



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 PM UTC

PDB ID : 1B52 / pdb_00001b52
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KTK
Authors : Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1999-01-11
Resolution : 2.30 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

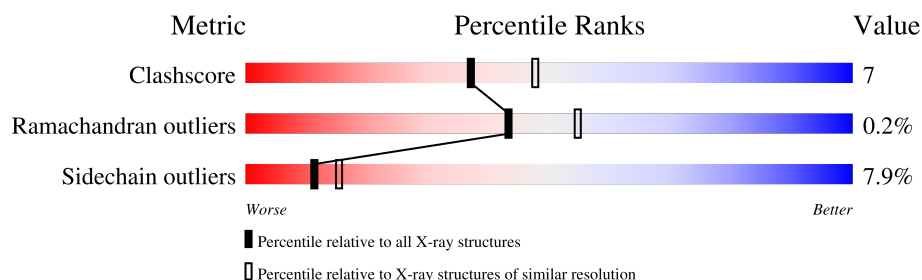
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	3	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4301 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.

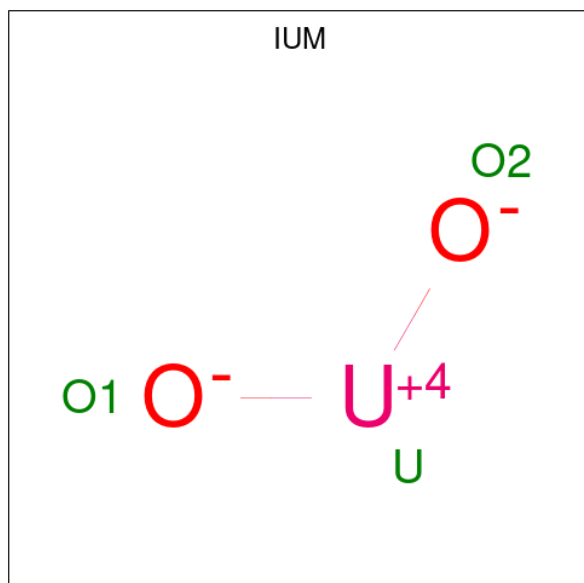
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	1	0	0
			4148	2656	697	790	5			

- Molecule 2 is a protein called PROTEIN (LYS-THR-LYS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			26	16	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.

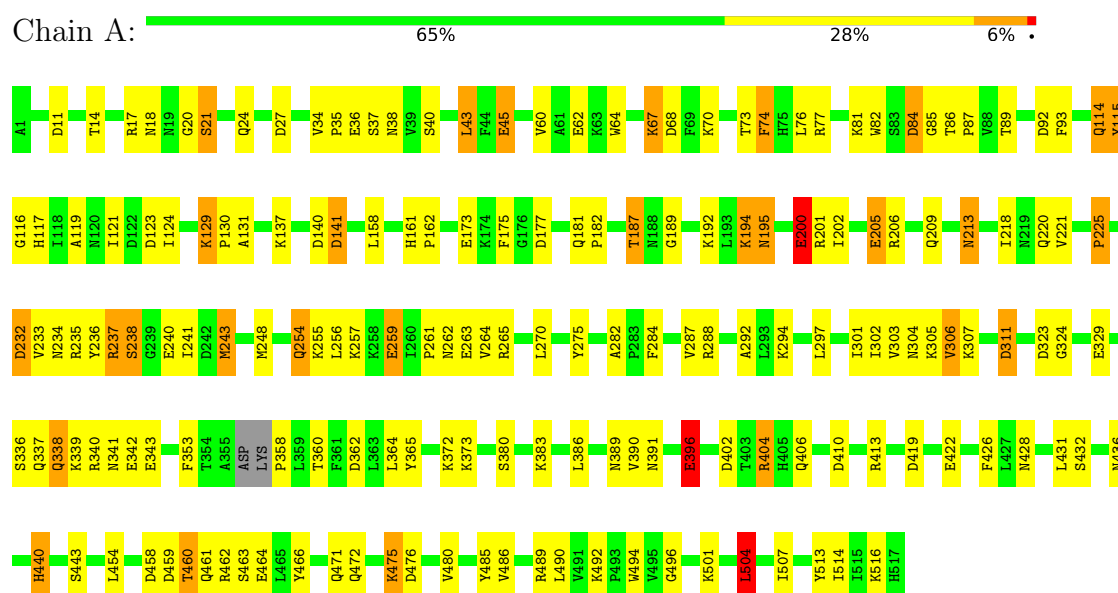
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total 122	O 122	0	0
4	B	3	Total 3	O 3	0	0

