



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:24 PM UTC

PDB ID : 2EFU / pdb_00002efu
Title : The crystal structure of D-amino acid amidase from Ochrobactrum anthropi SV3 complexed with L-phenylalanine
Authors : Okazaki, S.; Suzuki, A.; Mizushima, T.; Komeda, H.; Asano, Y.; Yamane, T.
Deposited on : 2007-02-26
Resolution : 2.30 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)
Xtrriage (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

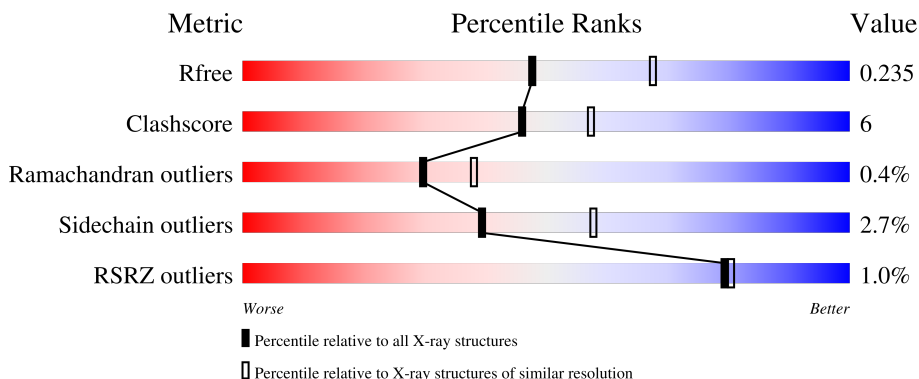
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



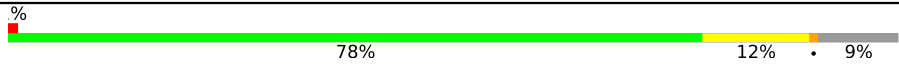
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	363	 87% 12% .
1	B	363	 2% 87% 10% ...
1	C	363	 87% 11% ..
1	D	363	 1% 83% 12% . .
1	E	363	 2% 83% 10% . 6%

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Mol	Chain	Length	Quality of chain
1	F	363	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a green segment representing 78%, a yellow segment representing 12%, and a grey segment representing 9%. A small red square is at the beginning of the bar, and a small black dot is at the end of the grey segment.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17915 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.

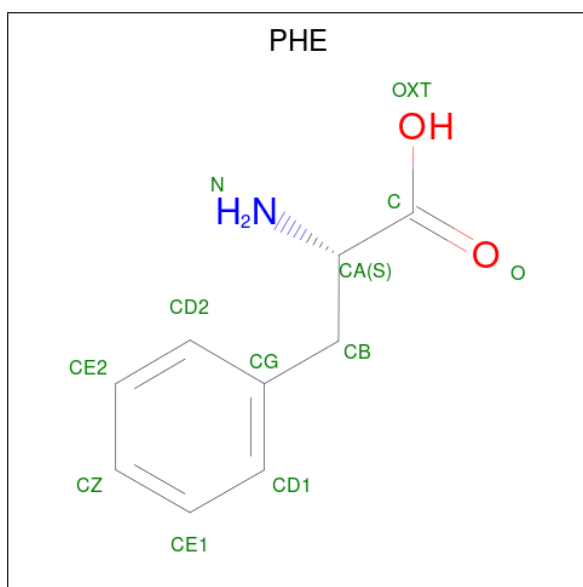
- Molecule 1 is a protein called D-Amino acid amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2819	1780	487	535	17	0	1	0
1	B	359	2806	1774	484	531	17	0	2	0
1	C	361	2805	1772	485	532	16	0	0	0
1	D	350	2726	1725	474	511	16	0	1	0
1	E	342	2665	1688	462	499	16	0	0	0
1	F	330	2589	1644	447	482	16	0	2	0

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Ba 4	0	0
2	B	2	Total 2	Ba 2	0	0
2	C	4	Total 4	Ba 4	0	0
2	D	5	Total 6	Ba 6	0	1
2	E	4	Total 4	Ba 4	0	0
2	F	6	Total 6	Ba 6	0	0

