



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:14 PM GMT

PDB ID : 1GQ3  
Title : STRUCTURE OF THE R105A MUTANT CATALYTIC TRIMER OF  
ESCHERICHIA COLI ASPARTATE TRANSCARBAMOYLASE AT 2.0-Å  
RESOLUTION  
Authors : Beernink, P.T.; Endrizzi, J.A.; Alber, T.; Schachman, H.K.  
Deposited on : 2001-11-19  
Resolution : 2.01 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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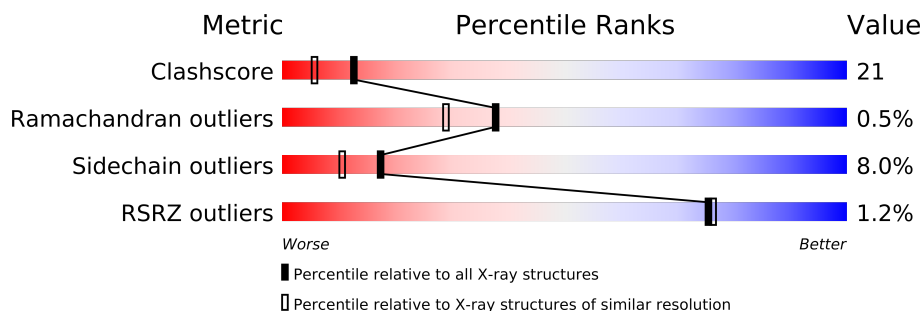
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.01 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	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  $\geq 3$ , 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	310	
1	B	310	
1	C	310	

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	CA	C	1310	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7331 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 ASPARTATE CARBAMOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2294	1455	399	431	9			
1	B	283	Total	C	N	O	S	0	0	0
			2184	1383	381	411	9			
1	C	308	Total	C	N	O	S	0	0	0
			2395	1515	418	453	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	ARG	ENGINEERED	UNP P00479
B	105	ALA	ARG	ENGINEERED	UNP P00479
C	105	ALA	ARG	ENGINEERED	UNP P00479

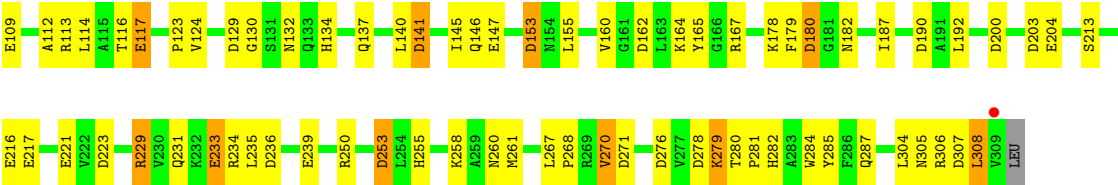
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	125	Total	O	0	0
			125	125		
3	C	204	Total	O	0	0
			204	204		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.03Å 81.10Å 211.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.29 – 2.01 18.29 – 2.01	Depositor EDS
% Data completeness (in resolution range)	89.8 (18.29-2.01) 88.8 (18.29-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	55.12 (at 2.00Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.195 , 0.281 0.192 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 97.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 57660 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: CA

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	13/2338 (0.6%)	1.15	36/3173 (1.1%)
1	B	0.74	6/2225 (0.3%)	1.10	35/3023 (1.2%)
1	C	0.79	11/2441 (0.5%)	1.14	39/3314 (1.2%)
All	All	0.78	30/7004 (0.4%)	1.13	110/9510 (1.2%)

