Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 10:33 am BST

PDB ID	:	9HYJ / pdb_00009hyj
Title	:	AlfB fucosidase in complex with Fucose
Authors	:	Marina, A.; Gallego del Sol, F.
Deposited on	:	2025-01-10
Resolution	:	2.25 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:

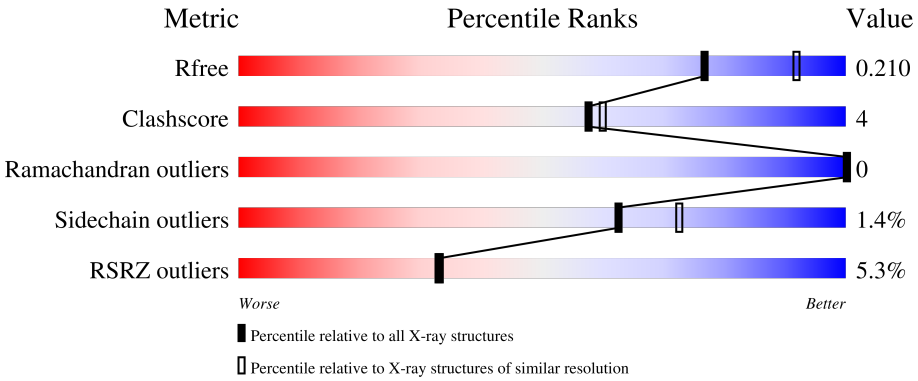
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	414	5% 87% 11% ·
1	B	414	6% 86% 12% ··
1	C	414	5% 86% 12% ··
1	D	414	4% 87% 11% ··
1	E	414	5% 87% 10% ··

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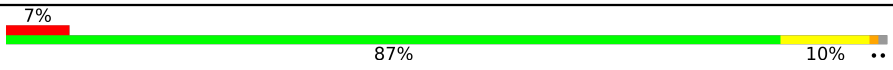
Mol	Chain	Length	Quality of chain
1	F	414	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20742 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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3293	2119	559	604	11			
1	B	410	Total	C	N	O	S	0	1	0
			3282	2112	558	601	11			
1	C	407	Total	C	N	O	S	0	0	0
			3257	2097	553	597	10			
1	D	409	Total	C	N	O	S	0	0	0
			3271	2104	556	601	10			
1	E	407	Total	C	N	O	S	0	1	0
			3266	2103	555	598	10			
1	F	410	Total	C	N	O	S	0	0	0
			3276	2109	556	601	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	SER	ASN	conflict	UNP A0A806EKD1
A	261	MET	VAL	conflict	UNP A0A806EKD1
A	346	LYS	ASN	conflict	UNP A0A806EKD1
B	196	SER	ASN	conflict	UNP A0A806EKD1
B	261	MET	VAL	conflict	UNP A0A806EKD1
B	346	LYS	ASN	conflict	UNP A0A806EKD1
C	196	SER	ASN	conflict	UNP A0A806EKD1
C	261	MET	VAL	conflict	UNP A0A806EKD1
C	346	LYS	ASN	conflict	UNP A0A806EKD1
D	196	SER	ASN	conflict	UNP A0A806EKD1
D	261	MET	VAL	conflict	UNP A0A806EKD1
D	346	LYS	ASN	conflict	UNP A0A806EKD1
E	196	SER	ASN	conflict	UNP A0A806EKD1
E	261	MET	VAL	conflict	UNP A0A806EKD1
E	346	LYS	ASN	conflict	UNP A0A806EKD1
F	196	SER	ASN	conflict	UNP A0A806EKD1
F	261	MET	VAL	conflict	UNP A0A806EKD1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LYS	ASN	conflict	UNP A0A806EKD1

- Molecule 2 is water.

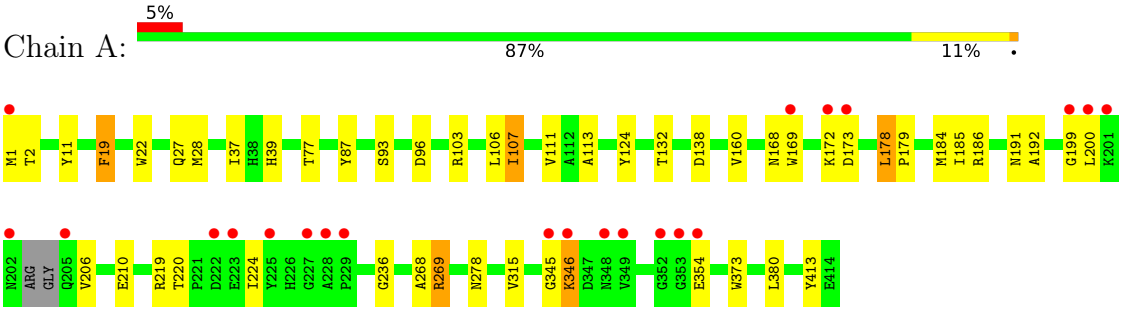
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	203	Total O 203 203	0	0
2	B	197	Total O 197 197	0	0
2	C	155	Total O 155 155	0	0
2	D	225	Total O 225 225	0	0
2	E	153	Total O 153 153	0	0
2	F	164	Total O 164 164	0	0

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.

