



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 09:31 PM EST

PDB ID : 5H4D  
Title : Crystal structure of hSIRT3 in complex with a specific agonist Amiodarone hydrochloride  
Authors : Zhang, S.; Fu, L.; Liu, J.; Liu, B.  
Deposited on : unknown  
Resolution : 3.21 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

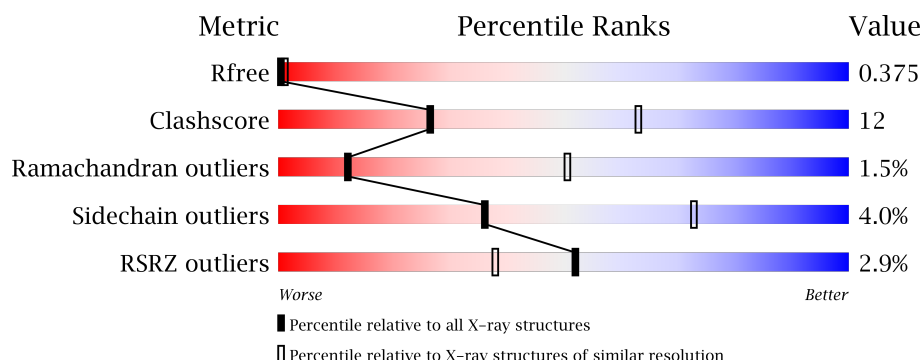
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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))
$R_{free}$	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

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.

Mol	Chain	Length	Quality of chain
1	A	271	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	H	271	<div> <div>3%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>
2	D	3	<div> <div>33%</div> <div>67%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	401	-	-	X	-
5	BBI	A	403	-	-	-	X
5	BBI	H	405	-	-	-	X
6	NAD	A	404	-	-	-	X
6	NAD	H	406	-	-	-	X
8	PEG	H	401	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4526 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	271	Total	C	N	O	S	0	0	0
			2127	1370	366	382	9			
1	H	271	Total	C	N	O	S	0	0	0
			2121	1364	366	382	9			

- Molecule 2 is a protein called ARG-HIS-LYS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			30	18	9	3			
2	C	3	Total	C	N	O	0	0	0
			30	18	9	3			

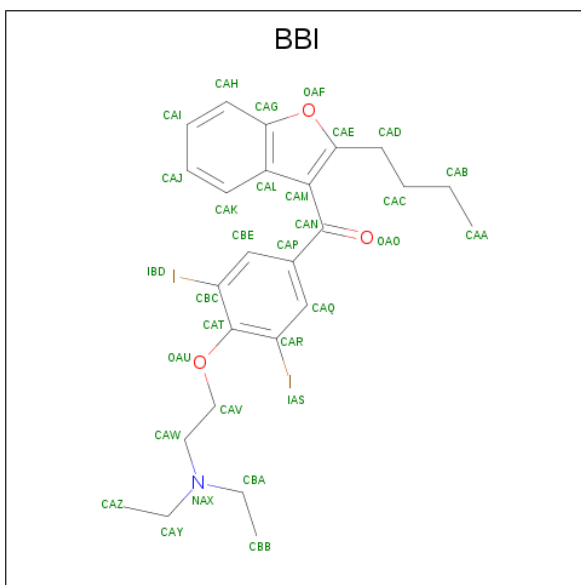
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

