Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 04:05 am BST

PDB ID	:	7BJ5
Title	:	Inulosucrase from Halalkalicoccus jeotgali
Authors	:	Ghauri, K.; Pijning, T.; Munawar, N.; Ali, H.; Ghauri, M.A.; Anwar, M.A.; Wallis, R.
Deposited on	:	2021-01-14
Resolution	:	2.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

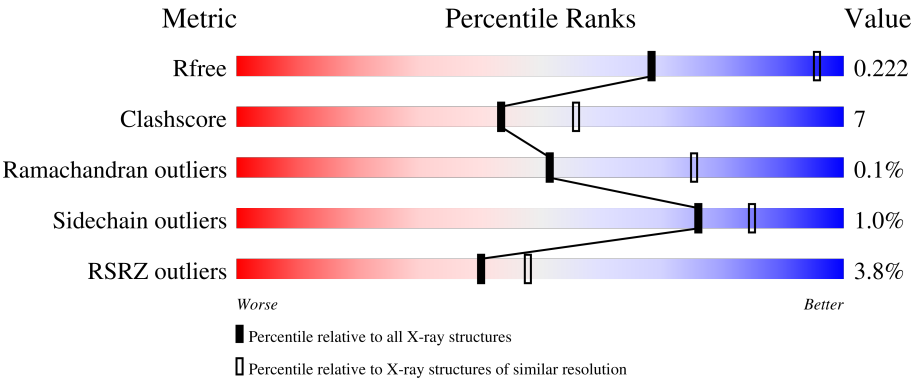
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	428	81% 14% 5%
1	B	428	7% 79% 16% 5%
1	C	428	% 83% 11% 5%
1	D	428	% 78% 16% • 5%
1	E	428	% 81% 14% 5%

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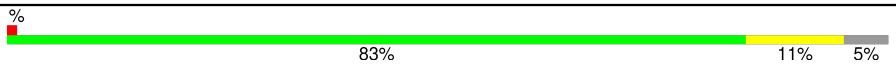
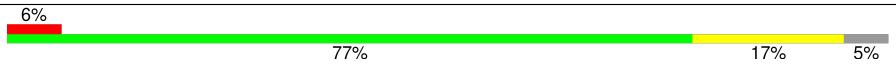
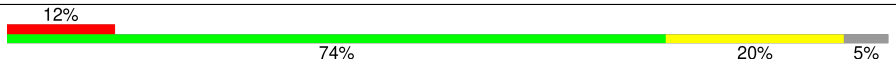
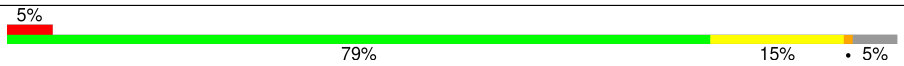
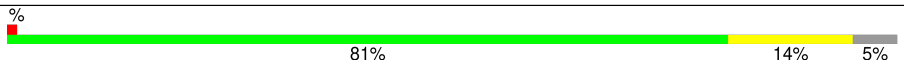
Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	
1	I	428	
1	J	428	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31875 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 Levansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	B	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	C	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	D	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	E	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	F	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	G	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	H	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	I	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			
1	J	406	Total	C	N	O	S	0	0	0
			3180	2013	546	617	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	11	Total	O	0	0
			11	11		
2	D	14	Total	O	0	0
			14	14		

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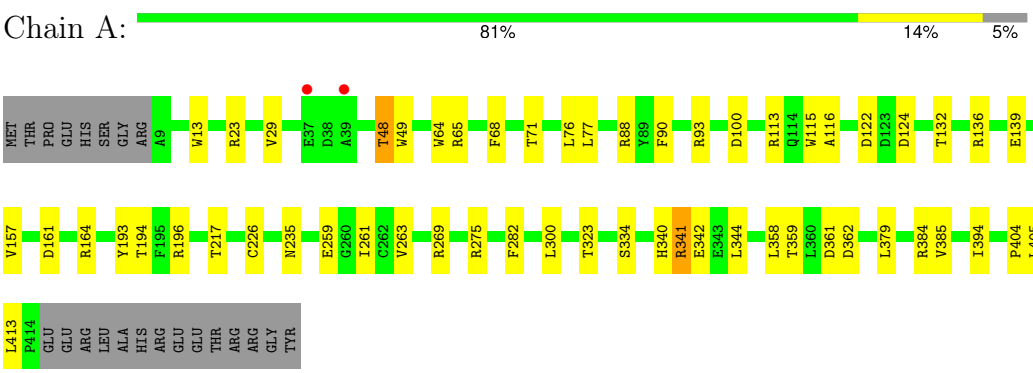
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	9	Total O 9 9	0	0
2	F	16	Total O 16 16	0	0
2	H	4	Total O 4 4	0	0
2	I	8	Total O 8 8	0	0
2	J	4	Total O 4 4	0	0

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.

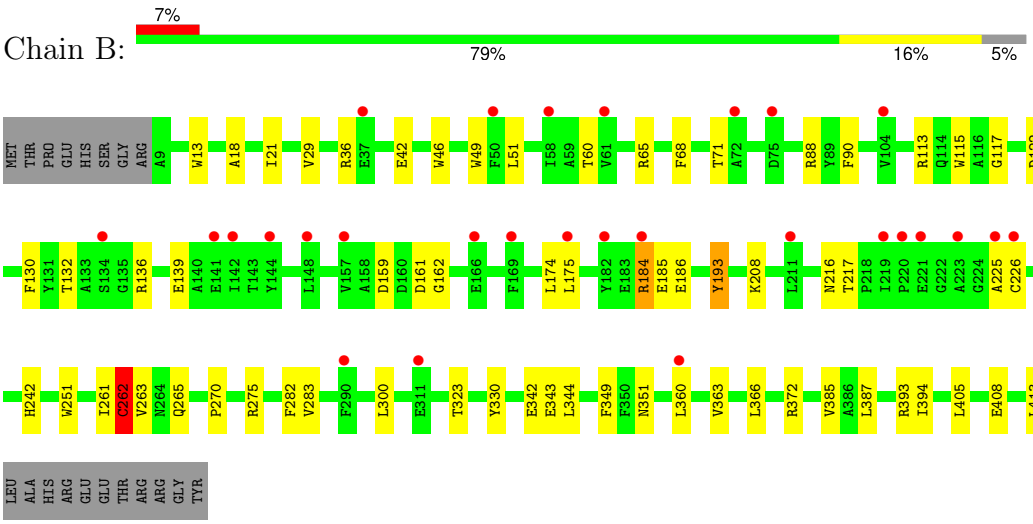
• Molecule 1: Levansucrase

Chain A:



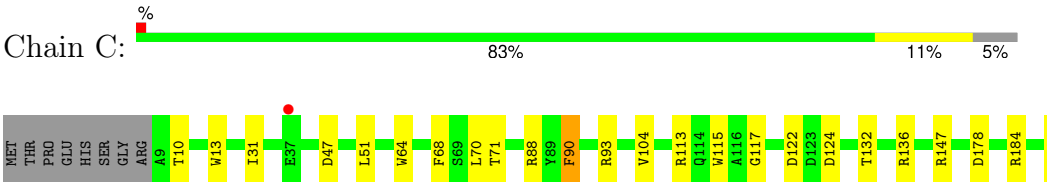
• Molecule 1: Levansucrase

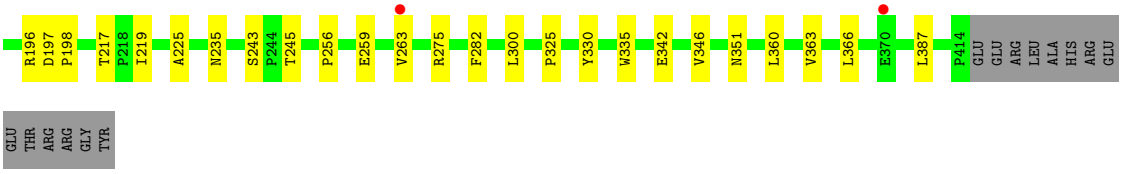
Chain B:



• Molecule 1: Levansucrase

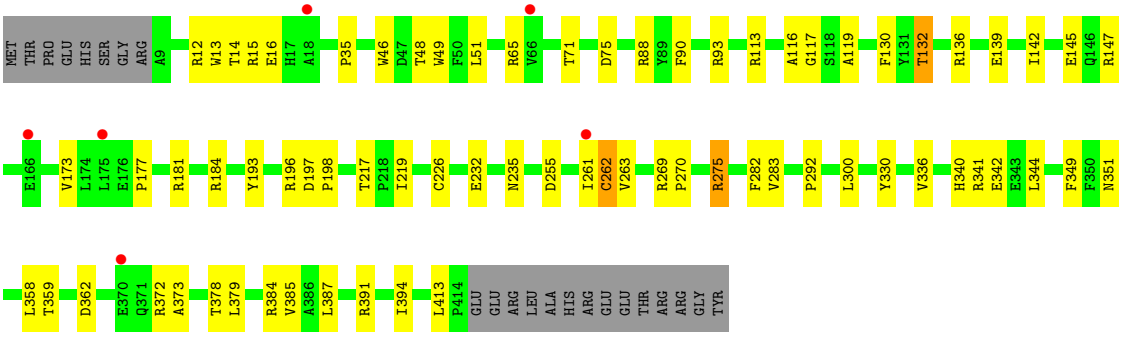
Chain C:





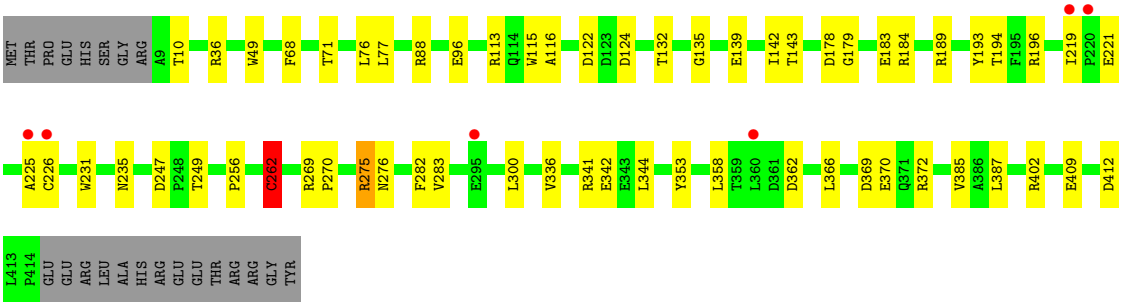
• Molecule 1: Levansucrase

Chain D:



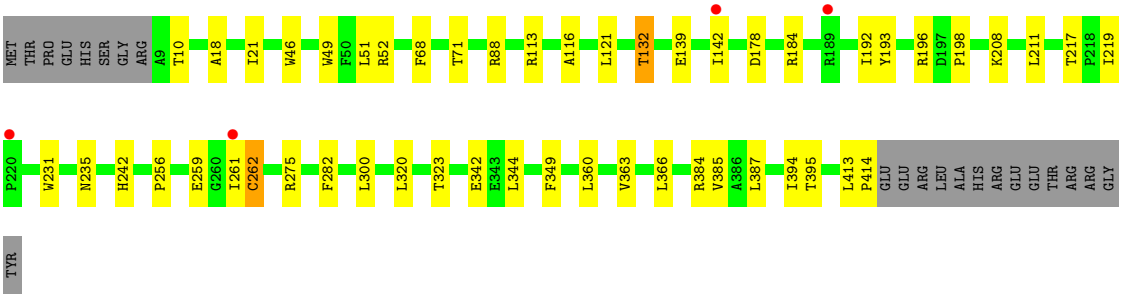
• Molecule 1: Levansucrase

Chain E:



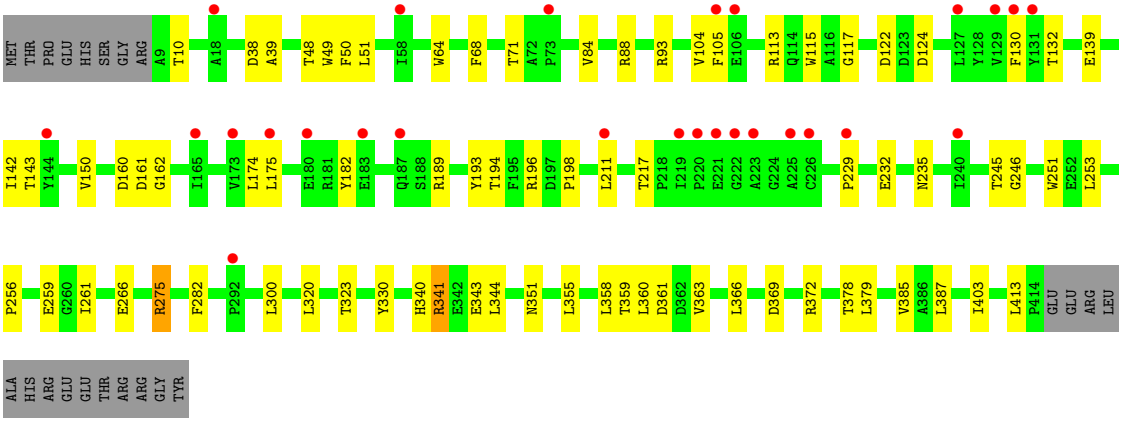
• Molecule 1: Levansucrase

Chain F:



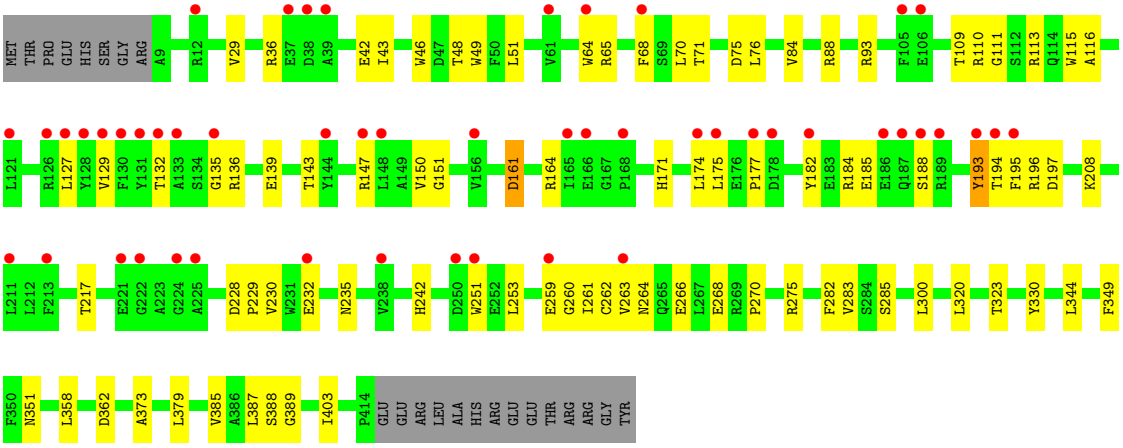
• Molecule 1: Levansucrase

Chain G:



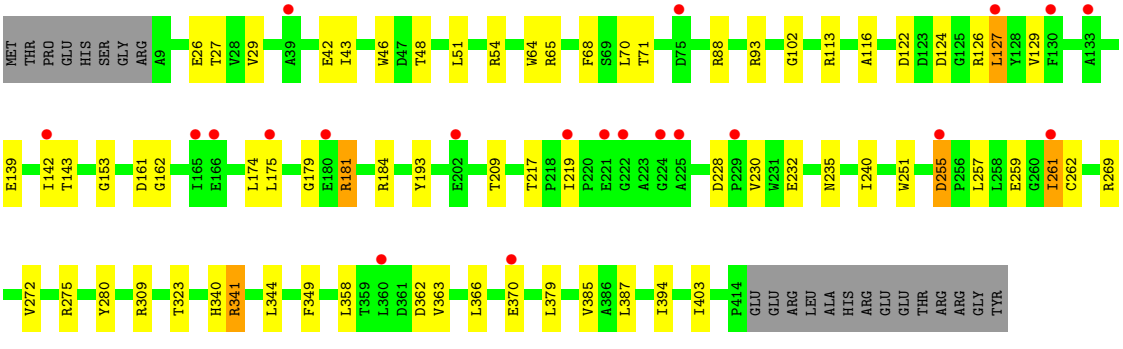
• Molecule 1: Levansucrase

Chain H:



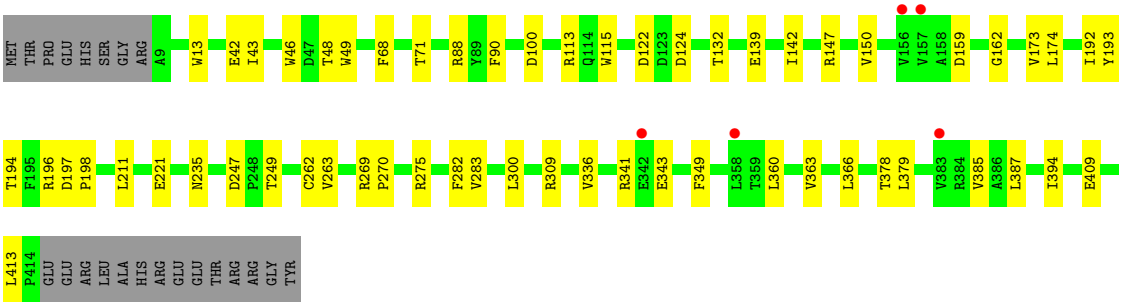
• Molecule 1: Levansucrase

Chain I:



• Molecule 1: Levansucrase

Chain J:


MET THR PRO GLU HIS SER GLY ARG A9 W13 E42 I43 W46 D47 T48 W49 F68 T71 R88 Y89 F90 D100 R113 Q114 W115 D122 D123 D124 T132 E139 I142 R147 V150 V156 V157 A158 D159 G162 V173 L174 I192 Y193
T194 F195 R196 D197 P198 L211 E221 N235 D247 P248 T249 C262 V263 R269 P270 R275 F282 V283 L300 R309 V336 R341 E342 E343 F349 L358 T359 L360 V363 L366 T378 L379 V383 R384 V385 A386 L387 I394 E409
L413 P414 GLU GLU ARG LEU ALA HIS ARG GLU GLU THR ARG ARG GLY TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.54Å 143.26Å 172.76Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	105.82 – 2.75 170.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	57.9 (105.82-2.75) 58.0 (170.95-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.228 0.181 , 0.222	Depositor DCC
R_{free} test set	4331 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31875	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6812e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.32	0/3274	0.54	0/4466
1	B	0.33	0/3274	0.57	3/4466 (0.1%)
1	C	0.32	0/3274	0.55	0/4466
1	D	0.33	0/3274	0.57	1/4466 (0.0%)
1	E	0.32	0/3274	0.56	2/4466 (0.0%)
1	F	0.33	0/3274	0.56	1/4466 (0.0%)
1	G	0.30	0/3274	0.55	0/4466
1	H	0.33	0/3274	0.60	2/4466 (0.0%)
1	I	0.30	0/3274	0.55	2/4466 (0.0%)
1	J	0.32	0/3274	0.55	1/4466 (0.0%)
All	All	0.32	0/32740	0.56	12/44660 (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	A	0	1
1	D	0	2
1	E	0	1
1	G	0	2
1	I	0	1
All	All	0	7