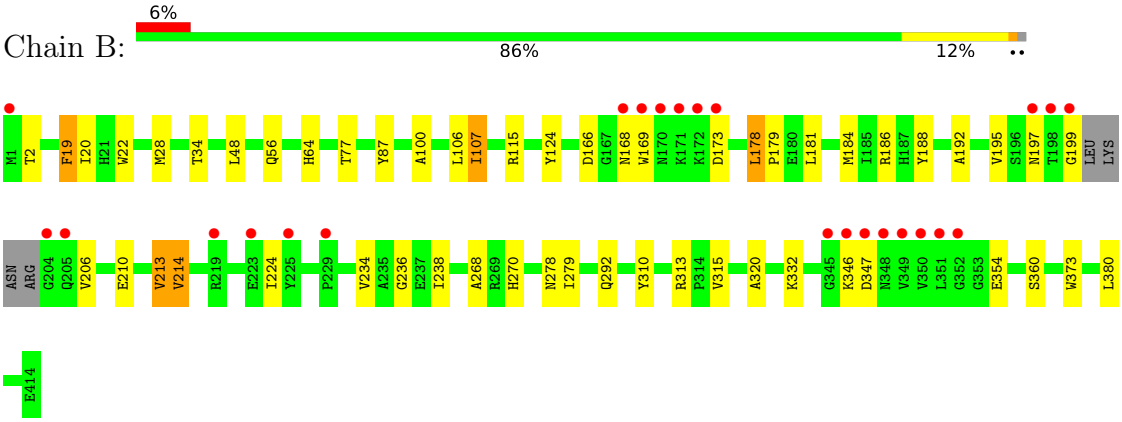
• Molecule 1: Alpha-L-fucosidase

Chain A:



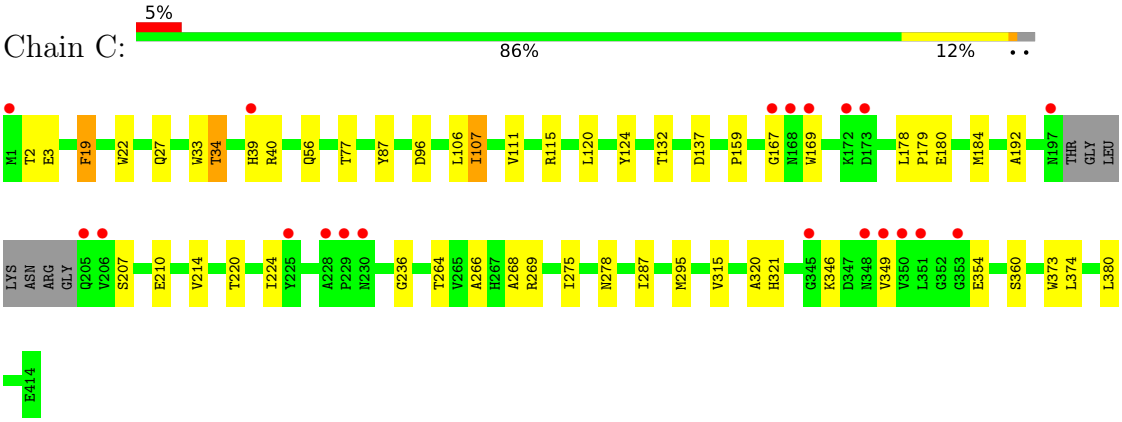
• Molecule 1: Alpha-L-fucosidase

Chain B:



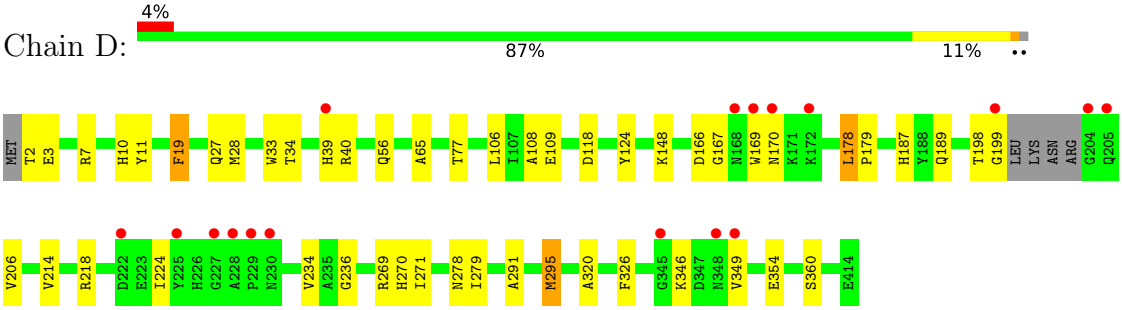
• Molecule 1: Alpha-L-fucosidase

Chain C:



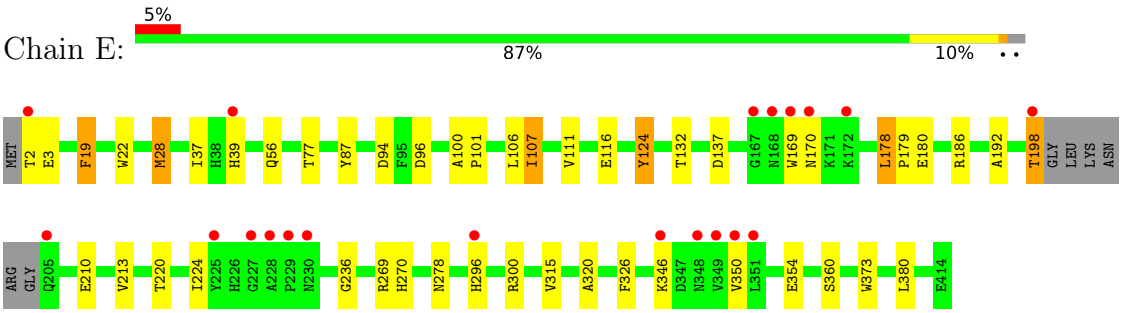
• Molecule 1: Alpha-L-fucosidase

Chain D:



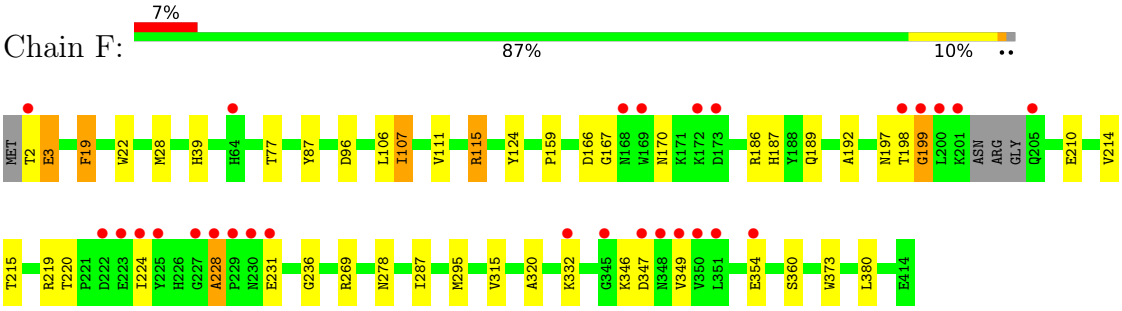
• Molecule 1: Alpha-L-fucosidase

Chain E:



• Molecule 1: Alpha-L-fucosidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	167.16Å 308.29Å 173.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.25 49.03 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.03-2.25) 99.9 (49.03-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.180 , 0.209 0.181 , 0.210	Depositor DCC
R_{free} test set	10595 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20742	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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 (i)

