



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:58 am BST

PDB ID : 2IE4  
Title : Structure of the Protein Phosphatase 2A Core Enzyme Bound to okadaic acid  
Authors : Xing, Y.; Xu, Y.; Chen, Y.; Jeffrey, P.D.; Chao, Y.; Shi, Y.  
Deposited on : 2006-09-17  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

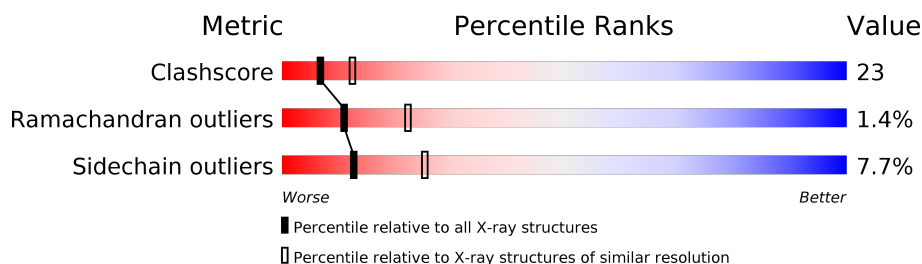
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 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	589	
2	C	309	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6972 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 Phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4527	2877	763	860	27			

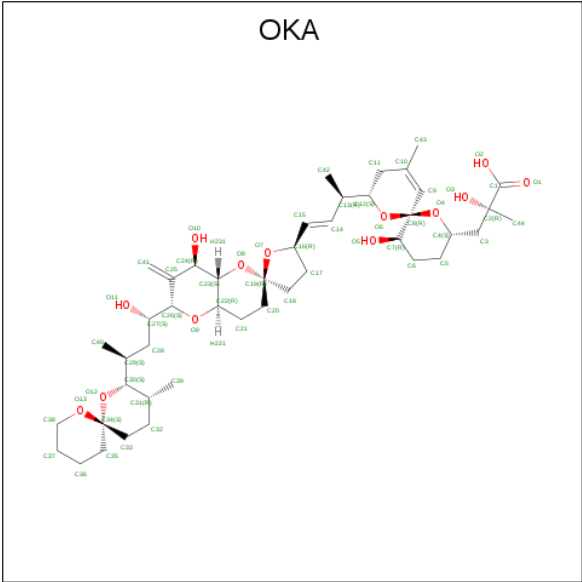
- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mn	0	0
			2	2		

- Molecule 4 is OKADAIC ACID (three-letter code: OKA) (formula: C<sub>44</sub>H<sub>68</sub>O<sub>13</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	C	O	0
			57	44	13	

- Molecule 5 is water.

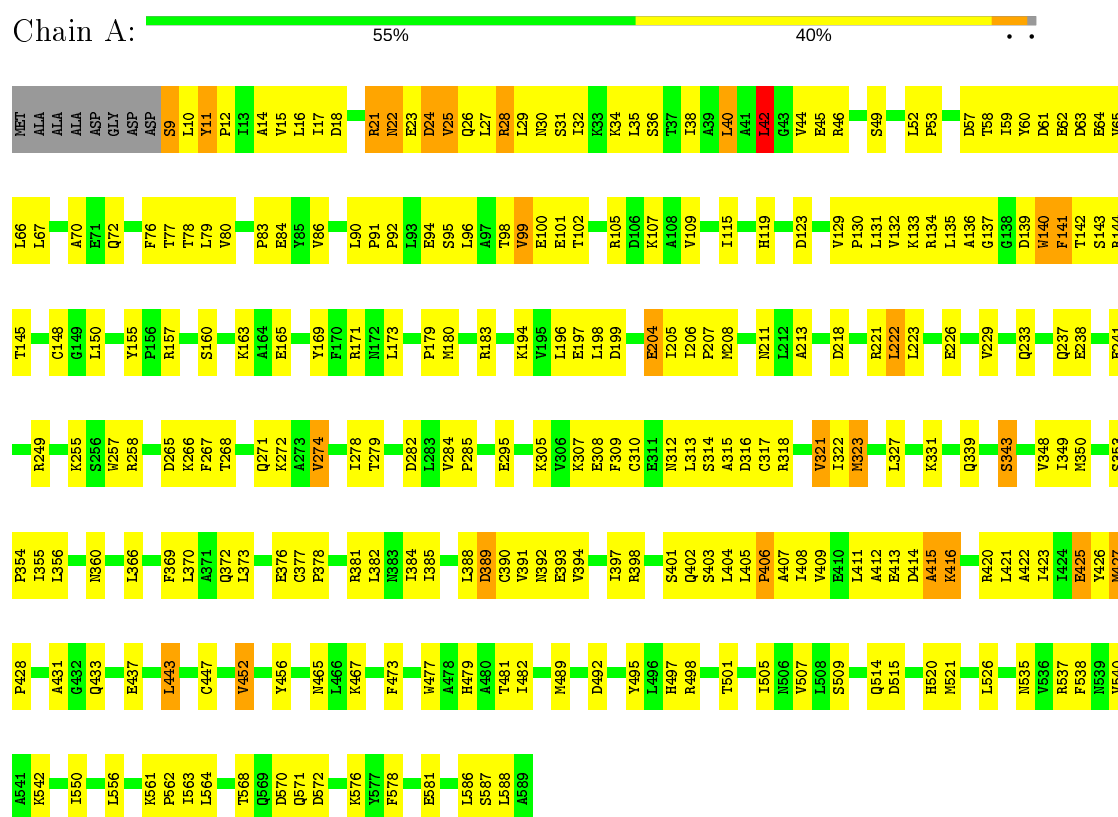
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	C	37	Total	O	0	0
			37	37		

