



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:19 PM UTC

PDB ID : 1RKM / pdb_00001rkm
Title : STRUCTURE OF OPPA
Authors : Sleight, S.H.; Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1997-03-25
Resolution : 2.40 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

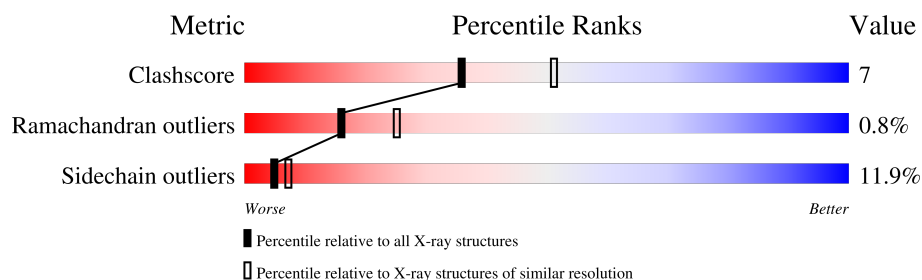
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	517	 51% 35% 12% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4291 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 OLIGO-PEPTIDE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	47	0	0
			4165	2666	700	794	5			

- Molecule 2 is water.

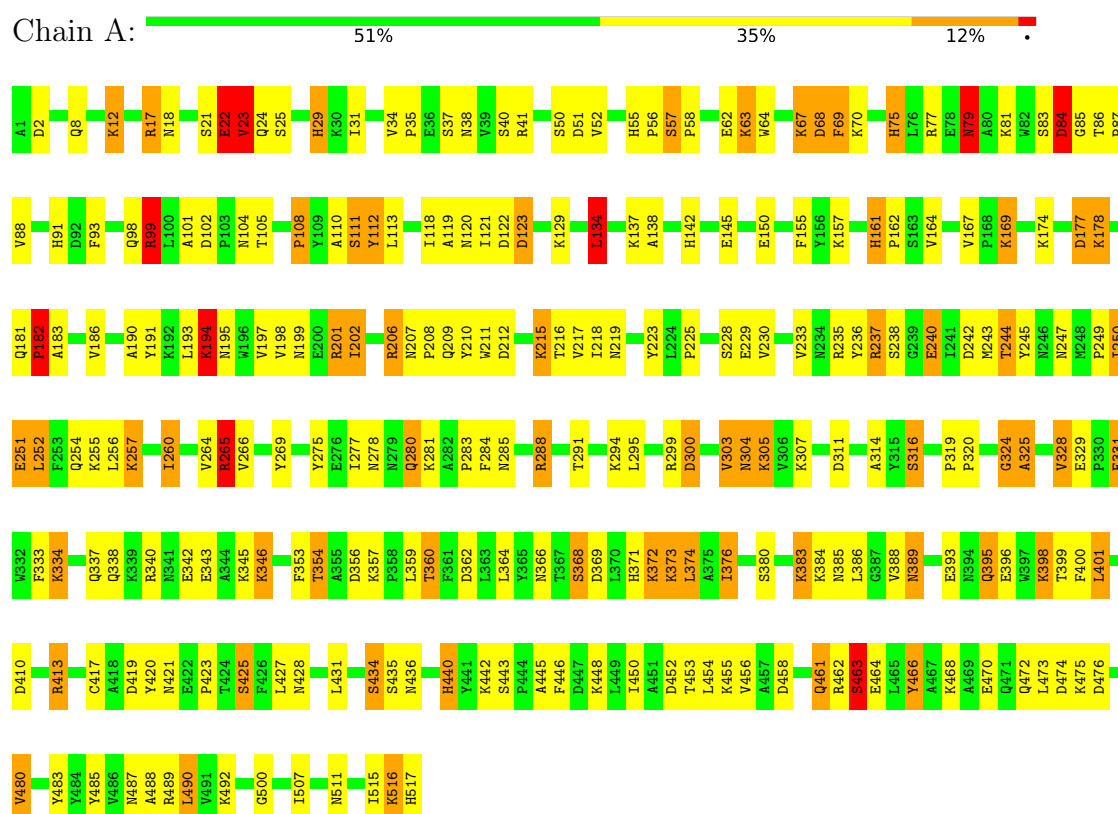
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: OLIGO-PEPTIDE BINDING PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.84Å 97.84Å 137.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.3 (20.00-2.40)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4291	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.18	12/4276 (0.3%)	2.38	248/5830 (4.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	21

