Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:21 PM GMT

PDB ID	:	1F6P
Title	:	CRYSTAL STRUCTURE ANALYSIS OF N-ACETYLNEURAMINATE LYASE FROM HAEMOPHILUS INFLUENZAE: CRYSTAL FORM III
Authors	:	Barbosa, J.A.R.G.; Smith, B.J.; DeGori, R.; Lawrence, M.C.
Deposited on	:	2000-06-22
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

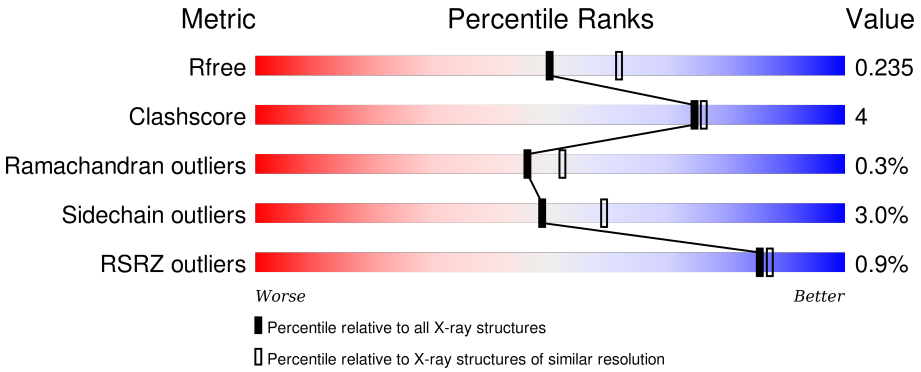
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 >=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 <=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	293	% 84% 15% •
1	B	293	% 78% 19% •
1	C	293	% 84% 14% •
1	D	293	% 81% 17% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9760 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-ACETYL NEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2290	1476	373	431	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	1	0
			2293	1477	373	433	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	SER	ASN	SEE REMARK 999	UNP P44539
A	229	LYS	ALA	SEE REMARK 999	UNP P44539
A	278	ALA	GLU	SEE REMARK 999	UNP P44539
A	281	VAL	LEU	SEE REMARK 999	UNP P44539
B	131	SER	ASN	SEE REMARK 999	UNP P44539
B	229	LYS	ALA	SEE REMARK 999	UNP P44539
B	278	ALA	GLU	SEE REMARK 999	UNP P44539
B	281	VAL	LEU	SEE REMARK 999	UNP P44539
C	131	SER	ASN	SEE REMARK 999	UNP P44539
C	229	LYS	ALA	SEE REMARK 999	UNP P44539
C	278	ALA	GLU	SEE REMARK 999	UNP P44539
C	281	VAL	LEU	SEE REMARK 999	UNP P44539
D	131	SER	ASN	SEE REMARK 999	UNP P44539
D	229	LYS	ALA	SEE REMARK 999	UNP P44539
D	278	ALA	GLU	SEE REMARK 999	UNP P44539
D	281	VAL	LEU	SEE REMARK 999	UNP P44539

- Molecule 2 is water.

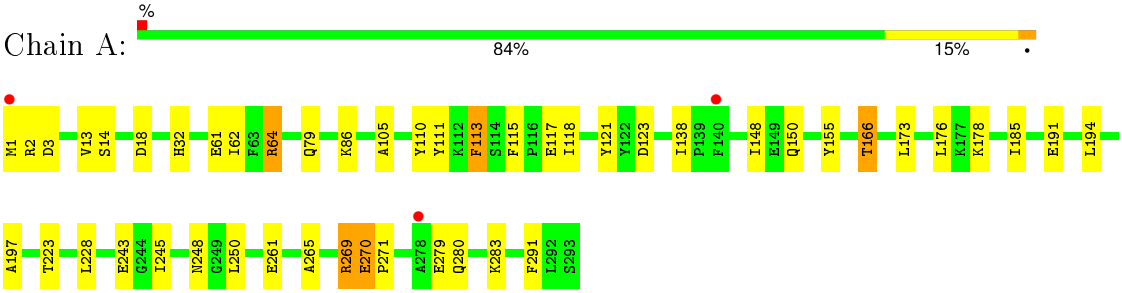
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	118	Total O 118 118	0	0
2	B	151	Total O 151 151	0	0
2	C	174	Total O 174 174	0	0
2	D	154	Total O 154 154	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

