



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:59 PM GMT

PDB ID : 1QB4  
Title : CRYSTAL STRUCTURE OF MN(2+)-BOUND PHOSPHOENOLPYRUVATE CARBOXYLASE  
Authors : Matsumura, H.; Terada, M.; Shirakata, S.; Inoue, T.; Yoshinaga, T.; Izui, K.; Kai, Y.  
Deposited on : 1999-04-30  
Resolution : 2.60 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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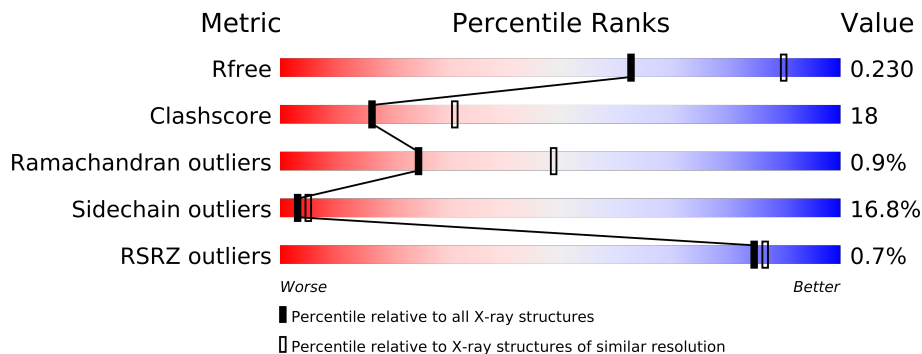
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	883	

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	MN	A	885	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6926 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.

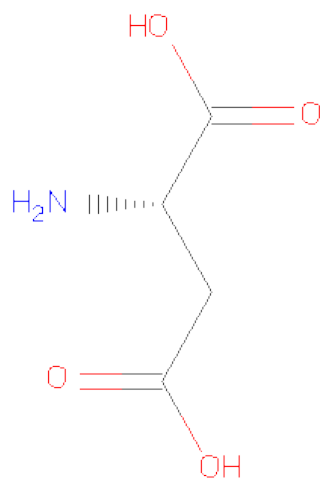
- Molecule 1 is a protein called PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	874	Total	C	N	O	S	0	0	1
			6835	4327	1194	1283	31			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is water.

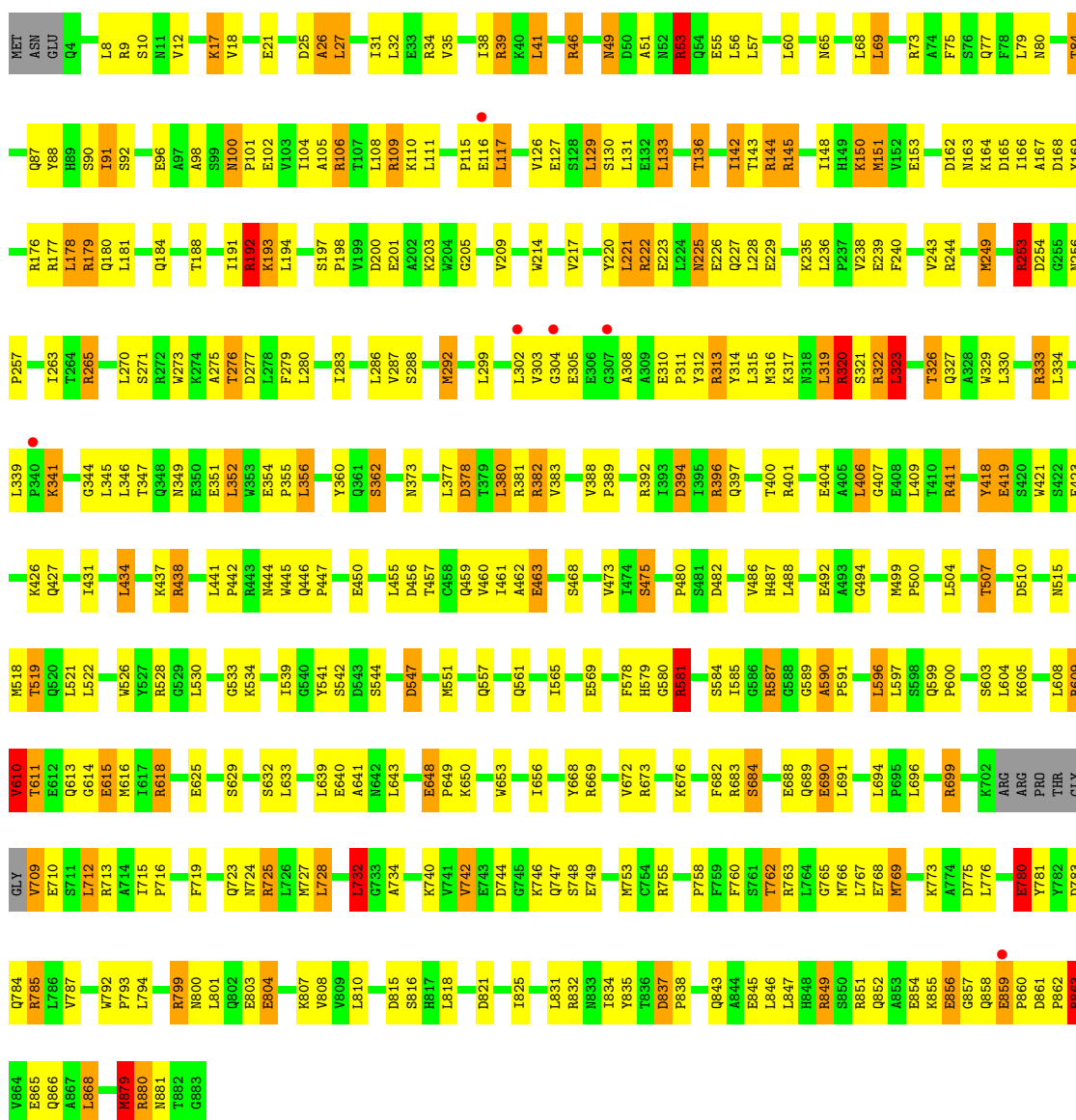
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total 81	O 81	0	0