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	GLN	CG-CD	14.71	1.88	1.52
1	A	448	LYS	CE-NZ	13.76	1.90	1.49
1	A	22	GLU	CG-CD	-11.51	1.23	1.52
1	A	174	LYS	CB-CG	10.54	1.84	1.52
1	A	475	LYS	CD-CE	-7.01	1.31	1.52
1	A	372	LYS	CE-NZ	6.96	1.70	1.49
1	A	288	ARG	CD-NE	-6.20	1.37	1.46
1	A	346	LYS	CD-CE	5.94	1.70	1.52
1	A	40	SER	CB-OG	5.73	1.53	1.42
1	A	398	LYS	CB-CG	5.50	1.69	1.52
1	A	480	VAL	N-CA	-5.35	1.42	1.46
1	A	329	GLU	C-O	-5.28	1.17	1.24

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ARG	CD-NE-CZ	24.20	158.29	124.40
1	A	300	ASP	CA-CB-CG	-15.02	97.58	112.60
1	A	240	GLU	CB-CG-CD	-14.49	87.97	112.60
1	A	235	ARG	CD-NE-CZ	13.96	143.95	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ASN	OD1-CG-ND2	-13.31	109.29	122.60
1	A	257	LYS	CG-CD-CE	-12.82	81.81	111.30
1	A	63	LYS	CG-CD-CE	12.40	139.83	111.30
1	A	177	ASP	CA-CB-CG	12.17	124.77	112.60
1	A	8	GLN	CG-CD-NE2	-11.89	98.56	116.40
1	A	265	ARG	NE-CZ-NH2	-11.35	108.99	119.20
1	A	284	PHE	CA-CB-CG	-10.83	102.97	113.80
1	A	22	GLU	CG-CD-OE1	-10.68	93.84	118.40
1	A	305	LYS	CG-CD-CE	10.60	135.69	111.30
1	A	75	HIS	CA-CB-CG	-10.22	103.58	113.80
1	A	38	ASN	OD1-CG-ND2	-10.13	112.47	122.60
1	A	41	ARG	NH1-CZ-NH2	9.83	132.08	119.30
1	A	174	LYS	CA-CB-CG	-9.79	94.51	114.10
1	A	475	LYS	CG-CD-CE	9.73	133.69	111.30
1	A	342	GLU	CA-CB-CG	9.71	133.51	114.10
1	A	201	ARG	CD-NE-CZ	9.48	137.67	124.40
1	A	75	HIS	CA-C-O	-9.11	111.06	120.54
1	A	340	ARG	CD-NE-CZ	-8.96	111.86	124.40
1	A	242	ASP	CA-CB-CG	-8.88	103.72	112.60
1	A	396	GLU	CA-CB-CG	8.87	131.84	114.10
1	A	265	ARG	CD-NE-CZ	-8.84	112.03	124.40
1	A	217	VAL	CA-C-O	-8.70	113.06	120.80
1	A	462	ARG	NE-CZ-NH2	-8.61	111.45	119.20
1	A	8	GLN	CG-CD-OE1	8.59	137.98	120.80
1	A	280	GLN	O-C-N	-8.46	112.00	122.24
1	A	386	LEU	N-CA-CB	-8.38	99.92	110.98
1	A	88	VAL	CA-C-O	-8.28	110.97	120.74
1	A	105	THR	N-CA-C	-8.27	102.97	113.23
1	A	247	ASN	CA-C-O	-8.15	111.57	120.30
1	A	83	SER	CA-C-O	-8.15	108.46	119.05
1	A	22	GLU	CB-CG-CD	8.10	126.36	112.60
1	A	120	ASN	CA-CB-CG	-8.06	104.54	112.60
1	A	41	ARG	NE-CZ-NH2	-8.00	112.00	119.20
1	A	395	GLN	OE1-CD-NE2	-7.99	114.61	122.60
1	A	285	ASN	N-CA-C	-7.86	103.67	113.18
1	A	371	HIS	CA-CB-CG	-7.84	105.96	113.80
1	A	201	ARG	NE-CZ-NH1	7.78	129.28	121.50
1	A	18	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	A	169	LYS	CA-C-N	7.64	132.29	120.82
1	A	169	LYS	C-N-CA	7.64	132.29	120.82
1	A	300	ASP	N-CA-C	7.62	120.26	111.11
1	A	137	LYS	CA-CB-CG	7.62	129.33	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	CD-NE-CZ	7.59	135.02	124.40
1	A	247	ASN	N-CA-CB	7.57	122.47	110.65
1	A	324	GLY	O-C-N	-7.41	113.78	122.45
1	A	461	GLN	OE1-CD-NE2	7.35	129.95	122.60
1	A	472	GLN	CA-C-O	-7.34	112.77	120.55
1	A	480	VAL	O-C-N	-7.34	114.17	120.92
1	A	314	ALA	N-CA-CB	-7.32	99.14	110.56