### 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 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.

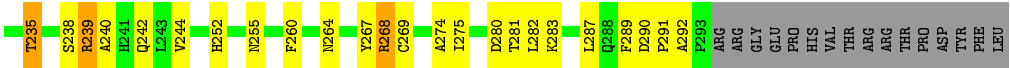
Note EDS was not executed.

- Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform



- Molecule 2: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.54Å 194.85Å 201.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (30.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.270 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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: OKA, MN

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	0.48	0/4601	0.72	5/6246 (0.1%)
2	C	0.53	0/2379	0.80	1/3227 (0.0%)
All	All	0.50	0/6980	0.75	6/9473 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	TYR	C-N-CA	-6.55	94.48	122.00
2	C	137	TYR	N-CA-C	-6.46	93.55	111.00
1	A	42	LEU	N-CA-C	-5.53	96.08	111.00
1	A	11	TYR	C-N-CD	5.37	139.68	128.40
1	A	11	TYR	N-CA-C	5.34	125.43	111.00
1	A	42	LEU	CA-CB-CG	5.17	127.20	115.30

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	4527	0	4633	227	0
2	C	2322	0	2224	97	0
3	C	2	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	57	0	67	1	0
5	A	27	0	0	0	0
5	C	37	0	0	2	0
All	All	6972	0	6924	322	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 23.

