



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:30 PM GMT

PDB ID : 1B3L  
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KGK  
Authors : Tame, J.R.H.; Wilkinson, A.J.  
Deposited on : 1998-12-11  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

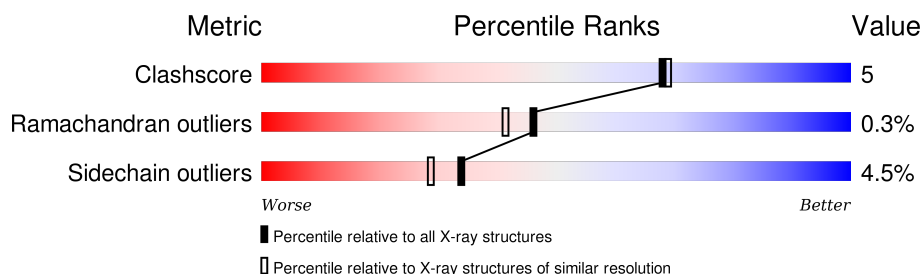
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	517	 75% 21% •
1	C	517	 84% 15% •
2	B	3	 100%
2	D	3	 67% 33%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8730 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.

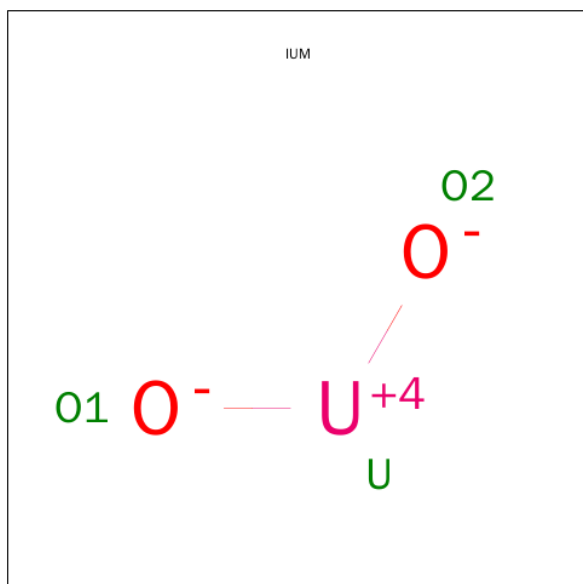
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	11	2	0
			4171	2671	700	795	5			
1	C	517	Total	C	N	O	S	8	4	0
			4173	2671	700	797	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			23	14	5	4			
2	D	3	Total	C	N	O	0	0	0
			23	14	5	4			

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



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

- Molecule 4 is water.

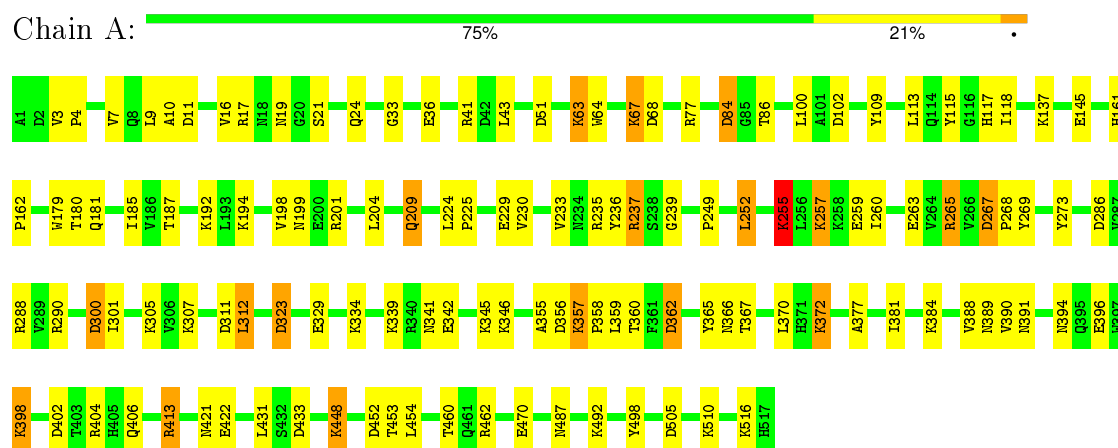
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	124	Total O 124 124	0	0
4	B	3	Total O 3 3	0	0
4	C	209	Total O 209 209	0	0
4	D	3	Total O 3 3	0	0