1	A	207	ASN	CA-C-O	7.27	125.60	119.71
1	A	87	PRO	CA-C-O	-7.27	112.59	121.31
1	A	178	LYS	CB-CA-C	7.27	122.84	110.56
1	A	142	HIS	CA-CB-CG	-7.22	106.58	113.80
1	A	195	ASN	OD1-CG-ND2	7.21	129.81	122.60
1	A	476	ASP	CA-CB-CG	-7.20	105.40	112.60
1	A	417	CYS	CA-C-O	-7.15	112.64	120.36
1	A	280	GLN	CA-C-O	7.11	127.78	119.32
1	A	177	ASP	CA-C-N	-7.09	111.31	122.65
1	A	177	ASP	C-N-CA	-7.09	111.31	122.65
1	A	210	TYR	CA-C-O	-7.08	113.41	121.19
1	A	396	GLU	CB-CG-CD	-7.04	100.64	112.60
1	A	112	TYR	CA-C-O	-7.02	112.17	120.10
1	A	384	LYS	O-C-N	-7.00	114.53	122.09
1	A	511	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	A	299	ARG	CA-C-O	6.95	127.95	120.10
1	A	111	SER	CA-CB-OG	-6.93	97.23	111.10
1	A	393	GLU	CB-CG-CD	6.93	124.38	112.60
1	A	362	ASP	CA-C-N	6.93	134.10	123.23
1	A	362	ASP	C-N-CA	6.93	134.10	123.23
1	A	288	ARG	CG-CD-NE	6.92	127.22	112.00
1	A	421	ASN	CA-C-O	-6.82	114.42	122.13
1	A	134	LEU	CA-C-O	-6.80	114.34	121.55
1	A	489	ARG	CD-NE-CZ	6.75	133.85	124.40
1	A	247	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	288	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	A	209	GLN	CB-CG-CD	-6.67	101.26	112.60
1	A	300	ASP	OD1-CG-OD2	6.64	138.83	122.90
1	A	104	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	419	ASP	CA-CB-CG	-6.53	106.07	112.60
1	A	247	ASN	O-C-N	6.53	130.84	123.27
1	A	257	LYS	CB-CA-C	6.51	122.90	109.95
1	A	121	ILE	O-C-N	-6.50	115.54	121.91
1	A	434	SER	O-C-N	-6.50	114.72	122.65
1	A	247	ASN	OD1-CG-ND2	6.49	129.09	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	ILE	O-C-N	-6.44	115.65	122.67
1	A	177	ASP	CA-C-O	6.40	127.17	119.43
1	A	217	VAL	CB-CA-C	-6.37	105.38	111.05
1	A	77	ARG	CD-NE-CZ	6.33	133.27	124.40
1	A	476	ASP	CB-CG-OD2	6.23	132.73	118.40
1	A	123	ASP	CA-CB-CG	-6.23	106.37	112.60
1	A	122	ASP	CA-C-O	-6.21	113.92	120.63
1	A	374	LEU	O-C-N	6.18	129.19	122.15
1	A	333	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	37	SER	CA-CB-OG	-6.12	98.86	111.10
1	A	120	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	A	466	TYR	CA-C-N	6.09	128.45	120.28
1	A	466	TYR	C-N-CA	6.09	128.45	120.28
1	A	63	LYS	CB-CG-CD	6.08	125.29	111.30
1	A	178	LYS	N-CA-C	-6.08	105.44	112.92
1	A	385	ASN	CB-CG-ND2	6.08	125.53	116.40
1	A	320	PRO	CB-CA-C	-6.08	103.22	111.85
1	A	369	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	353	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	468	LYS	CA-C-O	-6.02	114.04	120.42
1	A	464	GLU	CB-CG-CD	6.02	122.83	112.60
1	A	70	LYS	CB-CA-C	5.99	119.14	109.07
1	A	29	HIS	CA-CB-CG	-5.98	107.82	113.80
1	A	91	HIS	CA-CB-CG	-5.98	107.82	113.80
1	A	104	ASN	CB-CG-ND2	5.97	125.36	116.40
1	A	84	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	324	GLY	CA-C-O	5.97	125.92	119.06
1	A	194	LYS	O-C-N	-5.92	113.95	122.36
1	A	22	GLU	CA-C-N	-5.92	115.48	122.93
