Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 05:26 pm GMT

PDB ID	:	4BVH
Title	:	CRYSTAL STRUCTURE OF HUMAN SIRT3 IN COMPLEX WITH THE INHIBITOR EX-527 AND 2'-O-ACETYL-ADP-RIBOSE
Authors	:	Gertz, M.; Weyand, M.; Steegborn, C.
Deposited on	:	2013-06-25
Resolution	:	1.90 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:

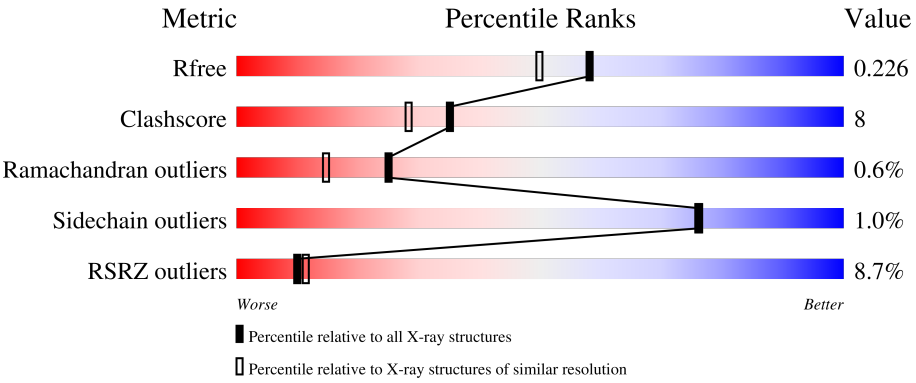
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	284	8% 80% 15%
1	B	284	12% 76% 18% 5%
1	C	284	5% 81% 13% 5%

2 Entry composition

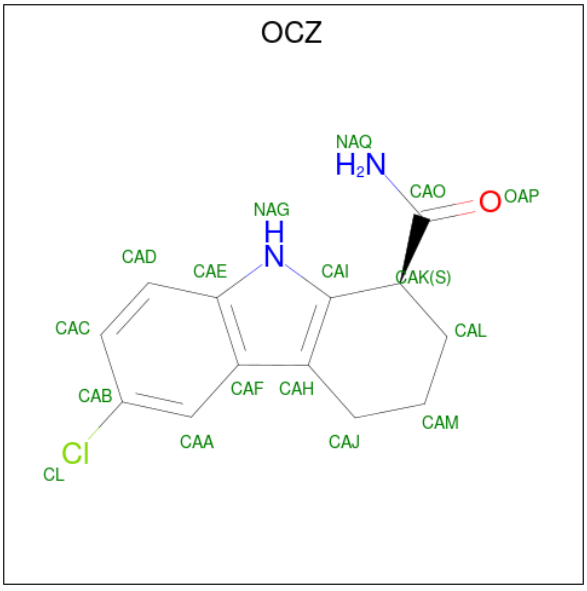
There are 10 unique types of molecules in this entry. The entry contains 7157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	8	0
			2177	1409	374	385	9			
1	B	271	Total	C	N	O	S	0	4	0
			2144	1384	366	384	10			
1	C	270	Total	C	N	O	S	0	7	0
			2149	1393	366	381	9			

- Molecule 2 is (1S)-6-chloro-2,3,4,9-tetrahydro-1H-carbazole-1- carboxamide (three-letter code: OCZ) (formula: $C_{13}H_{13}ClN_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
2	B	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		

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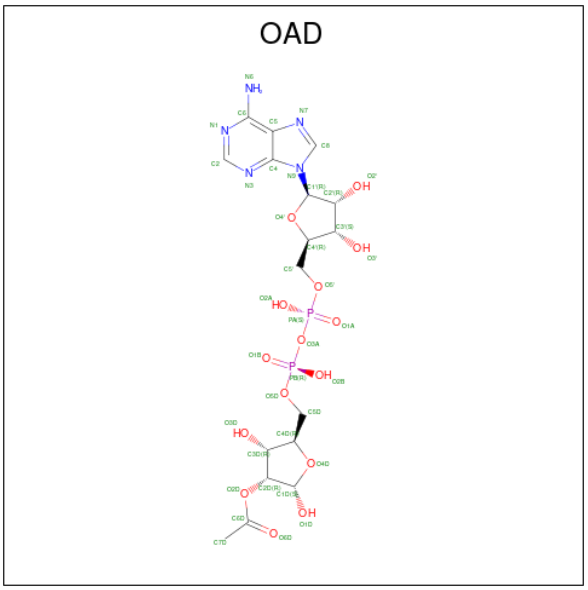
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		

- Molecule 3 is 2'-O-ACETYL ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: OAD) (formula: $C_{17}H_{25}N_5O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	17	5	15	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	5	15	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

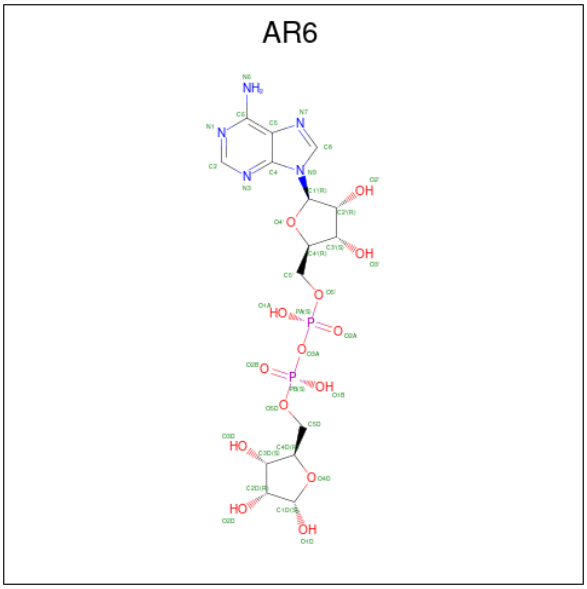
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

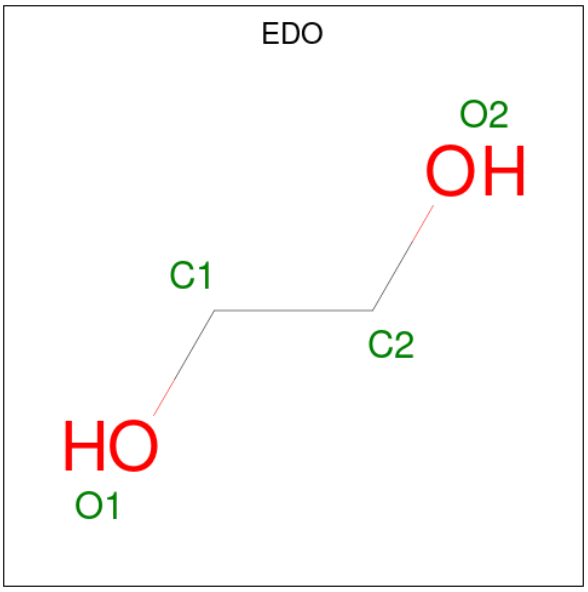
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



