



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:20 am GMT

PDB ID : 2EFX
Title : The crystal structure of D-amino acid amidase from Ochrobactrum anthropi SV3 complexed with L-phenylalanine amide
Authors : Okazaki, S.; Suzuki, A.; Mizushima, T.; Komeda, H.; Asano, Y.; Yamane, T.
Deposited on : 2007-02-26
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

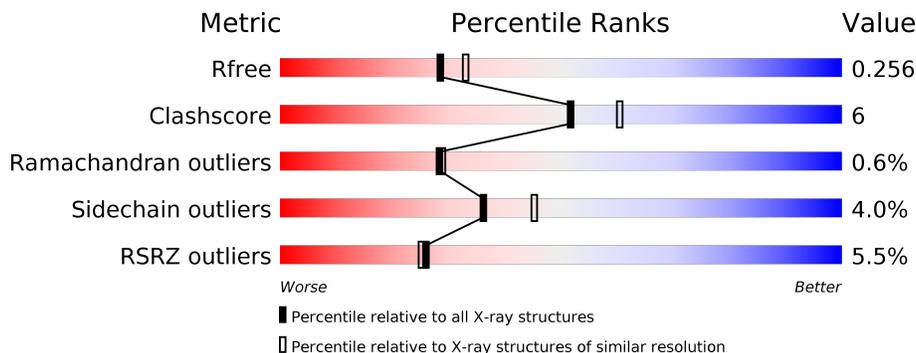
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	363	<p>88% 9% .</p>
1	B	363	<p>87% 12% .</p>
1	C	363	<p>85% 12% ..</p>
1	D	363	<p>85% 11% . .</p>
1	E	363	<p>82% 11% . 5%</p>
1	F	363	<p>21% 59% 22% . 18%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17426 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.

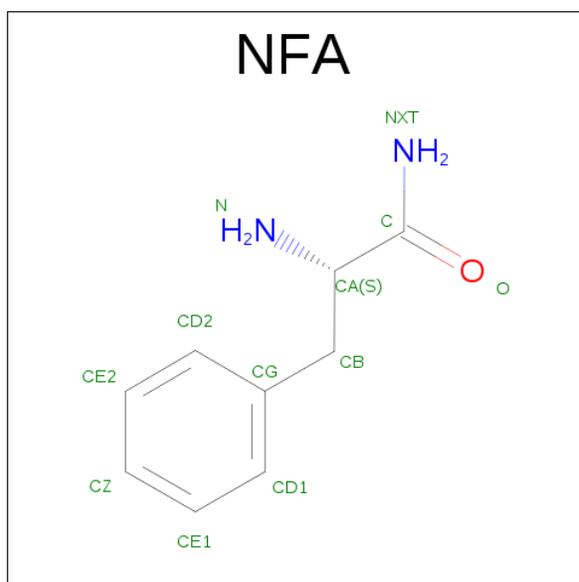
- Molecule 1 is a protein called D-amino acid amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2829	1785	490	538	16	0	2	0
1	B	362	2811	1775	486	534	16	0	0	0
1	C	358	2787	1762	482	527	16	0	0	0
1	D	350	2727	1725	472	514	16	0	1	0
1	E	345	2685	1699	466	504	16	0	0	0
1	F	296	2305	1461	401	430	13	0	2	0

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	4	Total 4	Ba 4	0	0
2	E	3	Total 3	Ba 3	0	0
2	B	4	Total 4	Ba 4	0	0
2	C	4	Total 4	Ba 4	0	0
2	A	4	Total 4	Ba 4	0	0
2	F	3	Total 3	Ba 3	0	0

- Molecule 3 is PHENYLALANINE AMIDE (three-letter code: NFA) (formula: C₉H₁₂N₂O).