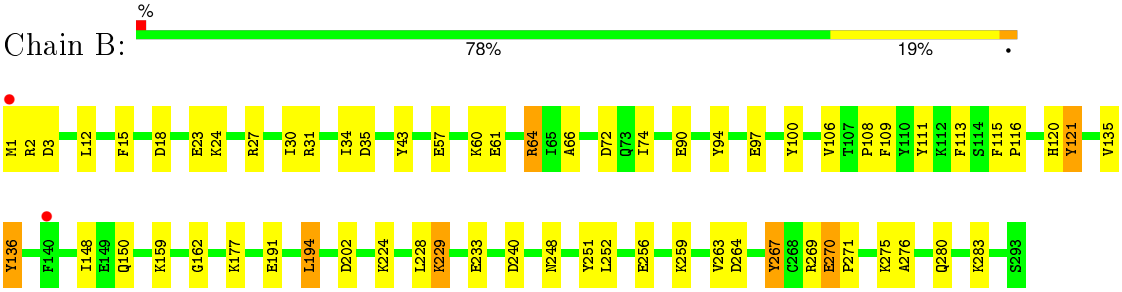
- Molecule 1: N-ACETYL NEURAMINATE LYASE

Chain A:



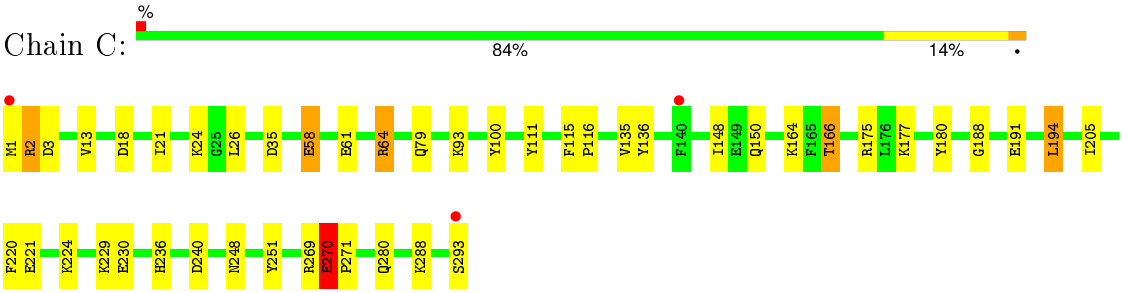
- Molecule 1: N-ACETYL NEURAMINATE LYASE

Chain B:



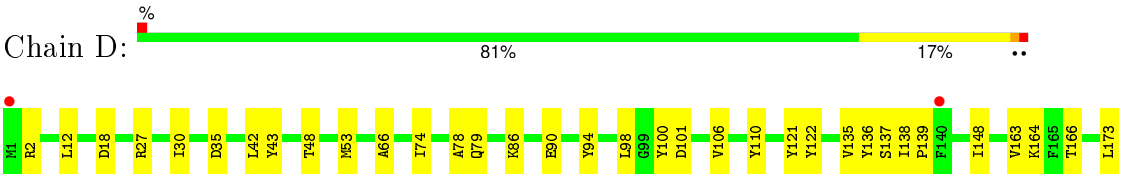
- Molecule 1: N-ACETYL NEURAMINATE LYASE

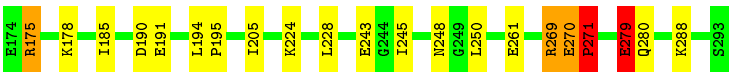
Chain C:



- Molecule 1: N-ACETYL NEURAMINATE LYASE

Chain D:




E174
R175
K178
I185
D190
E191
L194
P195
I205
K224
L228
E243
G244
I245
N248
G249
L250
E261
R269
E270
P271
E279
Q280
K288
S293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.10Å 116.81Å 129.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.25) 97.0 (19.90-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.26Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.261 0.173 , 0.235	Depositor DCC
R_{free} test set	2025 reflections (3.68%)	DCC
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 58180 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9760	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.94 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.8012e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.65	0/2330	1.60	21/3135 (0.7%)
1	B	0.69	0/2330	1.63	41/3135 (1.3%)
1	C	0.67	0/2330	1.50	21/3135 (0.7%)
1	D	0.67	0/2338	1.56	26/3146 (0.8%)
All	All	0.67	0/9328	1.57	109/12551 (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 (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ARG	CD-NE-CZ	25.49	159.28	123.60
1	B	27	ARG	NE-CZ-NH2	-16.65	111.97	120.30
1	B	64	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	D	269	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	A	291	PHE	CB-CG-CD1	-13.38	111.44	120.80
1	D	269	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	D	27	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	C	3	ASP	CB-CG-OD1	11.44	128.60	118.30
1	C	2	ARG	CD-NE-CZ	10.81	138.74	123.60
1	B	27	ARG	NE-CZ-NH1	10.56	125.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	27	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	269	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	B	271	PRO	N-CA-CB	9.93	115.22	103.30
1	D	101	ASP	CB-CG-OD2	9.79	127.11	118.30
1	A	291	PHE	CB-CG-CD2	9.47	127.43	120.80
1	B	31	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	D	191	GLU	OE1-CD-OE2	-9.37	112.06	123.30
1	B	64	ARG	CD-NE-CZ	9.33	136.67	123.60
1	C	271	PRO	N-CA-CB	9.30	114.45	103.30
1	C	269	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	B	31	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	191	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	C	270	GLU	CA-C-O	-8.47	102.30	120.10
1	B	270	GLU	CA-C-O	-8.40	102.45	120.10
1	D	175	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	B	251	TYR	CB-CG-CD2	-8.26	116.05	121.00
1	B	97	GLU	OE1-CD-OE2	-8.24	113.41	123.30
1	D	175	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	270	GLU	CA-C-O	-8.12	103.05	120.10
1	A	271	PRO	N-CA-CB	8.06	112.98	103.30
1	B	113	PHE	CB-CG-CD1	-8.04	115.17	120.80
1	D	137	SER	N-CA-CB	7.96	122.43	110.50
1	C	271	PRO	CA-N-CD	-7.76	100.64	111.50
1	D	271	PRO	N-CA-CB	7.75	112.59	103.30
1	A	113	PHE	CB-CG-CD1	-7.74	115.38	120.80
1	D	271	PRO	CA-N-CD	-7.72	100.69	111.50
1	D	270	GLU	CA-C-O	-7.69	103.95	120.10
1	C	111	TYR	CB-CG-CD1	-7.61	116.43	121.00
1	B	271	PRO	CA-N-CD	-7.51	100.99	111.50
1	D	2	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	C	240	ASP	CB-CG-OD1	7.43	124.99	118.30
1	C	35	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	3	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	191	GLU	OE1-CD-OE2	-7.18	114.69	123.30
1	B	264	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	3	ASP	CB-CG-OD1	7.15	124.73	118.30
1	B	269	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	43	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	D	137	SER	CB-CA-C	-6.91	96.96	110.10
1	A	271	PRO	CA-N-CD	-6.69	102.13	111.50
1	B	57	GLU	OE1-CD-OE2	6.68	131.31	123.30
1	B	72	ASP	CB-CG-OD1	6.66	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	PHE	CB-CG-CD1	-6.54	116.22	120.80
1	B	191	GLU	CG-CD-OE1	6.42	131.15	118.30
1	D	243	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	B	18	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	18	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	D	101	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	B	23	GLU	OE1-CD-OE2	-6.37	115.65	123.30
1	A	123	ASP	CB-CG-OD1	6.32	123.98	118.30
1	A	18	ASP	CB-CG-OD1	6.25	123.92	118.30
1	D	279	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	C	221	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	A	2	ARG	CD-NE-CZ	6.08	132.12	123.60
1	C	64	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	D	90	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	C	1	MET	CA-CB-CG	5.94	123.40	113.30
1	A	105	ALA	N-CA-CB	5.88	118.34	110.10
1	C	180	TYR	CB-CG-CD1	-5.81	117.52	121.00
1	D	43	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	A	18	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	D	269	ARG	CD-NE-CZ	5.74	131.64	123.60
1	B	267	TYR	CB-CG-CD1	5.73	124.44	121.00
1	B	90	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	113	PHE	CB-CG-CD2	5.69	124.78	120.80
1	B	2	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	35	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	240	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	43	TYR	CB-CG-CD1	5.56	124.34	121.00
1	A	2	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	109	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	155	TYR	CB-CG-CD1	5.53	124.32	121.00
1	A	64	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	C	18	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	243	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	B	121	TYR	CA-CB-CG	5.40	123.67	113.40
1	B	202	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	B	57	GLU	CG-CD-OE1	-5.33	107.64	118.30
1	D	2	ARG	NH1-CZ-NH2	5.28	125.20	119.40
1	D	191	GLU	CG-CD-OE1	5.26	128.83	118.30
1	C	100	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	C	191	GLU	CG-CD-OE1	5.24	128.79	118.30
1	C	175	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	D	224	LYS	CA-CB-CG	5.23	124.90	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	267	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	C	271	PRO	N-CD-CG	5.21	111.02	103.20
1	C	293	SER	CA-C-O	5.20	131.03	120.10
1	D	18	ASP	CA-C-N	5.19	126.58	116.20
1	B	111	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	191	GLU	CG-CD-OE1	5.17	128.64	118.30
1	C	58	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	B	100	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	B	150	GLN	CA-CB-CG	-5.11	102.16	113.40
1	D	122	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	B	251	TYR	CB-CG-CD1	5.04	124.03	121.00
1	B	35	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	135	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	B	269	ARG	CD-NE-CZ	5.01	130.61	123.60