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	262	CYS	CA-CB-SG	-8.28	99.09	114.00
1	D	262	CYS	CA-CB-SG	8.06	128.51	114.00
1	H	161	ASP	CB-CG-OD2	-6.79	112.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	161	ASP	CB-CG-OD1	6.56	124.20	118.30
1	I	261	ILE	CG1-CB-CG2	-6.15	97.87	111.40
1	E	226	CYS	CA-CB-SG	6.02	124.84	114.00
1	B	226	CYS	CA-CB-SG	5.66	124.19	114.00
1	I	181	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	184	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	262	CYS	CA-CB-SG	5.41	123.73	114.00
1	E	262	CYS	CA-CB-SG	5.39	123.71	114.00
1	J	262	CYS	CA-CB-SG	5.12	123.21	114.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	HIS	Peptide
1	D	275	ARG	Peptide
1	D	340	HIS	Peptide
1	E	275	ARG	Peptide
1	G	275	ARG	Peptide
1	G	340	HIS	Peptide
1	I	340	HIS	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	3180	0	2977	38	0
1	B	3180	0	2977	43	0
1	C	3180	0	2977	36	0
1	D	3180	0	2977	46	0
1	E	3180	0	2977	35	0
1	F	3180	0	2977	34	0
1	G	3180	0	2977	49	0
1	H	3180	0	2977	58	0
1	I	3180	0	2977	46	0
1	J	3180	0	2977	37	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	0	1	0
2	C	11	0	0	1	0
2	D	14	0	0	2	0
2	E	9	0	0	0	0
2	F	16	0	0	3	0
2	H	4	0	0	0	0
2	I	8	0	0	3	0
2	J	4	0	0	0	0
All	All	31875	0	29770	415	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 (415) 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:H:161:ASP:OD1	1:H:164:ARG:NH1	2.04	0.89
1:E:275:ARG:HD3	1:E:387:LEU:HD12	1.59	0.83
1:I:54:ARG:NH1	2:I:501:HOH:O	2.12	0.82
1:G:150:VAL:HG12	1:G:174:LEU:HD11	1.61	0.81
1:J:341:ARG:HH12	1:J:409:GLU:HG2	1.50	0.77
1:I:255:ASP:HB2	1:I:309:ARG:HH22	1.51	0.76
1:E:219:ILE:HD11	1:E:225:ALA:HB3	1.67	0.75
1:C:219:ILE:HD11	1:C:225:ALA:HB3	1.67	0.74
1:H:109:THR:HA	1:H:171:HIS:CE1	2.22	0.74
1:B:175:LEU:HD11	1:B:251:TRP:HB2	1.69	0.73
1:I:54:ARG:NH2	1:I:209:THR:OG1	2.20	0.73
1:A:341:ARG:HH12	1:A:409:GLU:HG2	1.53	0.72
1:J:132:THR:HG21	1:J:197:ASP:H	1.53	0.72
1:H:150:VAL:O	1:H:171:HIS:HB2	1.90	0.71
1:F:52:ARG:NH1	2:F:502:HOH:O	2.18	0.71
1:G:10:THR:HG21	1:G:256:PRO:HG2	1.73	0.71
1:C:10:THR:HG21	1:C:256:PRO:HG2	1.73	0.69
1:J:363:VAL:HA	1:J:366:LEU:HD13	1.73	0.69
1:B:372:ARG:NH2	1:J:221:GLU:OE2	2.25	0.68
1:J:159:ASP:OD1	1:J:162:GLY:N	2.25	0.68
1:D:181:ARG:NH1	1:D:255:ASP:OD1	2.28	0.67
1:F:10:THR:HG21	1:F:256:PRO:HG2	1.76	0.67
1:C:189:ARG:HH21	1:C:219:ILE:HG23	1.61	0.66
1:D:147:ARG:HE	1:D:173:VAL:HG21	1.61	0.65
1:D:261:ILE:O	1:D:262:CYS:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ARG:HH12	1:E:409:GLU:HG2	1.59	0.65
1:E:179:GLY:HA3	1:E:184:ARG:NH2	2.12	0.64
1:A:161:ASP:OD1	1:C:147:ARG:NH2	2.29	0.64
1:B:136:ARG:N	1:B:139:GLU:OE2	2.31	0.63
1:J:385:VAL:HG12	1:J:394:ILE:HD13	1.80	0.63
1:G:115:TRP:HB2	1:G:132:THR:HB	1.81	0.63
1:D:270:PRO:HB3	1:D:283:VAL:HG12	1.81	0.63
1:E:10:THR:HG21	1:E:256:PRO:HG2	1.79	0.63
1:H:174:LEU:HB3	1:H:175:LEU:HD12	1.81	0.62
1:E:96:GLU:OE2	1:E:402:ARG:NH1	2.32	0.62
1:H:175:LEU:HD11	1:H:251:TRP:HB2	1.80	0.62
1:J:115:TRP:HB2	1:J:132:THR:OG1	1.99	0.62
1:F:208:LYS:HE3	1:F:242:HIS:CE1	2.35	0.62
1:E:275:ARG:HH22	1:E:342:GLU:HA	1.65	0.62
1:G:229:PRO:O	1:G:232:GLU:HG2	2.00	0.62
1:F:385:VAL:HG12	1:F:394:ILE:HD13	1.82	0.62
1:B:275:ARG:HH22	1:B:342:GLU:HA	1.65	0.61
1:C:363:VAL:HA	1:C:366:LEU:HD13	1.82	0.61
1:H:320:LEU:HD11	1:H:323:THR:HB	1.83	0.61
1:F:414:PRO:O	2:F:501:HOH:O	2.16	0.61
1:B:184:ARG:HG2	1:B:186:GLU:OE1	2.01	0.60
1:D:132:THR:HG23	1:D:198:PRO:HD3	1.81	0.60
1:I:175:LEU:HD11	1:I:251:TRP:HB2	1.84	0.60
1:H:151:GLY:HA2	1:H:171:HIS:HB3	1.83	0.60
1:I:363:VAL:HA	1:I:366:LEU:HD13	1.83	0.60
1:C:132:THR:HG21	1:C:197:ASP:H	1.66	0.59
1:I:65:ARG:NH1	1:I:403:ILE:O	2.33	0.59
1:H:217:THR:HG21	1:H:259:GLU:OE2	2.02	0.59
1:A:341:ARG:NH1	1:A:409:GLU:HG2	2.18	0.59
1:C:132:THR:HG23	1:C:198:PRO:HD3	1.85	0.58
1:D:385:VAL:HG12	1:D:394:ILE:HD13	1.85	0.58
1:G:182:TYR:HD2	1:G:253:LEU:HD23	1.68	0.58
1:H:229:PRO:O	1:H:232:GLU:HG2	2.02	0.58
1:G:189:ARG:NH1	1:G:232:GLU:OE2	2.36	0.58
1:G:275:ARG:HD3	1:G:387:LEU:HD12	1.86	0.58
1:G:142:ILE:H	1:G:142:ILE:HD12	1.67	0.58
1:J:147:ARG:HE	1:J:173:VAL:HG21	1.69	0.58
1:I:27:THR:HA	1:I:394:ILE:HD13	1.86	0.57
1:J:247:ASP:OD2	1:J:249:THR:OG1	2.19	0.57
1:B:275:ARG:HD3	1:B:387:LEU:HD12	1.87	0.57
1:C:243:SER:OG	1:C:245:THR:O	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:LEU:HD23	1:G:251:TRP:CD1	2.40	0.57
1:A:139:GLU:OE2	1:A:142:ILE:HA	2.05	0.57
1:E:189:ARG:HD2	1:E:221:GLU:HG2	1.86	0.57
1:A:115:TRP:HB2	1:A:132:THR:HB	1.87	0.56
1:F:282:PHE:HB3	1:F:300:LEU:HD11	1.88	0.56
1:H:194:THR:HG21	1:H:266:GLU:HG2	1.88	0.56
1:D:275:ARG:HD3	1:D:387:LEU:HD12	1.88	0.56
1:F:275:ARG:HH22	1:F:342:GLU:HA	1.71	0.55
1:E:247:ASP:OD2	1:E:249:THR:OG1	2.20	0.55
1:B:235:ASN:HA	1:B:261:ILE:HD13	1.89	0.55
1:F:413:LEU:O	2:F:501:HOH:O	2.18	0.55
1:G:320:LEU:HD11	1:G:323:THR:HB	1.89	0.55
1:E:269:ARG:HH21	1:E:336:VAL:HG11	1.72	0.55
1:I:139:GLU:OE2	1:I:142:ILE:HA	2.07	0.55
1:H:136:ARG:O	1:H:139:GLU:HG3	2.06	0.55
1:B:363:VAL:HA	1:B:366:LEU:HD13	1.89	0.54
1:A:136:ARG:NH1	1:A:145:GLU:OE2	2.40	0.54
1:B:136:ARG:O	1:B:139:GLU:HG3	2.07	0.54
