



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:45 AM GMT

PDB ID : 2TBS
Title : COLD-ADAPTION OF ENZYMES: STRUCTURAL COMPARISON BETWEEN SALMON AND BOVINE TRYPSINS
Authors : Smalas, A.O.
Deposited on : 1994-01-14
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

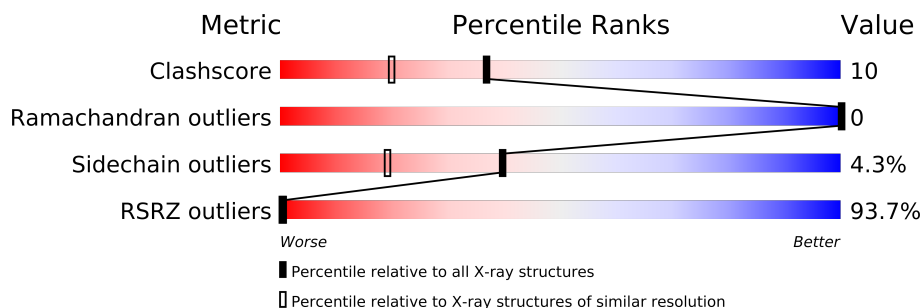
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	222	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	BEN	A	246	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1833 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	49	0	0
			1659	1034	277	330	18			

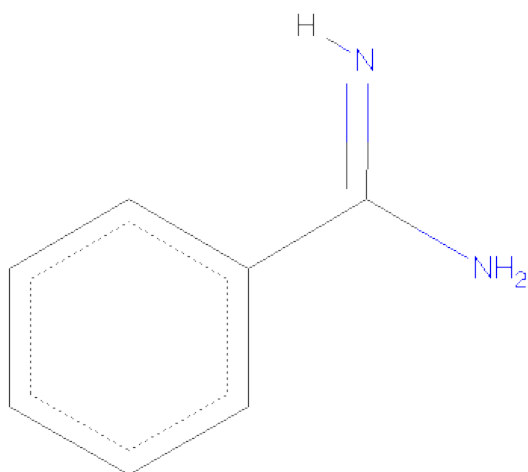
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	THR	CONFLICT	UNP P35031
A	153	ASP	ASN	CONFLICT	UNP P35031
A	170	ASP	ASN	CONFLICT	UNP P35031
A	235	SER	ASN	CONFLICT	UNP P35031

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		

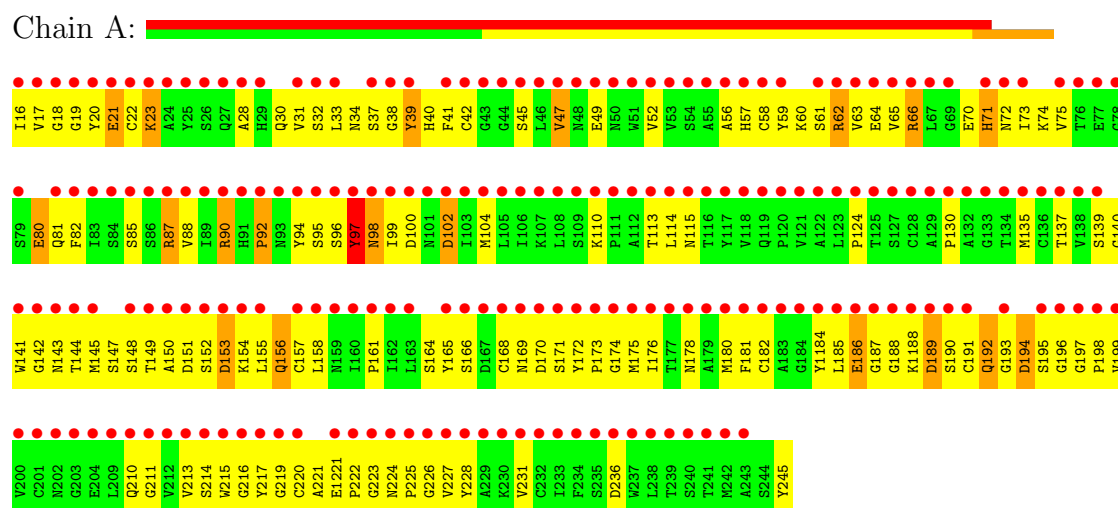
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total	O	0	0
			164	164		

3 Residue-property plots

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: TRYPSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.95Å 84.33Å 39.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80 42.17 – 1.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.80) 97.1 (42.17-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.83Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.508 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18298 reflections	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	1833	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BEN

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	1.03	2/1698 (0.1%)	1.72	35/2310 (1.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	TYR	CB-CG	-7.63	1.40	1.51
1	A	192	GLN	CG-CD	6.82	1.66	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	A	66	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	A	170	ASP	CB-CG-OD1	-8.26	110.86	118.30
1	A	87	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	A	62	ARG	CG-CD-NE	8.08	128.76	111.80
1	A	194	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	102	ASP	CB-CG-OD2	-7.97	111.12	118.30
1	A	71	HIS	N-CA-CB	7.96	124.94	110.60
1	A	47	VAL	N-CA-CB	-7.63	94.71	111.50
1	A	158	LEU	O-C-N	7.39	134.52	122.70
1	A	66	ARG	NE-CZ-NH2	-7.32	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	VAL	CB-CA-C	6.79	124.31	111.40
1	A	199	VAL	O-C-N	6.79	133.56	122.70
1	A	39	TYR	CB-CG-CD2	6.73	125.04	121.00
1	A	81	GLN	OE1-CD-NE2	6.64	137.17	121.90
1	A	153	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	23	LYS	N-CA-CB	6.31	121.97	110.60
1	A	62	ARG	N-CA-CB	6.18	121.73	110.60
1	A	62	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	A	49	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	A	181	PHE	CB-CG-CD2	-5.88	116.68	120.80
1	A	90	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	80	GLU	CG-CD-OE1	5.69	129.68	118.30
1	A	81	GLN	N-CA-CB	5.58	120.64	110.60
1	A	104	MET	CG-SD-CE	5.58	109.13	100.20
1	A	104	MET	O-C-N	5.56	131.60	122.70
1	A	52	VAL	O-C-N	5.52	131.53	122.70
1	A	236	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	80	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	A	189	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	156	GLN	O-C-N	5.31	131.20	122.70
1	A	104	MET	CA-CB-CG	5.30	122.32	113.30
1	A	210	GLN	CB-CG-CD	5.17	125.05	111.60
1	A	21	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	A	137	THR	O-C-N	5.08	130.83	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	ARG	Sidechain
1	A	90	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1659	0	1562	32	699
2	A	1	0	0	0	1
3	A	9	0	8	0	11
4	A	164	0	0	13	134
All	All	1833	0	1570	32	708

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:TYR:HB3	1:A:175:MET:HE3	1.24	1.16
1:A:172:TYR:HB3	1:A:175:MET:CE	1.86	1.04
1:A:192:GLN:HB2	4:A:342:HOH:O	1.67	0.93
1:A:110:LYS:HB3	4:A:443:HOH:O	1.77	0.85
1:A:175:MET:CE	4:A:336:HOH:O	2.28	0.82
1:A:175:MET:HE1	4:A:336:HOH:O	1.82	0.79
1:A:169:ASN:HD21	1:A:174:GLY:H	1.38	0.72
1:A:28:ALA:N	4:A:418:HOH:O	1.72	0.69
1:A:143:ASN:HB3	4:A:427:HOH:O	1.93	0.68
1:A:169:ASN:ND2	1:A:174:GLY:H	1.92	0.67
1:A:28:ALA:CB	4:A:418:HOH:O	2.43	0.65
1:A:98:ASN:HD22	1:A:98:ASN:H	1.46	0.64
1:A:28:ALA:HB3	4:A:418:HOH:O	2.04	0.57
1:A:98:ASN:N	1:A:98:ASN:HD22	2.02	0.56
1:A:172:TYR:CB	1:A:175:MET:HE3	2.17	0.55
1:A:172:TYR:CB	1:A:175:MET:CE	2.74	0.54
1:A:98:ASN:ND2	1:A:98:ASN:H	2.08	0.52
1:A:45:SER:OG	1:A:198:PRO:HB3	2.09	0.52
1:A:169:ASN:ND2	4:A:450:HOH:O	2.43	0.51
1:A:151:ASP:OD1	1:A:153:ASP:HB2	2.12	0.49
1:A:172:TYR:HB3	1:A:175:MET:HE2	1.86	0.49
1:A:135:MET:CE	1:A:161:PRO:HB3	2.44	0.47
1:A:41:PHE:CE1	1:A:60:LYS:HE3	2.50	0.47
1:A:215:TRP:HB2	4:A:384:HOH:O	2.16	0.46
1:A:135:MET:HE2	1:A:161:PRO:HB3	1.98	0.46
1:A:211:GLY:HA2	1:A:231:VAL:HG23	1.99	0.45
1:A:175:MET:HE2	4:A:336:HOH:O	2.02	0.43
1:A:124:PRO:O	4:A:422:HOH:O	2.21	0.43
1:A:64:GLU:OE2	1:A:66:ARG:NE	2.52	0.42
1:A:98:ASN:HB2	4:A:380:HOH:O	2.19	0.42
1:A:95:SER:HB3	1:A:98:ASN:HD21	1.84	0.42
1:A:33:LEU:HB3	1:A:63:VAL:HG21	2.02	0.41