- Molecule 3 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



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

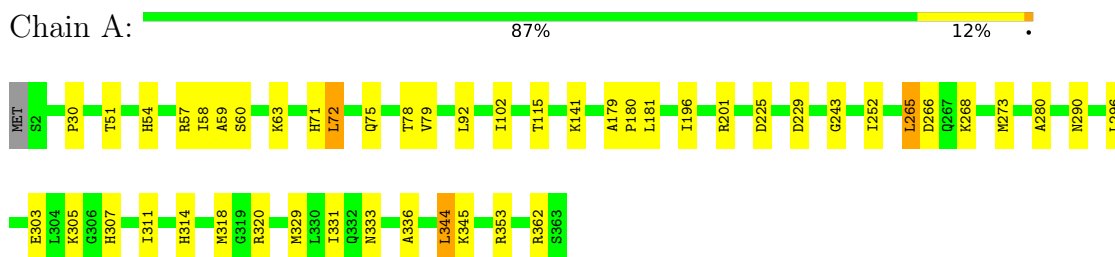
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	223	223	223	0	0
4	B	304	304	304	0	0
4	C	248	248	248	0	0
4	D	255	255	255	0	0
4	E	198	198	198	0	0
4	F	179	179	179	0	0

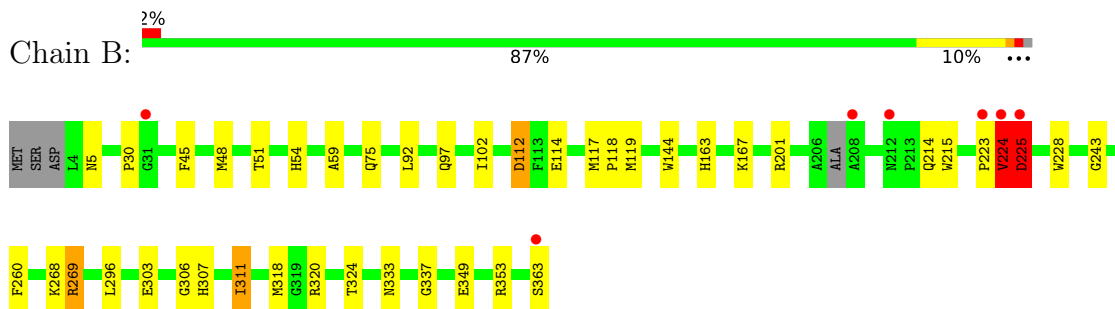
3 Residue-property plots

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 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.

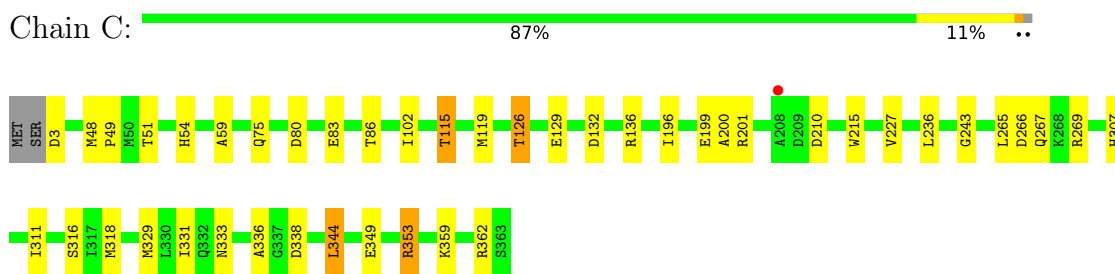
- Molecule 1: D-Amino acid amidase



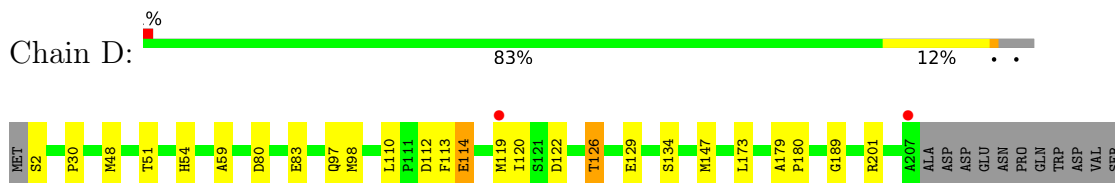
- Molecule 1: D-Amino acid amidase

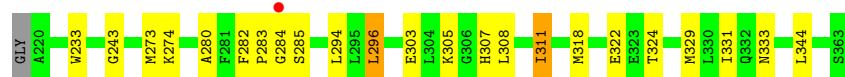


- Molecule 1: D-Amino acid amidase

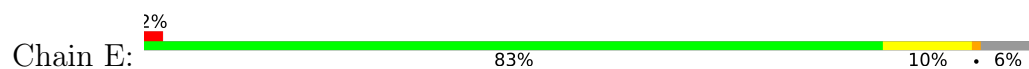


- Molecule 1: D-Amino acid amidase

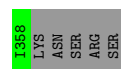
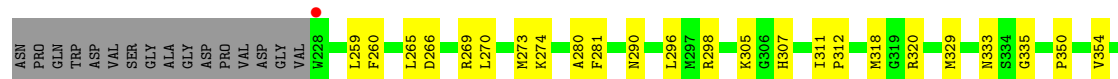
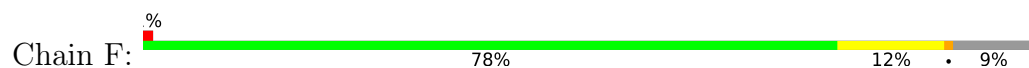