1	A	22	GLU	C-N-CA	-5.92	115.48	122.93
1	A	440	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	251	GLU	CB-CG-CD	5.90	122.63	112.60
1	A	485	TYR	CB-CA-C	-5.90	98.69	109.54
1	A	79	ASN	CB-CG-ND2	5.89	125.24	116.40
1	A	384	LYS	N-CA-C	5.89	117.50	111.14
1	A	374	LEU	CA-C-O	-5.87	114.19	120.42
1	A	164	VAL	O-C-N	5.87	128.03	122.05
1	A	399	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	120	ASN	CA-C-N	-5.85	113.18	120.56
1	A	120	ASN	C-N-CA	-5.85	113.18	120.56
1	A	436	ASN	CA-C-O	-5.78	112.80	119.56
1	A	85	GLY	N-CA-C	-5.76	107.14	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	VAL	CB-CA-C	5.75	118.66	110.84
1	A	250	ILE	N-CA-C	5.72	116.36	110.36
1	A	325	ALA	O-C-N	-5.72	116.50	123.19
1	A	24	GLN	CA-C-O	5.72	126.59	120.24
1	A	197	VAL	CA-C-N	5.69	132.22	121.97
1	A	197	VAL	C-N-CA	5.69	132.22	121.97
1	A	145	GLU	CA-C-O	5.68	126.63	120.32
1	A	207	ASN	CB-CA-C	5.68	115.55	110.44
1	A	228	SER	CA-C-O	5.68	126.45	120.54
1	A	2	ASP	CA-CB-CG	-5.67	106.92	112.60
1	A	428	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	119	ALA	O-C-N	-5.65	116.28	123.06
1	A	25	SER	CA-C-O	-5.65	114.66	120.99
1	A	473	LEU	CA-C-N	5.65	127.85	120.28
1	A	473	LEU	C-N-CA	5.65	127.85	120.28
1	A	515	ILE	CA-C-O	-5.64	114.42	120.85
1	A	41	ARG	CG-CD-NE	-5.63	99.62	112.00
1	A	420	TYR	CA-C-O	-5.61	115.44	121.45
1	A	93	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	389	ASN	CB-CG-ND2	5.61	124.81	116.40
1	A	376	ILE	CA-C-O	-5.59	115.24	121.17
1	A	41	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	67	LYS	CB-CG-CD	5.58	124.14	111.30
1	A	211	TRP	O-C-N	-5.58	115.69	122.22
1	A	342	GLU	CB-CG-CD	-5.58	103.11	112.60
1	A	56	PRO	CA-C-O	-5.55	115.27	121.32
1	A	266	VAL	CB-CA-C	-5.55	104.12	110.73
1	A	343	GLU	O-C-N	5.52	128.44	122.15
1	A	247	ASN	CB-CA-C	-5.50	101.03	110.16
1	A	264	VAL	O-C-N	-5.50	116.69	122.68
1	A	489	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	A	69	PHE	CA-C-O	-5.47	113.92	119.78
1	A	385	ASN	O-C-N	-5.47	114.91	122.46
1	A	110	ALA	CA-C-O	5.46	126.27	120.10
1	A	487	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	A	17	ARG	O-C-N	5.46	129.93	123.27
1	A	291	THR	O-C-N	5.44	128.36	122.15
1	A	181	GLN	CA-C-N	5.44	126.64	119.84
1	A	181	GLN	C-N-CA	5.44	126.64	119.84
1	A	329	GLU	OE1-CD-OE2	5.44	135.95	122.90
1	A	269	TYR	N-CA-CB	-5.42	101.43	111.13
1	A	202	ILE	N-CA-C	-5.41	100.33	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	GLN	CA-C-N	5.39	127.45	120.44
1	A	337	GLN	C-N-CA	5.39	127.45	120.44
1	A	79	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	A	462	ARG	NE-CZ-NH1	5.37	126.86	121.50
1	A	244	THR	CA-C-N	5.36	130.73	120.97
1	A	244	THR	C-N-CA	5.36	130.73	120.97
1	A	489	ARG	O-C-N	5.36	129.27	123.10
1	A	448	LYS	CD-CE-NZ	-5.36	94.75	111.90
1	A	12	LYS	CA-C-O	-5.35	114.97	120.54
1	A	463	SER	N-CA-CB	-5.35	101.52	110.39
