



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:03 pm GMT

PDB ID : 1RKM
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

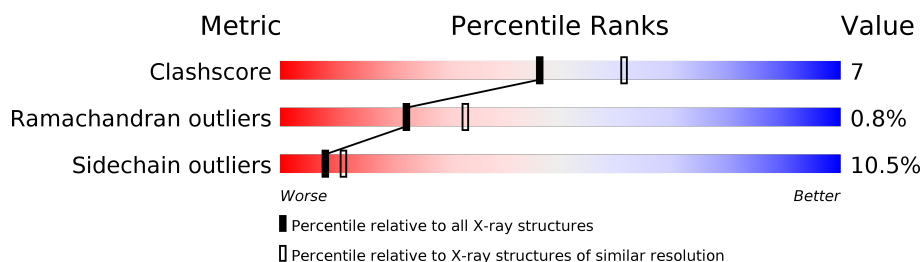
1 Overall quality at a glance

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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	

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.

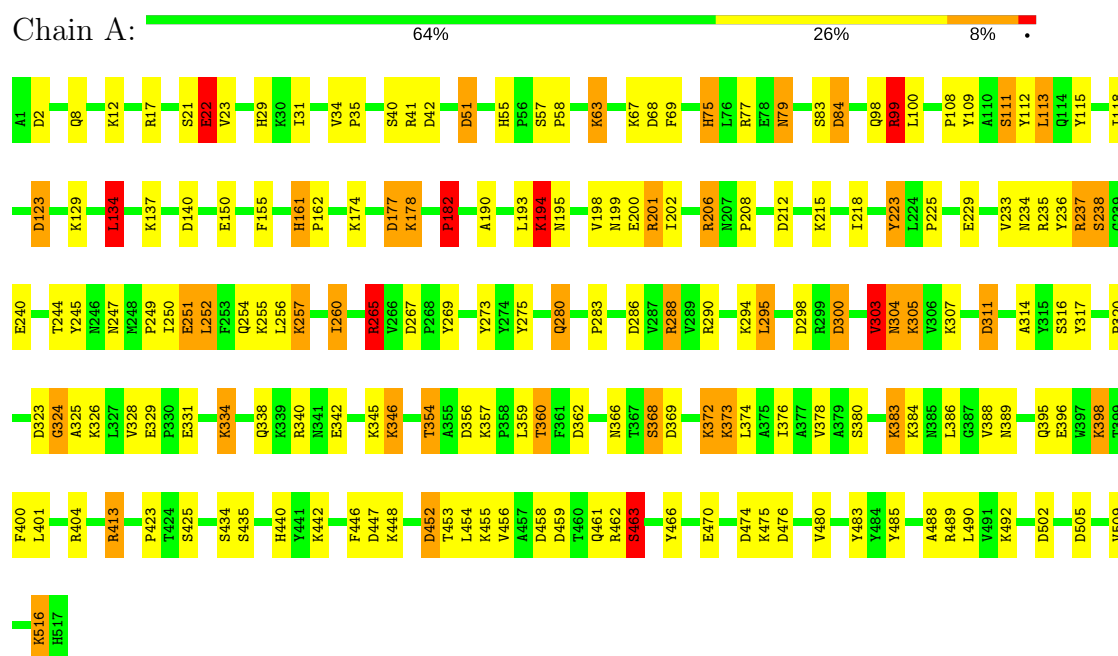
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

