



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 01:47 AM UTC

PDB ID : 1QB4 / pdb_00001qb4
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

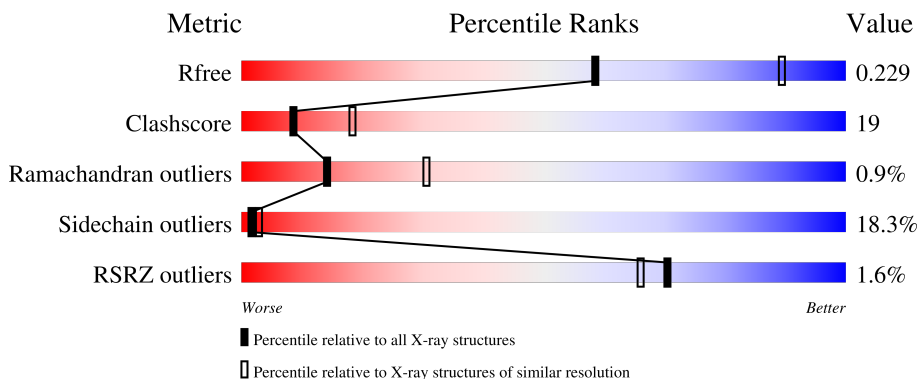
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	883	2% 47% 38% 12% ..

2 Entry composition [i](#)

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

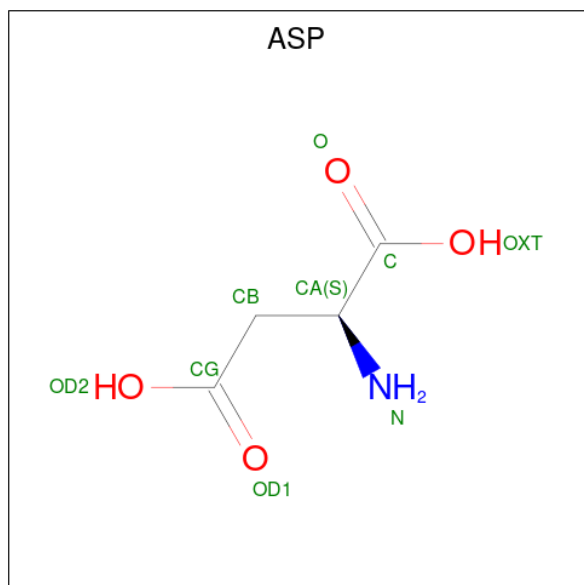
- Molecule 1 is a protein called PHOSPHOENOLPYRUVATE CARBOXYLASE.

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 (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



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

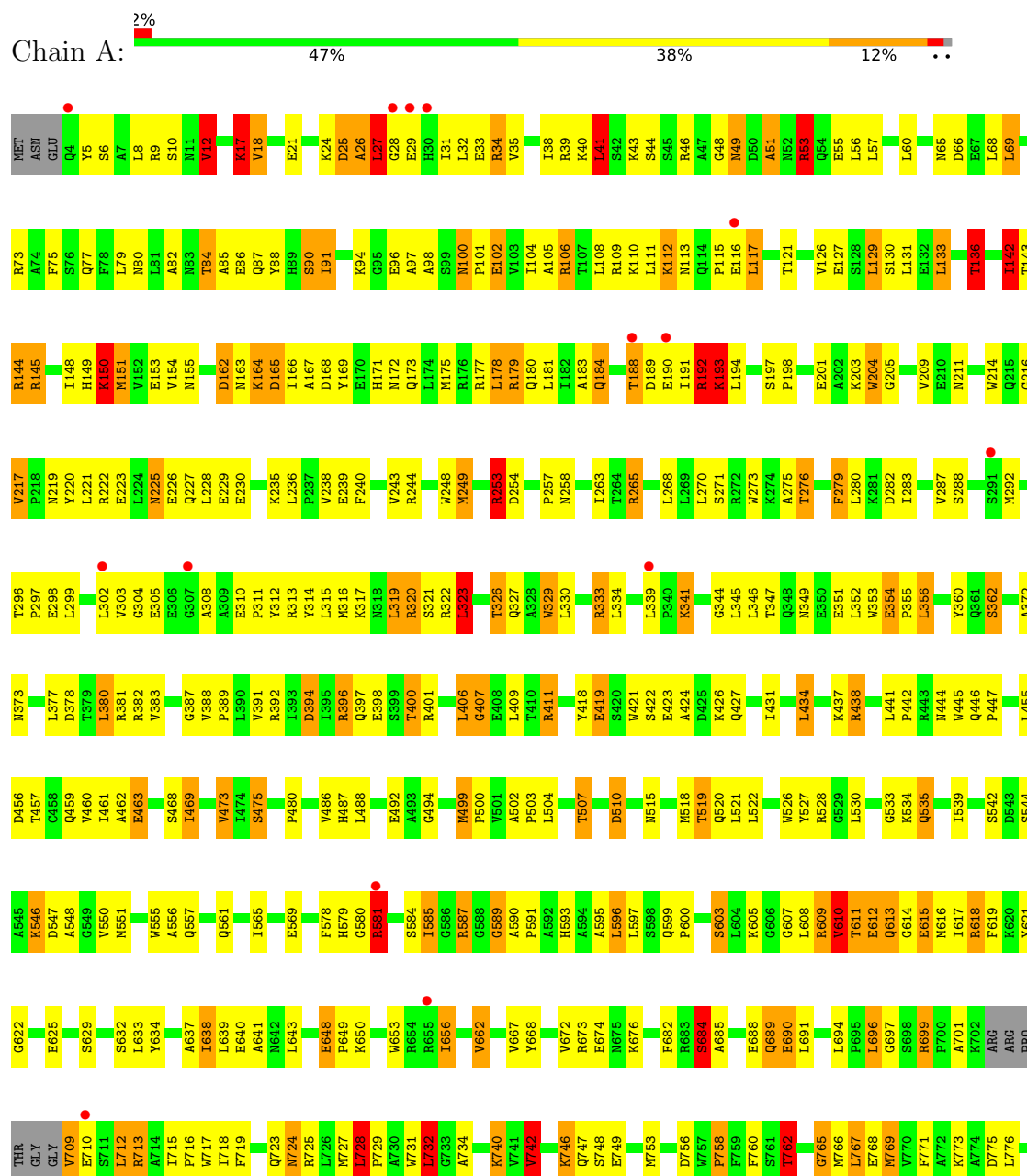
- Molecule 4 is water.