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2290	0	2332	19	0
1	B	2290	0	2332	22	0
1	C	2290	0	2332	15	0
1	D	2293	0	2332	26	0
2	A	118	0	0	0	0
2	B	151	0	0	0	0
2	C	174	0	0	2	0
2	D	154	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9760	0	9328	74	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 (74) 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:248:ASN:HD21	1:C:280:GLN:HA	1.58	0.67
1:B:229:LYS:O	1:B:233:GLU:HG3	1.95	0.67
1:B:267:TYR:HE2	1:B:275:LYS:HE2	1.61	0.65
1:C:61:GLU:OE1	1:C:64:ARG:NH2	2.27	0.63
1:A:61:GLU:CD	1:A:64:ARG:HH21	2.03	0.62
1:A:113:PHE:CE1	1:D:271:PRO:HG2	2.35	0.61
1:B:248:ASN:HD21	1:B:280:GLN:HA	1.65	0.61
1:A:248:ASN:HD21	1:A:280:GLN:HA	1.66	0.60
1:B:115:PHE:HB3	1:B:116:PRO:HD3	1.84	0.59
1:D:53:MET:SD	1:D:271:PRO:HD2	2.41	0.59
1:A:13:VAL:HG21	1:A:62:ILE:HD13	1.84	0.59
1:D:248:ASN:HD21	1:D:280:GLN:HA	1.69	0.58
1:D:173:LEU:HD11	1:D:185:ILE:HG21	1.86	0.57
1:C:166:THR:HG23	1:C:188:GLY:HA3	1.88	0.56
1:B:34:ILE:HG12	1:B:74:ILE:HD13	1.88	0.55
1:B:228:LEU:HD11	1:D:228:LEU:HD21	1.90	0.54
1:A:248:ASN:HB2	1:A:283:LYS:HE2	1.89	0.54
1:B:228:LEU:HD21	1:D:228:LEU:HD11	1.91	0.53
1:D:261:GLU:OE2	1:D:288:LYS:HE2	2.10	0.51
1:D:279:GLU:CD	1:D:279:GLU:H	2.14	0.51
1:D:135:VAL:HG23	1:D:163:VAL:HG23	1.93	0.51
1:C:251:TYR:HD1	2:C:433:HOH:O	1.94	0.50
1:A:32:HIS:CE1	1:A:261:GLU:HG3	2.46	0.50
1:C:220:PHE:CZ	1:C:224:LYS:HD2	2.47	0.50
1:D:42:LEU:HG	1:D:74:ILE:CD1	2.42	0.49
1:B:30:ILE:HD13	1:B:66:ALA:HA	1.94	0.49
1:C:24:LYS:HD3	2:C:446:HOH:O	2.12	0.48
1:D:42:LEU:HG	1:D:74:ILE:HD12	1.96	0.48
1:B:106:VAL:HA	1:B:136:TYR:HB3	1.96	0.48
1:D:12:LEU:HG	1:D:48:THR:HG22	1.95	0.47
1:B:252:LEU:HD13	1:B:276:ALA:HA	1.96	0.47
1:B:248:ASN:HB2	1:B:283:LYS:HE2	1.98	0.46
1:B:252:LEU:O	1:B:256:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TYR:HB2	1:A:113:PHE:CE2	2.52	0.45
1:D:194:LEU:N	1:D:195:PRO:HD2	2.31	0.45
1:D:245:ILE:CG2	1:D:250:LEU:HD12	2.46	0.45
1:A:173:LEU:CD1	1:A:185:ILE:HD13	2.46	0.45
1:A:115:PHE:CE1	1:A:150:GLN:HB3	2.52	0.45
1:D:106:VAL:HA	1:D:136:TYR:HB3	1.98	0.45
1:A:14:SER:HA	1:A:265:ALA:O	2.17	0.45