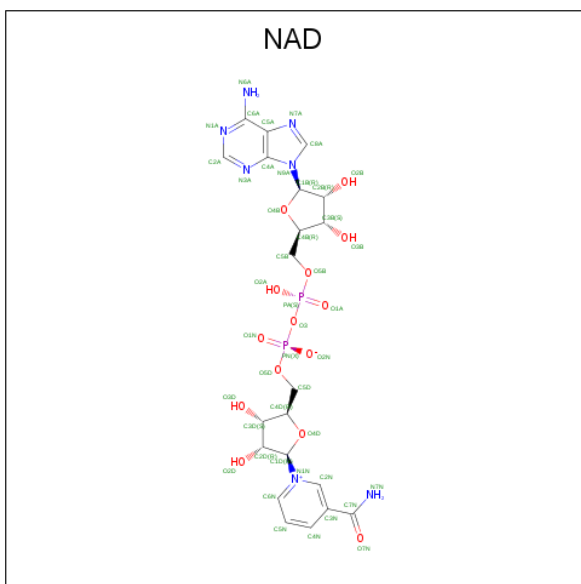
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is (2-butyl-1-benzofuran-3-yl){4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl}methanone (three-letter code: BBI) (formula: C<sub>25</sub>H<sub>29</sub>I<sub>2</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 25	I 2	N 1	O 3	0	0
5	H	1	Total 31	C 25	I 2	N 1	O 3	0	0

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



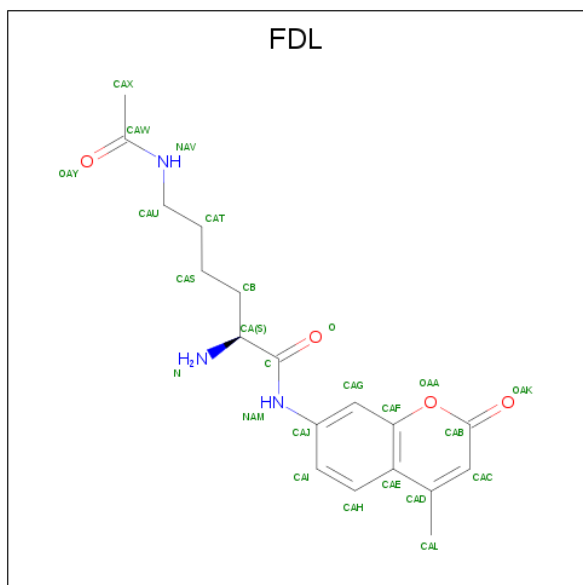
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 7 is N 6 -acetyl-N-(4-methyl-2-oxo-2H-chromen-7-yl)-L-lysine (three-letter code: FDL) (formula:  $C_{18}H_{23}N_3O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O		0	0
			25	18	3	4			
7	C	1	Total	C	N	O		0	0
			25	18	3	4			

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).

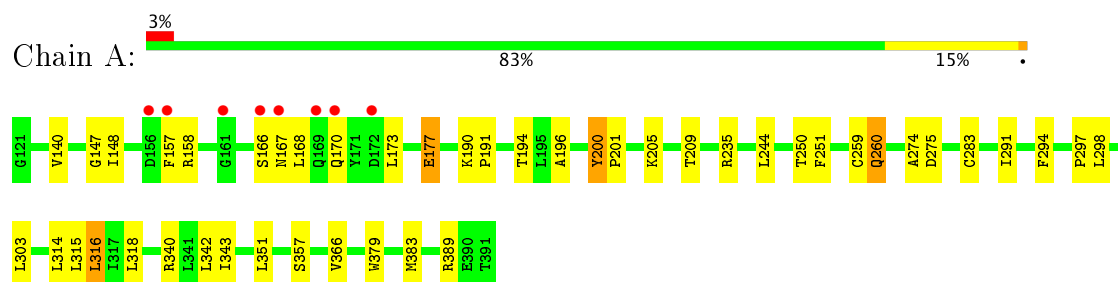


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			7	4	3		
8	H	1	Total	C	O	0	0
			7	4	3		

