Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 03:27 PM EDT

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 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:

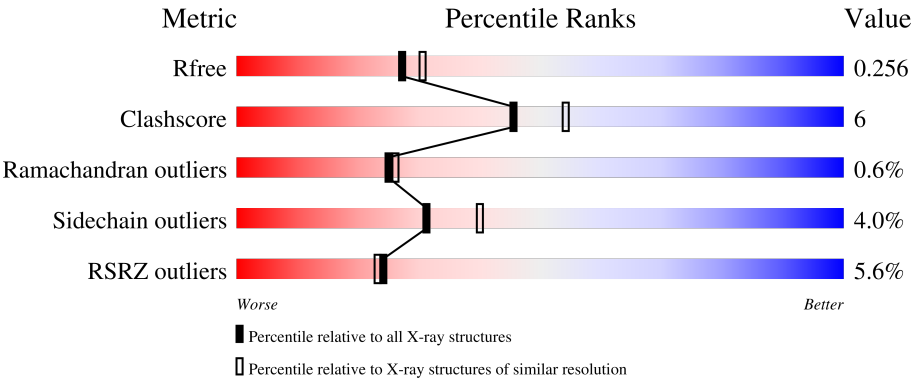
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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.



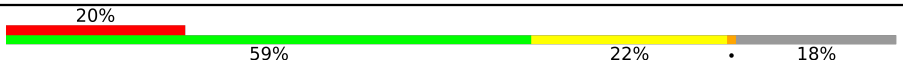
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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% 9% ·
1	B	363	4% 87% 12% ·
1	C	363	85% 12% ··
1	D	363	85% 11% · ·
1	E	363	4% 82% 11% · 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	363	

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.

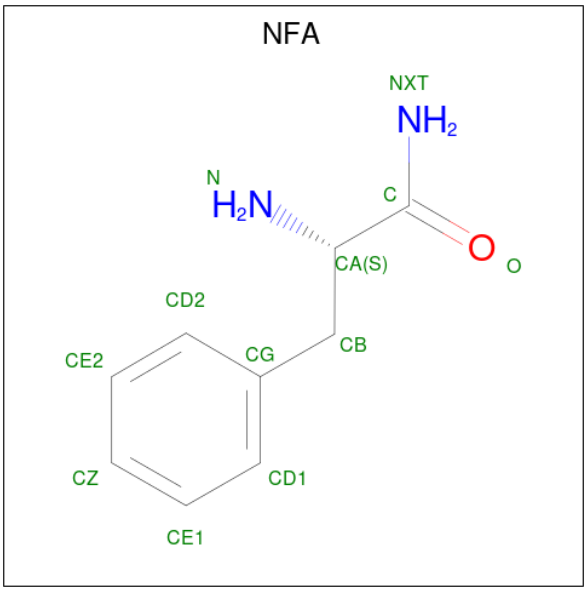
- Molecule 1 is a protein called D-amino acid amidase.

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

- Molecule 2 is BARIUM ION (three-letter code: 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 (three-letter code: NFA) (formula: $C_9H_{12}N_2O$).



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

- Molecule 4 is water.

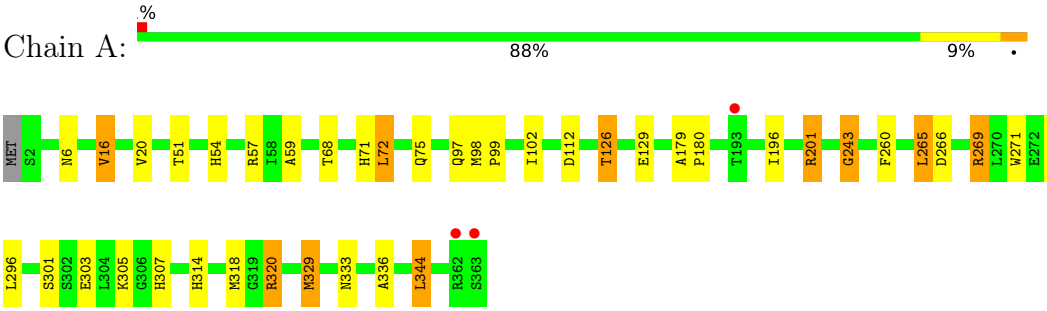
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	223	Total O 223 223	0	0
4	B	247	Total O 247 247	0	0
4	C	252	Total O 252 252	0	0
4	D	224	Total O 224 224	0	0
4	E	141	Total O 141 141	0	0
4	F	101	Total O 101 101	0	0

3 Residue-property plots (i)

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.

