



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:31 AM GMT

PDB ID : 2HJH  
Title : Crystal Structure of the Sir2 deacetylase  
Authors : Hall, B.E.; Ellenberger, T.E.  
Deposited on : 2006-06-30  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

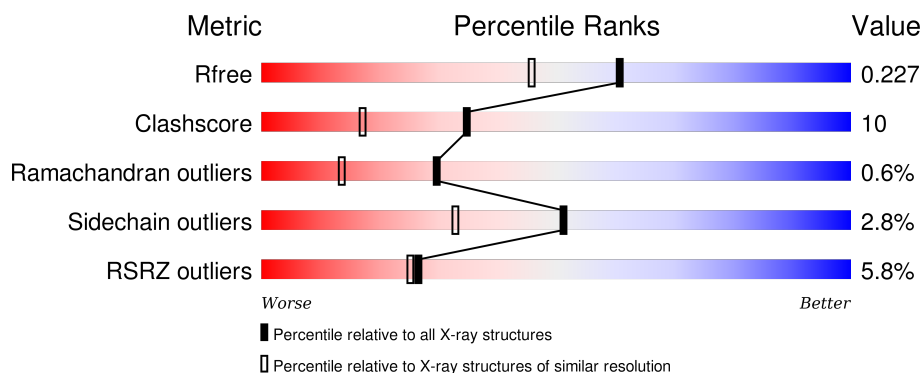
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	354	<div> <div>3%</div> <div>76% 15% 8%</div> </div>
1	B	354	<div> <div>7%</div> <div>75% 15% 8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NCA	A	900	-	-	-	X
4	NCA	B	901	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5747 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.

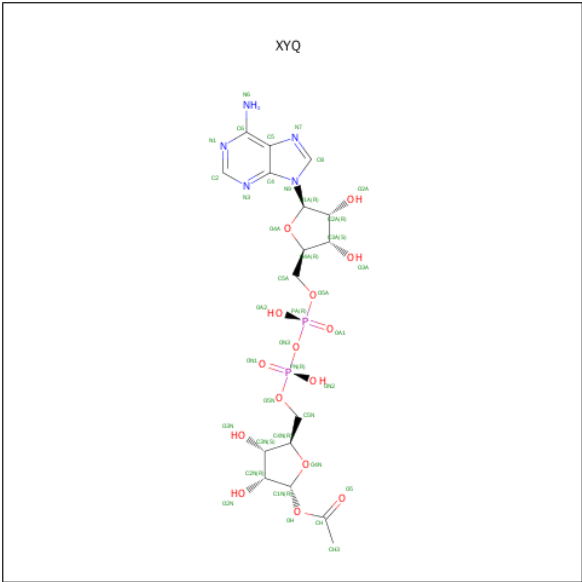
- Molecule 1 is a protein called NAD-dependent histone deacetylase SIR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se	0	1	0
			2595	1679	439	460	11	6			
1	B	326	Total	C	N	O	S	Se	0	0	0
			2539	1638	431	452	11	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

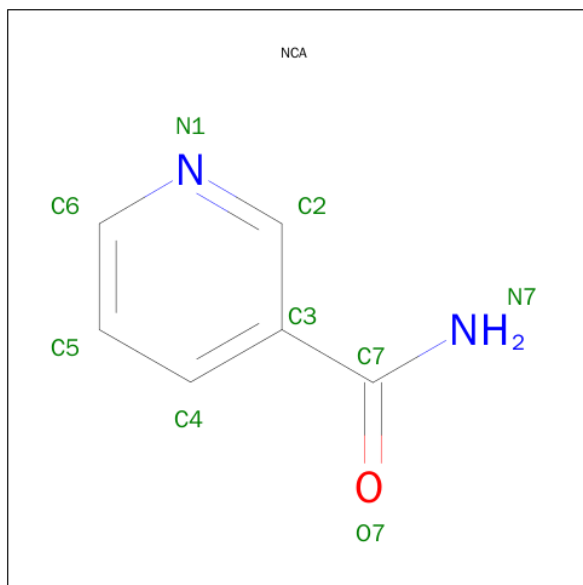
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2R,3R,4S,5R)-5-({[(R)-{[(R)-{(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}METHYL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL ACETATE (three-letter code: XYQ) (formula: C<sub>17</sub>H<sub>25</sub>N<sub>5</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			38	17	5	14	2		
3	B	1	Total	C	N	O	P	0	0
			38	17	5	14	2		

