



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:27 PM EDT

PDB ID : 1OLA / pdb_00001ola
Title : THE STRUCTURAL BASIS OF MULTISPECIFICITY IN THE OLIGOPEPTIDE-BINDING PROTEIN OPPA
Authors : Tame, J.; Wilkinson, A.J.
Deposited on : 1994-04-26
Resolution : 2.10 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) : 2.50

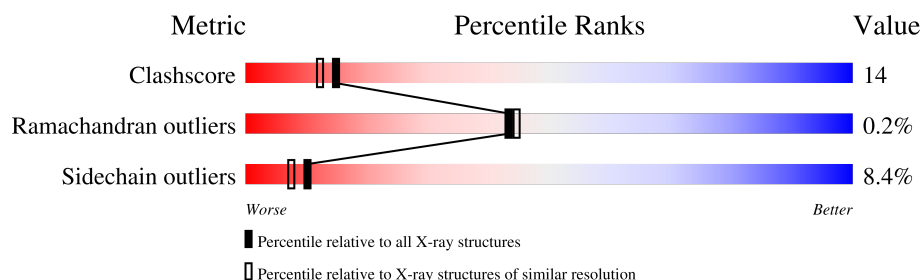
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	
2	B	4	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4463 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.

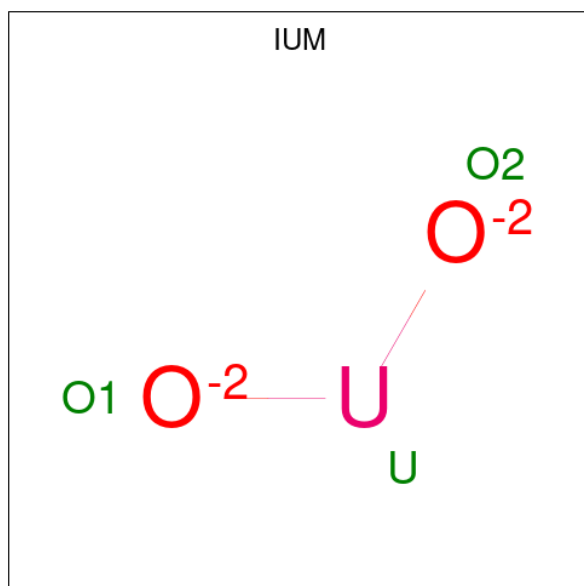
- Molecule 1 is a protein called OLIGO-PEPTIDE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4079	2603	681	790	5			

- Molecule 2 is a protein called PEPTIDE VAL-LYS-PRO-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			28	18	5	5			

- Molecule 3 is URANYL (VI) ION (CCD ID: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		

- Molecule 4 is water.

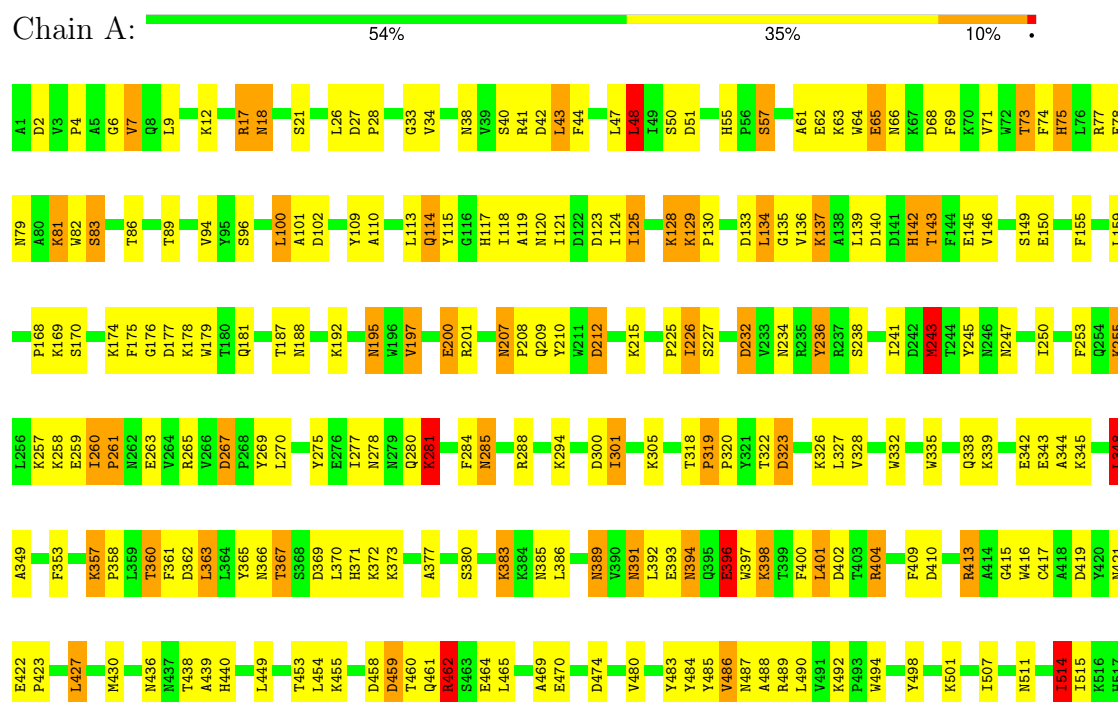
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	352	Total 352	O 352	0	0
4	B	2	Total 2	O 2	0	0

