



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 06:42 PM EDT

PDB ID : 1L5B  
Title : DOMAIN-SWAPPED CYANOVIRIN-N DIMER  
Authors : Barrientos, L.G.; Louis, J.M.; Botos, I.; Mori, T.; Han, Z.; O’Keefe, B.R.;  
Boyd, M.R.; Wlodawer, A.; Gronenborn, A.M.  
Deposited on : 2002-03-06  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

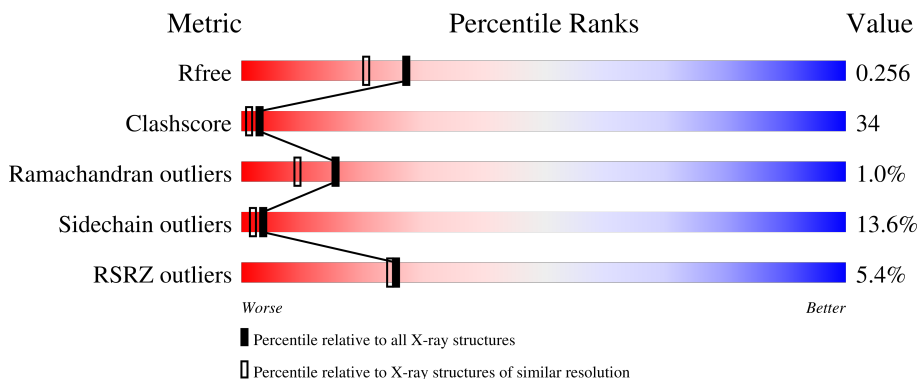
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	101	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4%      39%      39%      20%      •</p>
1	B	101	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">7%      34%      46%      17%      •</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1749 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.

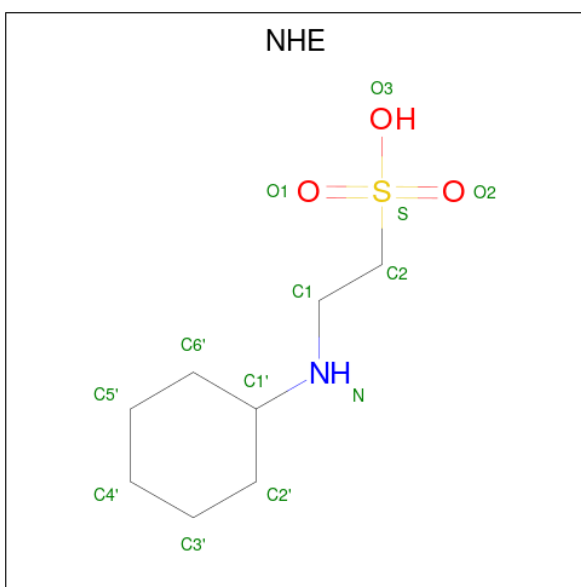
- Molecule 1 is a protein called cyanovirin-N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	101	770	470	133	163	4	0	0	0
1	B	101	770	470	133	163	4	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



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

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	101	Total 101	O 101	0	0
4	B	94	Total 94	O 94	0	0

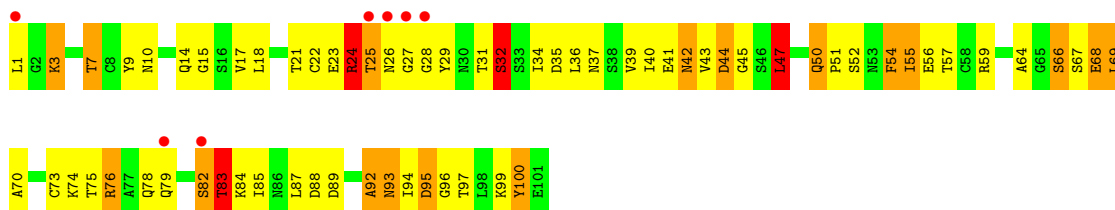
### 3 Residue-property plots [i](#)

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: cyanovirin-N



- Molecule 1: cyanovirin-N



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.97Å 61.97Å 148.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.00 19.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	76.7 (19.90-2.00) 76.7 (19.90-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.01Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.247 , 0.258 0.243 , 0.256	Depositor DCC
$R_{free}$ test set	1686 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtrriage
Anisotropy	0.505	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 70.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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: NA, 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	1.10	1/779 (0.1%)	2.31	42/1054 (4.0%)
1	B	1.02	1/779 (0.1%)	2.47	40/1054 (3.8%)
All	All	1.06	2/1558 (0.1%)	2.39	82/2108 (3.9%)