- Molecule 1: D-Amino acid amidase



- 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	77.47Å 123.27Å 116.16Å 90.00° 104.05° 90.00°	Depositor
Resolution (Å)	47.67 – 2.30 47.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.30) 100.0 (47.67-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.170 , 0.235 0.170 , 0.235	Depositor DCC
R_{free} test set	4735 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.0	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	0.95	EDS
Total number of atoms	17915	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
BA

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	0.60	0/2891	0.82	0/3921
1	B	0.66	0/2880	0.89	3/3904 (0.1%)
1	C	0.62	0/2877	0.84	0/3902
1	D	0.64	0/2797	0.85	3/3788 (0.1%)
1	E	0.58	0/2731	0.81	0/3697
1	F	0.63	0/2660	0.92	2/3602 (0.1%)
All	All	0.62	0/16836	0.86	8/22814 (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	2
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	114	GLU	N-CA-C	-17.98	90.78	113.43
1	B	311	ILE	N-CA-C	-8.05	102.59	109.19
1	D	311	ILE	N-CA-C	-7.35	103.17	109.19
1	D	311	ILE	CB-CA-C	5.89	115.10	109.33
1	D	189	GLY	N-CA-C	5.36	120.26	113.24
1	B	311	ILE	CB-CA-C	5.26	114.49	109.33
1	B	225	ASP	N-CA-C	5.21	121.89	110.80
1	F	113	PHE	N-CA-CB	5.05	117.63	110.16

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	224	VAL	Peptide
1	B	225	ASP	Peptide
1	F	113	PHE	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	2819	0	2719	31	0
1	B	2806	0	2711	26	0
1	C	2805	0	2706	27	0
1	D	2726	0	2651	35	0
1	E	2665	0	2587	32	0
1	F	2589	0	2522	43	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	1	0
2	D	6	0	0	0	0
2	E	4	0	0	0	0
2	F	6	0	0	0	0
3	A	12	0	8	1	0
3	B	12	0	8	0	0
3	C	12	0	8	0	0
3	D	12	0	8	0	0
3	E	12	0	8	0	0
3	F	12	0	8	0	0
4	A	223	0	0	4	0
4	B	304	0	0	7	0
4	C	248	0	0	4	0
4	D	255	0	0	2	0
4	E	198	0	0	1	0
4	F	179	0	0	4	0
All	All	17915	0	15944	186	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.