1	A	218	ILE	CA-CB-CG1	-5.34	101.32	110.40
1	A	68	ASP	CA-CB-CG	-5.32	107.28	112.60
1	A	206	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	A	52	VAL	CA-C-O	-5.32	114.73	120.47
1	A	219	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	167	VAL	N-CA-CB	5.30	118.63	111.21
1	A	81	LYS	CB-CG-CD	5.30	123.48	111.30
1	A	102	ASP	CA-C-O	5.28	124.18	119.59
1	A	319	PRO	CA-C-N	5.27	124.94	119.56
1	A	319	PRO	C-N-CA	5.27	124.94	119.56
1	A	500	GLY	N-CA-C	-5.27	107.71	115.30
1	A	52	VAL	N-CA-CB	5.27	120.31	110.77
1	A	337	GLN	CG-CD-NE2	5.27	124.31	116.40
1	A	275	TYR	N-CA-CB	5.26	118.81	110.55
1	A	329	GLU	CG-CD-OE2	-5.25	106.33	118.40
1	A	304	ASN	CB-CG-ND2	5.25	124.27	116.40
1	A	18	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	242	ASP	O-C-N	5.24	129.35	122.33
1	A	427	LEU	N-CA-C	5.23	118.76	112.38
1	A	431	LEU	CA-C-O	-5.23	115.44	121.19
1	A	183	ALA	CA-C-N	-5.22	112.88	121.92
1	A	183	ALA	C-N-CA	-5.22	112.88	121.92
1	A	245	TYR	CA-C-O	-5.22	115.82	121.87
1	A	52	VAL	CB-CA-C	-5.22	103.81	112.26
1	A	380	SER	N-CA-CB	-5.21	102.45	110.16
1	A	243	MET	CB-CA-C	-5.20	103.03	110.62
1	A	244	THR	CA-C-O	5.20	127.47	122.01
1	A	316	SER	CA-C-O	-5.20	115.85	121.36
1	A	490	LEU	CA-C-N	-5.19	116.19	123.10
1	A	490	LEU	C-N-CA	-5.19	116.19	123.10
1	A	328	VAL	CA-CB-CG1	5.19	119.22	110.40
1	A	278	ASN	CA-C-N	5.18	130.62	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASN	C-N-CA	5.18	130.62	120.99
1	A	191	TYR	CA-CB-CG	-5.17	104.59	113.90
1	A	119	ALA	CA-C-O	5.16	126.58	120.96
1	A	450	ILE	N-CA-C	-5.16	105.38	111.00
1	A	62	GLU	N-CA-C	-5.15	106.15	112.90
1	A	215	LYS	N-CA-CB	-5.15	102.38	110.46
1	A	104	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	346	LYS	CA-CB-CG	5.13	124.37	114.10
1	A	420	TYR	CA-C-N	-5.12	115.18	122.41
1	A	420	TYR	C-N-CA	-5.12	115.18	122.41
1	A	393	GLU	CA-CB-CG	5.12	124.34	114.10
1	A	84	ASP	CB-CG-OD1	5.11	130.16	118.40
1	A	50	SER	CA-C-O	-5.11	114.77	120.54
1	A	445	ALA	CA-C-N	5.11	127.39	120.44
1	A	445	ALA	C-N-CA	5.11	127.39	120.44
1	A	101	ALA	CA-C-O	-5.11	115.01	120.42
1	A	425	SER	CA-CB-OG	-5.10	100.89	111.10
1	A	325	ALA	CA-C-O	-5.10	115.14	120.80
1	A	138	ALA	CA-C-O	-5.10	115.24	120.54
1	A	380	SER	O-C-N	-5.09	116.35	122.15
1	A	25	SER	O-C-N	5.08	129.07	123.33
1	A	216	THR	N-CA-C	-5.07	102.78	110.28
1	A	277	ILE	O-C-N	5.05	128.29	123.14
1	A	364	LEU	O-C-N	-5.04	117.15	123.04
1	A	108	PRO	O-C-N	-5.03	116.08	122.17
1	A	446	PHE	CA-C-O	-5.03	115.52	120.70
1	A	206	ARG	N-CA-CB	-5.03	101.70	109.69
1	A	401	LEU	CA-C-O	5.03	126.10	120.82
1	A	443	SER	CA-CB-OG	-5.02	101.06	111.10
1	A	517	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	64	TRP	CA-C-O	-5.01	116.09	121.45
1	A	137	LYS	CA-C-N	-5.01	116.33	122.84
1	A	137	LYS	C-N-CA	-5.01	116.33	122.84
1	A	364	LEU	N-CA-CB	-5.00	102.19	109.95