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	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	TRP	CG-CD1	5.55	1.44	1.36
1	B	15	GLY	N-CA	5.47	1.54	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ASP	CB-CG-OD2	17.09	133.68	118.30
1	B	88	ASP	CB-CG-OD2	-14.70	105.07	118.30
1	B	89	ASP	CB-CG-OD1	-14.68	105.09	118.30
1	B	41	GLU	OE1-CD-OE2	-14.15	106.32	123.30
1	A	24	ARG	CD-NE-CZ	12.29	140.81	123.60
1	B	76	ARG	NE-CZ-NH2	-11.67	114.47	120.30
1	A	76	ARG	CD-NE-CZ	11.27	139.38	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ARG	NE-CZ-NH1	-10.18	115.21	120.30
1	B	24	ARG	NE-CZ-NH2	9.71	125.15	120.30
1	A	76	ARG	NE-CZ-NH1	-9.41	115.60	120.30
1	A	101	GLU	CA-C-O	-8.90	101.41	120.10
1	A	59	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	92	ALA	O-C-N	8.51	136.32	122.70
1	A	77	ALA	C-N-CA	8.48	142.89	121.70
1	B	92	ALA	CB-CA-C	-8.34	97.59	110.10
1	B	100	TYR	CB-CG-CD1	8.04	125.83	121.00
1	A	35	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	59	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	67	SER	C-N-CA	7.84	141.31	121.70
1	B	41	GLU	CG-CD-OE2	7.81	133.91	118.30
1	B	95	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	76	ARG	CD-NE-CZ	7.56	134.19	123.60
1	B	27	GLY	C-N-CA	7.39	137.81	122.30
1	A	1	LEU	CB-CA-C	7.25	123.97	110.20
1	A	78	GLN	CG-CD-OE1	7.15	135.90	121.60
1	A	39	VAL	CA-CB-CG1	7.05	121.48	110.90
1	A	3	LYS	O-C-N	-7.04	111.44	122.70
1	A	58	CYS	N-CA-CB	-6.98	98.04	110.60
1	A	95	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	78	GLN	OE1-CD-NE2	-6.69	106.52	121.90
1	A	3	LYS	N-CA-CB	-6.58	98.75	110.60
1	B	47	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	48	LYS	O-C-N	6.51	133.11	122.70
1	A	22	CYS	N-CA-CB	-6.49	98.91	110.60
1	B	68	GLU	OE1-CD-OE2	-6.47	115.54	123.30
1	A	81	VAL	CA-CB-CG2	6.33	120.39	110.90
1	A	9	TYR	CB-CG-CD2	6.23	124.74	121.00
1	B	44	ASP	CA-CB-CG	6.23	127.11	113.40
1	B	35	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	1	LEU	CA-C-O	6.22	133.16	120.10
1	B	83	THR	CA-CB-CG2	6.19	121.07	112.40
1	B	29	TYR	CB-CG-CD2	-6.19	117.28	121.00
1	B	1	LEU	C-N-CA	6.15	135.21	122.30
1	B	1	LEU	O-C-N	-6.14	112.77	123.20
1	B	67	SER	O-C-N	-6.04	113.03	122.70
1	A	85	ILE	CB-CA-C	-5.91	99.78	111.60
1	A	13	ILE	C-N-CA	5.73	136.01	121.70
1	B	88	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	54	PHE	CB-CG-CD1	5.66	124.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PHE	CB-CG-CD1	5.66	124.76	120.80
1	A	78	GLN	C-N-CA	5.66	135.84	121.70
1	B	14	GLN	CA-CB-CG	-5.63	101.02	113.40
1	A	61	THR	CA-CB-OG1	5.57	120.69	109.00
1	B	43	VAL	CA-CB-CG1	-5.57	102.55	110.90
1	B	73	CYS	N-CA-CB	-5.56	100.59	110.60
1	B	89	ASP	N-CA-CB	5.53	120.56	110.60
1	A	18	LEU	CB-CA-C	5.51	120.67	110.20
1	B	70	ALA	N-CA-CB	5.49	117.78	110.10
1	B	50	GLN	CA-CB-CG	5.47	125.44	113.40
1	A	47	LEU	CA-C-O	5.44	131.53	120.10
1	A	30	ASN	CB-CG-ND2	-5.42	103.69	116.70
1	B	68	GLU	CG-CD-OE2	5.42	129.13	118.30
1	A	19	THR	CA-C-O	-5.41	108.73	120.10
1	A	44	ASP	CA-C-N	5.41	127.01	116.20
1	A	85	ILE	N-CA-CB	5.37	123.16	110.80
1	B	59	ARG	NH1-CZ-NH2	5.37	125.31	119.40
1	A	42	ASN	CB-CG-OD1	-5.32	110.96	121.60
1	A	4	PHE	CB-CG-CD2	5.30	124.51	120.80
1	A	85	ILE	CA-CB-CG2	5.26	121.43	110.90
1	A	38	SER	N-CA-CB	-5.25	102.62	110.50
1	B	100	TYR	CG-CD2-CE2	5.23	125.49	121.30
1	B	84	LYS	CB-CA-C	-5.21	99.98	110.40
1	B	52	SER	N-CA-CB	5.20	118.30	110.50
1	A	19	THR	O-C-N	5.16	130.95	122.70
1	A	39	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	A	83	THR	CA-C-N	5.12	128.46	117.20
1	A	98	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	67	SER	N-CA-CB	-5.08	102.88	110.50
1	A	84	LYS	CB-CA-C	-5.03	100.34	110.40
1	B	32	SER	CB-CA-C	-5.03	100.55	110.10
1	A	3	LYS	CB-CA-C	5.02	120.45	110.40
1	A	24	ARG	CB-CG-CD	5.02	124.66	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	CYS	Mainchain
1	B	17	VAL	Mainchain
1	B	32	SER	Mainchain
1	B	66	SER	Mainchain