### 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: PHOSPHOENOLPYRUVATE CARBOXYLASE

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.75Å 248.41Å 83.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 29.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-2.60) 90.7 (29.86-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.223 , 0.261 0.197 , 0.230	Depositor DCC
$R_{free}$ test set	1092 reflections (3.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	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	1 of 34596 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	1/6969 (0.0%)	1.70	114/9462 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	GLU	CD-OE2	5.26	1.31	1.25

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	ARG	CD-NE-CZ	24.13	157.38	123.60
1	A	618	ARG	CD-NE-CZ	19.76	151.27	123.60
1	A	699	ARG	NE-CZ-NH1	17.61	129.11	120.30
1	A	401	ARG	NE-CZ-NH2	14.96	127.78	120.30
1	A	396	ARG	CD-NE-CZ	12.39	140.95	123.60
1	A	763	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	A	799	ARG	NE-CZ-NH2	-11.21	114.70	120.30
1	A	713	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	A	177	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	253	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	837	ASP	CB-CG-OD2	10.78	128.00	118.30
1	A	394	ASP	CB-CG-OD2	-10.29	109.04	118.30
1	A	396	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	A	856	GLU	CA-CB-CG	10.12	135.67	113.40
1	A	438	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	A	392	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	9	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	A	253	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	A	581	ARG	NE-CZ-NH2	9.39	124.99	120.30
1	A	277	ASP	CB-CG-OD2	9.29	126.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	A	401	ARG	NE-CZ-NH1	-9.21	115.69	120.30
1	A	785	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	192	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	A	313	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	A	858	GLN	C-N-CA	8.74	143.56	121.70
1	A	192	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	A	755	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	53	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	A	9	ARG	CD-NE-CZ	8.02	134.83	123.60
1	A	482	ASP	CB-CG-OD2	7.97	125.47	118.30
1	A	856	GLU	N-CA-CB	-7.96	96.27	110.60
1	A	179	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	265	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	200	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	192	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	A	580	GLY	C-N-CA	7.57	140.62	121.70
1	A	438	ARG	CD-NE-CZ	7.53	134.15	123.60
1	A	179	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	609	ARG	CD-NE-CZ	7.28	133.80	123.60
1	A	145	ARG	CD-NE-CZ	7.26	133.76	123.60
1	A	699	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
1	A	46	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	683	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	880	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	176	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	129	LEU	CA-CB-CG	6.86	131.09	115.30
1	A	166	ILE	N-CA-CB	6.84	126.53	110.80
1	A	728	LEU	CA-CB-CG	6.80	130.93	115.30
1	A	320	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	590	ALA	CB-CA-C	6.46	119.79	110.10
1	A	177	ARG	CD-NE-CZ	6.46	132.64	123.60
1	A	323	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	382	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	419	GLU	CA-CB-CG	6.28	127.20	113.40
1	A	404	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	A	468	SER	CB-CA-C	-6.09	98.52	110.10
1	A	88	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	A	322	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	609	ARG	CG-CD-NE	-6.04	99.11	111.80
1	A	378	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	411	ARG	NE-CZ-NH1	-6.04	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	ARG	CD-NE-CZ	6.04	132.05	123.60
1	A	401	ARG	CD-NE-CZ	-6.03	115.16	123.60
1	A	394	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	725	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	835	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	456	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	222	ARG	CG-CD-NE	5.76	123.90	111.80
1	A	401	ARG	CG-CD-NE	5.75	123.87	111.80
1	A	650	LYS	CA-CB-CG	5.73	126.00	113.40
1	A	394	ASP	CA-CB-CG	5.71	125.97	113.40
1	A	780	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	A	411	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	A	879	MET	CG-SD-CE	5.67	109.27	100.20
1	A	39	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	131	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	856	GLU	CA-C-N	-5.62	104.97	116.20
1	A	265	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	A	851	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	734	ALA	CB-CA-C	5.57	118.45	110.10
1	A	803	GLU	CA-CB-CG	5.57	125.65	113.40
1	A	109	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	96	GLU	CB-CA-C	5.54	121.47	110.40
1	A	551	MET	CA-CB-CG	5.51	122.67	113.30
1	A	581	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	A	418	TYR	CB-CG-CD2	5.49	124.30	121.00
1	A	127	GLU	CA-CB-CG	5.47	125.43	113.40
1	A	849	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	129	LEU	CB-CA-C	-5.46	99.82	110.20
1	A	475	SER	CB-CA-C	5.46	120.46	110.10
1	A	732	LEU	C-N-CA	-5.44	110.87	122.30
1	A	411	ARG	N-CA-CB	5.43	120.38	110.60
1	A	803	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	547	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	744	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	763	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	863	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	244	ARG	CA-CB-CG	5.25	124.95	113.40
1	A	610	VAL	CB-CA-C	-5.22	101.47	111.40
1	A	96	GLU	O-C-N	-5.18	114.41	122.70
1	A	9	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	A	411	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	450	GLU	OE1-CD-OE2	-5.15	117.12	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	A	411	ARG	NH1-CZ-NH2	5.08	124.99	119.40
1	A	423	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	A	257	PRO	O-C-N	-5.07	114.59	122.70
1	A	541	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	A	760	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	A	352	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	669	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	A	785	ARG	CD-NE-CZ	5.01	130.62	123.60
1	A	725	ARG	CD-NE-CZ	5.01	130.61	123.60