1:G:175:LEU:HD11	1:G:251:TRP:HB2	1.90	0.54
1:B:282:PHE:HB3	1:B:300:LEU:HD11	1.89	0.54
1:E:353:TYR:OH	1:H:36:ARG:NH2	2.41	0.54
1:B:174:LEU:HB3	1:B:175:LEU:HD12	1.90	0.54
1:B:185:GLU:HG3	1:B:193:TYR:CE1	2.43	0.54
1:H:109:THR:HA	1:H:171:HIS:HE1	1.69	0.53
1:A:269:ARG:NH1	1:A:334:SER:OG	2.37	0.53
1:I:261:ILE:HG22	1:I:262:CYS:SG	2.48	0.53
1:D:132:THR:HG21	1:D:196:ARG:HA	1.89	0.53
1:F:219:ILE:HD11	1:F:261:ILE:HD12	1.90	0.53
1:J:275:ARG:HD2	1:J:387:LEU:HD12	1.90	0.53
1:A:384:ARG:NH2	1:A:413:LEU:HD11	2.24	0.53
1:C:282:PHE:HB3	1:C:300:LEU:HD11	1.90	0.53
1:J:71:THR:HG21	1:J:88:ARG:HD3	1.90	0.53
1:D:359:THR:HG22	1:D:362:ASP:CG	2.30	0.52
1:J:132:THR:HG21	1:J:196:ARG:HB2	1.90	0.52
1:E:369:ASP:OD1	1:E:372:ARG:NH1	2.43	0.52
1:I:174:LEU:HB3	1:I:175:LEU:HD12	1.92	0.52
1:B:217:THR:OG1	1:B:261:ILE:HD11	2.09	0.52
1:H:275:ARG:HD3	1:H:387:LEU:HD12	1.92	0.52
1:G:182:TYR:CD2	1:G:253:LEU:HD23	2.44	0.52
1:C:275:ARG:HH22	1:C:342:GLU:HA	1.74	0.52
1:J:275:ARG:NH2	1:J:343:GLU:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:VAL:HA	1:F:366:LEU:HD13	1.92	0.52
1:J:132:THR:CG2	1:J:197:ASP:H	2.22	0.52
1:B:161:ASP:OD1	1:B:162:GLY:N	2.43	0.51
1:C:64:TRP:CZ3	1:C:93:ARG:HG3	2.45	0.51
1:G:363:VAL:HA	1:G:366:LEU:HD13	1.93	0.51
1:E:282:PHE:HB3	1:E:300:LEU:HD11	1.93	0.51
1:I:344:LEU:HB3	1:I:385:VAL:HG22	1.93	0.51
1:D:391:ARG:NH2	2:D:502:HOH:O	2.44	0.51
1:H:185:GLU:H	1:H:185:GLU:CD	2.13	0.51
1:A:269:ARG:HH11	1:A:334:SER:HG	1.58	0.51
1:E:358:LEU:HD22	1:E:362:ASP:HB3	1.93	0.51
1:I:240:ILE:HD12	1:I:257:LEU:HD11	1.92	0.51
1:E:344:LEU:HD22	1:E:387:LEU:HD11	1.93	0.51
1:D:358:LEU:HD22	1:D:362:ASP:HB3	1.93	0.51
1:E:116:ALA:HB1	1:E:269:ARG:NH1	2.26	0.50
1:H:136:ARG:HG2	1:H:147:ARG:HH22	1.76	0.50
1:D:14:THR:OG1	1:D:16:GLU:HG2	2.11	0.50
1:B:65:ARG:HH22	1:B:408:GLU:CD	2.13	0.50
1:D:71:THR:HG21	1:D:88:ARG:HD3	1.93	0.50
1:H:196:ARG:NH1	1:H:197:ASP:OD1	2.45	0.50
1:D:269:ARG:HH21	1:D:336:VAL:HG11	1.76	0.50
1:E:71:THR:HG21	1:E:88:ARG:HD2	1.93	0.50
1:J:270:PRO:HB3	1:J:283:VAL:HG12	1.92	0.50
1:C:275:ARG:HD3	1:C:387:LEU:HD12	1.94	0.50
1:G:369:ASP:OD1	1:G:372:ARG:NH1	2.45	0.50
1:H:151:GLY:HA2	1:H:171:HIS:CB	2.41	0.50
1:I:344:LEU:HD22	1:I:387:LEU:HD11	1.93	0.50
1:A:194:THR:HG22	1:A:196:ARG:HH12	1.76	0.50
1:D:12:ARG:NH2	2:D:501:HOH:O	2.28	0.50
1:G:359:THR:OG1	1:G:361:ASP:OD1	2.26	0.50
1:H:185:GLU:HA	1:H:188:SER:HB2	1.94	0.50
1:A:385:VAL:HG12	1:A:394:ILE:HD13	1.93	0.49
1:B:36:ARG:HH12	1:D:373:ALA:HB2	1.77	0.49
1:B:71:THR:HG21	1:B:88:ARG:HD3	1.94	0.49
1:A:13:TRP:O	1:A:263:VAL:HG21	2.12	0.49
1:D:136:ARG:NH1	1:D:145:GLU:OE2	2.44	0.49
1:F:132:THR:HG23	1:F:198:PRO:HD3	1.93	0.49
1:D:132:THR:HG21	1:D:196:ARG:CA	2.42	0.49
1:E:231:TRP:HB3	1:E:262:CYS:HB3	1.94	0.49
1:G:64:TRP:CZ3	1:G:93:ARG:HG3	2.48	0.49
1:D:219:ILE:HD11	1:D:261:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ARG:HH22	1:D:342:GLU:HA	1.77	0.49
1:I:275:ARG:HD3	1:I:387:LEU:HD12	1.94	0.49
1:F:275:ARG:HD3	1:F:387:LEU:HD12	1.94	0.49
1:B:115:TRP:HB2	1:B:132:THR:HB	1.94	0.49
1:D:282:PHE:HB3	1:D:300:LEU:HD11	1.95	0.49
1:F:139:GLU:OE2	1:F:142:ILE:HA	2.13	0.49
1:A:359:THR:OG1	1:A:361:ASP:OD1	2.24	0.48
1:F:71:THR:HG21	1:F:88:ARG:HD3	1.94	0.48
1:F:320:LEU:HD11	1:F:323:THR:HB	1.96	0.48
1:A:76:LEU:HD23	1:A:77:LEU:O	2.13	0.48
1:A:282:PHE:HB3	1:A:300:LEU:HD11	1.95	0.48
1:A:358:LEU:HD22	1:A:362:ASP:HB3	1.94	0.48
1:C:132:THR:HG21	1:C:196:ARG:HA	1.94	0.48
1:F:46:TRP:HB2	1:F:349:PHE:CE1	2.49	0.48
1:D:217:THR:OG1	1:D:261:ILE:HD11	2.13	0.48
1:G:282:PHE:HB3	1:G:300:LEU:HD11	1.96	0.48
1:I:142:ILE:HD12	1:I:142:ILE:H	1.78	0.48
1:C:189:ARG:NH1	2:C:504:HOH:O	2.45	0.48
1:J:343:GLU:OE1	1:J:413:LEU:HD11	2.14	0.48
1:F:132:THR:HG21	1:F:196:ARG:HA	1.94	0.48
1:C:132:THR:HG21	1:C:196:ARG:CA	2.44	0.48
1:E:235:ASN:N	1:E:235:ASN:OD1	2.47	0.48
1:B:42:GLU:OE1	1:B:42:GLU:N	2.40	0.48
1:G:38:ASP:OD1	1:G:39:ALA:N	2.47	0.48
1:H:282:PHE:HB3	1:H:300:LEU:HD11	1.95	0.48
1:F:18:ALA:HA	1:F:21:ILE:HG13	1.95	0.48
1:J:42:GLU:HG3	1:J:43:ILE:HG23	1.96	0.48
1:G:139:GLU:OE2	1:G:142:ILE:HA	2.14	0.47
1:H:29:VAL:HG22	1:H:323:THR:O	2.14	0.47
1:H:177:PRO:HG2	1:H:184:ARG:HD3	1.96	0.47
1:H:65:ARG:NH1	1:H:403:ILE:O	2.47	0.47
1:H:270:PRO:HB3	1:H:283:VAL:HG12	1.96	0.47
1:I:366:LEU:HD23	1:I:370:GLU:HB3	1.95	0.47
1:A:71:THR:HG21	1:A:88:ARG:HD2	1.96	0.47
1:A:341:ARG:H	1:A:341:ARG:HG3	1.39	0.47
1:D:139:GLU:OE2	1:D:142:ILE:HA	2.15	0.47
1:E:122:ASP:HB3	1:E:124:ASP:OD1	2.14	0.47
1:H:70:LEU:HD11	1:H:116:ALA:HA	1.96	0.47
1:B:122:ASP:HB3	1:B:124:ASP:OD1	2.14	0.47
1:B:235:ASN:OD1	1:B:235:ASN:N	2.47	0.47
1:G:93:ARG:NH2	1:G:160:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:TRP:CZ3	1:I:93:ARG:HG3	2.49	0.47
1:I:358:LEU:HD22	1:I:362:ASP:HB3	1.95	0.47
1:A:217:THR:OG1	1:A:261:ILE:HD11	2.15	0.47
1:H:136:ARG:HG2	1:H:147:ARG:NH2	2.29	0.47
1:H:110:ARG:H	1:H:171:HIS:HE1	1.62	0.47
1:J:341:ARG:NH1	1:J:409:GLU:HG2	2.23	0.47
1:C:47:ASP:HB2	1:C:70:LEU:HD23	1.97	0.47
1:G:71:THR:HG21	1:G:88:ARG:HD2	1.97	0.47
1:G:194:THR:HG21	1:G:266:GLU:HG2	1.96	0.47
1:G:245:THR:OG1	1:G:246:GLY:N	2.46	0.47