All (186) 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)
2:C:3001:BA:BA	4:C:3068:HOH:O	1.25	1.27
1:A:353:ARG:NH1	4:A:3239:HOH:O	1.92	1.02
1:F:265:LEU:CD1	1:F:273:MET:CE	2.38	1.02
1:F:265:LEU:HD12	1:F:273:MET:CE	1.92	0.99
1:A:51:THR:H	1:A:54:HIS:HD2	1.05	0.97
1:A:71:HIS:HD2	1:A:273:MET:HE3	1.31	0.93
1:F:204:MET:HA	1:F:205:HIS:HB2	1.52	0.92
1:A:353:ARG:HG2	4:A:3240:HOH:O	1.72	0.89
1:A:51:THR:H	1:A:54:HIS:CD2	1.92	0.86
1:E:51:THR:H	1:E:54:HIS:HD2	1.21	0.86
1:F:265:LEU:CD1	1:F:273:MET:HE2	2.06	0.85
1:C:51:THR:H	1:C:54:HIS:HD2	1.23	0.84
1:D:284:GLY:HA2	1:E:267:GLN:OE1	1.78	0.83
1:B:51:THR:H	1:B:54:HIS:HD2	1.25	0.83
1:F:51:THR:H	1:F:54:HIS:HD2	1.25	0.81
1:F:265:LEU:HD11	1:F:273:MET:CE	2.09	0.81
1:D:51:THR:H	1:D:54:HIS:HD2	1.28	0.80
1:C:126:THR:HG22	1:C:129:GLU:H	1.46	0.80
1:F:265:LEU:HD11	1:F:273:MET:HE2	1.64	0.79
1:A:71:HIS:CD2	1:A:273:MET:HE3	2.17	0.79
1:A:141:LYS:HE2	4:A:3105:HOH:O	1.84	0.77
1:E:75:GLN:NE2	1:E:266:ASP:H	1.83	0.76
1:C:210:ASP:HA	1:C:338:ASP:HB2	1.70	0.73
1:A:72:LEU:HD13	1:A:265:LEU:HD12	1.71	0.72
1:E:171:ASP:HB3	4:E:3125:HOH:O	1.88	0.71
1:E:75:GLN:HE22	1:E:265:LEU:HA	1.55	0.70
1:D:284:GLY:CA	1:E:267:GLN:OE1	2.39	0.70
1:C:267:GLN:HE22	1:E:284:GLY:H	1.37	0.70
1:F:265:LEU:CD1	1:F:273:MET:HE1	2.20	0.69
1:C:75:GLN:HE22	1:C:265:LEU:HA	1.58	0.69
1:F:265:LEU:HD12	1:F:273:MET:HE3	1.74	0.69
1:A:225:ASP:OD1	1:D:2:SER:N	2.27	0.68
1:B:51:THR:H	1:B:54:HIS:CD2	2.10	0.68
1:D:296:LEU:CD2	1:D:305:LYS:HD3	2.24	0.68
1:E:195:PRO:HB2	1:E:198:ARG:HG3	1.77	0.66
1:F:75:GLN:HE22	1:F:265:LEU:HA	1.61	0.65
1:E:75:GLN:HE22	1:E:266:ASP:H	1.44	0.65
1:B:167:LYS:HE3	4:B:3196:HOH:O	1.95	0.64
1:B:269:ARG:HD2	1:B:269:ARG:N	2.12	0.64
1:C:196:ILE:HG22	4:C:3114:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:HD2	1:A:273:MET:CE	2.08	0.63
1:D:296:LEU:HD22	1:D:305:LYS:HD3	1.80	0.63
1:A:57:ARG:H	1:A:314:HIS:HD2	1.46	0.62
1:D:51:THR:H	1:D:54:HIS:CD2	2.16	0.62
1:F:51:THR:H	1:F:54:HIS:CD2	2.12	0.62
1:B:214:GLN:HG2	1:B:337:GLY:O	2.00	0.62
1:F:270:LEU:O	1:F:274:LYS:HG2	2.00	0.61
1:C:336:ALA:H	1:C:344:LEU:HD13	1.67	0.60
1:E:51:THR:H	1:E:54:HIS:CD2	2.12	0.60
1:F:80:ASP:O	1:F:83:GLU:HG2	2.02	0.60
1:F:75:GLN:HG3	1:F:269:ARG:HD3	1.84	0.59
1:C:267:GLN:NE2	1:E:284:GLY:H	1.99	0.59
1:F:126:THR:HG21	4:F:3083:HOH:O	2.02	0.59
1:F:126:THR:HG22	1:F:129:GLU:H	1.68	0.59
1:C:75:GLN:NE2	1:C:266:ASP:H	2.02	0.58
1:A:75:GLN:NE2	1:A:266:ASP:H	2.01	0.58
1:C:51:THR:H	1:C:54:HIS:CD2	2.14	0.58
1:D:48:MET:HG3	4:D:3221:HOH:O	2.03	0.58
1:F:75:GLN:NE2	1:F:266:ASP:H	2.02	0.57
1:D:305:LYS:NZ	1:D:322:GLU:OE1	2.38	0.57
1:F:265:LEU:HD11	1:F:273:MET:HE1	1.85	0.57
1:A:75:GLN:HE22	1:A:266:ASP:H	1.52	0.57
1:F:265:LEU:HD12	1:F:273:MET:HE1	1.82	0.56
1:F:350:PRO:O	1:F:354:VAL:HG23	2.06	0.56
1:A:296:LEU:HD13	1:A:305:LYS:HE3	1.88	0.56
1:C:362:ARG:HD3	4:C:3234:HOH:O	2.04	0.56
1:F:205:HIS:HB2	1:F:335:GLY:O	2.06	0.56
1:B:201:ARG:O	1:B:333:ASN:HB2	2.07	0.54
1:B:5:ASN:HB3	4:B:3204:HOH:O	2.08	0.54
1:B:269:ARG:HD2	1:B:269:ARG:H	1.72	0.54
1:D:284:GLY:HA3	1:E:267:GLN:HE22	1.73	0.54
1:D:274:LYS:HD2	1:D:322:GLU:OE2	2.06	0.54
1:D:59:ALA:HB2	1:D:311:ILE:HB	1.90	0.53
1:F:296:LEU:HD13	1:F:305:LYS:HE3	1.91	0.53
1:F:320:ARG:HD3	4:F:3085:HOH:O	2.07	0.53
1:A:336:ALA:H	1:A:344:LEU:HD13	1.74	0.53
1:C:115:THR:HG22	4:C:3041:HOH:O	2.08	0.53
1:E:59:ALA:HB2	1:E:311:ILE:HB	1.91	0.53
1:E:201:ARG:O	1:E:333:ASN:HB2	2.08	0.52
1:B:163:HIS:HD2	4:B:3207:HOH:O	1.92	0.52
1:B:119:MET:HG3	1:B:215:TRP:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ASP:O	1:C:83:GLU:HG2	2.09	0.52
1:C:267:GLN:HE22	1:E:284:GLY:N	2.08	0.52
1:E:24:SER:HB2	1:E:50:MET:HE2	1.92	0.52
1:B:268:LYS:HE3	4:B:3162:HOH:O	2.08	0.52
1:C:269:ARG:N	1:C:269:ARG:HD2	2.25	0.51
1:F:75:GLN:CG	1:F:269:ARG:HD3	2.41	0.51
1:A:318:MET:HB3	1:A:329:MET:SD	2.51	0.51
1:C:132:ASP:O	1:C:136:ARG:HG2	2.11	0.50
1:F:269:ARG:N	1:F:269:ARG:HD2	2.26	0.50
1:B:48[A]:MET:HE2	4:B:3142:HOH:O	2.12	0.50
1:C:318:MET:HB3	1:C:329:MET:SD	2.51	0.50
1:D:273:MET:HE2	1:D:294:LEU:HG	1.93	0.50
1:D:201:ARG:O	1:D:333:ASN:HB2	2.12	0.49
1:A:329:MET:HE3	1:A:331:ILE:HD11	1.94	0.49
1:B:349:GLU:HB3	1:B:353:ARG:NH1	2.27	0.49
1:E:316:SER:HB3	1:E:331:ILE:HG23	1.95	0.49
1:B:353:ARG:NH1	4:B:3289:HOH:O	2.19	0.48
1:D:318:MET:HB3	1:D:329:MET:SD	2.53	0.48
1:F:48:MET:N	4:F:3197:HOH:O	2.45	0.48
1:F:205:HIS:CB	1:F:335:GLY:O	2.61	0.48
1:B:117:MET:HG3	1:B:118:PRO:HD2	1.95	0.48
1:B:45:PHE:CZ	1:B:224:VAL:HG12	2.49	0.48
1:D:126:THR:HG22	1:D:129:GLU:H	1.78	0.48
