Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:03 AM GMT

PDB ID	:	3NUZ
Title	:	Crystal structure of a putative acetyl xylan esterase (BF1801) from Bacteroides fragilis NCTC 9343 at 2.30 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2010-07-07
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

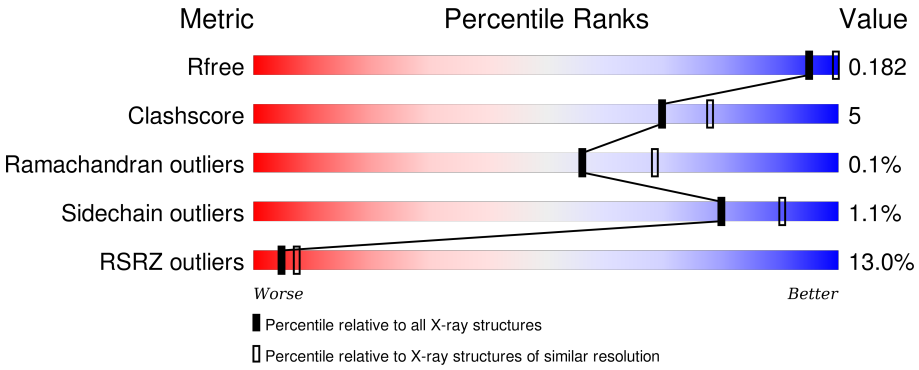
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	6% 86% 11% ·
1	B	398	5% 83% 15% ··
1	C	398	7% 89% 9% ·
1	D	398	5% 88% 10% ·
1	E	398	24% 82% 15% ·

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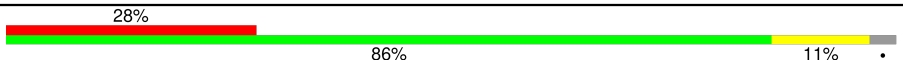
Mol	Chain	Length	Quality of chain
1	F	398	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19125 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 Putative acetyl xylan esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	Se	0	1	0
			3147	2027	540	566	4	10			
1	B	389	Total	C	N	O	S	Se	0	3	0
			3162	2038	542	568	4	10			
1	C	388	Total	C	N	O	S	Se	0	1	0
			3147	2028	541	564	4	10			
1	D	389	Total	C	N	O	S	Se	0	1	0
			3148	2029	539	566	4	10			
1	E	385	Total	C	N	O	S	Se	0	0	0
			3128	2017	536	561	4	10			
1	F	386	Total	C	N	O	S	Se	0	2	0
			3139	2026	535	564	4	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q5LEF1
B	0	GLY	-	EXPRESSION TAG	UNP Q5LEF1
C	0	GLY	-	EXPRESSION TAG	UNP Q5LEF1
D	0	GLY	-	EXPRESSION TAG	UNP Q5LEF1
E	0	GLY	-	EXPRESSION TAG	UNP Q5LEF1
F	0	GLY	-	EXPRESSION TAG	UNP Q5LEF1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	1
			62	62		
2	B	53	Total	O	0	0
			53	53		
2	C	55	Total	O	0	0
			55	55		

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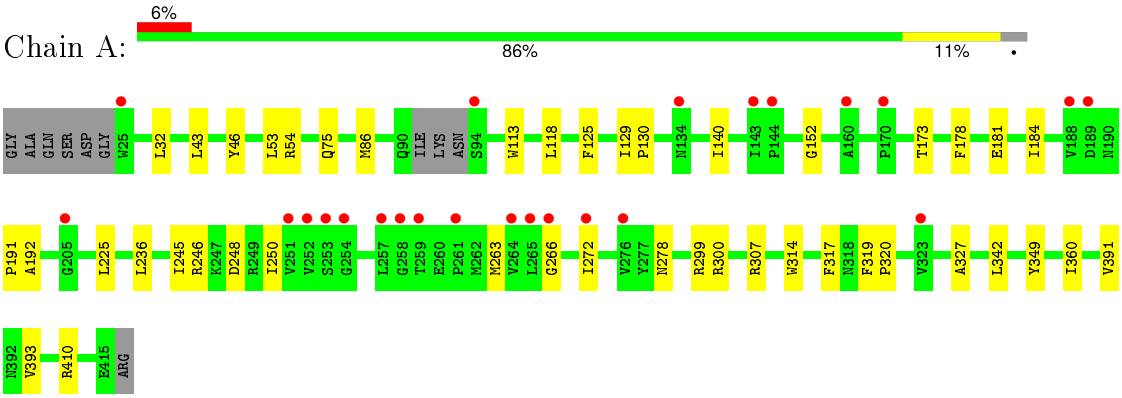
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	53	Total O 53 53	0	0
2	E	21	Total O 21 21	0	0
2	F	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