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



• Molecule 2: PEPTIDE VAL-LYS-PRO-GLY



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.50Å 74.50Å 70.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4463	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1/4190 (0.0%)	2.16	181/5723 (3.2%)
2	B	1.05	0/28	2.09	1/35 (2.9%)
All	All	1.18	1/4218 (0.0%)	2.15	182/5758 (3.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLN	N-CA	5.22	1.52	1.45

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ARG	CD-NE-CZ	12.12	141.36	124.40
1	A	459	ASP	N-CA-C	9.56	121.70	111.28
1	A	77	ARG	CD-NE-CZ	9.26	137.36	124.40
1	A	345	LYS	CA-C-O	8.99	130.52	120.90
1	A	207	ASN	CA-C-O	8.88	126.82	119.36
1	A	117	HIS	CA-CB-CG	-8.61	105.19	113.80
1	A	474	ASP	CA-C-N	8.59	131.61	120.44
1	A	474	ASP	C-N-CA	8.59	131.61	120.44
1	A	232	ASP	CA-CB-CG	8.55	121.15	112.60
1	A	369	ASP	CA-CB-CG	8.48	121.08	112.60
1	A	243	MET	N-CA-CB	8.48	124.59	110.77
1	A	7	VAL	N-CA-C	8.30	120.14	108.93
1	A	458	ASP	CA-C-N	8.24	131.32	120.28
1	A	458	ASP	C-N-CA	8.24	131.32	120.28
1	A	357	LYS	O-C-N	8.16	128.71	121.37
1	A	300	ASP	CA-CB-CG	-8.01	104.59	112.60
1	A	511	ASN	CA-CB-CG	8.01	120.61	112.60
1	A	120	ASN	O-C-N	7.95	130.38	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLU	O-C-N	7.89	126.76	121.71
1	A	400	PHE	CA-CB-CG	7.62	121.42	113.80
1	A	514	ILE	N-CA-CB	7.57	118.97	110.72
1	A	34	VAL	O-C-N	7.56	125.26	120.42
1	A	349	ALA	CA-C-O	7.52	128.71	120.82
1	A	278	ASN	CA-C-N	7.50	131.08	120.28
1	A	278	ASN	C-N-CA	7.50	131.08	120.28
1	A	77	ARG	CA-C-O	7.44	129.49	121.16
1	A	207	ASN	CB-CA-C	7.42	117.52	110.17
1	A	21	SER	CA-C-O	-7.23	113.54	121.28
1	A	129	LYS	O-C-N	7.21	128.00	121.80
1	A	21	SER	O-C-N	7.06	130.35	123.29
1	A	168	PRO	CA-C-N	7.01	132.34	121.19
1	A	168	PRO	C-N-CA	7.01	132.34	121.19
1	A	427	LEU	N-CA-C	6.96	119.76	111.33
1	A	260	ILE	CA-C-N	6.92	126.60	119.82
1	A	260	ILE	C-N-CA	6.92	126.60	119.82
1	A	188	ASN	O-C-N	6.89	129.74	122.23
1	A	267	ASP	O-C-N	6.87	126.91	121.55
1	A	68	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	43	LEU	N-CA-C	6.85	121.68	113.12
1	A	169	LYS	CA-C-N	6.83	130.28	120.79
1	A	169	LYS	C-N-CA	6.83	130.28	120.79
1	A	371	HIS	CA-CB-CG	-6.82	106.98	113.80
1	A	396	GLU	O-C-N	6.81	130.66	122.96
1	A	168	PRO	CB-CA-C	6.81	117.59	111.87
1	A	96	SER	CA-C-O	-6.80	113.70	120.70
1	A	348	LEU	O-C-N	6.77	129.87	122.15
1	A	128	LYS	CA-C-O	6.72	127.47	119.60
1	A	401	LEU	O-C-N	6.65	129.17	122.12
1	A	236	TYR	CA-C-N	6.64	129.18	120.28
1	A	236	TYR	C-N-CA	6.64	129.18	120.28
1	A	155	PHE	CA-CB-CG	-6.62	107.18	113.80
1	A	6	GLY	CA-C-N	6.61	130.42	120.77
1	A	6	GLY	C-N-CA	6.61	130.42	120.77
1	A	146	VAL	CA-C-O	6.56	127.21	120.39
