ND2	1:A:210:ARG:HH11	2.06	0.54
1:A:182:THR:HG23	4:A:391:HOH:O	2.07	0.54
1:A:175:ASN:CB	4:A:709:HOH:O	2.00	0.53
1:B:207:ASN:HA	1:B:210:ARG:HG3	1.89	0.53
1:B:207:ASN:HD22	1:B:210:ARG:HD2	1.73	0.52
1:B:112:LYS:HG2	1:B:145:TYR:OH	2.11	0.51
1:A:107:TYR:CZ	2:A:302[A]:GLU:HB2	2.47	0.50
1:B:206:ARG:O	1:B:210:ARG:CG	2.59	0.49
1:A:16:ARG:NH1	1:A:38:GLU:OE2	2.43	0.49
1:B:41:GLU:HG2	4:B:724:HOH:O	2.12	0.49
1:A:86:GLN:NE2	4:A:484:HOH:O	2.23	0.48
1:B:217:ARG:CD	4:B:343:HOH:O	2.33	0.48
1:A:48:ILE:HD12	4:A:628:HOH:O	2.13	0.48
1:A:89:ILE:CD1	1:A:161:LEU:HD23	2.44	0.48
1:B:107:TYR:CZ	2:B:302[B]:GLU:HB2	2.48	0.47
1:B:202:ARG:HG2	1:B:202:ARG:NH1	2.28	0.47
1:A:89:ILE:HD11	1:A:161:LEU:HD23	1.96	0.47
1:A:207:ASN:HD22	1:A:210:ARG:HD2	1.80	0.47
1:A:57:LEU:HD22	1:A:66:LEU:HD13	1.97	0.46
1:A:18:GLU:HG2	1:A:68:LEU:CD1	2.42	0.46
1:A:180:ASP:OD1	1:A:182:THR:HG22	2.15	0.46
1:A:81:GLN:HB3	1:A:133:PRO:HG2	1.98	0.46
1:B:54:LYS:O	1:B:58:ASP:HB2	2.16	0.46
1:B:203:ARG:HG3	4:B:479:HOH:O	2.15	0.45
1:B:8:ASP:O	1:B:12:ARG:HG3	2.17	0.45
1:A:89:ILE:CD1	1:A:161:LEU:CD2	2.95	0.45
1:A:94:PRO:HB2	1:A:169:LEU:HD23	1.98	0.45
1:B:207:ASN:HA	1:B:210:ARG:CD	2.46	0.45
1:A:119:ARG:HD2	1:A:119:ARG:HA	1.70	0.44
2:B:302[B]:GLU:HG3	4:B:329:HOH:O	2.16	0.44
1:A:64:HIS:CE1	4:A:468:HOH:O	2.71	0.44
1:A:145:TYR:HB2	1:A:147:MET:CE	2.45	0.43
2:A:302[B]:GLU:HG3	4:A:553:HOH:O	2.17	0.43
1:A:73:TYR:OH	1:A:255:ASN:ND2	2.52	0.43
1:A:115:ALA:HA	1:A:120:PHE:CD2	2.54	0.43
1:B:2:SER:N	4:B:509:HOH:O	2.51	0.42
1:B:11:LYS:HE2	4:B:520:HOH:O	2.19	0.42
1:A:107:TYR:CZ	2:A:302[B]:GLU:HB2	2.54	0.42
1:B:9:LYS:HE2	4:B:450:HOH:O	2.20	0.42
1:A:119:ARG:HH22	1:A:121:ARG:HD3	1.85	0.42
1:B:17:LEU:HD21	1:B:35:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:52:SER:O	1:B:55:HIS:HB3	2.20	0.42
1:A:2:SER:CB	4:A:487:HOH:O	2.65	0.41
1:A:155:GLU:HA	1:A:156:PRO:HD3	1.97	0.40
1:A:163:ARG:O	1:A:167:GLU:HG3	2.21	0.40
1:A:106:ARG:HD3	4:A:325:HOH:O	2.21	0.40
1:A:5:ILE:HD12	1:A:9:LYS:NZ	2.37	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	Distance(Å)	Clash(Å)
1:B:202:ARG:NH1	4:A:369:HOH:O[3_655]	1.55	0.65
1:B:202:ARG:CZ	4:A:369:HOH:O[3_655]	1.78	0.42
1:B:202:ARG:NH2	4:A:510:HOH:O[3_655]	1.99	0.21
4:A:718:HOH:O	4:B:331:HOH:O[3_545]	2.02	0.18
1:B:202:ARG:NH2	4:A:369:HOH:O[3_655]	2.04	0.16