1:H:51:LEU:HB2	1:H:68:PHE:HE1	1.80	0.47
1:B:18:ALA:HA	1:B:21:ILE:HG13	1.97	0.47
1:G:122:ASP:HB3	1:G:124:ASP:OD1	2.15	0.47
1:G:139:GLU:OE1	1:G:143:THR:HG22	2.15	0.47
1:I:161:ASP:OD1	1:I:162:GLY:N	2.47	0.47
1:C:117:GLY:HA2	1:C:198:PRO:HD2	1.96	0.46
1:D:48:THR:HG21	1:D:379:LEU:HD21	1.97	0.46
1:G:174:LEU:HB3	1:G:175:LEU:HD12	1.97	0.46
1:H:182:TYR:HD2	1:H:253:LEU:HD23	1.80	0.46
1:H:344:LEU:HD22	1:H:387:LEU:HD11	1.97	0.46
1:J:269:ARG:HH21	1:J:336:VAL:HG11	1.80	0.46
1:F:217:THR:HG21	1:F:259:GLU:OE2	2.16	0.46
1:G:49:TRP:CE2	1:G:68:PHE:HB2	2.50	0.46
1:G:51:LEU:HB2	1:G:68:PHE:HE2	1.81	0.46
1:G:150:VAL:CG1	1:G:174:LEU:HD11	2.38	0.46
1:H:111:GLY:HA2	1:H:135:GLY:O	2.16	0.46
1:H:235:ASN:N	1:H:235:ASN:OD1	2.47	0.46
1:F:235:ASN:OD1	1:F:235:ASN:N	2.49	0.46
1:D:132:THR:HG21	1:D:196:ARG:HB2	1.97	0.46
1:D:270:PRO:HA	1:D:282:PHE:O	2.16	0.46
1:E:341:ARG:NH1	1:E:409:GLU:HG2	2.28	0.46
1:I:181:ARG:NH1	1:I:255:ASP:HA	2.31	0.46
1:D:330:TYR:O	1:D:351:ASN:HB3	2.16	0.46
1:G:217:THR:HG21	1:G:259:GLU:OE2	2.16	0.46
1:G:235:ASN:OD1	1:G:235:ASN:N	2.49	0.46
1:H:193:TYR:CE2	1:H:195:PHE:HB2	2.50	0.46
1:A:90:PHE:CD1	1:A:100:ASP:HA	2.51	0.46
1:A:235:ASN:OD1	1:A:235:ASN:N	2.49	0.46
1:F:231:TRP:HB3	1:F:262:CYS:SG	2.55	0.46
1:H:193:TYR:CD1	1:H:193:TYR:C	2.89	0.46
1:H:344:LEU:HB3	1:H:385:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:ASP:HB3	1:I:124:ASP:OD1	2.15	0.46
1:I:139:GLU:OE1	1:I:143:THR:HG22	2.16	0.46
1:C:217:THR:HG21	1:C:259:GLU:OE2	2.16	0.45
1:H:264:ASN:ND2	1:H:285:SER:OG	2.49	0.45
1:J:13:TRP:O	1:J:263:VAL:HG21	2.16	0.45
1:J:192:ILE:HD12	1:J:192:ILE:H	1.81	0.45
1:J:282:PHE:HB3	1:J:300:LEU:HD11	1.98	0.45
1:H:208:LYS:HE2	1:H:242:HIS:NE2	2.31	0.45
1:J:360:LEU:HD23	1:J:360:LEU:HA	1.73	0.45
1:B:185:GLU:HG3	1:B:193:TYR:CZ	2.52	0.45
1:J:378:THR:OG1	1:J:379:LEU:N	2.50	0.45
1:D:117:GLY:HA3	1:D:130:PHE:O	2.16	0.45
1:D:235:ASN:OD1	1:D:235:ASN:N	2.48	0.45
1:I:344:LEU:HB3	1:I:385:VAL:CG2	2.46	0.45
1:C:330:TYR:O	1:C:351:ASN:HB3	2.16	0.45
1:E:115:TRP:HB2	1:E:132:THR:HB	1.99	0.45
1:E:139:GLU:OE1	1:E:142:ILE:HA	2.16	0.45
1:G:378:THR:OG1	1:G:379:LEU:N	2.49	0.45
1:H:46:TRP:HB2	1:H:349:PHE:CE1	2.52	0.45
1:I:179:GLY:HA2	1:I:184:ARG:HG3	1.97	0.45
1:C:115:TRP:HB2	1:C:132:THR:OG1	2.17	0.45
1:E:344:LEU:HB3	1:E:385:VAL:HG22	1.99	0.45
1:G:84:VAL:HG12	1:G:84:VAL:O	2.16	0.45
1:J:139:GLU:OE2	1:J:142:ILE:HD13	2.17	0.45
1:C:47:ASP:CB	1:C:70:LEU:HD23	2.47	0.45
1:C:122:ASP:HB3	1:C:124:ASP:OD1	2.17	0.45
1:C:360:LEU:HD23	1:C:360:LEU:HA	1.77	0.44
1:A:157:VAL:HG22	1:A:164:ARG:HB2	1.99	0.44
1:C:51:LEU:HB2	1:C:68:PHE:HE1	1.82	0.44
1:D:116:ALA:HB1	1:D:269:ARG:NH1	2.31	0.44
1:H:139:GLU:OE1	1:H:143:THR:HG22	2.18	0.44
1:J:49:TRP:CE2	1:J:68:PHE:HB2	2.52	0.44
1:F:360:LEU:HD23	1:F:360:LEU:HA	1.79	0.44
1:H:64:TRP:CZ3	1:H:93:ARG:HG3	2.52	0.44
1:H:84:VAL:HG12	1:H:84:VAL:O	2.18	0.44
1:J:122:ASP:HB3	1:J:124:ASP:OD1	2.16	0.44
1:E:270:PRO:HB3	1:E:283:VAL:HG12	2.00	0.44
1:F:344:LEU:HD22	1:F:387:LEU:HD11	1.99	0.44
1:F:384:ARG:O	1:F:395:THR:HG22	2.18	0.44
1:H:261:ILE:HG22	1:H:262:CYS:SG	2.58	0.44
1:F:49:TRP:CZ3	1:F:116:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:THR:HG21	1:H:379:LEU:HD21	1.99	0.44
1:I:71:THR:HG21	1:I:88:ARG:HD3	1.99	0.44
1:A:90:PHE:HD1	1:A:100:ASP:HA	1.81	0.44
1:A:161:ASP:HA	1:C:136:ARG:HH11	1.82	0.44
1:H:115:TRP:HB2	1:H:132:THR:HB	1.98	0.44
1:I:70:LEU:HD11	1:I:116:ALA:HA	2.00	0.44
1:I:235:ASN:OD1	1:I:235:ASN:N	2.51	0.44
1:J:235:ASN:N	1:J:235:ASN:OD1	2.51	0.44
1:H:330:TYR:O	1:H:351:ASN:HB3	2.18	0.44
1:J:269:ARG:HH21	1:J:336:VAL:CG1	2.31	0.44
1:J:198:PRO:HB2	1:J:211:LEU:HD11	2.00	0.44
1:A:29:VAL:HG22	1:A:323:THR:O	2.18	0.43
1:B:231:TRP:HB3	1:B:262:CYS:HB3	2.00	0.43
1:F:198:PRO:HB2	1:F:211:LEU:HD11	1.98	0.43
1:G:104:VAL:HG13	1:G:105:PHE:CD1	2.53	0.43
1:G:360:LEU:HA	1:G:360:LEU:HD23	1.75	0.43
1:A:48:THR:HG21	1:A:379:LEU:HD21	1.99	0.43
1:B:225:ALA:N	1:B:232:GLU:OE2	2.51	0.43
1:D:226:CYS:HB2	1:D:232:GLU:HG3	2.00	0.43
1:E:366:LEU:HB3	1:E:370:GLU:HB2	2.00	0.43
1:G:50:PHE:CE1	1:G:403:ILE:HG12	2.53	0.43
1:G:330:TYR:O	1:G:351:ASN:HB3	2.19	0.43
1:A:64:TRP:CZ3	1:A:93:ARG:HG3	2.53	0.43
1:A:344:LEU:HB3	1:A:385:VAL:CG2	2.48	0.43
1:B:159:ASP:HB2	1:B:161:ASP:OD1	2.18	0.43
1:D:49:TRP:CZ3	1:D:116:ALA:HA	2.53	0.43
1:G:355:LEU:O	1:G:358:LEU:HD13	2.17	0.43
1:I:219:ILE:HG21	1:I:232:GLU:HB3	1.99	0.43
1:F:132:THR:HG21	1:F:196:ARG:HB2	2.00	0.43
1:I:255:ASP:HB2	1:I:309:ARG:NH2	2.27	0.43
1:D:132:THR:HG21	1:D:197:ASP:H	1.83	0.43
1:E:36:ARG:NH2	1:H:373:ALA:O	2.52	0.43
1:G:198:PRO:HB2	1:G:211:LEU:HD11	2.01	0.43
1:G:344:LEU:HB3	1:G:385:VAL:CG2	2.48	0.43
1:I:48:THR:HG21	1:I:379:LEU:HD21	2.00	0.43
1:C:132:THR:HG21	1:C:196:ARG:HB2	2.00	0.43
1:I:42:GLU:HG3	1:I:43:ILE:HG13	2.00	0.43
1:I:126:ARG:HE	1:I:153:GLY:HA2	1.84	0.43
1:D:35:PRO:HG3	1:D:378:THR:HG21	1.99	0.43
1:D:269:ARG:HH21	1:D:336:VAL:CG1	2.32	0.43
1:D:344:LEU:HB3	1:D:385:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ARG:NH2	1:D:413:LEU:HD11	2.33	0.43
1:A:49:TRP:CZ3	1:A:116:ALA:HA	2.53	0.43
1:D:46:TRP:HB2	1:D:349:PHE:CE1	2.54	0.43