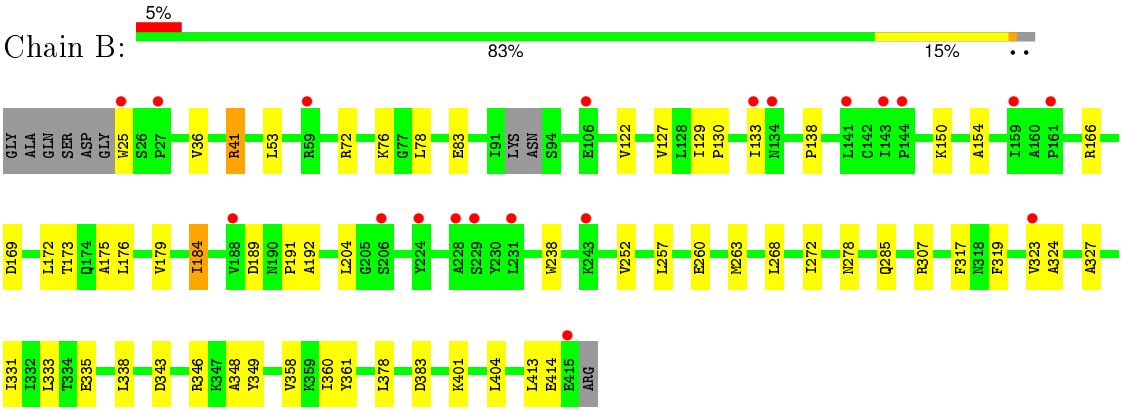
- Molecule 1: Putative acetyl xylan esterase

Chain A:



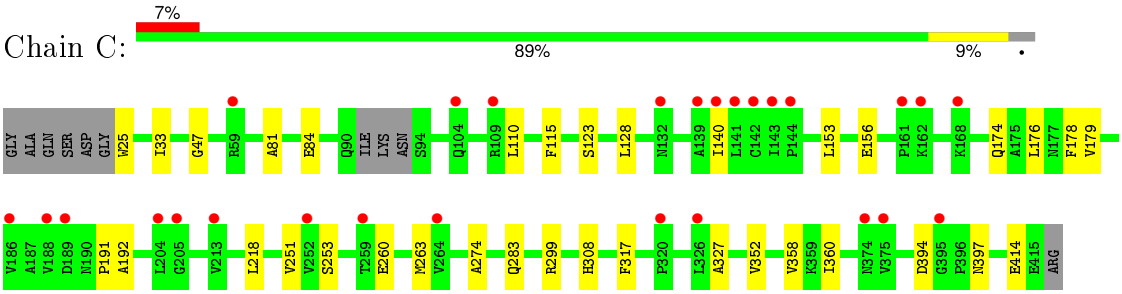
- Molecule 1: Putative acetyl xylan esterase

Chain B:



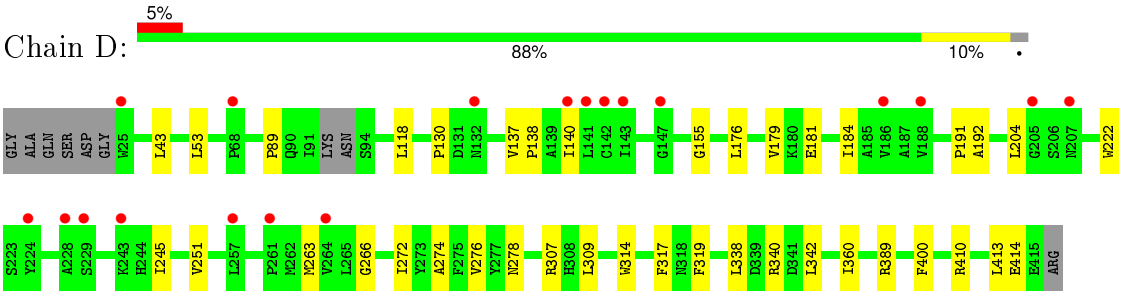
- Molecule 1: Putative acetyl xylan esterase

Chain C:



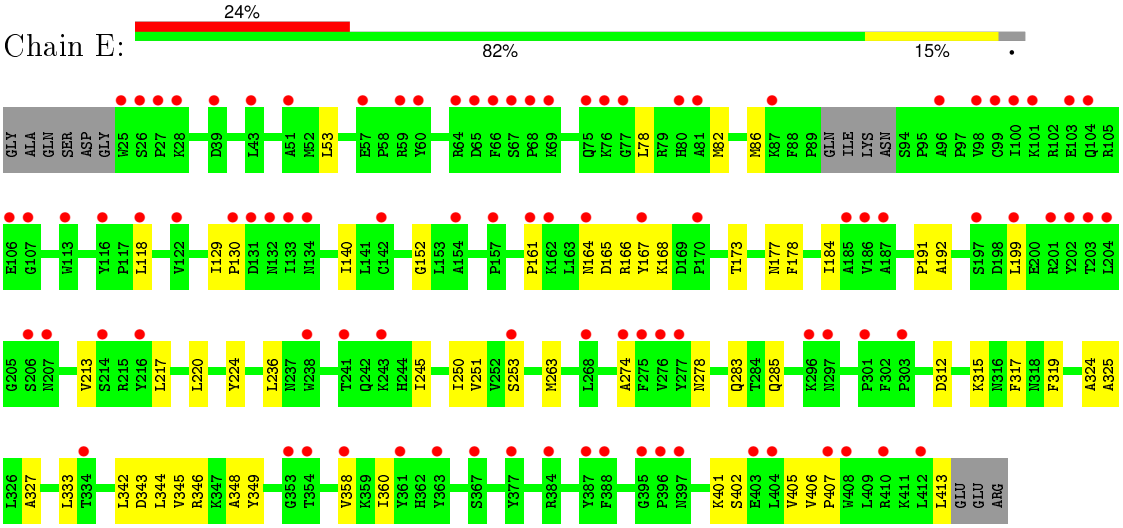
- Molecule 1: Putative acetyl xylan esterase