All (708) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:TRP:CG	1:A:220:CYS:CA[2.665]	0.27	1.93
1:A:141:TRP:CD2	1:A:220:CYS:N[2.665]	0.31	1.89
1:A:141:TRP:CD1	1:A:220:CYS:C[2.665]	0.34	1.86
1:A:165:TYR:CD2	4:A:339:HOH:O[3.556]	0.34	1.86
1:A:145:MET:SD	1:A:156:GLN:O[2.665]	0.38	1.82
1:A:40:HIS:C	1:A:215:TRP:O[2.665]	0.42	1.78
1:A:74:LYS:O	1:A:185:LEU:O[2.665]	0.42	1.78
1:A:40:HIS:CD2	3:A:246:BEN:C[2.665]	0.45	1.75
1:A:153:ASP:O	1:A:221:ALA:C[2.665]	0.50	1.70
1:A:192:GLN:NE2	1:A:197:GLY:N[2.665]	0.50	1.70
1:A:149:THR:N	4:A:301:HOH:O[2.665]	0.51	1.69
1:A:66:ARG:CG	1:A:217:TYR:CD2[2.665]	0.52	1.68
1:A:59:TYR:CD1	1:A:96:SER:CB[2.665]	0.53	1.67
1:A:187:GLY:O	4:A:375:HOH:O[2.665]	0.53	1.67
1:A:192:GLN:CA	1:A:194:ASP:CA[2.665]	0.53	1.67
1:A:34:ASN:CA	1:A:215:TRP:CZ3[2.665]	0.55	1.65
1:A:41:PHE:CB	1:A:215:TRP:N[2.665]	0.55	1.65
1:A:192:GLN:CG	1:A:194:ASP:O[2.665]	0.55	1.65
1:A:41:PHE:N	1:A:215:TRP:C[2.665]	0.61	1.59
1:A:151:ASP:OD1	1:A:1188:LYS:N[2.665]	0.64	1.56
1:A:145:MET:CB	1:A:156:GLN:CA[2.665]	0.65	1.55
1:A:37:SER:N	1:A:215:TRP:CZ2[2.665]	0.66	1.54
1:A:39:TYR:CD2	1:A:227:VAL:C[2.665]	0.68	1.52
1:A:32:SER:OG	1:A:217:TYR:N[2.665]	0.71	1.49
1:A:141:TRP:O	1:A:190:SER:O[2.665]	0.71	1.49
4:A:364:HOH:O	4:A:453:HOH:O[2.665]	0.71	1.49
1:A:60:LYS:CB	1:A:99:ILE:CA[2.665]	0.72	1.48
1:A:192:GLN:O	1:A:194:ASP:CB[2.665]	0.72	1.48
1:A:16:ILE:CB	1:A:144:THR:N[2.665]	0.75	1.45
1:A:40:HIS:NE2	3:A:246:BEN:C1[2.665]	0.77	1.43
1:A:61:SER:O	1:A:97:TYR:CB[2.665]	0.77	1.43
1:A:57:HIS:C	1:A:57:HIS:C[2.665]	0.78	1.42
1:A:41:PHE:CD1	1:A:215:TRP:CG[2.665]	0.79	1.41
1:A:195:SER:CB	4:A:415:HOH:O[2.665]	0.79	1.41
1:A:18:GLY:CA	1:A:150:ALA:C[2.665]	0.80	1.40
1:A:61:SER:CB	1:A:95:SER:OG[2.665]	0.80	1.40
1:A:71:HIS:C	1:A:1221:GLU:OE1[2.665]	0.80	1.40
1:A:70:GLU:OE2	1:A:224:ASN:OD1[2.665]	0.82	1.38
1:A:141:TRP:CE3	1:A:219:GLY:C[2.665]	0.82	1.38
1:A:31:VAL:O	4:A:340:HOH:O[2.665]	0.83	1.37
1:A:141:TRP:NE1	1:A:220:CYS:O[2.665]	0.83	1.37

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:TRP:CZ3	1:A:219:GLY:CA[2.665]	0.83	1.37
1:A:224:ASN:CB	4:A:330:HOH:O[2.665]	0.83	1.37
1:A:145:MET:CG	1:A:156:GLN:CA[2.665]	0.84	1.36
1:A:34:ASN:C	1:A:215:TRP:CH2[2.665]	0.85	1.35
1:A:225:PRO:C	4:A:451:HOH:O[2.665]	0.86	1.34
1:A:182:CYS:CB	4:A:368:HOH:O[2.665]	0.87	1.33
1:A:139:SER:C	4:A:459:HOH:O[2.665]	0.89	1.31
1:A:150:ALA:CB	4:A:452:HOH:O[2.665]	0.89	1.31
1:A:142:GLY:CA	1:A:191:CYS:N[2.665]	0.90	1.30
1:A:18:GLY:CA	1:A:150:ALA:O[2.665]	0.91	1.29
1:A:73:ILE:O	1:A:224:ASN:N[2.665]	0.92	1.28
1:A:18:GLY:C	1:A:150:ALA:O[2.665]	0.93	1.27
1:A:72:ASN:C	1:A:1221:GLU:C[2.665]	0.93	1.27
1:A:226:GLY:N	4:A:451:HOH:O[2.665]	0.93	1.27
1:A:34:ASN:CA	1:A:215:TRP:CE3[2.665]	0.94	1.26
1:A:38:GLY:CA	1:A:176:ILE:CD1[2.665]	0.94	1.26
1:A:73:ILE:CG2	4:A:305:HOH:O[2.665]	0.94	1.26
1:A:39:TYR:CD2	1:A:227:VAL:CA[2.665]	0.95	1.25
1:A:59:TYR:CE1	1:A:96:SER:OG[2.665]	0.95	1.25
1:A:19:GLY:C	1:A:147:SER:C[2.665]	0.97	1.23
1:A:191:CYS:O	1:A:193:GLY:C[2.665]	0.97	1.23
1:A:60:LYS:NZ	4:A:323:HOH:O[2.665]	0.98	1.22
1:A:64:GLU:CD	4:A:336:HOH:O[2.665]	0.98	1.22
1:A:72:ASN:O	1:A:222:PRO:N[2.665]	0.98	1.22
1:A:73:ILE:N	1:A:1221:GLU:CA[2.665]	0.98	1.22
1:A:34:ASN:ND2	1:A:172:TYR:CZ[2.665]	1.00	1.20
1:A:142:GLY:N	1:A:191:CYS:CB[2.665]	1.00	1.20
1:A:192:GLN:CB	1:A:194:ASP:O[2.665]	1.00	1.20
1:A:16:ILE:CB	1:A:143:ASN:C[2.665]	1.01	1.19
1:A:41:PHE:CA	1:A:215:TRP:N[2.665]	1.01	1.19
1:A:57:HIS:CA	1:A:57:HIS:O[2.665]	1.01	1.19
1:A:16:ILE:CD1	1:A:143:ASN:CB[2.665]	1.02	1.18
1:A:41:PHE:N	1:A:215:TRP:O[2.665]	1.02	1.18
1:A:62:ARG:N	1:A:98:ASN:N[2.665]	1.02	1.18
4:A:329:HOH:O	4:A:329:HOH:O[2.665]	1.02	1.18
1:A:16:ILE:N	1:A:143:ASN:O[2.665]	1.04	1.16
1:A:17:VAL:O	1:A:152:SER:N[2.665]	1.04	1.16
1:A:39:TYR:CE2	1:A:227:VAL:C[2.665]	1.04	1.16
1:A:82:PHE:CZ	4:A:344:HOH:O[2.665]	1.04	1.16
1:A:141:TRP:CD1	1:A:220:CYS:O[2.665]	1.04	1.16
1:A:16:ILE:CG1	1:A:143:ASN:CB[2.665]	1.05	1.15
1:A:19:GLY:C	1:A:147:SER:O[2.665]	1.05	1.15