1:H:49:TRP:CZ3	1:H:116:ALA:HA	2.54	0.43
1:I:26:GLU:OE1	2:I:502:HOH:O	2.21	0.43
1:J:150:VAL:HB	1:J:174:LEU:HD11	2.01	0.43
1:B:29:VAL:HG22	1:B:323:THR:O	2.19	0.42
1:C:13:TRP:O	1:C:263:VAL:HG21	2.18	0.42
1:C:235:ASN:N	1:C:235:ASN:OD1	2.50	0.42
1:B:13:TRP:O	1:B:263:VAL:HG21	2.19	0.42
1:D:13:TRP:O	1:D:263:VAL:HG21	2.18	0.42
1:E:194:THR:HG22	1:E:196:ARG:HH12	1.83	0.42
1:F:192:ILE:HD12	1:F:192:ILE:H	1.84	0.42
1:G:48:THR:HG21	1:G:379:LEU:HD21	2.01	0.42
1:I:29:VAL:HG22	1:I:323:THR:O	2.20	0.42
1:D:139:GLU:CD	1:D:142:ILE:HA	2.39	0.42
1:H:42:GLU:HG3	1:H:43:ILE:HG23	2.01	0.42
1:F:132:THR:HG21	1:F:196:ARG:CA	2.49	0.42
1:G:343:GLU:OE2	1:G:413:LEU:HD11	2.19	0.42
1:J:46:TRP:HB2	1:J:349:PHE:CE1	2.55	0.42
1:B:60:THR:HG21	1:B:405:LEU:HD11	2.02	0.42
1:B:343:GLU:OE1	1:B:413:LEU:HD11	2.20	0.42
1:B:360:LEU:HA	1:B:360:LEU:HD23	1.71	0.42
1:B:385:VAL:HG12	1:B:394:ILE:HD13	2.00	0.42
1:D:75:ASP:O	1:D:372:ARG:NE	2.46	0.42
1:F:178:ASP:O	1:F:184:ARG:NH2	2.49	0.42
1:G:341:ARG:H	1:G:341:ARG:HG3	1.47	0.42
1:A:217:THR:HG21	1:A:259:GLU:OE2	2.20	0.42
1:C:188:SER:HB2	1:C:193:TYR:HB3	2.02	0.42
1:E:76:LEU:HD23	1:E:77:LEU:O	2.19	0.42
1:I:116:ALA:HB1	1:I:269:ARG:NH1	2.35	0.42
1:A:122:ASP:HB3	1:A:124:ASP:OD1	2.20	0.42
1:B:393:ARG:NH1	2:B:501:HOH:O	2.52	0.42
1:D:177:PRO:O	1:D:184:ARG:HD3	2.19	0.42
1:H:111:GLY:HA2	1:H:135:GLY:C	2.40	0.42
1:I:181:ARG:O	1:I:217:THR:HG22	2.20	0.42
1:B:46:TRP:HB2	1:B:349:PHE:CE1	2.55	0.42
1:D:359:THR:HG23	1:D:362:ASP:H	1.84	0.42
1:H:196:ARG:NH2	1:H:268:GLU:OE2	2.53	0.42
1:I:181:ARG:NH2	1:I:255:ASP:OD1	2.52	0.42
1:J:194:THR:HG22	1:J:196:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LYS:HE3	1:B:242:HIS:NE2	2.35	0.42
1:E:344:LEU:HB3	1:E:385:VAL:CG2	2.50	0.42
1:H:344:LEU:HB3	1:H:385:VAL:CG2	2.50	0.42
1:H:358:LEU:HD22	1:H:362:ASP:HB3	2.00	0.42
1:C:275:ARG:NH2	1:C:342:GLU:HA	2.35	0.41
1:G:161:ASP:OD1	1:G:162:GLY:N	2.53	0.41
1:I:46:TRP:HB2	1:I:349:PHE:CE1	2.55	0.41
1:I:51:LEU:HB2	1:I:68:PHE:HE1	1.85	0.41
1:F:413:LEU:N	1:F:413:LEU:HD12	2.35	0.41
1:J:48:THR:HG21	1:J:379:LEU:HD21	2.01	0.41
1:D:15:ARG:NH2	1:D:292:PRO:O	2.53	0.41
1:E:135:GLY:HA2	1:E:143:THR:HG23	2.01	0.41
1:F:51:LEU:HD11	1:F:121:LEU:HB2	2.02	0.41
1:G:259:GLU:HB3	1:G:261:ILE:HD13	2.02	0.41
1:A:259:GLU:HB3	1:A:261:ILE:HD13	2.02	0.41
1:E:270:PRO:HA	1:E:282:PHE:O	2.21	0.41
1:I:26:GLU:CD	2:I:502:HOH:O	2.58	0.41
1:E:49:TRP:CE2	1:E:68:PHE:HB2	2.55	0.41
1:E:116:ALA:HB1	1:E:269:ARG:HH11	1.85	0.41
1:H:71:THR:HG21	1:H:88:ARG:HD2	2.00	0.41
1:C:31:ILE:HD13	1:C:325:PRO:HG3	2.01	0.41
1:D:65:ARG:NH1	1:D:93:ARG:O	2.52	0.41
1:J:90:PHE:CD2	1:J:100:ASP:HA	2.55	0.41
1:A:344:LEU:HB3	1:A:385:VAL:HG22	2.01	0.41
1:G:194:THR:HG22	1:G:196:ARG:HH12	1.86	0.41
1:H:75:ASP:OD1	1:H:76:LEU:N	2.54	0.41
1:H:388:SER:OG	1:H:389:GLY:N	2.54	0.41
1:I:127:LEU:HD21	1:I:129:VAL:HG23	2.02	0.41
1:B:216:ASN:ND2	1:B:265:GLN:OE1	2.51	0.41
1:B:372:ARG:HH22	1:J:221:GLU:CD	2.23	0.41
1:A:65:ARG:NH2	1:A:405:LEU:HG	2.35	0.41
1:A:275:ARG:HH22	1:A:342:GLU:HA	1.86	0.41
1:B:330:TYR:O	1:B:351:ASN:HB3	2.21	0.41
1:C:71:THR:HG21	1:C:88:ARG:HD2	2.03	0.41
1:F:139:GLU:OE2	1:F:142:ILE:HD13	2.20	0.41
1:H:260:GLY:O	1:H:263:VAL:HG22	2.20	0.41
1:I:259:GLU:HB2	1:I:261:ILE:CD1	2.50	0.41
1:B:49:TRP:CE2	1:B:68:PHE:HB2	2.55	0.41
1:B:117:GLY:HA3	1:B:130:PHE:O	2.21	0.41
1:D:51:LEU:HA	1:D:119:ALA:HB3	2.03	0.41
1:F:49:TRP:CE2	1:F:68:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:344:LEU:HB3	1:G:385:VAL:HG22	2.03	0.41
1:I:88:ARG:NH2	1:I:102:GLY:HA2	2.36	0.41
1:I:228:ASP:OD1	1:I:230:VAL:HG12	2.21	0.41
1:I:272:VAL:HA	1:I:280:TYR:O	2.21	0.41
1:I:341:ARG:H	1:I:341:ARG:HG3	1.48	0.41
1:B:51:LEU:HB2	1:B:68:PHE:HE1	1.86	0.40
1:B:344:LEU:HB3	1:B:385:VAL:CG2	2.52	0.40
1:C:90:PHE:CD1	1:C:90:PHE:N	2.90	0.40
1:C:335:TRP:HB3	1:C:346:VAL:HG12	2.03	0.40
1:C:335:TRP:HB3	1:C:346:VAL:CG1	2.52	0.40
1:G:117:GLY:HA3	1:G:130:PHE:O	2.21	0.40
1:G:379:LEU:HD23	1:G:379:LEU:HA	1.93	0.40
1:J:309:ARG:HH11	1:J:309:ARG:HD2	1.75	0.40
1:B:270:PRO:HB3	1:B:283:VAL:HG12	2.02	0.40
1:E:178:ASP:OD1	1:E:179:GLY:N	2.55	0.40
1:H:127:LEU:HD21	1:H:129:VAL:HG23	2.03	0.40
1:H:228:ASP:OD1	1:H:230:VAL:HG12	2.21	0.40
1:A:23:ARG:HG2	1:A:323:THR:HG21	2.04	0.40
1:A:49:TRP:CE2	1:A:68:PHE:HB2	2.56	0.40
1:A:404:PRO:HG3	1:A:410:LEU:HD21	2.04	0.40
1:C:178:ASP:O	1:C:184:ARG:NH1	2.53	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	404/428 (94%)	381 (94%)	22 (5%)	1 (0%)	47 69
1	B	404/428 (94%)	382 (95%)	22 (5%)	0	100 100
1	C	404/428 (94%)	380 (94%)	24 (6%)	0	100 100
1	D	404/428 (94%)	382 (95%)	21 (5%)	1 (0%)	47 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	404/428 (94%)	379 (94%)	24 (6%)	1 (0%)	47 69
1	F	404/428 (94%)	377 (93%)	27 (7%)	0	100 100
1	G	404/428 (94%)	383 (95%)	20 (5%)	1 (0%)	47 69
1	H	404/428 (94%)	379 (94%)	25 (6%)	0	100 100
1	I	404/428 (94%)	384 (95%)	19 (5%)	1 (0%)	47 69
1	J	404/428 (94%)	382 (95%)	22 (5%)	0	100 100
All	All	4040/4280 (94%)	3809 (94%)	226 (6%)	5 (0%)	51 75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	341	ARG
1	G	341	ARG
1	A	341	ARG
1	E	276	ASN
1	I	341	ARG