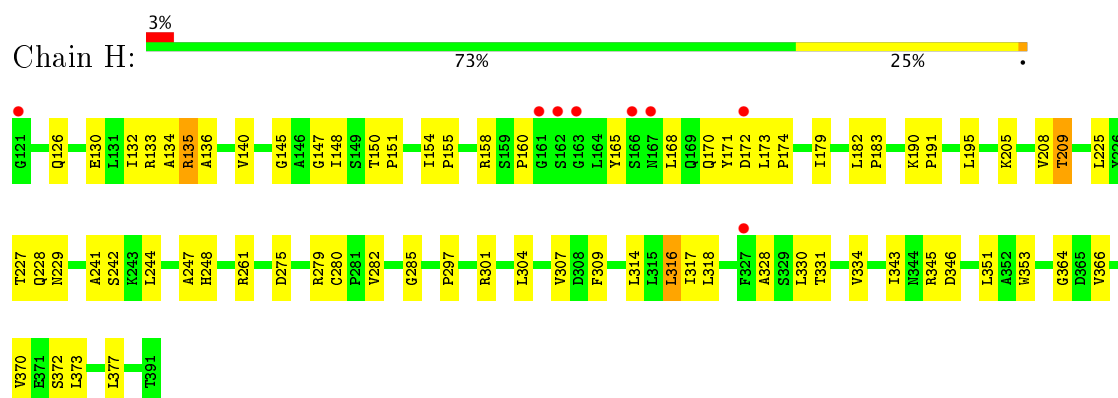
### 3 Residue-property plots [i](#)

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.

- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



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- Molecule 2: ARG-HIS-LYS



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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.56Å 114.56Å 123.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.32 – 3.21 38.66 – 3.21	Depositor EDS
% Data completeness (in resolution range)	59.2 (77.32-3.21) 59.2 (38.66-3.21)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.213 , 0.372 0.221 , 0.375	Depositor DCC
$R_{free}$ test set	285 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 10.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.349 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: ZN, NAD, BBI, MG, FDL, PEG

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	0.38	0/2182	0.58	0/2974
1	H	0.39	0/2175	0.63	0/2965
2	C	0.52	0/30	0.70	0/37
2	D	0.46	0/30	0.68	0/37
All	All	0.39	0/4417	0.61	0/6013

There are no bond length outliers.

There are no bond angle outliers.

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	2127	0	2137	30	0
1	H	2121	0	2130	54	0
2	C	30	0	35	2	0
2	D	30	0	35	2	1
3	A	1	0	0	2	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	29	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	31	0	29	14	0
6	A	44	0	26	2	0
6	H	44	0	26	10	0
7	C	25	0	21	3	0
7	D	25	0	21	6	0
8	H	14	0	20	8	0
All	All	4526	0	4509	105	1

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 12.