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:SER:CB	1:A:217:TYR:C[2.665]	1.05	1.15
1:A:38:GLY:O	1:A:182:CYS:SG[2.665]	1.05	1.15
1:A:72:ASN:C	1:A:1221:GLU:CA[2.665]	1.05	1.15
1:A:74:LYS:C	1:A:185:LEU:O[2.665]	1.05	1.15
1:A:151:ASP:CG	1:A:188:GLY:C[2.665]	1.05	1.15
1:A:153:ASP:C	1:A:221:ALA:CB[2.665]	1.05	1.15
1:A:32:SER:CB	1:A:217:TYR:CA[2.665]	1.06	1.14
1:A:73:ILE:C	1:A:1221:GLU:O[2.665]	1.06	1.14
1:A:190:SER:OG	4:A:416:HOH:O[2.665]	1.06	1.14
1:A:37:SER:N	1:A:215:TRP:CE2[2.665]	1.07	1.13
1:A:16:ILE:CA	1:A:143:ASN:C[2.665]	1.08	1.12
4:A:342:HOH:O	4:A:436:HOH:O[2.665]	1.08	1.12
1:A:20:TYR:C	1:A:145:MET:O[2.665]	1.09	1.11
1:A:37:SER:CA	1:A:215:TRP:CZ2[2.665]	1.09	1.11
1:A:37:SER:OG	1:A:215:TRP:NE1[2.665]	1.09	1.11
1:A:60:LYS:O	1:A:96:SER:C[2.665]	1.09	1.11
1:A:62:ARG:O	1:A:98:ASN:CA[2.665]	1.09	1.11
1:A:97:TYR:CD1	4:A:437:HOH:O[2.665]	1.09	1.11
1:A:145:MET:CG	1:A:156:GLN:N[2.665]	1.09	1.11
1:A:155:LEU:CA	4:A:359:HOH:O[2.665]	1.09	1.11
1:A:20:TYR:O	1:A:145:MET:O[2.665]	1.10	1.10
1:A:60:LYS:CD	1:A:99:ILE:O[2.665]	1.10	1.10
1:A:62:ARG:C	1:A:98:ASN:CA[2.665]	1.10	1.10
1:A:151:ASP:CB	1:A:188:GLY:O[2.665]	1.10	1.10
1:A:192:GLN:C	1:A:194:ASP:CB[2.665]	1.10	1.10
1:A:19:GLY:O	1:A:147:SER:C[2.665]	1.11	1.09
1:A:42:CYS:CB	4:A:324:HOH:O[2.665]	1.11	1.09
1:A:73:ILE:CA	1:A:1221:GLU:O[2.665]	1.11	1.09
1:A:39:TYR:CG	1:A:227:VAL:CA[2.665]	1.12	1.08
1:A:41:PHE:CD1	1:A:215:TRP:CB[2.665]	1.13	1.07
1:A:20:TYR:N	1:A:147:SER:CA[2.665]	1.14	1.06
1:A:73:ILE:N	1:A:1221:GLU:C[2.665]	1.14	1.06
1:A:60:LYS:CG	1:A:99:ILE:CA[2.665]	1.15	1.05
1:A:151:ASP:OD1	1:A:188:GLY:C[2.665]	1.15	1.05
1:A:191:CYS:O	1:A:194:ASP:N[2.665]	1.15	1.05
1:A:192:GLN:CA	1:A:194:ASP:C[2.665]	1.15	1.05
1:A:71:HIS:CA	1:A:1221:GLU:OE1[2.665]	1.16	1.04
1:A:85:SER:O	1:A:97:TYR:OH[2.665]	1.16	1.04
1:A:92:PRO:CB	1:A:148:SER:OG[2.664]	1.16	1.04
1:A:141:TRP:CZ2	4:A:407:HOH:O[2.665]	1.16	1.04
1:A:152:SER:OG	1:A:189:ASP:N[2.665]	1.16	1.04
1:A:32:SER:OG	1:A:216:GLY:C[2.665]	1.17	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:LYS:CB	1:A:99:ILE:N[2.665]	1.17	1.03
1:A:195:SER:CA	4:A:415:HOH:O[2.665]	1.17	1.03
1:A:57:HIS:CA	1:A:57:HIS:C[2.665]	1.18	1.02
1:A:57:HIS:CB	1:A:58:CYS:CA[2.665]	1.18	1.02
1:A:64:GLU:OE1	4:A:336:HOH:O[2.665]	1.18	1.02
1:A:66:ARG:CB	1:A:217:TYR:CD2[2.665]	1.18	1.02
1:A:34:ASN:ND2	1:A:172:TYR:CE2[2.665]	1.19	1.01
1:A:141:TRP:N	1:A:191:CYS:SG[2.665]	1.19	1.01
1:A:165:TYR:CG	4:A:339:HOH:O[3.556]	1.19	1.01
1:A:172:TYR:OH	4:A:315:HOH:O[2.665]	1.19	1.01
1:A:39:TYR:CE2	1:A:228:TYR:N[2.665]	1.20	1.00
1:A:61:SER:OG	1:A:95:SER:OG[2.665]	1.20	1.00
1:A:224:ASN:CA	4:A:330:HOH:O[2.665]	1.20	1.00
1:A:59:TYR:CA	1:A:94:TYR:OH[2.665]	1.21	0.99
1:A:97:TYR:CE1	4:A:437:HOH:O[2.665]	1.21	0.99
1:A:31:VAL:C	4:A:340:HOH:O[2.665]	1.22	0.98
1:A:34:ASN:C	1:A:215:TRP:CZ3[2.665]	1.22	0.98
1:A:64:GLU:CB	1:A:175:MET:SD[2.665]	1.22	0.98
1:A:153:ASP:O	1:A:221:ALA:O[2.665]	1.22	0.98
1:A:152:SER:CB	1:A:189:ASP:O[2.665]	1.23	0.97
1:A:192:GLN:C	1:A:194:ASP:CA[2.665]	1.24	0.96
2:A:247:CA:CA	4:A:351:HOH:O[2.665]	1.24	0.96
1:A:39:TYR:C	1:A:227:VAL:CG2[2.665]	1.25	0.95
1:A:64:GLU:OE2	4:A:336:HOH:O[2.665]	1.25	0.95
1:A:74:LYS:CE	1:A:225:PRO:CB[2.665]	1.25	0.95
1:A:140:GLY:C	1:A:191:CYS:SG[2.665]	1.25	0.95
1:A:145:MET:SD	1:A:156:GLN:C[2.665]	1.25	0.95
1:A:153:ASP:O	1:A:221:ALA:CA[2.665]	1.25	0.95
1:A:60:LYS:CG	1:A:99:ILE:C[2.665]	1.26	0.94
1:A:141:TRP:CD2	1:A:220:CYS:CA[2.665]	1.26	0.94
1:A:39:TYR:N	1:A:227:VAL:CG2[2.665]	1.27	0.93
1:A:57:HIS:C	1:A:57:HIS:O[2.665]	1.27	0.93
1:A:59:TYR:O	1:A:94:TYR:CE1[2.665]	1.27	0.93
1:A:59:TYR:CD1	1:A:96:SER:OG[2.665]	1.27	0.93
1:A:148:SER:C	4:A:301:HOH:O[2.665]	1.27	0.93
1:A:152:SER:OG	1:A:189:ASP:CA[2.665]	1.27	0.93
1:A:192:GLN:CD	1:A:197:GLY:N[2.665]	1.27	0.93
1:A:39:TYR:CA	1:A:227:VAL:CG2[2.665]	1.28	0.92
1:A:139:SER:CA	4:A:459:HOH:O[2.665]	1.28	0.92
1:A:140:GLY:N	4:A:459:HOH:O[2.665]	1.28	0.92
1:A:20:TYR:N	1:A:147:SER:N[2.665]	1.29	0.91
1:A:60:LYS:CA	1:A:95:SER:O[2.665]	1.29	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:ILE:CG1	1:A:143:ASN:CA[2_665]	1.30	0.90
1:A:60:LYS:C	1:A:95:SER:O[2_665]	1.30	0.90
1:A:72:ASN:O	1:A:1221:GLU:C[2_665]	1.30	0.90
1:A:34:ASN:N	1:A:215:TRP:CE3[2_665]	1.31	0.89
1:A:92:PRO:CA	1:A:148:SER:CB[2_664]	1.31	0.89
1:A:142:GLY:N	1:A:191:CYS:CA[2_665]	1.31	0.89
1:A:173:PRO:CD	4:A:363:HOH:O[2_665]	1.31	0.89
1:A:192:GLN:O	1:A:194:ASP:CG[2_665]	1.31	0.89
1:A:141:TRP:N	1:A:220:CYS:SG[2_665]	1.32	0.88
1:A:189:ASP:CG	4:A:458:HOH:O[2_665]	1.32	0.88
1:A:192:GLN:NE2	1:A:197:GLY:CA[2_665]	1.32	0.88
1:A:114:LEU:O	1:A:166:SER:OG[3_546]	1.33	0.87
1:A:141:TRP:CE3	1:A:220:CYS:N[2_665]	1.33	0.87
1:A:192:GLN:N	1:A:194:ASP:CA[2_665]	1.33	0.87
1:A:41:PHE:CB	1:A:214:SER:C[2_665]	1.34	0.86
1:A:57:HIS:CG	1:A:58:CYS:CA[2_665]	1.34	0.86
1:A:74:LYS:CG	1:A:1184:TYR:O[2_665]	1.34	0.86
1:A:75:VAL:N	1:A:222:PRO:CA[2_665]	1.34	0.86
1:A:143:ASN:N	1:A:194:ASP:OD2[2_665]	1.34	0.86
1:A:153:ASP:C	1:A:221:ALA:CA[2_665]	1.34	0.86
1:A:154:LYS:N	1:A:221:ALA:CB[2_665]	1.34	0.86
1:A:70:GLU:OE2	1:A:224:ASN:CG[2_665]	1.35	0.85
1:A:141:TRP:CE2	1:A:220:CYS:N[2_665]	1.35	0.85
1:A:222:PRO:O	4:A:327:HOH:O[2_665]	1.35	0.85
1:A:34:ASN:C	1:A:215:TRP:CZ2[2_665]	1.36	0.84
1:A:39:TYR:O	1:A:227:VAL:CG2[2_665]	1.36	0.84
1:A:187:GLY:C	4:A:375:HOH:O[2_665]	1.36	0.84
1:A:16:ILE:CD1	1:A:143:ASN:CG[2_665]	1.37	0.83
1:A:74:LYS:O	1:A:185:LEU:C[2_665]	1.37	0.83
1:A:85:SER:OG	1:A:97:TYR:CE1[2_665]	1.37	0.83
1:A:141:TRP:CB	1:A:220:CYS:CB[2_665]	1.37	0.83
1:A:141:TRP:CG	1:A:220:CYS:CB[2_665]	1.37	0.83
1:A:72:ASN:ND2	4:A:411:HOH:O[2_665]	1.38	0.82
1:A:73:ILE:N	1:A:1221:GLU:N[2_665]	1.38	0.82
1:A:73:ILE:CB	4:A:305:HOH:O[2_665]	1.38	0.82
1:A:97:TYR:CG	4:A:437:HOH:O[2_665]	1.38	0.82
1:A:151:ASP:CG	1:A:188:GLY:O[2_665]	1.38	0.82
1:A:16:ILE:CD1	1:A:143:ASN:CA[2_665]	1.39	0.81
1:A:114:LEU:O	1:A:166:SER:CB[3_546]	1.39	0.81
1:A:92:PRO:O	1:A:148:SER:O[2_664]	1.40	0.80
1:A:18:GLY:CA	1:A:151:ASP:N[2_665]	1.41	0.79
1:A:70:GLU:CD	1:A:224:ASN:OD1[2_665]	1.41	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:TRP:CG	1:A:220:CYS:C[2.665]	1.41	0.79
1:A:19:GLY:CA	1:A:147:SER:O[2.665]	1.42	0.78
1:A:19:GLY:C	1:A:147:SER:CA[2.665]	1.42	0.78
1:A:33:LEU:O	1:A:216:GLY:N[2.665]	1.42	0.78
1:A:74:LYS:N	1:A:1221:GLU:O[2.665]	1.42	0.78
1:A:102:ASP:OD2	4:A:328:HOH:O[2.665]	1.42	0.78
1:A:114:LEU:CB	4:A:401:HOH:O[3.546]	1.42	0.78
1:A:66:ARG:CG	1:A:217:TYR:CE2[2.665]	1.43	0.77
1:A:141:TRP:O	1:A:190:SER:C[2.665]	1.43	0.77
1:A:141:TRP:CH2	1:A:219:GLY:CA[2.665]	1.43	0.77
1:A:144:THR:O	1:A:156:GLN:OE1[2.665]	1.43	0.77
1:A:144:THR:CB	4:A:392:HOH:O[2.665]	1.43	0.77
1:A:189:ASP:OD1	4:A:458:HOH:O[2.665]	1.43	0.77
1:A:34:ASN:CB	1:A:215:TRP:CZ3[2.665]	1.44	0.76
1:A:20:TYR:CA	1:A:147:SER:CA[2.665]	1.45	0.75
1:A:41:PHE:N	1:A:215:TRP:CA[2.665]	1.45	0.75
1:A:16:ILE:O	1:A:144:THR:CG2[2.665]	1.46	0.74
1:A:72:ASN:C	1:A:222:PRO:N[2.665]	1.46	0.74
1:A:74:LYS:CB	1:A:1184:TYR:O[2.665]	1.46	0.74
1:A:192:GLN:CB	1:A:194:ASP:C[2.665]	1.46	0.74
1:A:41:PHE:CA	1:A:215:TRP:CA[2.665]	1.47	0.73
1:A:60:LYS:O	1:A:97:TYR:N[2.665]	1.47	0.73
1:A:141:TRP:NE1	1:A:220:CYS:C[2.665]	1.47	0.73
1:A:152:SER:OG	1:A:189:ASP:C[2.665]	1.47	0.73
1:A:155:LEU:CB	4:A:359:HOH:O[2.665]	1.47	0.73
1:A:20:TYR:O	1:A:145:MET:C[2.665]	1.48	0.72
1:A:41:PHE:CD1	1:A:215:TRP:CD1[2.665]	1.48	0.72
1:A:61:SER:N	1:A:95:SER:O[2.665]	1.48	0.72
1:A:66:ARG:NH2	1:A:171:SER:O[2.665]	1.48	0.72
1:A:72:ASN:OD1	1:A:187:GLY:CA[2.665]	1.48	0.72
1:A:191:CYS:C	1:A:193:GLY:C[2.665]	1.48	0.72
1:A:19:GLY:N	1:A:150:ALA:O[2.665]	1.49	0.71
1:A:57:HIS:N	1:A:57:HIS:O[2.665]	1.49	0.71
1:A:59:TYR:CG	1:A:96:SER:CB[2.665]	1.49	0.71
1:A:62:ARG:O	1:A:98:ASN:C[2.665]	1.49	0.71
1:A:20:TYR:N	1:A:147:SER:C[2.665]	1.50	0.70
1:A:37:SER:N	1:A:215:TRP:CH2[2.665]	1.50	0.70
1:A:59:TYR:C	1:A:94:TYR:OH[2.665]	1.50	0.70
1:A:75:VAL:CB	1:A:222:PRO:CB[2.665]	1.50	0.70
1:A:57:HIS:CB	1:A:58:CYS:N[2.665]	1.51	0.69
1:A:74:LYS:CG	4:A:304:HOH:O[2.665]	1.51	0.69
1:A:141:TRP:CD2	1:A:219:GLY:C[2.665]	1.51	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:ASP:CB	4:A:458:HOH:O[2_665]	1.51	0.69
1:A:225:PRO:O	4:A:451:HOH:O[2_665]	1.51	0.69
1:A:60:LYS:CD	1:A:99:ILE:C[2_665]	1.52	0.68
1:A:66:ARG:CB	1:A:217:TYR:CG[2_665]	1.52	0.68
1:A:16:ILE:O	1:A:144:THR:CB[2_665]	1.53	0.67
1:A:16:ILE:CG2	4:A:319:HOH:O[2_665]	1.53	0.67
1:A:59:TYR:O	1:A:94:TYR:CZ[2_665]	1.53	0.67
1:A:59:TYR:CZ	1:A:96:SER:N[2_665]	1.53	0.67
1:A:141:TRP:CD1	1:A:220:CYS:CA[2_665]	1.53	0.67
1:A:19:GLY:O	1:A:147:SER:O[2_665]	1.54	0.66
1:A:22:CYS:SG	1:A:145:MET:CE[2_665]	1.54	0.66
1:A:33:LEU:N	1:A:216:GLY:O[2_665]	1.54	0.66
1:A:38:GLY:N	1:A:176:ILE:CD1[2_665]	1.54	0.66
1:A:41:PHE:CE1	1:A:215:TRP:CG[2_665]	1.54	0.66
1:A:59:TYR:CE2	1:A:96:SER:N[2_665]	1.54	0.66
1:A:141:TRP:CA	1:A:220:CYS:CB[2_665]	1.54	0.66
1:A:151:ASP:OD1	1:A:1188:LYS:CA[2_665]	1.54	0.66
1:A:16:ILE:CA	1:A:144:THR:N[2_665]	1.55	0.65
1:A:16:ILE:CG2	1:A:144:THR:N[2_665]	1.55	0.65
1:A:34:ASN:O	1:A:215:TRP:CH2[2_665]	1.55	0.65
1:A:39:TYR:CD2	1:A:228:TYR:N[2_665]	1.55	0.65