Chain D:



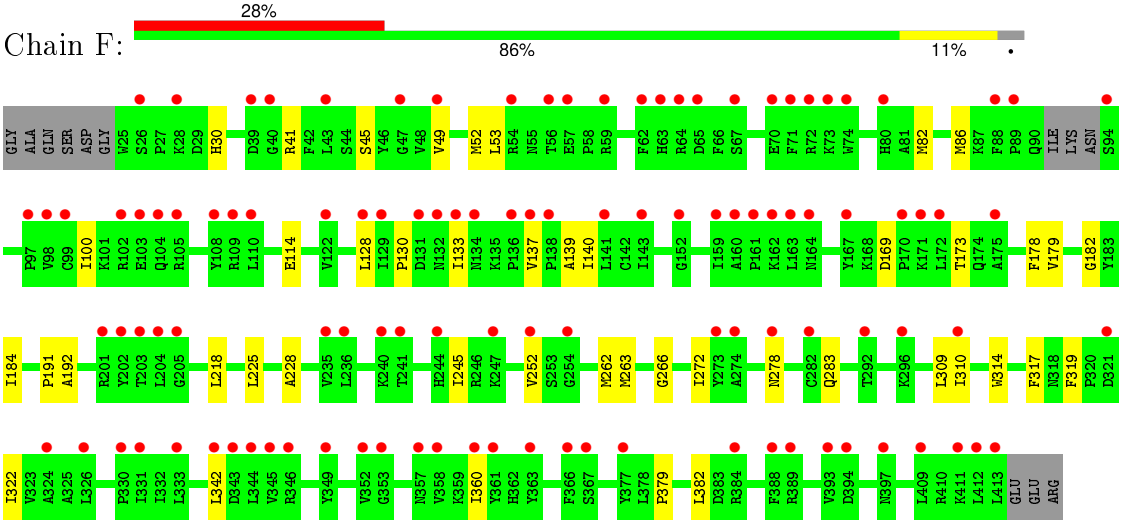
• Molecule 1: Putative acetyl xylan esterase

Chain E:



• Molecule 1: Putative acetyl xylan esterase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	125.61Å 125.61Å 162.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.66 – 2.30 29.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.66-2.30) 99.4 (29.66-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.152 , 0.182 0.154 , 0.182	Depositor DCC
R_{free} test set	6620 reflections (5.53%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.2	EDS
Estimated twinning fraction	0.382 for H, K, L 0.136 for -H, H+K, -L 0.162 for -H, -K, L 0.320 for K, H, -L 0.304 for -h,-k,l 0.460 for h,-h-k,-l 0.304 for -k,-h,-l	Xtriage
Reported twinning fraction	0.382 for H, K, L 0.136 for -H, H+K, -L 0.162 for -H, -K, L 0.320 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 126313 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	19125	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.44	0/3228	0.72	2/4364 (0.0%)
1	B	0.44	0/3249	0.71	2/4392 (0.0%)
1	C	0.45	0/3227	0.72	0/4360
1	D	0.44	0/3229	0.72	0/4366
1	E	0.45	0/3206	0.70	0/4332
1	F	0.43	0/3223	0.68	0/4357
All	All	0.44	0/19362	0.71	4/26171 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	72	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	307	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	41	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3147	0	3094	26	0
1	B	3162	0	3110	36	0
1	C	3147	0	3101	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3148	0	3091	22	0
1	E	3128	0	3093	43	0
1	F	3139	0	3096	33	0
2	A	62	0	0	0	0
2	B	53	0	0	0	0
2	C	55	0	0	0	0
2	D	53	0	0	2	0
2	E	21	0	0	0	0
2	F	10	0	0	0	0
All	All	19125	0	18585	170	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 5.