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PRO	Mainchain
1	A	112	TYR	Mainchain
1	A	134	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	155	PHE	Mainchain
1	A	161	HIS	Mainchain
1	A	182	PRO	Mainchain
1	A	190	ALA	Mainchain
1	A	194	LYS	Mainchain
1	A	22	GLU	Sidechain
1	A	237	ARG	Mainchain
1	A	283	PRO	Mainchain
1	A	325	ALA	Mainchain
1	A	376	ILE	Mainchain
1	A	425	SER	Mainchain
1	A	434	SER	Mainchain
1	A	442	LYS	Mainchain
1	A	463	SER	Mainchain
1	A	480	VAL	Mainchain
1	A	483	TYR	Mainchain
1	A	84	ASP	Mainchain
1	A	99	ARG	Mainchain

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	4165	0	4076	59	0
2	A	126	0	0	3	0
All	All	4291	0	4076	59	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 7.

All (59) 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:303:VAL:HG12	1:A:304:ASN:HD22	1.34	0.91
1:A:303:VAL:HG12	1:A:304:ASN:ND2	1.87	0.88
1:A:452:ASP:HA	1:A:455:LYS:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:THR:HB	1:A:389:ASN:HB2	1.77	0.67
1:A:331:GLU:HA	1:A:334:LYS:HE3	1.76	0.66
1:A:516:LYS:HD3	2:A:569:HOH:O	1.94	0.66
1:A:57:SER:HB2	1:A:58:PRO:CD	2.25	0.66
1:A:458:ASP:HB3	1:A:461:GLN:HB2	1.79	0.65
1:A:452:ASP:HA	1:A:455:LYS:CE	2.27	0.64
1:A:79:ASN:HD22	1:A:79:ASN:H	1.45	0.62
1:A:360:THR:HA	1:A:389:ASN:O	2.01	0.60
1:A:256:LEU:HD22	1:A:260:ILE:HD11	1.85	0.59
1:A:229:GLU:HB3	1:A:249:PRO:HD3	1.84	0.58
1:A:280:GLN:HG2	1:A:440:HIS:HB3	1.86	0.57
1:A:57:SER:HB2	1:A:58:PRO:HD2	1.88	0.55
1:A:23:VAL:HG22	1:A:202:ILE:HD11	1.88	0.54
1:A:17:ARG:HD3	1:A:223:TYR:CE1	2.43	0.54
1:A:359:LEU:HB3	1:A:388:VAL:HG12	1.90	0.52
1:A:307:LYS:NZ	1:A:311:ASP:OD2	2.42	0.52
1:A:413:ARG:HD3	1:A:413:ARG:C	2.35	0.51
1:A:236:TYR:CE2	1:A:492:LYS:HE2	2.45	0.51
1:A:265:ARG:O	1:A:488:ALA:HA	2.11	0.50
1:A:182:PRO:HG3	1:A:193:LEU:CD2	2.42	0.49
1:A:182:PRO:HG3	1:A:193:LEU:HD21	1.94	0.49
1:A:249:PRO:HG2	1:A:252:LEU:HB3	1.95	0.49
1:A:250:ILE:HD12	1:A:373:LYS:HE3	1.94	0.49
1:A:244:THR:HG23	1:A:490:LEU:HB2	1.95	0.48
1:A:294:LYS:NZ	1:A:474:ASP:O	2.47	0.48
1:A:316:SER:HB2	1:A:470:GLU:OE1	2.15	0.47
1:A:236:TYR:CZ	1:A:492:LYS:HE2	2.50	0.47
1:A:57:SER:CB	1:A:58:PRO:CD	2.91	0.46
1:A:29:HIS:ND1	1:A:99:ARG:NH1	2.63	0.46
1:A:75:HIS:HD2	2:A:539:HOH:O	1.98	0.45
1:A:383:LYS:HE3	1:A:389:ASN:ND2	2.31	0.45
1:A:456:VAL:HG11	1:A:461:GLN:HB3	1.98	0.45
1:A:453:THR:HG21	1:A:466:TYR:CE1	2.52	0.45
1:A:98:GLN:NE2	2:A:575:HOH:O	2.46	0.45
1:A:354:THR:HB	1:A:356:ASP:OD1	2.17	0.45
1:A:281:LYS:NZ	1:A:410:ASP:OD1	2.46	0.44
1:A:307:LYS:HG2	1:A:311:ASP:OD2	2.16	0.44
1:A:79:ASN:H	1:A:79:ASN:ND2	2.12	0.44
1:A:324:GLY:O	1:A:463:SER:HB2	2.18	0.44
1:A:113:LEU:HD22	1:A:118:ILE:HD13	1.98	0.44
1:A:251:GLU:H	1:A:251:GLU:HG2	1.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:O	1:A:208:PRO:HD3	2.17	0.44
1:A:212:ASP:OD1	1:A:215:LYS:HD3	2.18	0.44
1:A:51:ASP:OD1	1:A:55:HIS:N	2.32	0.43
1:A:373:LYS:HE2	1:A:373:LYS:HB2	1.62	0.43
1:A:401:LEU:HD23	1:A:401:LEU:HA	1.87	0.43
1:A:161:HIS:HA	1:A:162:PRO:HD3	1.79	0.43
1:A:84:ASP:CG	1:A:86:THR:HG1	2.25	0.43
1:A:395:GLN:HE21	1:A:400:PHE:HA	1.84	0.43
1:A:233:VAL:HG21	1:A:252:LEU:HD13	2.00	0.42
1:A:237:ARG:HD3	1:A:260:ILE:CD1	2.48	0.42
1:A:34:VAL:N	1:A:35:PRO:CD	2.82	0.42
1:A:374:LEU:HD23	1:A:374:LEU:HA	1.85	0.41
1:A:123:ASP:CB	1:A:129:LYS:HD2	2.51	0.41
1:A:68:ASP:O	1:A:69:PHE:HB2	2.21	0.40
1:A:366:ASN:HA	1:A:395:GLN:O	2.21	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	515/517 (100%)	492 (96%)	19 (4%)	4 (1%)	16	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	225	PRO
1	A	368	SER
1	A	182	PRO