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	6835	0	6833	248	0
2	A	1	0	0	0	0
3	A	9	0	3	2	0
4	A	81	0	0	3	0
All	All	6926	0	6836	248	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 18.

All (248) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:879:MET:HA	1:A:879:MET:CE	1.94	0.97
1:A:863:ARG:HG3	1:A:863:ARG:HH11	1.30	0.95
1:A:785:ARG:HH12	1:A:845:GLU:HG2	1.31	0.93
1:A:587:ARG:HB3	3:A:884:ASP:OXT	1.71	0.91
1:A:326:THR:HB	1:A:345:LEU:HD12	1.53	0.91
1:A:26:ALA:HB1	1:A:27:LEU:HD23	1.54	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:879:MET:HA	1:A:879:MET:HE3	1.54	0.89
1:A:49:ASN:HD22	1:A:51:ALA:H	1.21	0.88
1:A:84:THR:HG22	1:A:618:ARG:HH22	1.38	0.88
1:A:60:LEU:HB3	1:A:845:GLU:HG3	1.55	0.87
1:A:715:ILE:HB	1:A:716:PRO:HD3	1.57	0.87
1:A:53:ARG:HH21	1:A:781:TYR:HD1	1.24	0.86
1:A:776:LEU:HD22	1:A:799:ARG:HG2	1.60	0.83
1:A:126:VAL:HG12	1:A:236:LEU:HD21	1.62	0.81
1:A:68:LEU:HD11	1:A:849:ARG:HH11	1.45	0.81
1:A:378:ASP:O	1:A:382:ARG:HG3	1.81	0.80
1:A:526:TRP:CH2	1:A:530:LEU:HD22	2.16	0.80
1:A:507:THR:HG22	1:A:510:ASP:H	1.46	0.79
1:A:407:GLY:O	1:A:411:ARG:HD2	1.85	0.77
1:A:317:LYS:HG2	1:A:320:ARG:HH12	1.50	0.77
1:A:326:THR:HG21	1:A:346:LEU:H	1.50	0.75
1:A:49:ASN:ND2	1:A:51:ALA:H	1.85	0.74
1:A:68:LEU:HD22	1:A:846:LEU:HD21	1.69	0.74
1:A:837:ASP:HB3	1:A:838:PRO:HD3	1.67	0.74
1:A:287:VAL:O	1:A:313:ARG:HD3	1.90	0.72
1:A:863:ARG:HG3	1:A:863:ARG:NH1	2.01	0.72
1:A:585:ILE:HD13	1:A:596:LEU:HD12	1.74	0.70
1:A:236:LEU:HD13	1:A:240:PHE:CE2	2.28	0.68
1:A:299:LEU:HD11	1:A:315:LEU:HD11	1.74	0.68
1:A:715:ILE:HB	1:A:716:PRO:CD	2.24	0.67
1:A:126:VAL:CG1	1:A:236:LEU:HD21	2.25	0.67
1:A:329:TRP:CZ2	1:A:333:ARG:HD3	2.30	0.67
1:A:191:ILE:HG21	1:A:866:GLN:HG2	1.76	0.67
1:A:581:ARG:HG3	1:A:611:THR:HG21	1.77	0.66
1:A:80:ASN:O	1:A:84:THR:HG23	1.95	0.66
1:A:587:ARG:HD2	1:A:766:MET:SD	2.36	0.66
1:A:77:GLN:HA	1:A:77:GLN:NE2	2.11	0.65
1:A:672:VAL:HG13	1:A:709:VAL:HG11	1.77	0.65
1:A:21:GLU:HB3	1:A:179:ARG:HH21	1.60	0.65
1:A:303:VAL:HG13	1:A:314:TYR:CD1	2.33	0.64
1:A:613:GLN:HG2	1:A:616:MET:HB2	1.79	0.64
1:A:349:ASN:ND2	1:A:388:VAL:H	1.95	0.64
1:A:769:MET:HE3	1:A:881:ASN:O	1.97	0.64
1:A:515:ASN:O	1:A:519:THR:HG23	1.98	0.64
1:A:316:MET:HE1	1:A:356:LEU:HD11	1.80	0.63
1:A:117:LEU:HD21	1:A:643:LEU:HD22	1.82	0.62