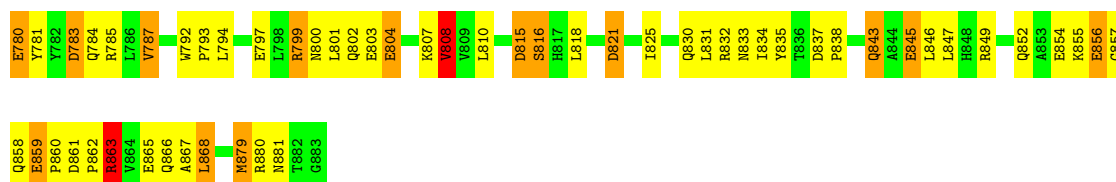
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		

3 Residue-property plots

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





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.75Å 248.41Å 83.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-2.60) 90.5 (20.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.261 0.195 , 0.229	Depositor DCC
R_{free} test set	1092 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6926	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.10	8/6969 (0.1%)	2.08	242/9462 (2.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	GLY	N-CA	8.38	1.51	1.44
1	A	581	ARG	N-CA	-7.31	1.37	1.46
1	A	396	ARG	CD-NE	-5.82	1.38	1.46
1	A	610	VAL	N-CA	-5.65	1.39	1.46
1	A	701	ALA	C-N	-5.29	1.25	1.33
1	A	217	VAL	CA-C	-5.20	1.48	1.52
1	A	699	ARG	NE-CZ	-5.19	1.27	1.33
1	A	502	ALA	CA-C	-5.07	1.48	1.52