1:A:181:LEU:O	4:A:3142:HOH:O	2.20	0.48
1:F:75:GLN:HE22	1:F:265:LEU:CA	2.27	0.48
1:F:201:ARG:O	1:F:333:ASN:HB2	2.13	0.47
1:D:285:SER:CB	1:D:308:LEU:HD22	2.44	0.47
1:F:280:ALA:HB2	1:F:290:ASN:OD1	2.15	0.47
1:B:75:GLN:HB3	1:B:269:ARG:HD3	1.96	0.47
1:D:296:LEU:HD22	1:D:305:LYS:CD	2.43	0.47
1:D:112:ASP:OD2	1:D:114:GLU:HB3	2.15	0.47
1:D:285:SER:HB3	1:D:308:LEU:HD22	1.96	0.47
1:A:58:ILE:HD13	1:A:252:ILE:HD11	1.97	0.46
1:F:298:ARG:NH2	4:F:3178:HOH:O	2.47	0.46
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.97	0.46
1:E:80:ASP:O	1:E:83:GLU:HG2	2.16	0.46
1:F:260:PHE:CG	1:F:320:ARG:HD2	2.51	0.46
1:B:59:ALA:HB2	1:B:311:ILE:HB	1.97	0.46
1:E:75:GLN:HE22	1:E:266:ASP:N	2.13	0.46
1:F:172:HIS:CE1	1:F:176:ARG:HD3	2.51	0.46
1:C:59:ALA:HB2	1:C:311:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:PRO:HG2	1:D:324:THR:O	2.15	0.45
1:B:223:PRO:HD3	1:B:228:TRP:CZ2	2.51	0.45
1:A:59:ALA:HB2	1:A:311:ILE:HB	1.97	0.45
1:B:306:GLY:HA3	1:B:318:MET:O	2.16	0.45
1:B:112:ASP:OD2	1:B:114[B]:GLU:HB2	2.17	0.45
1:D:284:GLY:C	4:D:3069:HOH:O	2.60	0.45
1:A:201:ARG:O	1:A:333:ASN:HB2	2.17	0.45
1:C:199:GLU:HG2	1:C:200:ALA:O	2.17	0.45
1:F:147:MET:HE3	1:F:280:ALA:HB1	1.97	0.45
1:D:282:PHE:CE2	1:D:283:PRO:O	2.70	0.45
1:D:98:MET:HE1	1:D:110:LEU:HD21	1.99	0.45
1:A:72:LEU:HD13	1:A:265:LEU:CD1	2.44	0.44
1:E:59:ALA:O	1:E:243:GLY:HA2	2.17	0.44
1:F:318:MET:HB3	1:F:329:MET:SD	2.57	0.44
1:E:66:ILE:HG13	1:E:241:ALA:O	2.17	0.44
1:F:311:ILE:O	1:F:312:PRO:C	2.60	0.44
1:A:78:THR:HG23	1:A:79:VAL:HG23	1.98	0.44
1:D:282:PHE:CD2	1:D:283:PRO:O	2.71	0.44
1:E:20:VAL:HG13	1:E:334:SER:HB2	2.00	0.44
1:B:30:PRO:HG3	1:B:324:THR:O	2.17	0.43
1:B:260:PHE:CB	1:B:320:ARG:HD2	2.48	0.43
1:C:316:SER:HB3	1:C:331:ILE:HG23	2.00	0.43
1:D:113:PHE:HB3	1:D:134:SER:OG	2.18	0.43
1:F:29:LEU:HB3	1:F:30:PRO:HD2	2.00	0.43
1:C:201:ARG:O	1:C:333:ASN:HB2	2.19	0.43
1:B:296:LEU:HD23	1:B:303:GLU:OE1	2.19	0.43
1:E:271:TRP:CD1	1:E:275:ASP:HB2	2.53	0.43
1:E:179:ALA:HB3	1:E:180:PRO:HD3	2.01	0.43
1:F:259:LEU:HD11	1:F:273:MET:HE1	2.01	0.43
1:A:296:LEU:HD11	1:A:303:GLU:OE2	2.19	0.42
1:D:283:PRO:HA	1:D:284:GLY:HA2	1.86	0.42
1:C:48:MET:HA	1:C:49:PRO:HD2	1.88	0.42
1:F:204:MET:CA	1:F:205:HIS:HB2	2.36	0.42
1:B:320:ARG:HD3	4:B:3212:HOH:O	2.19	0.42
1:C:3:ASP:O	1:C:3:ASP:CG	2.62	0.42
1:C:75:GLN:HE22	1:C:266:ASP:H	1.68	0.42
1:D:120:ILE:HG13	1:D:233:TRP:CG	2.55	0.42
1:A:201:ARG:HD3	1:A:229:ASP:OD2	2.20	0.42
1:E:30:PRO:HG3	1:E:324:THR:O	2.20	0.42
1:F:59:ALA:HB2	1:F:311:ILE:HB	2.02	0.42
1:B:102:ILE:HD12	1:B:144:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:MET:HB3	1:E:329:MET:SD	2.60	0.41
1:D:344:LEU:HD12	1:D:344:LEU:HA	1.87	0.41
1:A:30:PRO:CG	1:A:362:ARG:HH21	2.33	0.41
1:D:147:MET:HE3	1:D:280:ALA:HB1	2.03	0.41
1:E:265:LEU:HG	1:E:269:ARG:HB3	2.03	0.41
1:C:349:GLU:O	1:C:353:ARG:HG2	2.20	0.41
1:F:51:THR:N	1:F:54:HIS:HD2	2.05	0.41
1:A:60:SER:O	1:A:63:LYS:HB2	2.20	0.41
1:E:5:ASN:HD22	1:E:5:ASN:H	1.67	0.41
1:A:60:SER:HB3	3:A:2001:PHE:C	2.46	0.41
1:D:329:MET:HE3	1:D:331:ILE:HD11	2.02	0.41
1:D:296:LEU:HD13	1:D:303:GLU:OE2	2.21	0.41
1:A:268:LYS:HD3	1:F:281:PHE:CD2	2.55	0.41
1:D:179:ALA:HB3	1:D:180:PRO:HD3	2.03	0.41
1:E:196:ILE:H	1:E:196:ILE:HG13	1.63	0.41
1:F:260:PHE:CB	1:F:320:ARG:HD2	2.50	0.40
1:D:80:ASP:O	1:D:83:GLU:HG2	2.21	0.40
1:A:280:ALA:HB2	1:A:290:ASN:OD1	2.20	0.40
1:E:5:ASN:HD22	1:E:5:ASN:N	2.18	0.40
1:E:2:SER:OG	1:E:5:ASN:ND2	2.55	0.40
1:C:119:MET:CG	1:C:215:TRP:HB3	2.52	0.40
1:C:359:LYS:HE2	1:C:359:LYS:HB3	1.89	0.40
1:D:284:GLY:HA3	1:E:267:GLN:NE2	2.35	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	361/363 (99%)	353 (98%)	7 (2%)	1 (0%)	36 46
1	B	357/363 (98%)	342 (96%)	12 (3%)	3 (1%)	16 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	359/363 (99%)	348 (97%)	10 (3%)	1 (0%)	36	46
1	D	347/363 (96%)	332 (96%)	14 (4%)	1 (0%)	36	46
1	E	336/363 (93%)	326 (97%)	8 (2%)	2 (1%)	21	27
1	F	326/363 (90%)	314 (96%)	12 (4%)	0	100	100
All	All	2086/2178 (96%)	2015 (97%)	63 (3%)	8 (0%)	30	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	VAL
1	C	243	GLY
1	A	243	GLY
1	B	225	ASP
1	B	243	GLY
1	D	243	GLY
1	E	243	GLY
1	E	312	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	301/301 (100%)	291 (97%)	10 (3%)	33	50
1	B	300/301 (100%)	293 (98%)	7 (2%)	44	63
1	C	299/301 (99%)	290 (97%)	9 (3%)	36	53
1	D	291/301 (97%)	283 (97%)	8 (3%)	39	58
1	E	285/301 (95%)	279 (98%)	6 (2%)	47	66
1	F	277/301 (92%)	269 (97%)	8 (3%)	37	55
All	All	1753/1806 (97%)	1705 (97%)	48 (3%)	39	58