### 3 Residue-property plots

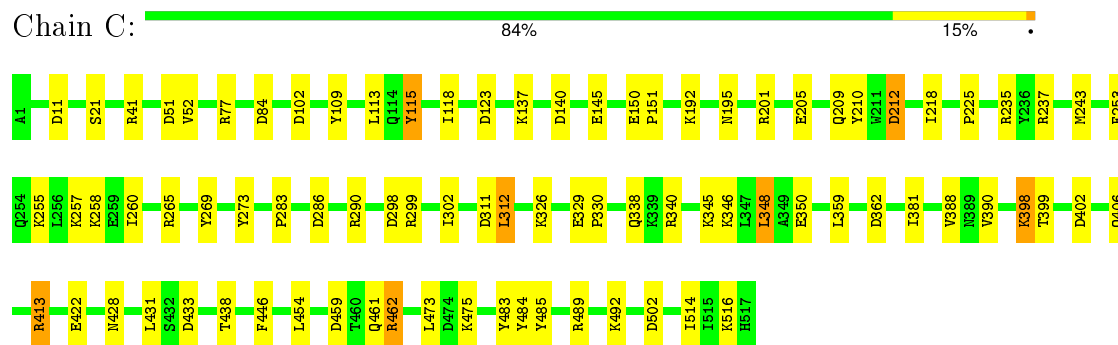
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



#### • Molecule 1: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



#### • Molecule 2: PROTEIN (LYS-GLY-LYS)



There are no outlier residues recorded for this chain.