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	ARG	CD-NE-CZ	23.56	157.38	124.40
1	A	618	ARG	CD-NE-CZ	19.19	151.27	124.40
1	A	166	ILE	N-CA-CB	14.50	126.53	110.72
1	A	858	GLN	CA-C-N	13.82	143.56	121.17
1	A	858	GLN	C-N-CA	13.82	143.56	121.17
1	A	580	GLY	CA-C-N	13.46	140.62	121.24
1	A	580	GLY	C-N-CA	13.46	140.62	121.24
1	A	394	ASP	CA-CB-CG	13.37	125.97	112.60
1	A	396	ARG	CD-NE-CZ	11.82	140.95	124.40
1	A	856	GLU	CA-CB-CG	10.78	135.67	114.10
1	A	856	GLU	N-CA-CB	-10.15	96.27	111.19
1	A	401	ARG	NE-CZ-NH2	9.53	127.78	119.20
1	A	193	LYS	N-CA-C	-8.87	102.59	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	CA-CB-CG	8.58	121.18	112.60
1	A	29	GLU	N-CA-C	-8.54	103.04	113.97
1	A	192	ARG	CD-NE-CZ	-8.37	112.68	124.40
1	A	724	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	A	696	LEU	CA-C-N	-8.05	113.03	122.77
1	A	696	LEU	C-N-CA	-8.05	113.03	122.77
1	A	815	ASP	CA-CB-CG	-8.03	104.57	112.60
1	A	607	GLY	N-CA-C	7.80	124.36	112.81
1	A	581	ARG	N-CA-C	7.70	120.91	109.59
1	A	535	GLN	CA-C-O	-7.66	112.14	121.11
1	A	699	ARG	NE-CZ-NH1	7.61	129.11	121.50
1	A	33	GLU	CA-C-N	7.55	130.40	120.28
1	A	33	GLU	C-N-CA	7.55	130.40	120.28
1	A	802	GLN	OE1-CD-NE2	-7.55	115.05	122.60
1	A	173	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	A	94	LYS	CA-C-N	7.50	129.66	120.51
1	A	94	LYS	C-N-CA	7.50	129.66	120.51
1	A	9	ARG	CD-NE-CZ	7.45	134.83	124.40
1	A	112	LYS	CA-C-N	-7.44	112.82	122.79
1	A	112	LYS	C-N-CA	-7.44	112.82	122.79
1	A	713	ARG	NE-CZ-NH2	7.44	125.89	119.20
1	A	808	VAL	CB-CA-C	-7.43	102.30	112.04
1	A	638	ILE	N-CA-CB	7.42	118.70	110.62
1	A	28	GLY	N-CA-C	7.33	121.84	110.91
1	A	550	VAL	N-CA-C	7.33	120.26	111.09
1	A	684	SER	CA-C-N	7.27	131.36	120.31
1	A	684	SER	C-N-CA	7.27	131.36	120.31
1	A	97	ALA	N-CA-C	7.22	121.35	111.54
1	A	88	TYR	CA-C-N	7.13	130.15	120.38
1	A	88	TYR	C-N-CA	7.13	130.15	120.38
1	A	189	ASP	CA-C-O	7.05	128.12	120.43
1	A	268	LEU	CA-C-O	7.04	128.02	120.55
1	A	85	ALA	N-CA-C	-7.02	103.56	111.14
1	A	411	ARG	N-CA-CB	6.98	120.38	110.12
1	A	438	ARG	CD-NE-CZ	6.96	134.15	124.40
1	A	662	VAL	N-CA-CB	6.88	119.38	110.57
1	A	613	GLN	CA-C-N	6.78	127.47	119.94
1	A	613	GLN	C-N-CA	6.78	127.47	119.94
1	A	66	ASP	CA-CB-CG	-6.77	105.83	112.60
1	A	88	TYR	O-C-N	-6.77	115.10	122.07
1	A	609	ARG	CD-NE-CZ	6.71	133.80	124.40
1	A	145	ARG	CD-NE-CZ	6.69	133.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	PRO	CA-C-O	-6.66	113.74	121.86
1	A	821	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	401	ARG	CD-NE-CZ	-6.60	115.16	124.40
1	A	51	ALA	CA-C-O	6.57	126.83	119.41
1	A	622	GLY	N-CA-C	6.57	122.01	113.27
1	A	419	GLU	CA-CB-CG	6.55	127.20	114.10
1	A	33	GLU	CA-C-O	-6.50	113.53	120.42
1	A	867	ALA	CA-C-N	6.46	128.84	120.44
1	A	867	ALA	C-N-CA	6.46	128.84	120.44
1	A	581	ARG	NE-CZ-NH2	6.44	124.99	119.20
1	A	216	GLY	CA-C-N	-6.41	115.20	120.33
1	A	216	GLY	C-N-CA	-6.41	115.20	120.33
1	A	257	PRO	O-C-N	-6.36	114.59	122.23
1	A	25	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	674	GLU	N-CA-C	6.36	118.29	111.36
1	A	546	LYS	CA-C-O	6.36	127.16	120.42
1	A	856	GLU	CA-C-O	6.30	127.53	121.67
1	A	411	ARG	CD-NE-CZ	-6.27	115.62	124.40
1	A	392	ARG	CA-C-O	-6.25	114.92	121.55
1	A	192	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	A	48	GLY	N-CA-C	6.23	122.49	115.08
1	A	527	TYR	CA-C-O	6.22	127.15	120.55
1	A	86	GLU	O-C-N	-6.20	115.68	122.07
1	A	713	ARG	CA-C-O	-6.17	114.24	121.46
1	A	475	SER	O-C-N	-6.17	115.58	122.86
1	A	881	ASN	CA-C-O	6.16	127.73	120.58