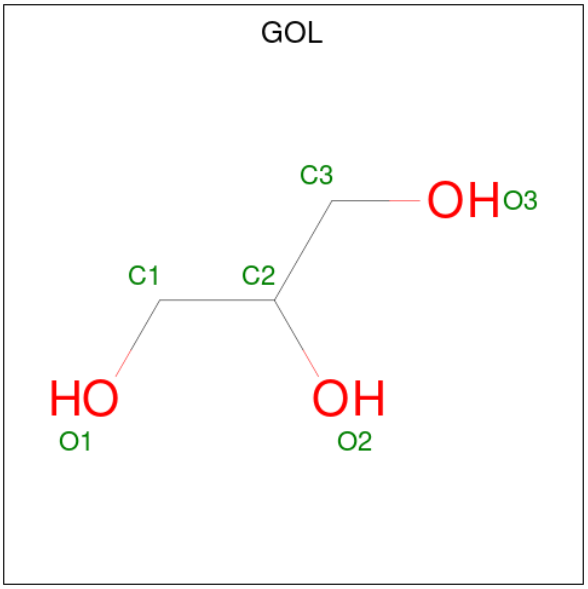
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 36 15 5 14 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

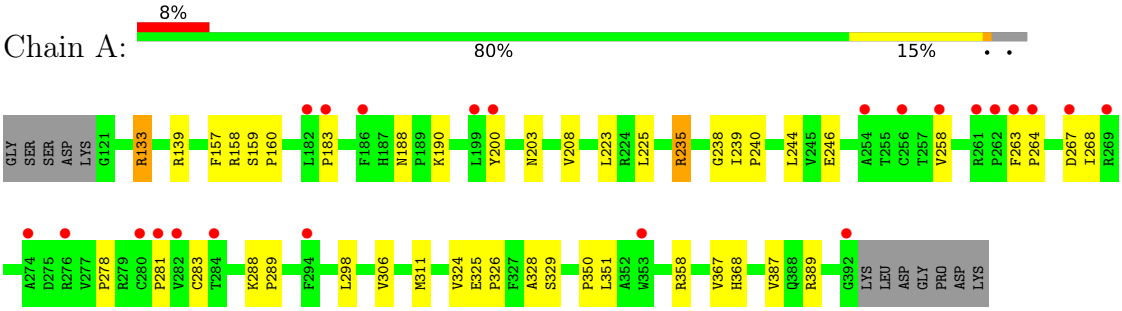
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	134	Total O 135 135	0	1
10	B	158	Total O 158 158	0	0
10	C	196	Total O 197 197	0	1

3 Residue-property plots (i)

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 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.

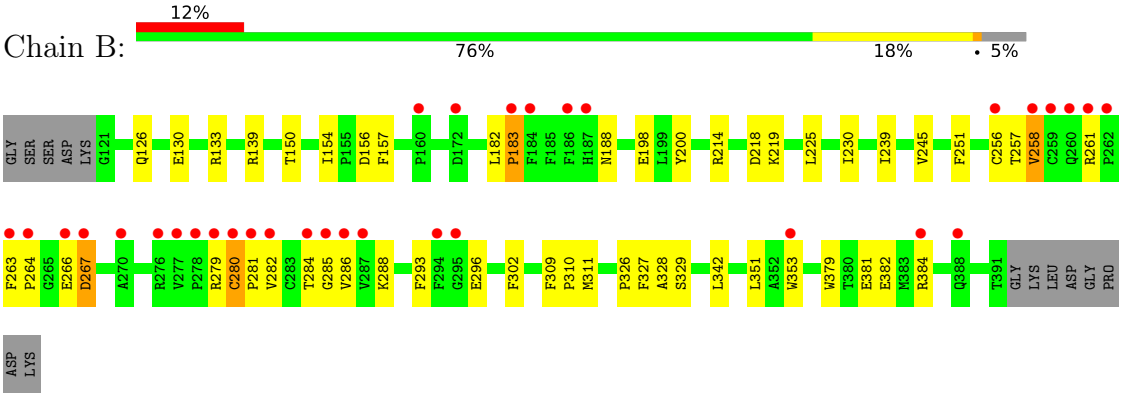
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain A:



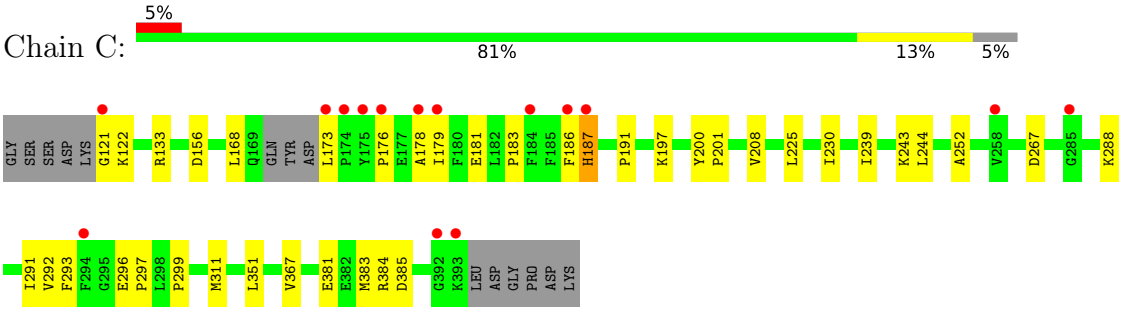
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain B:



• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.71Å 66.53Å 201.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.44 – 1.90 34.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.44-1.90) 99.9 (34.44-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.172 , 0.226 0.172 , 0.226	Depositor DCC
R_{free} test set	3415 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: EDO, GOL, CL, OCZ, ZN, OAD, NA, AR6

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	0.85	0/2256	0.94	4/3073 (0.1%)
1	B	0.93	1/2211 (0.0%)	1.02	6/3014 (0.2%)
1	C	1.04	1/2224 (0.0%)	1.01	5/3030 (0.2%)
All	All	0.95	2/6691 (0.0%)	0.99	15/9117 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	381	GLU	CD-OE1	5.17	1.31	1.25
1	B	353	TRP	CB-CG	5.06	1.59	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	235	ARG	NE-CZ-NH1	11.21	125.90	120.30
1	B	133	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	235	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	351	LEU	CA-CB-CG	-7.08	99.02	115.30
1	B	214	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	280	CYS	CA-CB-SG	6.75	126.16	114.00
1	A	351	LEU	CA-CB-CG	-6.24	100.95	115.30
1	C	244	LEU	CB-CG-CD2	-6.01	100.79	111.00
1	C	133	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	133	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	218	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	197	LYS	CD-CE-NZ	5.12	123.48	111.70
1	B	326	PRO	N-CA-C	5.08	125.30	112.10
1	A	158	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	2177	0	2224	34	0
1	B	2144	0	2169	44	0
1	C	2149	0	2194	35	0
2	A	17	0	13	0	0
2	B	17	0	13	0	0
2	C	17	0	13	0	0
3	A	39	0	23	1	0
3	C	39	0	23	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	36	0	21	2	0
8	B	8	0	12	0	0
8	C	12	0	18	0	0
9	C	6	0	8	2	0
10	A	135	0	0	10	0
10	B	158	0	0	6	0
10	C	197	0	0	5	0
All	All	7157	0	6731	110	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 8.