#### • Molecule 2: PROTEIN (LYS-GLY-LYS)





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.91 Å 74.80 Å 103.77 Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.8 (15.00-2.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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	1.19	4/4290 (0.1%)	1.48	43/5849 (0.7%)
1	C	0.95	1/4301 (0.0%)	1.53	52/5864 (0.9%)
2	B	1.06	0/22	1.19	0/24
2	D	1.66	0/22	1.84	0/24
All	All	1.08	5/8635 (0.1%)	1.51	95/11761 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	GLU	CG-CD	59.26	2.40	1.51
1	C	192	LYS	CD-CE	19.45	1.99	1.51
1	A	339	LYS	CD-CE	15.23	1.89	1.51
1	A	194	LYS	CD-CE	-9.99	1.26	1.51
1	A	192	LYS	CG-CD	5.15	1.70	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLU	CB-CG-CD	-17.41	67.20	114.20
1	A	413	ARG	NE-CZ-NH2	-15.57	112.51	120.30
1	C	413	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	A	339	LYS	CD-CE-NZ	-13.63	80.34	111.70
1	C	115	TYR	CB-CG-CD2	-11.12	114.33	121.00
1	A	194	LYS	CG-CD-CE	10.70	143.99	111.90
1	A	288	ARG	NE-CZ-NH2	10.41	125.50	120.30
1	C	273	TYR	CB-CG-CD1	10.28	127.17	121.00
1	A	290	ARG	NE-CZ-NH2	10.17	125.39	120.30
1	C	298	ASP	CB-CG-OD1	9.84	127.16	118.30
1	A	362	ASP	CB-CG-OD2	9.75	127.08	118.30
1	C	201	ARG	CD-NE-CZ	9.36	136.71	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	ASP	CB-CG-OD1	9.27	126.64	118.30
1	C	290	ARG	NE-CZ-NH2	9.25	124.93	120.30
1	A	115	TYR	CB-CG-CD2	-9.25	115.45	121.00
1	A	290	ARG	NE-CZ-NH1	-9.07	115.76	120.30
1	C	265	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	C	273	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	A	201	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	C	77	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	201	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	C	212	ASP	CB-CG-OD2	7.83	125.35	118.30
1	C	235	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	41	ARG	CD-NE-CZ	7.72	134.41	123.60
1	C	84	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	237	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	286	ASP	CB-CG-OD1	7.58	125.13	118.30
1	C	311	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	433	ASP	CB-CG-OD1	7.45	125.00	118.30
1	C	299	ARG	NE-CZ-NH1	-7.43	116.59	120.30
1	C	461	GLN	CA-CB-CG	7.19	129.21	113.40
1	A	235	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	115	TYR	CB-CG-CD1	7.08	125.25	121.00
1	A	109	TYR	CB-CG-CD2	7.03	125.22	121.00
1	A	77	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	255	LYS	CA-CB-CG	6.96	128.70	113.40
1	A	413	ARG	NH1-CZ-NH2	6.93	127.02	119.40
1	C	489	ARG	CD-NE-CZ	6.76	133.07	123.60
1	C	413	ARG	NH1-CZ-NH2	6.71	126.79	119.40
1	C	265	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	489	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	422	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	C	192	LYS	CG-CD-CE	-6.34	92.87	111.90
1	A	145	GLU	OE1-CD-OE2	6.20	130.74	123.30
1	A	102	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	413	ARG	CG-CD-NE	-6.17	98.85	111.80
1	C	115	TYR	CB-CG-CD1	6.16	124.70	121.00
1	C	102	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	192	LYS	CB-CG-CD	-6.09	95.78	111.60
1	C	446	PHE	CA-C-O	-5.97	107.56	120.10
1	A	235	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	77	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	484	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	433	ASP	CB-CG-OD1	5.84	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	C	109	TYR	CB-CG-CD2	5.81	124.49	121.00
1	A	505	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	339	LYS	CG-CD-CE	-5.74	94.67	111.90
1	A	265	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	C	438	THR	CA-CB-CG2	-5.71	104.40	112.40
1	C	362	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	286	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	51	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	273	TYR	CB-CG-CD1	5.64	124.39	121.00
1	C	205	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	C	348	LEU	CB-CG-CD2	5.63	120.56	111.00
1	C	483	TYR	CA-CB-CG	5.63	124.09	113.40
1	C	243	MET	CA-CB-CG	5.62	122.86	113.30
1	A	239	GLY	N-CA-C	5.53	126.92	113.10
1	C	237	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	462	ARG	CD-NE-CZ	5.48	131.27	123.60
1	C	492	LYS	CG-CD-CE	5.48	128.33	111.90
1	C	473	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	340	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	C	123	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	462	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	C	195	ASN	CB-CA-C	-5.38	99.64	110.40
1	A	267	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	100	LEU	O-C-N	-5.29	114.23	122.70
1	C	329	GLU	OE1-CD-OE2	5.28	129.64	123.30
1	C	422	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	A	300	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	C	312	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	485	TYR	CB-CA-C	-5.21	99.97	110.40
1	C	41	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	502	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	A	237	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	17	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	33	GLY	CA-C-O	5.08	129.74	120.60
1	A	109	TYR	CG-CD1-CE1	5.06	125.35	121.30
1	A	179	TRP	CA-CB-CG	5.05	123.30	113.70
1	A	404	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	346	LYS	CB-CG-CD	5.03	124.69	111.60
1	A	470	GLU	O-C-N	-5.02	114.67	122.70
1	A	84	ASP	CB-CG-OD1	5.00	122.81	118.30

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	4171	0	4084	54	0
1	C	4173	0	4084	23	0
2	B	23	0	31	0	0
2	D	23	0	31	2	0
3	C	1	0	0	0	0
4	A	124	0	0	1	0
4	B	3	0	0	0	0
4	C	209	0	0	2	0
4	D	3	0	0	0	0
All	All	8730	0	8230	77	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 5.