- Molecule 4 is NICOTINAMIDE (three-letter code: NCA) (formula: C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	2	1		
4	B	1	Total	C	N	O	0	0
			9	6	2	1		

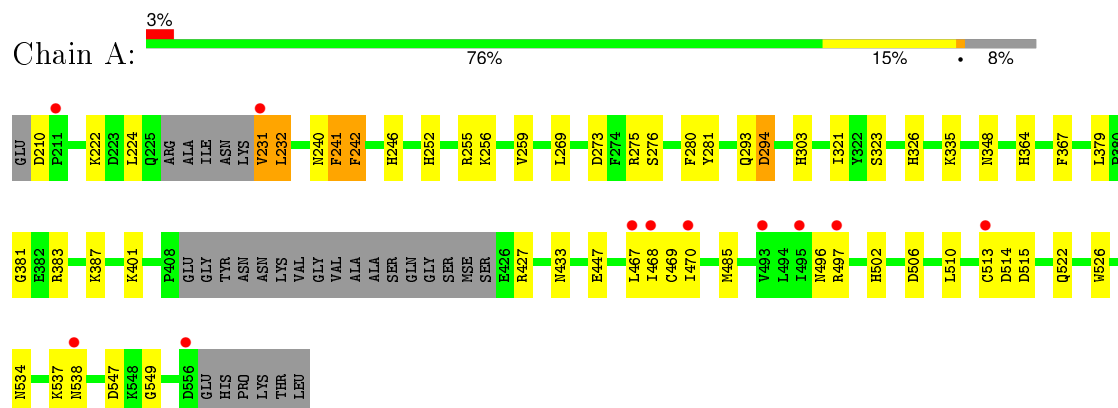
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	B	207	Total	O	0	0
			207	207		

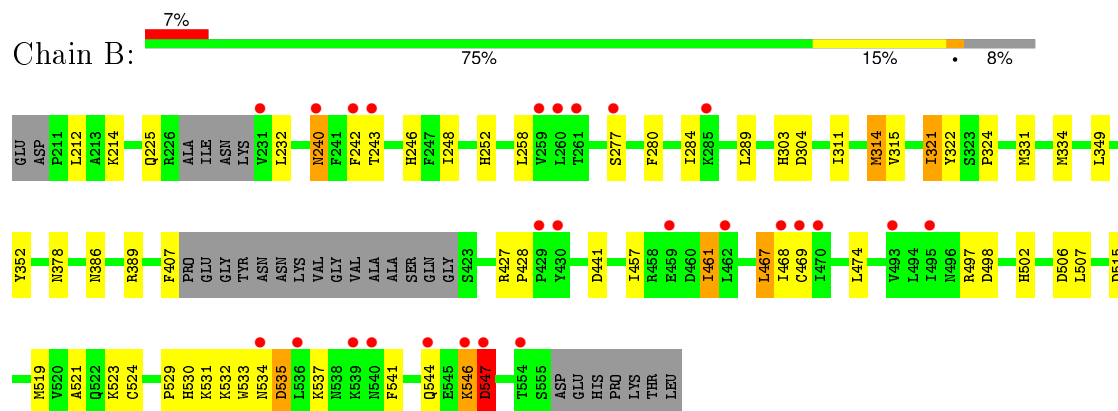
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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 histone deacetylase SIR2



- Molecule 1: NAD-dependent histone deacetylase SIR2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.35Å 89.57Å 94.51Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 29.87 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.85) 96.0 (29.87-1.85)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.171 , 0.215 0.188 , 0.227	Depositor DCC
$R_{free}$ test set	3497 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.0	EDS
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 69079 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: XYQ, ZN, NCA

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	1.14	2/2656 (0.1%)	1.03	7/3591 (0.2%)
1	B	0.98	2/2593 (0.1%)	0.96	7/3507 (0.2%)
All	All	1.06	4/5249 (0.1%)	1.00	14/7098 (0.2%)

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	1
1	B	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	MSE	SE-CE	6.13	2.31	1.95
1	B	315	VAL	CA-CB	5.32	1.66	1.54
1	A	447	GLU	CD-OE2	-5.25	1.19	1.25
1	A	256	LYS	CD-CE	5.10	1.64	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	506	ASP	CB-CG-OD2	9.84	127.16	118.30
1	B	304	ASP	CB-CG-OD2	8.02	125.52	118.30
1	A	506	ASP	CB-CG-OD2	7.23	124.80	118.30
1	A	497	ARG	NE-CZ-NH1	6.28	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	515	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	441	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	294	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	498	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	497	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	514	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	547	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	427	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	255	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	VAL	Peptide
1	B	225	GLN	Peptide
1	B	533	TRP	Peptide

## 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	2595	0	2601	48	1
1	B	2539	0	2502	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	38	0	20	7	0
3	B	38	0	20	1	0
4	A	9	0	6	1	0
4	B	9	0	6	2	0
5	A	310	0	0	13	1
5	B	207	0	0	7	1
All	All	5747	0	5155	103	2

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 10.