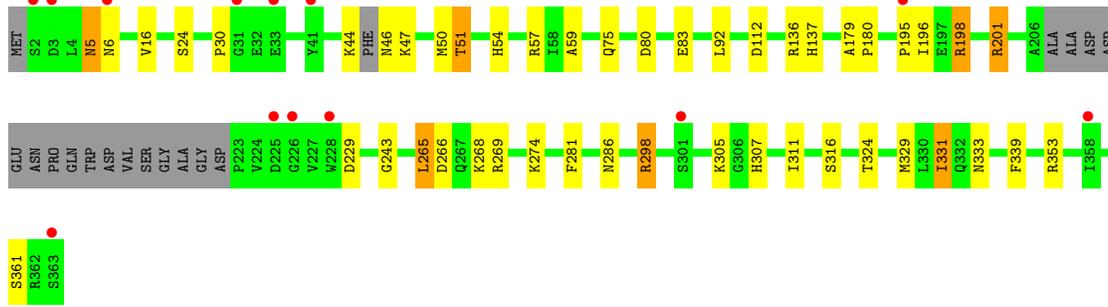
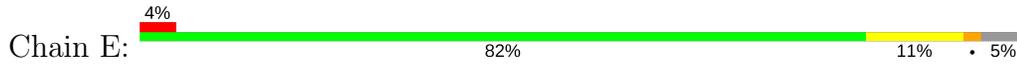
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	2	1		
3	B	1	Total	C	N	O	0	0
			12	9	2	1		
3	C	1	Total	C	N	O	0	0
			12	9	2	1		
3	D	1	Total	C	N	O	0	0
			12	9	2	1		
3	E	1	Total	C	N	O	0	0
			12	9	2	1		
3	F	1	Total	C	N	O	0	0
			12	9	2	1		

- Molecule 4 is water.

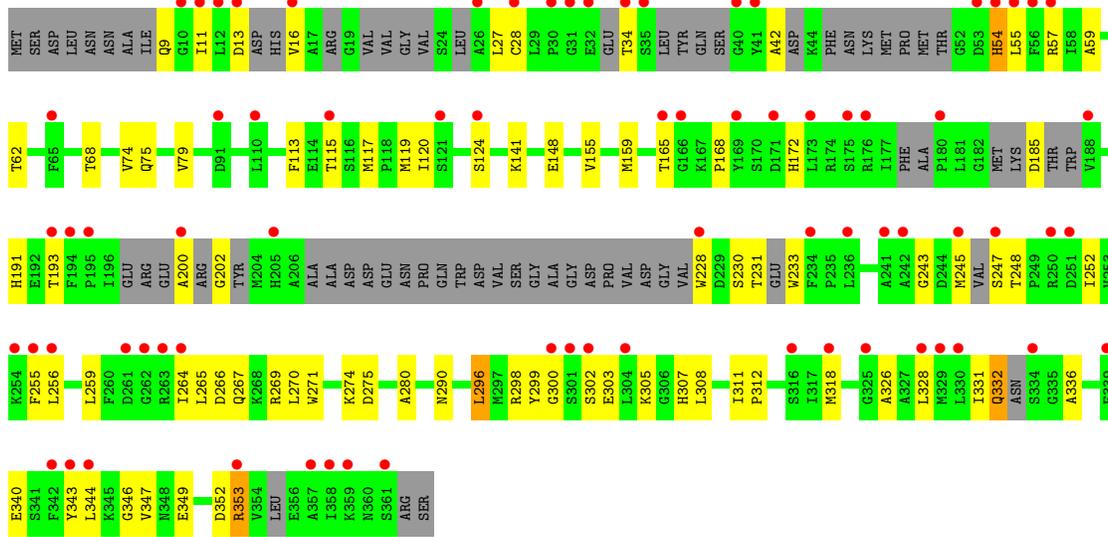
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	247	Total	O	0	0
			247	247		
4	C	252	Total	O	0	0
			252	252		
4	D	224	Total	O	0	0
			224	224		
4	E	141	Total	O	0	0
			141	141		
4	F	101	Total	O	0	0
			101	101		



● Molecule 1: D-amino acid amidase



● Molecule 1: D-amino acid amidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.71Å 123.40Å 115.48Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	19.82 – 2.20 19.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.82-2.20) 98.1 (19.82-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.21Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.256 0.187 , 0.256	Depositor DCC
R_{free} test set	5162 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	23.5	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17426	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: BA, NFA