5.1 Standard geometry (i)

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	1.00	9/3390 (0.3%)	1.09	9/4622 (0.2%)
1	B	0.93	6/3383 (0.2%)	1.11	8/4612 (0.2%)
1	C	0.95	4/3354 (0.1%)	1.10	10/4574 (0.2%)
1	D	1.03	12/3368 (0.4%)	1.12	5/4592 (0.1%)
1	E	0.85	2/3367 (0.1%)	1.11	12/4592 (0.3%)
1	F	0.83	2/3373 (0.1%)	1.11	11/4600 (0.2%)
All	All	0.93	35/20235 (0.2%)	1.11	55/27592 (0.2%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	271	ILE	C-O	-6.84	1.16	1.24
1	D	189	GLN	C-O	-6.39	1.16	1.24
1	C	268	ALA	C-O	-6.14	1.17	1.24
1	C	27	GLN	C-O	-5.97	1.17	1.24
1	D	109	GLU	C-O	-5.89	1.17	1.24
1	A	160	VAL	C-O	-5.65	1.17	1.24
1	E	178	LEU	C-O	-5.64	1.19	1.24
1	B	270	HIS	C-O	-5.63	1.17	1.24
1	D	269	ARG	C-O	-5.61	1.17	1.24
1	F	187	HIS	C-O	-5.56	1.17	1.24
1	B	100	ALA	C-O	-5.51	1.19	1.24
1	B	178	LEU	C-O	-5.48	1.19	1.24
1	A	184	MET	C-O	-5.47	1.17	1.24
1	A	113	ALA	C-O	-5.47	1.17	1.24
1	A	269	ARG	C-O	-5.46	1.17	1.24
1	A	178	LEU	C-O	-5.43	1.19	1.24
1	B	213	VAL	C-O	-5.43	1.18	1.24
1	D	178	LEU	C-O	-5.42	1.19	1.24
1	F	189	GLN	C-O	-5.42	1.17	1.24
1	E	213	VAL	C-O	-5.37	1.18	1.24
1	D	7	ARG	C-O	-5.36	1.17	1.24
1	D	108	ALA	C-O	-5.34	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	ALA	C-O	-5.33	1.17	1.23
1	A	185	ILE	C-O	-5.31	1.18	1.24
1	D	295	MET	C-O	-5.30	1.18	1.24
1	D	11	TYR	C-O	-5.28	1.18	1.24
1	B	64	HIS	C-O	-5.25	1.18	1.24
1	D	187	HIS	C-O	-5.22	1.18	1.24
1	C	266	ALA	C-O	-5.21	1.18	1.24
1	B	181	LEU	C-O	-5.15	1.18	1.24
1	A	11	TYR	C-O	-5.11	1.18	1.24
1	D	27	GLN	C-O	-5.05	1.18	1.24
1	D	106	LEU	C-O	-5.05	1.18	1.24
1	A	268	ALA	C-O	-5.03	1.18	1.24
1	A	93	SER	C-O	-5.01	1.17	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	220	THR	CA-C-N	8.85	128.50	118.85
1	E	220	THR	C-N-CA	8.85	128.50	118.85
1	C	220	THR	CA-C-N	8.71	128.35	118.85
1	C	220	THR	C-N-CA	8.71	128.35	118.85
1	F	215	THR	CA-CB-OG1	-7.57	98.25	109.60
1	F	332	LYS	CB-CG-CD	7.17	127.79	111.30
1	A	346	LYS	CB-CG-CD	6.84	127.03	111.30
1	F	228	ALA	CA-C-N	6.79	126.58	119.05
1	F	228	ALA	C-N-CA	6.79	126.58	119.05
1	B	310	TYR	N-CA-C	6.71	119.59	111.40
1	E	132	THR	CA-CB-OG1	-6.37	100.04	109.60
1	C	19	PHE	CA-CB-CG	6.29	120.09	113.80
1	B	313	ARG	CA-C-N	6.25	126.17	119.85
1	B	313	ARG	C-N-CA	6.25	126.17	119.85
1	E	19	PHE	CA-CB-CG	6.21	120.00	113.80
1	A	37	ILE	N-CA-C	6.14	116.92	110.72
1	C	315	VAL	N-CA-CB	-6.03	102.76	111.21
1	D	19	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	132	THR	CA-CB-OG1	-5.82	100.87	109.60
1	E	137	ASP	CA-CB-CG	5.74	118.34	112.60
1	C	111	VAL	N-CA-CB	5.72	119.16	110.58
1	E	111	VAL	N-CA-CB	5.69	119.11	110.58
1	F	19	PHE	CA-CB-CG	5.69	119.49	113.80
1	C	132	THR	CA-CB-OG1	-5.63	101.16	109.60
1	E	37	ILE	N-CA-C	5.60	116.33	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	315	VAL	N-CA-CB	-5.60	103.37	111.21
1	C	207	SER	N-CA-C	5.57	117.35	111.28
1	B	2	THR	CA-CB-OG1	-5.54	101.30	109.60
1	A	19	PHE	CA-CB-CG	5.52	119.32	113.80
1	D	170	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	315	VAL	N-CA-CB	-5.42	103.63	111.21
1	A	96	ASP	CA-CB-CG	5.40	118.00	112.60
1	E	170	ASN	CA-C-N	-5.38	115.26	122.42
1	E	170	ASN	C-N-CA	-5.38	115.26	122.42
1	D	118	ASP	CA-CB-CG	5.36	117.96	112.60
1	E	315	VAL	N-CA-CB	-5.33	103.75	111.21
1	A	2	THR	CA-CB-OG1	-5.32	101.63	109.60
1	F	3	GLU	CB-CA-C	5.31	116.35	108.87
1	F	115	ARG	CA-CB-CG	-5.27	103.56	114.10
1	A	315	VAL	N-CA-CB	-5.26	103.84	111.21
1	F	111	VAL	N-CA-CB	5.25	118.45	110.58
1	F	96	ASP	CA-CB-CG	5.23	117.83	112.60
1	E	94	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	34	THR	CA-CB-OG1	-5.16	101.87	109.60
1	D	166	ASP	CA-C-N	-5.15	111.32	121.41
1	D	166	ASP	C-N-CA	-5.15	111.32	121.41
1	A	138	ASP	CA-CB-CG	5.13	117.73	112.60
1	E	96	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	137	ASP	CB-CA-C	5.12	119.94	109.55
1	B	115	ARG	CA-CB-CG	-5.07	103.96	114.10
1	C	96	ASP	CA-CB-CG	5.06	117.66	112.60
1	F	199	GLY	N-CA-C	5.05	120.45	113.99
1	B	19	PHE	CA-CB-CG	5.03	118.83	113.80
1	C	34	THR	CA-CB-OG1	-5.02	102.07	109.60
1	A	413	TYR	N-CA-C	5.02	117.90	110.48

There are no chirality outliers.

There are no planarity outliers.

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	3293	0	3166	24	0
1	B	3282	0	3155	31	0
1	C	3257	0	3128	29	0
1	D	3271	0	3142	36	0
1	E	3266	0	3137	34	0
1	F	3276	0	3146	38	0
2	A	203	0	0	3	0
2	B	197	0	0	2	0
2	C	155	0	0	0	0
2	D	225	0	0	4	0
2	E	153	0	0	0	0
2	F	164	0	0	0	0
All	All	20742	0	18874	169	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 4.