## 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	770	0	741	57	0
1	B	770	0	743	66	0
2	A	1	0	0	0	0
3	A	13	0	16	2	0
4	A	101	0	0	11	0
4	B	94	0	0	14	0
All	All	1749	0	1500	101	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 34.

All (101) 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)
4:A:303:HOH:O	1:B:85:ILE:HB	1.44	1.16
1:B:32:SER:HB2	4:B:168:HOH:O	1.73	0.89
1:B:68:GLU:HG2	4:B:136:HOH:O	1.73	0.89
1:A:18:LEU:HD22	1:B:87:LEU:HD13	1.56	0.86
1:A:93:ASN:HD21	1:A:96:GLY:H	1.26	0.81
1:A:93:ASN:HD21	1:A:96:GLY:N	1.78	0.81
1:B:42:ASN:HD21	1:B:45:GLY:H	1.28	0.81
1:B:40:ILE:HD11	1:B:47:LEU:HG	1.62	0.81
1:B:93:ASN:HD21	1:B:96:GLY:H	1.26	0.80
1:A:30:ASN:ND2	1:B:96:GLY:O	2.17	0.75
1:B:42:ASN:HD21	1:B:45:GLY:N	1.88	0.72
1:B:56:GLU:HG3	4:B:122:HOH:O	1.90	0.70
1:A:39:VAL:HG22	1:B:100:TYR:CD2	2.27	0.69
1:B:40:ILE:CD1	1:B:47:LEU:HG	2.23	0.69
1:A:76:ARG:HG3	1:B:44:ASP:HB2	1.76	0.68
1:B:7:THR:HB	1:B:23:GLU:HB2	1.76	0.68
1:B:37:ASN:HB3	4:B:128:HOH:O	1.94	0.67
1:A:41:GLU:OE2	1:A:50:GLN:HG2	1.95	0.66
1:A:69:LEU:HD12	1:A:70:ALA:N	2.12	0.64
1:B:54:PHE:HB3	4:B:194:HOH:O	1.98	0.64
1:A:54:PHE:O	1:A:58:CYS:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PRO:O	4:B:189:HOH:O	2.14	0.63
1:A:96:GLY:HA2	1:B:22:CYS:HB2	1.79	0.63
1:B:99:LYS:HE2	4:B:160:HOH:O	1.98	0.63
1:B:75:THR:HG23	1:B:79:GLN:O	1.98	0.62
1:A:18:LEU:HD22	1:B:87:LEU:CD1	2.28	0.62
1:A:78:GLN:OE1	4:A:353:HOH:O	2.16	0.62
1:B:93:ASN:ND2	1:B:96:GLY:H	1.97	0.61
1:B:74:LYS:HG3	1:B:78:GLN:HA	1.82	0.61
1:A:26:ASN:OD1	1:A:27:GLY:N	2.31	0.60
1:A:74:LYS:HB3	3:A:301:NHE:H4'2	1.82	0.60
1:B:40:ILE:HD11	1:B:47:LEU:HB3	1.83	0.60
1:A:100:TYR:CD2	1:B:39:VAL:HG13	2.37	0.60
1:A:47:LEU:HB2	1:B:85:ILE:CG2	2.32	0.60
1:A:58:CYS:HG	1:A:73:CYS:HG	0.60	0.59
1:A:37:ASN:HB2	4:A:310:HOH:O	2.02	0.58
1:B:9:TYR:O	1:B:10:ASN:HB2	2.03	0.58
1:A:75:THR:O	1:A:78:GLN:NE2	2.37	0.57
1:A:39:VAL:HG22	1:B:100:TYR:CE2	2.41	0.56
1:A:57:THR:HG21	3:A:301:NHE:H3'1	1.88	0.56
1:B:21:THR:HA	1:B:31:THR:HA	1.89	0.55
1:A:85:ILE:HD13	1:A:85:ILE:N	2.23	0.54
1:A:24:ARG:HB2	1:A:26:ASN:ND2	2.22	0.54
1:B:64:ALA:O	1:B:68:GLU:OE1	2.27	0.53
1:A:58:CYS:SG	1:A:73:CYS:CB	2.97	0.53
1:A:78:GLN:HG3	4:A:400:HOH:O	2.09	0.52
1:A:18:LEU:CD2	1:B:87:LEU:HD13	2.36	0.52
1:B:85:ILE:O	1:B:85:ILE:HG13	2.10	0.51
1:B:93:ASN:HD21	1:B:96:GLY:N	2.01	0.51
1:A:55:ILE:HG13	4:A:308:HOH:O	2.11	0.51
1:A:22:CYS:HB2	4:A:309:HOH:O	2.09	0.51
4:A:303:HOH:O	1:B:85:ILE:CG2	2.56	0.51
