



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:11 PM UTC

PDB ID : 1F5Z / pdb_00001f5z
Title : CRYSTAL STRUCTURE ANALYSIS OF N-ACETYLNEURAMINATE
LYASE FROM HAEMOPHILUS INFLUENZAE: CRYSTAL FORM I
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Deposited on : 2000-06-18
Resolution : 1.88 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

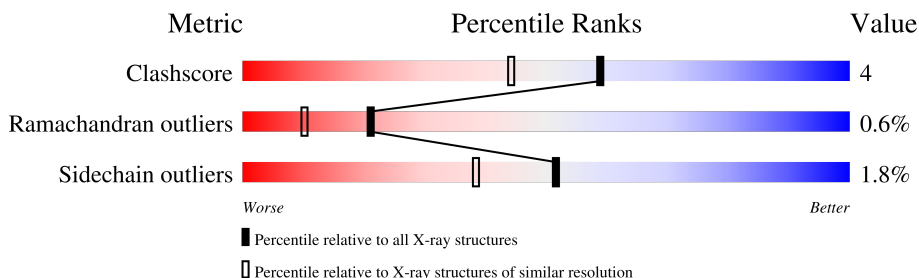
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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))
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	293	83% 15% .
1	B	293	82% 17% ..
1	C	293	81% 17% .
1	D	293	84% 14% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9946 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 N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	1	0
			2294	1478	373	433	10			
1	B	293	Total	C	N	O	S	0	0	0
			2290	1476	373	431	10			
1	C	293	Total	C	N	O	S	0	0	0
			2290	1476	373	431	10			
1	D	293	Total	C	N	O	S	0	0	0
			2290	1476	373	431	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	SER	ASN	variant	UNP P44539
A	229	LYS	ALA	variant	UNP P44539
A	278	ALA	GLU	variant	UNP P44539
A	281	VAL	LEU	variant	UNP P44539
B	131	SER	ASN	variant	UNP P44539
B	229	LYS	ALA	variant	UNP P44539
B	278	ALA	GLU	variant	UNP P44539
B	281	VAL	LEU	variant	UNP P44539
C	131	SER	ASN	variant	UNP P44539
C	229	LYS	ALA	variant	UNP P44539
C	278	ALA	GLU	variant	UNP P44539
C	281	VAL	LEU	variant	UNP P44539
D	131	SER	ASN	variant	UNP P44539
D	229	LYS	ALA	variant	UNP P44539
D	278	ALA	GLU	variant	UNP P44539
D	281	VAL	LEU	variant	UNP P44539

- Molecule 2 is water.

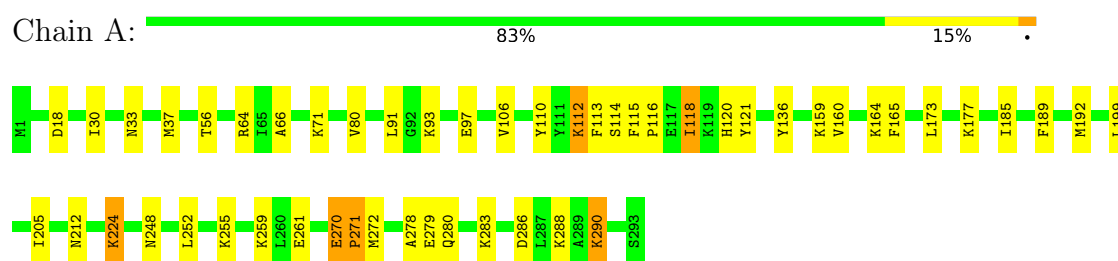
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	196	Total 196	O 196	0	0
2	B	193	Total 193	O 193	0	0
2	C	187	Total 187	O 187	0	0
2	D	206	Total 206	O 206	0	0