All (170) 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:E:184:ILE:HD11	1:E:245:ILE:HG12	1.54	0.89
1:A:184:ILE:HD11	1:A:245:ILE:HG12	1.54	0.87
1:B:129:ILE:HA	1:B:184:ILE:HG22	1.66	0.77
1:F:263:MSE:HE1	1:F:319:PHE:CD1	2.21	0.75
1:F:263:MSE:HE1	1:F:319:PHE:CE1	2.25	0.71
1:F:128:LEU:HD23	1:F:179:VAL:HG11	1.78	0.66
1:E:118:LEU:O	1:F:41:ARG:NH2	2.29	0.66
1:E:184:ILE:HD11	1:E:245:ILE:CG1	2.26	0.65
1:F:140[A]:ILE:HD13	1:F:178:PHE:CD2	2.31	0.65
1:D:184:ILE:HD11	1:D:245:ILE:HD11	1.77	0.65
1:A:184:ILE:HD11	1:A:245:ILE:CG1	2.27	0.64
1:A:140:ILE:HD13	1:A:178:PHE:CD2	2.33	0.64
1:A:43:LEU:HD23	1:B:122:VAL:HG13	1.80	0.63
1:F:140[A]:ILE:HD13	1:F:178:PHE:CE2	2.33	0.62
1:E:312:ASP:OD1	1:E:315:LYS:NZ	2.27	0.62
1:B:252:VAL:HG21	1:B:272:ILE:HD13	1.82	0.62
1:D:53:LEU:HD11	1:D:314:TRP:CE3	2.34	0.61
1:E:251:VAL:HG22	1:E:274:ALA:HB3	1.83	0.60
1:E:324:ALA:HB1	1:E:348:ALA:CB	2.32	0.59
1:B:76:LYS:NZ	1:C:414:GLU:O	2.35	0.59
1:F:53:LEU:HD11	1:F:314:TRP:CE3	2.38	0.59
1:E:263:MSE:HE1	1:E:319:PHE:CE1	2.37	0.59
1:D:176:LEU:O	1:D:179:VAL:HG12	2.03	0.58
1:F:86:MSE:HE1	1:F:225:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ALA:HB1	1:F:184:ILE:HD11	1.85	0.58
1:F:252:VAL:HG12	1:F:262:MSE:HG3	1.84	0.58
1:E:327:ALA:HB2	1:E:349:TYR:CD1	2.39	0.58
1:E:140:ILE:HD11	1:E:253:SER:HB2	1.85	0.57
1:A:181:GLU:OE1	1:A:410:ARG:NH1	2.38	0.57
1:B:150:LYS:NZ	1:B:189:ASP:OD2	2.36	0.57
1:E:191:PRO:O	1:E:192:ALA:HB3	2.05	0.57
1:A:118:LEU:O	1:B:41:ARG:NH2	2.38	0.56
1:B:324:ALA:HB1	1:B:348:ALA:CB	2.35	0.56
1:F:218:LEU:CD1	1:F:309:LEU:HD23	2.36	0.56
1:F:130:PRO:HD2	1:F:133:ILE:HD11	1.88	0.56
1:B:130:PRO:HD2	1:B:133:ILE:HD11	1.87	0.56
1:F:379:PRO:HG2	1:F:382:LEU:HD21	1.88	0.55
1:D:266:GLY:HA2	1:D:272:ILE:HD12	1.87	0.55
1:F:252:VAL:HG21	1:F:272:ILE:HD13	1.89	0.55
1:F:184:ILE:HD12	1:F:184:ILE:C	2.27	0.54
1:E:140:ILE:HD13	1:E:178:PHE:CE2	2.42	0.54
1:D:263:MSE:HE1	1:D:319:PHE:CD1	2.43	0.54
1:D:137:VAL:HG22	1:D:138:PRO:HD2	1.89	0.54
1:D:184:ILE:HD11	1:D:245:ILE:CD1	2.39	0.53
1:E:327:ALA:HB2	1:E:349:TYR:CE1	2.42	0.53
1:E:342:LEU:HB3	1:E:360:ILE:HD13	1.91	0.52
1:E:130:PRO:HD3	1:E:184:ILE:HG22	1.91	0.52
1:A:263:MSE:HE1	1:A:319:PHE:CD2	2.44	0.52
1:C:140:ILE:HD11	1:C:253:SER:HB2	1.91	0.52
1:E:130:PRO:CD	1:E:184:ILE:HG22	2.39	0.52
1:E:129:ILE:HA	1:E:184:ILE:HG22	1.92	0.52
1:F:266:GLY:HA2	1:F:272:ILE:HD12	1.91	0.52
1:A:86:MSE:HE1	1:A:225:LEU:HD23	1.91	0.51
1:D:191:PRO:O	1:D:192:ALA:HB3	2.09	0.51
1:D:89:PRO:HG2	1:D:118:LEU:HD21	1.92	0.51
1:C:327:ALA:HB1	1:C:352:VAL:HG21	1.92	0.51
1:C:128:LEU:N	1:C:128:LEU:HD12	2.26	0.51
1:B:343:ASP:OD1	1:B:346:ARG:NH1	2.44	0.51
1:C:260:GLU:HA	1:C:263:MSE:HE3	1.92	0.51
1:E:152:GLY:O	1:E:173:THR:HG22	2.11	0.51
