



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:40 PM UTC

PDB ID : 3RIG / pdb_00003rig
Title : Sirt5 is an NAD-dependent protein lysine demalonylase and desuccinylase
Authors : Zhou, Y.
Deposited on : 2011-04-13
Resolution : 2.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

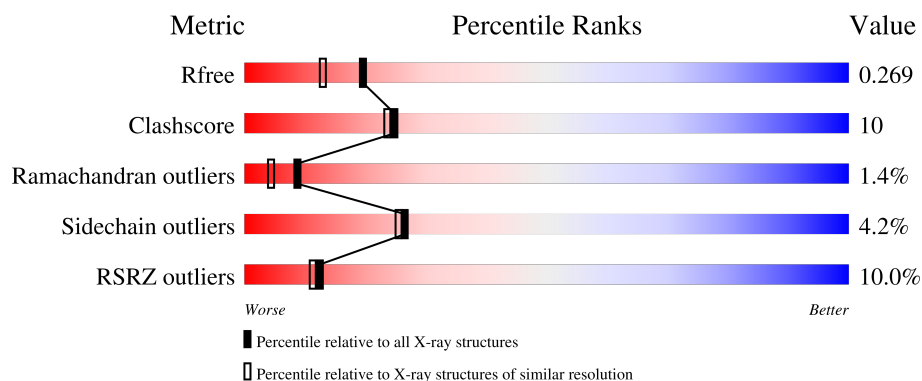
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	273	9% 78% 16% • 5%
1	B	273	11% 74% 18% • 5%
2	C	12	17% 33% 50%
2	D	12	17% 17% 17% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4339 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 deacetylase sirtuin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	5	0
			2027	1284	364	366	13			
1	B	258	Total	C	N	O	S	0	4	0
			2012	1273	365	362	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP Q9NXA8
A	31	SER	-	expression tag	UNP Q9NXA8
A	32	PHE	-	expression tag	UNP Q9NXA8
A	33	THR	-	expression tag	UNP Q9NXA8
B	30	GLY	-	expression tag	UNP Q9NXA8
B	31	SER	-	expression tag	UNP Q9NXA8
B	32	PHE	-	expression tag	UNP Q9NXA8
B	33	THR	-	expression tag	UNP Q9NXA8

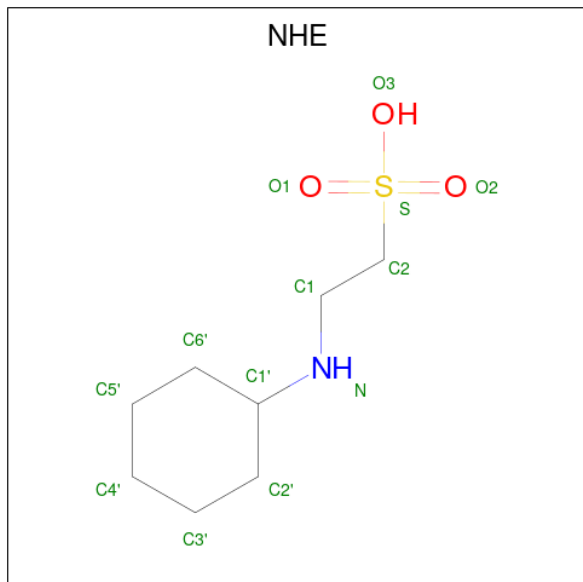
- Molecule 2 is a protein called peptide of histone 3 thioacetyl-lysine 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	S	0	0	0
			48	28	10	9	1			
2	D	6	Total	C	N	O	S	0	0	0
			48	28	10	9	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