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	1	0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	GLU	CD-OE2	6.24	1.32	1.25
1	B	50	GLU	CD-OE2	6.24	1.32	1.25
1	A	272	GLU	CD-OE2	6.19	1.32	1.25
1	A	86	GLU	CD-OE2	6.10	1.32	1.25
1	C	221	GLU	CD-OE2	5.96	1.32	1.25
1	A	60	GLU	CD-OE2	5.91	1.32	1.25
1	A	239	GLU	CD-OE2	5.91	1.32	1.25
1	A	37	GLU	CD-OE2	5.84	1.32	1.25
1	A	204	GLU	CD-OE2	5.78	1.32	1.25
1	A	117	GLU	CD-OE2	5.78	1.32	1.25
1	A	50	GLU	CD-OE2	5.75	1.31	1.25
1	C	109	GLU	CD-OE2	5.73	1.31	1.25
1	B	216	GLU	CD-OE2	5.73	1.31	1.25
1	C	60	GLU	CD-OE2	5.72	1.31	1.25
1	B	204	GLU	CD-OE2	5.72	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	GLU	CD-OE2	5.66	1.31	1.25
1	B	37	GLU	CD-OE2	5.64	1.31	1.25
1	A	147	GLU	CD-OE2	5.55	1.31	1.25
1	C	86	GLU	CD-OE2	5.49	1.31	1.25
1	B	221	GLU	CD-OE2	5.49	1.31	1.25
1	C	204	GLU	CD-OE2	5.45	1.31	1.25
1	A	217	GLU	CD-OE2	5.45	1.31	1.25
1	B	117	GLU	CD-OE2	5.43	1.31	1.25
1	C	117	GLU	CD-OE2	5.38	1.31	1.25
1	C	147	GLU	CD-OE2	5.36	1.31	1.25
1	A	221	GLU	CD-OE2	5.33	1.31	1.25
1	A	109	GLU	CD-OE2	5.29	1.31	1.25
1	C	216	GLU	CD-OE1	-5.14	1.20	1.25
1	C	233	GLU	CD-OE2	5.12	1.31	1.25
1	A	233	GLU	CD-OE2	5.04	1.31	1.25

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ASP	CB-CG-OD2	-12.01	107.49	118.30
1	B	153	ASP	CB-CG-OD1	8.92	126.33	118.30
1	C	307	ASP	CB-CG-OD2	-7.39	111.64	118.30
1	C	236	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	B	17	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	250	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	18	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	B	200	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	C	75	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	203	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	236	ASP	CB-CG-OD1	6.74	124.37	118.30
1	C	75	ASP	CB-CG-OD1	6.70	124.33	118.30
1	C	253	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	14	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	200	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	223	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	153	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	180	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	223	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	141	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	100	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	B	19	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	153	ASP	CB-CG-OD2	-6.37	112.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	203	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	18	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	14	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	18	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	271	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	276	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	153	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	162	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	75	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	278	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	14	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	19	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	141	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	190	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	18	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	296	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	153	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	141	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	278	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	19	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	190	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	19	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	100	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	253	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	271	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	C	180	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	190	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	129	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	B	190	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	236	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	153	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	278	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	278	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	129	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	180	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	203	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	253	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	14	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	162	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	C	203	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	276	ASP	CB-CG-OD2	-5.62	113.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	100	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	180	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	75	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	276	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	18	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	271	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	19	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	141	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	271	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	90	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	14	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	113	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	253	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	141	ASP	CB-CG-OD1	5.39	123.16	118.30
1	B	129	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	200	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	276	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	307	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	100	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	236	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	190	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	200	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	271	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	180	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	190	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	18	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	276	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	223	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	200	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	162	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	276	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	75	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	223	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	141	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	180	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	203	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	271	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	162	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	229	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	90	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	253	ASP	CB-CG-OD1	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	203	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	306	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	168	THR	CB

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	2294	0	2292	104	0
1	B	2184	0	2171	107	0
1	C	2395	0	2395	80	0
2	C	1	0	0	0	0
3	A	128	0	0	5	0
3	B	125	0	0	8	0
3	C	204	0	0	15	0
All	All	7331	0	6858	287	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 21.