1:D:130:PRO:HD2	1:D:184:ILE:HG22	1.93	0.50
1:F:218:LEU:HD13	1:F:309:LEU:HD23	1.91	0.50
1:D:181:GLU:OE1	1:D:410:ARG:NH1	2.45	0.50
1:E:140:ILE:HG21	1:E:178:PHE:CG	2.47	0.50
1:D:413:LEU:N	1:D:413:LEU:HD22	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ALA:HB1	1:B:348:ALA:HB2	1.93	0.50
1:E:263:MSE:HE1	1:E:319:PHE:CD1	2.47	0.49
1:B:327:ALA:HB2	1:B:349:TYR:CE1	2.47	0.49
1:B:78:LEU:HD23	1:B:78:LEU:C	2.33	0.49
1:A:130:PRO:HD2	1:A:184:ILE:HG22	1.95	0.49
1:B:335:GLU:OE2	1:B:401:LYS:NZ	2.45	0.49
1:E:220:LEU:HD12	1:F:52:MSE:HE2	1.95	0.49
1:D:251:VAL:HG22	1:D:274:ALA:HB3	1.94	0.49
1:E:161:PRO:O	1:E:164:ASN:ND2	2.46	0.49
1:E:345:VAL:HG12	1:E:358:VAL:HG21	1.95	0.48
1:E:401:LYS:O	1:E:405:VAL:HG23	2.14	0.48
1:E:324:ALA:HB1	1:E:348:ALA:HB2	1.94	0.48
1:B:138:PRO:HG3	1:B:413:LEU:HD12	1.96	0.47
1:F:45:SER:O	1:F:49:VAL:HG13	2.14	0.47
1:C:81:ALA:O	1:C:84:GLU:HB2	2.14	0.47
1:E:406:VAL:HB	1:E:407:PRO:HD3	1.96	0.47
1:B:191:PRO:O	1:B:192:ALA:HB3	2.14	0.47
1:E:78:LEU:HD13	1:E:325:ALA:HB2	1.96	0.47
1:E:140:ILE:HD11	1:E:253:SER:CB	2.46	0.46
1:A:391:VAL:HG23	1:A:393:VAL:HG23	1.97	0.46
1:C:191:PRO:O	1:C:192:ALA:HB3	2.15	0.46
1:B:154:ALA:HA	1:B:175:ALA:HB3	1.97	0.46
1:F:342:LEU:HB3	1:F:360:ILE:HD13	1.96	0.46
1:C:153:LEU:HD22	1:C:174:GLN:HB2	1.97	0.46
1:A:327:ALA:HB2	1:A:349:TYR:CE1	2.50	0.46
1:D:140:ILE:HD12	1:D:140:ILE:N	2.31	0.46
1:A:113:TRP:HB2	1:A:125:PHE:CE2	2.51	0.45
1:B:260:GLU:HA	1:B:263:MSE:HE3	1.98	0.45
1:A:130:PRO:CD	1:A:184:ILE:HG22	2.47	0.45
1:A:263:MSE:HE1	1:A:319:PHE:CE2	2.52	0.45
1:B:138:PRO:CG	1:B:413:LEU:HD12	2.46	0.45
1:F:310:ILE:N	1:F:310:ILE:HD12	2.32	0.45
1:B:176:LEU:O	1:B:179:VAL:HG12	2.17	0.45
1:E:167:TYR:O	1:E:168:LYS:CB	2.65	0.45
1:A:299:ARG:NH1	1:B:204:LEU:HD12	2.31	0.44
1:E:140:ILE:HA	1:E:251:VAL:O	2.16	0.44
1:F:184:ILE:HG12	1:F:245:ILE:HG12	2.00	0.44
1:B:129:ILE:HG23	1:B:184:ILE:CG2	2.48	0.44
1:B:257:LEU:HD22	1:B:307[A]:ARG:NH1	2.32	0.44
1:C:110:LEU:HD21	1:C:156:GLU:HG3	1.99	0.44
1:E:199:LEU:HD21	1:F:30:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ILE:HD13	1:E:178:PHE:CZ	2.53	0.44
1:C:251:VAL:HG22	1:C:274:ALA:HB3	1.99	0.44
1:E:165:ASP:OD1	1:E:166:ARG:N	2.45	0.43
1:A:129:ILE:HA	1:A:184:ILE:HG22	2.00	0.43
1:D:155:GLY:HA3	1:D:176:LEU:HD22	2.00	0.43
1:A:75:GLN:NE2	1:A:327:ALA:O	2.49	0.43
1:C:218:LEU:HB3	1:D:309:LEU:HD21	2.00	0.43
1:D:276:VAL:HG11	1:D:400:PHE:CZ	2.54	0.43
1:B:333:LEU:HD12	1:B:333:LEU:N	2.33	0.43
1:D:307:ARG:NH2	2:D:650:HOH:O	2.41	0.43
1:C:176:LEU:O	1:C:179:VAL:HG12	2.18	0.43
1:C:115:PHE:CZ	1:C:123:SER:HB3	2.54	0.43
1:B:319:PHE:O	1:B:323:VAL:HG23	2.18	0.43
1:B:129:ILE:HG23	1:B:184:ILE:HG21	2.01	0.43
1:B:333:LEU:HD13	1:B:360:ILE:HG12	2.01	0.43