1	A	391	ASN	CA-CB-CG	-6.54	106.06	112.60
1	A	209	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	A	338	GLN	OE1-CD-NE2	6.47	129.07	122.60
1	A	79	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	439	ALA	CA-C-O	6.36	127.20	119.31
1	A	383	LYS	CA-C-N	6.33	133.62	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	LYS	C-N-CA	6.33	133.62	121.54
1	A	261	PRO	N-CA-C	6.30	122.10	113.98
1	A	460	THR	O-C-N	6.28	129.30	122.15
1	A	33	GLY	CA-C-N	6.25	125.33	120.33
1	A	33	GLY	C-N-CA	6.25	125.33	120.33
1	A	50	SER	N-CA-CB	6.25	120.83	110.52
1	A	197	VAL	O-C-N	6.19	129.61	122.99
1	A	453	THR	CA-C-N	6.17	132.51	122.65
1	A	453	THR	C-N-CA	6.17	132.51	122.65
1	A	385	ASN	N-CA-C	6.14	120.50	112.89
1	A	83	SER	CA-CB-OG	-6.10	98.90	111.10
1	A	94	VAL	N-CA-CB	6.10	117.02	110.62
1	A	348	LEU	CA-C-O	-6.10	113.96	120.42
1	A	188	ASN	CA-C-O	-6.04	112.20	119.03
1	A	342	GLU	CA-C-O	6.04	126.95	120.55
1	A	159	LEU	N-CA-C	6.03	120.11	112.87
1	A	301	ILE	O-C-N	6.03	127.82	121.91
1	A	26	LEU	N-CA-C	-6.01	105.91	113.72
1	A	372	LYS	CA-C-N	5.99	128.62	120.54
1	A	372	LYS	C-N-CA	5.99	128.62	120.54
1	A	281	LYS	CA-CB-CG	5.96	126.01	114.10
1	A	82	TRP	CA-C-N	5.95	132.91	121.54
1	A	82	TRP	C-N-CA	5.95	132.91	121.54
1	A	17	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	A	371	HIS	N-CA-CB	5.92	118.83	110.12
1	A	48	LEU	CA-CB-CG	5.90	136.97	116.30
1	A	483	TYR	CA-C-N	5.90	130.62	122.77
1	A	483	TYR	C-N-CA	5.90	130.62	122.77
1	A	338	GLN	CB-CG-CD	-5.90	102.58	112.60
1	A	409	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	195	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	413	ARG	N-CA-C	-5.83	101.77	110.23
1	A	402	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	44	PHE	O-C-N	5.81	130.36	123.27
1	A	142	HIS	CA-CB-CG	-5.79	108.00	113.80
1	A	270	LEU	CB-CA-C	5.79	120.05	111.88
1	A	247	ASN	CA-C-O	-5.74	114.14	120.33
1	A	396	GLU	CA-CB-CG	5.71	125.52	114.10
1	A	389	ASN	N-CA-CB	5.65	119.85	110.47
1	A	69	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	389	ASN	O-C-N	5.65	130.25	123.13
1	A	462	ARG	CD-NE-CZ	-5.63	116.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	360	THR	CA-CB-OG1	-5.62	101.18	109.60
1	A	394	ASN	OD1-CG-ND2	5.61	128.21	122.60
1	A	367	THR	OG1-CB-CG2	5.60	120.50	109.30
1	A	485	TYR	CA-CB-CG	5.60	123.98	113.90
2	B	3	PRO	N-CA-CB	5.59	108.76	102.67
1	A	9	LEU	N-CA-C	5.56	117.92	110.35
1	A	430	MET	CA-C-N	5.54	128.57	120.71
1	A	430	MET	C-N-CA	5.54	128.57	120.71
1	A	81	LYS	O-C-N	5.53	129.86	123.17
1	A	343	GLU	O-C-N	5.52	127.76	122.07
1	A	82	TRP	N-CA-C	-5.50	103.13	110.55
1	A	62	GLU	CA-CB-CG	5.48	125.06	114.10
1	A	319	PRO	CB-CA-C	5.48	117.60	110.92
1	A	377	ALA	CA-C-N	5.47	127.57	120.56