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	92	LEU
1	A	102	ILE
1	A	115	THR
1	A	196	ILE
1	A	265	LEU
1	A	307	HIS
1	A	320	ARG
1	A	344	LEU
1	A	345	LYS
1	B	92	LEU
1	B	97	GLN
1	B	112	ASP
1	B	224	VAL
1	B	269	ARG
1	B	307	HIS
1	B	363	SER
1	C	86	THR
1	C	102	ILE
1	C	115	THR
1	C	126	THR
1	C	227	VAL
1	C	236	LEU
1	C	307	HIS
1	C	344	LEU
1	C	353	ARG
1	D	97	GLN
1	D	114	GLU
1	D	119	MET
1	D	122	ASP
1	D	126	THR
1	D	173	LEU
1	D	296	LEU
1	D	307	HIS
1	E	5	ASN
1	E	35	SER
1	E	196	ILE
1	E	265	LEU
1	E	307	HIS
1	E	353	ARG
1	F	6	ASN
1	F	23	VAL
1	F	78	THR

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Mol	Chain	Res	Type
1	F	114	GLU
1	F	124	SER
1	F	126	THR
1	F	184	LYS
1	F	307	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	ASN
1	A	46	ASN
1	A	54	HIS
1	A	71	HIS
1	A	75	GLN
1	A	205	HIS
1	A	267	GLN
1	A	314	HIS
1	B	5	ASN
1	B	46	ASN
1	B	54	HIS
1	B	163	HIS
1	B	267	GLN
1	B	360	ASN
1	C	6	ASN
1	C	54	HIS
1	C	75	GLN
1	C	128	GLN
1	C	137	HIS
1	C	191	HIS
1	C	267	GLN
1	C	360	ASN
1	D	54	HIS
1	D	97	GLN
1	D	191	HIS
1	D	348	ASN
1	D	360	ASN
1	E	5	ASN
1	E	46	ASN
1	E	54	HIS
1	E	75	GLN
1	E	137	HIS