All (77) 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:67:LYS:HD2	1:A:68:ASP:OD2	1.97	0.65
1:A:117:HIS:NE2	1:A:454:LEU:HD11	2.13	0.63
1:A:229:GLU:O	1:A:233:VAL:HG23	1.99	0.62
1:A:43:LEU:HD21	1:A:204:LEU:HD22	1.81	0.62
1:C:390:VAL:HG13	4:C:714:HOH:O	1.99	0.61
1:A:229:GLU:HB3	1:A:249:PRO:HD3	1.79	0.61
1:A:4:PRO:HD2	1:A:7:VAL:HG21	1.83	0.61
1:C:459:ASP:OD1	1:C:462:ARG:NH1	2.32	0.61
1:C:346:LYS:NZ	1:C:350:GLU:OE2	2.33	0.60
1:C:218:ILE:HD11	1:C:514:ILE:HG12	1.83	0.59
1:C:253:PHE:CE2	1:C:257:LYS:HD2	2.38	0.59
1:A:355:ALA:O	1:A:356:ASP:HB3	2.02	0.58
1:A:377:ALA:O	1:A:381:ILE:HG13	2.05	0.57
1:A:260:ILE:HD12	1:A:263:GLU:HB2	1.85	0.57
1:A:113:LEU:HD22	1:A:118:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21[A]:SER:HB3	4:C:672:HOH:O	2.04	0.56
1:A:236:TYR:O	1:A:492:LYS:NZ	2.34	0.55
1:A:24:GLN:HA	1:A:398:LYS:HE3	1.88	0.55
1:A:365:TYR:OH	1:A:372:LYS:HD3	2.05	0.55
1:A:24:GLN:HG3	1:A:36:GLU:OE2	2.06	0.54
1:A:255:LYS:HD2	1:A:259:GLU:OE1	2.10	0.51
1:A:323:ASP:HB2	1:A:421:ASN:OD1	2.10	0.51
1:A:233:VAL:HG11	1:A:252:LEU:HD12	1.93	0.51
1:C:302:ILE:HD11	1:C:381:ILE:HD12	1.91	0.51
1:A:3:VAL:HG11	1:A:9:LEU:HD21	1.93	0.50
1:A:4:PRO:O	1:A:7:VAL:HG23	2.11	0.50
1:A:301:ILE:HA	1:A:305:LYS:HD2	1.93	0.49
1:A:257:LYS:O	1:A:257:LYS:HG3	2.09	0.49
1:A:357:LYS:N	1:A:358:PRO:HD3	2.28	0.49
1:C:359:LEU:HB3	1:C:388:VAL:HG22	1.94	0.49
1:A:307:LYS:HD3	1:A:311:ASP:OD2	2.13	0.48
1:C:115:TYR:CE1	1:C:428:ASN:HB3	2.48	0.48
1:A:19:ASN:N	1:A:224:LEU:O	2.40	0.48
1:C:398:LYS:NZ	1:C:398:LYS:HB3	2.29	0.48
1:A:448:LYS:HD3	1:A:452:ASP:OD2	2.14	0.48
1:C:398:LYS:HG3	1:C:399:THR:N	2.28	0.47
1:A:402:ASP:OD2	1:A:406:GLN:NE2	2.47	0.47
1:C:137:LYS:HE2	1:C:145:GLU:OE1	2.14	0.47
1:C:218:ILE:CD1	1:C:514:ILE:HG12	2.44	0.47
1:A:161:HIS:CD2	1:A:162:PRO:HD2	2.50	0.47
1:A:307:LYS:HE2	1:A:370:LEU:HD11	1.97	0.47
1:A:63:LYS:HD3	1:A:64:TRP:N	2.30	0.47
1:A:265:ARG:NH2	1:A:498:TYR:O	2.49	0.46
1:C:269:TYR:HE2	2:D:3:LYS:HE3	1.80	0.46
1:C:113:LEU:HD22	1:C:118:ILE:HD12	1.97	0.45
1:C:210:TYR:CE2	1:C:212:ASP:HB3	2.52	0.45
1:A:360:THR:HA	1:A:389:ASN:O	2.16	0.45
1:A:453:THR:O	1:A:462:ARG:HD3	2.18	0.44
1:C:260:ILE:O	1:C:260:ILE:HG13	2.17	0.44
1:A:355:ALA:O	1:A:356:ASP:CB	2.64	0.43
1:A:84:ASP:OD1	1:A:86:THR:HG23	2.18	0.43
1:A:117:HIS:CD2	1:A:454:LEU:HD11	2.54	0.43
1:C:475:LYS:O	1:C:475:LYS:HG3	2.19	0.43
