



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:02 PM UTC

PDB ID : 2EFX / pdb_00002efx
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 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)
Xtriage (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

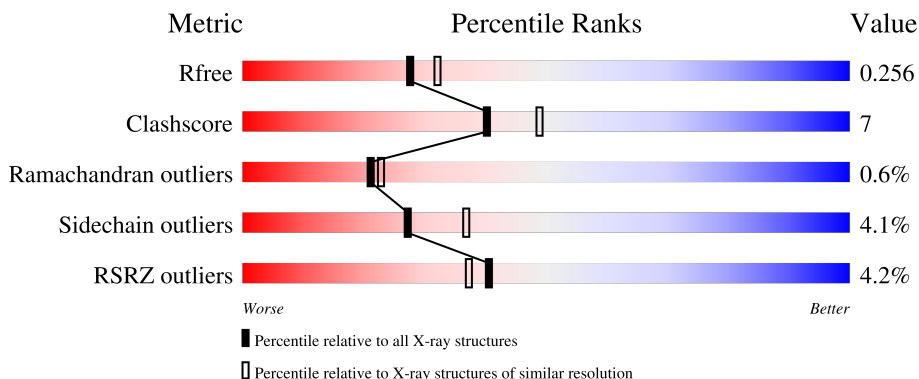
1 Overall quality at a glance i

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.



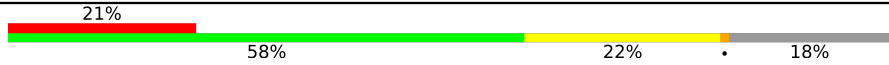
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 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	88% 10% .
1	B	363	% 85% 13% .
1	C	363	% 85% 13% ..
1	D	363	% 83% 13% . .
1	E	363	82% 11% . 5%

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Mol	Chain	Length	Quality of chain										
1	F	363	 <p>A horizontal bar chart showing the quality distribution of the chain. The bar is divided into four segments: red (21%), green (58%), yellow (22%), and grey (18%).</p> <table border="1"><thead><tr><th>Quality Category</th><th>Percentage</th></tr></thead><tbody><tr><td>Red</td><td>21%</td></tr><tr><td>Green</td><td>58%</td></tr><tr><td>Yellow</td><td>22%</td></tr><tr><td>Grey</td><td>18%</td></tr></tbody></table>	Quality Category	Percentage	Red	21%	Green	58%	Yellow	22%	Grey	18%
Quality Category	Percentage												
Red	21%												
Green	58%												
Yellow	22%												
Grey	18%												

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.

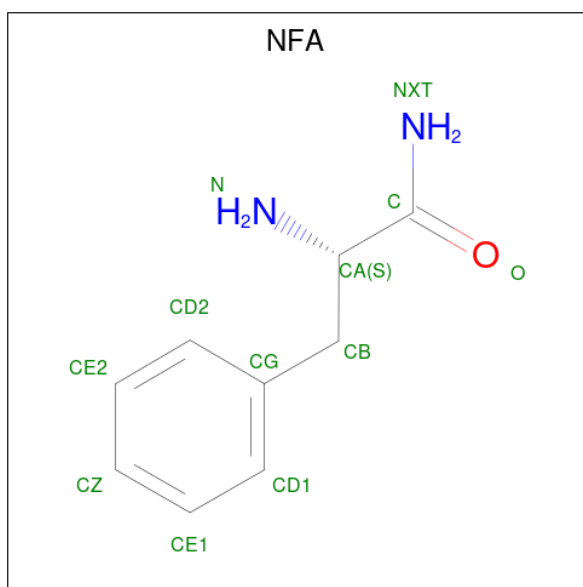
- Molecule 1 is a protein called D-amino acid amidase.

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 (CCD ID: BA) (formula: Ba).

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

- Molecule 3 is PHENYLALANINE AMIDE (CCD ID: NFA) (formula: C₉H₁₂N₂O).



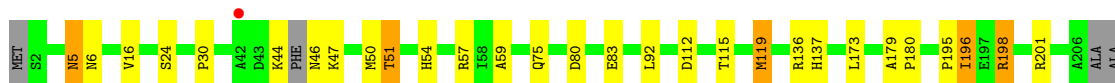
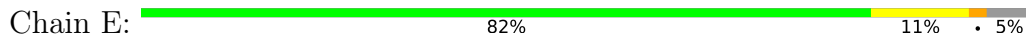
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	9	2	1	0	0
3	B	1	12	9	2	1	0	0
3	C	1	12	9	2	1	0	0
3	D	1	12	9	2	1	0	0
3	E	1	12	9	2	1	0	0
3	F	1	12	9	2	1	0	0

- Molecule 4 is water.