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Mol	Chain	Res	Type
1	E	163	HIS
1	E	205	HIS
1	E	348	ASN
1	F	6	ASN
1	F	54	HIS
1	F	75	GLN
1	F	97	GLN
1	F	163	HIS
1	F	205	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 26 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	PHE	A	2001	-	11,12,12	0.90	0	11,15,15	0.89	1 (9%)
3	PHE	C	2003	-	11,12,12	0.85	0	11,15,15	0.74	1 (9%)
3	PHE	B	2002	-	11,12,12	0.80	1 (9%)	11,15,15	0.74	1 (9%)
3	PHE	F	2006	2	11,12,12	0.84	0	11,15,15	1.05	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PHE	E	2005	-	11,12,12	0.82	0	11,15,15	0.75	1 (9%)
3	PHE	D	2004	2	11,12,12	0.78	1 (9%)	11,15,15	0.83	1 (9%)

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	PHE	A	2001	-	-	0/8/8/8	0/1/1/1
3	PHE	C	2003	-	-	0/8/8/8	0/1/1/1
3	PHE	B	2002	-	-	1/8/8/8	0/1/1/1
3	PHE	F	2006	2	-	4/8/8/8	0/1/1/1
3	PHE	E	2005	-	-	0/8/8/8	0/1/1/1
3	PHE	D	2004	2	-	0/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	PHE	OXT-C	-2.05	1.24	1.30
3	D	2004	PHE	OXT-C	-2.01	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2006	PHE	OXT-C-O	-3.44	116.28	124.08
3	A	2001	PHE	OXT-C-O	-2.89	117.53	124.08
3	D	2004	PHE	OXT-C-O	-2.64	118.08	124.08
3	B	2002	PHE	OXT-C-O	-2.34	118.78	124.08
3	C	2003	PHE	OXT-C-O	-2.28	118.90	124.08
3	E	2005	PHE	OXT-C-O	-2.19	119.12	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2006	PHE	C-CA-CB-CG
3	F	2006	PHE	OXT-C-CA-N
3	F	2006	PHE	N-CA-CB-CG
3	F	2006	PHE	O-C-CA-N
3	B	2002	PHE	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	PHE	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