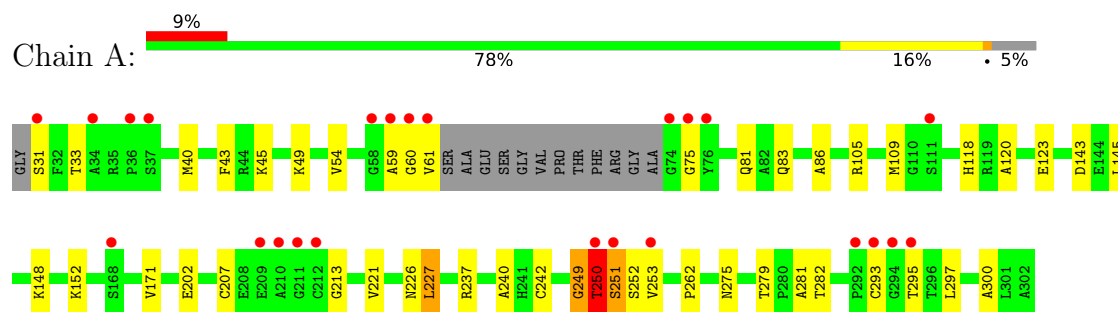
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	83	Total	O	0	0
			83	83		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

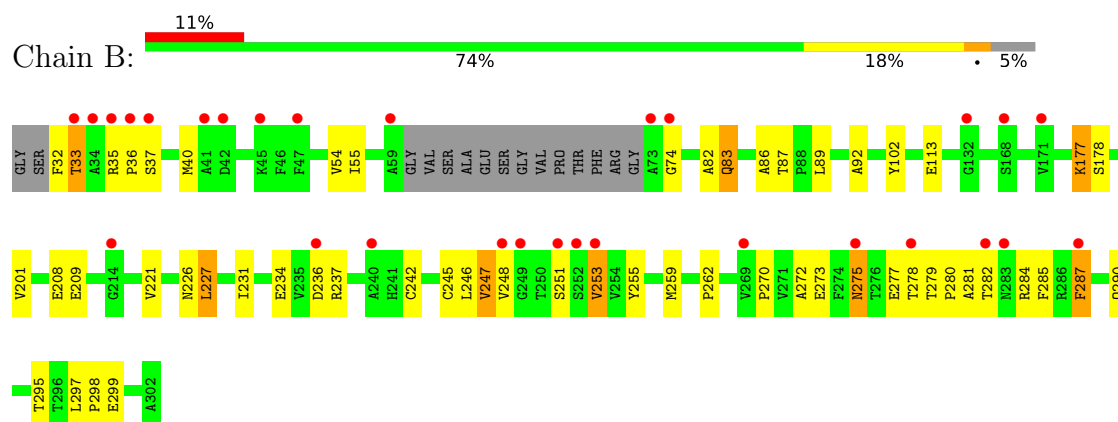
3 Residue-property plots

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.

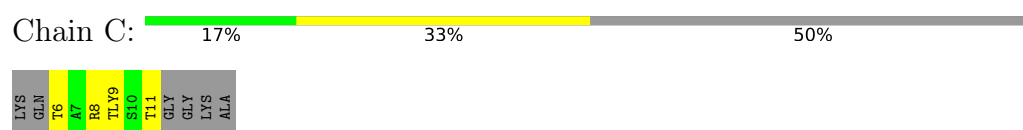
• Molecule 1: NAD-dependent deacetylase sirtuin-5



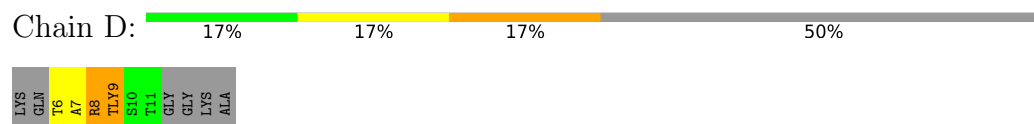
• Molecule 1: NAD-dependent deacetylase sirtuin-5