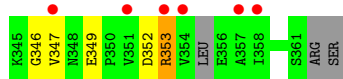
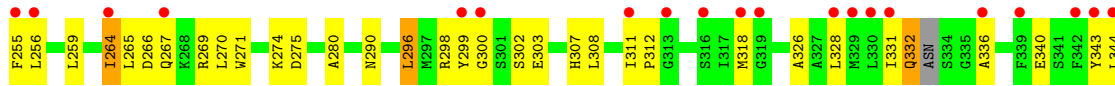
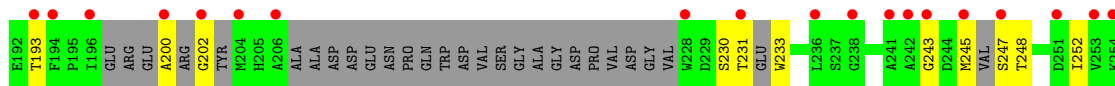
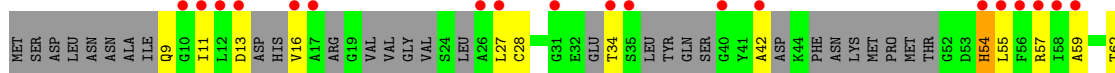
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	223	223	223	0	0
4	B	247	247	247	0	0
4	C	252	252	252	0	0
4	D	224	224	224	0	0
4	E	141	141	141	0	0
4	F	101	101	101	0	0



• 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) 97.9 (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 (4.91%)	wwPDB-VP
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 , 39.9	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: NFA, 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	0.69	0/2902	0.89	1/3936 (0.0%)
1	B	0.75	0/2883	0.95	6/3910 (0.2%)
1	C	0.74	0/2858	0.89	3/3874 (0.1%)
1	D	0.74	0/2795	0.91	3/3786 (0.1%)
1	E	0.68	0/2751	0.89	0/3724
1	F	0.64	0/2346	0.88	0/3146
All	All	0.71	0/16535	0.90	13/22376 (0.1%)

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 (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	PRO	CA-C-N	6.20	132.86	121.70
1	B	223	PRO	C-N-CA	6.20	132.86	121.70
1	C	311	ILE	CB-CA-C	6.03	115.24	109.33
1	B	189	GLY	N-CA-C	5.62	120.60	113.24
1	C	21	VAL	N-CA-C	5.57	115.77	110.42
1	D	284	GLY	CA-C-N	5.52	131.64	121.70
1	D	284	GLY	C-N-CA	5.52	131.64	121.70
1	C	311	ILE	N-CA-C	-5.46	104.71	109.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	ILE	N-CA-C	-5.45	104.72	109.19
1	B	225	ASP	N-CA-C	5.34	122.17	110.80
1	B	226	GLY	N-CA-C	-5.28	97.98	113.30
1	B	21	VAL	N-CA-C	5.17	115.39	110.42
1	A	189	GLY	N-CA-C	5.01	119.80	113.24

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	35	0
1	C	2787	0	2691	35	0
1	D	2727	0	2643	31	0
1	E	2685	0	2613	29	0
1	F	2305	0	2226	53	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	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	209	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 7.