1:A:40:HIS:C	1:A:215:TRP:C[2_665]	1.55	0.65
1:A:60:LYS:O	1:A:96:SER:O[2_665]	1.55	0.65
1:A:66:ARG:CG	1:A:217:TYR:CG[2_665]	1.55	0.65
1:A:73:ILE:N	1:A:1221:GLU:O[2_665]	1.55	0.65
1:A:82:PHE:CE1	4:A:344:HOH:O[2_665]	1.55	0.65
1:A:141:TRP:CZ3	1:A:219:GLY:C[2_665]	1.55	0.65
1:A:191:CYS:C	1:A:194:ASP:N[2_665]	1.55	0.65
1:A:17:VAL:CA	1:A:144:THR:CG2[2_665]	1.56	0.64
1:A:41:PHE:CG	1:A:215:TRP:CB[2_665]	1.56	0.64
1:A:59:TYR:CE1	1:A:96:SER:CB[2_665]	1.56	0.64
1:A:74:LYS:NZ	1:A:225:PRO:CB[2_665]	1.56	0.64
1:A:165:TYR:CB	4:A:455:HOH:O[3_556]	1.56	0.64
1:A:16:ILE:C	1:A:144:THR:CG2[2_665]	1.57	0.63
1:A:40:HIS:O	1:A:215:TRP:O[2_665]	1.57	0.63
1:A:97:TYR:CZ	4:A:437:HOH:O[2_665]	1.57	0.63
1:A:141:TRP:CB	1:A:220:CYS:CA[2_665]	1.57	0.63
1:A:32:SER:OG	1:A:217:TYR:CA[2_665]	1.58	0.62
1:A:41:PHE:CZ	1:A:99:ILE:CD1[2_665]	1.58	0.62
1:A:141:TRP:C	1:A:190:SER:O[2_665]	1.58	0.62
1:A:142:GLY:N	1:A:191:CYS:N[2_665]	1.58	0.62
1:A:16:ILE:N	1:A:143:ASN:C[2_665]	1.59	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:VAL:N	1:A:144:THR:CG2[2.665]	1.59	0.61
1:A:32:SER:CB	1:A:219:GLY:N[2.665]	1.59	0.61
1:A:62:ARG:O	1:A:98:ASN:O[2.665]	1.59	0.61
1:A:71:HIS:N	1:A:1221:GLU:OE1[2.665]	1.59	0.61
1:A:141:TRP:CD1	1:A:221:ALA:N[2.665]	1.59	0.61
1:A:213:VAL:CG2	4:A:460:HOH:O[2.665]	1.59	0.61
1:A:62:ARG:O	1:A:98:ASN:CB[2.665]	1.60	0.60
1:A:64:GLU:O	1:A:217:TYR:CE1[2.665]	1.60	0.60
1:A:72:ASN:N	1:A:1221:GLU:OE1[2.665]	1.60	0.60
1:A:182:CYS:SG	4:A:368:HOH:O[2.665]	1.60	0.60
1:A:33:LEU:CB	4:A:384:HOH:O[2.665]	1.61	0.59
1:A:37:SER:CB	1:A:215:TRP:NE1[2.665]	1.61	0.59
1:A:59:TYR:CB	1:A:94:TYR:OH[2.665]	1.61	0.59
1:A:61:SER:CA	1:A:95:SER:OG[2.665]	1.61	0.59
1:A:61:SER:O	1:A:97:TYR:CG[2.665]	1.61	0.59
1:A:18:GLY:N	1:A:150:ALA:O[2.665]	1.62	0.58
1:A:82:PHE:CE2	4:A:344:HOH:O[2.665]	1.63	0.57
1:A:141:TRP:CE3	1:A:219:GLY:O[2.665]	1.63	0.57
1:A:152:SER:OG	1:A:189:ASP:O[2.665]	1.63	0.57
1:A:191:CYS:O	1:A:193:GLY:CA[2.665]	1.63	0.57
1:A:224:ASN:CG	4:A:330:HOH:O[2.665]	1.63	0.57
4:A:364:HOH:O	4:A:364:HOH:O[2.665]	1.63	0.57
1:A:39:TYR:O	1:A:227:VAL:CB[2.665]	1.64	0.56
1:A:57:HIS:CD2	1:A:58:CYS:SG[2.665]	1.64	0.56
1:A:75:VAL:CA	1:A:222:PRO:CB[2.665]	1.64	0.56
1:A:145:MET:CB	1:A:156:GLN:CB[2.665]	1.64	0.56
1:A:192:GLN:CG	1:A:194:ASP:C[2.665]	1.64	0.56
1:A:192:GLN:NE2	1:A:196:GLY:C[2.665]	1.64	0.56
1:A:245:TYR:OH	4:A:388:HOH:O[1.554]	1.64	0.56
1:A:145:MET:CG	1:A:156:GLN:C[2.665]	1.65	0.55
1:A:153:ASP:CA	1:A:221:ALA:CB[2.665]	1.65	0.55
1:A:41:PHE:CG	1:A:215:TRP:N[2.665]	1.66	0.54
1:A:41:PHE:CD2	1:A:214:SER:O[2.665]	1.66	0.54
1:A:61:SER:N	1:A:95:SER:C[2.665]	1.66	0.54
1:A:64:GLU:CG	1:A:217:TYR:OH[2.665]	1.66	0.54
1:A:72:ASN:O	1:A:222:PRO:CD[2.665]	1.66	0.54
1:A:141:TRP:CG	1:A:220:CYS:N[2.665]	1.66	0.54
1:A:165:TYR:CE2	4:A:339:HOH:O[3.556]	1.66	0.54
1:A:40:HIS:CA	1:A:215:TRP:O[2.665]	1.67	0.53
1:A:64:GLU:CD	1:A:175:MET:CE[2.665]	1.67	0.53
1:A:66:ARG:NE	1:A:172:TYR:CD1[2.665]	1.67	0.53
1:A:59:TYR:O	1:A:94:TYR:OH[2.665]	1.68	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:62:ARG:C	1:A:98:ASN:CB[2.665]	1.68	0.52
1:A:71:HIS:C	1:A:1221:GLU:CD[2.665]	1.68	0.52
1:A:75:VAL:N	1:A:222:PRO:C[2.665]	1.68	0.52
1:A:39:TYR:CD1	1:A:227:VAL:CG1[2.665]	1.69	0.51
1:A:57:HIS:ND1	4:A:328:HOH:O[2.665]	1.69	0.51
1:A:60:LYS:CD	1:A:99:ILE:CB[2.665]	1.69	0.51
1:A:62:ARG:CA	1:A:98:ASN:CB[2.665]	1.69	0.51
1:A:140:GLY:CA	1:A:191:CYS:SG[2.665]	1.69	0.51
1:A:145:MET:N	1:A:156:GLN:CB[2.665]	1.69	0.51
1:A:150:ALA:CA	4:A:452:HOH:O[2.665]	1.69	0.51
1:A:62:ARG:CA	1:A:98:ASN:CA[2.665]	1.70	0.50
1:A:97:TYR:CD2	4:A:437:HOH:O[2.665]	1.70	0.50
1:A:144:THR:OG1	4:A:392:HOH:O[2.665]	1.70	0.50
1:A:16:ILE:CG1	1:A:143:ASN:C[2.665]	1.71	0.49
1:A:39:TYR:CE2	1:A:227:VAL:O[2.665]	1.71	0.49
1:A:62:ARG:CA	1:A:98:ASN:N[2.665]	1.71	0.49
1:A:151:ASP:OD2	1:A:188:GLY:CA[2.665]	1.71	0.49
1:A:153:ASP:C	1:A:221:ALA:C[2.665]	1.71	0.49
1:A:195:SER:C	4:A:415:HOH:O[2.665]	1.71	0.49
1:A:226:GLY:CA	4:A:451:HOH:O[2.665]	1.71	0.49
1:A:19:GLY:O	1:A:147:SER:CA[2.665]	1.72	0.48
1:A:57:HIS:CB	1:A:58:CYS:C[2.665]	1.72	0.48
1:A:59:TYR:N	1:A:94:TYR:OH[2.665]	1.72	0.48
1:A:71:HIS:CA	1:A:1221:GLU:CD[2.665]	1.72	0.48
1:A:73:ILE:CD1	1:A:189:ASP:OD2[2.665]	1.72	0.48
1:A:144:THR:O	1:A:156:GLN:CD[2.665]	1.72	0.48
1:A:151:ASP:CA	1:A:188:GLY:O[2.665]	1.72	0.48
1:A:153:ASP:OD1	1:A:1188:LYS:O[2.665]	1.72	0.48
1:A:192:GLN:CD	1:A:197:GLY:CA[2.665]	1.72	0.48
1:A:34:ASN:OD1	1:A:172:TYR:CG[2.665]	1.73	0.47
1:A:61:SER:C	1:A:98:ASN:N[2.665]	1.73	0.47
1:A:71:HIS:N	1:A:1221:GLU:CD[2.665]	1.73	0.47
1:A:80:GLU:OE2	4:A:351:HOH:O[2.665]	1.73	0.47
1:A:153:ASP:CG	1:A:1188:LYS:O[2.665]	1.73	0.47
1:A:18:GLY:N	1:A:150:ALA:C[2.665]	1.74	0.46
1:A:56:ALA:O	4:A:426:HOH:O[2.665]	1.74	0.46
1:A:192:GLN:CA	1:A:194:ASP:N[2.665]	1.74	0.46
1:A:16:ILE:CA	1:A:143:ASN:O[2.665]	1.75	0.45
1:A:17:VAL:C	1:A:152:SER:N[2.665]	1.75	0.45
1:A:30:GLN:NE2	4:A:431:HOH:O[2.665]	1.75	0.45
1:A:34:ASN:ND2	1:A:172:TYR:CE1[2.665]	1.75	0.45
1:A:85:SER:OG	1:A:97:TYR:CD1[2.665]	1.75	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:SER:N	4:A:398:HOH:O[2_665]	1.75	0.45
1:A:145:MET:CG	1:A:156:GLN:CB[2_665]	1.75	0.45
1:A:16:ILE:O	1:A:144:THR:CA[2_665]	1.76	0.44
1:A:37:SER:CA	1:A:215:TRP:CE2[2_665]	1.76	0.44
1:A:60:LYS:CB	1:A:99:ILE:C[2_665]	1.76	0.44
1:A:72:ASN:CB	1:A:222:PRO:CD[2_665]	1.76	0.44
1:A:102:ASP:CG	4:A:328:HOH:O[2_665]	1.76	0.44
1:A:150:ALA:CB	4:A:347:HOH:O[2_665]	1.76	0.44
1:A:151:ASP:CG	1:A:1188:LYS:N[2_665]	1.76	0.44
1:A:38:GLY:O	1:A:168:CYS:SG[2_665]	1.77	0.43
1:A:39:TYR:CE1	1:A:227:VAL:CG1[2_665]	1.77	0.43
1:A:73:ILE:CA	1:A:1221:GLU:C[2_665]	1.77	0.43
1:A:145:MET:CA	1:A:157:CYS:N[2_665]	1.77	0.43
1:A:172:TYR:CB	4:A:366:HOH:O[2_665]	1.77	0.43
1:A:173:PRO:N	4:A:363:HOH:O[2_665]	1.77	0.43
1:A:189:ASP:CA	4:A:458:HOH:O[2_665]	1.77	0.43
1:A:16:ILE:CB	1:A:143:ASN:CA[2_665]	1.78	0.42
1:A:17:VAL:CG2	4:A:325:HOH:O[2_665]	1.78	0.42
1:A:32:SER:C	1:A:216:GLY:O[2_665]	1.78	0.42
1:A:32:SER:CB	1:A:217:TYR:N[2_665]	1.78	0.42
1:A:34:ASN:N	1:A:215:TRP:CZ3[2_665]	1.78	0.42
1:A:39:TYR:CB	1:A:226:GLY:O[2_665]	1.78	0.42
1:A:42:CYS:SG	1:A:57:HIS:NE2[2_665]	1.78	0.42
1:A:62:ARG:N	1:A:98:ASN:CA[2_665]	1.78	0.42
1:A:97:TYR:CE2	4:A:437:HOH:O[2_665]	1.78	0.42
1:A:153:ASP:C	1:A:221:ALA:O[2_665]	1.78	0.42
1:A:153:ASP:OD1	4:A:311:HOH:O[2_665]	1.78	0.42
4:A:345:HOH:O	4:A:385:HOH:O[3_556]	1.78	0.42
1:A:21:GLU:N	1:A:145:MET:O[2_665]	1.79	0.41
1:A:57:HIS:O	1:A:58:CYS:N[2_665]	1.79	0.41
1:A:64:GLU:C	1:A:217:TYR:OH[2_665]	1.79	0.41
1:A:73:ILE:O	1:A:224:ASN:CA[2_665]	1.79	0.41
1:A:142:GLY:C	1:A:194:ASP:OD2[2_665]	1.79	0.41
1:A:153:ASP:O	1:A:1221:GLU:N[2_665]	1.79	0.41
1:A:155:LEU:CG	4:A:359:HOH:O[2_665]	1.79	0.41
1:A:193:GLY:N	1:A:195:SER:N[2_665]	1.79	0.41
1:A:17:VAL:O	1:A:152:SER:CA[2_665]	1.80	0.40
1:A:32:SER:N	4:A:340:HOH:O[2_665]	1.80	0.40
1:A:75:VAL:N	1:A:223:GLY:N[2_665]	1.80	0.40
1:A:141:TRP:CH2	4:A:407:HOH:O[2_665]	1.80	0.40
1:A:149:THR:CA	4:A:301:HOH:O[2_665]	1.80	0.40
1:A:153:ASP:CA	1:A:221:ALA:CA[2_665]	1.80	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:142:GLY:CA	1:A:191:CYS:CA[2_665]	1.81	0.39
1:A:192:GLN:N	1:A:194:ASP:N[2_665]	1.81	0.39
1:A:30:GLN:CD	4:A:431:HOH:O[2_665]	1.82	0.38
1:A:34:ASN:CA	1:A:215:TRP:CH2[2_665]	1.82	0.38
1:A:39:TYR:CD2	1:A:227:VAL:O[2_665]	1.82	0.38
1:A:59:TYR:CB	4:A:426:HOH:O[2_665]	1.82	0.38
1:A:71:HIS:O	1:A:1221:GLU:OE1[2_665]	1.82	0.38
1:A:92:PRO:CA	1:A:148:SER:OG[2_664]	1.82	0.38
1:A:141:TRP:CE3	1:A:219:GLY:CA[2_665]	1.82	0.38
1:A:41:PHE:O	1:A:214:SER:O[2_665]	1.83	0.37
1:A:57:HIS:C	1:A:57:HIS:CB[2_665]	1.83	0.37
1:A:60:LYS:CG	1:A:99:ILE:O[2_665]	1.83	0.37
1:A:66:ARG:NE	1:A:172:TYR:CE1[2_665]	1.83	0.37
1:A:74:LYS:C	1:A:223:GLY:N[2_665]	1.83	0.37
1:A:141:TRP:N	1:A:220:CYS:CB[2_665]	1.83	0.37
1:A:145:MET:CB	1:A:156:GLN:C[2_665]	1.83	0.37
1:A:34:ASN:C	1:A:215:TRP:CE3[2_665]	1.84	0.36
1:A:73:ILE:CG1	4:A:305:HOH:O[2_665]	1.84	0.36
1:A:151:ASP:OD2	1:A:188:GLY:C[2_665]	1.84	0.36
1:A:17:VAL:CG1	1:A:151:ASP:O[2_665]	1.85	0.35
1:A:34:ASN:C	1:A:215:TRP:CE2[2_665]	1.85	0.35
1:A:61:SER:C	1:A:97:TYR:CB[2_665]	1.85	0.35
1:A:70:GLU:O	1:A:1221:GLU:OE2[2_665]	1.85	0.35
1:A:73:ILE:CG1	4:A:302:HOH:O[2_665]	1.85	0.35
1:A:144:THR:O	1:A:156:GLN:CG[2_665]	1.85	0.35
1:A:19:GLY:N	1:A:144:THR:OG1[2_665]	1.86	0.34
1:A:39:TYR:CZ	1:A:228:TYR:N[2_665]	1.86	0.34
1:A:41:PHE:CG	1:A:214:SER:C[2_665]	1.86	0.34
1:A:192:GLN:C	1:A:194:ASP:C[2_665]	1.86	0.34
1:A:19:GLY:O	1:A:147:SER:CB[2_665]	1.87	0.33
1:A:32:SER:O	1:A:217:TYR:CD1[2_665]	1.87	0.33
1:A:33:LEU:C	1:A:215:TRP:CE3[2_665]	1.87	0.33
1:A:40:HIS:O	4:A:341:HOH:O[2_665]	1.87	0.33
1:A:41:PHE:CB	1:A:215:TRP:CA[2_665]	1.87	0.33
1:A:57:HIS:O	1:A:57:HIS:CB[2_665]	1.87	0.33
1:A:61:SER:OG	1:A:95:SER:CB[2_665]	1.87	0.33
1:A:70:GLU:OE1	1:A:224:ASN:OD1[2_665]	1.87	0.33
1:A:74:LYS:CA	4:A:304:HOH:O[2_665]	1.87	0.33
1:A:75:VAL:O	1:A:222:PRO:CB[2_665]	1.87	0.33
1:A:190:SER:CB	4:A:416:HOH:O[2_665]	1.87	0.33
1:A:191:CYS:C	1:A:193:GLY:O[2_665]	1.87	0.33
1:A:192:GLN:C	1:A:194:ASP:N[2_665]	1.87	0.33