• Molecule 2: peptide of histone 3 thioacetyl-lysine 9



• Molecule 2: peptide of histone 3 thioacetyl-lysine 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.54Å 67.88Å 156.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.00) 99.8 (30.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.256 0.231 , 0.269	Depositor DCC
R_{free} test set	2083 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4339	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	3/2093 (0.1%)	1.15	8/2836 (0.3%)
1	B	1.09	5/2075 (0.2%)	1.11	4/2814 (0.1%)
2	C	1.05	0/34	0.69	0/43
2	D	1.02	0/34	0.82	0/43
All	All	1.11	8/4236 (0.2%)	1.13	12/5736 (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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	VAL	CA-CB	6.20	1.60	1.54
1	B	201	VAL	CA-CB	5.68	1.62	1.54
1	A	86	ALA	CA-CB	5.51	1.59	1.52
1	B	92	ALA	CA-CB	5.47	1.61	1.53
1	B	270	PRO	N-CD	5.39	1.55	1.47
1	B	86	ALA	CA-CB	5.28	1.59	1.52
1	B	247	VAL	CA-CB	5.16	1.60	1.54
1	A	240	ALA	N-CA	5.07	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	THR	N-CA-C	-14.85	85.68	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	GLY	N-CA-C	-8.72	103.66	111.95
1	B	287	PHE	N-CA-C	6.54	119.83	109.50
1	B	247	VAL	CB-CA-C	6.14	119.49	110.77
1	A	249	GLY	O-C-N	-6.12	114.74	122.70
1	A	250	THR	O-C-N	-5.94	115.66	123.21
1	A	249	GLY	N-CA-C	5.62	126.50	113.18
1	A	59	ALA	N-CA-C	5.52	118.06	111.71
1	A	250	THR	CA-C-N	5.23	131.12	121.70
1	A	250	THR	C-N-CA	5.23	131.12	121.70
1	B	209	GLU	N-CA-C	5.11	117.05	108.73
1	B	102	TYR	CA-CB-CG	-5.06	104.79	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	GLY	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	2027	0	2011	38	0
1	B	2012	0	1994	36	0
2	C	48	0	49	1	0
2	D	48	0	49	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	17	0	0
4	B	13	0	17	1	0
5	A	91	0	0	3	0
5	B	83	0	0	4	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	4339	0	4137	81	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 10.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:HA	1:A:251:SER:HB2	1.38	1.05
1:B:83:GLN:HE21	1:B:83:GLN:H	1.16	0.92
1:A:250:THR:CA	1:A:251:SER:HB2	1.99	0.92
2:D:6:THR:HG23	2:D:7:ALA:H	1.36	0.89
2:D:8:ARG:HH11	2:D:8:ARG:HG3	1.36	0.89
1:A:61:VAL:CG1	1:A:145:LEU:HD12	2.04	0.87
1:B:273:GLU:OE2	1:B:282:THR:OG1	1.93	0.87
1:A:250:THR:HB	1:A:275:ASN:ND2	1.95	0.81
1:A:61:VAL:HG22	1:A:118:HIS:HE2	1.48	0.78
1:A:295:THR:HG23	1:B:295:THR:OG1	1.84	0.78
1:A:120:ALA:O	1:A:123[B]:GLU:HG3	1.83	0.78
2:D:8:ARG:HH11	2:D:8:ARG:CG	1.97	0.77
1:B:278:THR:HG21	5:B:306:HOH:O	1.84	0.75
1:B:281:ALA:O	1:B:284:ARG:HB2	1.87	0.75
1:B:87[B]:THR:HG23	5:B:351:HOH:O	1.87	0.73
1:A:61:VAL:HG11	1:A:145:LEU:HD12	1.72	0.70
1:B:87[B]:THR:CG2	5:B:351:HOH:O	2.42	0.67
1:B:40:MET:HG2	1:B:299:GLU:OE2	1.95	0.66
1:A:105:ARG:NH2	5:A:372:HOH:O	2.29	0.65
1:B:177:LYS:HE3	1:B:178:SER:H	1.61	0.64
1:A:120:ALA:HA	1:A:123[B]:GLU:HG2	1.80	0.63