1:A:254:ASP:O	1:A:699:ARG:NH1	2.32	0.62
1:A:105:ALA:HB2	1:A:227:GLN:OE1	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:780:GLU:HG3	1:A:799:ARG:NH1	2.15	0.61
1:A:487:HIS:CE1	1:A:530:LEU:HD21	2.35	0.61
1:A:459:GLN:O	1:A:463:GLU:HB2	2.01	0.61
1:A:236:LEU:HD13	1:A:240:PHE:CD2	2.35	0.61
1:A:35:VAL:HG13	1:A:75:PHE:CE2	2.35	0.61
1:A:462:ALA:HB1	1:A:494:GLY:O	2.02	0.60
1:A:569:GLU:OE2	1:A:605:LYS:NZ	2.30	0.60
1:A:854:GLU:O	1:A:856:GLU:N	2.34	0.60
1:A:879:MET:HA	1:A:879:MET:HE2	1.82	0.60
1:A:225:ASN:ND2	1:A:235:LYS:HB3	2.17	0.60
1:A:319:LEU:HD22	1:A:323:LEU:HD22	1.83	0.60
1:A:377:LEU:O	1:A:381:ARG:HG3	2.01	0.60
1:A:46:ARG:HH22	1:A:775:ASP:CG	2.05	0.60
1:A:299:LEU:HD11	1:A:315:LEU:CD1	2.32	0.59
1:A:310:GLU:HG3	1:A:313:ARG:HB3	1.83	0.59
1:A:742:VAL:HG22	1:A:747:GLN:HG3	1.85	0.58
1:A:163:ASN:ND2	1:A:164:LYS:O	2.38	0.57
1:A:193:LYS:HE3	1:A:193:LYS:H	1.69	0.57
1:A:98:ALA:HB1	1:A:629:SER:OG	2.05	0.57
1:A:305:GLU:H	1:A:308:ALA:HB2	1.70	0.56
1:A:326:THR:CG2	1:A:346:LEU:H	2.18	0.56
1:A:238:VAL:HG21	1:A:360:TYR:CZ	2.41	0.56
1:A:102:GLU:OE2	1:A:109:ARG:NH2	2.39	0.56
1:A:322:ARG:HG3	1:A:344:GLY:O	2.06	0.55
1:A:584:SER:O	1:A:587:ARG:HG3	2.06	0.55
1:A:133:LEU:N	1:A:133:LEU:HD22	2.21	0.55
1:A:68:LEU:HD11	1:A:849:ARG:NH1	2.18	0.55
1:A:26:ALA:CB	1:A:27:LEU:HD23	2.34	0.55
1:A:87:GLN:HE22	1:A:618:ARG:HE	1.55	0.55
1:A:205:GLY:O	1:A:209:VAL:HG23	2.06	0.55
1:A:356:LEU:HB3	1:A:380:LEU:CD1	2.36	0.55
1:A:326:THR:HG21	1:A:346:LEU:N	2.22	0.54
1:A:271:SER:HB3	1:A:389:PRO:O	2.07	0.54
1:A:193:LYS:CE	1:A:193:LYS:H	2.19	0.54
1:A:193:LYS:N	1:A:193:LYS:HE3	2.23	0.54
1:A:727:MET:CE	1:A:773:LYS:HB2	2.38	0.54
1:A:115:PRO:O	1:A:116:GLU:HB2	2.08	0.54
1:A:668:TYR:HA	1:A:732:LEU:HD13	1.90	0.54
1:A:84:THR:HG22	1:A:618:ARG:NH2	2.16	0.54
1:A:581:ARG:HG3	1:A:611:THR:CG2	2.38	0.53
1:A:396:ARG:HG3	1:A:473:VAL:HG12	1.88	0.53
1:A:354:GLU:HB2	1:A:355:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:LEU:HD13	1:A:643:LEU:HD12	1.90	0.53
1:A:352:LEU:HD23	1:A:383:VAL:HG22	1.91	0.52
1:A:317:LYS:HG2	1:A:320:ARG:NH1	2.21	0.52
1:A:800:ASN:HD22	1:A:800:ASN:N	2.07	0.52
1:A:35:VAL:HA	1:A:75:PHE:CZ	2.45	0.52
1:A:142:ILE:HD13	1:A:191:ILE:HD12	1.92	0.51
1:A:373:ASN:OD1	1:A:377:LEU:HD22	2.10	0.51