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:PHE:N	1:A:216:GLY:N[2.665]	1.88	0.32
1:A:75:VAL:CG2	1:A:186:GLU:O[2.665]	1.88	0.32
1:A:151:ASP:OD1	1:A:188:GLY:O[2.665]	1.88	0.32
1:A:19:GLY:C	1:A:147:SER:N[2.665]	1.89	0.31
1:A:20:TYR:C	1:A:145:MET:C[2.665]	1.89	0.31
1:A:42:CYS:SG	4:A:324:HOH:O[2.665]	1.89	0.31
1:A:60:LYS:CD	1:A:99:ILE:CA[2.665]	1.89	0.31
1:A:142:GLY:CA	1:A:190:SER:C[2.665]	1.89	0.31
1:A:145:MET:CA	1:A:156:GLN:CA[2.665]	1.89	0.31
1:A:192:GLN:CA	1:A:194:ASP:CB[2.665]	1.89	0.31
1:A:16:ILE:CA	1:A:143:ASN:CA[2.665]	1.90	0.30
1:A:18:GLY:C	1:A:150:ALA:C[2.665]	1.90	0.30
1:A:39:TYR:CB	1:A:227:VAL:CA[2.665]	1.90	0.30
1:A:39:TYR:CG	1:A:227:VAL:CB[2.665]	1.90	0.30
1:A:41:PHE:CE1	1:A:215:TRP:CB[2.665]	1.90	0.30
1:A:59:TYR:CD2	1:A:94:TYR:CE2[2.665]	1.90	0.30
1:A:71:HIS:O	1:A:1221:GLU:CD[2.665]	1.90	0.30
1:A:141:TRP:C	1:A:191:CYS:CB[2.665]	1.90	0.30
1:A:144:THR:C	1:A:156:GLN:CB[2.665]	1.90	0.30
1:A:145:MET:CA	1:A:156:GLN:CB[2.665]	1.90	0.30
1:A:60:LYS:CG	1:A:99:ILE:CB[2.665]	1.91	0.29
1:A:65:VAL:N	1:A:217:TYR:OH[2.665]	1.91	0.29
1:A:72:ASN:CA	1:A:1221:GLU:CA[2.665]	1.91	0.29
1:A:72:ASN:CA	1:A:222:PRO:CD[2.665]	1.91	0.29
1:A:74:LYS:CB	4:A:304:HOH:O[2.665]	1.91	0.29
1:A:75:VAL:C	1:A:222:PRO:CB[2.665]	1.91	0.29
1:A:115:ASN:ND2	4:A:463:HOH:O[3.546]	1.91	0.29
1:A:139:SER:CB	4:A:459:HOH:O[2.665]	1.91	0.29
4:A:412:HOH:O	4:A:433:HOH:O[2.665]	1.91	0.29
1:A:41:PHE:CG	1:A:215:TRP:CA[2.665]	1.92	0.28
1:A:61:SER:O	1:A:97:TYR:CA[2.665]	1.92	0.28
1:A:95:SER:CB	4:A:398:HOH:O[2.665]	1.92	0.28
1:A:114:LEU:CG	4:A:401:HOH:O[3.546]	1.92	0.28
1:A:192:GLN:CB	1:A:194:ASP:CA[2.665]	1.92	0.28
1:A:34:ASN:ND2	1:A:172:TYR:CD2[2.665]	1.93	0.27
1:A:59:TYR:CD1	1:A:96:SER:CA[2.665]	1.93	0.27
1:A:66:ARG:CB	1:A:217:TYR:CB[2.665]	1.93	0.27
1:A:85:SER:O	1:A:97:TYR:CZ[2.665]	1.93	0.27
1:A:151:ASP:C	1:A:188:GLY:O[2.665]	1.93	0.27
1:A:190:SER:N	4:A:458:HOH:O[2.665]	1.93	0.27
1:A:192:GLN:O	1:A:194:ASP:OD2[2.665]	1.93	0.27
1:A:192:GLN:OE1	1:A:197:GLY:O[2.665]	1.93	0.27