1:B:177:LYS:HE3	1:B:177:LYS:HA	1.82	0.61
1:A:221:VAL:HG11	1:A:227:LEU:HD22	1.82	0.61
1:A:250:THR:CA	1:A:251:SER:CB	2.78	0.61
1:A:61:VAL:HG11	1:A:143:ASP:OD2	2.02	0.59
1:A:61:VAL:CG1	1:A:145:LEU:CD1	2.80	0.59
1:B:236:ASP:OD2	5:B:337:HOH:O	2.17	0.59
1:B:253:VAL:HG11	1:B:280:PRO:HG2	1.83	0.58
1:A:61:VAL:HG13	1:A:118:HIS:CE1	2.41	0.56
1:B:275:ASN:HB3	1:B:277:GLU:O	2.06	0.56
1:A:237:ARG:NH2	5:A:374:HOH:O	2.39	0.56
1:B:87[B]:THR:HG22	1:B:89:LEU:H	1.71	0.56
1:A:120:ALA:HA	1:A:123[B]:GLU:CG	2.36	0.56
1:B:32:PHE:O	1:B:33:THR:HB	2.05	0.55
1:B:83:GLN:H	1:B:83:GLN:NE2	1.95	0.55
1:A:61:VAL:HG22	1:A:118:HIS:NE2	2.21	0.54
1:A:293:CYS:O	1:A:297:LEU:HB2	2.07	0.54
1:A:250:THR:HG23	1:A:252:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:THR:HG23	2:D:7:ALA:N	2.16	0.53
1:A:54:VAL:HG23	1:A:242:CYS:HB3	1.90	0.53
1:A:250:THR:HG22	1:A:250:THR:O	2.10	0.52
1:A:250:THR:HB	1:A:275:ASN:HD21	1.71	0.52
1:B:234:GLU:OE1	1:B:237:ARG:NH1	2.43	0.52
1:A:250:THR:HA	1:A:251:SER:CB	2.25	0.51
2:D:8:ARG:HG3	2:D:8:ARG:NH1	2.15	0.51
1:A:207:CYS:O	1:A:213:GLY:HA2	2.11	0.50
1:A:250:THR:HG21	1:A:279:THR:HG21	1.92	0.50
1:B:54:VAL:HG23	1:B:242:CYS:HB3	1.94	0.50
1:A:45:LYS:O	1:A:49:LYS:HG2	2.13	0.49
1:B:35[B]:ARG:HB2	1:B:36:PRO:HD3	1.94	0.49
1:B:221:VAL:HG11	1:B:227:LEU:HD22	1.95	0.48
2:D:6:THR:CG2	2:D:7:ALA:H	2.18	0.48
1:B:281:ALA:HB1	1:B:285:PHE:CZ	2.48	0.47
1:B:177:LYS:HA	1:B:177:LYS:CE	2.44	0.47
1:A:81:GLN:HE21	1:A:83:GLN:HE21	1.64	0.46
2:D:8:ARG:CG	2:D:8:ARG:NH1	2.67	0.46
1:B:248:VAL:HG11	1:B:297:LEU:HD11	1.98	0.46
1:B:259:MET:C	1:B:262:PRO:HD2	2.41	0.46
1:B:226:ASN:OD1	2:D:8:ARG:NH1	2.49	0.45
1:B:35[B]:ARG:HB2	1:B:36:PRO:CD	2.46	0.45
1:B:87[B]:THR:HG22	1:B:89:LEU:N	2.32	0.45
1:A:81:GLN:NE2	1:A:83:GLN:HE21	2.14	0.45
1:A:40:MET:HE1	1:A:300:ALA:HB2	1.98	0.44
1:B:279:THR:HB	1:B:280:PRO:HD2	2.00	0.43
1:A:109:MET:HE2	5:A:367:HOH:O	2.18	0.43
1:A:281:ALA:O	1:A:282:THR:C	2.62	0.43
1:A:226:ASN:OD1	2:C:8:ARG:HG3	2.19	0.42
1:A:148:LYS:HE3	1:A:148:LYS:HB2	1.76	0.42
1:B:55:ILE:HG12	1:B:246:LEU:HB2	2.02	0.42
1:B:54:VAL:O	1:B:245:CYS:HA	2.20	0.42
1:B:273:GLU:OE1	1:B:279:THR:OG1	2.29	0.41
1:B:177:LYS:HE3	1:B:178:SER:N	2.31	0.41
1:B:272:ALA:HA	1:B:287:PHE:HB2	2.03	0.41
1:B:255:TYR:O	2:D:9:TLY:HA	2.20	0.41
1:A:43:PHE:CD2	1:A:43:PHE:C	2.99	0.41
2:D:8:ARG:HH11	2:D:8:ARG:CB	2.34	0.41
1:A:81:GLN:HE21	1:A:83:GLN:NE2	2.18	0.40
1:A:202:GLU:H	1:A:202:GLU:CD	2.29	0.40
1:B:82:ALA:HB1	4:B:2002:NHE:HC21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:HG13	1:B:273:GLU:HG3	2.03	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	261/273 (96%)	255 (98%)	3 (1%)	3 (1%)	11	7
1	B	258/273 (94%)	245 (95%)	9 (4%)	4 (2%)	7	3
2	C	3/12 (25%)	3 (100%)	0	0	100	100
2	D	3/12 (25%)	3 (100%)	0	0	100	100
All	All	525/570 (92%)	506 (96%)	12 (2%)	7 (1%)	9	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	251	SER
1	B	33	THR
1	B	253	VAL
1	B	251	SER
1	B	74	GLY
1	A	60	GLY