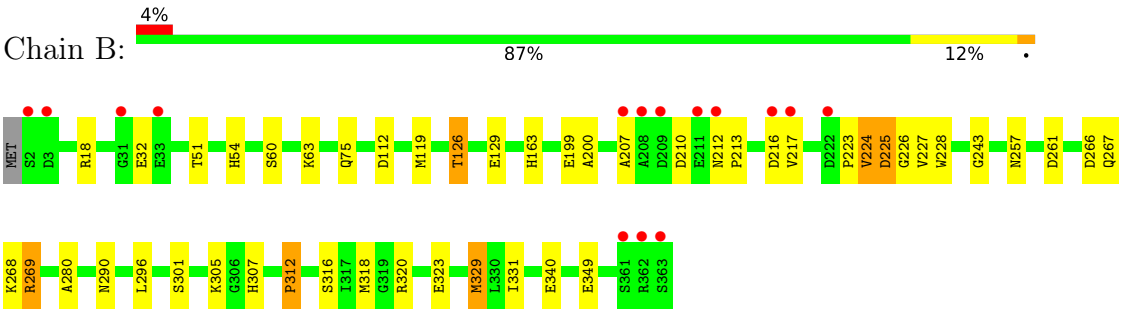
• Molecule 1: D-amino acid amidase

Chain A:



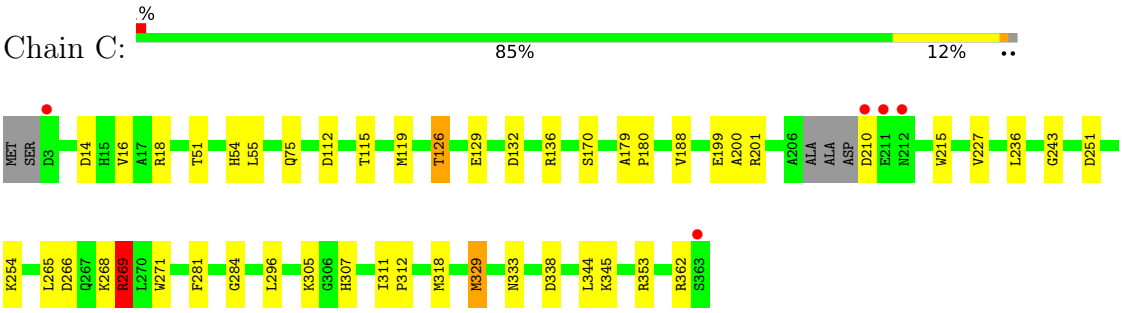
• Molecule 1: D-amino acid amidase

Chain B:



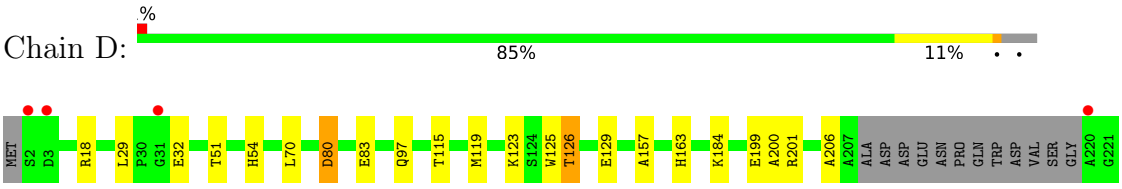
• Molecule 1: D-amino acid amidase

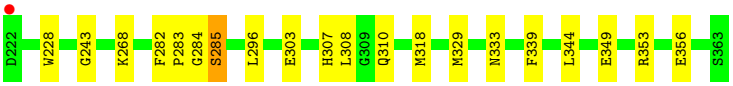
Chain C:



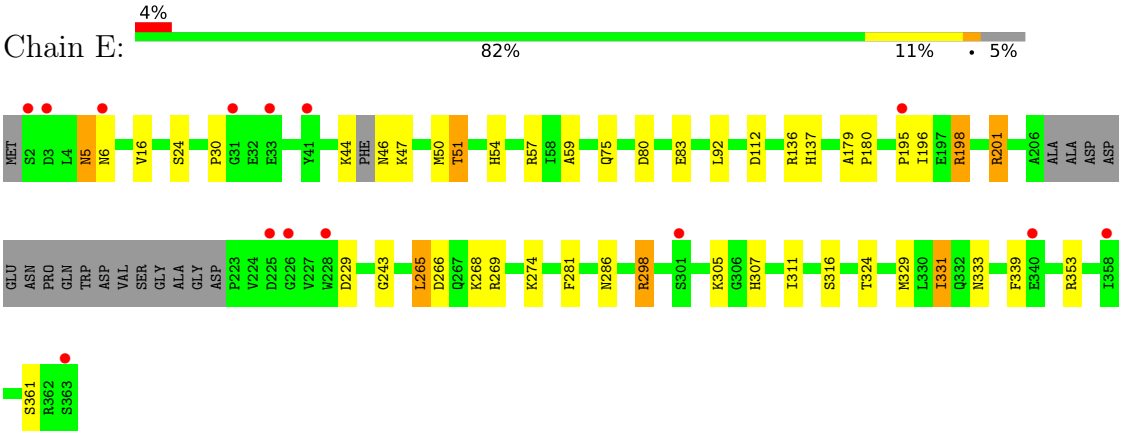
• Molecule 1: D-amino acid amidase

Chain D:

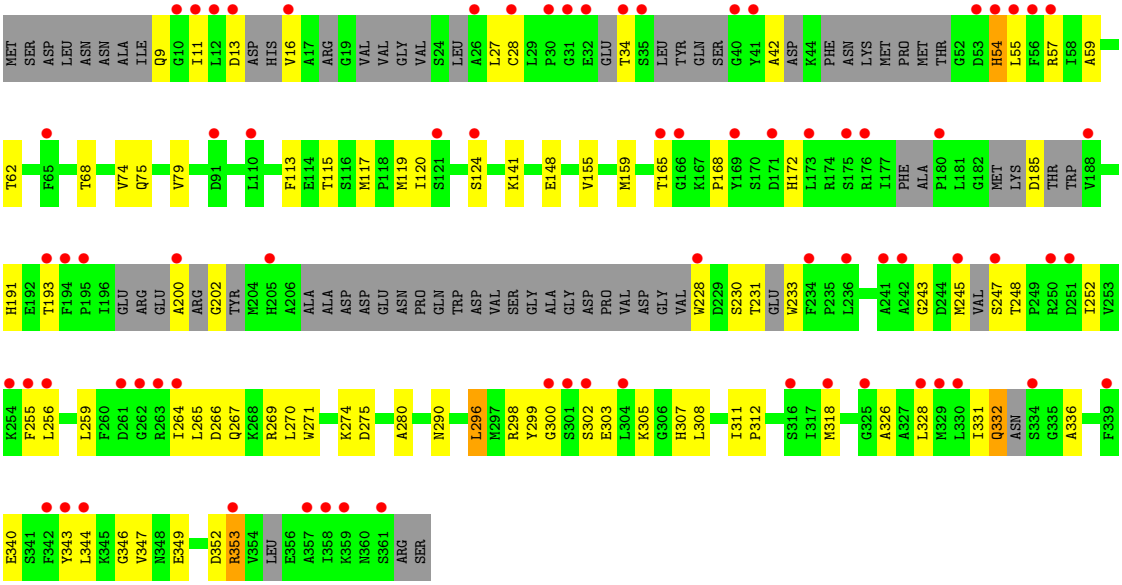




• Molecule 1: D-amino acid amidase



• Molecule 1: D-amino acid amidase



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.45 (at 2.21Å)	Xtriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	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(^{o})	Ideal(^{o})
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.