All (287) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:THR:HG22	1:A:282:HIS:H	1.21	1.04
1:B:8:HIS:HD2	1:B:124:VAL:H	1.06	1.00
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.32	0.92
1:A:219:MET:HB3	1:A:256:ASN:HD21	1.35	0.92
1:A:280:THR:HG23	1:A:281:PRO:HD2	1.54	0.87
1:C:8:HIS:HD2	1:C:124:VAL:H	1.21	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:THR:HG22	1:A:282:HIS:N	1.94	0.82
1:C:8:HIS:CD2	1:C:124:VAL:H	1.98	0.81
1:B:8:HIS:CD2	1:B:124:VAL:H	1.96	0.81
1:A:233:GLU:OE2	1:A:234:ARG:HD3	1.82	0.80
1:A:134:HIS:HB2	1:A:135:PRO:HD2	1.65	0.78
1:A:280:THR:CG2	1:A:282:HIS:H	1.97	0.78
1:B:7:LYS:CE	1:B:7:LYS:HA	2.12	0.78
1:B:133:GLN:CD	1:B:167:ARG:HB3	2.03	0.78
1:A:106:HIS:ND1	1:A:107:PRO:HD2	1.98	0.78
1:B:160:VAL:HG21	1:B:225:LEU:HD11	1.63	0.77
1:B:276:ASP:HA	1:B:279:LYS:HE3	1.64	0.77
1:C:255:HIS:HB3	3:C:2167:HOH:O	1.85	0.77
1:A:31:LYS:NZ	1:A:291:ASN:HD21	1.83	0.76
1:B:106:HIS:ND1	1:B:107:PRO:HD2	2.01	0.75
1:A:189:PRO:HG2	1:A:192:LEU:HD12	1.68	0.75
1:A:2:ASN:HB3	1:A:306:ARG:O	1.87	0.75
1:B:249:LEU:HD11	1:B:254:LEU:HD21	1.69	0.74
1:A:200:ASP:HA	3:A:2083:HOH:O	1.85	0.74
1:A:8:HIS:CD2	1:A:124:VAL:H	2.06	0.73
1:A:219:MET:HB3	1:A:256:ASN:ND2	2.02	0.73
1:A:199:LEU:HD11	3:A:2081:HOH:O	1.88	0.73
1:C:155:LEU:H	1:C:182:ASN:HD22	1.37	0.72
1:C:153:ASP:OD1	1:C:179:PHE:HB3	1.88	0.72
1:C:280:THR:HB	1:C:281:PRO:HD2	1.72	0.72
1:B:146:GLN:NE2	1:B:151:ARG:HA	2.04	0.72
1:A:114:LEU:HD11	1:A:118:PHE:HE2	1.52	0.72
1:B:167:ARG:NH1	1:B:170:HIS:HD2	1.88	0.71
1:B:7:LYS:HA	1:B:7:LYS:HE2	1.71	0.71
1:B:292:GLY:O	1:B:296:ARG:HG3	1.91	0.70
1:A:106:HIS:HE1	1:A:108:GLN:HG3	1.57	0.70
1:C:235:LEU:HD12	1:C:239:GLU:CB	2.22	0.69
1:B:158:ALA:HB2	1:B:222:VAL:HG11	1.73	0.69
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.28	0.69
1:A:170:HIS:O	1:A:174:GLN:HG3	1.91	0.69
1:B:254:LEU:HD23	1:B:254:LEU:N	2.07	0.68
1:A:51:ALA:HB2	1:A:75:ASP:HB2	1.76	0.68
1:B:59:PHE:O	1:B:63:MET:HG3	1.93	0.68
1:C:279:LYS:HG2	3:C:2185:HOH:O	1.93	0.68
1:A:216:GLU:H	1:A:216:GLU:CD	1.95	0.67
1:B:214:SER:OG	1:B:216:GLU:HG2	1.95	0.67
1:C:235:LEU:HD12	1:C:239:GLU:HB2	1.75	0.67
1:B:205:LYS:HB2	1:B:207:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:12:ILE:O	1:C:178:LYS:NZ	2.28	0.66
1:C:279:LYS:HD2	3:C:2190:HOH:O	1.96	0.66
1:B:276:ASP:HA	1:B:279:LYS:CE	2.26	0.66
1:A:239:GLU:OE2	1:A:239:GLU:HA	1.97	0.65
1:C:8:HIS:CD2	1:C:123:PRO:HA	2.32	0.65
1:A:194:MET:SD	1:A:195:PRO:HD2	2.37	0.65
1:B:183:ARG:NH1	1:B:184:PHE:O	2.30	0.65
1:B:7:LYS:NZ	1:B:8:HIS:H	1.94	0.65
1:C:54:ARG:HB3	3:C:2049:HOH:O	1.96	0.65
1:C:38:LEU:HD11	1:C:305:ASN:ND2	2.11	0.64
1:C:35:GLN:NE2	3:C:2031:HOH:O	2.30	0.64
1:B:106:HIS:HB3	1:B:111:ALA:HB3	1.80	0.64
1:A:8:HIS:HD2	1:A:124:VAL:H	1.45	0.64
1:A:239:GLU:O	1:A:243:VAL:HG13	1.97	0.63
1:B:216:GLU:CD	1:B:216:GLU:H	2.01	0.63
1:B:205:LYS:CB	1:B:207:ILE:HD12	2.28	0.63
1:B:54:ARG:HG3	1:C:94:VAL:HG11	1.80	0.63
1:B:33:ASN:HB3	3:B:2020:HOH:O	1.99	0.62
1:A:250:ARG:HG3	1:A:250:ARG:NH1	2.05	0.62
1:A:250:ARG:HH11	1:A:250:ARG:CG	2.09	0.62
1:A:7:LYS:NZ	3:A:2002:HOH:O	2.29	0.62
1:B:106:HIS:CG	1:B:107:PRO:HD2	2.35	0.62
1:C:155:LEU:H	1:C:182:ASN:ND2	1.97	0.62
1:B:106:HIS:CE1	1:B:108:GLN:HG3	2.34	0.61