1:B:361:TYR:CZ	1:B:404:LEU:HD22	2.53	0.43
1:B:331:ILE:HG23	1:B:358:VAL:HG23	2.01	0.43
1:E:343:ASP:OD1	1:E:346:ARG:NH1	2.52	0.43
1:A:53:LEU:HD11	1:A:314:TRP:CE3	2.54	0.43
1:A:342:LEU:HD22	1:A:360:ILE:HD13	2.00	0.42
1:E:82:MSE:SE	1:E:86:MSE:HE3	2.69	0.42
1:A:266:GLY:HA2	1:A:272:ILE:HD12	2.01	0.42
1:E:78:LEU:HD13	1:E:325:ALA:CB	2.50	0.42
1:F:169:ASP:O	1:F:173:THR:HG23	2.19	0.42
1:A:46:TYR:CZ	1:A:300:ARG:HD2	2.54	0.42
1:E:177:ASN:ND2	1:E:402:SER:OG	2.52	0.42
1:E:217:LEU:HD13	1:E:224:TYR:HA	2.01	0.42
1:F:139:ALA:HB2	1:F:245:ILE:HG23	2.02	0.42
1:B:83:GLU:HG2	1:B:268:LEU:HD22	2.02	0.42
1:C:140:ILE:HD13	1:C:178:PHE:CZ	2.55	0.42
1:A:319:PHE:HB2	1:A:320:PRO:HD3	2.00	0.42
1:D:338:LEU:HD23	1:D:340:ARG:CZ	2.50	0.42
1:D:389:ARG:NE	2:D:750:HOH:O	2.52	0.42
1:E:53:LEU:HD11	1:E:285:GLN:HG3	2.02	0.42
1:F:82:MSE:HE1	1:F:322:ILE:HD13	2.01	0.42
1:F:100:ILE:HD13	1:F:114:GLU:HG3	2.02	0.42
1:B:53:LEU:HD11	1:B:285:GLN:HG3	2.02	0.42
1:C:33:ILE:HG21	1:C:47:GLY:HA2	2.02	0.42
1:F:140[B]:ILE:HD12	1:F:178:PHE:CG	2.55	0.41
1:E:344:LEU:C	1:E:344:LEU:HD23	2.41	0.41
1:F:137:VAL:HG21	1:F:182:GLY:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:HD22	1:B:378:LEU:HD21	2.02	0.41
1:B:257:LEU:HD22	1:B:307[A]:ARG:CZ	2.50	0.41
1:B:166:ARG:HB2	1:B:172:LEU:HD12	2.02	0.41
1:A:191:PRO:O	1:A:192:ALA:HB3	2.19	0.41
1:F:191:PRO:HG2	1:F:228:ALA:HB2	2.03	0.41
1:B:127:VAL:HG21	1:B:238:TRP:CH2	2.55	0.41
1:B:169:ASP:O	1:B:173:THR:HG23	2.20	0.41
1:E:191:PRO:O	1:E:192:ALA:CB	2.69	0.41
1:A:236:LEU:HD11	1:A:250:ILE:HG21	2.03	0.41
1:C:299:ARG:NH1	1:D:204:LEU:HD12	2.36	0.41
1:F:218:LEU:HD11	1:F:309:LEU:HD23	2.03	0.41
1:C:358:VAL:HG22	1:C:360:ILE:HG13	2.02	0.41
1:C:140:ILE:HD13	1:C:178:PHE:CE2	2.56	0.41
1:E:213:VAL:HG13	1:F:49:VAL:HG11	2.02	0.41
1:D:342:LEU:HB3	1:D:360:ILE:HD13	2.01	0.41
1:C:260:GLU:OE2	1:C:308:HIS:ND1	2.46	0.41
1:E:236:LEU:CD1	1:E:250:ILE:HG21	2.51	0.41
1:E:333:LEU:N	1:E:333:LEU:HD12	2.36	0.41
1:A:152:GLY:O	1:A:173:THR:HG22	2.21	0.41
1:F:191:PRO:O	1:F:192:ALA:HB3	2.20	0.40
1:A:246:ARG:HG2	1:A:248:ASP:OD1	2.20	0.40
1:B:383:ASP:C	1:B:383:ASP:OD1	2.60	0.40
1:C:394:ASP:OD2	1:C:397:ASN:ND2	2.48	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	385/398 (97%)	366 (95%)	19 (5%)	0	100 100
1	B	388/398 (98%)	373 (96%)	14 (4%)	1 (0%)	46 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	385/398 (97%)	370 (96%)	15 (4%)	0	100 100
1	D	386/398 (97%)	369 (96%)	16 (4%)	1 (0%)	46 57
1	E	381/398 (96%)	362 (95%)	19 (5%)	0	100 100
1	F	384/398 (96%)	367 (96%)	17 (4%)	0	100 100
All	All	2309/2388 (97%)	2207 (96%)	100 (4%)	2 (0%)	56 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	GLU
1	D	414	GLU