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	0.54	0/2902	0.66	0/3936
1	B	0.58	0/2883	0.70	1/3910 (0.0%)
1	C	0.60	0/2858	0.66	1/3874 (0.0%)
1	D	0.60	0/2795	0.67	1/3786 (0.0%)
1	E	0.52	0/2751	0.63	0/3724
1	F	0.51	0/2346	0.61	0/3146
All	All	0.56	0/16535	0.66	3/22376 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	GLY	N-CA-C	-6.05	97.98	113.10
1	D	80	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	269	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	225	ASP	Peptide
1	D	283	PRO	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	2829	0	2719	31	0
1	B	2811	0	2711	34	0
1	C	2787	0	2691	32	0
1	D	2727	0	2643	28	0
1	E	2685	0	2613	30	0
1	F	2305	0	2226	52	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
3	E	12	0	12	0	0
3	F	12	0	12	1	0
4	A	223	0	0	0	0
4	B	247	0	0	6	0
4	C	252	0	0	2	0
4	D	224	0	0	4	0
4	E	141	0	0	2	0
4	F	101	0	0	5	0
All	All	17426	0	15675	202	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 6.

The worst 5 of 202 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:F:68:THR:HG23	1:F:265:LEU:HD11	1.30	1.13
1:D:282:PHE:O	1:D:285:SER:HB3	1.63	0.98
1:E:51:THR:H	1:E:54:HIS:HD2	1.16	0.89
1:A:51:THR:H	1:A:54:HIS:HD2	1.19	0.87
1:B:51:THR:H	1:B:54:HIS:HD2	1.20	0.86

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	362/363 (100%)	350 (97%)	11 (3%)	1 (0%)	44 49
1	B	360/363 (99%)	338 (94%)	19 (5%)	3 (1%)	22 21
1	C	354/363 (98%)	343 (97%)	10 (3%)	1 (0%)	44 49
1	D	347/363 (96%)	334 (96%)	11 (3%)	2 (1%)	28 29
1	E	339/363 (93%)	327 (96%)	11 (3%)	1 (0%)	44 49
1	F	264/363 (73%)	243 (92%)	17 (6%)	4 (2%)	12 9
All	All	2026/2178 (93%)	1935 (96%)	79 (4%)	12 (1%)	28 29

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	300	GLY
1	B	224	VAL
1	D	285	SER
1	F	243	GLY
1	E	243	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	302/301 (100%)	288 (95%)	14 (5%)	31	39
1	B	300/301 (100%)	292 (97%)	8 (3%)	50	62
1	C	298/301 (99%)	286 (96%)	12 (4%)	36	45
1	D	291/301 (97%)	285 (98%)	6 (2%)	59	72
1	E	288/301 (96%)	273 (95%)	15 (5%)	27	32
1	F	245/301 (81%)	231 (94%)	14 (6%)	24	28
All	All	1724/1806 (96%)	1655 (96%)	69 (4%)	36	45

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	344	LEU
1	D	184	LYS
1	F	305	LYS
1	C	353	ARG
1	D	115	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	46	ASN
1	C	348	ASN
1	E	205	HIS
1	C	54	HIS
1	C	360	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 22 are monoatomic - leaving 6 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	NFA	A	2001	-	12,12,12	0.82	0	15,15,15	1.14	2 (13%)
3	NFA	B	2002	-	12,12,12	0.63	0	15,15,15	0.96	1 (6%)
3	NFA	C	2003	-	12,12,12	0.68	0	15,15,15	1.28	2 (13%)
3	NFA	D	2004	-	12,12,12	0.55	0	15,15,15	1.18	2 (13%)
3	NFA	E	2005	-	12,12,12	0.67	0	15,15,15	0.79	0
3	NFA	F	2006	-	12,12,12	0.68	0	15,15,15	0.60	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
3	NFA	A	2001	-	-	0/7/8/8	0/1/1/1
3	NFA	B	2002	-	-	0/7/8/8	0/1/1/1
3	NFA	C	2003	-	-	0/7/8/8	0/1/1/1
3	NFA	D	2004	-	-	0/7/8/8	0/1/1/1
3	NFA	E	2005	-	-	0/7/8/8	0/1/1/1
3	NFA	F	2006	-	-	0/7/8/8	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	2001	NFA	CG-CB-CA	-3.12	107.84	114.33
3	D	2004	NFA	CG-CB-CA	-2.23	109.69	114.33
3	B	2002	NFA	CG-CB-CA	-2.21	109.74	114.33
3	C	2003	NFA	CG-CB-CA	-2.21	109.74	114.33
3	A	2001	NFA	CB-CA-C	2.22	112.84	108.57