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	214/217 (99%)	209 (98%)	5 (2%)	44	49
1	B	211/217 (97%)	201 (95%)	10 (5%)	23	22
2	C	4/7 (57%)	2 (50%)	2 (50%)	0	0
2	D	4/7 (57%)	3 (75%)	1 (25%)	0	0
All	All	433/448 (97%)	415 (96%)	18 (4%)	26	25

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	152	LYS
1	A	227	LEU
1	A	250	THR
1	A	253	VAL
1	B	37	SER
1	B	83	GLN
1	B	113	GLU
1	B	177	LYS
1	B	208	GLU
1	B	227	LEU
1	B	231	ILE
1	B	275	ASN
1	B	290	GLN
1	B	298	PRO
2	C	6	THR
2	C	11	THR
2	D	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	83	GLN
1	A	94	ASN
1	A	131	GLN
1	A	263	GLN
1	A	275	ASN
1	A	288	HIS

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Mol	Chain	Res	Type
1	A	290	GLN
1	B	83	GLN
1	B	195	GLN
1	B	275	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	TLY	C	9	2	10,11,12	2.20	2 (20%)	5,12,14	1.60	1 (20%)
2	TLY	D	9	2	10,11,12	2.62	3 (30%)	5,12,14	1.11	0

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
2	TLY	C	9	2	-	0/9/10/12	-
2	TLY	D	9	2	-	0/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	TLY	CX-SX	-5.59	1.56	1.67
2	C	9	TLY	CY-CX	4.75	1.53	1.50
2	D	9	TLY	CY-CX	4.65	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9	TLY	CX-SX	-4.62	1.58	1.67
2	D	9	TLY	CB-CA	3.13	1.58	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	TLY	CY-CX-SX	2.64	124.03	121.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9	TLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	NHE	B	2002	-	13,13,13	1.62	3 (23%)	16,17,17	2.01	6 (37%)
4	NHE	A	2001	-	13,13,13	1.21	2 (15%)	16,17,17	1.73	3 (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
4	NHE	B	2002	-	-	0/7/15/15	0/1/1/1
4	NHE	A	2001	-	-	0/7/15/15	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	NHE	O2-S	2.97	1.53	1.45
4	A	2001	NHE	O2-S	2.63	1.52	1.45
4	B	2002	NHE	C3'-C2'	2.60	1.59	1.53
4	A	2001	NHE	C6'-C1'	2.32	1.57	1.52
4	B	2002	NHE	C2-S	2.15	1.80	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	NHE	O2-S-C2	5.03	114.34	106.73
4	B	2002	NHE	O2-S-C2	4.74	113.89	106.73
4	B	2002	NHE	O1-S-C2	3.25	111.64	106.73