All (322) 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)
2:C:45:VAL:HA	2:C:156:THR:HG22	1.31	1.07
1:A:99:VAL:HG12	1:A:100:GLU:H	1.15	1.04
1:A:102:THR:HA	1:A:105:ARG:HG3	1.44	0.99
1:A:526:LEU:HD22	1:A:563:ILE:HG13	1.43	0.98
2:C:103:LEU:HB3	2:C:111:ILE:CD1	2.00	0.90
1:A:323:MET:HE3	1:A:327:LEU:HD22	1.56	0.88
1:A:99:VAL:HG12	1:A:100:GLU:N	1.91	0.86
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.42	0.85
1:A:205:ILE:HD13	1:A:208:MET:HE2	1.58	0.85
2:C:268:ARG:HH11	2:C:268:ARG:CB	1.90	0.84
2:C:175:ASP:H	2:C:179:HIS:HD2	1.28	0.80
1:A:77:THR:HG23	1:A:86:VAL:HG12	1.63	0.80
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.62	0.80
2:C:45:VAL:HA	2:C:156:THR:CG2	2.12	0.79
1:A:99:VAL:CG1	1:A:100:GLU:H	1.95	0.78
2:C:176:THR:CG2	2:C:179:HIS:H	1.97	0.78
1:A:94:GLU:OE1	1:A:131:LEU:HD13	1.84	0.77
1:A:102:THR:HA	1:A:105:ARG:CG	2.16	0.76
1:A:59:ILE:HG23	1:A:66:LEU:HD21	1.67	0.76
1:A:339:GLN:O	1:A:343:SER:HB2	1.86	0.75
1:A:274:VAL:HG13	1:A:278:ILE:HB	1.67	0.75
1:A:381:ARG:HD2	1:A:426:TYR:OH	1.87	0.74
1:A:70:ALA:HB2	1:A:96:LEU:HD13	1.68	0.74
2:C:158:LEU:HD21	2:C:161:GLY:HA2	1.71	0.73
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.71	0.73
1:A:180:MET:HG3	1:A:183:ARG:NH2	2.04	0.73
2:C:268:ARG:HH11	2:C:268:ARG:HB3	1.52	0.73
1:A:194:LYS:HD2	1:A:194:LYS:O	1.89	0.72
1:A:323:MET:CE	1:A:327:LEU:HD22	2.19	0.72
2:C:188:GLU:HG3	2:C:189:VAL:N	2.03	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ALA:O	1:A:221:ARG:HD2	1.89	0.72
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.71	0.72
1:A:102:THR:HG22	1:A:105:ARG:NH1	2.04	0.72
1:A:21:ARG:C	1:A:22:ASN:HD22	1.94	0.71
2:C:176:THR:HG23	2:C:179:HIS:H	1.54	0.71
1:A:514:GLN:HG3	1:A:550:ILE:O	1.90	0.71
2:C:204:ASP:O	2:C:252:HIS:HE1	1.74	0.70
2:C:281:THR:HG22	2:C:283:LYS:HE3	1.72	0.70
1:A:94:GLU:OE1	1:A:134:ARG:NH2	2.20	0.70
1:A:136:ALA:O	1:A:144:ARG:HD2	1.91	0.70
2:C:103:LEU:HB3	2:C:111:ILE:HD13	1.74	0.69
1:A:155:TYR:CE1	1:A:163:LYS:HB3	2.27	0.69
2:C:176:THR:HG22	2:C:179:HIS:CG	2.27	0.69
1:A:27:LEU:HD13	1:A:32:ILE:HD11	1.74	0.69
1:A:148:CYS:SG	1:A:173:LEU:HD13	2.34	0.68
1:A:131:LEU:O	1:A:131:LEU:HD12	1.93	0.68
1:A:414:ASP:CG	1:A:415:ALA:H	1.97	0.68
1:A:129:VAL:HB	1:A:130:PRO:HD3	1.74	0.68
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.74	0.68
2:C:176:THR:HG23	2:C:178:ASP:N	2.09	0.68
2:C:225:SER:OG	2:C:252:HIS:HD2	1.77	0.67
1:A:23:GLU:HG3	1:A:26:GLN:CD	2.15	0.67
1:A:388:LEU:H	1:A:433:GLN:HE22	1.43	0.67
2:C:174:ILE:HD11	2:C:183:LEU:HD11	1.77	0.67
1:A:29:LEU:C	1:A:31:SER:H	1.98	0.66
1:A:36:SER:O	1:A:40:LEU:HD23	1.96	0.65
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.27	0.65
1:A:12:PRO:HB2	1:A:42:LEU:HD11	1.77	0.65
2:C:68:LEU:HD21	2:C:275:ILE:CD1	2.27	0.65
1:A:389:ASP:O	1:A:393:GLU:HG3	1.97	0.65
2:C:275:ILE:HG22	2:C:287:LEU:HB2	1.77	0.64
1:A:323:MET:HE3	1:A:327:LEU:CD2	2.27	0.64
1:A:23:GLU:HG3	1:A:26:GLN:OE1	1.96	0.64
2:C:67:GLU:HB2	2:C:292:ALA:HB2	1.78	0.64
1:A:222:LEU:HD23	1:A:223:LEU:N	2.12	0.63
1:A:317:CYS:O	1:A:321:VAL:HG13	1.99	0.63
1:A:38:ILE:O	1:A:42:LEU:HD22	1.98	0.63
2:C:281:THR:HG22	2:C:281:THR:O	1.98	0.63
1:A:310:CYS:HB3	1:A:322:ILE:HD11	1.81	0.62
2:C:45:VAL:HG22	2:C:156:THR:HG21	1.81	0.62
2:C:264:ASN:ND2	2:C:267:TYR:HA	2.15	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:ASP:HB3	2:C:291:PRO:HD2	1.81	0.62
1:A:416:LYS:H	1:A:416:LYS:HD3	1.64	0.62
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.29	0.62
1:A:183:ARG:NH1	1:A:183:ARG:HG3	2.12	0.61
1:A:427:MET:HE3	1:A:427:MET:HA	1.81	0.61
2:C:68:LEU:HD21	2:C:275:ILE:HD11	1.82	0.61
1:A:268:THR:HG21	1:A:308:GLU:HB3	1.82	0.61
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.65	0.61