All (105) 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)
5:H:405:BB1:H25	5:H:405:BB1:H30	1.42	1.00
7:D:101:FDL:OAY	5:H:405:BB1:H23	1.69	0.93
1:A:259:CYS:HG	3:A:401:ZN:ZN	0.71	0.90
1:H:228:GLN:O	6:H:406:NAD:O2D	1.95	0.85
1:H:241:ALA:O	8:H:401:PEG:H21	1.80	0.80
1:H:228:GLN:O	6:H:406:NAD:C2D	2.31	0.78
5:H:405:BB1:IBD	5:H:405:BB1:H18	2.58	0.74
5:H:405:BB1:H24	6:H:406:NAD:H4D	1.71	0.72
1:H:366:VAL:HG23	6:H:406:NAD:C2A	2.22	0.70
1:H:158:ARG:CZ	5:H:405:BB1:H28	2.23	0.69
1:H:248:HIS:CD2	6:H:406:NAD:O3D	2.46	0.69
1:A:259:CYS:SG	3:A:401:ZN:ZN	1.81	0.68
1:H:134:ALA:O	1:H:136:ALA:N	2.27	0.68
7:D:101:FDL:O	7:D:101:FDL:H7	1.97	0.63
1:H:366:VAL:HG23	6:H:406:NAD:H2A	1.81	0.62
1:A:158:ARG:HD3	5:A:403:BB1:H25	1.80	0.62
7:D:101:FDL:CAI	7:D:101:FDL:O	2.45	0.61
1:H:228:GLN:O	6:H:406:NAD:H2D	2.00	0.61
5:A:403:BB1:IAS	5:A:403:BB1:H19	2.74	0.58
1:A:366:VAL:HG23	6:A:404:NAD:C2A	2.34	0.57
1:H:140:VAL:HG22	1:H:314:LEU:HD23	1.85	0.57
1:A:168:LEU:HB3	1:A:173:LEU:HD12	1.86	0.57
5:A:403:BB1:CAW	5:A:403:BB1:IAS	3.23	0.57
7:C:101:FDL:H7	7:C:101:FDL:O	2.04	0.57
1:H:317:ILE:HD13	1:H:351:LEU:HD11	1.87	0.56
1:H:209:THR:HG23	1:H:370:VAL:HG21	1.88	0.55
1:H:173:LEU:HD11	1:H:179:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:ILE:HG22	1:H:209:THR:HG21	1.89	0.54
1:A:342:LEU:HD22	1:A:351:LEU:HD12	1.89	0.54
1:H:345:ARG:HA	1:H:364:GLY:O	2.07	0.53
1:A:147:GLY:HA2	6:A:404:NAD:C8A	2.37	0.53
1:H:316:LEU:HD22	1:H:318:LEU:HG	1.90	0.52
1:H:261:ARG:CZ	1:H:282:VAL:HG11	2.40	0.52
5:H:405:BBI:H24	6:H:406:NAD:C4D	2.37	0.52
1:H:145:GLY:O	1:H:229:ASN:ND2	2.41	0.52
1:A:148:ILE:HG22	1:A:209:THR:HG21	1.92	0.51
1:H:158:ARG:NE	5:H:405:BBI:H28	2.25	0.51
5:H:405:BBI:CBE	5:H:405:BBI:H13	2.41	0.51
1:H:309:PHE:CE2	1:H:330:LEU:HB3	2.46	0.51
1:A:294:PHE:HZ	5:A:403:BBI:H22	1.75	0.51
1:A:251:PHE:CE2	1:A:291:ILE:HD11	2.47	0.50
1:H:171:TYR:O	1:H:173:LEU:N	2.44	0.50
7:C:101:FDL:O	7:C:101:FDL:CAI	2.57	0.49
2:D:3:LYS:O	7:D:101:FDL:C	2.59	0.49
1:H:331:THR:O	1:H:334:VAL:HG22	2.12	0.49
1:H:229:ASN:HA	6:H:406:NAD:H2N	1.92	0.49
7:D:101:FDL:OAY	5:H:405:BBI:CBB	2.52	0.48
1:H:182:LEU:HB2	1:H:183:PRO:HD3	1.95	0.48
1:A:379:TRP:O	1:A:383:MET:HB2	2.13	0.48
5:H:405:BBI:IBD	5:H:405:BBI:CAW	3.31	0.48
1:H:316:LEU:HD22	1:H:318:LEU:CD2	2.44	0.47
1:H:126:GLN:O	1:H:130:GLU:HG2	2.14	0.47
1:A:260:GLN:HE21	1:A:260:GLN:HA	1.80	0.47