3 Residue-property plots

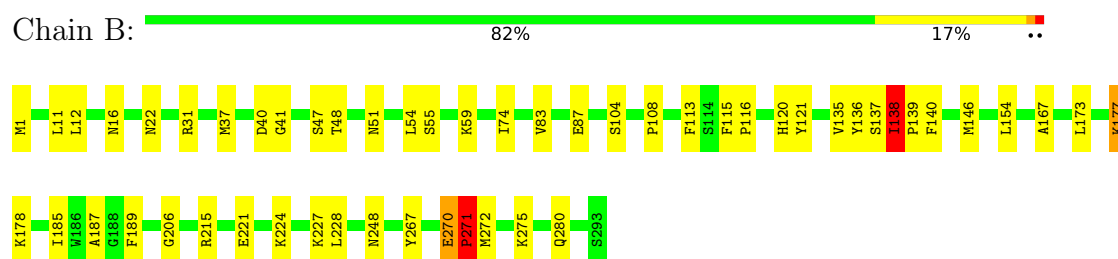
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

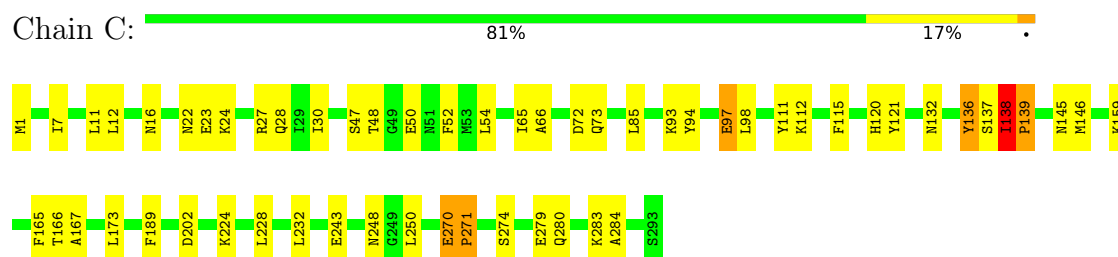
• Molecule 1: N-ACETYLNEURAMINATE LYASE



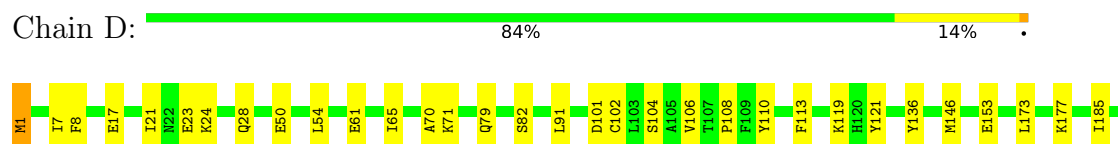
• Molecule 1: N-ACETYLNEURAMINATE LYASE



• Molecule 1: N-ACETYLNEURAMINATE LYASE



• Molecule 1: N-ACETYLNEURAMINATE LYASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.75Å 109.78Å 133.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.88	Depositor
% Data completeness (in resolution range)	74.0 (20.00-1.88)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9946	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	0.69	0/2339	1.67	26/3147 (0.8%)
1	B	0.73	0/2330	1.65	26/3135 (0.8%)
1	C	0.72	0/2330	1.66	34/3135 (1.1%)
1	D	0.70	0/2330	1.58	26/3135 (0.8%)
All	All	0.71	0/9329	1.64	112/12552 (0.9%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	GLU	CA-C-O	-17.02	102.64	119.49
1	D	270	GLU	CA-C-O	-12.85	102.55	120.16
1	B	270	GLU	CA-C-O	-12.80	102.62	120.16
1	C	270	GLU	CA-C-O	-11.81	103.98	120.16
1	A	270	GLU	CA-C-N	11.08	133.69	119.84
1	A	270	GLU	C-N-CA	11.08	133.69	119.84
1	A	271	PRO	N-CA-CB	10.74	114.53	103.25
1	A	270	GLU	O-C-N	10.48	130.93	121.18
1	C	137	SER	CA-C-N	9.98	140.60	122.13
1	C	137	SER	C-N-CA	9.98	140.60	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	PRO	CA-N-CD	-9.13	99.22	112.00
1	B	270	GLU	CA-C-N	8.65	130.66	119.84
1	B	270	GLU	C-N-CA	8.65	130.66	119.84
1	C	271	PRO	N-CD-CG	8.59	114.11	103.80
1	A	120	HIS	CA-C-O	8.47	129.53	120.55
1	C	271	PRO	N-CA-CB	7.71	111.08	102.60
1	C	271	PRO	CA-N-CD	-7.61	100.85	111.50
1	B	221	GLU	CB-CG-CD	7.38	125.15	112.60
1	C	138	ILE	N-CA-C	7.38	124.83	108.88
1	C	250	LEU	N-CA-C	7.35	119.99	111.02
1	B	271	PRO	N-CA-CB	7.23	110.84	103.25
1	A	224	LYS	CA-CB-CG	7.15	128.41	114.10
1	D	70	ALA	CA-C-O	-6.88	111.67	119.79
1	C	115	PHE	CA-CB-CG	-6.78	107.02	113.80
1	A	64	ARG	CD-NE-CZ	6.77	133.88	124.40
1	A	33	ASN	OD1-CG-ND2	6.74	129.34	122.60