1:A:32:ILE:O	1:A:35:LEU:HB2	2.00	0.60
1:A:339:GLN:NE2	1:A:377:CYS:HB2	2.16	0.60
1:A:412:ALA:O	1:A:420:ARG:HD2	2.01	0.60
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.83	0.60
1:A:307:LYS:NZ	1:A:307:LYS:HB3	2.17	0.59
1:A:180:MET:HG3	1:A:183:ARG:HH21	1.65	0.59
1:A:136:ALA:O	1:A:144:ARG:CD	2.51	0.59
1:A:509:SER:O	1:A:550:ILE:HD13	2.02	0.59
1:A:282:ASP:O	1:A:285:PRO:HD2	2.02	0.59
2:C:204:ASP:HB2	2:C:219:THR:HB	1.85	0.59
1:A:409:VAL:O	1:A:413:GLU:HG2	2.03	0.58
2:C:71:ILE:CD1	2:C:289:PHE:HB3	2.32	0.58
1:A:115:ILE:O	1:A:119:HIS:HD2	1.85	0.58
1:A:427:MET:CE	1:A:443:LEU:HG	2.32	0.58
2:C:118:HIS:HA	2:C:123:ILE:HG21	1.86	0.58
1:A:205:ILE:HD13	1:A:208:MET:CE	2.31	0.58
2:C:176:THR:HG23	2:C:178:ASP:H	1.67	0.58
1:A:77:THR:HG23	1:A:86:VAL:CG1	2.33	0.58
1:A:105:ARG:HH22	1:A:145:THR:HG21	1.69	0.57
1:A:29:LEU:HD11	1:A:64:GLU:HG2	1.85	0.57
1:A:431:ALA:HB1	1:A:473:PHE:CZ	2.38	0.57
2:C:103:LEU:HB3	2:C:111:ILE:HD11	1.81	0.57
1:A:427:MET:HG2	1:A:447:CYS:SG	2.45	0.57
1:A:58:THR:O	1:A:58:THR:HG22	2.05	0.57
2:C:10:LEU:HD11	2:C:105:VAL:HG12	1.87	0.57
1:A:29:LEU:O	1:A:31:SER:N	2.35	0.57
2:C:45:VAL:CA	2:C:156:THR:HG22	2.22	0.56
1:A:398:ARG:O	1:A:402:GLN:HB2	2.06	0.56
2:C:281:THR:CG2	2:C:281:THR:O	2.53	0.56
2:C:71:ILE:CG2	2:C:287:LEU:HD13	2.36	0.56
1:A:165:GLU:O	1:A:169:TYR:HD1	1.88	0.56
1:A:356:LEU:O	1:A:360:ASN:HB2	2.06	0.56
1:A:241:GLU:OE2	1:A:249:ARG:NH2	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.41	0.56
1:A:144:ARG:HG2	1:A:173:LEU:HD21	1.87	0.56
2:C:175:ASP:H	2:C:179:HIS:CD2	2.18	0.56
1:A:38:ILE:HD12	1:A:38:ILE:N	2.21	0.56
1:A:586:LEU:O	1:A:587:SER:HB2	2.05	0.55
1:A:271:GLN:HE22	1:A:309:PHE:HA	1.71	0.55
1:A:38:ILE:H	1:A:38:ILE:HD12	1.71	0.55
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.36	0.55
1:A:12:PRO:HB2	1:A:42:LEU:CD1	2.36	0.55
1:A:204:GLU:O	1:A:208:MET:HG3	2.07	0.55
2:C:268:ARG:HB3	2:C:268:ARG:NH1	2.19	0.55
2:C:44:ASN:O	2:C:156:THR:HG22	2.07	0.55
1:A:179:PRO:C	1:A:183:ARG:HH12	2.10	0.54
2:C:229:ASN:ND2	2:C:255:ASN:HB3	2.22	0.54
2:C:76:PRO:HB2	2:C:110:ARG:HG3	1.90	0.54
1:A:136:ALA:O	1:A:144:ARG:CG	2.55	0.54
1:A:571:GLN:HG2	1:A:572:ASP:N	2.23	0.54
1:A:456:TYR:CG	2:C:73:GLY:HA2	2.42	0.54
1:A:42:LEU:HB3	1:A:46:ARG:HB3	1.89	0.54
1:A:21:ARG:C	1:A:22:ASN:ND2	2.61	0.54
2:C:162:GLN:HB3	2:C:235:THR:OG1	2.08	0.54
1:A:22:ASN:N	1:A:22:ASN:HD22	2.05	0.54
1:A:570:ASP:O	1:A:576:LYS:HE3	2.08	0.54
2:C:158:LEU:O	2:C:158:LEU:HD23	2.08	0.54
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.37	0.54
1:A:492:ASP:O	1:A:498:ARG:HD3	2.08	0.54
1:A:542:LYS:HE2	1:A:578:PHE:CD1	2.43	0.54
2:C:50:CYS:HB2	2:C:51:PRO:HA	1.90	0.54
1:A:427:MET:HE1	1:A:443:LEU:HG	1.90	0.53
1:A:60:TYR:O	1:A:62:GLU:N	2.41	0.53
2:C:124:THR:HB	2:C:129:PHE:HB3	1.89	0.53
2:C:203:PRO:HD2	2:C:239:ARG:CZ	2.39	0.53
1:A:373:LEU:HD11	1:A:385:ILE:CD1	2.39	0.53
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.91	0.53
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.90	0.53
1:A:229:VAL:O	1:A:233:GLN:HG3	2.08	0.53
1:A:542:LYS:HE2	1:A:578:PHE:CE1	2.44	0.53
2:C:103:LEU:C	2:C:111:ILE:HD12	2.30	0.53
1:A:59:ILE:HG22	1:A:59:ILE:O	2.08	0.52
2:C:264:ASN:HA	2:C:269:CYS:O	2.10	0.52
1:A:100:GLU:O	1:A:101:GLU:C	2.48	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:THR:O	2:C:282:LEU:HB2	2.08	0.52
1:A:350:MET:CE	1:A:369:PHE:HB2	2.39	0.52
1:A:373:LEU:HD11	1:A:385:ILE:HD11	1.91	0.52
1:A:481:THR:HG22	1:A:481:THR:O	2.09	0.52
1:A:378:PRO:HA	1:A:381:ARG:NH1	2.24	0.52
2:C:264:ASN:HD22	2:C:267:TYR:HA	1.75	0.52
2:C:103:LEU:O	2:C:111:ILE:HD12	2.10	0.51
1:A:102:THR:HG22	1:A:105:ARG:HH12	1.75	0.51
1:A:136:ALA:O	1:A:144:ARG:HG3	2.10	0.51