1:B:54:PHE:CB	4:B:194:HOH:O	2.57	0.51
1:B:82:SER:O	1:B:83:THR:CB	2.57	0.51
1:A:13:ILE:HA	1:A:17:VAL:O	2.12	0.50
1:B:76:ARG:HB2	4:B:185:HOH:O	2.11	0.50
1:B:74:LYS:CG	1:B:78:GLN:HA	2.42	0.50
1:A:47:LEU:HB2	1:B:85:ILE:HG23	1.94	0.50
1:A:47:LEU:HG	1:B:83:THR:HG23	1.93	0.49
1:B:36:LEU:HD23	1:B:36:LEU:N	2.27	0.49
1:A:15:GLY:HA3	4:A:348:HOH:O	2.13	0.49
1:A:34:ILE:HG13	1:A:35:ASP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:THR:HB	4:B:130:HOH:O	2.13	0.48
1:A:47:LEU:HG	1:B:83:THR:CG2	2.44	0.48
1:B:97:THR:HG21	4:B:156:HOH:O	2.13	0.47
1:A:28:GLY:HA3	4:A:370:HOH:O	2.15	0.47
1:A:55:ILE:HD12	1:A:56:GLU:HG3	1.97	0.47
1:A:39:VAL:CG2	1:B:100:TYR:CD2	2.97	0.46
1:A:55:ILE:HD12	1:A:56:GLU:CG	2.44	0.46
1:B:34:ILE:HD13	1:B:34:ILE:HG21	1.78	0.46
1:A:56:GLU:HG3	4:A:308:HOH:O	2.15	0.46
1:B:94:ILE:CG1	1:B:99:LYS:HD3	2.46	0.46
1:B:28:GLY:N	4:B:143:HOH:O	2.19	0.45
1:B:3:LYS:HD3	4:B:188:HOH:O	2.17	0.45
1:B:69:LEU:HD12	1:B:85:ILE:HD11	1.97	0.45
1:A:23:GLU:HG3	1:A:29:TYR:CE2	2.52	0.44
1:A:8:CYS:CB	1:A:22:CYS:SG	3.06	0.44
1:A:95:ASP:OD1	1:B:24:ARG:NE	2.50	0.44
1:A:2:GLY:O	1:B:92:ALA:HA	2.18	0.44
1:A:69:LEU:HD12	1:A:70:ALA:H	1.81	0.44
1:A:42:ASN:HD22	1:B:57:THR:CB	2.30	0.44
1:A:58:CYS:SG	1:A:73:CYS:HB3	2.58	0.43
1:A:85:ILE:CD1	1:B:47:LEU:HD23	2.48	0.43
1:B:25:THR:CB	4:B:130:HOH:O	2.65	0.43
1:A:18:LEU:HD23	1:A:36:LEU:HD21	2.01	0.43
1:A:62:GLN:N	1:A:70:ALA:O	2.52	0.43
1:B:55:ILE:H	1:B:55:ILE:HG13	1.51	0.43
1:A:69:LEU:HB2	1:A:87:LEU:HD21	2.00	0.43
1:B:92:ALA:N	1:B:99:LYS:O	2.42	0.42
1:B:93:ASN:ND2	1:B:96:GLY:N	2.66	0.42
1:B:50:GLN:HA	1:B:51:PRO:HD3	1.95	0.41
1:A:93:ASN:HD21	1:A:96:GLY:CA	2.34	0.41
1:B:85:ILE:HD13	1:B:85:ILE:HG21	1.67	0.41
1:A:25:THR:HG23	1:B:95:ASP:OD2	2.21	0.41
1:A:40:ILE:HD12	1:B:85:ILE:CD1	2.51	0.41
1:A:100:TYR:CE2	1:B:39:VAL:HG13	2.56	0.41
1:A:26:ASN:CG	1:A:27:GLY:H	2.21	0.41
1:B:75:THR:O	1:B:76:ARG:C	2.58	0.40
1:A:41:GLU:O	1:A:47:LEU:HA	2.20	0.40
1:A:76:ARG:HG3	1:B:44:ASP:CB	2.48	0.40
4:A:310:HOH:O	1:B:55:ILE:HG13	2.20	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	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15	9
1	B	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	9
All	All	198/202 (98%)	174 (88%)	22 (11%)	2 (1%)	15	9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	A	27	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	88/88 (100%)	78 (89%)	10 (11%)	5	3
1	B	88/88 (100%)	74 (84%)	14 (16%)	2	1
All	All	176/176 (100%)	152 (86%)	24 (14%)	3	2