All (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
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:A:71:HIS:HD2	1:A:273:MET:HE3	1.41	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: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: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:A:71:HIS:CD2	1:A:273:MET:HE3	2.23	0.73
1:C:126:THR:HG22	1:C:129:GLU:H	1.55	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:68:THR:HA	1:A:273:MET:HE1	1.84	0.58
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: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:C:119:MET:HE3	1:C:312:PRO:HD3	1.87	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:24:SER:HB2	1:E:50:MET:HE2	1.94	0.49
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
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: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:B:225:ASP:O	1:B:225:ASP:CG	2.52	0.46
1:E:75:GLN:HE22	1:E:266:ASP:N	2.12	0.46
1:B:119:MET:HE3	1:B:312:PRO:HG3	1.98	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:68:THR:CA	1:A:273:MET:HE1	2.47	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:C:119:MET:CE	1:C:312:PRO:HD3	2.47	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: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:60:SER:OG	1:B:63:LYS:NZ	2.48	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: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
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: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: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: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:C:119:MET:HE1	1:C:215:TRP:NE1	2.34	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:B:119:MET:HE2	1:B:312:PRO:HG3	1.98	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:274:LYS:O	1:E:305:LYS:NZ	2.40	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: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
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:C:311:ILE:O	1:C:312:PRO:C	2.59	0.40
1:E:50:MET:HE3	1:E:51:THR:O	2.21	0.40
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: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: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%)	41	46
1	B	360/363 (99%)	338 (94%)	19 (5%)	3 (1%)	19	19
1	C	354/363 (98%)	343 (97%)	10 (3%)	1 (0%)	41	46
1	D	347/363 (96%)	334 (96%)	11 (3%)	2 (1%)	25	26
1	E	339/363 (93%)	327 (96%)	11 (3%)	1 (0%)	41	46
1	F	264/363 (73%)	243 (92%)	17 (6%)	4 (2%)	10	8
All	All	2026/2178 (93%)	1935 (96%)	79 (4%)	12 (1%)	25	26

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%)	288 (95%)	14 (5%)	27	34
1	B	300/301 (100%)	292 (97%)	8 (3%)	44	57
1	C	298/301 (99%)	286 (96%)	12 (4%)	31	40
1	D	291/301 (97%)	285 (98%)	6 (2%)	53	67
1	E	288/301 (96%)	273 (95%)	15 (5%)	23	28
1	F	245/301 (81%)	231 (94%)	14 (6%)	20	24
All	All	1724/1806 (96%)	1655 (96%)	69 (4%)	31	40

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	16	VAL
1	A	72	LEU
1	A	97	GLN
1	A	112	ASP
1	A	126	THR
1	A	196	ILE
1	A	201	ARG
1	A	265	LEU
1	A	269	ARG
1	A	307	HIS
1	A	320	ARG
1	A	329	MET
1	A	344	LEU
1	B	112	ASP
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	B	329	MET
1	C	16	VAL
1	C	112	ASP
1	C	115	THR
1	C	126	THR
1	C	227	VAL
1	C	236	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	269	ARG
1	C	307	HIS
1	C	329	MET
1	C	344	LEU
1	C	353	ARG
1	C	362	ARG
1	D	97	GLN
1	D	115	THR
1	D	119	MET
1	D	126	THR
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	198	ARG
1	E	201	ARG
1	E	265	LEU
1	E	268	LYS
1	E	298	ARG
1	E	307	HIS
1	E	329	MET
1	E	331	ILE
1	E	353	ARG
1	E	361	SER
1	F	34	THR
1	F	54	HIS
1	F	115	THR
1	F	117	MET
1	F	124	SER
1	F	193	THR
1	F	228	TRP
1	F	296	LEU
1	F	305	LYS
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 (29)