1	C	97	GLU	CA-CB-CG	6.59	127.28	114.10
1	B	206	GLY	CA-C-O	6.52	127.12	121.19
1	D	82	SER	N-CA-CB	-6.52	100.02	111.49
1	C	27	ARG	CD-NE-CZ	6.30	133.22	124.40
1	A	118	ILE	CA-C-O	6.21	127.76	121.17
1	D	91	LEU	CA-C-N	6.20	126.86	119.98
1	D	91	LEU	C-N-CA	6.20	126.86	119.98
1	D	291	PHE	N-CA-C	6.15	121.84	113.97
1	B	271	PRO	CA-N-CD	-6.15	103.39	112.00
1	C	139	PRO	N-CA-C	6.12	121.50	113.86
1	D	271	PRO	CA-N-CD	-6.11	102.94	111.50
1	A	212	ASN	CA-C-N	6.10	126.86	120.03
1	A	212	ASN	C-N-CA	6.10	126.86	120.03
1	D	79	GLN	CB-CG-CD	6.06	122.90	112.60
1	B	11	LEU	N-CA-C	6.00	118.90	109.96
1	C	279	GLU	CA-C-O	-5.99	114.20	120.55
1	B	104	SER	CA-C-O	-5.97	114.14	121.06
1	D	50	GLU	CA-C-N	5.97	128.55	120.38
1	D	50	GLU	C-N-CA	5.97	128.55	120.38
1	D	8	PHE	CA-CB-CG	5.92	119.72	113.80
1	C	50	GLU	CA-C-N	5.91	128.48	120.38
1	C	50	GLU	C-N-CA	5.91	128.48	120.38
1	D	279	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	71	LYS	CB-CA-C	-5.88	109.24	117.23
1	A	160	VAL	N-CA-CB	5.85	118.51	111.31
1	C	121	TYR	CA-CB-CG	5.85	124.43	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	LEU	N-CA-C	5.79	117.59	111.28
1	C	72	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	31	ARG	CD-NE-CZ	5.76	132.47	124.40
1	B	40	ASP	CA-CB-CG	-5.72	106.88	112.60
1	C	16	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	C	54	LEU	N-CA-C	5.70	118.97	110.14
1	D	271	PRO	N-CA-CB	5.69	108.86	102.60
1	C	28	GLN	CA-C-O	-5.69	114.52	120.55
1	C	111	TYR	CA-C-O	-5.67	115.12	121.81
1	D	146	MET	CA-C-N	-5.65	117.40	122.43
1	D	146	MET	C-N-CA	-5.65	117.40	122.43
1	D	102	CYS	CA-CB-SG	5.64	127.38	114.40
1	D	290	LYS	N-CA-C	5.62	117.48	111.36
1	B	87	GLU	N-CA-CB	5.62	118.47	110.16
1	B	138	ILE	N-CA-C	5.61	121.00	108.88
1	B	54	LEU	N-CA-C	5.61	119.11	110.42
1	C	165	PHE	N-CA-CB	-5.60	102.01	110.35
1	A	272	MET	CA-C-O	-5.59	115.04	121.47
1	C	202	ASP	CA-CB-CG	-5.55	107.05	112.60
1	C	11	LEU	N-CA-C	5.54	118.22	109.96
1	D	104	SER	CA-C-O	-5.52	114.81	120.99
1	A	18	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	290	LYS	N-CA-C	5.51	117.37	111.36