1:D:94:TYR:CE2	1:D:98:LEU:HD11	2.53	0.44
1:B:194:LEU:C	1:B:194:LEU:HD12	2.38	0.44
1:C:194:LEU:HD12	1:C:194:LEU:C	2.37	0.44
1:D:138:ILE:N	1:D:139:PRO:HD3	2.33	0.44
1:B:224:LYS:HD2	1:B:224:LYS:HA	1.87	0.43
1:C:21:ILE:HD11	1:C:58:GLU:HB3	2.01	0.43
1:B:61:GLU:OE1	1:B:64:ARG:NH2	2.44	0.43
1:A:269:ARG:NH2	1:D:86:LYS:HD2	2.34	0.43
1:B:259:LYS:HA	1:B:263:VAL:O	2.18	0.43
1:A:197:ALA:HB3	1:A:223:THR:HG21	1.99	0.43
1:D:175:ARG:NH2	1:D:178:LYS:HG2	2.33	0.42
1:B:120:HIS:HE1	1:C:270:GLU:OE1	2.01	0.42
1:A:245:ILE:CG2	1:A:250:LEU:HD12	2.50	0.42
1:A:86:LYS:HD2	1:D:269:ARG:NH2	2.34	0.42
1:D:135:VAL:CG2	1:D:163:VAL:HB	2.50	0.42
1:D:30:ILE:HD13	1:D:66:ALA:HA	2.01	0.42
1:A:118:ILE:O	1:A:121:TYR:HB3	2.20	0.42
1:C:115:PHE:N	1:C:116:PRO:CD	2.84	0.41
1:B:108:PRO:HD3	1:B:121:TYR:CE1	2.55	0.41
1:B:135:VAL:HG22	1:B:162:GLY:O	2.20	0.41
1:A:138:ILE:HD12	1:A:166:THR:HG21	2.03	0.41
1:D:78:ALA:HB2	1:D:100:TYR:CD2	2.55	0.41
1:A:178:LYS:HB2	1:C:236:HIS:ND1	2.36	0.41
1:A:148:ILE:HD11	1:A:176:LEU:N	2.36	0.41
1:B:148:ILE:HA	1:B:148:ILE:HD13	1.92	0.41
1:C:164:LYS:HE3	1:C:205:ILE:CG2	2.51	0.40
1:C:13:VAL:HA	1:C:26:LEU:HD13	2.02	0.40
1:D:148:ILE:HD12	1:D:148:ILE:HG23	1.77	0.40
1:B:60:LYS:HB3	1:B:94:TYR:CE2	2.56	0.40
1:A:117:GLU:HB3	1:D:271:PRO:O	2.21	0.40
1:C:115:PHE:CG	1:C:150:GLN:NE2	2.90	0.40
1:B:115:PHE:N	1:B:116:PRO:CD	2.85	0.40
1:D:164:LYS:HG3	1:D:205:ILE:HD12	2.03	0.40
1:C:148:ILE:HD13	1:C:148:ILE:HA	1.94	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	291/293 (99%)	283 (97%)	7 (2%)	1 (0%)	46 52
1	B	291/293 (99%)	283 (97%)	8 (3%)	0	100 100
1	C	291/293 (99%)	284 (98%)	7 (2%)	0	100 100
1	D	292/293 (100%)	287 (98%)	3 (1%)	2 (1%)	26 26
All	All	1165/1172 (99%)	1137 (98%)	25 (2%)	3 (0%)	46 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	D	110	TYR
1	D	271	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	242/242 (100%)	236 (98%)	6 (2%)	55 66
1	B	242/242 (100%)	234 (97%)	8 (3%)	45 56
1	C	242/242 (100%)	232 (96%)	10 (4%)	37 44
1	D	243/242 (100%)	238 (98%)	5 (2%)	61 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	969/968 (100%)	940 (97%)	29 (3%)	48 59