1	A	756	ASP	N-CA-C	6.15	120.92	113.17
1	A	96	GLU	O-C-N	-6.14	114.41	122.39
1	A	468	SER	CB-CA-C	-6.13	98.52	110.11
1	A	593	HIS	CA-CB-CG	6.10	119.90	113.80
1	A	171	HIS	CA-C-O	6.09	127.20	120.63
1	A	548	ALA	N-CA-C	6.09	121.46	113.30
1	A	718	ILE	N-CA-C	6.08	116.26	110.42
1	A	136	THR	CA-CB-OG1	-6.08	100.49	109.60
1	A	581	ARG	CD-NE-CZ	-6.07	115.90	124.40
1	A	423	GLU	O-C-N	-6.01	115.18	122.22
1	A	760	PHE	CA-CB-CG	-6.01	107.79	113.80
1	A	12	VAL	N-CA-CB	6.00	118.70	110.54
1	A	253	ARG	CA-C-O	5.99	126.45	119.32
1	A	142	ILE	N-CA-C	5.97	122.05	113.16
1	A	830	GLN	CA-C-N	5.96	128.52	120.65
1	A	830	GLN	C-N-CA	5.96	128.52	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	ARG	NH1-CZ-NH2	-5.96	111.56	119.30
1	A	650	LYS	CA-CB-CG	5.95	126.00	114.10
1	A	833	ASN	CB-CG-ND2	5.95	125.32	116.40
1	A	475	SER	CB-CA-C	5.94	120.46	109.54
1	A	82	ALA	O-C-N	-5.92	115.97	122.07
1	A	400	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	762	THR	O-C-N	-5.92	115.85	122.12
1	A	177	ARG	CD-NE-CZ	5.89	132.64	124.40
1	A	728	LEU	O-C-N	-5.87	114.57	121.32
1	A	329	TRP	CA-C-N	-5.86	111.84	120.28
1	A	329	TRP	C-N-CA	-5.86	111.84	120.28
1	A	609	ARG	CG-CD-NE	-5.86	99.11	112.00
1	A	742	VAL	N-CA-C	-5.84	104.82	110.72
1	A	282	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	422	SER	CA-C-N	5.83	128.67	120.28
1	A	422	SER	C-N-CA	5.83	128.67	120.28
1	A	424	ALA	CA-C-N	5.83	128.56	120.29
1	A	424	ALA	C-N-CA	5.83	128.56	120.29
1	A	613	GLN	CA-C-O	5.82	127.59	121.19
1	A	401	ARG	NE-CZ-NH1	-5.80	115.69	121.50
1	A	354	GLU	CB-CG-CD	-5.80	102.75	112.60
1	A	551	MET	CA-C-N	5.78	127.96	120.44
1	A	551	MET	C-N-CA	5.78	127.96	120.44
1	A	166	ILE	O-C-N	5.78	129.53	122.95
1	A	803	GLU	CA-CB-CG	5.78	125.65	114.10
1	A	53	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	503	PRO	O-C-N	5.73	130.35	123.13
1	A	18	VAL	CA-C-N	5.71	127.87	120.44
1	A	18	VAL	C-N-CA	5.71	127.87	120.44
1	A	710	GLU	N-CA-C	-5.69	105.06	112.23
1	A	279	PHE	O-C-N	-5.69	115.57	122.22
1	A	595	ALA	N-CA-C	5.68	117.47	111.28
1	A	638	ILE	CB-CA-C	-5.68	104.71	111.81
1	A	717	TRP	N-CA-C	-5.68	104.72	111.03
1	A	127	GLU	CA-CB-CG	5.67	125.43	114.10
1	A	279	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	765	GLY	CA-C-N	5.63	128.60	120.38
1	A	765	GLY	C-N-CA	5.63	128.60	120.38
1	A	799	ARG	CA-C-O	5.63	126.39	120.42
1	A	835	TYR	CA-C-N	5.62	130.24	120.68
1	A	835	TYR	C-N-CA	5.62	130.24	120.68
1	A	731	TRP	CA-C-N	5.62	132.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	731	TRP	C-N-CA	5.62	132.26	121.54
1	A	724	ASN	CA-C-O	5.60	126.26	119.31
1	A	190	GLU	CA-C-O	-5.60	114.22	120.66
1	A	5	TYR	CA-C-N	5.59	128.09	120.54
1	A	5	TYR	C-N-CA	5.59	128.09	120.54
1	A	556	ALA	CA-C-N	-5.59	112.35	120.29
1	A	556	ALA	C-N-CA	-5.59	112.35	120.29
1	A	113	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	A	637	ALA	CA-C-O	-5.59	114.92	120.90
1	A	843	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	833	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	149	HIS	CA-C-O	-5.53	114.66	120.63
1	A	162	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	18	VAL	CA-C-O	-5.53	115.52	121.27
1	A	154	VAL	CA-C-N	5.53	128.14	120.29
1	A	154	VAL	C-N-CA	5.53	128.14	120.29
1	A	729	PRO	CB-CA-C	-5.50	103.07	112.64
1	A	783	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	265	ARG	CD-NE-CZ	-5.48	116.72	124.40
1	A	129	LEU	CB-CA-C	-5.47	99.82	109.62
1	A	863	ARG	CD-NE-CZ	5.47	132.05	124.40
1	A	520	GLN	N-CA-C	-5.46	105.24	111.14