1:A:407:ALA:O	1:A:411:LEU:HG	2.09	0.51
1:A:556:LEU:HD22	1:A:588:LEU:HD11	1.91	0.51
1:A:180:MET:HA	1:A:183:ARG:CZ	2.40	0.51
1:A:194:LYS:CD	1:A:194:LYS:O	2.58	0.51
2:C:166:LEU:N	2:C:166:LEU:HD23	2.26	0.51
1:A:94:GLU:CD	1:A:131:LEU:HD13	2.31	0.51
1:A:109:VAL:HG13	1:A:150:LEU:HD21	1.93	0.51
2:C:176:THR:HG22	2:C:179:HIS:H	1.73	0.51
1:A:105:ARG:NH2	1:A:145:THR:CG2	2.74	0.51
1:A:356:LEU:HB3	1:A:360:ASN:HB3	1.92	0.51
2:C:209:TRP:CE2	2:C:224:ILE:HD13	2.46	0.51
2:C:68:LEU:CD2	2:C:275:ILE:HD12	2.41	0.51
1:A:381:ARG:O	1:A:385:ILE:HG12	2.10	0.51
1:A:98:THR:HG22	1:A:98:THR:O	2.10	0.51
1:A:197:GLU:CD	1:A:197:GLU:H	2.13	0.50
1:A:452:VAL:HG22	1:A:497:HIS:CE1	2.47	0.50
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.45	0.50
1:A:44:VAL:HG13	1:A:45:GLU:H	1.76	0.50
1:A:29:LEU:C	1:A:31:SER:N	2.65	0.50
2:C:48:VAL:O	2:C:159:VAL:HA	2.10	0.50
1:A:12:PRO:O	1:A:15:VAL:HG23	2.12	0.50
1:A:218:ASP:OD2	1:A:258:ARG:HD3	2.11	0.50
1:A:196:LEU:HD11	1:A:205:ILE:HD11	1.92	0.50
2:C:186:LEU:O	2:C:186:LEU:HD13	2.12	0.50
2:C:103:LEU:CB	2:C:111:ILE:HD13	2.42	0.50
2:C:36:LYS:O	2:C:40:THR:OG1	2.30	0.50
1:A:18:ASP:C	1:A:18:ASP:OD1	2.50	0.49
1:A:421:LEU:O	1:A:421:LEU:HD12	2.12	0.49
1:A:96:LEU:HA	1:A:99:VAL:HG23	1.94	0.49
1:A:370:LEU:HD21	1:A:403:SER:O	2.12	0.49
1:A:413:GLU:O	1:A:413:GLU:HG3	2.13	0.49
1:A:105:ARG:NH1	1:A:105:ARG:HG3	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ALA:O	1:A:425:GLU:HG2	2.12	0.49
1:A:356:LEU:HB3	1:A:360:ASN:CB	2.43	0.49
1:A:392:ASN:HD21	1:A:397:ILE:HA	1.78	0.49
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.77	0.49
1:A:26:GLN:HG2	1:A:27:LEU:N	2.27	0.48
1:A:537:ARG:O	1:A:540:VAL:HB	2.12	0.48
2:C:171:SER:HB2	2:C:197:ASP:CB	2.43	0.48
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.49	0.48
2:C:268:ARG:CB	2:C:268:ARG:NH1	2.70	0.48
1:A:401:SER:O	1:A:405:LEU:HB2	2.13	0.48
1:A:238:GLU:H	1:A:238:GLU:CD	2.15	0.48
1:A:265:ASP:O	1:A:305:LYS:HE2	2.13	0.48
1:A:129:VAL:O	1:A:132:VAL:N	2.47	0.48
2:C:45:VAL:HG22	2:C:156:THR:CG2	2.44	0.48
1:A:196:LEU:CD1	1:A:205:ILE:HD11	2.45	0.47
1:A:45:GLU:H	1:A:45:GLU:CD	2.17	0.47
2:C:68:LEU:HD21	2:C:275:ILE:HD12	1.96	0.47
1:A:155:TYR:CE2	1:A:163:LYS:HD3	2.50	0.47
1:A:373:LEU:HD13	1:A:384:ILE:HG21	1.95	0.47
2:C:68:LEU:HG	2:C:275:ILE:HD12	1.96	0.47
2:C:202:ASP:OD1	2:C:242:GLN:HG3	2.14	0.47
1:A:130:PRO:O	1:A:134:ARG:HG3	2.14	0.47
1:A:183:ARG:CG	1:A:183:ARG:HH11	2.20	0.47
2:C:115:ARG:HB2	2:C:153:LEU:HB2	1.96	0.47
1:A:24:ASP:C	1:A:25:VAL:HG23	2.34	0.47
1:A:414:ASP:CG	1:A:415:ALA:N	2.67	0.47
2:C:174:ILE:HD13	2:C:180:ILE:HG12	1.97	0.47
2:C:186:LEU:C	2:C:186:LEU:HD22	2.35	0.47
2:C:187:GLN:NE2	5:C:537:HOH:O	2.48	0.46
1:A:354:PRO:HD3	1:A:390:CYS:SG	2.55	0.46
1:A:405:LEU:HB3	1:A:406:PRO:CD	2.44	0.46
2:C:118:HIS:CE1	2:C:123:ILE:HD11	2.50	0.46
2:C:128:GLY:O	2:C:129:PHE:C	2.53	0.46
2:C:264:ASN:OD1	2:C:269:CYS:O	2.33	0.46
1:A:226:GLU:OE2	1:A:266:LYS:HE3	2.16	0.46
2:C:174:ILE:HD11	2:C:194:PRO:HB2	1.97	0.46
1:A:180:MET:HA	1:A:183:ARG:NH2	2.31	0.46
1:A:279:THR:O	1:A:284:VAL:HG23	2.15	0.46
1:A:564:LEU:O	1:A:568:THR:HG23	2.15	0.46
1:A:62:GLU:HB3	1:A:65:VAL:HB	1.98	0.46
2:C:83:MET:HE3	2:C:240:ALA:HB2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:CYS:O	2:C:36:LYS:HG3	2.16	0.45
2:C:244:VAL:HG22	2:C:260:PHE:HB2	1.97	0.45
2:C:268:ARG:HH11	2:C:268:ARG:HB2	1.78	0.45
2:C:171:SER:HB2	2:C:197:ASP:HB2	1.97	0.45
1:A:313:LEU:HD13	1:A:321:VAL:HG22	1.99	0.45
1:A:42:LEU:HD13	1:A:42:LEU:N	2.32	0.45
2:C:42:GLU:HB3	2:C:46:GLN:OE1	2.17	0.45
1:A:505:ILE:HG23	1:A:521:MET:HB3	1.99	0.45
1:A:99:VAL:CG1	1:A:100:GLU:N	2.62	0.45
1:A:404:LEU:HD11	1:A:408:ILE:HD11	1.98	0.45