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
3	F	2006	NFA	1	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, 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	362/363 (99%)	-0.29	3 (0%) 86 85	13, 23, 36, 50	0
1	B	362/363 (99%)	-0.21	14 (3%) 40 38	12, 20, 42, 59	0
1	C	358/363 (98%)	-0.34	5 (1%) 75 73	10, 19, 38, 55	0
1	D	350/363 (96%)	-0.41	4 (1%) 80 79	10, 19, 35, 51	0
1	E	345/363 (95%)	0.10	13 (3%) 41 39	13, 30, 48, 61	0
1	F	296/363 (81%)	1.20	75 (25%) 1 1	18, 50, 70, 79	0
All	All	2073/2178 (95%)	-0.03	114 (5%) 26 25	10, 24, 56, 79	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	SER	6.9
1	F	342	PHE	6.2
1	F	11	ILE	5.8
1	F	55	LEU	5.6
1	B	363	SER	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q < 0.9
3	NFA	E	2005	12/12	0.86	0.18	1.47	32,34,37,37	0
3	NFA	C	2003	12/12	0.92	0.13	1.37	21,24,25,25	0
3	NFA	B	2002	12/12	0.94	0.12	0.88	30,31,32,32	0
3	NFA	D	2004	12/12	0.92	0.14	0.68	20,22,23,23	0
3	NFA	A	2001	12/12	0.94	0.12	0.62	27,28,28,30	0
3	NFA	F	2006	12/12	0.81	0.21	0.29	57,57,57,57	0
2	BA	A	3003	1/1	0.99	0.08	-0.80	19,19,19,19	1
2	BA	E	3011	1/1	0.86	0.10	-1.10	44,44,44,44	1
2	BA	C	3001	1/1	1.00	0.05	-2.56	20,20,20,20	1
2	BA	C	3012	1/1	0.97	0.04	-	35,35,35,35	1
2	BA	D	3020	1/1	0.73	0.19	-	65,65,65,65	1
2	BA	F	3022	1/1	0.94	0.09	-	45,45,45,45	1
2	BA	C	3005	1/1	1.00	0.03	-	36,36,36,36	1
2	BA	A	3017	1/1	0.84	0.16	-	69,69,69,69	1
2	BA	F	3018	1/1	0.99	0.04	-	40,40,40,40	1
2	BA	E	3019	1/1	0.83	0.11	-	64,64,64,64	1
2	BA	B	3002	1/1	0.99	0.05	-	31,31,31,31	1
2	BA	C	3010	1/1	0.94	0.15	-	48,48,48,48	1
2	BA	D	3015	1/1	0.98	0.06	-	54,54,54,54	1
2	BA	B	3007	1/1	0.90	0.08	-	64,64,64,64	1
2	BA	D	3013	1/1	0.92	0.11	-	36,36,36,36	1
2	BA	E	3014	1/1	0.82	0.13	-	65,65,65,65	1
2	BA	D	3016	1/1	0.86	0.14	-	64,64,64,64	1
2	BA	F	3006	1/1	0.94	0.11	-	51,51,51,51	1
2	BA	A	3004	1/1	0.96	0.12	-	42,42,42,42	1
2	BA	A	3008	1/1	0.95	0.15	-	32,32,32,32	1
2	BA	B	3009	1/1	0.93	0.08	-	37,37,37,37	1
2	BA	B	3021	1/1	0.87	0.14	-	65,65,65,65	1

6.5 Other polymers [i](#)

There are no such residues in this entry.