All (169) 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:A:39:HIS:NE2	1:B:346:LYS:HD3	1.83	0.94
1:E:39:HIS:CE1	1:F:346:LYS:HE3	2.03	0.93
1:E:39:HIS:CE1	1:F:346:LYS:HG3	2.05	0.91
1:E:186:ARG:HD2	1:E:210:GLU:OE1	1.70	0.90
1:D:279:ILE:HD11	1:D:295:MET:CE	2.03	0.88
1:D:279:ILE:HD11	1:D:295:MET:HE2	1.57	0.86
1:B:186:ARG:HD2	1:B:210:GLU:OE1	1.75	0.86
1:D:167:GLY:HA2	1:D:169:TRP:NE1	1.91	0.85
1:C:167:GLY:HA2	1:C:169:TRP:NE1	1.93	0.83
1:A:186:ARG:HD2	1:A:210:GLU:OE1	1.79	0.81
1:F:186:ARG:HD2	1:F:210:GLU:OE1	1.82	0.80
1:D:167:GLY:HA2	1:D:169:TRP:CE2	2.18	0.78
1:C:167:GLY:HA2	1:C:169:TRP:CE2	2.18	0.77
1:D:279:ILE:CD1	1:D:295:MET:HE2	2.15	0.77
1:C:39:HIS:HB2	1:D:346:LYS:HZ3	1.48	0.76
1:D:291:ALA:O	1:D:295:MET:HG2	1.90	0.71
1:B:87:TYR:HB3	1:B:107:ILE:HG12	1.72	0.71
1:E:39:HIS:HE1	1:F:346:LYS:CE	2.04	0.71
1:E:39:HIS:HE1	1:F:346:LYS:HE3	1.54	0.71
1:C:87:TYR:HB3	1:C:107:ILE:HG12	1.73	0.70
1:A:39:HIS:NE2	1:B:346:LYS:CD	2.55	0.70
1:E:87:TYR:HB3	1:E:107:ILE:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:MET:HA	1:D:28:MET:HE2	1.75	0.68
1:A:87:TYR:HB3	1:A:107:ILE:HG12	1.75	0.68
1:D:10:HIS:CE1	2:D:502:HOH:O	2.46	0.68
1:A:224:ILE:HD13	1:A:236:GLY:HA3	1.77	0.67
1:C:39:HIS:HB2	1:D:346:LYS:NZ	2.10	0.66
1:B:346:LYS:HE3	1:B:347:ASP:OD2	1.96	0.66
1:F:87:TYR:HB3	1:F:107:ILE:HG12	1.78	0.66
1:C:34:THR:OG1	1:C:40:ARG:NH1	2.30	0.65
1:D:279:ILE:CD1	1:D:295:MET:CE	2.75	0.65
1:B:224:ILE:HD13	1:B:236:GLY:HA3	1.78	0.64
1:C:115:ARG:NH2	1:C:159:PRO:O	2.29	0.64
1:E:39:HIS:CE1	1:F:346:LYS:CE	2.77	0.64
1:C:224:ILE:HD13	1:C:236:GLY:HA3	1.79	0.63
1:F:224:ILE:HD13	1:F:236:GLY:HA3	1.79	0.63
1:A:172:LYS:O	1:A:173:ASP:HB2	1.97	0.63
1:D:224:ILE:HD13	1:D:236:GLY:HA3	1.79	0.63
1:E:198:THR:HG22	1:E:198:THR:O	1.98	0.63
1:E:186:ARG:NH2	1:E:192:ALA:O	2.31	0.63
1:E:346:LYS:HE3	1:F:39:HIS:CE1	2.34	0.63
1:E:224:ILE:HD13	1:E:236:GLY:HA3	1.80	0.63
1:C:346:LYS:HE3	1:D:39:HIS:HB2	1.80	0.62
1:E:169:TRP:NE1	1:F:349:VAL:HG22	2.13	0.62
1:F:198:THR:O	1:F:198:THR:HG23	2.00	0.61
2:A:615:HOH:O	1:C:321:HIS:HE1	1.82	0.61
1:D:169:TRP:HD1	1:D:198:THR:HG23	1.66	0.59
1:E:39:HIS:CE1	1:F:346:LYS:CG	2.84	0.59
1:F:346:LYS:HE2	1:F:347:ASP:OD2	2.03	0.58
1:F:186:ARG:NH2	1:F:192:ALA:O	2.37	0.58
1:A:345:GLY:O	1:A:346:LYS:HG2	2.05	0.56
1:A:224:ILE:CD1	1:A:236:GLY:HA3	2.35	0.56
1:E:224:ILE:CD1	1:E:236:GLY:HA3	2.37	0.55
1:D:224:ILE:CD1	1:D:236:GLY:HA3	2.37	0.55
1:B:168:ASN:HB3	1:B:169:TRP:HE3	1.71	0.55
1:F:224:ILE:CD1	1:F:236:GLY:HA3	2.36	0.55
1:B:224:ILE:CD1	1:B:236:GLY:HA3	2.36	0.54
1:E:100:ALA:HB1	1:E:101:PRO:HD2	1.89	0.54
1:B:166:ASP:OD1	1:B:197:ASN:ND2	2.37	0.54
1:C:224:ILE:CD1	1:C:236:GLY:HA3	2.38	0.53
1:C:124:TYR:C	1:C:124:TYR:CD1	2.87	0.53