1:A:235:ARG:HG3	1:A:244:LEU:CD1	2.45	0.47
1:H:150:THR:HG22	1:H:154:ILE:O	2.15	0.47
5:A:403:BBI:IAS	5:A:403:BBI:H18	2.85	0.46
1:H:147:GLY:HA2	6:H:406:NAD:C8A	2.46	0.46
1:H:261:ARG:NH2	1:H:282:VAL:HG11	2.30	0.46
1:H:301:ARG:NE	8:H:401:PEG:H22	2.31	0.46
1:A:190:LYS:O	1:A:194:THR:N	2.48	0.46
1:A:316:LEU:HD22	1:A:318:LEU:HG	1.98	0.46
1:A:298:LEU:HD12	2:C:2:HIS:HB3	1.97	0.45
1:A:274:ALA:O	1:A:275:ASP:HB2	2.17	0.45
2:D:3:LYS:HA	1:H:297:PRO:HA	1.99	0.45
1:H:225:LEU:HD23	1:H:244:LEU:CD2	2.47	0.45
1:H:280:CYS:N	1:H:285:GLY:O	2.46	0.45
1:H:242:SER:O	8:H:401:PEG:O1	2.35	0.44
5:H:405:BBI:CBB	5:H:405:BBI:H30	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:HA	2:C:3:LYS:HA	2.00	0.44
7:C:101:FDL:H1	7:C:101:FDL:H6	1.75	0.44
1:A:177:GLU:HG2	5:A:403:BBI:IBD	2.87	0.44
1:H:301:ARG:HE	8:H:401:PEG:C2	2.31	0.44
1:H:301:ARG:HE	8:H:401:PEG:H22	1.81	0.44
1:A:251:PHE:CD2	1:A:291:ILE:HD11	2.53	0.44
1:H:160:PRO:HA	1:H:165:TYR:CE1	2.52	0.44
5:H:405:BBI:CBB	5:H:405:BBI:CAZ	2.87	0.44
1:A:318:LEU:HD21	1:A:343:ILE:HD12	2.00	0.43
1:A:173:LEU:HD11	1:A:191:PRO:HB3	1.99	0.43
1:H:168:LEU:HD23	1:H:171:TYR:CD2	2.53	0.43
1:H:343:ILE:HD11	1:H:373:LEU:HD22	2.00	0.43
1:A:318:LEU:HD23	1:A:343:ILE:HB	2.00	0.43
1:A:303:LEU:HD21	1:H:307:VAL:HG13	2.01	0.43
1:H:301:ARG:NH2	1:H:304:LEU:HD11	2.34	0.42
1:A:196:ALA:O	1:A:200:TYR:N	2.52	0.42
1:A:140:VAL:HG22	1:A:314:LEU:HD23	2.00	0.42
1:H:132:ILE:O	1:H:135:ARG:NH2	2.52	0.42
1:H:150:THR:OG1	1:H:151:PRO:HD3	2.20	0.42
1:H:190:LYS:N	1:H:191:PRO:CD	2.83	0.42
5:H:405:BBI:CAV	5:H:405:BBI:IAS	3.38	0.42
1:H:160:PRO:HA	1:H:165:TYR:CD1	2.55	0.42
1:A:315:LEU:HB3	1:A:340:ARG:HA	2.01	0.42
1:H:241:ALA:O	8:H:401:PEG:C2	2.59	0.42
1:H:301:ARG:NE	8:H:401:PEG:C2	2.82	0.41
1:H:279:ARG:HA	1:H:285:GLY:O	2.20	0.41
1:H:133:ARG:HG3	1:H:377:LEU:HD23	2.03	0.41
5:H:405:BBI:H17	5:H:405:BBI:IAS	2.91	0.41
1:A:190:LYS:N	1:A:191:PRO:CD	2.84	0.41
1:H:316:LEU:HD13	1:H:318:LEU:HD11	2.02	0.41
7:D:101:FDL:H6	7:D:101:FDL:H1	1.71	0.41
1:A:140:VAL:CG2	1:A:314:LEU:HD23	2.51	0.41
1:H:353:TRP:CE3	1:H:353:TRP:HA	2.56	0.41
1:H:227:THR:O	1:H:247:ALA:HB3	2.21	0.41
1:H:244:LEU:C	8:H:401:PEG:H11	2.42	0.41
1:A:259:CYS:SG	1:A:283:CYS:SG	3.20	0.40
1:H:150:THR:N	1:H:151:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:ARG:NE	5:A:403:BBI:OAO[5_555]	2.15	0.05