1	A	377	ALA	C-N-CA	5.47	127.57	120.56
1	A	361	PHE	CA-C-N	5.46	130.25	122.72
1	A	361	PHE	C-N-CA	5.46	130.25	122.72
1	A	404	ARG	CB-CA-C	5.43	119.50	110.81
1	A	486	VAL	N-CA-C	-5.42	100.66	108.89
1	A	373	LYS	CA-C-N	5.41	127.47	120.44
1	A	373	LYS	C-N-CA	5.41	127.47	120.44
1	A	140	ASP	N-CA-C	-5.40	101.64	108.45
1	A	57	SER	CB-CA-C	5.39	118.33	109.97
1	A	343	GLU	CA-C-N	5.38	127.43	120.44
1	A	343	GLU	C-N-CA	5.38	127.43	120.44
1	A	28	PRO	CA-C-N	5.37	132.10	122.38
1	A	28	PRO	C-N-CA	5.37	132.10	122.38
1	A	212	ASP	CA-CB-CG	-5.37	107.23	112.60
1	A	226	ILE	CA-C-N	5.37	130.53	121.14
1	A	226	ILE	C-N-CA	5.37	130.53	121.14
1	A	89	THR	CA-C-N	5.34	127.97	120.28
1	A	89	THR	C-N-CA	5.34	127.97	120.28
1	A	344	ALA	CA-C-O	-5.33	115.22	120.82
1	A	253	PHE	CB-CA-C	5.32	119.33	110.81
1	A	238	SER	N-CA-C	-5.32	105.38	111.07
1	A	73	THR	O-C-N	5.32	129.44	123.27
1	A	178	LYS	CB-CA-C	5.31	119.57	110.01
1	A	255	LYS	CA-C-N	5.31	128.17	120.79
1	A	255	LYS	C-N-CA	5.31	128.17	120.79
1	A	12	LYS	CA-C-O	-5.29	114.51	120.43
1	A	42	ASP	CA-CB-CG	5.27	117.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	TYR	N-CA-C	5.27	117.52	110.35
1	A	27	ASP	CA-C-N	5.26	124.93	119.56
1	A	27	ASP	C-N-CA	5.26	124.93	119.56
1	A	245	TYR	O-C-N	-5.26	116.80	122.79
1	A	75	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	18	ASN	CA-C-O	-5.25	115.07	121.05
1	A	259	GLU	CA-CB-CG	5.25	124.59	114.10
1	A	47	LEU	CB-CA-C	5.24	119.11	110.88
1	A	201	ARG	CA-C-O	5.24	126.86	121.10
1	A	419	ASP	CA-C-O	5.24	124.90	119.14
1	A	386	LEU	N-CA-CB	-5.23	102.74	111.06
1	A	114	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	125	ILE	CA-C-N	5.22	127.80	120.28
1	A	125	ILE	C-N-CA	5.22	127.80	120.28
1	A	102	ASP	O-C-N	5.21	125.84	121.31
1	A	461	GLN	N-CA-C	-5.21	105.60	111.28
1	A	419	ASP	N-CA-C	-5.21	107.10	113.50
1	A	436	ASN	O-C-N	5.18	128.82	122.34
1	A	114	GLN	CB-CG-CD	5.15	121.36	112.60
1	A	363	LEU	CA-C-O	-5.15	114.95	120.46
1	A	61	ALA	N-CA-C	-5.15	102.07	110.20
1	A	389	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	94	VAL	CA-C-N	5.14	127.16	120.28
1	A	94	VAL	C-N-CA	5.14	127.16	120.28
1	A	322	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	234	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	A	27	ASP	O-C-N	5.11	125.93	121.18
1	A	86	THR	CB-CA-C	5.09	116.75	109.11
1	A	34	VAL	CA-C-O	-5.04	115.31	118.69
1	A	137	LYS	CA-CB-CG	5.04	124.18	114.10
1	A	38	ASN	O-C-N	5.03	127.25	122.07
1	A	195	ASN	N-CA-CB	-5.02	102.19	111.53
1	A	270	LEU	N-CA-CB	-5.02	104.13	110.45
1	A	370	LEU	CA-C-N	5.02	127.00	120.28
1	A	370	LEU	C-N-CA	5.02	127.00	120.28
1	A	51	ASP	N-CA-C	-5.01	102.59	110.36
1	A	358	PRO	N-CA-C	5.00	119.17	111.57
1	A	438	THR	CA-CB-CG2	5.00	119.00	110.50