1:C:2:ASN:HB2	1:C:308:LEU:HD13	1.81	0.61
1:C:54:ARG:HG3	1:C:55:THR:N	2.14	0.61
1:C:7:LYS:HD3	3:C:2004:HOH:O	2.01	0.61
1:A:31:LYS:HZ2	1:A:291:ASN:HD21	1.47	0.60
1:A:146:GLN:HE21	1:A:151:ARG:HA	1.66	0.60
1:A:98:TYR:CZ	1:C:58:SER:HB2	2.37	0.60
1:A:106:HIS:CE1	1:A:108:GLN:HG3	2.36	0.60
1:B:183:ARG:HH12	1:B:210:SER:N	2.00	0.60
1:C:15:LEU:O	1:C:178:LYS:NZ	2.28	0.60
1:A:243:VAL:O	1:A:246:GLN:HG3	2.01	0.59
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.66	0.59
1:B:133:GLN:OE1	1:B:167:ARG:HB3	2.00	0.59
1:B:164:LYS:HD3	1:B:165:TYR:CE1	2.38	0.59
1:A:168:THR:HB	3:A:2069:HOH:O	2.02	0.58
1:B:160:VAL:CG2	1:B:225:LEU:HD11	2.30	0.58
1:A:114:LEU:HD11	1:A:118:PHE:CE2	2.36	0.58
1:A:167:ARG:HB3	1:A:167:ARG:NH1	2.18	0.58
1:A:136:THR:HG22	1:A:299:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:165:TYR:HE2	1:C:235:LEU:HD13	1.67	0.58
1:A:29:LYS:HD2	1:A:29:LYS:O	2.02	0.58
1:C:134:HIS:HD2	3:C:2110:HOH:O	1.86	0.58
1:B:146:GLN:HE21	1:B:151:ARG:HA	1.69	0.58
1:B:163:LEU:O	1:B:170:HIS:HE1	1.86	0.58
1:C:75:ASP:HB3	1:C:78:ASN:ND2	2.19	0.58
1:B:253:ASP:C	1:B:254:LEU:HD23	2.24	0.57
1:C:8:HIS:HD2	1:C:124:VAL:N	1.99	0.57
1:A:214:SER:HB2	1:A:216:GLU:OE1	2.04	0.57
1:A:233:GLU:CG	1:A:234:ARG:HH11	2.18	0.57
1:A:8:HIS:CD2	1:A:116:THR:HG22	2.39	0.57
1:A:114:LEU:CD1	1:A:118:PHE:HE2	2.17	0.57
1:C:279:LYS:HE2	3:C:2185:HOH:O	2.04	0.57
1:B:274:ALA:O	1:B:277:VAL:HG23	2.04	0.56
1:B:183:ARG:NH2	1:B:210:SER:OG	2.30	0.56
1:A:261:MET:O	1:A:282:HIS:HD2	1.88	0.56
1:C:261:MET:O	1:C:282:HIS:HD2	1.88	0.56
1:C:229:ARG:HG3	1:C:270:VAL:HG23	1.85	0.56
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.87	0.56
1:A:153:ASP:HB2	1:A:180:ASP:O	2.06	0.56
1:A:232:LYS:NZ	1:A:237:PRO:HA	2.20	0.56
1:A:280:THR:HG23	1:A:281:PRO:CD	2.29	0.56
1:B:218:VAL:HG23	1:B:222:VAL:HG13	1.88	0.56
1:A:232:LYS:HZ1	1:A:237:PRO:HA	1.72	0.55
1:A:134:HIS:HB2	1:A:135:PRO:CD	2.34	0.55
1:C:231:GLN:O	1:C:235:LEU:HD23	2.06	0.55
1:A:284:TRP:HA	1:A:287:GLN:OE1	2.06	0.55
1:B:199:LEU:HD11	3:B:2094:HOH:O	2.06	0.55
1:A:140:LEU:HD12	1:A:140:LEU:C	2.26	0.55
1:B:167:ARG:HG3	1:B:167:ARG:NH1	2.21	0.55
1:A:50:GLU:O	1:A:50:GLU:HG3	2.06	0.55
1:B:156:HIS:HB3	1:B:185:TYR:HE1	1.71	0.55
1:B:106:HIS:HB3	1:B:111:ALA:CB	2.37	0.54
1:C:250:ARG:O	1:C:253:ASP:HB2	2.07	0.54
1:A:31:LYS:HG3	1:A:294:PHE:CE2	2.42	0.54
1:C:50:GLU:HA	3:C:2044:HOH:O	2.07	0.54
1:C:35:GLN:NE2	1:C:38:LEU:HD13	2.22	0.54
1:B:8:HIS:HD2	1:B:124:VAL:N	1.90	0.54
1:B:12:ILE:O	1:B:15:LEU:HB2	2.08	0.53
1:A:233:GLU:HG3	1:A:234:ARG:HH11	1.73	0.53
1:B:134:HIS:HB2	1:B:135:PRO:HD2	1.91	0.53
1:B:29:LYS:HE2	3:B:2016:HOH:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:LEU:CD2	1:A:261:MET:HE3	2.38	0.53
1:C:260:ASN:H	1:C:260:ASN:HD22	1.56	0.53
1:C:235:LEU:HD12	1:C:239:GLU:HB3	1.90	0.53
1:B:146:GLN:HE21	1:B:151:ARG:CA	2.22	0.53
1:B:31:LYS:HD2	1:B:294:PHE:CD2	2.44	0.53
1:C:114:LEU:O	1:C:117:GLU:HB2	2.09	0.53
1:C:2:ASN:HB2	1:C:308:LEU:CD1	2.39	0.53
1:A:243:VAL:HA	1:A:246:GLN:HE21	1.74	0.52
1:A:12:ILE:O	1:A:15:LEU:HB2	2.09	0.52
1:B:4:LEU:HD12	1:B:302:LEU:HD13	1.90	0.52
1:B:183:ARG:NH1	1:B:210:SER:N	2.58	0.52
1:A:230:VAL:HG12	1:A:230:VAL:O	2.09	0.51
1:A:232:LYS:HA	1:A:240:TYR:CE1	2.46	0.51
1:C:192:LEU:HD21	1:C:235:LEU:HD11	1.93	0.51