All (209) 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:A:71:HIS:HD2	1:A:273:MET:HE3	1.34	0.92
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
1:B:163:HIS:HD2	4:B:3035:HOH:O	1.58	0.86
1:C:51:THR:H	1:C:54:HIS:HD2	1.21	0.86
1:C:75:GLN:NE2	1:C:266:ASP:H	1.75	0.84
1:E:51:THR:H	1:E:54:HIS:CD2	1.95	0.84
1:A:71:HIS:CD2	1:A:273:MET:HE3	2.15	0.82
1:D:51:THR:H	1:D:54:HIS:HD2	1.24	0.81
1:F:68:THR:HG23	1:F:265:LEU:CD1	2.10	0.81
1:C:210:ASP:HA	1:C:338:ASP:HB2	1.62	0.81
1:A:71:HIS:HD2	1:A:273:MET:CE	1.95	0.79
1:B:32:GLU:HG3	4:B:3122:HOH:O	1.82	0.78
1:B:75:GLN:HB3	1:B:269:ARG:HD3	1.66	0.78
1:A:126:THR:HG22	1:A:129:GLU:H	1.48	0.76
1:C:119:MET:HE3	1:C:312:PRO:HD3	1.68	0.76
1:E:6:ASN:HB3	4:E:3132:HOH:O	1.84	0.76
1:A:57:ARG:H	1:A:314:HIS:HD2	1.30	0.76
1:E:75:GLN:NE2	1:E:266:ASP:H	1.84	0.76
1:E:46:ASN:N	1:E:47:LYS:HA	2.02	0.75
1:C:75:GLN:HE22	1:C:265:LEU:HA	1.53	0.73
1:C:126:THR:HG22	1:C:129:GLU:H	1.55	0.72
1:E:24:SER:HB2	1:E:50:MET:HE2	1.71	0.72
1:B:51:THR:H	1:B:54:HIS:CD2	2.06	0.70
1:F:55:LEU:HD23	1:F:248:THR:HG23	1.72	0.69
1:A:51:THR:H	1:A:54:HIS:CD2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:PHE:O	1:D:285:SER:CB	2.40	0.68
1:F:165:THR:HG21	1:F:172:HIS:HB2	1.75	0.68
1:A:99:PRO:O	1:A:102:ILE:HG13	1.94	0.68
1:C:51:THR:H	1:C:54:HIS:CD2	2.08	0.68
4:C:3161:HOH:O	1:E:339:PHE:HB2	1.93	0.67
1:F:9:GLN:NE2	1:F:13:ASP:OD2	2.28	0.67
1:E:75:GLN:HE22	1:E:266:ASP:H	1.42	0.66
1:E:75:GLN:HE22	1:E:265:LEU:HA	1.60	0.66
1:B:119:MET:CE	1:B:312:PRO:HG3	2.27	0.65
1:F:11:ILE:HG21	1:F:353:ARG:HB3	1.79	0.65
1:D:284:GLY:HA2	1:D:285:SER:HB3	1.79	0.64
1:C:119:MET:HE2	1:C:215:TRP:NE1	2.12	0.64
1:E:196:ILE:HD12	1:E:196:ILE:H	1.63	0.64
1:A:301:SER:HA	1:B:323:GLU:HG2	1.77	0.64
1:A:98:MET:HB3	1:A:102:ILE:HD11	1.79	0.63
1:C:75:GLN:HE22	1:C:266:ASP:H	1.46	0.63
1:C:119:MET:HE2	1:C:215:TRP:CE2	2.34	0.63
1:A:296:LEU:HD13	1:A:305:LYS:HE3	1.81	0.62
1:E:201:ARG:HD3	1:E:229:ASP:OD2	1.99	0.62
1:B:119:MET:SD	1:B:217:VAL:HG12	2.39	0.62
1:B:126:THR:HG23	4:B:3038:HOH:O	2.00	0.62
1:D:126:THR:HG22	1:D:129:GLU:H	1.64	0.61
1:C:14:ASP:O	1:C:18:ARG:HG3	1.99	0.61
1:C:119:MET:HE2	1:C:215:TRP:CD1	2.36	0.61
1:D:339:PHE:HA	1:D:344:LEU:HD23	1.81	0.61
1:A:179:ALA:HB3	1:A:180:PRO:HD3	1.83	0.60
1:F:141:LYS:NZ	1:F:148:GLU:OE1	2.34	0.60
1:A:68:THR:HA	1:A:273:MET:HE1	1.83	0.60
1:F:298:ARG:HH11	1:F:298:ARG:HG3	1.66	0.60
1:D:125:TRP:HE3	1:D:129:GLU:HG2	1.67	0.59
1:B:18:ARG:NH1	1:B:349:GLU:OE1	2.37	0.58
1:E:80:ASP:O	1:E:83:GLU:HG2	2.03	0.58
1:F:270:LEU:HG	1:F:274:LYS:HE3	1.84	0.58
1:C:119:MET:HE3	1:C:312:PRO:CD	2.34	0.58
1:D:296:LEU:HD11	1:D:303:GLU:HB3	1.86	0.58
1:F:296:LEU:CD1	1:F:303:GLU:HB2	2.34	0.58
1:E:195:PRO:HB2	1:E:198:ARG:HG3	1.86	0.57
1:E:201:ARG:O	1:E:333:ASN:HB2	2.05	0.57
1:E:30:PRO:HG3	1:E:324:THR:O	2.05	0.57
1:F:346:GLY:HA2	1:F:349:GLU:OE2	2.04	0.56
1:F:259:LEU:HD12	1:F:265:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD13	1:C:305:LYS:HE3	1.87	0.56
1:C:132:ASP:O	1:C:136:ARG:HG2	2.06	0.56
1:F:11:ILE:HG21	1:F:353:ARG:CB	2.36	0.56
1:E:46:ASN:N	1:E:47:LYS:CA	2.69	0.56