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	4079	0	3889	109	0
2	B	28	0	34	7	0
3	A	2	0	0	0	0
4	A	352	0	0	29	2
4	B	2	0	0	1	0
All	All	4463	0	3923	111	2

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 14.

All (111) 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:427:LEU:HD23	4:A:764:HOH:O	1.18	1.31
1:A:383:LYS:CA	4:A:858:HOH:O	1.86	1.22
1:A:226:ILE:HG13	4:A:849:HOH:O	1.58	1.01
1:A:192:LYS:CA	4:A:778:HOH:O	2.10	0.99
1:A:149:SER:HA	4:A:686:HOH:O	1.67	0.93
1:A:142:HIS:CD2	4:A:685:HOH:O	2.24	0.90
1:A:109:TYR:HA	4:A:852:HOH:O	1.70	0.89
1:A:142:HIS:HD2	4:A:685:HOH:O	1.54	0.88
1:A:396:GLU:OE2	1:A:398:LYS:HE2	1.79	0.82
1:A:335:TRP:CD2	1:A:339:LYS:HD3	2.22	0.75
1:A:392:LEU:O	4:A:722:HOH:O	2.06	0.73
1:A:226:ILE:CG1	4:A:849:HOH:O	2.26	0.71
1:A:281:LYS:NZ	4:A:696:HOH:O	2.24	0.71
1:A:455:LYS:HD3	4:A:838:HOH:O	1.91	0.71
1:A:208:PRO:O	4:A:833:HOH:O	2.10	0.68
1:A:17:ARG:HD3	1:A:243:MET:HG3	1.76	0.67
1:A:124:ILE:HD13	1:A:129:LYS:HB2	1.77	0.66
1:A:417:CYS:SG	2:B:3:PRO:HG3	2.36	0.65
1:A:301:ILE:HA	1:A:305:LYS:HD2	1.79	0.64
2:B:4:GLY:HA3	4:B:328:HOH:O	1.98	0.64
1:A:391:ASN:HB2	4:A:868:HOH:O	1.97	0.63
1:A:41:ARG:HG2	4:A:666:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:HB3	1:A:129:LYS:HG3	1.81	0.62
1:A:66:ASN:HA	1:A:71:VAL:O	2.00	0.62
1:A:139:LEU:HB2	1:A:143:THR:HB	1.82	0.61
1:A:176:GLY:O	1:A:179:TRP:HD1	1.83	0.61
1:A:83:SER:HB2	1:A:187:THR:H	1.65	0.60
1:A:260:ILE:N	1:A:261:PRO:CD	2.63	0.60
1:A:323:ASP:O	1:A:423:PRO:HD3	2.02	0.60
1:A:404:ARG:O	1:A:440:HIS:HE1	1.85	0.60
1:A:255:LYS:CA	4:A:845:HOH:O	2.51	0.58
1:A:335:TRP:CG	1:A:339:LYS:HD3	2.37	0.58
1:A:263:GLU:O	1:A:490:LEU:HA	2.04	0.58
1:A:501:LYS:CA	4:A:840:HOH:O	2.52	0.57
1:A:17:ARG:HD2	4:A:557:HOH:O	2.05	0.55
1:A:40:SER:HB2	4:A:566:HOH:O	2.04	0.55
1:A:265:ARG:O	1:A:488:ALA:HA	2.06	0.55
1:A:124:ILE:HD12	1:A:130:PRO:O	2.07	0.55
1:A:226:ILE:HD13	1:A:226:ILE:N	2.20	0.55
1:A:427:LEU:CD2	4:A:764:HOH:O	2.03	0.55
1:A:197:VAL:HG12	1:A:200:GLU:HB2	1.89	0.55
1:A:207:ASN:ND2	4:A:681:HOH:O	2.35	0.55
1:A:285:ASN:N	1:A:285:ASN:HD22	2.06	0.54
1:A:43:LEU:O	1:A:187:THR:HB	2.08	0.53
1:A:396:GLU:OE2	1:A:398:LYS:CE	2.53	0.53
1:A:130:PRO:HD2	1:A:133:ASP:OD2	2.08	0.52
1:A:416:TRP:HE3	2:B:2:LYS:HD3	1.75	0.52
1:A:489:ARG:NH2	4:A:655:HOH:O	2.26	0.52
1:A:269:TYR:HB2	1:A:487:ASN:HB2	1.92	0.51
1:A:267:ASP:OD2	4:A:572:HOH:O	2.19	0.51
1:A:294:LYS:HE3	1:A:332:TRP:CE2	2.46	0.51
1:A:416:TRP:CE3	2:B:2:LYS:HD3	2.46	0.51
1:A:100:LEU:HD13	1:A:113:LEU:HG	1.91	0.51
1:A:323:ASP:HB2	1:A:421:ASN:OD1	2.11	0.50
1:A:422:GLU:HG2	4:A:712:HOH:O	2.11	0.50