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	338/340 (99%)	335 (99%)	3 (1%)	84 93
1	B	339/340 (100%)	334 (98%)	5 (2%)	72 85
1	C	338/340 (99%)	335 (99%)	3 (1%)	84 93
1	D	337/340 (99%)	333 (99%)	4 (1%)	78 89
1	E	338/340 (99%)	334 (99%)	4 (1%)	78 89
1	F	338/340 (99%)	335 (99%)	3 (1%)	84 93
All	All	2028/2040 (99%)	2006 (99%)	22 (1%)	80 90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	278	ASN
1	A	317	PHE
1	B	25	TRP
1	B	36	VAL

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Mol	Chain	Res	Type
1	B	184	ILE
1	B	278	ASN
1	B	317	PHE
1	C	25	TRP
1	C	283	GLN
1	C	317	PHE
1	D	43	LEU
1	D	222	TRP
1	D	278	ASN
1	D	317	PHE
1	E	278	ASN
1	E	283	GLN
1	E	317	PHE
1	E	413	LEU
1	F	278	ASN
1	F	283	GLN
1	F	317	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	E	55	ASN
1	E	164	ASN
1	E	177	ASN
1	F	392	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	378/398 (94%)	0.53	24 (6%) 23 31	18, 31, 44, 51	0
1	B	379/398 (95%)	0.59	20 (5%) 30 39	19, 32, 44, 52	0
1	C	378/398 (94%)	0.57	27 (7%) 19 26	18, 31, 43, 51	0
1	D	379/398 (95%)	0.56	19 (5%) 32 41	18, 31, 43, 58	0
1	E	375/398 (94%)	1.40	94 (25%) 1 1	28, 36, 46, 53	0
1	F	376/398 (94%)	1.55	111 (29%) 1 1	27, 37, 47, 56	0
All	All	2265/2388 (94%)	0.86	295 (13%) 5 7	18, 34, 45, 58	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	137	VAL	8.7
1	F	324	ALA	6.9
1	E	25	TRP	6.3
1	E	51	ALA	5.4
1	E	133	ILE	5.4
1	F	132	ASN	5.3
1	F	159	ILE	5.2
1	F	133	ILE	5.2
1	F	129	ILE	5.0
1	E	98	VAL	5.0
1	D	205	GLY	5.0
1	F	204	LEU	4.8
1	F	205	GLY	4.6
1	F	162	LYS	4.6
1	F	254	GLY	4.5
1	F	247	LYS	4.5
1	E	59	ARG	4.5
1	E	361	TYR	4.5
1	F	296	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	77	GLY	4.5
1	F	361	TYR	4.4
1	B	415	GLU	4.4
1	E	243	LYS	4.4
1	A	170	PRO	4.3
1	E	301	PRO	4.3
1	E	132	ASN	4.3
1	F	393	VAL	4.2
1	E	296	LYS	4.2
1	F	134	ASN	4.2
1	F	65	ASP	4.2
1	E	358	VAL	4.2
1	F	273	TYR	4.2
1	F	110	LEU	4.1
1	E	130	PRO	4.1
1	F	236	LEU	4.1
1	C	143	ILE	4.0
1	E	27	PRO	4.0
1	F	349	TYR	4.0
1	E	122	VAL	4.0
1	F	136	PRO	3.9
1	E	404	LEU	3.9
1	C	141	LEU	3.8
1	F	412	LEU	3.8
1	E	353	GLY	3.7
1	D	132	ASN	3.6
1	F	358	VAL	3.6
1	F	274	ALA	3.6
1	E	43	LEU	3.6
1	E	134	ASN	3.6
1	C	109	ARG	3.5
1	E	69	LYS	3.5
1	E	238	TRP	3.5
1	E	396	PRO	3.5
1	F	171	LYS	3.5
1	F	72	ARG	3.5
1	E	412	LEU	3.5
1	A	25	TRP	3.4
1	E	157	PRO	3.4
1	E	204	LEU	3.4
1	F	413	LEU	3.4
1	D	224	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	62	PHE	3.4
1	E	185	ALA	3.4
1	F	163	LEU	3.3
1	E	303	PRO	3.3
1	E	241	THR	3.3
1	F	164	ASN	3.3
1	E	104	GLN	3.3
1	E	395	GLY	3.3
1	F	366	PHE	3.3
1	F	73	LYS	3.3
1	C	259	THR	3.3
1	E	100	ILE	3.2
1	F	67	SER	3.2
1	F	70	GLU	3.2
1	D	25	TRP	3.2
1	E	67	SER	3.2
1	F	344	LEU	3.2
1	A	188	VAL	3.2
1	F	104	GLN	3.2
1	B	161	PRO	3.2
1	F	40	GLY	3.2
1	F	203	THR	3.2
1	E	80	HIS	3.1
1	C	204	LEU	3.1
1	F	326	LEU	3.1
1	F	108	TYR	3.1
1	F	98	VAL	3.1
1	F	352	VAL	3.1
1	A	134	ASN	3.1
1	E	354	THR	3.1
1	F	353	GLY	3.1
1	A	252	VAL	3.1
1	C	213	VAL	3.1
1	E	367	SER	3.1
1	F	88	PHE	3.1
1	B	25	TRP	3.1
1	F	47	GLY	3.0
1	F	63	HIS	3.0
1	F	74	TRP	3.0
1	F	26	SER	3.0
1	E	68	PRO	3.0
1	F	143	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	170	PRO	3.0
1	E	65	ASP	2.9
1	E	118	LEU	2.9
1	F	80	HIS	2.9
1	A	276	VAL	2.9
1	F	160	ALA	2.9
1	F	54	ARG	2.9