1:A:724:ASN:O	1:A:725:ARG:HB2	2.11	0.51
1:A:354:GLU:CB	1:A:355:PRO:HD3	2.40	0.51
1:A:104:ILE:HD11	1:A:632:SER:CB	2.41	0.51
1:A:236:LEU:HD13	1:A:240:PHE:HE2	1.74	0.50
1:A:625:GLU:HA	1:A:625:GLU:OE2	2.10	0.50
1:A:487:HIS:ND1	1:A:530:LEU:HD21	2.26	0.50
1:A:279:PHE:O	1:A:283:ILE:HG12	2.11	0.50
1:A:783:ASP:HA	1:A:787:VAL:HG23	1.93	0.50
1:A:322:ARG:O	1:A:326:THR:HG23	2.11	0.50
1:A:804:GLU:O	1:A:808:VAL:HG23	2.11	0.50
1:A:214:TRP:CE2	1:A:382:ARG:HD3	2.47	0.49
1:A:111:LEU:HD13	1:A:643:LEU:CD1	2.42	0.49
1:A:815:ASP:OD1	1:A:816:SER:N	2.42	0.49
1:A:27:LEU:HD12	1:A:31:ILE:HD11	1.95	0.48
1:A:349:ASN:HD21	1:A:388:VAL:H	1.59	0.48
1:A:522:LEU:O	1:A:528:ARG:HD3	2.13	0.48
1:A:460:VAL:O	1:A:461:ILE:C	2.50	0.48
1:A:394:ASP:OD2	1:A:609:ARG:NH2	2.47	0.48
1:A:406:LEU:HD21	1:A:488:LEU:HD23	1.96	0.48
1:A:445:TRP:CE3	1:A:447:PRO:HG3	2.48	0.48
1:A:273:TRP:O	1:A:276:THR:HG22	2.14	0.48
1:A:648:GLU:HG3	1:A:649:PRO:HD2	1.96	0.48
1:A:837:ASP:HB3	1:A:838:PRO:CD	2.41	0.47
1:A:349:ASN:HD22	1:A:388:VAL:HG23	1.78	0.47
1:A:201:GLU:O	1:A:249:MET:HE2	2.15	0.47
1:A:579:HIS:CE1	1:A:599:GLN:HE22	2.32	0.47
1:A:459:GLN:NE2	1:A:463:GLU:OE2	2.47	0.47
1:A:418:TYR:CE2	1:A:426:LYS:HD3	2.50	0.47
1:A:394:ASP:CG	1:A:609:ARG:HH22	2.18	0.47
1:A:77:GLN:NE2	1:A:77:GLN:CA	2.74	0.47
1:A:832:ARG:HH22	3:A:884:ASP:CG	2.19	0.46
1:A:860:PRO:HB2	1:A:865:GLU:OE2	2.15	0.46
1:A:77:GLN:HE21	1:A:77:GLN:CA	2.29	0.46
1:A:406:LEU:HD12	1:A:409:LEU:HD23	1.97	0.46
1:A:480:PRO:HB3	1:A:521:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:ASN:C	1:A:49:ASN:HD22	2.18	0.46
1:A:275:ALA:O	1:A:279:PHE:HB2	2.16	0.46
1:A:518:MET:HE2	1:A:518:MET:HB3	1.71	0.46
1:A:17:LYS:O	1:A:18:VAL:C	2.54	0.46
1:A:533:GLY:O	1:A:534:LYS:HG3	2.15	0.46
1:A:87:GLN:O	1:A:91:ILE:HD13	2.16	0.46
1:A:825:ILE:HG12	4:A:946:HOH:O	2.15	0.46
1:A:773:LYS:HD3	1:A:879:MET:HE2	1.98	0.46
1:A:292:MET:SD	1:A:292:MET:N	2.88	0.46
1:A:475:SER:HA	1:A:504:LEU:HB3	1.98	0.46
1:A:303:VAL:HG13	1:A:314:TYR:HD1	1.78	0.46
1:A:253:ARG:HG3	1:A:397:GLN:NE2	2.31	0.46
1:A:229:GLU:HB2	1:A:235:LYS:HG2	1.98	0.46
1:A:100:ASN:C	1:A:100:ASN:HD22	2.19	0.46
1:A:615:GLU:CG	1:A:719:PHE:HZ	2.29	0.46
1:A:184:GLN:HG2	4:A:893:HOH:O	2.16	0.46
1:A:457:THR:HB	4:A:920:HOH:O	2.16	0.45
1:A:84:THR:HG21	1:A:151:MET:HE1	1.98	0.45