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: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



• Molecule 2: PROTEIN (LYS-THR-LYS)



There are no outlier residues recorded for this chain.

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 A	Depositor
Cell constants a, b, c, α , β , γ	106.35 Å 76.80 Å 69.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	98.5 (15.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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: 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	0.99	2/4258 (0.0%)	1.98	110/5804 (1.9%)
2	B	1.05	0/25	1.49	0/29
All	All	0.99	2/4283 (0.0%)	1.98	110/5833 (1.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	PHE	C-O	-23.39	0.95	1.24
1	A	410	ASP	CG-OD2	-5.42	1.15	1.25

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	PHE	CA-C-O	19.65	141.80	120.38
1	A	353	PHE	O-C-N	-14.62	106.04	123.29
1	A	265	ARG	CD-NE-CZ	14.07	144.10	124.40
1	A	195	ASN	CA-CB-CG	11.16	123.76	112.60
1	A	114	GLN	CB-CG-CD	9.48	128.71	112.60
1	A	77	ARG	CD-NE-CZ	8.42	136.19	124.40
1	A	460	THR	CA-C-O	8.41	129.33	120.42
1	A	284	PHE	CA-CB-CG	-8.06	105.74	113.80
1	A	93	PHE	CA-CB-CG	-7.88	105.92	113.80
1	A	21	SER	O-C-N	-7.76	115.97	123.26
1	A	471	GLN	OE1-CD-NE2	-7.61	114.99	122.60
1	A	476	ASP	CA-CB-CG	-7.58	105.03	112.60
1	A	288	ARG	CD-NE-CZ	7.48	134.87	124.40
1	A	489	ARG	NE-CZ-NH2	-7.47	112.47	119.20
1	A	410	ASP	CA-CB-CG	-7.44	105.16	112.60
1	A	302	ILE	CB-CG1-CD1	-7.38	98.30	113.80
1	A	301	ILE	CA-C-N	-7.12	111.45	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ILE	C-N-CA	-7.12	111.45	120.56
1	A	292	ALA	CA-C-O	-7.10	113.03	120.55
1	A	140	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	40	SER	CA-C-O	-6.88	113.26	120.55
1	A	413	ARG	CD-NE-CZ	6.83	133.96	124.40
1	A	200	GLU	CB-CG-CD	6.80	124.17	112.60
1	A	475	LYS	CA-C-O	-6.75	112.20	119.97
1	A	460	THR	CA-C-N	6.63	129.17	120.28
1	A	460	THR	C-N-CA	6.63	129.17	120.28
1	A	440	HIS	CA-CB-CG	-6.58	107.22	113.80
1	A	458	ASP	N-CA-CB	-6.56	99.44	111.37
1	A	432	SER	O-C-N	6.55	129.07	122.12
1	A	288	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	A	27	ASP	N-CA-C	-6.54	101.40	109.65
1	A	342	GLU	CB-CA-C	-6.48	100.70	110.88
1	A	259	GLU	N-CA-C	6.48	118.42	111.36
1	A	177	ASP	CA-CB-CG	-6.43	106.17	112.60
1	A	158	LEU	CB-CA-C	-6.40	96.93	110.31
1	A	475	LYS	N-CA-CB	6.38	120.16	110.28