1	A	24	LYS	N-CA-C	-5.46	105.02	110.97
1	A	192	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	A	27	LEU	CA-C-N	-5.44	113.15	121.09
1	A	27	LEU	C-N-CA	-5.44	113.15	121.09
1	A	12	VAL	O-C-N	5.44	127.14	121.87
1	A	400	THR	N-CA-CB	-5.43	101.92	110.06
1	A	244	ARG	CA-CB-CG	5.42	124.95	114.10
1	A	155	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	499	MET	N-CA-CB	-5.42	103.14	110.23
1	A	746	LYS	N-CA-CB	5.41	118.32	110.47
1	A	222	ARG	CG-CD-NE	5.41	123.90	112.00
1	A	401	ARG	CG-CD-NE	5.40	123.87	112.00
1	A	34	ARG	CA-C-N	5.39	128.46	120.74
1	A	34	ARG	C-N-CA	5.39	128.46	120.74
1	A	398	GLU	N-CA-CB	5.39	118.65	110.45
1	A	258	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	204	TRP	CB-CA-C	5.37	119.98	110.85
1	A	650	LYS	N-CA-C	-5.36	101.91	109.96
1	A	612	GLU	O-C-N	-5.32	116.26	122.96
1	A	353	TRP	CA-C-O	5.31	126.91	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	LYS	N-CA-C	-5.31	105.18	110.97
1	A	96	GLU	CB-CA-C	5.29	121.47	110.32
1	A	179	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	165	ASP	CA-C-N	-5.27	115.57	122.37
1	A	165	ASP	C-N-CA	-5.27	115.57	122.37
1	A	762	THR	N-CA-CB	-5.27	102.37	110.12
1	A	219	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	473	VAL	CA-C-O	-5.27	114.73	120.84
1	A	685	ALA	N-CA-C	5.27	117.93	111.82
1	A	41	LEU	CA-C-N	5.26	127.77	120.29
1	A	41	LEU	C-N-CA	5.26	127.77	120.29
1	A	220	TYR	N-CA-C	-5.23	105.47	111.07
1	A	279	PHE	CA-C-O	5.22	126.00	120.10
1	A	610	VAL	CB-CA-C	-5.22	101.47	110.30
1	A	510	ASP	N-CA-C	-5.21	105.60	111.28
1	A	456	ASP	O-C-N	-5.21	116.60	122.12
1	A	136	THR	N-CA-CB	-5.20	102.49	111.55
1	A	164	LYS	N-CA-C	-5.20	104.02	110.41
1	A	90	SER	CA-CB-OG	-5.19	100.72	111.10
1	A	150	LYS	CA-C-N	5.18	127.22	120.28
1	A	150	LYS	C-N-CA	5.18	127.22	120.28
1	A	771	PHE	N-CA-C	-5.18	105.81	111.82
1	A	188	THR	CA-C-O	-5.18	116.17	122.64
1	A	603	SER	N-CA-C	5.17	121.81	110.80
1	A	387	GLY	CA-C-O	5.17	129.56	120.57
1	A	248	TRP	N-CA-C	-5.16	106.67	113.17
1	A	179	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	211	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	265	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	589	GLY	N-CA-C	5.15	121.17	111.80
1	A	372	ALA	CA-C-O	-5.13	115.43	120.82
1	A	767	LEU	CA-C-O	5.13	125.86	120.42
1	A	617	ILE	N-CA-C	5.12	115.33	110.42
1	A	44	SER	CA-C-N	5.11	127.38	120.38
1	A	44	SER	C-N-CA	5.11	127.38	120.38
1	A	230	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	121	THR	N-CA-C	-5.11	105.72	111.28
1	A	407	GLY	O-C-N	-5.10	116.07	122.70
1	A	740	LYS	CA-C-O	5.10	126.17	120.82
1	A	175	MET	O-C-N	-5.09	116.27	122.22
1	A	6	SER	CA-C-N	5.09	127.09	120.28
1	A	6	SER	C-N-CA	5.09	127.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	734	ALA	CA-C-N	5.06	125.60	119.98
1	A	734	ALA	C-N-CA	5.06	125.60	119.98
1	A	172	ASN	N-CA-CB	-5.06	102.68	110.12
1	A	619	PHE	O-C-N	-5.05	115.49	122.46
1	A	758	PRO	CA-C-N	5.05	127.30	120.38
1	A	758	PRO	C-N-CA	5.05	127.30	120.38
1	A	746	LYS	CA-CB-CG	5.05	124.20	114.10
1	A	612	GLU	CA-C-O	5.04	126.43	120.58
1	A	555	TRP	CB-CA-C	5.03	119.41	110.85
1	A	323	LEU	CA-C-O	5.03	125.75	120.42
1	A	689	GLN	CA-C-N	5.03	127.43	120.29
1	A	689	GLN	C-N-CA	5.03	127.43	120.29
1	A	667	VAL	O-C-N	-5.03	117.00	121.87
1	A	787	VAL	N-CA-C	5.02	116.19	108.71
1	A	40	LYS	CA-C-N	5.01	127.50	120.28
1	A	40	LYS	C-N-CA	5.01	127.50	120.28
1	A	797	GLU	O-C-N	-5.01	116.91	122.07
1	A	172	ASN	OD1-CG-ND2	5.01	127.61	122.60
1	A	799	ARG	NE-CZ-NH2	-5.00	114.70	119.20