1	F	389	ARG	2.9
1	E	203	THR	2.9
1	F	71	PHE	2.9
1	B	134	ASN	2.9
1	A	258	GLY	2.9
1	F	56	THR	2.9
1	F	122	VAL	2.8
1	F	330	PRO	2.8
1	B	188	VAL	2.8
1	B	323	VAL	2.8
1	E	76	LYS	2.8
1	E	131	ASP	2.8
1	E	397	ASN	2.8
1	E	388	PHE	2.8
1	E	28	LYS	2.8
1	F	43	LEU	2.8
1	C	142	CYS	2.8
1	F	89	PRO	2.8
1	F	97	PRO	2.8
1	F	357	ASN	2.8
1	F	170	PRO	2.8
1	F	345	VAL	2.7
1	A	257	LEU	2.7
1	F	388	PHE	2.7
1	C	320	PRO	2.7
1	E	408	TRP	2.7
1	F	241	THR	2.7
1	B	206	SER	2.7
1	D	143	ILE	2.7
1	F	310	ILE	2.7
1	F	342	LEU	2.7
1	F	244	HIS	2.7
1	C	188	VAL	2.7
1	D	68	PRO	2.7
1	E	101	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	105	ARG	2.7
1	A	143	ILE	2.7
1	F	333	LEU	2.7
1	E	202	TYR	2.7
1	F	292	THR	2.7
1	C	162	LYS	2.7
1	A	261	PRO	2.7
1	F	411	LYS	2.7
1	E	107	GLY	2.7
1	E	410	ARG	2.7
1	C	264	VAL	2.7
1	D	229	SER	2.6
1	E	206	SER	2.6
1	F	201	ARG	2.6
1	A	254	GLY	2.6
1	F	360	ILE	2.6
1	C	186	VAL	2.6
1	D	188	VAL	2.6
1	F	141	LEU	2.6
1	B	143	ILE	2.6
1	E	64	ARG	2.6
1	E	164	ASN	2.6
1	E	197	SER	2.6
1	F	346	ARG	2.6
1	F	409	LEU	2.6
1	F	161	PRO	2.5
1	F	343	ASP	2.5
1	E	207	ASN	2.5
1	C	205	GLY	2.5
1	E	214	SER	2.5
1	F	59	ARG	2.5
1	D	142	CYS	2.5
1	C	168	LYS	2.5
1	E	167	TYR	2.5
1	F	102	ARG	2.5
1	E	66	PHE	2.5
1	F	384	ARG	2.5
1	A	259	THR	2.5
1	B	224	TYR	2.5
1	E	106	GLU	2.5
1	B	159	ILE	2.5
1	C	132	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	276	VAL	2.5
1	A	94	SER	2.4
1	B	106	GLU	2.4
1	E	268	LEU	2.4
1	E	387	TYR	2.4
1	F	167	TYR	2.4
1	D	264	VAL	2.4
1	B	243	LYS	2.4
1	E	57	GLU	2.4
1	E	253	SER	2.4
1	C	395	GLY	2.4
1	E	87	LYS	2.4
1	F	363	TYR	2.4
1	D	243	LYS	2.4
1	E	161	PRO	2.4
1	B	231	LEU	2.4
1	D	257	LEU	2.4
1	D	207	ASN	2.4
1	A	160	ALA	2.4
1	E	384	ARG	2.4
1	C	252	VAL	2.4
1	E	113	TRP	2.4
1	E	99	CYS	2.4
1	E	201	ARG	2.4
1	E	403	GLU	2.3
1	F	172	LEU	2.3
1	E	363	TYR	2.3
1	A	264	VAL	2.3
1	F	331	ILE	2.3
1	E	103	GLU	2.3
1	B	59	ARG	2.3
1	C	59	ARG	2.3
1	E	26	SER	2.3
1	E	116	TYR	2.3
1	E	186	VAL	2.3
1	F	109	ARG	2.3
1	F	321	ASP	2.3
1	C	374	ASN	2.3
1	E	81	ALA	2.3
1	E	162	LYS	2.3
1	E	407	PRO	2.3
1	F	99	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	138	PRO	2.3
1	C	139	ALA	2.3
1	F	175	ALA	2.3
1	F	235	VAL	2.3
1	E	275	PHE	2.3
1	F	39	ASP	2.3
1	F	131	ASP	2.3
1	A	272	ILE	2.2
1	A	253	SER	2.2
1	F	202	TYR	2.2
1	F	367	SER	2.2
1	F	377	TYR	2.2
1	A	265	LEU	2.2
1	C	144	PRO	2.2
1	B	228	ALA	2.2
1	D	140	ILE	2.2
1	D	228	ALA	2.2
1	E	154	ALA	2.2
1	E	216	TYR	2.2
1	F	282	CYS	2.2
1	F	394	ASP	2.2
1	B	133	ILE	2.2
1	C	375	VAL	2.2
1	F	28	LYS	2.2
1	D	261	PRO	2.2
1	F	94	SER	2.2
1	E	277	TYR	2.2
1	B	229	SER	2.2
1	E	187	ALA	2.2
1	C	104	GLN	2.1
1	B	27	PRO	2.1
1	B	141	LEU	2.1
1	E	199	LEU	2.1
1	F	128	LEU	2.1
1	A	251	VAL	2.1
1	E	377	TYR	2.1
1	C	326	LEU	2.1
1	A	144	PRO	2.1
1	F	152	GLY	2.1
1	F	240	LYS	2.1
1	F	278	ASN	2.1
1	F	49	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	142	CYS	2.1
1	D	141	LEU	2.1
1	E	96	ALA	2.1
1	E	39	ASP	2.1
1	E	75	GLN	2.1
1	F	252	VAL	2.1
1	A	266	GLY	2.0
1	E	297	ASN	2.0
1	E	274	ALA	2.0
1	B	144	PRO	2.0
1	F	57	GLU	2.0
1	A	323	VAL	2.0
1	D	147	GLY	2.0
1	C	189	ASP	2.0
1	E	60	TYR	2.0
1	C	161	PRO	2.0
1	F	64	ARG	2.0
1	A	205	GLY	2.0
1	C	140	ILE	2.0
1	F	397	ASN	2.0
1	A	189	ASP	2.0
1	D	186	VAL	2.0
1	E	334	THR	2.0
1	F	103	GLU	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.