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

5.1 Standard geometry

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	1.02	11/4276 (0.3%)	2.05	119/5830 (2.0%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLU	CG-CD	-19.12	1.23	1.51
1	A	448	LYS	CE-NZ	16.63	1.90	1.49
1	A	8	GLN	CG-CD	16.42	1.88	1.51
1	A	174	LYS	CB-CG	11.67	1.84	1.52
1	A	40	SER	CB-OG	8.73	1.53	1.42
1	A	372	LYS	CE-NZ	8.47	1.70	1.49
1	A	475	LYS	CD-CE	-7.93	1.31	1.51
1	A	346	LYS	CD-CE	7.61	1.70	1.51
1	A	398	LYS	CB-CG	6.07	1.69	1.52
1	A	288	ARG	CD-NE	-5.22	1.37	1.46
1	A	396	GLU	CB-CG	-5.02	1.42	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ARG	CD-NE-CZ	24.78	158.29	123.60
1	A	265	ARG	NE-CZ-NH2	-22.62	108.99	120.30
1	A	201	ARG	NE-CZ-NH1	17.96	129.28	120.30
1	A	462	ARG	NE-CZ-NH2	-17.70	111.45	120.30
1	A	41	ARG	NE-CZ-NH2	-16.59	112.00	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ASP	CB-CG-OD2	16.04	132.73	118.30
1	A	235	ARG	CD-NE-CZ	14.53	143.95	123.60
1	A	288	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	A	489	ARG	NE-CZ-NH1	13.37	126.98	120.30
1	A	84	ASP	CB-CG-OD1	13.17	130.16	118.30
1	A	462	ARG	NE-CZ-NH1	13.13	126.86	120.30
1	A	51	ASP	CB-CG-OD1	12.61	129.65	118.30
1	A	22	GLU	CG-CD-OE1	-12.23	93.84	118.30
1	A	206	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	A	275	TYR	CB-CG-CD2	-11.60	114.04	121.00
1	A	41	ARG	NH1-CZ-NH2	11.53	132.08	119.40
1	A	300	ASP	CB-CG-OD2	-11.20	108.22	118.30
1	A	265	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	A	404	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	A	235	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	329	GLU	OE1-CD-OE2	10.54	135.95	123.30
1	A	459	ASP	CB-CG-OD2	-10.17	109.15	118.30
1	A	201	ARG	CD-NE-CZ	10.05	137.67	123.60
1	A	257	LYS	CG-CD-CE	-10.03	81.81	111.90
1	A	240	GLU	CB-CG-CD	-9.72	87.97	114.20
1	A	201	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	63	LYS	CG-CD-CE	9.31	139.83	111.90
1	A	51	ASP	CB-CG-OD2	-9.26	109.97	118.30
1	A	267	ASP	CB-CG-OD2	9.17	126.55	118.30
1	A	342	GLU	CA-CB-CG	9.14	133.51	113.40
1	A	223	TYR	CB-CG-CD1	-9.11	115.53	121.00
1	A	459	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	41	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	A	84	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	A	174	LYS	CA-CB-CG	-8.59	94.51	113.40
1	A	340	ARG	CD-NE-CZ	-8.38	111.86	123.60
1	A	396	GLU	CA-CB-CG	8.38	131.84	113.40
1	A	502	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	A	265	ARG	CD-NE-CZ	-8.27	112.03	123.60
1	A	275	TYR	CB-CG-CD1	8.23	125.94	121.00
1	A	8	GLN	CG-CD-OE1	8.19	137.98	121.60
1	A	300	ASP	OD1-CG-OD2	8.18	138.83	123.30
1	A	99	ARG	CD-NE-CZ	8.16	135.02	123.60
1	A	369	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	305	LYS	CG-CD-CE	7.93	135.69	111.90
1	A	314	ALA	N-CA-CB	-7.83	99.14	110.10
1	A	362	ASP	CB-CG-OD2	-7.72	111.35	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	8	GLN	CG-CD-NE2	-7.56	98.56	116.70
1	A	447	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	206	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	448	LYS	CD-CE-NZ	-7.37	94.75	111.70
1	A	288	ARG	CG-CD-NE	7.34	127.22	111.80
1	A	273	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	A	489	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	273	TYR	CB-CG-CD1	7.27	125.36	121.00
1	A	475	LYS	CG-CD-CE	7.26	133.69	111.90
1	A	137	LYS	CA-CB-CG	7.24	129.33	113.40
1	A	300	ASP	CA-CB-CG	-7.19	97.58	113.40
1	A	404	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	489	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	77	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	140	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	123	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	452	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	280	GLN	O-C-N	-6.68	112.00	122.70
1	A	109	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	247	ASN	N-CA-CB	6.59	122.47	110.60
1	A	298	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	311	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	42	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	290	ARG	NE-CZ-NH2	6.43	123.51	120.30
1	A	22	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	A	257	LYS	CB-CA-C	6.25	122.90	110.40
1	A	505	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	326	LYS	CD-CE-NZ	-6.23	97.37	111.70
1	A	178	LYS	CB-CA-C	6.22	122.84	110.40
1	A	286	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	300	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	A	509	VAL	CA-CB-CG2	-6.00	101.90	110.90
1	A	463	SER	N-CA-CB	-5.99	101.52	110.50
1	A	329	GLU	CG-CD-OE2	-5.99	106.33	118.30
1	A	295	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	75	HIS	CA-CB-CG	-5.90	103.58	113.60
1	A	100	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	A	485	TYR	CB-CA-C	-5.86	98.69	110.40
1	A	41	ARG	CG-CD-NE	-5.80	99.62	111.80
1	A	134	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	115	TYR	CB-CG-CD2	-5.65	117.61	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLY	O-C-N	-5.57	113.78	122.70
1	A	463	SER	CB-CA-C	5.57	120.69	110.10
1	A	323	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	328	VAL	CA-CB-CG1	5.55	119.22	110.90
1	A	83	SER	CA-C-O	-5.54	108.46	120.10
1	A	304	ASN	OD1-CG-ND2	-5.48	109.29	121.90
1	A	194	LYS	O-C-N	-5.47	113.95	122.70
1	A	476	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	317	TYR	CG-CD2-CE2	5.46	125.67	121.30
1	A	340	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	A	251	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	A	378	VAL	CA-CB-CG2	-5.38	102.83	110.90
1	A	380	SER	N-CA-CB	-5.37	102.45	110.50
1	A	505	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	A	177	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	245	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	63	LYS	CB-CG-CD	5.27	125.29	111.60
1	A	386	LEU	N-CA-CB	-5.24	99.92	110.40
1	A	265	ARG	NH1-CZ-NH2	5.23	125.15	119.40
1	A	111	SER	CA-CB-OG	-5.17	97.23	111.20
1	A	177	ASP	CA-CB-CG	5.17	124.77	113.40
1	A	303	VAL	CA-CB-CG2	5.11	118.56	110.90
1	A	384	LYS	O-C-N	-5.11	114.53	122.70
1	A	446	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	A	505	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	218	ILE	CA-CB-CG1	-5.09	101.32	111.00
1	A	269	TYR	N-CA-CB	-5.09	101.43	110.60
1	A	113	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	A	247	ASN	O-C-N	5.09	130.84	122.70
1	A	396	GLU	CB-CG-CD	-5.02	100.64	114.20