1:B:119:MET:HG2	1:B:216:ASP:O	2.06	0.55
1:D:163:HIS:HD2	4:D:3137:HOH:O	1.87	0.55
1:E:5:ASN:HD22	1:E:5:ASN:N	2.02	0.55
1:B:119:MET:SD	1:B:217:VAL:HA	2.46	0.55
1:D:349:GLU:HG2	4:D:3152:HOH:O	2.06	0.55
1:B:126:THR:HG21	4:B:3181:HOH:O	2.06	0.55
1:B:119:MET:HE3	1:B:312:PRO:HG3	1.88	0.54
1:C:199:GLU:HG2	1:C:200:ALA:O	2.08	0.54
1:A:57:ARG:H	1:A:314:HIS:CD2	2.19	0.54
1:F:27:LEU:HD11	1:F:326:ALA:HB1	1.91	0.54
1:E:179:ALA:HB3	1:E:180:PRO:HD3	1.90	0.53
1:D:125:TRP:CE3	1:D:129:GLU:HG2	2.44	0.52
1:A:75:GLN:NE2	1:A:266:ASP:H	2.08	0.52
1:C:75:GLN:HE22	1:C:265:LEU:CA	2.22	0.52
1:F:74:VAL:HA	1:F:79:VAL:O	2.09	0.52
1:C:269:ARG:N	1:C:269:ARG:HD2	2.25	0.52
1:E:136:ARG:HG2	1:E:137:HIS:CE1	2.45	0.52
1:A:336:ALA:H	1:A:344:LEU:HD13	1.73	0.51
1:A:265:LEU:HG	1:A:269:ARG:HB3	1.93	0.51
1:B:225:ASP:HB2	4:B:3160:HOH:O	2.10	0.51
1:B:318:MET:HB3	1:B:329:MET:SD	2.52	0.50
1:B:225:ASP:O	1:B:225:ASP:CG	2.52	0.50
1:F:248:THR:O	1:F:252:ILE:HG12	2.11	0.50
1:F:264:ILE:HB	1:F:265:LEU:HD12	1.93	0.50
1:F:27:LEU:HD13	1:F:328:LEU:HB3	1.94	0.50
1:B:119:MET:SD	1:B:217:VAL:CG1	2.99	0.50
1:F:252:ILE:O	1:F:255:PHE:HB3	2.12	0.50
1:D:201:ARG:O	1:D:333:ASN:HB2	2.11	0.50
1:E:316:SER:HB3	1:E:331:ILE:HG23	1.93	0.49
1:F:308:LEU:HG	4:F:3120:HOH:O	2.11	0.49
1:A:201:ARG:O	1:A:333:ASN:HB2	2.12	0.49
1:C:269:ARG:NH2	4:C:3255:HOH:O	2.37	0.49
1:D:296:LEU:HD21	1:D:303:GLU:OE1	2.12	0.49
1:D:282:PHE:CE2	1:D:308:LEU:HD11	2.48	0.49
1:D:310:GLN:HG2	1:D:344:LEU:HD11	1.94	0.49
1:D:206:ALA:HB2	1:D:228:TRP:CZ3	2.48	0.49
1:B:296:LEU:HG	1:B:305:LYS:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:HIS:CD2	4:D:3137:HOH:O	2.63	0.48
1:A:16:VAL:HB	1:A:20:VAL:O	2.12	0.48
1:E:59:ALA:HB2	1:E:311:ILE:HB	1.94	0.48
1:B:340:GLU:HG2	1:F:267[A]:GLN:NE2	2.28	0.48
1:A:72:LEU:HD13	1:A:265:LEU:CD1	2.44	0.48
1:A:252:ILE:HG13	1:A:329:MET:HE2	1.95	0.48
1:F:68:THR:CG2	1:F:265:LEU:HD11	2.21	0.47
1:A:318:MET:HB3	1:A:329:MET:SD	2.55	0.47
1:F:11:ILE:HG13	4:F:3066:HOH:O	2.14	0.47
1:F:75:GLN:HG3	1:F:269:ARG:HG2	1.96	0.47
1:D:318:MET:HB3	1:D:329:MET:SD	2.54	0.47
1:F:62:THR:HG23	1:F:245:MET:HG3	1.96	0.47
1:E:75:GLN:HE22	1:E:266:ASP:N	2.12	0.46
1:C:284:GLY:O	1:C:345:LYS:HG3	2.15	0.46
1:C:75:GLN:HE22	1:C:266:ASP:N	2.11	0.46
1:F:42:ALA:HB2	1:F:54:HIS:ND1	2.30	0.46
1:B:60:SER:OG	1:B:63:LYS:NZ	2.48	0.46
1:D:18:ARG:NH1	1:D:349:GLU:OE1	2.48	0.46
1:F:296:LEU:HD11	1:F:303:GLU:HB2	1.98	0.46
1:F:352:ASP:HB3	4:F:3053:HOH:O	2.16	0.46
1:F:168:PRO:HB3	1:F:191:HIS:CG	2.51	0.46
1:D:29:LEU:HD12	1:D:32:GLU:OE1	2.16	0.46
1:A:71:HIS:CD2	1:A:273:MET:CE	2.85	0.45
1:F:59:ALA:HB2	1:F:311:ILE:HB	1.97	0.45
1:A:59:ALA:O	1:A:243:GLY:HA2	2.16	0.45
1:E:44:LYS:HE3	4:E:3128:HOH:O	2.15	0.45
1:A:296:LEU:HD11	1:A:303:GLU:OE2	2.16	0.45
1:F:185:ASP:O	1:F:247:SER:HA	2.17	0.45
1:A:75:GLN:HE22	1:A:265:LEU:HA	1.82	0.45
1:B:207:ALA:HA	1:B:210:ASP:HB3	1.98	0.45
1:C:311:ILE:O	1:C:312:PRO:C	2.59	0.44
1:F:13:ASP:HA	1:F:16:VAL:HG22	1.99	0.44
1:F:230:SER:HB2	1:F:233:TRP:CG	2.53	0.44
1:F:271:TRP:CD1	1:F:275:ASP:HB2	2.53	0.44
1:B:199:GLU:HG2	1:B:200:ALA:O	2.18	0.44
1:B:316:SER:HB3	1:B:331:ILE:HG23	1.99	0.44