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	79	GLN
1	A	166	THR
1	A	194	LEU
1	A	228	LEU
1	A	279	GLU
1	B	1	MET
1	B	12	LEU
1	B	24	LYS
1	B	136	TYR
1	B	159	LYS
1	B	177	LYS
1	B	194	LEU
1	B	229	LYS
1	C	2	ARG
1	C	79	GLN
1	C	93	LYS
1	C	136	TYR
1	C	166	THR
1	C	177	LYS
1	C	194	LEU
1	C	229	LYS
1	C	230	GLU
1	C	288	LYS
1	D	79	GLN
1	D	121	TYR
1	D	166	THR
1	D	190	ASP
1	D	279	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	ASN
1	B	51	ASN
1	B	120	HIS

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Mol	Chain	Res	Type
1	B	248	ASN
1	C	51	ASN
1	C	150	GLN
1	C	248	ASN
1	D	120	HIS
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 carbohydrates 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

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^{th} 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	293/293 (100%)	-0.39	3 (1%)	84	85	13, 23, 36, 59	0
1	B	293/293 (100%)	-0.45	2 (0%)	89	90	11, 19, 34, 59	0
1	C	293/293 (100%)	-0.51	3 (1%)	84	85	12, 20, 34, 62	0
1	D	293/293 (100%)	-0.51	2 (0%)	89	90	12, 20, 32, 48	0
All	All	1172/1172 (100%)	-0.47	10 (0%)	85	87	11, 20, 35, 62	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.4
1	C	1	MET	6.4
1	B	1	MET	5.0
1	B	140	PHE	4.2
1	C	140	PHE	3.9
1	A	140	PHE	3.5
1	D	140	PHE	3.4
1	A	278	ALA	2.2
1	D	1	MET	2.1
1	C	293	SER	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.