All (103) 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:314:MSE:SE	1:B:314:MSE:CE	2.31	1.28
1:B:407:PHE:C	5:B:1398:HOH:O	2.04	0.94
1:B:378:ASN:HB3	5:B:1422:HOH:O	1.72	0.88
1:B:546:LYS:O	1:B:547:ASP:HB2	1.73	0.87
1:B:427:ARG:HB3	1:B:428:PRO:HD2	1.58	0.86
1:A:467:LEU:HD21	1:A:469:CYS:SG	2.15	0.86
1:B:530:HIS:HD2	1:B:532:LYS:H	1.22	0.84
1:A:485:MSE:HE1	1:B:212:LEU:HD11	1.62	0.81
1:A:383:ARG:NH1	5:A:1527:HOH:O	2.14	0.79
1:B:534:ASN:O	1:B:535:ASP:CB	2.34	0.75
1:B:467:LEU:HD21	1:B:469:CYS:SG	2.27	0.73
1:B:242:PHE:O	1:B:507:LEU:HD13	1.90	0.72
1:B:519:MSE:HG3	1:B:541:PHE:CD1	2.24	0.72
1:A:348:ASN:ND2	5:A:1509:HOH:O	2.23	0.71
1:A:280:PHE:HB2	4:A:900:NCA:H6	1.72	0.70
1:B:240:ASN:N	1:B:240:ASN:ND2	2.44	0.66
1:A:241:PHE:HA	1:A:246:HIS:CD2	2.30	0.66
1:A:231:VAL:HG22	1:A:232:LEU:HA	1.78	0.66
1:B:467:LEU:C	1:B:467:LEU:HD23	2.17	0.65
1:B:519:MSE:HG3	1:B:541:PHE:CG	2.32	0.65
1:B:240:ASN:H	1:B:240:ASN:ND2	1.93	0.65
1:B:546:LYS:O	1:B:547:ASP:CB	2.45	0.64
1:A:515:ASP:OD2	5:A:1500:HOH:O	2.16	0.63
1:A:210:ASP:N	5:A:1395:HOH:O	2.32	0.61
1:B:427:ARG:HB3	1:B:428:PRO:CD	2.30	0.60
1:A:242:PHE:H	1:A:246:HIS:HD2	1.50	0.60
1:A:467:LEU:HD23	1:A:467:LEU:C	2.22	0.59
1:A:513:CYS:HG	3:A:1222:XYQ:C2	2.15	0.59
1:A:326:HIS:HE1	5:A:1231:HOH:O	1.85	0.59
1:B:240:ASN:HD22	1:B:240:ASN:N	2.02	0.58
1:A:522:GLN:HE21	1:A:537:LYS:HA	1.69	0.58
1:A:240:ASN:O	1:A:241:PHE:HB2	2.04	0.57
4:B:901:NCA:H5	5:B:1289:HOH:O	2.04	0.57
1:A:513:CYS:SG	3:A:1222:XYQ:N1	2.71	0.57
1:B:457:ILE:HG13	1:B:461:ILE:HD13	1.87	0.56
1:B:386:ASN:ND2	1:B:389:ARG:HH11	2.04	0.56
1:A:323:SER:H	1:A:326:HIS:HD2	1.53	0.56
1:A:485:MSE:CE	1:B:212:LEU:HD11	2.33	0.56
1:A:252:HIS:HE1	5:A:1342:HOH:O	1.87	0.56
1:A:275:ARG:HG3	5:A:1371:HOH:O	2.06	0.56
1:B:386:ASN:HD22	1:B:389:ARG:HH11	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:CYS:SG	3:A:1222:XYQ:C2	2.94	0.55
1:A:242:PHE:O	1:A:549:GLY:HA2	2.07	0.55
3:B:1222:XYQ:CH3	5:B:1268:HOH:O	2.54	0.54
1:A:534:ASN:HA	1:A:537:LYS:HE3	1.89	0.54
1:B:519:MSE:HE3	1:B:523:LYS:CE	2.38	0.53
1:B:530:HIS:CD2	1:B:532:LYS:H	2.14	0.52
1:B:519:MSE:HE3	1:B:523:LYS:HD2	1.93	0.51
1:B:322:TYR:CE2	5:B:1371:HOH:O	2.63	0.50
1:A:383:ARG:HG3	1:A:383:ARG:HH11	1.77	0.50
1:B:242:PHE:CE2	1:B:246:HIS:HE1	2.30	0.50