1	A	323	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	364	LEU	CA-C-O	6.33	127.83	120.80
1	A	386	LEU	N-CA-CB	-6.32	101.01	111.06
1	A	187	THR	N-CA-C	6.27	119.40	109.81
1	A	115	TYR	N-CA-CB	6.25	119.31	110.12
1	A	436	ASN	CA-C-O	6.25	126.88	119.56
1	A	386	LEU	CB-CA-C	6.18	118.63	109.29
1	A	311	ASP	CA-C-O	-6.18	114.70	121.87
1	A	485	TYR	CA-CB-CG	6.13	124.93	113.90
1	A	45	GLU	CB-CG-CD	6.12	123.01	112.60
1	A	117	HIS	CA-CB-CG	-6.11	107.69	113.80
1	A	426	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	343	GLU	CG-CD-OE1	6.07	132.36	118.40
1	A	413	ARG	CG-CD-NE	-6.05	98.70	112.00
1	A	43	LEU	N-CA-C	6.01	120.64	113.12
1	A	419	ASP	N-CA-C	-6.01	106.10	113.50
1	A	195	ASN	CA-C-O	6.01	128.19	121.40
1	A	141	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	195	ASN	N-CA-CB	5.98	122.10	111.69
1	A	404	ARG	CA-C-O	-5.90	114.62	120.82
1	A	362	ASP	CB-CG-OD2	5.87	131.90	118.40
1	A	202	ILE	N-CA-C	-5.86	99.69	108.12
1	A	175	PHE	N-CA-C	5.84	120.27	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	SER	CA-C-O	-5.83	114.33	120.63
1	A	516	LYS	CA-C-O	-5.83	114.61	120.96
1	A	306	VAL	CB-CA-C	5.83	118.25	111.55
1	A	362	ASP	CB-CG-OD1	-5.81	105.03	118.40
1	A	504	LEU	CD1-CG-CD2	-5.78	98.09	110.80
1	A	463	SER	CA-CB-OG	-5.67	99.76	111.10
1	A	232	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	137	LYS	CA-CB-CG	5.64	125.38	114.10
1	A	297	LEU	CA-C-N	-5.62	115.54	122.84
1	A	297	LEU	C-N-CA	-5.62	115.54	122.84
1	A	275	TYR	CA-C-O	5.60	126.36	120.54
1	A	431	LEU	CA-C-N	5.57	128.01	120.38
1	A	431	LEU	C-N-CA	5.57	128.01	120.38
1	A	340	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	A	84	ASP	O-C-N	-5.53	115.24	122.59
1	A	189	GLY	O-C-N	-5.50	117.52	122.96
1	A	485	TYR	N-CA-C	5.50	117.78	110.53
1	A	304	ASN	CA-C-O	-5.49	112.50	119.31
1	A	461	GLN	N-CA-C	-5.47	105.32	111.28
1	A	82	TRP	N-CA-C	-5.47	103.31	110.53
1	A	116	GLY	CA-C-N	5.46	129.88	122.19
1	A	116	GLY	C-N-CA	5.46	129.88	122.19
1	A	460	THR	O-C-N	-5.44	115.95	122.15
1	A	341	ASN	CA-C-N	5.42	127.48	120.44
1	A	341	ASN	C-N-CA	5.42	127.48	120.44
1	A	74	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	282	ALA	CA-C-O	-5.39	114.56	120.17
1	A	432	SER	CB-CA-C	-5.37	101.55	110.68
1	A	38	ASN	CA-CB-CG	-5.34	107.26	112.60
1	A	489	ARG	NH1-CZ-NH2	5.30	126.19	119.30
1	A	60	VAL	CA-C-O	-5.27	115.47	120.95
1	A	486	VAL	N-CA-C	-5.26	100.90	108.89