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	314	HIS
1	B	54	HIS
1	B	163	HIS
1	B	267	GLN
1	B	348	ASN
1	B	360	ASN
1	C	46	ASN
1	C	54	HIS
1	C	75	GLN
1	C	348	ASN
1	C	360	ASN
1	D	6	ASN
1	D	54	HIS
1	D	163	HIS
1	D	360	ASN
1	E	5	ASN
1	E	6	ASN
1	E	54	HIS
1	E	75	GLN
1	E	205	HIS
1	F	75	GLN
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 monosaccharides 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	0.52	0	15,15,15	1.02	2 (13%)
3	NFA	A	2001	-	12,12,12	0.76	0	15,15,15	1.05	1 (6%)
3	NFA	B	2002	-	12,12,12	0.59	0	15,15,15	0.93	1 (6%)
3	NFA	C	2003	-	12,12,12	0.62	0	15,15,15	1.08	2 (13%)
3	NFA	F	2006	-	12,12,12	0.63	0	15,15,15	0.52	0
3	NFA	E	2005	-	12,12,12	0.60	0	15,15,15	0.77	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	D	2004	-	-	0/8/8/8	0/1/1/1
3	NFA	A	2001	-	-	3/8/8/8	0/1/1/1
3	NFA	B	2002	-	-	3/8/8/8	0/1/1/1
3	NFA	C	2003	-	-	3/8/8/8	0/1/1/1
3	NFA	F	2006	-	-	0/8/8/8	0/1/1/1
3	NFA	E	2005	-	-	0/8/8/8	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2003	NFA	CB-CA-C	3.03	116.16	109.09
3	A	2001	NFA	CG-CB-CA	-3.02	107.84	114.13
3	D	2004	NFA	CB-CA-C	2.28	114.42	109.09
3	D	2004	NFA	CG-CB-CA	-2.13	109.69	114.13
3	B	2002	NFA	CG-CB-CA	-2.11	109.74	114.13
3	C	2003	NFA	CG-CB-CA	-2.11	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.