1:A:17:ARG:CD	1:A:243:MET:HG3	2.41	0.50
1:A:64:TRP:HB3	1:A:74:PHE:CD2	2.47	0.50
1:A:137:LYS:HE3	1:A:145:GLU:OE1	2.13	0.49
1:A:494:TRP:O	1:A:515:ILE:HG13	2.12	0.49
1:A:275:TYR:CD1	1:A:363:LEU:HD11	2.47	0.49
1:A:320:PRO:HD3	1:A:484:TYR:CZ	2.47	0.49
1:A:285:ASN:HD22	1:A:285:ASN:H	1.61	0.48
1:A:18:ASN:ND2	1:A:232:ASP:OD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASP:OD1	1:A:215:LYS:CE	2.62	0.48
1:A:498:TYR:HE1	1:A:507:ILE:HD11	1.79	0.48
1:A:514:ILE:N	1:A:514:ILE:HD13	2.27	0.48
1:A:114:GLN:HA	1:A:121:ILE:HG21	1.96	0.48
1:A:277:ILE:CG2	1:A:284:PHE:HB3	2.44	0.48
1:A:360:THR:HA	1:A:389:ASN:O	2.14	0.48
1:A:78:GLU:HG3	4:A:719:HOH:O	2.15	0.47
1:A:65:GLU:CD	1:A:75:HIS:HE1	2.22	0.47
1:A:48:LEU:HB3	1:A:57:SER:O	2.16	0.46
1:A:123:ASP:CB	1:A:129:LYS:HG3	2.44	0.46
1:A:115:TYR:CD1	1:A:115:TYR:N	2.82	0.45
1:A:4:PRO:HG2	1:A:7:VAL:HG21	1.97	0.45
1:A:417:CYS:HB2	2:B:1:VAL:HG23	1.98	0.45
1:A:449:LEU:HD13	1:A:469:ALA:HA	1.98	0.45
1:A:415:GLY:O	2:B:3:PRO:HD2	2.17	0.45
1:A:277:ILE:HD11	1:A:480:VAL:HG23	1.99	0.44
1:A:134:LEU:HD13	1:A:136:VAL:HG13	2.00	0.44
1:A:260:ILE:N	1:A:261:PRO:HD3	2.32	0.44
1:A:119:ALA:HB3	1:A:135:GLY:HA3	1.99	0.43
1:A:118:ILE:CG2	1:A:134:LEU:HD22	2.48	0.43
1:A:174:LYS:HB2	4:A:739:HOH:O	2.17	0.43
1:A:250:ILE:HA	4:A:803:HOH:O	2.17	0.43
1:A:236:TYR:O	1:A:492:LYS:NZ	2.39	0.43
1:A:236:TYR:OH	1:A:263:GLU:HB3	2.19	0.43
1:A:360:THR:HG23	1:A:389:ASN:HB2	2.01	0.42
1:A:366:ASN:O	1:A:367:THR:C	2.61	0.42
1:A:462:ARG:HH11	1:A:462:ARG:HD2	1.49	0.42
1:A:55:HIS:HD2	4:A:725:HOH:O	2.02	0.42
1:A:327:LEU:HD22	1:A:470:GLU:HG3	2.01	0.42
1:A:210:TYR:CE2	1:A:212:ASP:HB3	2.55	0.42
1:A:362:ASP:O	1:A:410:ASP:HB2	2.20	0.42
1:A:365:TYR:CZ	1:A:394:ASN:HB3	2.54	0.42
1:A:64:TRP:HA	1:A:73:THR:O	2.20	0.42
1:A:174:LYS:HD3	1:A:175:PHE:CZ	2.55	0.42
1:A:285:ASN:H	1:A:285:ASN:ND2	2.18	0.42
1:A:348:LEU:HD22	1:A:353:PHE:HD2	1.85	0.42
1:A:397:TRP:CE2	1:A:401:LEU:HD11	2.55	0.42
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.88	0.41
1:A:236:TYR:HA	1:A:241:ILE:HB	2.01	0.41
1:A:101:ALA:HB2	1:A:113:LEU:HD12	2.03	0.41
4:A:568:HOH:O	2:B:2:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD22	1:A:110:ALA:HA	2.03	0.41
1:A:128:LYS:HB3	1:A:128:LYS:HE2	1.90	0.41
1:A:318:THR:HA	1:A:319:PRO:HD3	1.94	0.41
1:A:4:PRO:HB2	1:A:7:VAL:HG23	2.02	0.41
1:A:64:TRP:C	1:A:65:GLU:CG	2.93	0.40
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.94	0.40
1:A:4:PRO:CG	1:A:7:VAL:HG21	2.50	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:665:HOH:O	4:A:665:HOH:O[2_555]	1.50	0.70
4:A:857:HOH:O	4:A:857:HOH:O[2_545]	1.91	0.29