## 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	262/298 (88%)	256 (98%)	6 (2%)	0	100	100
1	B	262/298 (88%)	259 (99%)	3 (1%)	0	100	100
All	All	524/596 (88%)	515 (98%)	9 (2%)	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	229/259 (88%)	220 (96%)	9 (4%)	43	23
1	B	229/259 (88%)	218 (95%)	11 (5%)	35	15
All	All	458/518 (88%)	438 (96%)	20 (4%)	40	18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	29	THR
1	A	48	ILE
1	A	112	LYS
1	A	161	LEU
1	A	182	THR
1	A	197	LEU
1	A	215	GLU
1	A	236	ASP
1	B	5	ILE
1	B	29	THR
1	B	48	ILE
1	B	51	GLU
1	B	58	ASP
1	B	175	ASN
1	B	182	THR
1	B	197	LEU
1	B	206	ARG
1	B	215	GLU
1	B	240	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	175	ASN
1	A	207	ASN
1	B	55	HIS
1	B	75	ASN
1	B	81	GLN
1	B	86	GLN
1	B	175	ASN
1	B	207	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 2 are 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$
2	GLU	A	302[A]	-	9,9,9	1.21	1 (11%)	11,11,11	1.00	1 (9%)
2	GLU	A	302[B]	-	9,9,9	1.22	1 (11%)	11,11,11	1.14	0
2	GLU	B	302[A]	-	9,9,9	1.22	1 (11%)	11,11,11	1.58	1 (9%)
2	GLU	B	302[B]	-	9,9,9	1.10	1 (11%)	11,11,11	1.28	1 (9%)

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
2	GLU	A	302[A]	-	-	0/9/9/9	0/0/0/0
2	GLU	A	302[B]	-	-	0/9/9/9	0/0/0/0
2	GLU	B	302[A]	-	-	0/9/9/9	0/0/0/0
2	GLU	B	302[B]	-	-	0/9/9/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302[B]	GLU	OXT-C	-2.35	1.21	1.30
2	A	302[A]	GLU	CB-CG	-2.20	1.45	1.52
2	B	302[A]	GLU	CB-CG	-2.16	1.45	1.52
2	B	302[B]	GLU	CB-CG	-2.07	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302[A]	GLU	C-CA-N	3.88	115.78	109.36
2	B	302[B]	GLU	OXT-C-CA	2.52	122.53	116.88
2	A	302[A]	GLU	C-CA-N	2.21	113.02	109.36

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/298 (88%)	-0.11	2 (0%) 83 81	17, 26, 40, 46	0
1	B	264/298 (88%)	-0.16	7 (2%) 52 44	14, 23, 38, 50	0
All	All	528/596 (88%)	-0.13	9 (1%) 67 62	14, 24, 39, 50	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	ILE	3.6
1	B	5	ILE	3.5
1	B	6	TYR	3.1
1	A	265	PRO	2.6
1	B	23	HIS	2.5
1	B	55	HIS	2.3
1	B	7	TRP	2.3
1	B	2	SER	2.1
1	A	12	ARG	2.0

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

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

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	NA	B	299	1/1	0.12	4.41	20,20,20,20	0
2	GLU	B	302[A]	10/10	0.15	2.97	20,23,24,25	10
2	GLU	B	302[B]	10/10	0.15	2.92	19,24,25,26	10
2	GLU	A	302[A]	10/10	0.15	1.75	26,28,30,32	10
2	GLU	A	302[B]	10/10	0.15	1.75	20,24,27,29	10
3	NA	A	299	1/1	0.14	0.75	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.