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:HIS:CA	1:A:1221:GLU:OE2[2_665]	1.94	0.26
1:A:39:TYR:C	1:A:227:VAL:CB[2_665]	1.95	0.25
1:A:60:LYS:CE	1:A:99:ILE:O[2_665]	1.95	0.25
1:A:145:MET:CB	1:A:156:GLN:N[2_665]	1.95	0.25
1:A:192:GLN:OE1	1:A:197:GLY:N[2_665]	1.95	0.25
1:A:16:ILE:CA	1:A:142:GLY:O[2_665]	1.96	0.24
1:A:19:GLY:O	1:A:148:SER:N[2_665]	1.96	0.24
1:A:32:SER:OG	1:A:216:GLY:O[2_665]	1.96	0.24
1:A:41:PHE:CA	1:A:214:SER:C[2_665]	1.96	0.24
1:A:66:ARG:CD	1:A:217:TYR:CD2[2_665]	1.96	0.24
1:A:70:GLU:OE2	1:A:224:ASN:ND2[2_665]	1.96	0.24
1:A:92:PRO:CB	1:A:148:SER:CB[2_664]	1.96	0.24
1:A:60:LYS:C	1:A:95:SER:C[2_665]	1.97	0.23
1:A:66:ARG:CZ	1:A:172:TYR:CD1[2_665]	1.97	0.23
1:A:102:ASP:OD1	4:A:328:HOH:O[2_665]	1.97	0.23
1:A:141:TRP:C	1:A:190:SER:C[2_665]	1.97	0.23
1:A:30:GLN:OE1	4:A:431:HOH:O[2_665]	1.98	0.22
1:A:40:HIS:N	1:A:227:VAL:N[2_665]	1.98	0.22
1:A:40:HIS:CA	1:A:216:GLY:CA[2_665]	1.98	0.22
1:A:41:PHE:C	1:A:215:TRP:CA[2_665]	1.98	0.22
1:A:92:PRO:O	1:A:148:SER:C[2_664]	1.98	0.22
1:A:37:SER:N	1:A:215:TRP:CD2[2_665]	1.99	0.21
1:A:41:PHE:CE1	1:A:215:TRP:CD1[2_665]	1.99	0.21
1:A:59:TYR:C	1:A:94:TYR:CZ[2_665]	1.99	0.21
1:A:153:ASP:N	1:A:221:ALA:CB[2_665]	1.99	0.21
1:A:62:ARG:N	1:A:98:ASN:ND2[2_665]	2.00	0.20
1:A:75:VAL:O	1:A:222:PRO:O[2_665]	2.00	0.20
1:A:113:THR:CG2	4:A:463:HOH:O[3_546]	2.00	0.20
1:A:141:TRP:CE2	4:A:407:HOH:O[2_665]	2.00	0.20
1:A:151:ASP:CG	1:A:188:GLY:CA[2_665]	2.00	0.20
1:A:192:GLN:CA	1:A:194:ASP:O[2_665]	2.00	0.20
1:A:192:GLN:O	1:A:194:ASP:CA[2_665]	2.00	0.20
1:A:34:ASN:O	1:A:215:TRP:CZ2[2_665]	2.01	0.19
1:A:34:ASN:O	1:A:215:TRP:CZ3[2_665]	2.01	0.19
1:A:34:ASN:CG	1:A:172:TYR:CD1[2_665]	2.01	0.19
1:A:41:PHE:CA	1:A:215:TRP:C[2_665]	2.01	0.19
1:A:41:PHE:CD2	1:A:214:SER:C[2_665]	2.01	0.19
1:A:153:ASP:O	1:A:221:ALA:CB[2_665]	2.01	0.19
1:A:191:CYS:CB	1:A:194:ASP:OD1[2_665]	2.01	0.19
1:A:16:ILE:C	1:A:144:THR:N[2_665]	2.02	0.18
1:A:60:LYS:CA	1:A:99:ILE:N[2_665]	2.02	0.18
1:A:60:LYS:C	1:A:96:SER:C[2_665]	2.02	0.18