## 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	269/271 (99%)	234 (87%)	33 (12%)	2 (1%)	25	68
1	H	269/271 (99%)	240 (89%)	23 (9%)	6 (2%)	8	41
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	540/548 (98%)	476 (88%)	56 (10%)	8 (2%)	12	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	135	ARG
1	H	172	ASP
1	A	157	PHE
1	H	275	ASP
1	H	328	ALA
1	H	155	PRO
1	H	174	PRO
1	A	201	PRO

### 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	235/235 (100%)	224 (95%)	11 (5%)	30	68
1	H	234/235 (100%)	226 (97%)	8 (3%)	42	76
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	475/476 (100%)	456 (96%)	19 (4%)	36	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	167	ASN
1	A	170	GLN
1	A	177	GLU
1	A	200	TYR
1	A	205	LYS
1	A	250	THR
1	A	260	GLN
1	A	316	LEU
1	A	357	SER
1	A	389	ARG
1	H	170	GLN
1	H	195	LEU
1	H	205	LYS
1	H	208	VAL
1	H	209	THR
1	H	316	LEU
1	H	346	ASP
1	H	372	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	GLN
1	A	170	GLN
1	A	260	GLN
1	H	248	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
5	BBI	A	403	-	27,33,33	3.33	4 (14%)	36,45,45	1.39	7 (19%)
6	NAD	A	404	-	41,48,48	0.94	2 (4%)	43,73,73	1.38	3 (6%)
7	FDL	C	101	2	25,26,26	1.62	2 (8%)	27,35,35	1.96	5 (18%)
7	FDL	D	101	2	25,26,26	1.62	2 (8%)	27,35,35	1.98	5 (18%)
8	PEG	H	401	-	6,6,6	0.43	0	5,5,5	0.40	0
8	PEG	H	403	-	6,6,6	0.55	0	5,5,5	0.20	0
5	BBI	H	405	-	27,33,33	3.12	4 (14%)	36,45,45	1.02	1 (2%)
6	NAD	H	406	-	41,48,48	1.00	2 (4%)	43,73,73	1.46	4 (9%)

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
5	BBI	A	403	-	-	0/18/22/22	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAD	A	404	-	-	0/22/62/62	0/5/5/5
7	FDL	C	101	2	-	0/16/16/16	0/2/2/2
7	FDL	D	101	2	-	0/16/16/16	0/2/2/2
8	PEG	H	401	-	-	0/4/4/4	0/0/0/0
8	PEG	H	403	-	-	0/4/4/4	0/0/0/0
5	BBI	H	405	-	-	0/18/22/22	0/2/3/3
6	NAD	H	406	-	-	0/22/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	BBI	CAM-CAN	-15.39	1.33	1.50
5	H	405	BBI	CAM-CAN	-14.23	1.34	1.50
7	C	101	FDL	CAL-CAD	-5.95	1.39	1.51
7	D	101	FDL	CAL-CAD	-5.74	1.40	1.51
5	A	403	BBI	CAP-CAN	-5.65	1.39	1.49
5	H	405	BBI	CAP-CAN	-5.57	1.39	1.49
7	D	101	FDL	CAJ-NAM	-4.22	1.33	1.41
5	A	403	BBI	CAK-CAL	-4.10	1.33	1.42
7	C	101	FDL	CAJ-NAM	-3.71	1.34	1.41
5	H	405	BBI	CAK-CAL	-3.45	1.35	1.42
6	A	404	NAD	O4D-C1D	2.02	1.44	1.41
5	A	403	BBI	CAD-CAE	2.37	1.54	1.51
5	H	405	BBI	CAD-CAE	2.74	1.54	1.51
6	H	406	NAD	O4B-C1B	2.77	1.45	1.41
6	A	404	NAD	C5A-C4A	3.41	1.48	1.40
6	H	406	NAD	C5A-C4A	3.41	1.48	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	404	NAD	N3A-C2A-N1A	-6.54	123.16	128.86
7	D	101	FDL	CAJ-NAM-C	-6.45	114.69	127.29
6	H	406	NAD	N3A-C2A-N1A	-6.02	123.61	128.86
7	C	101	FDL	CAJ-NAM-C	-4.49	118.54	127.29
6	A	404	NAD	C4A-C5A-N7A	-3.49	106.04	109.41
6	H	406	NAD	C4A-C5A-N7A	-3.03	106.48	109.41
7	C	101	FDL	OAA-CAF-CAE	-2.99	118.31	121.20
5	A	403	BBI	CAL-CAM-CAN	-2.33	120.01	125.12
5	A	403	BBI	CAK-CAL-CAM	-2.31	130.76	135.53
5	A	403	BBI	CAQ-CAR-IAS	-2.21	114.51	118.61
5	A	403	BBI	CAM-CAN-CAP	-2.20	116.39	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	406	NAD	C1B-N9A-C4A	-2.19	122.84	126.64
7	D	101	FDL	CAH-CAE-CAD	-2.07	119.69	123.66
7	D	101	FDL	OAA-CAF-CAE	-2.05	119.22	121.20
6	A	404	NAD	C2A-N1A-C6A	2.10	122.44	118.77
5	H	405	BBI	OAQ-CAN-CAM	2.16	121.91	119.54
7	C	101	FDL	OAA-CAB-CAC	2.34	122.33	119.27
6	H	406	NAD	C4D-O4D-C1D	2.48	112.40	109.77
5	A	403	BBI	CAT-CBC-IBD	2.61	124.04	119.42
7	D	101	FDL	OAA-CAF-CAG	2.63	119.14	116.03
5	A	403	BBI	CAK-CAL-CAG	2.93	122.23	120.38
7	C	101	FDL	OAA-CAF-CAG	3.09	119.70	116.03
5	A	403	BBI	CAT-CAR-IAS	3.48	125.57	119.42
7	D	101	FDL	CAD-CAE-CAF	5.86	121.72	118.04
7	C	101	FDL	CAD-CAE-CAF	6.60	122.18	118.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	BBI	6	1
6	A	404	NAD	2	0
7	C	101	FDL	3	0
7	D	101	FDL	6	0
8	H	401	PEG	8	0
5	H	405	BBI	14	0
6	H	406	NAD	10	0