All (110) 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:B:257:THR:HB	10:B:2096:HOH:O	1.25	1.31
1:A:235:ARG:HD2	1:B:130:GLU:OE2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ARG:HD3	10:A:2130:HOH:O	1.74	0.86
1:A:208[A]:VAL:HG23	10:A:2042:HOH:O	1.75	0.85
1:B:286:VAL:HG12	10:B:2100:HOH:O	1.78	0.83
1:C:178:ALA:HA	1:C:181:GLU:HG3	1.60	0.82
1:C:208[B]:VAL:HG11	1:C:367:VAL:HG13	1.62	0.81
1:A:133:ARG:NH1	10:A:2013:HOH:O	2.13	0.81
1:B:258:VAL:CG2	1:B:285:GLY:HA3	2.12	0.78
1:B:382:GLU:HG3	10:B:2153:HOH:O	1.84	0.77
1:B:258:VAL:HG23	1:B:285:GLY:HA3	1.71	0.72
1:C:168:LEU:HD13	1:C:179:ILE:CG2	2.21	0.70
1:B:230:ILE:HD12	1:B:251:PHE:CE2	2.26	0.69
1:B:139:ARG:HH11	1:B:311[A]:MET:HE3	1.57	0.69
1:C:239[A]:ILE:HD11	10:C:2064:HOH:O	1.94	0.68
1:A:225:LEU:HD12	1:A:239[B]:ILE:HD13	1.77	0.67
1:C:173:LEU:CD1	1:C:179:ILE:HG23	2.24	0.67
1:C:168:LEU:HD13	1:C:179:ILE:HG21	1.76	0.67
1:B:139:ARG:NH1	1:B:311[A]:MET:CE	2.59	0.66
1:A:225:LEU:CD1	1:A:239[B]:ILE:HD13	2.26	0.65
1:B:264:PRO:O	1:B:267:ASP:HB2	1.96	0.65
1:C:267:ASP:OD1	9:C:1397:GOL:H12	1.96	0.65
1:C:208[B]:VAL:CG1	1:C:367:VAL:HG13	2.26	0.64
1:B:198:GLU:HB3	1:C:311:MET:HG2	1.79	0.63
1:B:230:ILE:HD12	1:B:251:PHE:HE2	1.63	0.63
1:C:173:LEU:HD11	1:C:179:ILE:HG23	1.80	0.62
1:A:311:MET:CE	1:A:311:MET:HA	2.28	0.62
1:B:327:PHE:HB2	10:B:2071:HOH:O	2.00	0.62
1:C:121:GLY:O	1:C:122:LYS:HG2	2.00	0.61
1:C:288:LYS:HE2	1:C:293:PHE:CE1	2.35	0.61
1:B:263:PHE:CZ	1:B:281:PRO:HD2	2.35	0.61
1:C:201:PRO:HD3	10:C:2047:HOH:O	2.00	0.61
1:C:288:LYS:HE2	1:C:293:PHE:HE1	1.66	0.61
1:B:288:LYS:HE2	1:B:293:PHE:CE1	2.35	0.61
1:C:186:PHE:O	1:C:187:HIS:HB3	2.01	0.60
1:C:186:PHE:O	1:C:187:HIS:CB	2.49	0.60
1:C:239[A]:ILE:CD1	10:C:2064:HOH:O	2.47	0.59
1:C:183:PRO:O	1:C:186:PHE:O	2.21	0.59
1:C:156:ASP:OD2	3:C:1395:OAD:H8	2.03	0.59
1:B:139:ARG:NH1	1:B:311[A]:MET:HE1	2.17	0.59
1:C:173:LEU:HD11	1:C:179:ILE:CG2	2.33	0.58
1:B:258:VAL:HG21	1:B:285:GLY:HA3	1.87	0.57
1:B:381:GLU:HG3	1:B:384:ARG:HH12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139[B]:ARG:NH1	10:A:2017:HOH:O	2.27	0.55
1:B:263:PHE:CE1	1:B:281:PRO:HD2	2.42	0.54
1:C:292:VAL:HG21	1:C:299:PRO:HD3	1.90	0.54
1:A:157:PHE:CE2	3:A:1394:OAD:HR'3	2.42	0.53
1:C:168:LEU:HD13	1:C:179:ILE:HG23	1.89	0.52
1:B:139:ARG:HH11	1:B:311[A]:MET:CE	2.18	0.52
1:B:288:LYS:HE2	1:B:293:PHE:CD1	2.46	0.51
1:B:150:THR:HA	1:B:154:ILE:O	2.11	0.50
1:C:384:ARG:HH21	1:C:385[A]:ASP:CG	2.15	0.50
1:C:178:ALA:CA	1:C:181:GLU:HG3	2.37	0.50
1:A:324:VAL:HG12	1:A:325:GLU:O	2.11	0.50
1:C:173:LEU:HD21	10:C:2036:HOH:O	2.12	0.49
1:A:240:PRO:HA	1:B:126:GLN:HE22	1.77	0.49
1:A:368:HIS:HD2	10:A:2118:HOH:O	1.94	0.49
1:A:208[B]:VAL:HG21	1:A:367:VAL:HG13	1.94	0.49
1:C:225:LEU:CD1	1:C:239[A]:ILE:HD13	2.43	0.49
1:A:239[B]:ILE:HD11	10:A:2044:HOH:O	2.13	0.48
1:B:329:SER:HB2	10:B:2119:HOH:O	2.13	0.48
1:A:188:ASN:OD1	1:A:190:LYS:HB2	2.13	0.48
1:A:311:MET:HA	1:A:311:MET:HE2	1.94	0.48
1:B:280:CYS:O	1:B:284:THR:HA	2.14	0.48
1:C:168:LEU:HD11	1:C:179:ILE:HD13	1.95	0.47
1:B:279:ARG:HA	1:B:285:GLY:O	2.15	0.47
1:B:327:PHE:O	1:B:328:ALA:C	2.53	0.47
1:A:325:GLU:CD	1:A:329:SER:HG	2.18	0.47
1:A:288:LYS:NZ	1:A:289:PRO:O	2.48	0.46
1:B:261:ARG:NH2	1:B:282:VAL:HG11	2.30	0.46
1:B:261:ARG:HD2	1:B:263:PHE:CE1	2.50	0.45
1:B:245:VAL:HG11	1:B:302:PHE:HA	1.98	0.45
1:A:358:ARG:NH2	10:A:2111:HOH:O	2.46	0.45
1:A:203:ASN:OD1	1:A:203:ASN:N	2.42	0.45
1:B:261:ARG:HH21	1:B:282:VAL:HG11	1.82	0.45
1:B:225:LEU:HD12	1:B:239[B]:ILE:HD13	1.98	0.45
1:C:178:ALA:HA	1:C:181:GLU:CG	2.40	0.45
1:A:183:PRO:HB2	10:A:2033:HOH:O	2.18	0.44
1:A:239[B]:ILE:CD1	10:A:2044:HOH:O	2.65	0.44
1:B:156:ASP:OD2	7:B:1393:AR6:H8	2.17	0.44
1:B:257:THR:HG22	1:B:286:VAL:O	2.18	0.44
1:B:157:PHE:CE1	7:B:1393:AR6:H3D	2.52	0.44
1:B:219:LYS:HD3	1:B:379:TRP:CZ2	2.53	0.44
1:B:182:LEU:N	1:B:183:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208[B]:VAL:CG2	1:A:367:VAL:HG13	2.49	0.43
1:A:244[B]:LEU:HG	1:A:246:GLU:HG3	2.01	0.43
1:B:382:GLU:CG	10:B:2153:HOH:O	2.53	0.43
1:C:296:GLU:HB3	1:C:297:PRO:HD2	2.00	0.43
1:A:258:VAL:HB	1:A:283:CYS:SG	2.59	0.43
1:C:383:MET:HA	1:C:383:MET:HE2	2.01	0.43
1:B:256:CYS:SG	1:B:258:VAL:N	2.82	0.42
1:C:252:ALA:HA	10:C:2050[B]:HOH:O	2.18	0.42
1:B:309:PHE:N	1:B:310:PRO:CD	2.82	0.42
1:C:176:PRO:O	1:C:179:ILE:HG12	2.20	0.42
1:A:298:LEU:HD11	1:A:326:PRO:HG3	2.02	0.42
1:C:230:ILE:HG21	1:C:291:ILE:HG23	2.00	0.42
1:A:268:ILE:HD12	1:A:278:PRO:HB3	2.01	0.42
1:A:139[B]:ARG:HB3	1:A:223[B]:LEU:HD12	2.01	0.42
1:A:263:PHE:CE2	1:A:281:PRO:HD2	2.54	0.42
1:B:293:PHE:O	1:B:296:GLU:HB2	2.20	0.42
1:A:238:GLY:HA2	10:A:2061:HOH:O	2.19	0.42
1:B:342:LEU:HB2	1:B:351:LEU:HD22	2.02	0.41
1:A:208[B]:VAL:HG12	1:A:387:VAL:HG21	2.03	0.41
1:A:159:SER:HA	1:A:160:PRO:HD3	1.96	0.41
1:B:256:CYS:SG	1:B:280:CYS:HB2	2.61	0.41
1:B:280:CYS:N	1:B:285:GLY:O	2.45	0.41
1:C:267:ASP:OD1	9:C:1397:GOL:C1	2.66	0.41
1:A:264:PRO:HG2	1:A:267:ASP:OD2	2.22	0.40
1:C:243[B]:LYS:HA	1:C:243[B]:LYS:HD3	1.84	0.40
1:A:328:ALA:O	1:A:350:PRO:HG2	2.21	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	278/284 (98%)	265 (95%)	13 (5%)	0	100 100
1	B	273/284 (96%)	261 (96%)	8 (3%)	4 (2%)	10 3
1	C	273/284 (96%)	267 (98%)	5 (2%)	1 (0%)	34 24
All	All	824/852 (97%)	793 (96%)	26 (3%)	5 (1%)	25 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	GLU
1	C	187	HIS
1	B	188	ASN
1	B	183	PRO
1	B	258	VAL