1:D:167:GLY:HA2	1:D:169:TRP:CD1	2.43	0.53
1:E:124:TYR:C	1:E:124:TYR:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:VAL:HG21	1:D:33:TRP:CZ3	2.45	0.52
1:A:124:TYR:C	1:A:124:TYR:CD1	2.88	0.52
1:B:332:LYS:HB2	2:B:664:HOH:O	2.10	0.52
1:F:28:MET:HA	1:F:28:MET:HE2	1.91	0.52
1:B:195:VAL:HG22	1:B:213:VAL:HB	1.92	0.52
1:E:169:TRP:CE2	1:F:349:VAL:HG22	2.44	0.52
1:D:169:TRP:HD1	1:D:198:THR:CG2	2.23	0.51
1:A:39:HIS:NE2	1:B:346:LYS:CE	2.74	0.51
1:E:39:HIS:ND1	1:F:346:LYS:HE3	2.25	0.51
1:B:77:THR:HA	1:B:124:TYR:HB3	1.93	0.50
1:D:124:TYR:C	1:D:124:TYR:CD1	2.89	0.50
1:E:28:MET:HA	1:E:28:MET:HE2	1.93	0.50
1:E:39:HIS:HE1	1:F:346:LYS:CG	2.23	0.50
1:B:124:TYR:C	1:B:124:TYR:CD1	2.89	0.50
1:A:168:ASN:HB3	1:A:169:TRP:HE3	1.77	0.50
1:C:167:GLY:HA2	1:C:169:TRP:CD1	2.45	0.50
1:F:287:ILE:HG21	1:F:295:MET:HE1	1.93	0.50
1:A:39:HIS:CD2	1:B:346:LYS:HE2	2.46	0.50
1:A:28:MET:HA	1:A:28:MET:HE2	1.93	0.49
1:D:34:THR:OG1	1:D:40:ARG:NH1	2.39	0.49
1:F:199:GLY:HA3	1:F:214:VAL:HG22	1.95	0.49
1:F:166:ASP:OD1	1:F:197:ASN:ND2	2.43	0.49
1:D:10:HIS:ND1	2:D:502:HOH:O	2.35	0.49
1:E:346:LYS:HE3	1:F:39:HIS:HE1	1.75	0.49
1:B:186:ARG:NH2	1:B:192:ALA:O	2.45	0.48
1:F:124:TYR:C	1:F:124:TYR:CD1	2.91	0.48
1:E:269:ARG:HA	1:E:269:ARG:HD2	1.61	0.47
1:B:184:MET:HE3	1:B:188:TYR:HD2	1.80	0.47
1:B:206:VAL:HG11	1:B:234:VAL:HG21	1.97	0.47
1:D:65:ALA:HB1	1:D:295:MET:HE3	1.97	0.47
1:B:199:GLY:O	1:B:206:VAL:HA	2.14	0.46
1:A:27:GLN:HG3	2:A:608:HOH:O	2.15	0.46
1:B:28:MET:HE3	1:B:48:LEU:HD11	1.97	0.46
1:C:320:ALA:HB2	1:C:360:SER:HB2	1.96	0.46
1:A:186:ARG:NH2	1:A:192:ALA:O	2.45	0.46
1:E:320:ALA:HB2	1:E:360:SER:HB2	1.98	0.46
1:A:178:LEU:N	1:A:179:PRO:CD	2.78	0.46
1:D:169:TRP:HB3	1:D:198:THR:HG21	1.97	0.46
1:F:320:ALA:HB2	1:F:360:SER:HB2	1.99	0.46
1:F:115:ARG:NH2	1:F:159:PRO:HD2	2.31	0.45
1:B:178:LEU:N	1:B:179:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296[B]:HIS:CE1	1:E:300:ARG:HH21	2.34	0.45
1:B:166:ASP:HA	1:B:197:ASN:HB2	1.98	0.45
1:A:77:THR:HA	1:A:124:TYR:HB3	1.99	0.45
1:C:77:THR:HA	1:C:124:TYR:HB3	1.98	0.45
1:E:19:PHE:HB3	1:E:278:ASN:HA	1.99	0.45
1:A:19:PHE:HB3	1:A:278:ASN:HA	1.99	0.44
1:A:199:GLY:O	1:A:206:VAL:HA	2.16	0.44
1:B:173:ASP:OD1	1:B:173:ASP:N	2.45	0.44
1:D:199:GLY:HA3	1:D:214:VAL:HG22	1.98	0.44
1:D:206:VAL:HG11	1:D:234:VAL:HG21	1.98	0.44
1:C:287:ILE:HG21	1:C:295:MET:HE1	1.99	0.44
1:C:33:TRP:CZ3	1:D:349:VAL:HG21	2.52	0.44
1:D:279:ILE:HD11	1:D:295:MET:SD	2.58	0.44
1:C:269:ARG:HA	1:C:269:ARG:HD2	1.82	0.43
1:C:178:LEU:N	1:C:179:PRO:CD	2.82	0.43
1:C:19:PHE:HB3	1:C:278:ASN:HA	2.00	0.43
1:E:270:HIS:HB2	1:E:326:PHE:CE1	2.54	0.43
1:F:2:THR:HG22	1:F:3:GLU:H	1.84	0.43
1:B:320:ALA:HB2	1:B:360:SER:HB2	2.00	0.43