1	A	329	GLU	CB-CA-C	-5.16	101.15	109.67
1	A	362	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	391	ASN	O-C-N	-5.16	117.44	123.27
1	A	287	VAL	O-C-N	-5.16	116.66	121.87
1	A	396	GLU	CA-C-N	5.15	129.37	121.19
1	A	396	GLU	C-N-CA	5.15	129.37	121.19
1	A	472	GLN	CA-C-O	5.13	125.86	120.42
1	A	390	VAL	N-CA-C	5.12	115.34	108.17
1	A	254	GLN	CA-CB-CG	5.11	124.32	114.10
1	A	464	GLU	CA-C-O	-5.10	115.02	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	VAL	N-CA-CB	-5.09	104.33	111.25
1	A	119	ALA	CA-C-O	5.04	126.90	121.55
1	A	358	PRO	N-CA-CB	5.04	108.54	103.00
1	A	342	GLU	N-CA-CB	5.03	117.31	110.01
1	A	213	ASN	O-C-N	-5.03	116.79	122.12
1	A	324	GLY	CA-C-N	-5.01	113.50	122.07
1	A	324	GLY	C-N-CA	-5.01	113.50	122.07
1	A	70	LYS	CB-CA-C	5.01	117.14	109.03
1	A	337	GLN	OE1-CD-NE2	5.01	127.61	122.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4148	0	4059	59	0
2	B	26	0	35	0	0
3	A	2	0	0	0	0
4	A	122	0	0	4	0
4	B	3	0	0	0	0
All	All	4301	0	4094	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:37:SER:HB2	4:A:578:HOH:O	1.70	0.90
1:A:17:ARG:HG2	1:A:243:MET:HG3	1.68	0.75
1:A:402:ASP:HB2	4:A:641:HOH:O	1.91	0.69
1:A:129:LYS:HB3	1:A:130:PRO:HD2	1.76	0.67
1:A:236:TYR:CZ	1:A:492:LYS:HD3	2.31	0.66
1:A:206:ARG:HD3	1:A:213:ASN:OD1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HG3	1:A:205:GLU:HG2	1.79	0.65
1:A:365:TYR:OH	1:A:372:LYS:HG3	2.01	0.60
1:A:248:MET:HA	1:A:248:MET:HE2	1.84	0.59
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.37	0.58
1:A:234:ASN:ND2	4:A:615:HOH:O	2.08	0.57
1:A:200:GLU:O	1:A:201:ARG:HB3	2.05	0.56
1:A:238:SER:OG	1:A:240:GLU:HG3	2.06	0.56
1:A:236:TYR:CE2	1:A:492:LYS:HD3	2.40	0.55
1:A:263:GLU:O	1:A:490:LEU:HA	2.05	0.55
1:A:67:LYS:O	1:A:68:ASP:HB2	2.09	0.53
1:A:85:GLY:HA2	1:A:209:GLN:NE2	2.25	0.51
1:A:235:ARG:HB2	1:A:241:ILE:HD12	1.93	0.50
1:A:270:LEU:HD12	1:A:504:LEU:CD2	2.42	0.49
1:A:396:GLU:HB2	4:A:634:HOH:O	2.12	0.49
1:A:192:LYS:HG2	1:A:205:GLU:O	2.12	0.49
1:A:194:LYS:HG3	1:A:205:GLU:CG	2.42	0.48
1:A:181:GLN:NE2	1:A:182:PRO:HD2	2.30	0.47
1:A:459:ASP:OD1	1:A:462:ARG:NH1	2.47	0.47
1:A:89:THR:O	1:A:92:ASP:HB2	2.14	0.47
1:A:114:GLN:HA	1:A:121:ILE:HG21	1.95	0.47
1:A:43:LEU:O	1:A:187:THR:HB	2.15	0.47
1:A:129:LYS:HB3	1:A:130:PRO:CD	2.44	0.47
1:A:89:THR:HB	1:A:141:ASP:O	2.16	0.46
1:A:422:GLU:OE2	1:A:466:TYR:OH	2.34	0.45
1:A:338:GLN:HG3	1:A:339:LYS:N	2.30	0.45
1:A:18:ASN:HD22	1:A:232:ASP:CG	2.24	0.45