1	B	227	LYS	CA-C-N	5.45	127.58	120.28
1	B	227	LYS	C-N-CA	5.45	127.58	120.28
1	D	270	GLU	CB-CA-C	5.44	120.89	110.17
1	C	284	ALA	CA-C-O	5.43	126.31	120.55
1	B	215	ARG	CD-NE-CZ	5.38	131.93	124.40
1	B	187	ALA	CA-C-O	-5.37	115.14	121.16
1	D	274	SER	N-CA-C	5.37	117.21	111.36
1	A	80	VAL	CA-C-N	5.36	126.28	120.44
1	A	80	VAL	C-N-CA	5.36	126.28	120.44
1	B	271	PRO	N-CA-C	5.36	123.52	112.47
1	B	272	MET	CA-C-O	-5.35	115.73	121.56
1	B	47	SER	CB-CA-C	-5.33	102.28	110.81
1	C	136	TYR	CB-CA-C	-5.33	100.23	110.24
1	D	240	ASP	CA-C-O	5.32	126.06	120.42
1	B	83	VAL	N-CA-C	-5.32	105.10	112.50
1	D	71	LYS	CB-CA-C	-5.31	110.44	116.54
1	C	73	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	278	ALA	CA-C-N	5.20	127.25	120.28
1	A	278	ALA	C-N-CA	5.20	127.25	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	228	LEU	N-CA-C	5.18	117.66	111.71
1	C	54	LEU	N-CA-CB	-5.16	102.91	110.85
1	A	112	LYS	CA-C-O	-5.15	116.45	122.37
1	D	7	ILE	CB-CA-C	-5.13	103.94	110.98
1	C	52	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	290	LYS	CB-CA-C	-5.12	102.14	110.85
1	A	252	LEU	CA-C-O	-5.12	115.12	120.55
1	B	104	SER	CA-CB-OG	-5.12	100.87	111.10
1	D	101	ASP	CA-CB-CG	-5.11	107.49	112.60
1	C	7	ILE	N-CA-C	5.09	115.67	107.73
1	D	54	LEU	N-CA-C	5.08	117.98	110.46
1	D	269	ARG	CD-NE-CZ	5.08	131.50	124.40
1	C	243	GLU	CA-C-N	5.03	125.57	119.98
1	C	243	GLU	C-N-CA	5.03	125.57	119.98
1	B	55	SER	CA-C-O	-5.03	115.87	121.81
1	A	115	PHE	CA-CB-CG	-5.03	108.77	113.80
1	B	121	TYR	CA-CB-CG	5.01	122.92	113.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	GLU	Mainchain,Peptide
1	B	270	GLU	Mainchain,Peptide
1	C	270	GLU	Mainchain,Peptide
1	D	270	GLU	Mainchain,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	2294	0	2334	26	0
1	B	2290	0	2332	24	0
1	C	2290	0	2332	21	0
1	D	2290	0	2332	18	0
2	A	196	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	193	0	0	1	0
2	C	187	0	0	2	0
2	D	206	0	0	2	0
All	All	9946	0	9330	82	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 4.