1:C:210:GLU:HA	1:C:210:GLU:OE1	2.19	0.43
1:C:264:THR:HG22	1:C:275:ILE:CD1	2.49	0.43
1:F:228:ALA:HB3	1:F:231:GLU:HG3	2.01	0.43
1:D:320:ALA:HB2	1:D:360:SER:HB2	2.01	0.42
1:E:350:VAL:O	1:E:350:VAL:HG13	2.18	0.42
1:B:199:GLY:HA3	1:B:214:VAL:HG22	2.00	0.42
1:D:77:THR:HA	1:D:124:TYR:HB3	2.01	0.42
1:F:219:ARG:O	1:F:220:THR:C	2.62	0.42
1:A:191:ASN:ND2	2:A:513:HOH:O	2.51	0.42
1:B:19:PHE:HB3	1:B:278:ASN:HA	2.01	0.42
1:B:22:TRP:CZ3	1:B:106:LEU:HD13	2.54	0.42
1:D:19:PHE:HB3	1:D:278:ASN:HA	2.01	0.42
1:E:22:TRP:CZ3	1:E:106:LEU:HD13	2.55	0.42
1:A:22:TRP:CZ3	1:A:106:LEU:HD13	2.55	0.42
1:A:219:ARG:O	1:A:220:THR:C	2.63	0.42
1:E:169:TRP:CZ2	1:F:349:VAL:HG13	2.55	0.42
1:C:2:THR:HG22	1:C:3:GLU:H	1.85	0.42
1:D:270:HIS:HB2	1:D:326:PHE:CE1	2.54	0.42
1:D:148:LYS:NZ	2:D:509:HOH:O	2.51	0.42
1:E:373:TRP:CD1	1:E:380:LEU:HD21	2.55	0.41
1:F:19:PHE:HB3	1:F:278:ASN:HA	2.01	0.41
1:E:178:LEU:N	1:E:179:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:THR:HG22	1:F:3:GLU:N	2.35	0.41
1:D:2:THR:HG22	1:D:3:GLU:N	2.35	0.41
1:D:218:ARG:HB2	2:D:536:HOH:O	2.19	0.41
1:A:269:ARG:HA	1:A:269:ARG:HD2	1.88	0.41
1:C:22:TRP:CZ3	1:C:106:LEU:HD13	2.55	0.41
1:E:2:THR:HG22	1:E:3:GLU:N	2.35	0.41
1:F:22:TRP:CZ3	1:F:106:LEU:HD13	2.55	0.41
1:C:2:THR:HG22	1:C:3:GLU:N	2.35	0.41
1:A:373:TRP:CD1	1:A:380:LEU:HD21	2.56	0.41
1:B:373:TRP:CD1	1:B:380:LEU:HD21	2.56	0.41
1:D:178:LEU:N	1:D:179:PRO:CD	2.84	0.41
1:D:279:ILE:HD13	1:D:279:ILE:HG21	1.90	0.41
1:B:238:ILE:HD11	1:B:268:ALA:HB2	2.01	0.41
1:F:77:THR:HA	1:F:124:TYR:HB3	2.03	0.41
1:F:167:GLY:HA3	1:F:170:ASN:ND2	2.35	0.41
1:B:20:ILE:HD13	1:B:279:ILE:HG12	2.02	0.41
1:F:269:ARG:HA	1:F:269:ARG:HD2	1.80	0.41
1:B:292:GLN:HG3	2:B:613:HOH:O	2.20	0.40
1:C:184:MET:HE3	1:C:184:MET:HB3	1.95	0.40
1:F:373:TRP:CD1	1:F:380:LEU:HD21	2.56	0.40
1:C:374:LEU:HD23	1:C:374:LEU:HA	1.93	0.40
1:E:39:HIS:NE2	1:F:346:LYS:HG3	2.36	0.40
1:C:373:TRP:CD1	1:C:380:LEU:HD21	2.56	0.40
1:E:77:THR:HA	1:E:124:TYR:HB3	2.03	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	408/414 (99%)	396 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	407/414 (98%)	397 (98%)	10 (2%)	0	100	100
1	C	403/414 (97%)	391 (97%)	12 (3%)	0	100	100
1	D	405/414 (98%)	394 (97%)	11 (3%)	0	100	100
1	E	404/414 (98%)	395 (98%)	9 (2%)	0	100	100
1	F	406/414 (98%)	396 (98%)	10 (2%)	0	100	100
All	All	2433/2484 (98%)	2369 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	343/346 (99%)	337 (98%)	6 (2%)	56	66
1	B	342/346 (99%)	338 (99%)	4 (1%)	67	76
1	C	339/346 (98%)	333 (98%)	6 (2%)	54	64
1	D	341/346 (99%)	339 (99%)	2 (1%)	84	89
1	E	341/346 (99%)	333 (98%)	8 (2%)	45	54
1	F	341/346 (99%)	339 (99%)	2 (1%)	84	89
All	All	2047/2076 (99%)	2019 (99%)	28 (1%)	62	72