1:A:477:TRP:CH2	1:A:482:ILE:HD12	2.52	0.45
2:C:274:ALA:HA	2:C:287:LEU:O	2.17	0.44
1:A:141:PHE:CD1	1:A:141:PHE:C	2.89	0.44
1:A:80:VAL:CG1	1:A:80:VAL:O	2.66	0.44
1:A:92:PRO:O	1:A:95:SER:HB3	2.18	0.44
1:A:34:LYS:O	1:A:38:ILE:CD1	2.65	0.44
1:A:66:LEU:HD22	1:A:96:LEU:HD21	1.99	0.44
2:C:71:ILE:HG23	2:C:287:LEU:HD13	2.00	0.44
1:A:107:LYS:HD3	1:A:107:LYS:HA	1.85	0.44
1:A:255:LYS:HD3	1:A:255:LYS:HA	1.78	0.44
1:A:388:LEU:H	1:A:433:GLN:NE2	2.11	0.44
1:A:570:ASP:O	1:A:576:LYS:CE	2.65	0.44
1:A:378:PRO:O	1:A:382:LEU:HB2	2.18	0.44
2:C:174:ILE:HG13	2:C:194:PRO:HB3	1.99	0.44
1:A:353:SER:N	1:A:354:PRO:HD2	2.33	0.43
1:A:427:MET:HE2	1:A:443:LEU:HG	1.98	0.43
2:C:89:ARG:HH21	4:C:401:OKA:H32	1.83	0.43
1:A:42:LEU:HB3	1:A:46:ARG:CB	2.48	0.43
1:A:9:SER:HB2	1:A:14:ALA:HB2	1.99	0.43
1:A:572:ASP:OD2	2:C:110:ARG:NH2	2.51	0.43
1:A:62:GLU:O	1:A:64:GLU:N	2.51	0.43
1:A:35:LEU:HB3	1:A:72:GLN:HG2	2.01	0.43
1:A:135:LEU:O	1:A:143:SER:O	2.36	0.43
1:A:21:ARG:HD2	1:A:26:GLN:OE1	2.18	0.43
2:C:144:LYS:HE3	2:C:148:ASP:OD2	2.19	0.43
1:A:381:ARG:CD	1:A:426:TYR:OH	2.61	0.43
1:A:489:MET:HB2	1:A:501:THR:OG1	2.18	0.43
2:C:57:ASP:OD1	2:C:57:ASP:N	2.52	0.43
2:C:165:CYS:HA	2:C:238:SER:O	2.19	0.43
2:C:31:LEU:HD21	2:C:102:ALA:HA	2.01	0.43
1:A:416:LYS:HD3	1:A:416:LYS:N	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:HIS:HE1	2:C:118:HIS:CD2	2.37	0.42
1:A:17:ILE:HG22	1:A:18:ASP:N	2.34	0.42
1:A:204:GLU:C	1:A:207:PRO:HD2	2.39	0.42
1:A:381:ARG:HG3	1:A:426:TYR:OH	2.19	0.42
1:A:179:PRO:C	1:A:183:ARG:NH1	2.72	0.42
1:A:28:ARG:HB3	1:A:31:SER:CB	2.49	0.42
2:C:103:LEU:CB	2:C:111:ILE:CD1	2.84	0.42
1:A:46:ARG:HA	1:A:49:SER:OG	2.19	0.42
2:C:176:THR:HG23	2:C:179:HIS:N	2.28	0.42
2:C:176:THR:CG2	2:C:179:HIS:N	2.73	0.42
1:A:405:LEU:HA	1:A:405:LEU:HD12	1.89	0.42
1:A:67:LEU:HA	1:A:67:LEU:HD12	1.86	0.42
2:C:158:LEU:CD2	2:C:161:GLY:HA2	2.45	0.42
2:C:66:MET:HA	2:C:66:MET:HE2	2.01	0.42
1:A:372:GLN:OE1	1:A:384:ILE:HD11	2.20	0.42
1:A:411:LEU:CB	1:A:423:ILE:HG13	2.49	0.42
1:A:390:CYS:O	1:A:394:VAL:HG23	2.19	0.42
2:C:158:LEU:HD21	2:C:161:GLY:CA	2.43	0.42
1:A:139:ASP:O	1:A:140:TRP:C	2.59	0.42
1:A:9:SER:HB2	1:A:10:LEU:H	1.69	0.41
1:A:171:ARG:HH22	1:A:204:GLU:HG2	1.85	0.41
1:A:105:ARG:NH2	1:A:142:THR:HB	2.35	0.41
1:A:66:LEU:HD22	1:A:96:LEU:CD2	2.50	0.41
1:A:83:PRO:HA	1:A:86:VAL:HG13	2.02	0.41
1:A:327:LEU:HG	1:A:331:LYS:HE3	2.01	0.41
1:A:44:VAL:HG23	1:A:80:VAL:C	2.41	0.41
2:C:283:LYS:HA	2:C:283:LYS:HE2	2.03	0.41
1:A:413:GLU:O	1:A:414:ASP:HB2	2.21	0.41
1:A:349:ILE:HG23	1:A:350:MET:N	2.36	0.41
1:A:355:ILE:HG22	1:A:355:ILE:O	2.21	0.41
1:A:100:GLU:O	1:A:102:THR:N	2.54	0.41
1:A:373:LEU:HD13	1:A:384:ILE:CG2	2.51	0.41
1:A:481:THR:O	1:A:481:THR:CG2	2.68	0.41
1:A:479:HIS:CE1	1:A:520:HIS:CD2	3.09	0.41
1:A:40:LEU:CD2	1:A:40:LEU:N	2.83	0.40
1:A:498:ARG:O	1:A:501:THR:HB	2.21	0.40
1:A:171:ARG:HH22	1:A:204:GLU:CG	2.34	0.40
2:C:177:LEU:O	2:C:181:ARG:HG3	2.20	0.40
1:A:133:LYS:O	1:A:137:GLY:N	2.49	0.40
2:C:49:ARG:NH2	5:C:504:HOH:O	2.41	0.40
1:A:257:TRP:CB	1:A:295:GLU:HG3	2.51	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HG21	1:A:308:GLU:CG	2.52	0.40
1:A:272:LYS:HE3	1:A:312:ASN:ND2	2.36	0.40
1:A:314:SER:O	1:A:315:ALA:C	2.60	0.40
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.86	0.40
1:A:42:LEU:H	1:A:42:LEU:HD13	1.85	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	579/589 (98%)	511 (88%)	56 (10%)	12 (2%)	7	13
2	C	286/309 (93%)	256 (90%)	30 (10%)	0	100	100
All	All	865/898 (96%)	767 (89%)	86 (10%)	12 (1%)	11	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	63	ASP
1	A	99	VAL
1	A	318	ARG
1	A	415	ALA
1	A	21	ARG
1	A	30	ASN
1	A	84	GLU
1	A	140	TRP
1	A	376	GLU
1	A	348	VAL
1	A	25	VAL