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
1	A	155	PHE	Mainchain
1	A	161	HIS	Mainchain
1	A	182	PRO	Mainchain
1	A	190	ALA	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	58	0
2	A	126	0	0	3	0
All	All	4291	0	4076	58	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 (58) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:236:TYR:CE2	1:A:492:LYS:HE2	2.45	0.51
1:A:307:LYS:NZ	1:A:311:ASP:OD2	2.42	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:413:ARG:C	1:A:413:ARG:HD3	2.35	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:354:THR:HB	1:A:356:ASP:OD1	2.17	0.45
1:A:98:GLN:NE2	2:A:575:HOH:O	2.46	0.45
1:A:307:LYS:HG2	1:A:311:ASP:OD2	2.16	0.44
1:A:324:GLY:O	1:A:463:SER:HB2	2.18	0.44
1:A:79:ASN:H	1:A:79:ASN:ND2	2.12	0.44
1:A:113:LEU:HD22	1:A:118:ILE:HD13	1.98	0.44
1:A:251:GLU:HG2	1:A:251:GLU:H	1.51	0.44
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:234:ASN:O	1:A:238:SER:OG	2.36	0.43
1:A:373:LYS:HE2	1:A:373:LYS:HB2	1.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.87	0.43
1:A:161:HIS:HA	1:A:162:PRO:HD3	1.79	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%)	22	33

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%)	407 (90%)	48 (10%)	8 11

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	22	GLU
1	A	31	ILE
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	177	ASP
1	A	178	LYS
1	A	194	LYS
1	A	195	ASN
1	A	198	VAL
1	A	199	ASN
1	A	200	GLU
1	A	201	ARG
1	A	238	SER
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
1	A	295	LEU
1	A	300	ASP
1	A	303	VAL
1	A	305	LYS
1	A	320	PRO
1	A	334	LYS
1	A	338	GLN
1	A	345	LYS
1	A	346	LYS
1	A	354	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

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	75	HIS
1	A	79	ASN
1	A	280	GLN
1	A	304	ASN
1	A	309	GLN
1	A	389	ASN
1	A	395	GLN
1	A	440	HIS
1	A	487	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.