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	362/363 (99%)	-0.19	0 100 100	12, 27, 39, 54	1 (0%)
1	B	359/363 (98%)	-0.42	7 (1%) 66 68	9, 17, 44, 55	2 (0%)
1	C	361/363 (99%)	-0.31	1 (0%) 90 90	10, 22, 40, 46	0
1	D	350/363 (96%)	-0.43	3 (0%) 81 82	9, 19, 37, 52	1 (0%)
1	E	342/363 (94%)	-0.02	6 (1%) 67 69	12, 28, 49, 59	0
1	F	330/363 (90%)	0.09	4 (1%) 76 77	16, 30, 43, 54	2 (0%)
All	All	2104/2178 (96%)	-0.22	21 (0%) 79 80	9, 24, 44, 59	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6	ASN	2.9
1	F	48	MET	2.8
1	F	228	TRP	2.8
1	B	208	ALA	2.7
1	D	207	ALA	2.7
1	E	363	SER	2.6
1	E	339	PHE	2.6
1	B	363	SER	2.4
1	E	46	ASN	2.3
1	E	45	PHE	2.3
1	B	223	PRO	2.3
1	D	284	GLY	2.3
1	B	212	ASN	2.2
1	E	226	GLY	2.2
1	C	208	ALA	2.2
1	B	224	VAL	2.2
1	D	119	MET	2.2
1	B	31	GLY	2.1
1	E	48	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	225	ASP	2.1
1	F	31	GLY	2.1

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 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(Å ²)	Q<0.9
2	BA	E	3018	1/1	0.75	0.14	50,50,50,50	1
3	PHE	F	2006	12/12	0.77	0.16	40,42,42,42	0
3	PHE	E	2005	12/12	0.82	0.13	33,38,40,40	0
2	BA	A	3020	1/1	0.82	0.23	46,46,46,46	1
2	BA	A	3009	1/1	0.83	0.27	48,48,48,48	1
3	PHE	D	2004	12/12	0.83	0.13	37,40,43,43	0
2	BA	D	3014	1/1	0.85	0.41	45,45,45,45	1
2	BA	F	3021	1/1	0.87	0.22	42,42,42,42	1
2	BA	B	3010	1/1	0.87	0.34	49,49,49,49	1
3	PHE	C	2003	12/12	0.88	0.12	36,38,39,39	0
3	PHE	A	2001	12/12	0.89	0.10	31,33,33,33	0
3	PHE	B	2002	12/12	0.89	0.10	33,34,35,35	0
2	BA	D	3022	1/1	0.90	0.15	53,53,53,53	1
2	BA	D	3017	1/1	0.91	0.09	57,57,57,57	1
2	BA	E	3019	1/1	0.91	0.22	48,48,48,48	1
2	BA	A	3004	1/1	0.91	0.07	62,62,62,62	1
2	BA	E	3012	1/1	0.92	0.08	44,44,44,44	1
2	BA	F	3016	1/1	0.93	0.06	48,48,48,48	1
2	BA	C	3013	1/1	0.94	0.18	46,46,46,46	1
2	BA	F	3007	1/1	0.95	0.16	67,67,67,67	1
2	BA	C	3011	1/1	0.95	0.05	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BA	E	3024	1/1	0.95	0.05	44,44,44,44	1
2	BA	F	3008	1/1	0.96	0.14	24,24,24,24	1
2	BA	F	3006	1/1	0.97	0.04	30,30,30,30	1
2	BA	F	3025	1/1	0.98	0.03	36,36,36,36	1
2	BA	D	3023[A]	1/1	0.99	0.04	33,33,33,33	1
2	BA	D	3023[B]	1/1	0.99	0.04	39,39,39,39	1
2	BA	C	3005	1/1	0.99	0.04	22,22,22,22	1
2	BA	D	3015	1/1	0.99	0.07	52,52,52,52	1
2	BA	B	3002	1/1	0.99	0.03	32,32,32,32	1
2	BA	A	3003	1/1	0.99	0.05	21,21,21,21	1
2	BA	C	3001	1/1	1.00	0.01	27,27,27,27	1

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.