There are no chirality outliers.

There are no planarity outliers.

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	6835	0	6835	259	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	6838	259	0

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 19.

All (259) 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:879:MET:HA	1:A:879:MET:HE3	1.25	1.14
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
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:68:LEU:HD11	1:A:849:ARG:HH11	1.45	0.81
1:A:126:VAL:HG12	1:A:236:LEU:HD21	1.62	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:316:MET:HE1	1:A:356:LEU:HD11	1.70	0.73
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: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:715:ILE:HB	1:A:716:PRO:CD	2.24	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:NE2	1:A:77:GLN:HA	2.11	0.65
1:A:581:ARG:CD	1:A:581:ARG:H	2.08	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:46:ARG:HH22	1:A:775:ASP:CG	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:515:ASN:O	1:A:519:THR:HG23	1.98	0.64
1:A:769:MET:HE3	1:A:773:LYS:HD2	1.79	0.62
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:201:GLU:O	1:A:249:MET:HE2	2.00	0.62
1:A:105:ALA:HB2	1:A:227:GLN:OE1	2.00	0.61
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:35:VAL:HG13	1:A:75:PHE:CE2	2.35	0.61
1:A:236:LEU:HD13	1:A:240:PHE:CD2	2.35	0.61
1:A:462:ALA:HB1	1:A:494:GLY:O	2.02	0.60
1:A:854:GLU:O	1:A:856:GLU:N	2.34	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: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:773:LYS:HD3	1:A:879:MET:HE2	1.85	0.58
1:A:163:ASN:ND2	1:A:164:LYS:O	2.38	0.57
1:A:98:ALA:HB1	1:A:629:SER:OG	2.05	0.57
1:A:193:LYS:HE3	1:A:193:LYS:H	1.69	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:133:LEU:N	1:A:133:LEU:HD22	2.21	0.55
1:A:584:SER:O	1:A:587:ARG:HG3	2.06	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:193:LYS:H	1:A:193:LYS:CE	2.19	0.54
1:A:271:SER:HB3	1:A:389:PRO:O	2.07	0.54
1:A:326:THR:HG21	1:A:346:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HE3	1:A:193:LYS:N	2.23	0.54
1:A:115:PRO:O	1:A:116:GLU:HB2	2.08	0.54
1:A:727:MET:CE	1:A:773:LYS:HB2	2.38	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:396:ARG:HG3	1:A:473:VAL:HG12	1.88	0.53
1:A:581:ARG:HG3	1:A:611:THR:CG2	2.38	0.53
1:A:354:GLU:HB2	1:A:355:PRO:HD3	1.90	0.53
1:A:460:VAL:O	1:A:461:ILE:C	2.50	0.53
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:569:GLU:OE2	1:A:605:LYS:NZ	2.30	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:394:ASP:CG	1:A:609:ARG:HH22	2.18	0.52
1:A:769:MET:HE3	1:A:773:LYS:CD	2.40	0.51
1:A:142:ILE:HD13	1:A:191:ILE:HD12	1.92	0.51
1:A:581:ARG:H	1:A:581:ARG:HD2	1.75	0.51
1:A:832:ARG:HH22	3:A:884:ASP:CG	2.19	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:49:ASN:HD22	1:A:49:ASN:C	2.18	0.51
1:A:17:LYS:O	1:A:18:VAL:C	2.54	0.51
1:A:104:ILE:HD11	1:A:632:SER:CB	2.41	0.51
1:A:354:GLU:CB	1:A:355:PRO:HD3	2.40	0.51
1:A:236:LEU:HD13	1:A:240:PHE:HE2	1.74	0.50
1:A:625:GLU:OE2	1:A:625:GLU:HA	2.10	0.50
1:A:100:ASN:C	1:A:100:ASN:HD22	2.19	0.50
1:A:279:PHE:O	1:A:283:ILE:HG12	2.11	0.50
1:A:487:HIS:ND1	1:A:530:LEU:HD21	2.26	0.50
1:A:84:THR:HG21	1:A:151:MET:HE3	1.92	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:111:LEU:HD13	1:A:643:LEU:CD1	2.42	0.49
1:A:214:TRP:CE2	1:A:382:ARG:HD3	2.47	0.49
1:A:333:ARG:O	1:A:334:LEU:C	2.55	0.49
1:A:253:ARG:O	1:A:254:ASP:C	2.52	0.49
1:A:815:ASP:OD1	1:A:816:SER:N	2.42	0.49
1:A:656:ILE:HB	1:A:753:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:518:MET:HE1	1:A:535:GLN:NE2	2.28	0.48
1:A:522:LEU:O	1:A:528:ARG:HD3	2.13	0.48
1:A:394:ASP:OD2	1:A:609:ARG:NH2	2.47	0.48
1:A:854:GLU:C	1:A:856:GLU:H	2.22	0.48
1:A:406:LEU:HD21	1:A:488:LEU:HD23	1.96	0.48
1:A:273:TRP:O	1:A:276:THR:HG22	2.14	0.48
1:A:445:TRP:CE3	1:A:447:PRO:HG3	2.48	0.48
1:A:648:GLU:HG3	1:A:649:PRO:HD2	1.96	0.48
1:A:203:LYS:HZ3	1:A:270:LEU:CD1	2.27	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:579:HIS:CE1	1:A:599:GLN:HE22	2.32	0.47
1:A:418:TYR:CE2	1:A:426:LYS:HD3	2.50	0.47
1:A:459:GLN:NE2	1:A:463:GLU:OE2	2.47	0.47
1:A:77:GLN:NE2	1:A:77:GLN:CA	2.74	0.47
1:A:860:PRO:HB2	1:A:865:GLU:OE2	2.15	0.46