All (82) 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:C:139:PRO:HD2	1:C:167:ALA:HB2	1.60	0.83
1:A:248:ASN:HD21	1:A:280:GLN:HA	1.48	0.77
1:A:248:ASN:HB2	1:A:283:LYS:HD3	1.69	0.74
1:C:248:ASN:HB2	1:C:283:LYS:HD3	1.75	0.68
1:D:248:ASN:HD21	1:D:280:GLN:HA	1.61	0.66
1:A:173:LEU:HD11	1:A:185:ILE:HG21	1.80	0.64
1:B:120:HIS:HD2	2:B:395:HOH:O	1.80	0.64
1:C:248:ASN:HD21	1:C:280:GLN:HA	1.63	0.63
1:B:173:LEU:HD11	1:B:185:ILE:HG21	1.81	0.62
1:D:194:LEU:HD13	1:D:223:THR:OG1	2.00	0.60
1:C:93:LYS:O	1:C:97:GLU:HG3	2.05	0.56
1:C:138:ILE:O	1:C:138:ILE:HG23	2.03	0.56
1:A:93:LYS:O	1:A:97:GLU:HG3	2.05	0.55
1:B:138:ILE:O	1:B:138:ILE:HG23	2.07	0.54
1:C:24:LYS:HD2	2:C:371:HOH:O	2.08	0.54
1:A:261:GLU:OE2	1:A:288:LYS:HE2	2.07	0.53
1:B:267:TYR:CD2	1:B:275:LYS:HG2	2.43	0.53
1:D:173:LEU:HD12	1:D:185:ILE:HD13	1.91	0.53
1:D:177:LYS:HE2	1:D:185:ILE:HD12	1.89	0.53
1:B:51:ASN:ND2	1:B:59:LYS:HG2	2.24	0.52
1:B:177:LYS:HD3	1:B:185:ILE:HD12	1.91	0.52
1:A:106:VAL:HA	1:A:136:TYR:HB3	1.91	0.51
1:A:189:PHE:HD2	1:A:192:MET:CE	2.24	0.51
1:A:136:TYR:CD1	1:A:164:LYS:HD3	2.46	0.51
1:D:21:ILE:HD12	1:D:61:GLU:OE1	2.12	0.50
1:A:112:LYS:HE2	2:A:455:HOH:O	2.11	0.50
1:C:23:GLU:HG3	1:C:65:ILE:HD13	1.95	0.49
1:C:120:HIS:HD2	2:C:457:HOH:O	1.96	0.49
1:C:1:MET:HE2	1:C:132:ASN:ND2	2.28	0.48
1:A:271:PRO:HG2	1:D:113:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLY:HA2	1:B:74:ILE:HB	1.96	0.48
1:D:108:PRO:HD3	1:D:121:TYR:CE1	2.49	0.48
1:A:255:LYS:O	1:A:259:LYS:HG3	2.13	0.48
1:C:94:TYR:CE2	1:C:98:LEU:HD11	2.49	0.47
1:D:106:VAL:HA	1:D:136:TYR:HB3	1.96	0.47
1:A:113:PHE:CE1	1:D:271:PRO:HG2	2.50	0.47
1:A:177:LYS:HE2	1:A:185:ILE:HD12	1.96	0.47
1:A:164:LYS:HE2	1:A:205:ILE:HB	1.96	0.47
1:B:136:TYR:CD2	1:B:138:ILE:HG22	2.50	0.47
1:B:248:ASN:HD21	1:B:280:GLN:HA	1.80	0.47
1:C:1:MET:HE2	1:C:132:ASN:HD21	1.80	0.47
1:B:173:LEU:HD12	1:B:185:ILE:HD13	1.95	0.46
1:B:173:LEU:CD1	1:B:185:ILE:HG21	2.46	0.46
1:B:12:LEU:HG	1:B:48:THR:HG22	1.96	0.46
1:B:115:PHE:N	1:B:116:PRO:CD	2.80	0.45
1:A:56:THR:HG23	1:A:91:LEU:HD21	1.98	0.45
1:D:177:LYS:HA	1:D:177:LYS:HD3	1.75	0.45
1:B:178:LYS:HE3	1:D:240:ASP:OD2	2.16	0.45
1:B:139:PRO:CD	1:B:167:ALA:HB2	2.47	0.45
1:B:37:MET:HA	1:B:37:MET:HE2	1.99	0.45
1:A:165:PHE:CD2	1:A:173:LEU:HD13	2.52	0.44
1:C:30:ILE:HD13	1:C:66:ALA:HA	1.98	0.44
1:A:30:ILE:HD13	1:A:66:ALA:HA	1.99	0.44
1:C:224:LYS:HA	1:C:224:LYS:HD2	1.78	0.44
1:B:136:TYR:HD2	1:B:138:ILE:HG22	1.81	0.44