1:A:31:LYS:HZ1	1:A:291:ASN:HD21	1.55	0.51
1:C:165:TYR:CD2	1:C:235:LEU:HD22	2.46	0.51
1:B:229:ARG:HA	3:B:2106:HOH:O	2.09	0.51
1:B:220:ALA:N	3:B:2102:HOH:O	2.42	0.51
1:A:232:LYS:HA	1:A:240:TYR:CD1	2.46	0.51
1:C:8:HIS:HD2	1:C:123:PRO:HA	1.75	0.50
1:B:125:LEU:N	1:B:125:LEU:HD12	2.26	0.50
1:B:247:PHE:C	1:B:248:VAL:HG12	2.31	0.50
1:C:267:LEU:HB3	1:C:268:PRO:HA	1.92	0.50
1:A:31:LYS:NZ	1:A:147:GLU:OE1	2.45	0.50
1:A:167:ARG:HB3	1:A:167:ARG:HH11	1.77	0.50
1:A:48:PHE:HB2	1:A:74:SER:HA	1.94	0.50
1:A:8:HIS:HD2	1:A:124:VAL:N	2.10	0.49
1:B:214:SER:HB2	1:B:216:GLU:OE1	2.11	0.49
1:A:232:LYS:HE3	1:A:237:PRO:N	2.27	0.49
1:A:8:HIS:CD2	1:A:124:VAL:N	2.79	0.49
1:A:31:LYS:HZ2	1:A:291:ASN:ND2	2.10	0.49
1:C:108:GLN:NE2	1:C:108:GLN:HA	2.28	0.49
1:C:37:GLU:O	1:C:38:LEU:C	2.50	0.48
1:C:235:LEU:HD13	1:C:239:GLU:OE1	2.13	0.48
1:C:304:LEU:HD22	3:C:2002:HOH:O	2.13	0.48
1:C:17:ARG:NE	3:C:2128:HOH:O	2.46	0.48
1:B:12:ILE:HD12	1:B:15:LEU:HD22	1.96	0.48
1:B:114:LEU:O	1:B:117:GLU:HB2	2.14	0.48
1:B:191:ALA:C	1:B:192:LEU:HD23	2.33	0.48
1:B:39:LEU:HB3	1:B:42:LYS:HG3	1.95	0.48
1:B:7:LYS:HZ3	1:B:8:HIS:H	1.60	0.48
1:A:6:GLN:HA	1:A:123:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:MET:HE3	1:A:254:LEU:HD23	1.96	0.47
1:A:13:ASN:C	1:A:15:LEU:H	2.17	0.47
1:A:106:HIS:CE1	1:A:107:PRO:HD2	2.49	0.47
1:C:59:PHE:O	1:C:63:MET:HG3	2.14	0.47
1:C:231:GLN:HB3	1:C:234:ARG:HG3	1.95	0.47
1:C:75:ASP:HB3	1:C:78:ASN:HD21	1.79	0.47
1:B:8:HIS:CD2	1:B:123:PRO:HA	2.50	0.47
1:B:160:VAL:HG13	1:B:187:ILE:HB	1.96	0.47
1:A:158:ALA:HB3	1:A:225:LEU:HD12	1.96	0.47
1:A:214:SER:OG	1:A:217:GLU:HG2	2.14	0.46
1:A:232:LYS:HD3	1:A:240:TYR:CD1	2.50	0.46
1:B:189:PRO:O	1:B:192:LEU:N	2.44	0.46
1:A:233:GLU:CG	1:A:234:ARG:NH1	2.79	0.46
1:C:153:ASP:OD1	1:C:180:ASP:N	2.29	0.46
1:C:112:ALA:O	1:C:116:THR:HG23	2.16	0.46
1:A:232:LYS:HE3	1:A:237:PRO:HA	1.97	0.46
1:A:8:HIS:HD2	1:A:124:VAL:HB	1.81	0.46
1:B:54:ARG:NH1	3:B:2028:HOH:O	2.48	0.46
1:C:281:PRO:HD2	3:C:2194:HOH:O	2.15	0.46
1:B:184:PHE:O	1:B:209:TRP:HA	2.16	0.46
1:B:154:ASN:HA	1:B:181:GLY:O	2.16	0.46
1:A:232:LYS:O	1:A:233:GLU:C	2.54	0.46
1:C:130:GLY:O	1:C:167:ARG:HD3	2.16	0.46
1:A:219:MET:CE	1:A:254:LEU:HD23	2.46	0.45
1:B:167:ARG:HA	1:B:170:HIS:CD2	2.51	0.45
1:B:174:GLN:HG2	1:B:201:MET:HE2	1.98	0.45
1:B:186:PHE:CE1	1:B:194:MET:HE2	2.51	0.45
1:C:35:GLN:HE22	1:C:38:LEU:HD13	1.81	0.45
1:C:93:SER:O	1:C:96:SER:OG	2.29	0.45
1:A:163:LEU:O	1:A:170:HIS:NE2	2.49	0.45
1:C:35:GLN:HE21	1:C:35:GLN:HB3	1.48	0.45
1:A:164:LYS:HB2	1:A:193:ALA:O	2.17	0.45
1:A:266:PRO:O	1:A:267:LEU:HB2	2.16	0.45
1:A:232:LYS:CE	1:A:237:PRO:HA	2.48	0.44
1:A:305:ASN:O	1:A:306:ARG:C	2.54	0.44
1:C:50:GLU:HB2	1:C:107:PRO:HD3	1.99	0.44
1:C:141:ASP:O	1:C:145:ILE:HG13	2.17	0.44
1:A:232:LYS:HE3	1:A:237:PRO:CA	2.48	0.44
1:C:164:LYS:NZ	1:C:239:GLU:OE2	2.51	0.44
1:B:183:ARG:HH11	1:B:209:TRP:HA	1.82	0.44
1:A:31:LYS:HG3	1:A:294:PHE:CD2	2.53	0.44
1:C:280:THR:HB	1:C:281:PRO:CD	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:ALA:HB2	1:B:304:LEU:HD21	2.00	0.44
1:B:146:GLN:NE2	1:B:151:ARG:CA	2.78	0.43
1:B:167:ARG:O	1:B:170:HIS:HB2	2.18	0.43
1:B:186:PHE:CE1	1:B:194:MET:CE	3.01	0.43
1:B:255:HIS:ND1	1:B:255:HIS:N	2.66	0.43
1:C:61:THR:O	1:C:65:ARG:HG2	2.19	0.43