1:A:77:GLN:CA	1:A:77:GLN:HE21	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
1:A:275:ALA:O	1:A:279:PHE:HB2	2.16	0.46
1:A:533:GLY:O	1:A:534:LYS:HG3	2.15	0.46
1:A:469:ILE:CG2	1:A:499:MET:HE1	2.45	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: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:184:GLN:HG2	4:A:893:HOH:O	2.16	0.46
1:A:229:GLU:HB2	1:A:235:LYS:HG2	1.98	0.46
1:A:253:ARG:HG3	1:A:397:GLN:NE2	2.31	0.46
1:A:615:GLU:CG	1:A:719:PHE:HZ	2.29	0.46
1:A:457:THR:HB	4:A:920:HOH:O	2.16	0.45
1:A:41:LEU:HD21	1:A:55:GLU:HG3	1.98	0.45
1:A:116:GLU:OE1	1:A:116:GLU:HA	2.15	0.45
1:A:142:ILE:HG23	1:A:143:THR:HG23	1.99	0.45
1:A:723:GLN:HB3	1:A:843:GLN:HE22	1.81	0.45
1:A:228:LEU:CD1	1:A:236:LEU:HG	2.47	0.45
1:A:341:LYS:CB	1:A:345:LEU:HD22	2.46	0.45
1:A:561:GLN:O	1:A:565:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:HB3	1:A:787:VAL:HG22	1.98	0.45
1:A:599:GLN:O	1:A:600:PRO:C	2.57	0.45
1:A:34:ARG:O	1:A:38:ILE:HG13	2.17	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:690:GLU:HG3	1:A:847:LEU:HD21	1.98	0.45
1:A:769:MET:HE3	1:A:773:LYS:CE	2.46	0.45
1:A:27:LEU:CD1	1:A:31:ILE:HD11	2.47	0.45
1:A:192:ARG:HE	1:A:192:ARG:HB3	1.75	0.44
1:A:265:ARG:HH11	1:A:265:ARG:HD2	1.49	0.44
1:A:557:GLN:HG3	1:A:561:GLN:HE21	1.82	0.44
1:A:110:LYS:HE2	1:A:640:GLU:OE1	2.18	0.44
1:A:217:VAL:O	1:A:221:LEU:HD12	2.18	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
1:A:742:VAL:CG2	1:A:747:GLN:HG3	2.47	0.44
1:A:163:ASN:HD22	1:A:164:LYS:N	2.15	0.43
1:A:612:GLU:OE2	1:A:634:TYR:OH	2.27	0.43
1:A:861:ASP:OD2	1:A:862:PRO:HD2	2.18	0.43
1:A:183:ALA:O	1:A:184:GLN:C	2.59	0.43
1:A:144:ARG:HH11	1:A:144:ARG:HD2	1.62	0.43
1:A:612:GLU:OE2	1:A:621:TYR:OH	2.33	0.43
1:A:346:LEU:HA	1:A:351:GLU:OE2	2.19	0.43
1:A:696:LEU:HD23	1:A:696:LEU:HA	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:469:ILE:HG21	1:A:499:MET:HE1	2.00	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:198:PRO:HB2	1:A:263:ILE:HG21	2.01	0.43
1:A:728:LEU:CD1	1:A:728:LEU:C	2.92	0.43
1:A:765:GLY:O	1:A:768:GLU:HB2	2.18	0.43
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.86	0.43
1:A:17:LYS:HD2	1:A:17:LYS:HA	1.59	0.42
1:A:142:ILE:HD13	1:A:191:ILE:CD1	2.48	0.42
1:A:378:ASP:HB3	1:A:382:ARG:NH1	2.34	0.42
1:A:578:PHE:CD1	1:A:609:ARG:HG2	2.54	0.42
1:A:150:LYS:NZ	1:A:150:LYS:HA	2.34	0.42
1:A:442:PRO:HB2	1:A:445:TRP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:GLN:O	1:A:188:THR:N	2.38	0.42
1:A:329:TRP:CE2	1:A:333:ARG:HD3	2.55	0.42
1:A:611:THR:O	1:A:611:THR:HG22	2.19	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:69:LEU:HD22	1:A:73:ARG:HG3	2.01	0.42
1:A:783:ASP:HA	1:A:787:VAL:CG2	2.48	0.42
1:A:879:MET:CE	1:A:879:MET:CA	2.76	0.42
1:A:539:ILE:HG21	1:A:557:GLN:HG3	2.02	0.41
1:A:333:ARG:CZ	1:A:333:ARG:HB3	2.49	0.41
1:A:167:ALA:HB1	1:A:169:TYR:CE2	2.56	0.41
1:A:441:LEU:HA	1:A:442:PRO:HD3	1.82	0.41
1:A:863:ARG:HH11	1:A:863:ARG:CG	2.16	0.41
1:A:102:GLU:O	1:A:106:ARG:HG3	2.21	0.41
1:A:254:ASP:CG	1:A:713:ARG:HH22	2.29	0.41
1:A:515:ASN:O	1:A:519:THR:CG2	2.66	0.41
1:A:296:THR:O	1:A:297:PRO:C	2.61	0.41
1:A:8:LEU:O	1:A:12:VAL:HG13	2.21	0.41
1:A:203:LYS:NZ	1:A:270:LEU:HD11	2.34	0.41
1:A:225:ASN:HD21	1:A:235:LYS:HB3	1.85	0.41
1:A:411:ARG:HH11	1:A:411:ARG:HD3	1.50	0.41
1:A:585:ILE:HD13	1:A:596:LEU:CD1	2.46	0.41
1:A:625:GLU:OE2	1:A:625:GLU:CA	2.68	0.41
1:A:859:GLU:HA	1:A:860:PRO:HD2	1.85	0.41
1:A:164:LYS:O	1:A:165:ASP:HB2	2.21	0.41
1:A:178:LEU:HD23	1:A:178:LEU:HA	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:79:LEU:HD12	1:A:79:LEU:O	2.21	0.41
1:A:445:TRP:HZ3	1:A:455:LEU:HD11	1.85	0.41
1:A:276:THR:CG2	1:A:327:GLN:HB2	2.52	0.40
1:A:742:VAL:HG22	1:A:747:GLN:CG	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLN:NE2	1:A:618:ARG:HE	2.16	0.40
1:A:145:ARG:HD2	1:A:145:ARG:HA	1.79	0.40
1:A:499:MET:HA	1:A:500:PRO:HD3	1.93	0.40
1:A:597:LEU:HD12	1:A:641:ALA:HB2	2.03	0.40
1:A:46:ARG:NH2	1:A:775:ASP:OD2	2.39	0.40
1:A:191:ILE:HG22	1:A:192:ARG:O	2.21	0.40
1:A:312:TYR:OH	1:A:362:SER:HB2	2.21	0.40
1:A:615:GLU:HG2	1:A:719:PHE:HZ	1.86	0.40
1:A:837:ASP:CB	1:A:838:PRO:CD	3.00	0.40
1:A:326:THR:HG21	1:A:346:LEU:HB2	2.03	0.40
1:A:589:GLY:HA2	1:A:633:LEU:HD13	2.03	0.40
1:A:682:PHE:HE2	1:A:712:LEU:HD21	1.87	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%)	14	30