1:B:330:LEU:C	1:B:330:LEU:HD23	2.41	0.44
1:F:16:VAL:HG21	4:F:3093:HOH:O	2.16	0.44
1:F:336:ALA:HB2	1:F:343:TYR:HB2	1.98	0.44
1:B:267:GLN:HE21	1:B:267:GLN:HB3	1.63	0.44
1:F:299:TYR:N	1:F:302:SER:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLN:NE2	1:C:266:ASP:N	2.56	0.44
1:C:201:ARG:O	1:C:333:ASN:HB2	2.16	0.44
1:D:273:MET:HE2	1:D:294:LEU:HG	2.00	0.44
1:F:57:ARG:HB3	1:F:311:ILE:HG21	1.99	0.44
1:A:271:TRP:CD1	1:A:275:ASP:HB2	2.53	0.44
1:B:280:ALA:HB2	1:B:290:ASN:OD1	2.18	0.44
1:C:119:MET:HE1	3:C:2003:NFA:HE1	1.99	0.44
1:B:223:PRO:HB3	1:B:227:VAL:O	2.16	0.43
1:F:332:GLN:HG3	1:F:347:VAL:HG23	2.00	0.43
1:B:266:ASP:OD1	1:B:269:ARG:HD2	2.19	0.43
1:C:170:SER:HB3	1:C:188:VAL:HG11	2.00	0.43
1:B:329:MET:HE3	1:B:331:ILE:HD11	1.99	0.43
1:C:251:ASP:HA	1:C:254:LYS:HG3	2.00	0.43
1:F:54:HIS:HB2	1:F:200:ALA:HB2	1.99	0.43
1:D:353:ARG:NH1	1:D:356:GLU:OE1	2.51	0.43
1:F:155:VAL:O	1:F:159:MET:HG3	2.18	0.43
1:D:51:THR:H	1:D:54:HIS:CD2	2.15	0.42
1:B:257:ASN:O	1:B:261:ASP:HB2	2.19	0.42
1:F:202:GLY:HA3	1:F:231:THR:OG1	2.19	0.42
1:C:268:LYS:HD3	1:E:281:PHE:CD2	2.54	0.42
1:D:80:ASP:O	1:D:83:GLU:HG2	2.19	0.42
1:C:55:LEU:HB2	1:C:199:GLU:HA	2.02	0.42
1:F:265:LEU:HD23	1:F:269:ARG:HB3	2.02	0.42
1:C:179:ALA:HB3	1:C:180:PRO:HD3	2.00	0.42
1:C:318:MET:HB3	1:C:329:MET:SD	2.60	0.42
1:B:223:PRO:HD3	1:B:228:TRP:CZ2	2.55	0.42
1:C:269:ARG:HD2	1:C:269:ARG:H	1.85	0.42
1:D:147:MET:HE3	1:D:280:ALA:HB1	2.01	0.42
1:E:57:ARG:HB3	1:E:311:ILE:HG21	2.01	0.42
1:B:126:THR:HG22	1:B:129:GLU:H	1.84	0.42
1:F:256:LEU:HD11	1:F:318:MET:HG3	2.01	0.42
1:C:281:PHE:CD2	1:D:268:LYS:HD3	2.55	0.41
1:F:336:ALA:HB3	1:F:344:LEU:HB2	2.01	0.41
1:C:266:ASP:OD1	1:C:269:ARG:HD2	2.20	0.41
1:F:75:GLN:HE22	1:F:265:LEU:HG	1.84	0.41
1:F:119:MET:HG3	3:F:2006:NFA:HXT2	1.85	0.41
1:A:75:GLN:HE21	1:A:269:ARG:HB2	1.86	0.41
1:E:119:MET:HE3	1:E:119:MET:HB2	1.96	0.41
1:F:27:LEU:HD12	1:F:28:CYS:H	1.86	0.41
1:F:113:PHE:HA	4:F:3103:HOH:O	2.20	0.41
1:A:260:PHE:CD1	1:A:320:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ALA:HB2	1:F:290:ASN:OD1	2.20	0.41
1:A:75:GLN:HE22	1:A:266:ASP:H	1.68	0.41
1:D:70:LEU:HD22	1:D:157:ALA:HB1	2.02	0.41
1:A:75:GLN:HG2	1:A:266:ASP:OD2	2.21	0.41
1:F:120:ILE:HG12	1:F:233:TRP:CD2	2.56	0.41
1:C:271:TRP:CD2	1:E:281:PHE:HB2	2.56	0.41
1:D:123:LYS:HE3	1:D:125:TRP:CE2	2.57	0.41
1:D:199:GLU:HG2	1:D:200:ALA:O	2.21	0.41
1:E:286:ASN:HB3	1:E:298:ARG:O	2.21	0.40
1:E:75:GLN:HE21	1:E:269:ARG:HB2	1.87	0.40
1:F:167:LYS:HD2	1:F:171:ASP:CG	2.46	0.40
1:F:298:ARG:HG3	1:F:298:ARG:NH1	2.34	0.40
1:B:212:ASN:HA	1:B:213:PRO:HD2	1.79	0.40
1:B:268:LYS:HE3	4:B:3264:HOH:O	2.20	0.40
1:D:64:SER:HB2	1:D:318:MET:HE1	2.03	0.40
1:D:126:THR:HG23	4:D:3175:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/363 (100%)	350 (97%)	11 (3%)	1 (0%)	36	42
1	B	360/363 (99%)	338 (94%)	19 (5%)	3 (1%)	16	16
1	C	354/363 (98%)	343 (97%)	10 (3%)	1 (0%)	36	42
1	D	347/363 (96%)	334 (96%)	11 (3%)	2 (1%)	21	23
1	E	339/363 (93%)	327 (96%)	11 (3%)	1 (0%)	36	42
1	F	264/363 (73%)	243 (92%)	17 (6%)	4 (2%)	8	6
All	All	2026/2178 (93%)	1935 (96%)	79 (4%)	12 (1%)	21	23