1:C:8:HIS:HE1	3:C:2101:HOH:O	2.01	0.43
1:B:167:ARG:HD2	1:B:167:ARG:HA	1.77	0.43
1:A:150:GLY:O	1:A:151:ARG:HB3	2.18	0.43
1:B:15:LEU:HA	1:B:15:LEU:HD12	1.72	0.43
1:B:31:LYS:HD2	1:B:294:PHE:CE2	2.54	0.43
1:A:219:MET:HG2	1:A:253:ASP:O	2.19	0.43
1:B:13:ASN:C	1:B:15:LEU:H	2.20	0.43
1:C:258:LYS:HB3	1:C:260:ASN:ND2	2.33	0.43
1:B:205:LYS:HB3	1:B:207:ILE:CD1	2.49	0.43
1:A:53:THR:N	1:B:80:SER:OG	2.46	0.43
1:A:12:ILE:HG23	1:A:13:ASN:N	2.34	0.43
1:B:194:MET:HG3	1:B:195:PRO:HD2	2.01	0.43
1:C:5:TYR:CD1	1:C:306:ARG:HA	2.54	0.42
1:B:106:HIS:CE1	1:B:107:PRO:HD2	2.52	0.42
1:C:260:ASN:H	1:C:260:ASN:ND2	2.17	0.42
1:B:218:VAL:HG23	1:B:222:VAL:CG1	2.50	0.42
1:C:38:LEU:CD1	1:C:305:ASN:ND2	2.80	0.42
1:B:194:MET:SD	1:B:195:PRO:HD2	2.59	0.42
1:B:108:GLN:HB3	1:B:108:GLN:HE21	1.74	0.42
1:C:17:ARG:NH2	3:C:2128:HOH:O	2.51	0.42
1:A:219:MET:SD	1:A:261:MET:HE3	2.58	0.42
1:B:136:THR:OG1	1:B:296:ARG:NE	2.47	0.42
1:B:261:MET:O	1:B:262:LYS:HD3	2.20	0.42
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.53	0.42
1:B:215:ILE:CG2	1:B:219:MET:CE	2.98	0.42
1:C:160:VAL:HG22	1:C:187:ILE:HB	2.02	0.42
1:B:162:ASP:CG	1:B:192:LEU:HD13	2.40	0.42
1:C:229:ARG:NH2	1:C:233:GLU:OE2	2.53	0.42
1:B:75:ASP:O	1:B:78:ASN:OD1	2.38	0.42
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.49	0.42
1:B:106:HIS:ND1	1:B:107:PRO:CD	2.79	0.42
1:A:154:ASN:ND2	1:A:180:ASP:O	2.53	0.41
1:B:166:GLY:O	1:B:169:VAL:HG22	2.20	0.41
1:B:273:ILE:HG23	1:B:277:VAL:HG21	2.02	0.41
1:B:48:PHE:CD2	1:B:105:ALA:HB3	2.55	0.41
1:C:84:LYS:NZ	3:C:2072:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:165:TYR:CE2	1:C:235:LEU:HD13	2.50	0.41
1:A:53:THR:OG1	1:B:79:THR:HB	2.20	0.41
1:B:5:TYR:CD1	1:B:6:GLN:HG2	2.56	0.41
1:A:143:PHE:HD1	1:A:291:ASN:HB3	1.86	0.41
1:A:243:VAL:HA	1:A:246:GLN:NE2	2.35	0.41
1:B:12:ILE:HD12	1:B:15:LEU:CD2	2.51	0.41
1:A:280:THR:CG2	1:A:281:PRO:N	2.82	0.41
1:C:98:TYR:HB2	1:C:99:VAL:HG13	2.01	0.41
1:B:220:ALA:HB3	3:B:2102:HOH:O	2.21	0.41
1:B:291:ASN:HA	1:B:291:ASN:HD22	1.61	0.41
1:A:192:LEU:HD11	1:A:234:ARG:HB3	2.02	0.41
1:B:167:ARG:HD2	1:B:170:HIS:CD2	2.56	0.41
1:C:229:ARG:HH22	1:C:233:GLU:CD	2.24	0.41
1:A:153:ASP:OD1	1:A:154:ASN:ND2	2.53	0.41
1:B:132:ASN:HA	3:B:2068:HOH:O	2.21	0.41
1:B:7:LYS:HZ1	1:B:8:HIS:H	1.65	0.41
1:C:233:GLU:CD	1:C:233:GLU:H	2.22	0.41
1:A:4:LEU:HA	1:A:4:LEU:HD12	1.76	0.41
1:A:262:LYS:HE3	3:A:2104:HOH:O	2.21	0.41
1:C:8:HIS:CE1	1:C:116:THR:HB	2.56	0.40
1:A:164:LYS:HD3	1:A:165:TYR:CE1	2.57	0.40
1:B:167:ARG:HH11	1:B:170:HIS:HD2	1.65	0.40
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.82	0.40
1:B:264:LEU:N	1:B:264:LEU:HD23	2.36	0.40
1:C:54:ARG:HH21	1:C:137:GLN:NE2	2.19	0.40
1:B:263:VAL:C	1:B:264:LEU:HD23	2.41	0.40
1:C:284:TRP:CZ2	1:C:287:GLN:HG2	2.56	0.40
1:C:137:GLN:O	1:C:140:LEU:HG	2.22	0.40
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.82	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	288/310 (93%)	268 (93%)	20 (7%)	0	100	100
1	B	277/310 (89%)	256 (92%)	19 (7%)	2 (1%)	30	20
1	C	306/310 (99%)	294 (96%)	10 (3%)	2 (1%)	30	20
All	All	871/930 (94%)	818 (94%)	49 (6%)	4 (0%)	38	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	VAL
1	C	270	VAL
1	B	167	ARG
1	C	132	ASN