1:A:142:ILE:HG23	1:A:143:THR:HG23	1.99	0.45
1:A:116:GLU:OE1	1:A:116:GLU:HA	2.15	0.45
1:A:41:LEU:HD21	1:A:55:GLU:HG3	1.98	0.45
1:A:253:ARG:O	1:A:254:ASP:C	2.52	0.45
1:A:723:GLN:HB3	1:A:843:GLN:HE22	1.81	0.45
1:A:341:LYS:CB	1:A:345:LEU:HD22	2.46	0.45
1:A:228:LEU:CD1	1:A:236:LEU:HG	2.47	0.45
1:A:684:SER:HB3	1:A:787:VAL:HG22	1.98	0.45
1:A:561:GLN:O	1:A:565:ILE:HG13	2.16	0.45
1:A:356:LEU:HB3	1:A:380:LEU:HD13	1.98	0.45
1:A:694:LEU:HD11	1:A:868:LEU:HD13	1.98	0.45
1:A:34:ARG:O	1:A:38:ILE:HG13	2.17	0.45
1:A:333:ARG:O	1:A:334:LEU:C	2.55	0.45
1:A:690:GLU:HG3	1:A:847:LEU:HD21	1.98	0.45
1:A:27:LEU:CD1	1:A:31:ILE:HD11	2.47	0.45
1:A:192:ARG:HB3	1:A:192:ARG:HE	1.75	0.44
1:A:557:GLN:HG3	1:A:561:GLN:HE21	1.82	0.44
1:A:265:ARG:HD2	1:A:265:ARG:HH11	1.49	0.44
1:A:217:VAL:O	1:A:221:LEU:HD12	2.18	0.44
1:A:110:LYS:HE2	1:A:640:GLU:OE1	2.18	0.44
1:A:742:VAL:CG2	1:A:747:GLN:HG3	2.47	0.44
1:A:136:THR:HG22	1:A:614:GLY:N	2.33	0.44
1:A:653:TRP:CD1	1:A:753:MET:HG3	2.52	0.44
1:A:682:PHE:CZ	1:A:688:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:854:GLU:C	1:A:856:GLU:H	2.22	0.43
1:A:163:ASN:HD22	1:A:164:LYS:N	2.15	0.43
1:A:286:LEU:HD13	1:A:316:MET:HE2	1.99	0.43
1:A:861:ASP:OD2	1:A:862:PRO:HD2	2.18	0.43
1:A:203:LYS:HZ3	1:A:270:LEU:CD1	2.31	0.43
1:A:144:ARG:HH11	1:A:144:ARG:HD2	1.62	0.43
1:A:346:LEU:HA	1:A:351:GLU:OE2	2.19	0.43
1:A:696:LEU:HA	1:A:696:LEU:HD23	1.86	0.43
1:A:310:GLU:N	1:A:311:PRO:HD3	2.33	0.43
1:A:427:GLN:O	1:A:431:ILE:HG13	2.18	0.43
1:A:434:LEU:HG	1:A:526:TRP:CH2	2.54	0.43
1:A:616:MET:SD	1:A:880:ARG:HB3	2.59	0.43
1:A:65:ASN:HA	1:A:68:LEU:HD12	2.01	0.43
1:A:765:GLY:O	1:A:768:GLU:HB2	2.18	0.43
1:A:198:PRO:HB2	1:A:263:ILE:HG21	2.01	0.43
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.86	0.43
1:A:378:ASP:HB3	1:A:382:ARG:NH1	2.34	0.42
1:A:142:ILE:HD13	1:A:191:ILE:CD1	2.48	0.42
1:A:578:PHE:CD1	1:A:609:ARG:HG2	2.54	0.42
1:A:17:LYS:HA	1:A:17:LYS:HD2	1.59	0.42
1:A:442:PRO:HB2	1:A:445:TRP:HB2	2.01	0.42
1:A:150:LYS:HA	1:A:150:LYS:NZ	2.34	0.42
1:A:611:THR:HG22	1:A:611:THR:O	2.19	0.42
1:A:77:GLN:HA	1:A:77:GLN:HE21	1.83	0.42
1:A:341:LYS:HB2	1:A:345:LEU:HD22	2.00	0.42
1:A:837:ASP:CB	1:A:838:PRO:HD3	2.44	0.42
1:A:329:TRP:CE2	1:A:333:ARG:HD3	2.55	0.42
1:A:184:GLN:O	1:A:188:THR:N	2.38	0.42