All (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
1	F	266	ASP
1	F	312	PRO
1	A	243	GLY
1	B	243	GLY
1	B	312	PRO
1	C	243	GLY
1	D	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%)	290 (96%)	12 (4%)	28	38
1	B	300/301 (100%)	291 (97%)	9 (3%)	36	49
1	C	298/301 (99%)	289 (97%)	9 (3%)	36	49
1	D	291/301 (97%)	283 (97%)	8 (3%)	39	53
1	E	288/301 (96%)	270 (94%)	18 (6%)	16	19
1	F	245/301 (81%)	231 (94%)	14 (6%)	18	23
All	All	1724/1806 (96%)	1654 (96%)	70 (4%)	27	37

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	72	LEU
1	A	97	GLN
1	A	102	ILE
1	A	115	THR

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Mol	Chain	Res	Type
1	A	126	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	36	LEU
1	B	102	ILE
1	B	114	GLU
1	B	126	THR
1	B	224	VAL
1	B	269	ARG
1	B	301	SER
1	B	307	HIS
1	B	320	ARG
1	C	16	VAL
1	C	23	VAL
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	D	97	GLN
1	D	102	ILE
1	D	115	THR
1	D	119	MET
1	D	126	THR
1	D	173	LEU
1	D	184	LYS
1	D	307	HIS
1	E	5	ASN
1	E	16	VAL
1	E	51	THR
1	E	92	LEU
1	E	112	ASP
1	E	115	THR
1	E	119	MET
1	E	173	LEU
1	E	196	ILE