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	455/455 (100%)	401 (88%)	54 (12%)	5 7

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	22	GLU
1	A	23	VAL
1	A	31	ILE
1	A	57	SER
1	A	63	LYS
1	A	67	LYS
1	A	79	ASN
1	A	111	SER
1	A	134	LEU
1	A	150	GLU
1	A	157	LYS
1	A	169	LYS
1	A	177	ASP
1	A	178	LYS
1	A	186	VAL
1	A	194	LYS
1	A	198	VAL
1	A	199	ASN
1	A	201	ARG
1	A	230	VAL
1	A	238	SER
1	A	240	GLU
1	A	252	LEU
1	A	254	GLN
1	A	255	LYS
1	A	257	LYS
1	A	260	ILE
1	A	265	ARG
1	A	288	ARG

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Mol	Chain	Res	Type
1	A	295	LEU
1	A	300	ASP
1	A	303	VAL
1	A	305	LYS
1	A	328	VAL
1	A	331	GLU
1	A	334	LYS
1	A	338	GLN
1	A	345	LYS
1	A	346	LYS
1	A	354	THR
1	A	357	LYS
1	A	360	THR
1	A	368	SER
1	A	372	LYS
1	A	373	LYS
1	A	383	LYS
1	A	398	LYS
1	A	413	ARG
1	A	423	PRO
1	A	435	SER
1	A	454	LEU
1	A	463	SER
1	A	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	79	ASN
1	A	195	ASN
1	A	304	ASN
1	A	309	GLN
1	A	337	GLN
1	A	341	ASN
1	A	391	ASN
1	A	395	GLN
1	A	440	HIS
1	A	487	ASN
1	A	506	ASN

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](#)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.