5.3.2 Protein sidechains (i)

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	243/245 (99%)	240 (99%)	3 (1%)	71 70
1	B	239/245 (98%)	237 (99%)	2 (1%)	81 82
1	C	240/245 (98%)	237 (99%)	3 (1%)	69 68
All	All	722/735 (98%)	714 (99%)	8 (1%)	76 73

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	A	200	TYR
1	A	306	VAL
1	B	200	TYR
1	B	267	ASP
1	C	191	PRO
1	C	200[A]	TYR
1	C	200[B]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	305	HIS
1	A	368	HIS
1	B	126	GLN
1	B	354	HIS
1	B	388	GLN
1	C	126	GLN
1	C	388	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
8	EDO	C	1398	-	3,3,3	0.48	0	2,2,2	1.16	0
9	GOL	C	1397	-	5,5,5	1.04	0	5,5,5	0.98	0
2	OCZ	A	1393	-	17,19,19	3.35	10 (58%)	18,28,28	1.62	4 (22%)
2	OCZ	C	1394	-	17,19,19	3.74	11 (64%)	18,28,28	1.10	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	AR6	B	1393	-	34,39,39	1.10	2 (5%)	40,60,60	1.85	10 (25%)
8	EDO	C	1396	-	3,3,3	0.50	0	2,2,2	0.42	0
3	OAD	A	1394	-	36,42,42	1.62	9 (25%)	42,64,64	2.17	9 (21%)
8	EDO	B	1394	-	3,3,3	0.51	0	2,2,2	0.56	0
8	EDO	B	1395	-	3,3,3	0.73	0	2,2,2	0.54	0
8	EDO	C	1399	-	3,3,3	0.55	0	2,2,2	0.28	0
2	OCZ	B	1392	-	17,19,19	4.59	9 (52%)	18,28,28	1.67	3 (16%)
3	OAD	C	1395	-	36,42,42	1.45	10 (27%)	42,64,64	1.94	6 (14%)

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
8	EDO	C	1398	-	-	0/1/1/1	-
9	GOL	C	1397	-	-	2/4/4/4	-
2	OCZ	A	1393	-	-	2/4/14/14	0/3/3/3
2	OCZ	C	1394	-	-	3/4/14/14	0/3/3/3
7	AR6	B	1393	-	-	3/18/54/54	0/4/4/4
8	EDO	C	1396	-	-	0/1/1/1	-
3	OAD	A	1394	-	-	4/22/58/58	0/4/4/4
8	EDO	B	1394	-	-	0/1/1/1	-
8	EDO	B	1395	-	-	1/1/1/1	-
8	EDO	C	1399	-	-	1/1/1/1	-
2	OCZ	B	1392	-	-	4/4/14/14	0/3/3/3
3	OAD	C	1395	-	-	4/22/58/58	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1392	OCZ	CAI-CAK	-15.37	1.46	1.51
2	C	1394	OCZ	CAI-CAK	-11.47	1.47	1.51
2	A	1393	OCZ	CAI-CAK	-7.99	1.48	1.51
2	B	1392	OCZ	CAK-CAO	-7.19	1.46	1.53
2	A	1393	OCZ	CAK-CAO	-6.07	1.47	1.53
2	C	1394	OCZ	CAB-CL	5.71	1.86	1.74
2	A	1393	OCZ	CAB-CL	5.28	1.86	1.74
2	B	1392	OCZ	CAA-CAB	4.13	1.44	1.36
3	A	1394	OAD	C2-N3	4.03	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1394	OCZ	CAK-CAO	-4.01	1.49	1.53
2	A	1393	OCZ	CAJ-CAH	-3.56	1.45	1.51
7	B	1393	AR6	O4'-C4'	-3.44	1.37	1.45
2	C	1394	OCZ	CAA-CAB	3.43	1.43	1.36
2	A	1393	OCZ	CAA-CAF	-3.25	1.35	1.42
3	C	1395	OAD	C3'-C4'	3.22	1.61	1.53
3	A	1394	OAD	C5-C4	-2.97	1.33	1.40
2	B	1392	OCZ	CAB-CL	2.96	1.80	1.74
2	A	1393	OCZ	CAF-CAE	-2.88	1.34	1.42
3	A	1394	OAD	C8-N7	-2.85	1.29	1.34
2	C	1394	OCZ	CAM-CAJ	2.85	1.61	1.51
2	A	1393	OCZ	CAM-CAJ	2.78	1.61	1.51
3	C	1395	OAD	O3D-C3D	2.74	1.49	1.43
3	C	1395	OAD	C5-C4	-2.70	1.33	1.40
3	C	1395	OAD	C2-N3	2.63	1.36	1.32
7	B	1393	AR6	O5D-C5D	-2.63	1.34	1.44
2	B	1392	OCZ	CAO-NAQ	2.63	1.39	1.32
3	A	1394	OAD	O3'-C3'	-2.56	1.37	1.43
2	C	1394	OCZ	CAD-CAC	2.51	1.41	1.36
2	C	1394	OCZ	CAA-CAF	-2.44	1.37	1.42
3	C	1395	OAD	O2D-C6D	2.43	1.40	1.35
2	A	1393	OCZ	CAM-CAL	2.42	1.59	1.53
3	A	1394	OAD	O4D-C1D	2.39	1.46	1.43
2	B	1392	OCZ	CAF-CAE	-2.38	1.36	1.42
2	C	1394	OCZ	CAF-CAE	-2.36	1.36	1.42
3	A	1394	OAD	O3D-C3D	2.36	1.48	1.43
2	A	1393	OCZ	CAD-CAE	-2.34	1.37	1.41
3	A	1394	OAD	O2'-C2'	2.30	1.48	1.43
2	B	1392	OCZ	CAL-CAK	2.27	1.60	1.54
3	C	1395	OAD	C2-N1	2.26	1.38	1.33
3	C	1395	OAD	C2'-C1'	2.24	1.57	1.53
2	C	1394	OCZ	CAO-NAQ	2.22	1.38	1.32
3	C	1395	OAD	O4'-C1'	2.22	1.44	1.41
2	B	1392	OCZ	CAD-CAE	-2.21	1.38	1.41
2	C	1394	OCZ	CAJ-CAH	-2.16	1.47	1.51
3	C	1395	OAD	PB-O1B	-2.15	1.43	1.50
2	A	1393	OCZ	CAA-CAB	2.11	1.40	1.36
3	C	1395	OAD	C6-N6	2.09	1.41	1.34
3	A	1394	OAD	C2'-C1'	2.05	1.56	1.53
2	C	1394	OCZ	CAL-CAK	2.04	1.59	1.54
2	B	1392	OCZ	CAA-CAF	-2.03	1.38	1.42
3	A	1394	OAD	C6-C5	-2.03	1.35	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1395	OAD	N3-C2-N1	-6.88	117.93	128.68
3	A	1394	OAD	O1D-C1D-O4D	-6.56	102.73	111.13
3	A	1394	OAD	N3-C2-N1	-6.40	118.67	128.68
7	B	1393	AR6	C5D-C4D-C3D	-5.89	93.10	115.18
3	A	1394	OAD	C2D-O2D-C6D	5.28	125.89	117.72
3	C	1395	OAD	O2D-C6D-C7D	4.94	120.19	111.09
3	C	1395	OAD	O4'-C1'-C2'	-4.45	100.42	106.93
3	A	1394	OAD	C1D-C2D-C3D	-3.98	99.72	104.09
3	C	1395	OAD	C1D-C2D-C3D	-3.94	99.77	104.09
7	B	1393	AR6	N3-C2-N1	-3.78	122.77	128.68
3	A	1394	OAD	O4'-C1'-C2'	-3.76	101.43	106.93
2	B	1392	OCZ	CAD-CAC-CAB	-3.74	114.88	119.21
3	C	1395	OAD	C4-C5-N7	-3.32	105.94	109.40
3	A	1394	OAD	O2D-C6D-C7D	3.27	117.10	111.09
2	B	1392	OCZ	CAM-CAJ-CAH	3.18	117.31	112.49
3	C	1395	OAD	C2D-O2D-C6D	3.13	122.57	117.72
2	A	1393	OCZ	CAD-CAC-CAB	-3.10	115.61	119.21
2	A	1393	OCZ	OAP-CAO-NAQ	-3.08	117.64	123.00
7	B	1393	AR6	O4D-C4D-C5D	-2.94	99.71	109.37
2	A	1393	OCZ	CAL-CAK-CAI	2.88	111.65	106.19
2	B	1392	OCZ	CAL-CAK-CAI	2.80	111.49	106.19
3	A	1394	OAD	C4-C5-N7	-2.76	106.53	109.40
7	B	1393	AR6	C2'-C3'-C4'	2.55	107.61	102.64
7	B	1393	AR6	O3'-C3'-C4'	-2.45	103.97	111.05
3	A	1394	OAD	C5'-C4'-C3'	-2.36	106.35	115.18
7	B	1393	AR6	O2'-C2'-C1'	-2.33	102.23	110.85
3	A	1394	OAD	O2D-C2D-C1D	2.30	114.93	108.37
2	C	1394	OCZ	CAL-CAK-CAI	2.25	110.46	106.19
7	B	1393	AR6	O2'-C2'-C3'	2.20	118.95	111.82
7	B	1393	AR6	C1D-C2D-C3D	-2.11	99.66	102.30
7	B	1393	AR6	O5D-PB-O2B	-2.10	100.87	109.07
2	A	1393	OCZ	CAM-CAL-CAK	-2.05	106.43	111.50
7	B	1393	AR6	O3D-C3D-C2D	2.02	118.36	111.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1393	OCZ	CAI-CAK-CAO-OAP
2	B	1392	OCZ	CAI-CAK-CAO-NAQ
3	A	1394	OAD	O6D-C6D-O2D-C2D