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Mol	Chain	Res	Type
1	E	198	ARG
1	E	265	LEU
1	E	268	LYS
1	E	298	ARG
1	E	301	SER
1	E	307	HIS
1	E	331	ILE
1	E	353	ARG
1	E	361	SER
1	F	34	THR
1	F	54	HIS
1	F	102	ILE
1	F	115	THR
1	F	117	MET
1	F	124	SER
1	F	193	THR
1	F	264	ILE
1	F	296	LEU
1	F	307	HIS
1	F	331	ILE
1	F	332	GLN
1	F	340	GLU
1	F	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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	191	HIS
1	A	205	HIS
1	A	314	HIS
1	A	348	ASN
1	B	46	ASN
1	B	54	HIS
1	B	163	HIS
1	B	214	GLN
1	B	267	GLN

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Mol	Chain	Res	Type
1	B	310	GLN
1	B	360	ASN
1	C	46	ASN
1	C	54	HIS
1	C	75	GLN
1	C	128	GLN
1	C	360	ASN
1	D	6	ASN
1	D	54	HIS
1	D	97	GLN
1	D	163	HIS
1	D	360	ASN
1	E	5	ASN
1	E	54	HIS
1	E	75	GLN
1	E	205	HIS
1	F	75	GLN
1	F	137	HIS
1	F	163	HIS
1	F	240	ASN
1	F	348	ASN
1	F	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 oligosaccharides 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	D	2004	-	12,12,12	0.56	0	15,15,15	0.98	1 (6%)
3	NFA	B	2002	-	12,12,12	0.64	0	15,15,15	0.97	1 (6%)
3	NFA	F	2006	-	12,12,12	0.69	0	15,15,15	0.52	0
3	NFA	A	2001	-	12,12,12	0.83	0	15,15,15	1.05	1 (6%)
3	NFA	E	2005	-	12,12,12	0.66	0	15,15,15	0.80	0
3	NFA	C	2003	-	12,12,12	0.66	0	15,15,15	1.01	2 (13%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	NFA	CG-CB-CA	-3.07	107.84	114.13
3	C	2003	NFA	CB-CA-C	2.60	116.16	109.27
3	D	2004	NFA	CG-CB-CA	-2.17	109.69	114.13
3	B	2002	NFA	CG-CB-CA	-2.15	109.74	114.13
3	C	2003	NFA	CG-CB-CA	-2.15	109.74	114.13