1:A:388:VAL:HB	1:A:389:PRO:HD3	2.00	0.42
1:A:547:ASP:OD1	1:A:673:ARG:NH2	2.53	0.42
1:A:758:PRO:O	1:A:762:THR:HB	2.19	0.42
1:A:783:ASP:HA	1:A:787:VAL:CG2	2.48	0.42
1:A:69:LEU:HD22	1:A:73:ARG:HG3	2.01	0.42
1:A:539:ILE:HG21	1:A:557:GLN:HG3	2.02	0.41
1:A:333:ARG:HB3	1:A:333:ARG:CZ	2.49	0.41
1:A:863:ARG:CG	1:A:863:ARG:HH11	2.16	0.41
1:A:441:LEU:HA	1:A:442:PRO:HD3	1.82	0.41
1:A:167:ALA:HB1	1:A:169:TYR:CE2	2.56	0.41
1:A:515:ASN:O	1:A:519:THR:CG2	2.66	0.41
1:A:102:GLU:O	1:A:106:ARG:HG3	2.21	0.41
1:A:411:ARG:HD3	1:A:411:ARG:HH11	1.50	0.41
1:A:585:ILE:HD13	1:A:596:LEU:CD1	2.46	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:225:ASN:HD21	1:A:235:LYS:HB3	1.85	0.41
1:A:625:GLU:CA	1:A:625:GLU:OE2	2.68	0.41
1:A:859:GLU:HA	1:A:860:PRO:HD2	1.85	0.41
1:A:203:LYS:NZ	1:A:270:LEU:HD11	2.34	0.41
1:A:8:LEU:O	1:A:12:VAL:HG13	2.21	0.41
1:A:164:LYS:O	1:A:165:ASP:HB2	2.21	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.97	0.41
1:A:590:ALA:N	1:A:591:PRO:CD	2.84	0.41
1:A:108:LEU:HD11	1:A:228:LEU:HD23	2.01	0.41
1:A:421:TRP:O	1:A:426:LYS:HE2	2.21	0.41
1:A:792:TRP:N	1:A:793:PRO:CD	2.84	0.41
1:A:445:TRP:HZ3	1:A:455:LEU:HD11	1.85	0.41
1:A:79:LEU:O	1:A:79:LEU:HD12	2.21	0.41
1:A:773:LYS:HB3	1:A:879:MET:HE1	2.03	0.40
1:A:742:VAL:HG22	1:A:747:GLN:CG	2.49	0.40
1:A:276:THR:CG2	1:A:327:GLN:HB2	2.52	0.40
1:A:53:ARG:NH1	1:A:784:GLN:OE1	2.55	0.40
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.94	0.40
1:A:608:LEU:HD11	1:A:610:VAL:HG22	2.04	0.40
1:A:87:GLN:NE2	1:A:618:ARG:HE	2.16	0.40
1:A:597:LEU:HD12	1:A:641:ALA:HB2	2.03	0.40
1:A:145:ARG:HA	1:A:145:ARG:HD2	1.79	0.40
1:A:499:MET:HA	1:A:500:PRO:HD3	1.93	0.40
1:A:837:ASP:CB	1:A:838:PRO:CD	3.00	0.40
1:A:191:ILE:HG22	1:A:192:ARG:O	2.21	0.40
1:A:46:ARG:NH2	1:A:775:ASP:OD2	2.39	0.40
1:A:599:GLN:O	1:A:600:PRO:C	2.57	0.40
1:A:615:GLU:HG2	1:A:719:PHE:HZ	1.86	0.40
1:A:312:TYR:OH	1:A:362:SER:HB2	2.21	0.40
1:A:326:THR:HG21	1:A:346:LEU:HB2	2.03	0.40
1:A:682:PHE:HE2	1:A:712:LEU:HD21	1.87	0.40
1:A:589:GLY:HA2	1:A:633:LEU:HD13	2.03	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	870/883 (98%)	802 (92%)	60 (7%)	8 (1%)	25	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	732	LEU
1	A	26	ALA
1	A	304	GLY
1	A	603	SER
1	A	855	LYS
1	A	101	PRO
1	A	857	GLY
1	A	148	ILE