1:A:367:PHE:O	1:A:381:GLY:HA3	2.11	0.50
3:A:1222:XYQ:CH3	5:A:1322:HOH:O	2.59	0.50
1:A:281:TYR:CZ	1:A:293:GLN:HG3	2.47	0.49
1:B:467:LEU:HD23	1:B:468:ILE:N	2.27	0.49
1:A:273:ASP:OD2	1:A:276:SER:OG	2.30	0.49
1:B:457:ILE:O	1:B:461:ILE:HB	2.13	0.48
1:A:246:HIS:HE1	5:A:1393:HOH:O	1.95	0.48
1:A:513:CYS:HG	3:A:1222:XYQ:C6	2.23	0.48
1:A:467:LEU:HD23	1:A:468:ILE:N	2.29	0.48
1:B:248:ILE:HD13	1:B:523:LYS:HB3	1.96	0.48
1:B:352:TYR:C	5:B:1371:HOH:O	2.51	0.48
1:A:293:GLN:NE2	5:A:1478:HOH:O	2.45	0.48
1:B:311:ILE:HD12	1:B:311:ILE:C	2.35	0.47
1:B:252:HIS:NE2	5:B:1387:HOH:O	2.14	0.47
1:B:474:LEU:O	1:B:502:HIS:HE1	1.98	0.47
1:A:259:VAL:CG1	1:A:470[B]:ILE:HD12	2.45	0.47
1:A:231:VAL:HG22	1:A:232:LEU:CA	2.44	0.46
1:A:496:ASN:O	1:A:510:LEU:HA	2.16	0.46
1:A:502:HIS:HD2	5:A:1391:HOH:O	1.98	0.45
1:A:335:LYS:NZ	1:A:526:TRP:CG	2.85	0.45
1:A:275:ARG:NE	3:A:1222:XYQ:OA1	2.49	0.45
1:B:467:LEU:CD2	1:B:467:LEU:C	2.84	0.45
1:A:502:HIS:CD2	5:A:1391:HOH:O	2.70	0.45
1:B:280:PHE:CB	4:B:901:NCA:O7	2.65	0.44
1:B:386:ASN:ND2	1:B:389:ARG:NH1	2.65	0.44
1:B:243:THR:O	1:B:507:LEU:HD22	2.17	0.44
1:B:232:LEU:N	1:B:232:LEU:CD1	2.81	0.44
1:B:519:MSE:HE3	1:B:523:LYS:CD	2.48	0.43
1:A:269:LEU:HB3	1:A:321:ILE:HD12	2.01	0.43
1:A:222:LYS:HE3	1:A:364:HIS:CE1	2.54	0.43
1:B:331:MSE:HA	1:B:334:MSE:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1222:XYQ:CH3	5:A:1479:HOH:O	2.65	0.43
1:B:334:MSE:HE1	1:B:529:PRO:HG3	1.99	0.43
1:B:530:HIS:CD2	1:B:531:LYS:N	2.86	0.43
1:B:243:THR:OG1	1:B:246:HIS:CG	2.72	0.43
1:A:534:ASN:OD1	1:A:537:LYS:HE3	2.18	0.43
1:B:519:MSE:HE3	1:B:523:LYS:HE2	2.01	0.42
1:A:224:LEU:HD13	1:A:293:GLN:OE1	2.19	0.42
1:B:474:LEU:O	1:B:502:HIS:CE1	2.72	0.42
1:B:242:PHE:CD2	1:B:242:PHE:N	2.88	0.42
1:A:485:MSE:HG2	1:B:214:LYS:HB3	2.02	0.42
1:B:322:TYR:N	1:B:322:TYR:CD2	2.88	0.42
1:A:281:TYR:OH	1:A:293:GLN:HG3	2.20	0.41
1:B:427:ARG:CB	1:B:428:PRO:CD	2.91	0.41
1:A:242:PHE:N	1:A:246:HIS:HD2	2.17	0.41
1:A:259:VAL:HG13	1:A:470[B]:ILE:HD12	2.02	0.41
1:A:303:HIS:O	1:A:433:ASN:HB2	2.20	0.41
1:A:224:LEU:HD22	1:A:293:GLN:OE1	2.20	0.41
1:B:284:ILE:CG2	1:B:289:LEU:HD22	2.51	0.41
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.87	0.40
1:B:521:ALA:O	1:B:524:CYS:HB2	2.21	0.40
1:B:321:ILE:O	1:B:349:LEU:HD22	2.21	0.40