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	NFA	O-C-CA-CB
3	B	2002	NFA	NXT-C-CA-CB
3	C	2003	NFA	O-C-CA-CB
3	C	2003	NFA	NXT-C-CA-CB
3	A	2001	NFA	O-C-CA-CB
3	A	2001	NFA	NXT-C-CA-CB
3	A	2001	NFA	O-C-CA-N
3	B	2002	NFA	O-C-CA-N
3	C	2003	NFA	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2006	NFA	1	0
3	C	2003	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%)	-0.37	0 100 100	12, 23, 36, 50	2 (0%)
1	B	362/363 (99%)	-0.39	5 (1%) 73 71	12, 20, 42, 59	0
1	C	358/363 (98%)	-0.48	3 (0%) 82 80	10, 19, 38, 55	0
1	D	350/363 (96%)	-0.49	2 (0%) 85 83	10, 19, 35, 51	1 (0%)
1	E	345/363 (95%)	-0.02	1 (0%) 90 88	13, 30, 48, 61	0
1	F	296/363 (81%)	1.26	77 (26%) 1 1	17, 50, 70, 79	2 (0%)
All	All	2073/2178 (95%)	-0.12	88 (4%) 40 37	10, 24, 56, 79	5 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	16	VAL	5.0
1	F	267[A]	GLN	4.8
1	F	342	PHE	4.2
1	F	56	PHE	4.1
1	F	55	LEU	3.8
1	F	241	ALA	3.8
1	F	182	GLY	3.7
1	F	27	LEU	3.6
1	F	17	ALA	3.6
1	F	200	ALA	3.6
1	C	363	SER	3.5
1	F	354	VAL	3.5
1	F	328	LEU	3.5
1	F	12	LEU	3.4
1	F	339	PHE	3.4
1	F	343	TYR	3.4
1	F	202	GLY	3.2
1	B	216	ASP	3.2
1	F	54	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	26	ALA	3.1
1	F	344	LEU	3.1
1	F	255	PHE	3.0
1	F	300	GLY	3.0
1	F	136[A]	ARG	2.9
1	F	196	ILE	2.9
1	F	40	GLY	2.8
1	B	207	ALA	2.8
1	F	319	GLY	2.8
1	F	42	ALA	2.8
1	B	119	MET	2.8
1	F	177	ILE	2.8
1	F	247	SER	2.7
1	F	169	TYR	2.7
1	F	206	ALA	2.7
1	F	228	TRP	2.7
1	F	31	GLY	2.6
1	F	57	ARG	2.6
1	F	34	THR	2.6
1	F	245	MET	2.6
1	F	331	ILE	2.6
1	F	236	LEU	2.5
1	E	42	ALA	2.5
1	F	251	ASP	2.5
1	F	316	SER	2.5
1	F	10	GLY	2.5
1	F	65	PHE	2.4
1	F	189	GLY	2.4
1	F	243	GLY	2.4
1	F	358	ILE	2.4
1	F	311	ILE	2.4
1	F	59	ALA	2.4
1	F	194	PHE	2.4
1	F	264	ILE	2.4
1	F	171	ASP	2.3
1	F	35	SER	2.3
1	F	204	MET	2.3
1	F	329	MET	2.3
1	F	58	ILE	2.3
1	F	238	GLY	2.3
1	F	193	THR	2.3
1	F	347	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	173	LEU	2.3
1	F	181	LEU	2.3
1	D	284	GLY	2.3
1	F	336	ALA	2.3
1	F	254	LYS	2.3
1	F	351	VAL	2.3
1	F	353	ARG	2.2
1	D	2	SER	2.2
1	B	217	VAL	2.2
1	F	188	VAL	2.2
1	F	256	LEU	2.2
1	F	313	GLY	2.2
1	F	253	VAL	2.2
1	F	242	ALA	2.2
1	F	357	ALA	2.2
1	C	210	ASP	2.1
1	F	318	MET	2.1
1	F	330	LEU	2.1
1	C	3	ASP	2.1
1	F	13	ASP	2.1
1	F	231	THR	2.1
1	F	172	HIS	2.1
1	F	299	TYR	2.1
1	F	117	MET	2.0
1	F	11	ILE	2.0
1	F	133	PHE	2.0
1	B	225	ASP	2.0

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
3	NFA	F	2006	12/12	0.77	0.15	57,57,57,57	0
2	BA	E	3011	1/1	0.82	0.12	44,44,44,44	1
2	BA	B	3021	1/1	0.82	0.10	65,65,65,65	1
2	BA	D	3020	1/1	0.83	0.35	65,65,65,65	1
3	NFA	E	2005	12/12	0.84	0.10	32,34,37,37	0
2	BA	B	3007	1/1	0.85	0.19	64,64,64,64	1
2	BA	E	3014	1/1	0.85	0.09	65,65,65,65	1
2	BA	D	3013	1/1	0.86	0.17	36,36,36,36	1
2	BA	E	3019	1/1	0.86	0.10	64,64,64,64	1
2	BA	F	3022	1/1	0.89	0.17	45,45,45,45	1
3	NFA	D	2004	12/12	0.89	0.08	20,22,23,23	0
3	NFA	A	2001	12/12	0.90	0.09	27,28,28,30	0
2	BA	A	3017	1/1	0.91	0.09	69,69,69,69	1
2	BA	D	3016	1/1	0.91	0.08	64,64,64,64	1
3	NFA	C	2003	12/12	0.91	0.09	21,24,25,25	0
2	BA	B	3009	1/1	0.92	0.14	37,37,37,37	1
3	NFA	B	2002	12/12	0.93	0.07	30,31,32,32	0
2	BA	A	3008	1/1	0.95	0.18	32,32,32,32	1
2	BA	F	3006	1/1	0.96	0.04	51,51,51,51	1
2	BA	C	3010	1/1	0.96	0.08	48,48,48,48	1
2	BA	A	3004	1/1	0.97	0.04	42,42,42,42	1
2	BA	D	3015	1/1	0.98	0.06	54,54,54,54	1
2	BA	C	3012	1/1	0.98	0.08	35,35,35,35	1
2	BA	C	3005	1/1	0.99	0.02	36,36,36,36	1
2	BA	F	3018	1/1	0.99	0.03	40,40,40,40	1
2	BA	B	3002	1/1	0.99	0.02	31,31,31,31	1
2	BA	C	3001	1/1	1.00	0.01	20,20,20,20	1
2	BA	A	3003	1/1	1.00	0.06	19,19,19,19	1

6.5 Other polymers

There are no such residues in this entry.