### 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	725/747 (97%)	603 (83%)	122 (17%)	3	5

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	17	LYS
1	A	25	ASP
1	A	27	LEU
1	A	32	LEU
1	A	39	ARG
1	A	41	LEU
1	A	49	ASN
1	A	53	ARG
1	A	56	LEU
1	A	57	LEU
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	84	THR
1	A	90	SER
1	A	91	ILE
1	A	92	SER
1	A	100	ASN
1	A	106	ARG
1	A	117	LEU
1	A	129	LEU
1	A	130	SER
1	A	133	LEU
1	A	136	THR
1	A	142	ILE
1	A	144	ARG
1	A	150	LYS
1	A	151	MET
1	A	153	GLU
1	A	162	ASP
1	A	168	ASP
1	A	178	LEU
1	A	180	GLN
1	A	181	LEU
1	A	192	ARG
1	A	193	LYS
1	A	194	LEU
1	A	197	SER
1	A	220	TYR
1	A	221	LEU
1	A	222	ARG
1	A	223	GLU
1	A	225	ASN
1	A	226	GLU
1	A	239	GLU
1	A	243	VAL
1	A	249	MET
1	A	253	ARG
1	A	256	ASN
1	A	276	THR
1	A	280	LEU
1	A	288	SER
1	A	292	MET
1	A	302	LEU
1	A	319	LEU

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	321	SER
1	A	323	LEU
1	A	326	THR
1	A	330	LEU
1	A	333	ARG
1	A	339	LEU
1	A	341	LYS
1	A	347	THR
1	A	356	LEU
1	A	362	SER
1	A	380	LEU
1	A	400	THR
1	A	406	LEU
1	A	419	GLU
1	A	434	LEU
1	A	437	LYS
1	A	438	ARG
1	A	444	ASN
1	A	446	GLN
1	A	463	GLU
1	A	486	VAL
1	A	492	GLU
1	A	507	THR
1	A	519	THR
1	A	542	SER
1	A	544	SER
1	A	581	ARG
1	A	587	ARG
1	A	596	LEU
1	A	610	VAL
1	A	611	THR
1	A	615	GLU
1	A	639	LEU
1	A	648	GLU
1	A	656	ILE
1	A	676	LYS
1	A	684	SER
1	A	689	GLN
1	A	690	GLU
1	A	691	LEU
1	A	709	VAL

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Mol	Chain	Res	Type
1	A	712	LEU
1	A	728	LEU
1	A	732	LEU
1	A	740	LYS
1	A	742	VAL
1	A	746	LYS
1	A	748	SER
1	A	749	GLU
1	A	762	THR
1	A	767	LEU
1	A	769	MET
1	A	780	GLU
1	A	794	LEU
1	A	801	LEU
1	A	804	GLU
1	A	807	LYS
1	A	810	LEU
1	A	818	LEU
1	A	821	ASP
1	A	831	LEU
1	A	834	ILE
1	A	852	GLN
1	A	859	GLU
1	A	863	ARG
1	A	868	LEU
1	A	879	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	49	ASN
1	A	54	GLN
1	A	65	ASN
1	A	77	GLN
1	A	87	GLN
1	A	100	ASN
1	A	113	ASN
1	A	163	ASN
1	A	225	ASN
1	A	256	ASN
1	A	266	HIS

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Mol	Chain	Res	Type
1	A	327	GLN
1	A	349	ASN
1	A	364	GLN
1	A	535	GLN
1	A	557	GLN
1	A	561	GLN
1	A	599	GLN
1	A	800	ASN
1	A	843	GLN

### 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	ASP	A	884	-	8,8,8	1.21	1 (12%)	10,10,10	1.45	1 (10%)

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	ASP	A	884	-	-	0/8/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	884	ASP	OXT-C	2.90	1.40	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	884	ASP	OXT-C-O	-2.89	117.55	124.07

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	874/883 (98%)	-0.44	6 (0%) 84 86	18, 40, 70, 93	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	3.2
1	A	302	LEU	2.9
1	A	859	GLU	2.8
1	A	116	GLU	2.7
1	A	304	GLY	2.6
1	A	340	PRO	2.3

### 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( $\text{\AA}^2$ )	Q<0.9
2	MN	A	885	1/1	0.28	7.87	20,20,20,20	0
3	ASP	A	884	9/9	0.11	-0.24	36,38,44,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.