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:SER:N	1:A:95:SER:OG[2_665]	2.02	0.18
1:A:72:ASN:C	1:A:222:PRO:CD[2_665]	2.02	0.18
1:A:152:SER:CB	1:A:189:ASP:C[2_665]	2.02	0.18
1:A:18:GLY:CA	1:A:151:ASP:CA[2_665]	2.03	0.17
1:A:34:ASN:CG	1:A:172:TYR:CE1[2_665]	2.03	0.17
1:A:34:ASN:OD1	1:A:172:TYR:CD2[2_665]	2.03	0.17
1:A:37:SER:O	1:A:180:MET:SD[2_665]	2.03	0.17
1:A:41:PHE:C	1:A:215:TRP:N[2_665]	2.03	0.17
1:A:143:ASN:O	4:A:325:HOH:O[2_665]	2.03	0.17
1:A:152:SER:CB	1:A:189:ASP:N[2_665]	2.03	0.17
1:A:16:ILE:CD1	1:A:143:ASN:ND2[2_665]	2.04	0.16
1:A:64:GLU:OE2	1:A:175:MET:CE[2_665]	2.04	0.16
1:A:66:ARG:CA	1:A:217:TYR:CD2[2_665]	2.04	0.16
1:A:95:SER:CA	4:A:398:HOH:O[2_665]	2.04	0.16
1:A:139:SER:O	4:A:459:HOH:O[2_665]	2.04	0.16
1:A:142:GLY:CA	1:A:194:ASP:OD2[2_665]	2.04	0.16
1:A:151:ASP:CB	1:A:188:GLY:C[2_665]	2.04	0.16
1:A:19:GLY:O	1:A:147:SER:OG[2_665]	2.05	0.15
1:A:32:SER:CA	1:A:219:GLY:N[2_665]	2.05	0.15
1:A:39:TYR:CG	1:A:227:VAL:C[2_665]	2.05	0.15
1:A:62:ARG:N	1:A:98:ASN:CB[2_665]	2.05	0.15
1:A:73:ILE:CB	1:A:224:ASN:O[2_665]	2.05	0.15
1:A:145:MET:CA	1:A:156:GLN:C[2_665]	2.05	0.15
1:A:145:MET:CG	1:A:156:GLN:O[2_665]	2.05	0.15
1:A:145:MET:CE	1:A:156:GLN:O[2_665]	2.05	0.15
1:A:150:ALA:N	4:A:452:HOH:O[2_665]	2.05	0.15
1:A:34:ASN:C	1:A:215:TRP:CD2[2_665]	2.06	0.14
1:A:41:PHE:O	1:A:214:SER:C[2_665]	2.06	0.14
1:A:42:CYS:N	3:A:246:BEN:C4[2_665]	2.06	0.14
1:A:42:CYS:O	4:A:384:HOH:O[2_665]	2.06	0.14
1:A:61:SER:OG	1:A:98:ASN:ND2[2_665]	2.06	0.14
1:A:74:LYS:N	4:A:304:HOH:O[2_665]	2.06	0.14
1:A:113:THR:OG1	1:A:164:SER:CB[3_546]	2.06	0.14
1:A:149:THR:OG1	4:A:369:HOH:O[2_666]	2.06	0.14
1:A:192:GLN:CD	1:A:194:ASP:O[2_665]	2.06	0.14
1:A:40:HIS:ND1	3:A:246:BEN:C2[2_665]	2.07	0.13
1:A:41:PHE:N	1:A:215:TRP:N[2_665]	2.07	0.13
1:A:60:LYS:CE	1:A:99:ILE:CG2[2_665]	2.07	0.13
1:A:62:ARG:CB	1:A:98:ASN:CB[2_665]	2.07	0.13
1:A:73:ILE:N	1:A:1221:GLU:CB[2_665]	2.07	0.13
1:A:189:ASP:C	4:A:458:HOH:O[2_665]	2.07	0.13
1:A:191:CYS:O	1:A:193:GLY:O[2_665]	2.07	0.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:327:HOH:O	4:A:351:HOH:O[2.665]	2.07	0.13
1:A:32:SER:OG	1:A:217:TYR:C[2.665]	2.08	0.12
1:A:34:ASN:ND2	1:A:172:TYR:OH[2.665]	2.08	0.12
1:A:37:SER:CB	1:A:215:TRP:CE2[2.665]	2.08	0.12
1:A:42:CYS:SG	1:A:57:HIS:CE1[2.665]	2.08	0.12
1:A:60:LYS:N	1:A:96:SER:CA[2.665]	2.08	0.12
1:A:72:ASN:O	1:A:1221:GLU:CA[2.665]	2.08	0.12
1:A:75:VAL:N	1:A:222:PRO:CB[2.665]	2.08	0.12
1:A:75:VAL:N	1:A:185:LEU:O[2.665]	2.08	0.12
1:A:75:VAL:O	1:A:222:PRO:C[2.665]	2.08	0.12
1:A:114:LEU:CD1	4:A:401:HOH:O[3.546]	2.08	0.12
1:A:151:ASP:O	1:A:188:GLY:O[2.665]	2.08	0.12
1:A:224:ASN:ND2	4:A:330:HOH:O[2.665]	2.08	0.12
1:A:17:VAL:CB	1:A:152:SER:CA[2.665]	2.09	0.11
1:A:40:HIS:ND1	3:A:246:BEN:N2[2.665]	2.09	0.11
1:A:41:PHE:C	1:A:214:SER:C[2.665]	2.09	0.11
1:A:42:CYS:CA	3:A:246:BEN:C3[2.665]	2.09	0.11
1:A:66:ARG:NH2	1:A:171:SER:C[2.665]	2.09	0.11
1:A:74:LYS:NZ	1:A:225:PRO:CG[2.665]	2.09	0.11
1:A:88:VAL:CG2	1:A:97:TYR:CA[2.665]	2.09	0.11
1:A:113:THR:CG2	1:A:164:SER:CB[3.546]	2.09	0.11
1:A:141:TRP:CE2	1:A:220:CYS:O[2.665]	2.09	0.11
1:A:149:THR:CG2	4:A:369:HOH:O[2.666]	2.09	0.11
1:A:245:TYR:CZ	4:A:388:HOH:O[1.554]	2.09	0.11
1:A:39:TYR:C	1:A:227:VAL:N[2.665]	2.10	0.10
1:A:39:TYR:CD2	1:A:227:VAL:N[2.665]	2.10	0.10
1:A:40:HIS:CD2	3:A:246:BEN:C6[2.665]	2.10	0.10
1:A:141:TRP:C	1:A:191:CYS:CA[2.665]	2.10	0.10
1:A:32:SER:CA	1:A:217:TYR:CA[2.665]	2.11	0.09
1:A:34:ASN:CA	1:A:215:TRP:CD2[2.665]	2.11	0.09
1:A:39:TYR:CD2	1:A:227:VAL:CB[2.665]	2.11	0.09
1:A:75:VAL:CA	1:A:222:PRO:CA[2.665]	2.11	0.09
1:A:144:THR:CA	4:A:392:HOH:O[2.665]	2.11	0.09
1:A:18:GLY:O	1:A:150:ALA:O[2.665]	2.12	0.08
1:A:39:TYR:CE2	1:A:228:TYR:CA[2.665]	2.12	0.08
1:A:40:HIS:CD2	3:A:246:BEN:C2[2.665]	2.12	0.08
1:A:59:TYR:CE1	1:A:96:SER:CA[2.665]	2.12	0.08
1:A:73:ILE:C	1:A:224:ASN:N[2.665]	2.12	0.08
1:A:155:LEU:CD1	4:A:359:HOH:O[2.665]	2.12	0.08
1:A:165:TYR:CD2	4:A:374:HOH:O[3.556]	2.12	0.08
1:A:192:GLN:OE1	1:A:197:GLY:CA[2.665]	2.12	0.08
1:A:192:GLN:OE1	1:A:197:GLY:C[2.665]	2.12	0.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:342:HOH:O	4:A:365:HOH:O[2.665]	2.12	0.08
1:A:17:VAL:O	1:A:151:ASP:C[2.665]	2.13	0.07
1:A:20:TYR:N	1:A:147:SER:O[2.665]	2.13	0.07
1:A:34:ASN:CG	1:A:172:TYR:CZ[2.665]	2.13	0.07
1:A:40:HIS:NE2	3:A:246:BEN:N2[2.665]	2.13	0.07
1:A:41:PHE:CE1	1:A:99:ILE:CD1[2.665]	2.13	0.07
1:A:60:LYS:CA	1:A:99:ILE:CA[2.665]	2.13	0.07
1:A:113:THR:OG1	4:A:349:HOH:O[3.546]	2.13	0.07
1:A:141:TRP:CA	1:A:220:CYS:SG[2.665]	2.13	0.07
1:A:156:GLN:OE1	4:A:347:HOH:O[2.665]	2.13	0.07
1:A:16:ILE:CB	1:A:144:THR:CA[2.665]	2.14	0.06
1:A:41:PHE:C	1:A:214:SER:O[2.665]	2.14	0.06
1:A:41:PHE:CG	1:A:215:TRP:CG[2.665]	2.14	0.06
1:A:62:ARG:C	1:A:98:ASN:N[2.665]	2.14	0.06
1:A:70:GLU:C	1:A:1221:GLU:OE2[2.665]	2.14	0.06
1:A:74:LYS:C	1:A:185:LEU:C[2.665]	2.14	0.06
1:A:92:PRO:C	1:A:148:SER:CB[2.664]	2.14	0.06
1:A:141:TRP:N	1:A:191:CYS:CB[2.665]	2.14	0.06
1:A:153:ASP:OD2	1:A:1188:LYS:O[2.665]	2.14	0.06
1:A:191:CYS:C	1:A:194:ASP:CA[2.665]	2.14	0.06
1:A:16:ILE:CB	1:A:143:ASN:O[2.665]	2.15	0.05
1:A:32:SER:CA	1:A:216:GLY:O[2.665]	2.15	0.05
1:A:34:ASN:CG	1:A:172:TYR:CG[2.665]	2.15	0.05
1:A:37:SER:OG	1:A:215:TRP:CD1[2.665]	2.15	0.05
1:A:59:TYR:CD2	1:A:96:SER:N[2.665]	2.15	0.05
1:A:144:THR:C	4:A:392:HOH:O[2.665]	2.15	0.05
1:A:145:MET:CE	1:A:156:GLN:C[2.665]	2.15	0.05
1:A:151:ASP:CB	4:A:433:HOH:O[2.665]	2.15	0.05
1:A:155:LEU:C	4:A:359:HOH:O[2.665]	2.15	0.05
1:A:20:TYR:CA	1:A:147:SER:C[2.665]	2.16	0.04
1:A:20:TYR:CB	1:A:148:SER:N[2.665]	2.16	0.04
1:A:32:SER:CA	4:A:340:HOH:O[2.665]	2.16	0.04
1:A:41:PHE:CZ	1:A:99:ILE:CG2[2.665]	2.16	0.04
1:A:61:SER:CB	1:A:95:SER:CB[2.665]	2.16	0.04
1:A:62:ARG:N	1:A:97:TYR:C[2.665]	2.16	0.04
1:A:70:GLU:C	1:A:1221:GLU:CD[2.665]	2.16	0.04
1:A:72:ASN:C	1:A:1221:GLU:CB[2.665]	2.16	0.04
1:A:72:ASN:C	1:A:1221:GLU:O[2.665]	2.16	0.04
1:A:75:VAL:CG2	4:A:428:HOH:O[2.665]	2.16	0.04
1:A:141:TRP:CZ3	1:A:219:GLY:N[2.665]	2.16	0.04
1:A:142:GLY:N	1:A:190:SER:C[2.665]	2.16	0.04
1:A:144:THR:O	4:A:392:HOH:O[2.665]	2.16	0.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:GLY:CA	4:A:375:HOH:O[2_665]	2.16	0.04
1:A:192:GLN:CA	1:A:195:SER:N[2_665]	2.16	0.04
1:A:245:TYR:CE2	4:A:388:HOH:O[1_554]	2.16	0.04
1:A:17:VAL:O	1:A:152:SER:CB[2_665]	2.17	0.03
1:A:40:HIS:CG	3:A:246:BEN:C1[2_665]	2.17	0.03
1:A:41:PHE:CE2	1:A:99:ILE:CG2[2_665]	2.17	0.03
1:A:57:HIS:CB	1:A:59:TYR:N[2_665]	2.17	0.03
1:A:59:TYR:CG	1:A:96:SER:CA[2_665]	2.17	0.03
1:A:59:TYR:CE1	1:A:96:SER:N[2_665]	2.17	0.03
1:A:60:LYS:CB	1:A:100:ASP:N[2_665]	2.17	0.03
1:A:61:SER:C	1:A:97:TYR:CA[2_665]	2.17	0.03
1:A:66:ARG:CD	1:A:172:TYR:CE1[2_665]	2.17	0.03
1:A:72:ASN:O	1:A:222:PRO:CA[2_665]	2.17	0.03
1:A:73:ILE:O	1:A:223:GLY:C[2_665]	2.17	0.03
1:A:195:SER:OG	4:A:415:HOH:O[2_665]	2.17	0.03
1:A:16:ILE:C	1:A:144:THR:CB[2_665]	2.18	0.02
1:A:18:GLY:N	1:A:151:ASP:N[2_665]	2.18	0.02
1:A:32:SER:CB	1:A:217:TYR:O[2_665]	2.18	0.02
1:A:33:LEU:O	1:A:215:TRP:CE3[2_665]	2.18	0.02
1:A:39:TYR:CB	1:A:226:GLY:C[2_665]	2.18	0.02
1:A:40:HIS:O	1:A:227:VAL:N[2_665]	2.18	0.02
1:A:40:HIS:CE1	3:A:246:BEN:C3[2_665]	2.18	0.02
1:A:41:PHE:CA	1:A:215:TRP:O[2_665]	2.18	0.02
1:A:73:ILE:CA	1:A:1221:GLU:CA[2_665]	2.18	0.02
1:A:73:ILE:CG2	1:A:217:TYR:O[2_665]	2.18	0.02
1:A:74:LYS:CA	1:A:185:LEU:O[2_665]	2.18	0.02
1:A:75:VAL:CB	1:A:222:PRO:CG[2_665]	2.18	0.02
1:A:144:THR:O	1:A:156:GLN:CB[2_665]	2.18	0.02
1:A:153:ASP:CB	1:A:188:GLY:N[2_665]	2.18	0.02
1:A:182:CYS:CA	4:A:368:HOH:O[2_665]	2.18	0.02
1:A:20:TYR:CA	1:A:147:SER:N[2_665]	2.19	0.01
1:A:37:SER:OG	1:A:215:TRP:CE2[2_665]	2.19	0.01
1:A:62:ARG:N	1:A:98:ASN:CG[2_665]	2.19	0.01
1:A:64:GLU:OE1	1:A:175:MET:CE[2_665]	2.19	0.01
1:A:71:HIS:N	1:A:1221:GLU:OE2[2_665]	2.19	0.01
1:A:85:SER:C	1:A:97:TYR:OH[2_665]	2.19	0.01
1:A:175:MET:CE	4:A:366:HOH:O[2_665]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	220/222 (99%)	213 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	185/185 (100%)	177 (96%)	8 (4%)	40	19