## 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	271/271 (100%)	-0.02	8 (2%)	51	36	14, 31, 105, 122	0
1	H	271/271 (100%)	-0.05	8 (2%)	51	36	13, 29, 67, 108	0
2	C	3/3 (100%)	0.08	0	100	100	37, 37, 43, 48	0
2	D	3/3 (100%)	-0.23	0	100	100	35, 35, 40, 52	0
All	All	548/548 (100%)	-0.03	16 (2%)	52	38	13, 30, 79, 122	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	GLY	8.3
1	A	172	ASP	6.2
1	H	163	GLY	5.0
1	H	167	ASN	4.2
1	A	167	ASN	4.1
1	A	166	SER	3.7
1	H	162	SER	3.1
1	H	166	SER	3.1
1	A	157	PHE	3.0
1	A	169	GLN	2.7
1	H	327	PHE	2.7
1	H	121	GLY	2.7
1	A	170	GLN	2.3
1	H	161	GLY	2.1
1	A	156	ASP	2.1
1	H	172	ASP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	BBI	H	405	31/31	0.79	0.45	3.96	81,108,155,189	0
6	NAD	A	404	44/44	0.79	0.56	3.21	77,101,112,117	0
6	NAD	H	406	44/44	0.84	0.35	2.14	62,68,73,74	0
8	PEG	H	401	7/7	0.90	0.27	1.93	20,20,21,22	0
8	PEG	H	403	7/7	0.88	0.25	1.39	33,34,36,36	0
5	BBI	A	403	31/31	0.73	0.43	1.31	88,124,178,212	0
7	FDL	C	101	25/25	0.94	0.24	0.63	26,27,31,31	0
7	FDL	D	101	25/25	0.95	0.22	0.06	21,23,26,27	0
4	MG	H	404	1/1	0.90	0.23	-0.06	2,2,2,2	0
3	ZN	A	401	1/1	0.99	0.10	-2.35	28,28,28,28	0
3	ZN	H	402	1/1	0.99	0.06	-3.31	29,29,29,29	0
4	MG	A	402	1/1	0.94	0.13	-	2,2,2,2	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.