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Mol	Chain	Res	Type	Atoms
3	A	1394	OAD	C7D-C6D-O2D-C2D
3	C	1395	OAD	O6D-C6D-O2D-C2D
3	C	1395	OAD	C7D-C6D-O2D-C2D
9	C	1397	GOL	C1-C2-C3-O3
7	B	1393	AR6	O4D-C4D-C5D-O5D
8	B	1395	EDO	O1-C1-C2-O2
2	C	1394	OCZ	CAL-CAK-CAO-NAQ
7	B	1393	AR6	C3D-C4D-C5D-O5D
2	B	1392	OCZ	CAI-CAK-CAO-OAP
2	C	1394	OCZ	CAI-CAK-CAO-OAP
9	C	1397	GOL	O1-C1-C2-C3
8	C	1399	EDO	O1-C1-C2-O2
2	B	1392	OCZ	CAL-CAK-CAO-NAQ
2	A	1393	OCZ	CAL-CAK-CAO-OAP
2	B	1392	OCZ	CAL-CAK-CAO-OAP
2	C	1394	OCZ	CAL-CAK-CAO-OAP
3	A	1394	OAD	O4'-C4'-C5'-O5'
3	C	1395	OAD	O4'-C4'-C5'-O5'
3	A	1394	OAD	C5D-O5D-PB-O1B
3	C	1395	OAD	C5D-O5D-PB-O1B
7	B	1393	AR6	O4'-C4'-C5'-O5'

There are no ring outliers.

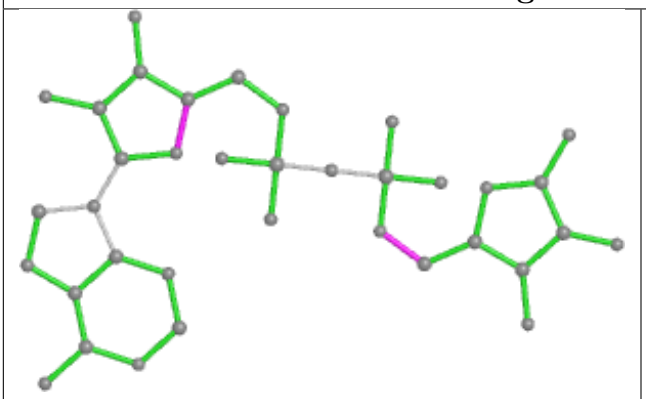
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1397	GOL	2	0
7	B	1393	AR6	2	0
3	A	1394	OAD	1	0
3	C	1395	OAD	1	0

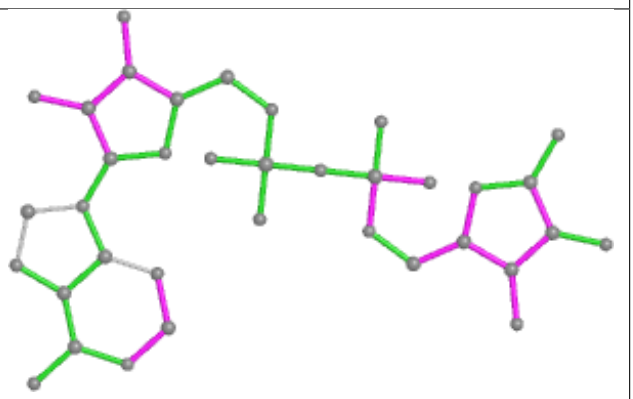
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