### 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	247/260 (95%)	224 (91%)	23 (9%)	13	7
1	B	235/260 (90%)	210 (89%)	25 (11%)	10	5
1	C	259/260 (100%)	248 (96%)	11 (4%)	40	34
All	All	741/780 (95%)	682 (92%)	59 (8%)	17	10

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	LEU
1	A	11	SER
1	A	14	ASP
1	A	16	SER
1	A	29	LYS
1	A	59	PHE
1	A	146	GLN
1	A	168	THR
1	A	171	SER
1	A	194	MET

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Mol	Chain	Res	Type
1	A	232	LYS
1	A	233	GLU
1	A	235	LEU
1	A	236	ASP
1	A	239	GLU
1	A	244	LYS
1	A	246	GLN
1	A	250	ARG
1	A	261	MET
1	A	279	LYS
1	A	285	TYR
1	A	305	ASN
1	B	2	ASN
1	B	7	LYS
1	B	15	LEU
1	B	24	LEU
1	B	29	LYS
1	B	35	GLN
1	B	59	PHE
1	B	74	SER
1	B	80	SER
1	B	108	GLN
1	B	140	LEU
1	B	146	GLN
1	B	167	ARG
1	B	168	THR
1	B	187	ILE
1	B	190	ASP
1	B	218	VAL
1	B	227	MET
1	B	248	VAL
1	B	261	MET
1	B	269	ARG
1	B	270	VAL
1	B	278	ASP
1	B	279	LYS
1	B	285	TYR
1	C	11	SER
1	C	13	ASN
1	C	35	GLN
1	C	59	PHE
1	C	78	ASN