### 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	508/512 (99%)	468 (92%)	40 (8%)	12	24
2	C	254/274 (93%)	235 (92%)	19 (8%)	13	27
All	All	762/786 (97%)	703 (92%)	59 (8%)	13	25

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	TYR
1	A	16	LEU
1	A	22	ASN
1	A	24	ASP
1	A	28	ARG
1	A	40	LEU
1	A	42	LEU
1	A	57	ASP
1	A	76	PHE
1	A	78	THR
1	A	79	LEU
1	A	123	ASP
1	A	141	PHE
1	A	157	ARG
1	A	160	SER
1	A	198	LEU
1	A	199	ASP
1	A	204	GLU
1	A	211	ASN
1	A	222	LEU
1	A	237	GLN
1	A	267	PHE
1	A	274	VAL
1	A	316	ASP
1	A	321	VAL
1	A	323	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	343	SER
1	A	366	LEU
1	A	389	ASP
1	A	406	PRO
1	A	416	LYS
1	A	425	GLU
1	A	427	MET
1	A	437	GLU
1	A	443	LEU
1	A	452	VAL
1	A	495	TYR
1	A	515	ASP
1	A	581	GLU
2	C	31	LEU
2	C	40	THR
2	C	43	SER
2	C	47	GLU
2	C	52	VAL
2	C	57	ASP
2	C	110	ARG
2	C	134	LEU
2	C	135	ARG
2	C	144	LYS
2	C	156	THR
2	C	158	LEU
2	C	160	ASP
2	C	186	LEU
2	C	188	GLU
2	C	235	THR
2	C	239	ARG
2	C	268	ARG
2	C	280	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	119	HIS
1	A	237	GLN
1	A	271	GLN
1	A	288	GLN
1	A	339	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	364	HIS
1	A	392	ASN
1	A	402	GLN
1	A	433	GLN
1	A	465	ASN
1	A	479	HIS
1	A	506	ASN
1	A	520	HIS
2	C	12	GLN
2	C	16	GLN
2	C	122	GLN
2	C	179	HIS
2	C	187	GLN
2	C	191	HIS
2	C	252	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OKA	C	401	-	57,63,63	1.45	4 (7%)	67,97,97	1.70	12 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OKA	C	401	-	-	3/26/129/129	0/7/7/7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	OKA	C8-C9	-8.61	1.39	1.50
4	C	401	OKA	C41-C25	3.98	1.39	1.32
4	C	401	OKA	C15-C14	2.50	1.39	1.32
4	C	401	OKA	C16-C15	-2.46	1.39	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	OKA	C7-C8-C9	-6.42	106.96	113.98
4	C	401	OKA	C11-C12-C13	-3.90	106.93	116.14
4	C	401	OKA	C21-C20-C19	-3.58	107.51	111.73
4	C	401	OKA	C23-C24-C25	-3.55	106.12	112.08
4	C	401	OKA	C29-C30-C31	-3.46	110.32	116.50
4	C	401	OKA	O8-C23-C22	2.66	113.31	109.42
4	C	401	OKA	C43-C10-C11	2.58	120.56	116.16
4	C	401	OKA	C19-O8-C23	-2.54	110.75	114.27
4	C	401	OKA	O12-C30-C29	2.53	109.97	106.12
4	C	401	OKA	C38-O13-C34	-2.43	111.38	113.92
4	C	401	OKA	O5-C7-C8	-2.30	107.48	110.92
4	C	401	OKA	O6-C8-O4	2.11	111.37	106.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