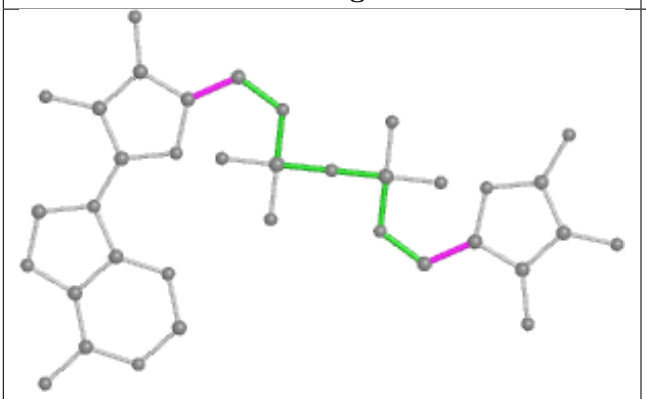
Ligand AR6 B 1393



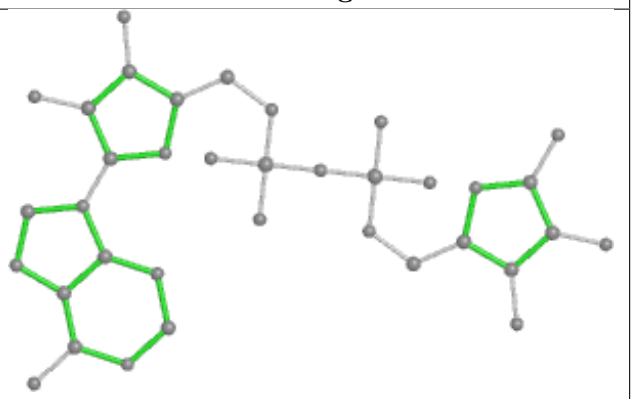
Bond lengths



Bond angles

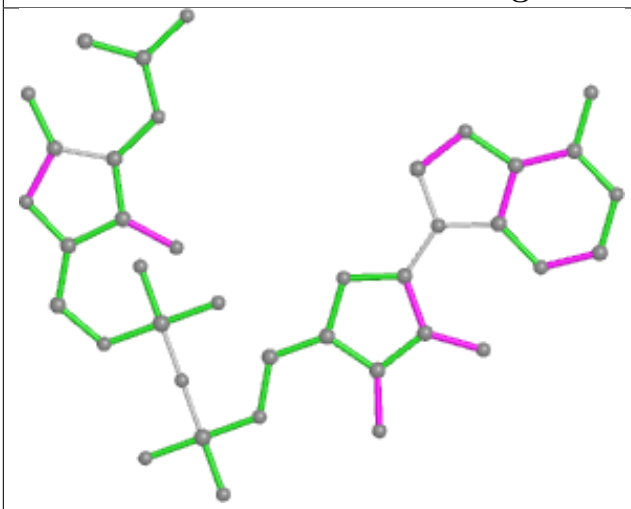


Torsions

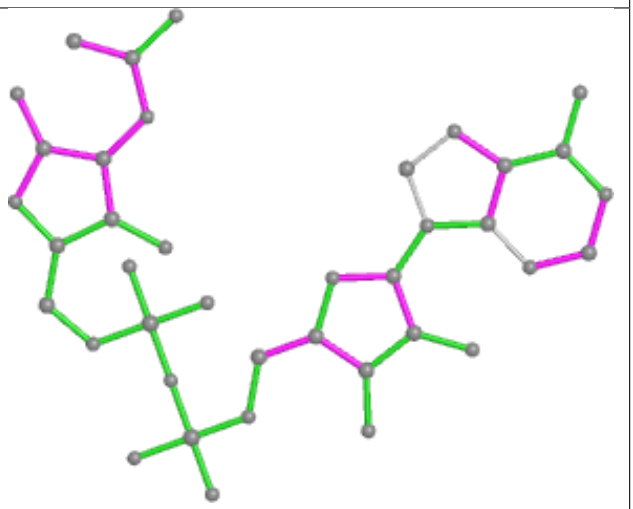


Rings

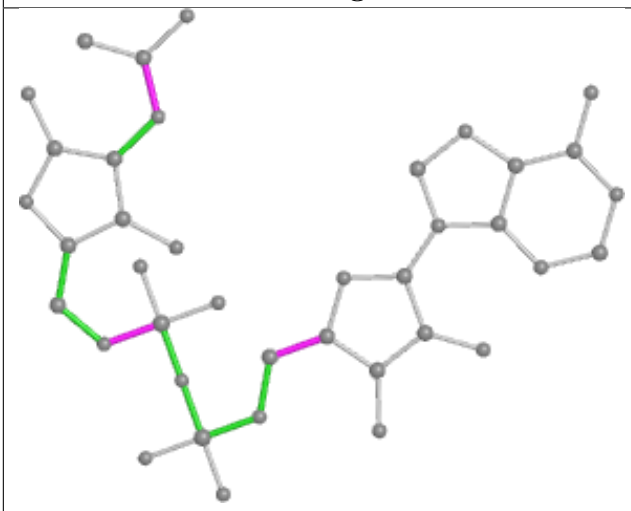
Ligand OAD A 1394



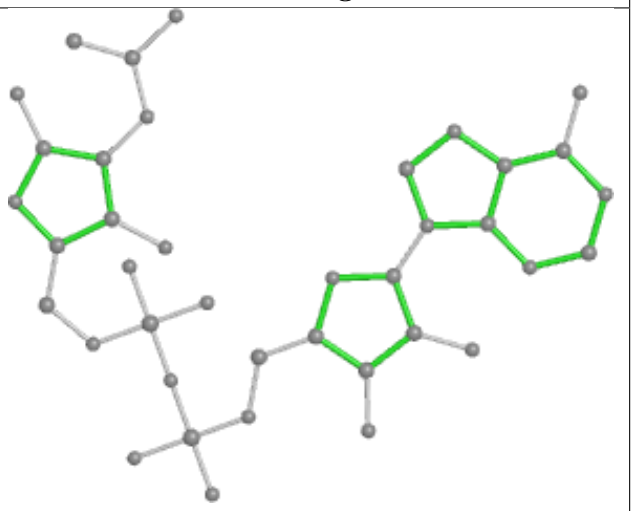
Bond lengths



Bond angles

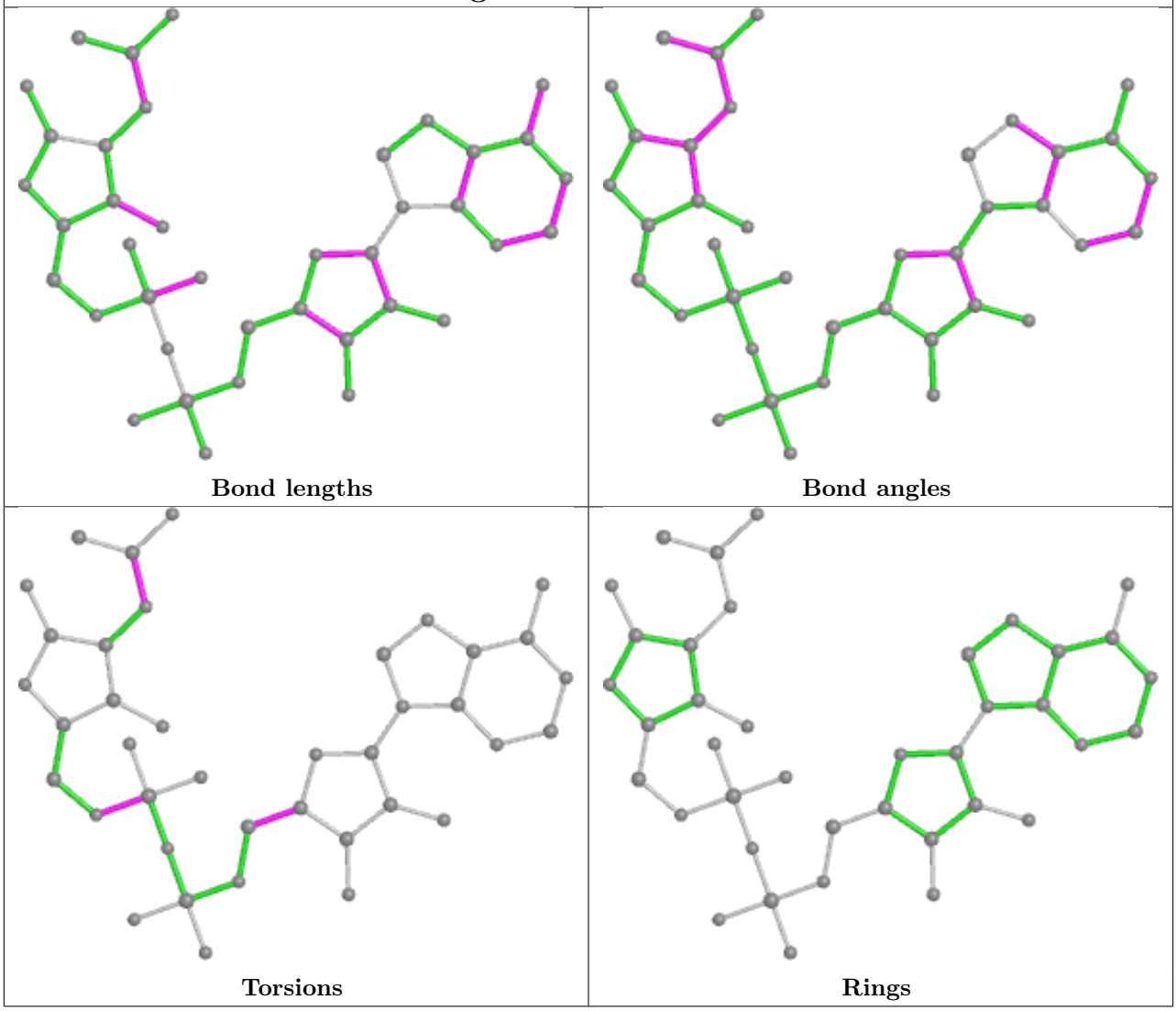


Torsions



Rings

Ligand OAD C 1395



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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	272/284 (95%)	0.29	23 (8%) 10 12	10, 26, 58, 88	0
1	B	271/284 (95%)	0.38	33 (12%) 4 4	10, 25, 59, 85	4 (1%)
1	C	270/284 (95%)	0.05	15 (5%) 24 27	8, 18, 44, 69	1 (0%)
All	All	813/852 (95%)	0.24	71 (8%) 10 11	8, 22, 56, 88	5 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	PRO	11.6
1	C	175	TYR	6.1
1	C	121	GLY	6.1
1	A	294	PHE	5.9
1	A	281	PRO	5.5
1	B	282	VAL	5.3
1	B	284	THR	5.2
1	B	256	CYS	5.0
1	A	263	PHE	4.8
1	A	264	PRO	4.8
1	A	284	THR	4.8
1	B	263	PHE	4.7
1	A	282	VAL	4.6
1	A	261	ARG	4.5
1	A	262	PRO	4.2
1	A	267	ASP	4.2
1	B	261	ARG	4.1
1	B	259	CYS	4.1
1	C	174	PRO	4.1
1	B	270	ALA	3.9
1	B	278	PRO	3.8
1	C	294	PHE	3.8
1	B	186	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	173	LEU	3.6
1	B	295	GLY	3.5
1	B	160	PRO	3.5
1	A	258	VAL	3.4
1	A	269	ARG	3.4
1	B	187	HIS	3.4
1	C	178	ALA	3.4
1	B	287	VAL	3.4
1	A	186	PHE	3.4
1	C	393	LYS	3.3
1	A	353	TRP	3.3
1	B	280	CYS	3.2
1	B	262	PRO	3.2
1	C	176	PRO	3.2
1	B	277	VAL	3.2
1	B	258	VAL	3.1
1	A	256	CYS	3.0