1:A:359:LEU:HB3	1:A:388:VAL:HG12	2.01	0.42
1:A:10:ALA:HA	1:A:516:LYS:HG3	2.01	0.42
1:A:362:ASP:OD1	1:A:391:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:N	1:A:312:LEU:HD22	2.35	0.42
1:A:43:LEU:O	1:A:187:THR:HB	2.20	0.42
1:A:365:TYR:CZ	1:A:394:ASN:HB3	2.54	0.42
1:A:329:GLU:OE1	1:A:334:LYS:NZ	2.53	0.42
1:A:198:VAL:O	1:A:199:ASN:HB2	2.19	0.42
1:C:269:TYR:OH	2:D:3:LYS:HE2	2.19	0.42
1:A:16:VAL:CG1	1:A:224:LEU:HD11	2.50	0.41
1:A:267:ASP:HB3	1:A:268:PRO:CD	2.50	0.41
1:A:3:VAL:HA	1:A:4:PRO:HD3	1.75	0.41
1:A:269:TYR:HB2	1:A:487:ASN:HB2	2.00	0.41
1:A:180:THR:HA	1:A:185:ILE:HD12	2.02	0.41
1:C:150:GLU:HB3	1:C:151:PRO:HD2	2.01	0.41
1:A:267:ASP:HB3	1:A:268:PRO:HD2	2.03	0.41
1:A:357:LYS:N	1:A:358:PRO:CD	2.84	0.41
1:A:209:GLN:HE21	1:A:209:GLN:HA	1.85	0.41
1:A:341:ASN:O	1:A:345:LYS:HE3	2.21	0.41
1:A:516:LYS:HA	4:A:633:HOH:O	2.21	0.41
1:A:366:ASN:O	1:A:367:THR:C	2.59	0.41
1:C:402:ASP:OD2	1:C:406:GLN:NE2	2.53	0.40
1:C:258:LYS:HE3	1:C:258:LYS:HB2	1.78	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	517/517 (100%)	488 (94%)	27 (5%)	2 (0%)	39	33
1	C	519/517 (100%)	509 (98%)	9 (2%)	1 (0%)	52	48
2	B	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1038/1040 (100%)	999 (96%)	36 (4%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	51	ASP
1	C	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	457/455 (100%)	431 (94%)	26 (6%)	25	19
1	C	459/455 (101%)	444 (97%)	15 (3%)	45	43
2	B	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	920/914 (101%)	879 (96%)	41 (4%)	34	29

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	21	SER
1	A	63	LYS
1	A	67	LYS
1	A	137	LYS
1	A	181	GLN
1	A	209	GLN
1	A	230	VAL
1	A	237	ARG
1	A	252	LEU
1	A	255	LYS
1	A	257	LYS
1	A	300	ASP
1	A	312	LEU
1	A	323	ASP
1	A	342	GLU
1	A	357	LYS

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Mol	Chain	Res	Type
1	A	372	LYS
1	A	384	LYS
1	A	390	VAL
1	A	398	LYS
1	A	413	ARG
1	A	431	LEU
1	A	448	LYS
1	A	460	THR
1	A	510	LYS
1	C	11	ASP
1	C	209	GLN
1	C	255	LYS
1	C	283	PRO
1	C	312	LEU
1	C	326	LYS
1	C	330	PRO
1	C	338	GLN
1	C	345	LYS
1	C	348	LEU
1	C	398	LYS
1	C	413	ARG
1	C	431	LEU
1	C	454	LEU
1	C	516	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	181	GLN
1	A	199	ASN
1	A	209	GLN
1	A	254	GLN
1	A	406	GLN
1	C	199	ASN
1	C	209	GLN
1	C	461	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.