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	329/348 (94%)	325 (99%)	4 (1%)	71 82
1	B	329/348 (94%)	325 (99%)	4 (1%)	71 82
1	C	329/348 (94%)	325 (99%)	4 (1%)	71 82
1	D	329/348 (94%)	325 (99%)	4 (1%)	71 82
1	E	329/348 (94%)	324 (98%)	5 (2%)	65 78
1	F	329/348 (94%)	326 (99%)	3 (1%)	78 87
1	G	329/348 (94%)	327 (99%)	2 (1%)	86 90
1	H	329/348 (94%)	327 (99%)	2 (1%)	86 90
1	I	329/348 (94%)	325 (99%)	4 (1%)	71 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	329/348 (94%)	327 (99%)	2 (1%)	86 90
All	All	3290/3480 (94%)	3256 (99%)	34 (1%)	76 85

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	113	ARG
1	A	193	TYR
1	A	226	CYS
1	B	90	PHE
1	B	113	ARG
1	B	193	TYR
1	B	262	CYS
1	C	90	PHE
1	C	104	VAL
1	C	113	ARG
1	C	193	TYR
1	D	90	PHE
1	D	113	ARG
1	D	132	THR
1	D	193	TYR
1	E	113	ARG
1	E	183	GLU
1	E	193	TYR
1	E	262	CYS
1	E	412	ASP
1	F	113	ARG
1	F	132	THR
1	F	193	TYR
1	G	113	ARG
1	G	193	TYR
1	H	113	ARG
1	H	193	TYR
1	I	113	ARG
1	I	127	LEU
1	I	193	TYR
1	I	255	ASP
1	J	113	ARG
1	J	193	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	242	HIS
1	F	242	HIS
1	G	242	HIS
1	H	171	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	406/428 (94%)	0.34	2 (0%) 91 94	20, 45, 78, 99	0
1	B	406/428 (94%)	0.62	29 (7%) 16 19	19, 66, 106, 133	0
1	C	406/428 (94%)	0.36	3 (0%) 87 91	23, 48, 83, 94	0
1	D	406/428 (94%)	0.36	6 (1%) 73 81	18, 42, 75, 94	0
1	E	406/428 (94%)	0.47	6 (1%) 73 81	25, 46, 85, 114	0
1	F	406/428 (94%)	0.43	4 (0%) 82 87	26, 50, 89, 114	0
1	G	406/428 (94%)	0.66	27 (6%) 17 21	27, 67, 108, 140	0
1	H	406/428 (94%)	0.83	50 (12%) 4 4	22, 75, 131, 161	0
1	I	406/428 (94%)	0.58	21 (5%) 27 33	28, 66, 107, 126	0
1	J	406/428 (94%)	0.39	5 (1%) 79 85	27, 50, 81, 97	0
All	All	4060/4280 (94%)	0.50	153 (3%) 40 48	18, 54, 102, 161	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	225	ALA	5.3
1	B	220	PRO	5.2
1	G	106	GLU	4.6
1	H	148	LEU	4.6
1	H	127	LEU	4.5
1	G	229	PRO	4.4
1	H	165	ILE	4.3
1	H	38	ASP	3.9
1	H	186	GLU	3.8
1	H	106	GLU	3.8
1	B	142	ILE	3.8
1	I	75	ASP	3.7
1	B	141	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	126	ARG	3.7
1	G	223	ALA	3.7
1	I	219	ILE	3.7
1	H	156	VAL	3.7
1	H	251	TRP	3.6
1	B	221	GLU	3.6
1	I	224	GLY	3.6
1	E	226	CYS	3.6
1	H	147	ARG	3.6
1	I	130	PHE	3.6
1	H	259	GLU	3.5
1	B	37	GLU	3.4
1	E	225	ALA	3.4
1	F	220	PRO	3.3
1	G	225	ALA	3.3
1	H	213	PHE	3.3
1	D	166	GLU	3.3
1	H	61	VAL	3.3
1	H	131	TYR	3.2
1	H	68	PHE	3.2
1	H	144	TYR	3.2
1	G	180	GLU	3.1
1	H	166	GLU	3.1
1	G	130	PHE	3.1
1	H	130	PHE	3.1
1	B	166	GLU	3.1
1	B	134	SER	3.0
1	H	187	GLN	3.0
1	G	129	VAL	2.9
1	G	165	ILE	2.9
1	I	127	LEU	2.9
1	B	169	PHE	2.9
1	G	105	PHE	2.8
1	I	39	ALA	2.8
1	H	182	TYR	2.8
1	E	220	PRO	2.8
1	G	175	LEU	2.8
1	B	148	LEU	2.7
1	E	295	GLU	2.7
1	H	175	LEU	2.7
1	H	194	THR	2.7
1	B	184	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	360	LEU	2.7
1	I	225	ALA	2.7
1	H	222	GLY	2.7
1	A	37	GLU	2.7
1	G	211	LEU	2.7
1	H	178	ASP	2.7
1	B	223	ALA	2.6
1	H	211	LEU	2.6
1	I	175	LEU	2.6
1	H	37	GLU	2.6
1	B	219	ILE	2.6
1	G	131	TYR	2.6
1	G	240	ILE	2.6
1	H	12	ARG	2.6
1	G	226	CYS	2.6
1	G	58	ILE	2.6
1	I	370	GLU	2.5
1	G	219	ILE	2.5
1	G	292	PRO	2.5
1	F	142	ILE	2.5
1	B	226	CYS	2.5
1	H	105	PHE	2.4
1	H	250	ASP	2.4
1	H	133	ALA	2.4
1	G	127	LEU	2.4
1	H	174	LEU	2.4
1	H	128	TYR	2.4
1	B	61	VAL	2.4
1	I	221	GLU	2.4
1	H	193	TYR	2.4
1	B	127	LEU	2.4
1	H	121	LEU	2.4
1	F	189	ARG	2.4
1	H	39	ALA	2.4
1	I	261	ILE	2.4
1	G	173	VAL	2.3
1	H	238	VAL	2.3
1	G	73	PRO	2.3
1	C	370	GLU	2.3
1	G	222	GLY	2.3
1	H	129	VAL	2.3
1	I	255	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	232	GLU	2.3
1	A	39	ALA	2.3
1	B	211	LEU	2.3
1	E	219	ILE	2.3
1	D	370	GLU	2.3
1	H	64	TRP	2.3
1	H	195	PHE	2.3
1	H	221	GLU	2.3
1	I	229	PRO	2.3
1	I	222	GLY	2.3
1	B	144	TYR	2.3
1	H	189	ARG	2.3
1	J	342	GLU	2.2
1	G	18	ALA	2.2
1	I	165	ILE	2.2
1	G	187	GLN	2.2
1	G	144	TYR	2.2
1	C	37	GLU	2.2
1	I	360	LEU	2.2
1	D	18	ALA	2.2
1	I	142	ILE	2.2
1	J	156	VAL	2.2
1	H	188	SER	2.2
1	I	133	ALA	2.2
1	B	75	ASP	2.2
1	B	290	PHE	2.2
1	H	177	PRO	2.2
1	B	104	VAL	2.2
1	B	311	GLU	2.2
1	I	166	GLU	2.2
1	B	72	ALA	2.2
1	B	50	PHE	2.2
1	D	66	VAL	2.1
1	G	221	GLU	2.1
1	E	360	LEU	2.1
1	H	168	PRO	2.1
1	B	225	ALA	2.1
1	I	202	GLU	2.1
1	J	383	VAL	2.1
1	G	183	GLU	2.1
1	B	182	TYR	2.1
1	F	261	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	220	PRO	2.1
1	H	224	GLY	2.1
1	J	157	VAL	2.1
1	H	132	THR	2.1
1	I	180	GLU	2.1
1	D	261	ILE	2.0
1	H	135	GLY	2.0
1	D	175	LEU	2.0
1	B	157	VAL	2.0
1	C	263	VAL	2.0
1	B	58	ILE	2.0
1	B	175	LEU	2.0
1	J	358	LEU	2.0
1	H	263	VAL	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.