1	B	279	ARG	2.9
1	A	254	ALA	2.9
1	B	286	VAL	2.9
1	B	184	PHE	2.8
1	C	258	VAL	2.8
1	C	285	GLY	2.7
1	B	285	GLY	2.7
1	B	260	GLN	2.6
1	B	267	ASP	2.6
1	B	294	PHE	2.5
1	A	183	PRO	2.5
1	B	183	PRO	2.5
1	B	384	ARG	2.4
1	A	280	CYS	2.4
1	C	187	HIS	2.4
1	B	353	TRP	2.3
1	B	172	ASP	2.3
1	A	392	GLY	2.3
1	C	184	PHE	2.3
1	A	276	ARG	2.3
1	A	274	ALA	2.3
1	B	264	PRO	2.3
1	C	186	PHE	2.2
1	A	199	LEU	2.2
1	A	200	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	388	GLN	2.2
1	B	276	ARG	2.2
1	B	266	GLU	2.1
1	C	179	ILE	2.1
1	C	392	GLY	2.1
1	A	182	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	C	1399	4/4	0.69	0.14	56,58,58,60	0
8	EDO	B	1395	4/4	0.70	0.21	42,44,49,51	0
4	ZN	B	1396	1/1	0.76	0.11	87,87,87,87	0
6	CL	B	1397	1/1	0.79	0.12	72,72,72,72	0
9	GOL	C	1397	6/6	0.81	0.17	28,32,34,38	0
8	EDO	B	1394	4/4	0.86	0.14	47,51,52,53	0
8	EDO	C	1396	4/4	0.90	0.11	41,41,42,43	0
2	OCZ	A	1393	17/17	0.93	0.10	16,23,30,33	0
5	NA	A	1396	1/1	0.93	0.14	33,33,33,33	0
8	EDO	C	1398	4/4	0.94	0.11	30,31,31,33	0
4	ZN	A	1395	1/1	0.96	0.07	42,42,42,42	0
2	OCZ	B	1392	17/17	0.96	0.08	13,20,24,31	0
2	OCZ	C	1394	17/17	0.97	0.10	10,12,17,24	0
4	ZN	C	1400	1/1	0.98	0.04	27,27,27,27	0
7	AR6	B	1393	36/36	0.98	0.09	15,18,36,44	0
3	OAD	A	1394	39/39	0.98	0.09	15,18,39,50	3
6	CL	A	1397	1/1	0.98	0.14	56,56,56,56	0

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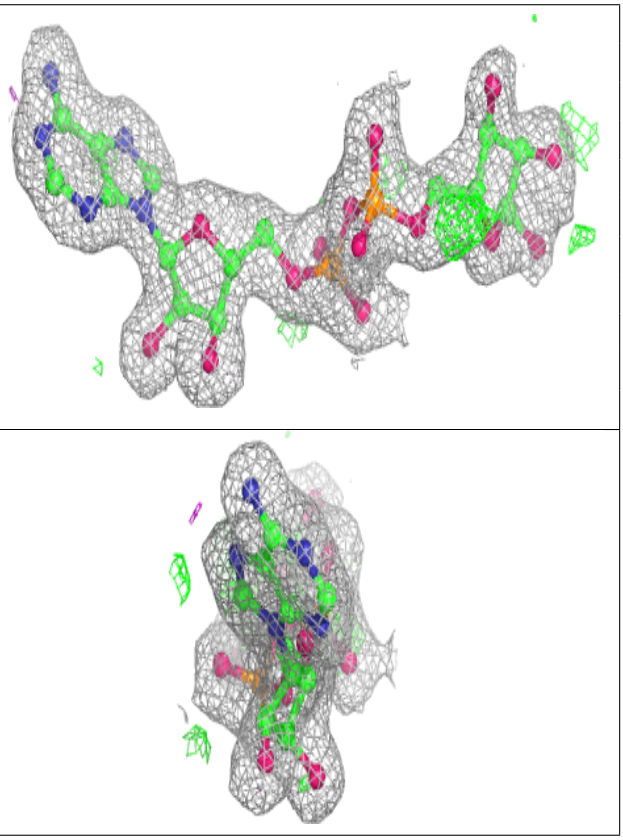
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OAD	C	1395	39/39	0.99	0.07	9,11,23,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