4	A	2001	NHE	O2-S-O1	-3.17	103.52	113.82
4	B	2002	NHE	O3-S-O2	-2.98	103.94	111.40
4	B	2002	NHE	O3-S-C2	2.54	110.97	106.00
4	B	2002	NHE	O2-S-O1	-2.24	106.54	113.82
4	B	2002	NHE	C6'-C1'-C2'	-2.04	107.28	110.80
4	A	2001	NHE	O3-S-C2	2.03	109.97	106.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2002	NHE	1	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, 95th 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	260/273 (95%)	0.51	24 (9%) 14 13	19, 36, 67, 83	8 (3%)
1	B	258/273 (94%)	0.65	29 (11%) 10 9	16, 43, 81, 119	4 (1%)
2	C	5/12 (41%)	0.87	0 100 100	36, 39, 43, 48	0
2	D	5/12 (41%)	1.28	0 100 100	36, 43, 46, 48	0
All	All	528/570 (92%)	0.59	53 (10%) 12 11	16, 39, 74, 119	12 (2%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	ALA	7.6
1	A	250	THR	5.5
1	B	36	PRO	5.2
1	A	59	ALA	4.9
1	A	74	GLY	4.8
1	A	294	GLY	4.6
1	A	293	CYS	4.4
1	B	278	THR	4.1
1	A	210	ALA	4.0
1	B	33	THR	3.9
1	A	61	VAL	3.8
1	B	73	ALA	3.8
1	B	35[A]	ARG	3.5
1	B	59	ALA	3.5
1	A	31	SER	3.5
1	B	34	ALA	3.4
1	B	269	VAL	3.3
1	B	282	THR	3.3
1	B	168	SER	3.3
1	B	283	ASN	3.2
1	B	251	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	75	GLY	3.2
1	B	253	VAL	3.0
1	B	252	SER	3.0
1	A	295	THR	3.0
1	A	60	GLY	2.9
1	B	47	PHE	2.9
1	A	211	GLY	2.9
1	A	212	CYS	2.8
1	A	58	GLY	2.8
1	B	240	ALA	2.7
1	B	42	ASP	2.7
1	A	251	SER	2.6
1	B	132	GLY	2.6
1	A	37	SER	2.6
1	B	74	GLY	2.6
1	A	111	SER	2.6
1	B	275	ASN	2.5
1	A	292	PRO	2.5
1	B	236	ASP	2.5
1	B	249	GLY	2.4
1	B	37	SER	2.4
1	A	168	SER	2.3
1	A	36	PRO	2.3
1	A	76	TYR	2.3
1	A	209	GLU	2.2
1	B	287	PHE	2.2
1	A	253	VAL	2.2
1	B	41	ALA	2.2
1	B	171	VAL	2.1
1	B	214	GLY	2.1
1	B	248	VAL	2.1
1	B	45	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
2	TLY	D	9	12/13	0.96	0.08	24,27,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TLY	C	9	12/13	0.97	0.06	21,25,31,31	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
4	NHE	A	2001	13/13	0.96	0.07	25,31,33,33	0
3	ZN	B	1002	1/1	0.97	0.05	61,61,61,61	0
4	NHE	B	2002	13/13	0.97	0.07	24,32,34,34	0
3	ZN	A	1001	1/1	0.98	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.