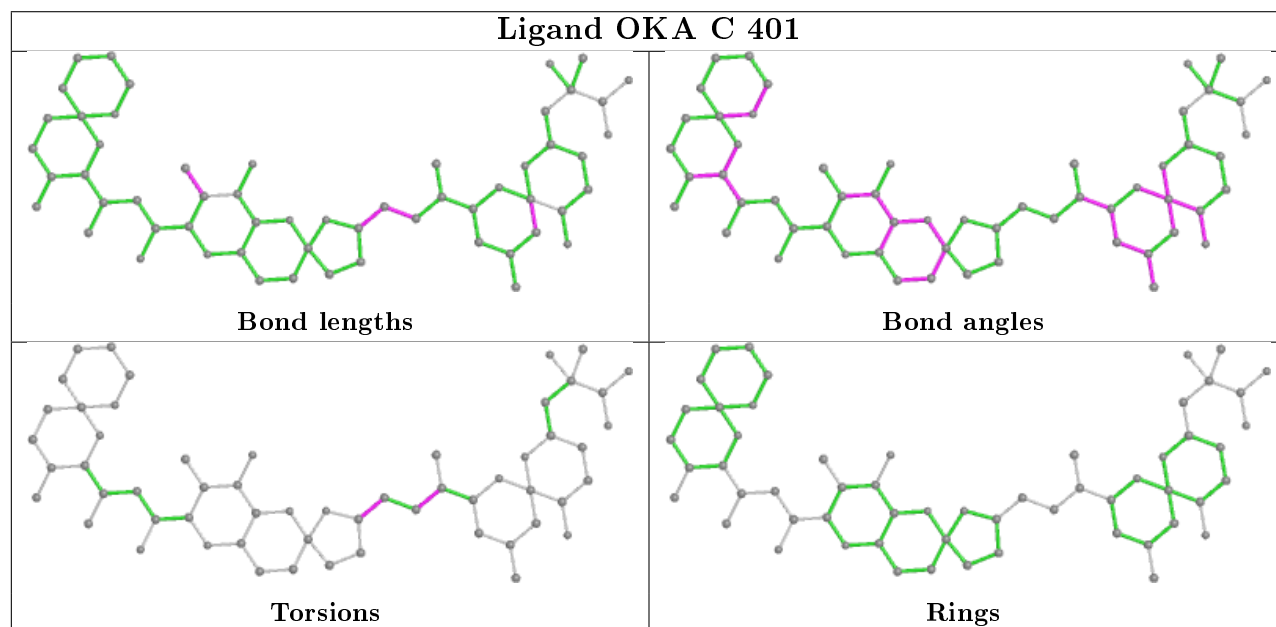
Mol	Chain	Res	Type	Atoms
4	C	401	OKA	C14-C15-C16-C17
4	C	401	OKA	C14-C15-C16-O7
4	C	401	OKA	C42-C13-C14-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	OKA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.