1:B:135:VAL:HG11	1:B:154:LEU:HD13	2.00	0.44
1:B:140:PHE:CE2	1:C:112:LYS:HE2	2.52	0.44
1:A:37:MET:HA	1:A:37:MET:HE2	2.00	0.43
1:C:1:MET:CE	1:C:132:ASN:HD21	2.32	0.42
1:C:166:THR:HG22	1:C:166:THR:O	2.19	0.42
1:D:119:LYS:HE2	1:D:153:GLU:O	2.19	0.42
1:C:136:TYR:HD2	1:C:138:ILE:HB	1.85	0.42
1:D:24:LYS:O	1:D:28:GLN:HG3	2.19	0.42
1:D:177:LYS:HD2	2:D:397:HOH:O	2.19	0.42
1:B:16:ASN:OD1	1:B:22:ASN:HB2	2.20	0.41
1:C:139:PRO:HB3	1:C:145:ASN:ND2	2.35	0.41
1:A:118:ILE:O	1:A:121:TYR:HB3	2.21	0.41
1:A:189:PHE:CD2	1:A:192:MET:CE	3.04	0.41
1:C:12:LEU:HG	1:C:48:THR:HG22	2.03	0.41
1:A:113:PHE:CZ	1:D:271:PRO:HG2	2.56	0.41
1:A:114:SER:OG	1:A:116:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD23	1:C:232:LEU:HD13	2.02	0.41
1:A:279:GLU:CD	1:A:279:GLU:H	2.28	0.41
1:B:271:PRO:HD3	1:C:85:LEU:HB2	2.02	0.41
1:D:17:GLU:OE2	1:D:275:LYS:HE2	2.21	0.41
1:D:23:GLU:HG3	1:D:65:ILE:HD13	2.03	0.41
1:A:286:ASP:OD2	1:A:290:LYS:HE2	2.21	0.41
1:D:1:MET:HG2	2:D:436:HOH:O	2.21	0.41
1:B:177:LYS:HD2	1:B:177:LYS:HA	1.93	0.40
1:B:267:TYR:HD2	1:B:275:LYS:HG2	1.84	0.40
1:B:108:PRO:HB2	1:B:113:PHE:CE2	2.56	0.40
1:A:173:LEU:CD1	1:A:185:ILE:HG21	2.49	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	292/293 (100%)	284 (97%)	7 (2%)	1 (0%)	36	26
1	B	291/293 (99%)	282 (97%)	7 (2%)	2 (1%)	18	7
1	C	291/293 (99%)	283 (97%)	6 (2%)	2 (1%)	18	7
1	D	291/293 (99%)	283 (97%)	6 (2%)	2 (1%)	18	7
All	All	1165/1172 (99%)	1132 (97%)	26 (2%)	7 (1%)	21	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	271	PRO
1	C	271	PRO
1	D	271	PRO
1	B	138	ILE

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Mol	Chain	Res	Type
1	D	110	TYR
1	A	110	TYR
1	C	138	ILE

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	243/242 (100%)	241 (99%)	2 (1%)	73	68
1	B	242/242 (100%)	236 (98%)	6 (2%)	42	26
1	C	242/242 (100%)	236 (98%)	6 (2%)	42	26
1	D	242/242 (100%)	239 (99%)	3 (1%)	63	53
All	All	969/968 (100%)	952 (98%)	17 (2%)	51	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	A	224	LYS
1	B	1	MET
1	B	137	SER
1	B	146	MET
1	B	177	LYS
1	B	189	PHE
1	B	224	LYS
1	C	47	SER
1	C	146	MET
1	C	159	LYS
1	C	173	LEU
1	C	189	PHE
1	C	274	SER
1	D	1	MET
1	D	194	LEU
1	D	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	120	HIS
1	A	248	ASN
1	B	51	ASN
1	B	120	HIS
1	B	145	ASN
1	B	248	ASN
1	C	120	HIS
1	C	132	ASN
1	C	248	ASN
1	D	51	ASN
1	D	132	ASN
1	D	248	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.