All (2) 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)
1:A:294:ASP:OD2	5:B:1410:HOH:O[1_655]	2.14	0.06
5:A:1377:HOH:O	5:A:1448:HOH:O[2_647]	2.19	0.01

## 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	320/354 (90%)	308 (96%)	10 (3%)	2 (1%)	30	13
1	B	320/354 (90%)	312 (98%)	6 (2%)	2 (1%)	30	13
All	All	640/708 (90%)	620 (97%)	16 (2%)	4 (1%)	30	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	535	ASP
1	A	241	PHE
1	A	242	PHE
1	B	547	ASP

### 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	291/313 (93%)	285 (98%)	6 (2%)	61	45
1	B	277/313 (88%)	267 (96%)	10 (4%)	42	21
All	All	568/626 (91%)	552 (97%)	16 (3%)	51	33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	LEU
1	A	379	LEU
1	A	387	LYS
1	A	401	LYS
1	A	538	ASN
1	A	547	ASP
1	B	240	ASN
1	B	277	SER
1	B	303	HIS
1	B	321	ILE
1	B	324	PRO
1	B	461	ILE

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Mol	Chain	Res	Type
1	B	467	LEU
1	B	537	LYS
1	B	544	GLN
1	B	546	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	246	HIS
1	A	326	HIS
1	A	344	GLN
1	A	348	ASN
1	A	502	HIS
1	A	522	GLN
1	B	240	ASN
1	B	252	HIS
1	B	386	ASN
1	B	502	HIS
1	B	530	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	XYQ	A	1222	1	34,41,42	1.61	4 (11%)	43,62,64	3.65	18 (41%)
4	NCA	A	900	-	9,9,9	1.13	0	11,11,11	2.13	2 (18%)
3	XYQ	B	1222	1	34,41,42	1.44	5 (14%)	43,62,64	3.37	14 (32%)
4	NCA	B	901	-	9,9,9	0.47	0	11,11,11	1.36	2 (18%)