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%)	493 (96%)	21 (4%)	1 (0%)	43	44
2	B	2/4 (50%)	2 (100%)	0	0	100	100
All	All	517/521 (99%)	495 (96%)	21 (4%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	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	437/455 (96%)	401 (92%)	36 (8%)	10	8
2	B	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	440/458 (96%)	403 (92%)	37 (8%)	10	7

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	63	LYS
1	A	65	GLU
1	A	81	LYS
1	A	100	LEU
1	A	125	ILE
1	A	134	LEU
1	A	143	THR
1	A	170	SER
1	A	177	ASP
1	A	195	ASN
1	A	200	GLU
1	A	227	SER
1	A	243	MET
1	A	257	LYS
1	A	258	LYS
1	A	280	GLN
1	A	281	LYS
1	A	285	ASN
1	A	288	ARG
1	A	323	ASP
1	A	326	LYS
1	A	328	VAL
1	A	348	LEU
1	A	357	LYS
1	A	380	SER
1	A	393	GLU

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Mol	Chain	Res	Type
1	A	396	GLU
1	A	398	LYS
1	A	413	ARG
1	A	454	LEU
1	A	459	ASP
1	A	462	ARG
1	A	464	GLU
1	A	486	VAL
1	A	514	ILE
2	B	1	VAL

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	24	GLN
1	A	75	HIS
1	A	91	HIS
1	A	117	HIS
1	A	142	HIS
1	A	184	ASN
1	A	195	ASN
1	A	207	ASN
1	A	280	GLN
1	A	285	ASN
1	A	391	ASN
1	A	440	HIS

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

Of 2 ligands modelled in this entry, 2 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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.