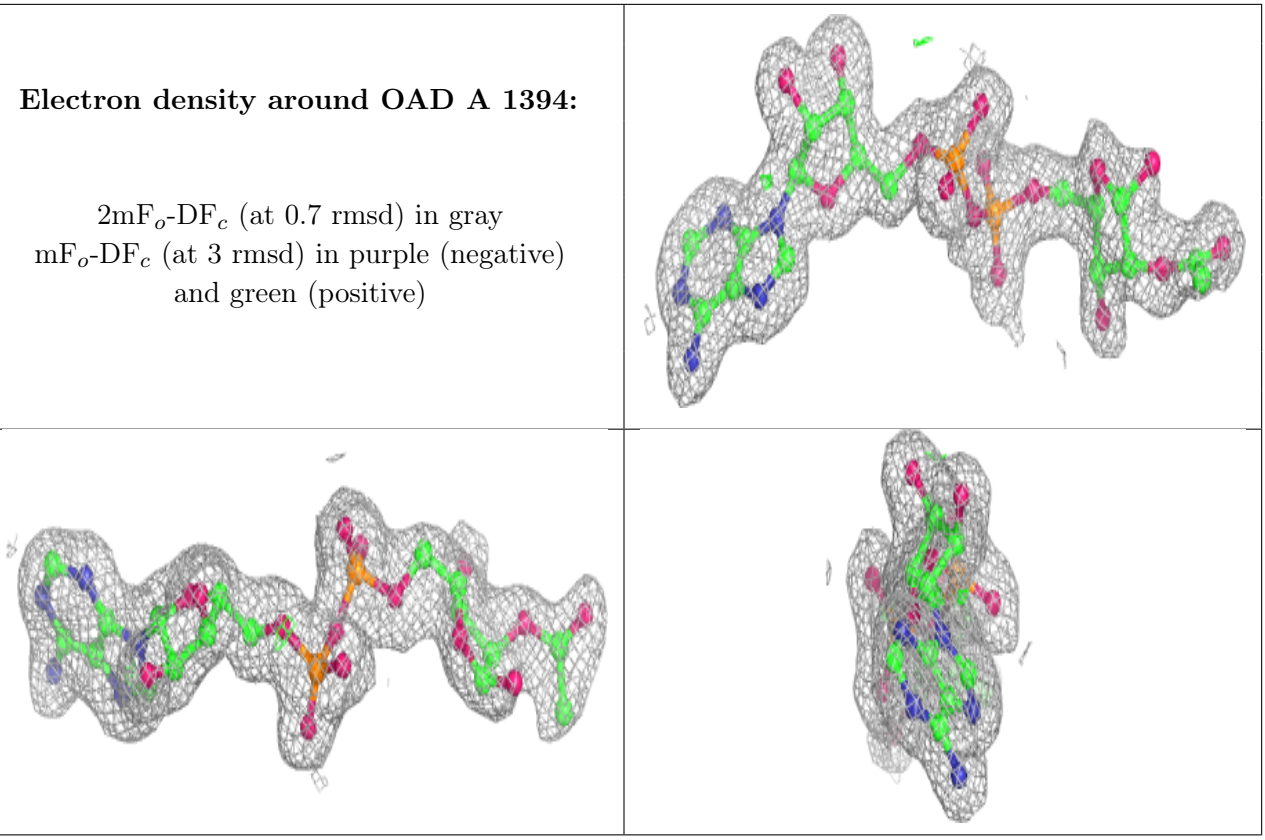
Electron density around AR6 B 1393:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



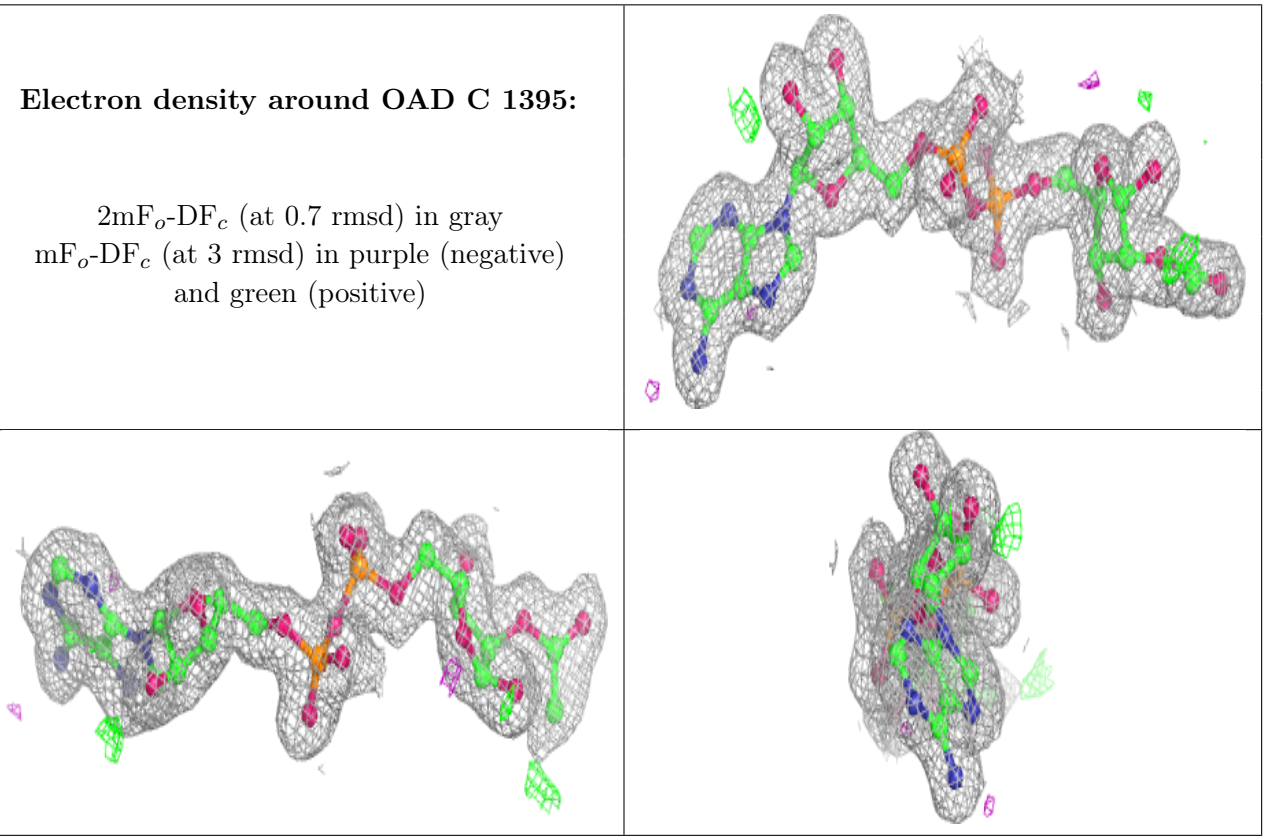
Electron density around OAD A 1394:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OAD C 1395:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.