1:A:20:GLY:O	1:A:21:SER:HB3	2.16	0.45
1:A:86:THR:HB	1:A:87:PRO:CD	2.46	0.45
1:A:257:LYS:HZ2	1:A:264:VAL:HG11	1.82	0.44
1:A:360:THR:HA	1:A:389:ASN:O	2.17	0.44
1:A:492:LYS:HG3	1:A:494:TRP:CZ2	2.53	0.44
1:A:124:ILE:HD13	1:A:131:ALA:HA	2.00	0.44
1:A:218:ILE:HD11	1:A:514:ILE:HG12	2.00	0.44
1:A:123:ASP:HB3	1:A:129:LYS:HG3	2.00	0.44
1:A:64:TRP:HA	1:A:73:THR:O	2.18	0.44
1:A:218:ILE:HD11	1:A:514:ILE:CD1	2.48	0.44
1:A:257:LYS:O	1:A:261:PRO:HD3	2.17	0.43
1:A:129:LYS:CB	1:A:130:PRO:HD2	2.45	0.43
1:A:129:LYS:CB	1:A:130:PRO:CD	2.97	0.43
1:A:307:LYS:NZ	1:A:311:ASP:OD2	2.47	0.43
1:A:24:GLN:HG3	1:A:36:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:NH1	1:A:259:GLU:OE1	2.51	0.43
1:A:294:LYS:HA	1:A:480:VAL:HG13	2.00	0.43
1:A:64:TRP:HB3	1:A:74:PHE:CD2	2.55	0.42
1:A:496:GLY:HA3	1:A:513:TYR:CE1	2.54	0.42
1:A:303:VAL:HG13	1:A:311:ASP:HB2	2.02	0.41
1:A:233:VAL:HG11	1:A:256:LEU:HD11	2.02	0.41
1:A:404:ARG:O	1:A:440:HIS:HE1	2.03	0.41
1:A:34:VAL:N	1:A:35:PRO:CD	2.84	0.41
1:A:161:HIS:CD2	1:A:162:PRO:HD2	2.56	0.41
1:A:14:THR:HG22	1:A:220:GLN:HB3	2.04	0.40
1:A:84:ASP:OD1	1:A:84:ASP:C	2.64	0.40
1:A:233:VAL:HG22	1:A:490:LEU:HD11	2.04	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	511/517 (99%)	480 (94%)	30 (6%)	1 (0%)	43	55
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	512/520 (98%)	481 (94%)	30 (6%)	1 (0%)	43	55

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	453/455 (100%)	417 (92%)	36 (8%)	11	15
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	456/458 (100%)	420 (92%)	36 (8%)	11	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	45	GLU
1	A	62	GLU
1	A	67	LYS
1	A	76	LEU
1	A	81	LYS
1	A	129	LYS
1	A	173	GLU
1	A	194	LYS
1	A	195	ASN
1	A	200	GLU
1	A	205	GLU
1	A	221	VAL
1	A	225	PRO
1	A	237	ARG
1	A	238	SER
1	A	243	MET
1	A	254	GLN
1	A	255	LYS
1	A	262	ASN
1	A	305	LYS
1	A	306	VAL
1	A	336	SER
1	A	338	GLN
1	A	373	LYS
1	A	380	SER
1	A	383	LYS

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Mol	Chain	Res	Type
1	A	396	GLU
1	A	406	GLN
1	A	443	SER
1	A	454	LEU
1	A	460	THR
1	A	475	LYS
1	A	501	LYS
1	A	504	LEU
1	A	507	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	142	HIS
1	A	161	HIS
1	A	181	GLN
1	A	199	ASN
1	A	209	GLN
1	A	262	ASN
1	A	279	ASN
1	A	308	ASN
1	A	389	ASN
1	A	440	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 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.