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%)	592 (82%)	133 (18%)	2 3

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	VAL
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	43	LYS
1	A	49	ASN
1	A	53	ARG
1	A	56	LEU
1	A	57	LEU
1	A	69	LEU
1	A	84	THR
1	A	90	SER
1	A	91	ILE
1	A	100	ASN
1	A	102	GLU
1	A	106	ARG
1	A	112	LYS
1	A	117	LEU
1	A	129	LEU
1	A	130	SER
1	A	131	LEU
1	A	133	LEU
1	A	136	THR
1	A	142	ILE
1	A	144	ARG
1	A	150	LYS

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Mol	Chain	Res	Type
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	184	GLN
1	A	192	ARG
1	A	193	LYS
1	A	194	LEU
1	A	197	SER
1	A	204	TRP
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	276	THR
1	A	280	LEU
1	A	288	SER
1	A	298	GLU
1	A	302	LEU
1	A	319	LEU
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	391	VAL
1	A	400	THR
1	A	406	LEU
1	A	419	GLU

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Mol	Chain	Res	Type
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	469	ILE
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	546	LYS
1	A	581	ARG
1	A	585	ILE
1	A	587	ARG
1	A	596	LEU
1	A	610	VAL
1	A	611	THR
1	A	615	GLU
1	A	638	ILE
1	A	639	LEU
1	A	648	GLU
1	A	656	ILE
1	A	662	VAL
1	A	676	LYS
1	A	684	SER
1	A	689	GLN
1	A	690	GLU
1	A	691	LEU
1	A	709	VAL
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

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Mol	Chain	Res	Type
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	808	VAL
1	A	810	LEU
1	A	816	SER
1	A	818	LEU
1	A	821	ASP
1	A	831	LEU
1	A	834	ILE
1	A	845	GLU
1	A	852	GLN
1	A	859	GLU
1	A	863	ARG
1	A	868	LEU
1	A	879	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	54	GLN
1	A	77	GLN
1	A	87	GLN
1	A	100	ASN
1	A	163	ASN
1	A	225	ASN
1	A	231	ASN
1	A	256	ASN
1	A	266	HIS
1	A	327	GLN
1	A	349	ASN
1	A	364	GLN
1	A	446	GLN
1	A	513	ASN
1	A	535	GLN
1	A	557	GLN
1	A	561	GLN
1	A	599	GLN

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Mol	Chain	Res	Type
1	A	800	ASN
1	A	817	HIS
1	A	843	GLN
1	A	866	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	7,8,8	1.38	1 (14%)	6,10,10	1.61	2 (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	ASP	A	884	-	-	0/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	884	ASP	OXT-C	3.05	1.40	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	884	ASP	OXT-C-O	-2.88	117.55	124.08
3	A	884	ASP	OD2-CG-CB	2.00	120.23	114.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	884	ASP	2	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	874/883 (98%)	-0.32	14 (1%) 70 66	18, 40, 70, 93	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	3.5
1	A	190	GLU	3.4
1	A	291	SER	3.0
1	A	710	GLU	2.4
1	A	116	GLU	2.3
1	A	4	GLN	2.2
1	A	339	LEU	2.2
1	A	655	ARG	2.2
1	A	28	GLY	2.2
1	A	581	ARG	2.1
1	A	188	THR	2.1
1	A	302	LEU	2.1
1	A	29	GLU	2.0
1	A	30	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	885	1/1	0.90	0.36	20,20,20,20	0
3	ASP	A	884	9/9	0.96	0.08	36,38,44,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.