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

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	362/363 (99%)	-0.29	3 (0%) 86 85	13, 23, 36, 50	0
1	B	362/363 (99%)	-0.20	15 (4%) 37 35	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	5 (1%) 75 73	10, 19, 35, 51	0
1	E	345/363 (95%)	0.11	14 (4%) 37 35	13, 30, 48, 61	0
1	F	296/363 (81%)	1.20	74 (25%) 0 0	18, 50, 70, 79	0
All	All	2073/2178 (95%)	-0.02	116 (5%) 24 23	10, 24, 56, 79	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	SER	7.0
1	F	342	PHE	6.2
1	F	11	ILE	5.8
1	B	363	SER	5.7
1	F	55	LEU	5.6
1	F	31	GLY	5.2
1	E	31	GLY	5.0
1	F	40	GLY	4.9
1	E	2	SER	4.4
1	F	56	PHE	4.4
1	F	16	VAL	4.4
1	F	328	LEU	4.3
1	F	300	GLY	4.3
1	E	363	SER	4.1
1	B	362	ARG	4.0
1	F	353	ARG	4.0
1	F	339	PHE	3.9
1	F	250	ARG	3.9
1	F	54	HIS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	363	SER	3.8
1	F	195	PRO	3.7
1	F	53	ASP	3.7
1	B	31	GLY	3.7
1	F	41	TYR	3.6
1	B	2	SER	3.5
1	B	207	ALA	3.4
1	F	228	TRP	3.4
1	F	171	ASP	3.3
1	E	226	GLY	3.3
1	F	358	ILE	3.3
1	F	193	THR	3.3
1	F	343	TYR	3.3
1	F	57	ARG	3.3
1	C	210	ASP	3.3
1	D	31	GLY	3.2
1	E	6	ASN	3.2
1	D	222	ASP	3.2
1	B	212	ASN	3.2
1	F	241	ALA	3.1
1	F	12	LEU	3.1
1	B	33	GLU	3.0
1	F	344	LEU	3.0
1	F	254	LYS	3.0
1	F	166	GLY	3.0
1	B	3	ASP	2.9
1	F	316	SER	2.9
1	F	26	ALA	2.9
1	F	175	SER	2.9
1	E	33	GLU	2.9
1	F	91	ASP	2.9
1	B	216	ASP	2.8
1	F	357	ALA	2.8
1	F	124	SER	2.8
1	F	34	THR	2.8
1	C	212	ASN	2.8
1	F	28	CYS	2.8
1	F	173	LEU	2.7
1	F	236	LEU	2.7
1	F	255	PHE	2.7
1	B	361	SER	2.7
1	B	208	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	251	ASP	2.7
1	B	217	VAL	2.7
1	F	302	SER	2.6
1	F	256	LEU	2.6
1	B	211	GLU	2.6
1	F	10	GLY	2.6
1	F	318	MET	2.6
1	F	329	MET	2.5
1	F	30	PRO	2.5
1	F	304	LEU	2.5
1	D	3	ASP	2.5
1	C	211	GLU	2.5
1	E	228	TRP	2.4
1	F	188	VAL	2.4
1	F	165	THR	2.4
1	F	169	TYR	2.4
1	E	41	TYR	2.4
1	E	225	ASP	2.4
1	F	261	ASP	2.3
1	E	195	PRO	2.3
1	F	205	HIS	2.3
1	F	35	SER	2.3
1	F	242	ALA	2.3
1	E	301	SER	2.3
1	F	262	GLY	2.3
1	F	264	ILE	2.3
1	F	65	PHE	2.3
1	F	180	PRO	2.3
1	F	200	ALA	2.3
1	F	263	ARG	2.2
1	F	194	PHE	2.2
1	F	361	SER	2.2
1	F	325	GLY	2.2
1	E	3	ASP	2.2
1	F	121	SER	2.2
1	F	13	ASP	2.2
1	F	234	PHE	2.2
1	F	245	MET	2.2
1	F	334	SER	2.2
1	F	176	ARG	2.1
1	A	362	ARG	2.1
1	E	358	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	110	LEU	2.1
1	F	330	LEU	2.1
1	F	32	GLU	2.1
1	D	220	ALA	2.1
1	D	2	SER	2.1
1	A	193	THR	2.1
1	B	209	ASP	2.1
1	F	301	SER	2.1
1	F	359	LYS	2.1
1	E	340	GLU	2.0
1	F	247	SER	2.0
1	B	222	ASP	2.0
1	C	3	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 monosaccharides 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, 95^{th} 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	D	3020	1/1	0.73	0.19	65,65,65,65	1
3	NFA	F	2006	12/12	0.81	0.22	57,57,57,57	0
2	BA	E	3019	1/1	0.82	0.11	64,64,64,64	1
2	BA	E	3014	1/1	0.82	0.12	65,65,65,65	1
2	BA	A	3017	1/1	0.84	0.16	69,69,69,69	1
2	BA	E	3011	1/1	0.85	0.11	44,44,44,44	1
3	NFA	E	2005	12/12	0.86	0.19	32,34,37,37	0
2	BA	D	3016	1/1	0.86	0.14	64,64,64,64	1
2	BA	B	3021	1/1	0.87	0.14	65,65,65,65	1
2	BA	B	3007	1/1	0.90	0.08	64,64,64,64	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NFA	D	2004	12/12	0.92	0.14	20,22,23,23	0
2	BA	D	3013	1/1	0.92	0.11	36,36,36,36	1
3	NFA	C	2003	12/12	0.92	0.13	21,24,25,25	0
2	BA	B	3009	1/1	0.93	0.08	37,37,37,37	1
2	BA	F	3006	1/1	0.94	0.11	51,51,51,51	1
2	BA	F	3022	1/1	0.94	0.09	45,45,45,45	1
3	NFA	A	2001	12/12	0.94	0.12	27,28,28,30	0
3	NFA	B	2002	12/12	0.94	0.12	30,31,32,32	0
2	BA	A	3008	1/1	0.95	0.15	32,32,32,32	1
2	BA	C	3010	1/1	0.95	0.14	48,48,48,48	1
2	BA	A	3004	1/1	0.96	0.12	42,42,42,42	1
2	BA	C	3012	1/1	0.97	0.04	35,35,35,35	1
2	BA	D	3015	1/1	0.98	0.06	54,54,54,54	1
2	BA	A	3003	1/1	0.99	0.08	19,19,19,19	1
2	BA	F	3018	1/1	0.99	0.03	40,40,40,40	1
2	BA	B	3002	1/1	0.99	0.05	31,31,31,31	1
2	BA	C	3001	1/1	1.00	0.05	20,20,20,20	1
2	BA	C	3005	1/1	1.00	0.03	36,36,36,36	1

6.5 Other polymers (i)

There are no such residues in this entry.