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	20	SER
1	A	24	ARG
1	A	34	ILE

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Mol	Chain	Res	Type
1	A	62	GLN
1	A	69	LEU
1	A	78	GLN
1	A	83	THR
1	A	85	ILE
1	A	93	ASN
1	B	3	LYS
1	B	7	THR
1	B	18	LEU
1	B	24	ARG
1	B	25	THR
1	B	32	SER
1	B	42	ASN
1	B	47	LEU
1	B	55	ILE
1	B	66	SER
1	B	69	LEU
1	B	82	SER
1	B	83	THR
1	B	93	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	78	GLN
1	A	93	ASN
1	B	6	GLN
1	B	42	ASN
1	B	78	GLN
1	B	93	ASN

### 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NHE	A	301	-	13,13,13	4.14	9 (69%)	16,17,17	3.22	8 (50%)

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	NHE	A	301	-	-	1/7/15/15	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NHE	O1-S	7.55	1.67	1.45
3	A	301	NHE	O2-S	7.24	1.66	1.45
3	A	301	NHE	O3-S	5.56	1.67	1.47
3	A	301	NHE	C3'-C2'	-4.43	1.41	1.53
3	A	301	NHE	C5'-C6'	-4.39	1.41	1.53
3	A	301	NHE	C2'-C1'	-4.16	1.42	1.52
3	A	301	NHE	C6'-C1'	-3.27	1.44	1.52
3	A	301	NHE	C4'-C5'	-2.38	1.42	1.51
3	A	301	NHE	C4'-C3'	-2.35	1.42	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NHE	O1-S-C2	5.95	114.08	106.92
3	A	301	NHE	C6'-C1'-C2'	5.09	119.64	110.82
3	A	301	NHE	C3'-C2'-C1'	4.74	120.04	111.11
3	A	301	NHE	C5'-C6'-C1'	4.69	119.94	111.11
3	A	301	NHE	C4'-C3'-C2'	4.33	120.24	111.42
3	A	301	NHE	C4'-C5'-C6'	4.12	119.82	111.42
3	A	301	NHE	C5'-C4'-C3'	2.97	120.32	111.18
3	A	301	NHE	C6'-C1'-N	2.78	122.49	110.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NHE	C2'-C1'-N-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NHE	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	101/101 (100%)	0.23	4 (3%) 38 37	25, 39, 53, 67	0
1	B	101/101 (100%)	0.35	7 (6%) 16 16	28, 42, 57, 73	0
All	All	202/202 (100%)	0.29	11 (5%) 25 24	25, 41, 56, 73	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	GLY	10.0
1	B	26	ASN	5.1
1	A	25	THR	4.5
1	B	28	GLY	3.7
1	A	77	ALA	2.8
1	A	26	ASN	2.7
1	A	27	GLY	2.7
1	B	1	LEU	2.3
1	B	25	THR	2.3
1	B	79	GLN	2.3
1	B	82	SER	2.2

### 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	A	302	1/1	0.76	0.15	60,60,60,60	0
3	NHE	A	301	13/13	0.91	0.23	39,48,50,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.