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Mol	Chain	Res	Type
1	C	79	THR
1	C	146	GLN
1	C	213	SER
1	C	279	LYS
1	C	285	TYR
1	C	308	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	13	ASN
1	A	21	ASN
1	A	35	GLN
1	A	146	GLN
1	A	154	ASN
1	A	174	GLN
1	A	231	GLN
1	A	246	GLN
1	A	260	ASN
1	A	282	HIS
1	A	291	ASN
1	B	8	HIS
1	B	108	GLN
1	B	132	ASN
1	B	146	GLN
1	B	170	HIS
1	B	291	ASN
1	C	8	HIS
1	C	13	ASN
1	C	35	GLN
1	C	78	ASN
1	C	132	ASN
1	C	133	GLN
1	C	134	HIS
1	C	137	GLN
1	C	174	GLN
1	C	182	ASN
1	C	260	ASN
1	C	282	HIS
1	C	305	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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	294/310 (94%)	-0.22	3 (1%) 79 80	15, 29, 63, 84	0
1	B	283/310 (91%)	-0.19	5 (1%) 65 66	15, 30, 63, 82	0
1	C	308/310 (99%)	-0.49	2 (0%) 86 88	13, 23, 48, 70	0
All	All	885/930 (95%)	-0.30	10 (1%) 75 78	13, 27, 59, 84	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	2.9
1	B	78	ASN	2.8
1	A	306	ARG	2.7
1	B	165	TYR	2.7
1	B	191	ALA	2.5
1	C	78	ASN	2.1
1	B	121	ASN	2.1
1	B	279	LYS	2.1
1	C	309	VAL	2.0
1	A	238	SER	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
2	CA	C	1310	1/1	0.28	8.53	1,1,1,1	0

## 6.5 Other polymers

There are no such residues in this entry.