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	103	ARG
1	A	107	ILE
1	A	111	VAL
1	A	200	LEU
1	A	354	GLU
1	B	56	GLN
1	B	107	ILE

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Mol	Chain	Res	Type
1	B	214	VAL
1	B	354	GLU
1	C	56	GLN
1	C	107	ILE
1	C	120	LEU
1	C	180	GLU
1	C	214	VAL
1	C	354	GLU
1	D	56	GLN
1	D	354	GLU
1	E	28	MET
1	E	56	GLN
1	E	107	ILE
1	E	116	GLU
1	E	124	TYR
1	E	180	GLU
1	E	198	THR
1	E	354	GLU
1	F	107	ILE
1	F	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	187	HIS
1	A	191	ASN
1	A	366	GLN
1	A	410	GLN
1	B	27	GLN
1	B	43	HIS
1	B	191	ASN
1	B	270	HIS
1	B	296	HIS
1	B	366	GLN
1	B	410	GLN
1	C	168	ASN
1	C	170	ASN
1	C	191	ASN
1	C	230	ASN
1	C	292	GLN
1	C	410	GLN

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Mol	Chain	Res	Type
1	D	147	GLN
1	D	168	ASN
1	D	191	ASN
1	D	296	HIS
1	D	366	GLN
1	D	372	HIS
1	D	410	GLN
1	E	27	GLN
1	E	39	HIS
1	E	147	GLN
1	E	187	HIS
1	E	366	GLN
1	E	372	HIS
1	E	410	GLN
1	F	27	GLN
1	F	230	ASN
1	F	410	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides 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 (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	412/414 (99%)	-0.29	22 (5%)	33	33	19, 30, 76, 116	0
1	B	410/414 (99%)	-0.32	24 (5%)	29	29	19, 30, 74, 135	1 (0%)
1	C	407/414 (98%)	-0.19	20 (4%)	36	35	21, 34, 71, 134	0
1	D	409/414 (98%)	-0.44	17 (4%)	41	41	19, 28, 67, 112	0
1	E	407/414 (98%)	-0.11	20 (4%)	36	35	18, 35, 77, 123	1 (0%)
1	F	410/414 (99%)	-0.14	28 (6%)	25	24	23, 33, 82, 150	0
All	All	2455/2484 (98%)	-0.25	131 (5%)	33	33	18, 32, 75, 150	2 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	169	TRP	9.4
1	F	228	ALA	8.2
1	A	202	ASN	7.8
1	F	169	TRP	7.1
1	F	225	TYR	6.9
1	B	169	TRP	6.2
1	D	225	TYR	6.1
1	F	229	PRO	6.1
1	A	169	TRP	6.0
1	C	225	TYR	6.0
1	E	225	TYR	5.9
1	C	229	PRO	5.7
1	B	198	THR	5.3
1	E	198	THR	5.2
1	F	201	LYS	5.2
1	E	168	ASN	5.1
1	C	1	MET	5.1
1	A	172	LYS	5.0
1	B	199	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	201	LYS	4.8
1	A	1	MET	4.8
1	A	200	LEU	4.6
1	F	349	VAL	4.5
1	B	204	GLY	4.5
1	E	167	GLY	4.4
1	D	204	GLY	4.4
1	D	228	ALA	4.3
1	A	225	TYR	4.2
1	E	205	GLN	4.2
1	D	199	GLY	4.1
1	B	172	LYS	4.1
1	C	228	ALA	4.0
1	E	229	PRO	3.9
1	A	346	LYS	3.9
1	E	172	LYS	3.8
1	F	350	VAL	3.8
1	F	173	ASP	3.7
1	B	350	VAL	3.7
1	E	346	LYS	3.7
1	D	229	PRO	3.6
1	B	1	MET	3.6
1	A	228	ALA	3.6
1	F	2	THR	3.6
1	F	172	LYS	3.5
1	A	229	PRO	3.5
1	C	353	GLY	3.5
1	A	222	ASP	3.4
1	F	200	LEU	3.4
1	A	199	GLY	3.4
1	D	172	LYS	3.3
1	A	345	GLY	3.3
1	D	227	GLY	3.3
1	E	170	ASN	3.2
1	B	229	PRO	3.2
1	F	198	THR	3.2
1	A	349	VAL	3.2
1	A	353	GLY	3.2
1	B	347	ASP	3.2
1	C	345	GLY	3.2
1	E	228	ALA	3.1
1	F	227	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	349	VAL	3.1
1	A	352	GLY	3.1
1	B	225	TYR	3.1
1	F	199	GLY	3.0
1	C	350	VAL	3.0
1	C	205	GLN	3.0
1	B	345	GLY	3.0
1	E	350	VAL	3.0
1	C	349	VAL	2.9
1	C	39	HIS	2.9
1	D	348	ASN	2.9
1	B	349	VAL	2.8
1	C	197	ASN	2.8
1	E	227	GLY	2.8
1	B	348	ASN	2.8
1	C	168	ASN	2.7
1	C	348	ASN	2.7
1	F	223	GLU	2.7
1	D	39	HIS	2.7
1	F	205	GLN	2.7
1	C	351	LEU	2.7
1	E	2	THR	2.7
1	F	224	ILE	2.7
1	F	230	ASN	2.6
1	D	349	VAL	2.6
1	A	223	GLU	2.6
1	B	351	LEU	2.6
1	A	348	ASN	2.6
1	C	173	ASP	2.6
1	B	173	ASP	2.5
1	F	222	ASP	2.5
1	B	205	GLN	2.5
1	D	170	ASN	2.5
1	D	345	GLY	2.4
1	C	206	VAL	2.4
1	F	64	HIS	2.4
1	F	347	ASP	2.4
1	F	332	LYS	2.4
1	F	348	ASN	2.4
1	C	169	TRP	2.4
1	E	348	ASN	2.4
1	B	170	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	227	GLY	2.3
1	D	205	GLN	2.3
1	F	351	LEU	2.3
1	A	205	GLN	2.3
1	B	168	ASN	2.3
1	D	222	ASP	2.3
1	C	230	ASN	2.2
1	B	219	ARG	2.2
1	B	352	GLY	2.2
1	F	231	GLU	2.2
1	E	230	ASN	2.2
1	A	354	GLU	2.2
1	F	354	GLU	2.1
1	D	169	TRP	2.1
1	E	351	LEU	2.1
1	F	168	ASN	2.1
1	C	172	LYS	2.1
1	F	345	GLY	2.1
1	E	39	HIS	2.1
1	D	168	ASN	2.1
1	B	223	GLU	2.1
1	B	171	LYS	2.1
1	E	296[A]	HIS	2.0
1	B	346	LYS	2.0
1	B	197	ASN	2.0
1	D	230	ASN	2.0
1	A	173	ASP	2.0
1	C	167	GLY	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.