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
3	XYQ	A	1222	1	-	1/21/57/58	0/4/4/4
4	NCA	A	900	-	-	0/4/4/4	0/1/1/1
3	XYQ	B	1222	1	-	2/21/57/58	0/4/4/4
4	NCA	B	901	-	-	0/4/4/4	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1222	XYQ	C5-C4	-2.87	1.34	1.40
3	A	1222	XYQ	C5-C4	-2.27	1.35	1.40
3	B	1222	XYQ	O4N-C4N	-2.23	1.39	1.45
3	B	1222	XYQ	C2-N3	2.02	1.35	1.32
3	A	1222	XYQ	OH-C1N	2.48	1.44	1.40
3	A	1222	XYQ	O4A-C1A	3.52	1.45	1.41
3	B	1222	XYQ	OH-C1N	3.64	1.46	1.40
3	B	1222	XYQ	C4-N3	4.79	1.42	1.35
3	A	1222	XYQ	C4-N3	5.01	1.43	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1222	XYQ	N3-C2-N1	-15.20	117.25	128.89
3	B	1222	XYQ	O4N-C1N-OH	-14.04	95.22	111.77
3	A	1222	XYQ	O4N-C1N-OH	-13.37	96.01	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1222	XYQ	N3-C2-N1	-11.65	119.97	128.89
3	B	1222	XYQ	C1A-N9-C4	-3.79	121.22	126.94
3	B	1222	XYQ	C4-C5-N7	-3.37	106.38	109.48
3	A	1222	XYQ	O3A-C3A-C4A	-3.31	101.14	111.05
3	B	1222	XYQ	O3N-C3N-C4N	-3.09	101.80	111.05
4	A	900	NCA	O7-C7-C3	-2.96	116.35	119.59
3	B	1222	XYQ	O3A-C3A-C2A	-2.89	102.43	111.83
3	A	1222	XYQ	PA-ON3-PN	-2.58	125.49	132.73
3	A	1222	XYQ	C1A-N9-C4	-2.51	123.15	126.94
3	B	1222	XYQ	O3A-C3A-C4A	-2.49	103.57	111.05
3	B	1222	XYQ	O5A-PA-OA1	-2.48	99.99	109.62
3	A	1222	XYQ	C5N-C4N-C3N	-2.32	105.99	115.21
3	A	1222	XYQ	O3N-C3N-C4N	-2.29	104.18	111.05
4	B	901	NCA	C3-C2-N1	-2.10	120.49	123.52
3	A	1222	XYQ	OH-C1N-C2N	-2.10	104.11	107.84
3	A	1222	XYQ	C5A-C4A-C3A	-2.05	107.09	115.21
3	A	1222	XYQ	C2N-C3N-C4N	2.06	106.85	102.61
3	A	1222	XYQ	ON2-PN-ON1	2.12	124.00	112.53
3	B	1222	XYQ	C2A-C3A-C4A	2.22	107.17	102.61
3	A	1222	XYQ	O2N-C2N-C1N	2.27	118.00	111.67
3	B	1222	XYQ	O4N-C4N-C3N	2.28	109.73	105.15
3	B	1222	XYQ	O2N-C2N-C1N	2.28	118.02	111.67
3	A	1222	XYQ	OH-CH-CH3	2.35	118.43	109.86
4	B	901	NCA	C6-N1-C2	2.48	121.41	116.84
3	A	1222	XYQ	C2A-C3A-C4A	2.54	107.82	102.61
3	B	1222	XYQ	OH-CH-CH3	3.05	120.98	109.86
3	A	1222	XYQ	C2-N1-C6	3.11	124.33	118.77
3	A	1222	XYQ	N6-C6-N1	3.22	126.12	119.20
3	A	1222	XYQ	O4N-C1N-C2N	3.61	109.85	104.78
3	B	1222	XYQ	C2A-C1A-N9	4.40	121.01	114.29
3	B	1222	XYQ	O4N-C1N-C2N	4.60	111.25	104.78
4	A	900	NCA	C3-C7-N7	5.38	123.71	117.82
3	A	1222	XYQ	C2A-C1A-N9	6.04	123.51	114.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1222	XYQ	CH-OH-C1N-C2N
3	A	1222	XYQ	CH-OH-C1N-O4N
3	B	1222	XYQ	CH-OH-C1N-O4N

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1222	XYQ	7	0
4	A	900	NCA	1	0
3	B	1222	XYQ	1	0
4	B	901	NCA	2	0

## 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<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	319/354 (90%)	-0.01	11 (3%) 49 46	17, 24, 43, 66	3 (0%)
1	B	319/354 (90%)	0.37	26 (8%) 14 14	21, 34, 49, 62	0
All	All	638/708 (90%)	0.18	37 (5%) 26 25	17, 30, 48, 66	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	7.8
1	B	536	LEU	5.7
1	B	462	LEU	5.1
1	B	430	TYR	4.5
1	B	231	VAL	4.1
1	A	538	ASN	3.9
1	B	470	ILE	3.8
1	B	242	PHE	3.7
1	A	211	PRO	3.6
1	B	285	LYS	3.5
1	B	540	ASN	3.5
1	B	240	ASN	3.4
1	A	513	CYS	3.4
1	B	544	GLN	3.3
1	B	495	ILE	3.0
1	B	468	ILE	3.0
1	A	497	ARG	3.0
1	A	556	ASP	2.9
1	A	468	ILE	2.9
1	B	277	SER	2.8
1	B	243	THR	2.7
1	B	554	THR	2.6
1	B	493	VAL	2.6
1	B	469	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	470[A]	ILE	2.3
1	B	259	VAL	2.3
1	B	546	LYS	2.3
1	B	429	PRO	2.3
1	B	260	LEU	2.2
1	B	261	THR	2.2
1	A	493	VAL	2.2
1	B	534	ASN	2.1
1	A	495	ILE	2.1
1	B	459	GLU	2.1
1	A	467	LEU	2.1
1	B	539	LYS	2.0
1	B	547	ASP	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 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( $\text{\AA}^2$ )	Q<0.9
4	NCA	B	901	9/9	0.68	0.72	25.48	124,125,126,126	9
4	NCA	A	900	9/9	0.45	0.35	10.75	81,83,86,86	0
2	ZN	A	800	1/1	1.00	0.07	0.11	32,32,32,32	0
2	ZN	B	800	1/1	1.00	0.06	-0.56	31,31,31,31	0
3	XYQ	A	1222	38/39	0.97	0.07	-0.86	17,21,25,25	0
3	XYQ	B	1222	38/39	0.97	0.07	-1.20	20,29,37,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.