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	47	VAL
1	A	92	PRO
1	A	97	TYR
1	A	98	ASN
1	A	130	PRO
1	A	178	ASN
1	A	186	GLU

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	27	GLN
1	A	93	ASN
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	210	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BEN	A	246	1	9,9,9	5.03	3 (33%)	11,11,11	3.99	9 (81%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	A	246	1	-	0/4/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	BEN	C1-C	-14.23	1.34	1.49
3	A	246	BEN	C-N1	2.71	1.35	1.27
3	A	246	BEN	C4-C3	2.34	1.44	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	BEN	C5-C4-C3	-6.68	106.06	119.97
3	A	246	BEN	C4-C3-C2	5.48	129.30	120.17
3	A	246	BEN	C4-C5-C6	5.37	129.11	120.17
3	A	246	BEN	N2-C-N1	-4.32	109.83	121.04
3	A	246	BEN	C1-C-N2	3.85	124.07	117.99
3	A	246	BEN	C3-C2-C1	-3.70	115.52	120.32
3	A	246	BEN	C6-C1-C2	3.21	123.22	118.63
3	A	246	BEN	C5-C6-C1	-2.82	116.65	120.32
3	A	246	BEN	C6-C1-C	-2.13	115.11	120.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/222 (99%)	4.49	206 (93%) 0 0	6, 15, 27, 46	9 (4%)

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	13.7
1	A	240	SER	11.5
1	A	168	CYS	10.5
1	A	17	VAL	8.9
1	A	83	ILE	8.8
1	A	134	THR	8.1
1	A	225	PRO	8.0
1	A	1184	TYR	8.0
1	A	160	ILE	7.8
1	A	65	VAL	7.7
1	A	117	TYR	7.6
1	A	203	GLY	7.5
1	A	25	TYR	7.5
1	A	89	ILE	7.5
1	A	115	ASN	7.4
1	A	63	VAL	7.4
1	A	114	LEU	7.4
1	A	118	VAL	7.2
1	A	142	GLY	7.2
1	A	94	TYR	7.2
1	A	191	CYS	7.2
1	A	107	LYS	7.2
1	A	241	THR	7.1
1	A	97	TYR	7.1
1	A	138	VAL	7.1
1	A	169	ASN	7.0
1	A	213	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	116	THR	6.7
1	A	111	PRO	6.6
1	A	204	GLU	6.6
1	A	149	THR	6.5
1	A	39	TYR	6.4
1	A	202	ASN	6.4
1	A	176	ILE	6.2
1	A	234	PHE	6.2
1	A	125	THR	6.2
1	A	71	HIS	6.1
1	A	113	THR	6.0
1	A	49	GLU	6.0
1	A	165	TYR	6.0
1	A	175	MET	5.9
1	A	121	VAL	5.9
1	A	119	GLN	5.8
1	A	110	LYS	5.7
1	A	193	GLY	5.7
1	A	148	SER	5.7
1	A	150	ALA	5.7
1	A	209	LEU	5.7
1	A	20	TYR	5.6
1	A	170	ASP	5.6
1	A	123	LEU	5.6
1	A	98	ASN	5.6
1	A	162	ILE	5.6
1	A	100	ASP	5.5
1	A	152	SER	5.5
1	A	128	CYS	5.5
1	A	141	TRP	5.5
1	A	59	TYR	5.4
1	A	233	ILE	5.4
1	A	42	CYS	5.4
1	A	46	LEU	5.4
1	A	105	LEU	5.4
1	A	178	ASN	5.4
1	A	239	THR	5.3
1	A	99	ILE	5.3
1	A	52	VAL	5.3
1	A	103	ILE	5.3
1	A	33	LEU	5.3
1	A	217	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	82	PHE	5.2
1	A	212	VAL	5.2
1	A	56	ALA	5.2
1	A	96	SER	5.2
1	A	157	CYS	5.2
1	A	243	ALA	5.2
1	A	75	VAL	5.1
1	A	237	TRP	5.1
1	A	18	GLY	5.1
1	A	24	ALA	5.1
1	A	106	ILE	5.1
1	A	90	ARG	5.0
1	A	101	ASN	5.0
1	A	88	VAL	5.0
1	A	120	PRO	4.9
1	A	108	LEU	4.8
1	A	127	SER	4.8
1	A	129	ALA	4.7
1	A	85	SER	4.7
1	A	26	SER	4.7
1	A	224	ASN	4.7
1	A	231	VAL	4.7
1	A	223	GLY	4.7
1	A	181	PHE	4.6
1	A	229	ALA	4.6
1	A	87	ARG	4.6
1	A	1188	LYS	4.6
1	A	236	ASP	4.6
1	A	41	PHE	4.5
1	A	37	SER	4.5
1	A	172	TYR	4.5
1	A	135	MET	4.4
1	A	45	SER	4.4
1	A	155	LEU	4.4
1	A	102	ASP	4.4
1	A	183	ALA	4.4
1	A	163	LEU	4.4
1	A	214	SER	4.4
1	A	47	VAL	4.4
1	A	137	THR	4.4
1	A	44	GLY	4.4
1	A	50	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	38	GLY	4.3
1	A	158	LEU	4.3
1	A	51	TRP	4.2
1	A	228	TYR	4.2
1	A	109	SER	4.2
1	A	67	LEU	4.2
1	A	190	SER	4.2
1	A	72	ASN	4.1
1	A	92	PRO	4.1
1	A	200	VAL	4.1
1	A	215	TRP	4.1
1	A	133	GLY	4.1
1	A	53	VAL	4.0
1	A	112	ALA	4.0
1	A	136	CYS	4.0
1	A	210	GLN	4.0
1	A	28	ALA	3.9
1	A	242	MET	3.9
1	A	27	GLN	3.9
1	A	144	THR	3.9
1	A	132	ALA	3.9
1	A	198	PRO	3.8
1	A	154	LYS	3.8
1	A	235	SER	3.8
1	A	91	HIS	3.7
1	A	199	VAL	3.7
1	A	84	SER	3.7
1	A	54	SER	3.7
1	A	95	SER	3.6
1	A	185	LEU	3.6
1	A	43	GLY	3.6
1	A	104	MET	3.5
1	A	159	ASN	3.5
1	A	61	SER	3.5
1	A	31	VAL	3.4
1	A	220	CYS	3.4
1	A	66	ARG	3.4
1	A	124	PRO	3.4
1	A	179	ALA	3.4
1	A	182	CYS	3.4
1	A	184	GLY	3.3
1	A	195	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	186	GLU	3.3
1	A	167	ASP	3.3
1	A	48	ASN	3.3
1	A	139	SER	3.3
1	A	189	ASP	3.3
1	A	81	GLN	3.3
1	A	161	PRO	3.3
1	A	29	HIS	3.3
1	A	69	GLY	3.2
1	A	196	GLY	3.2
1	A	76	THR	3.2
1	A	93	ASN	3.2
1	A	22	CYS	3.2
1	A	174	GLY	3.1
1	A	143	ASN	3.1
1	A	21	GLU	3.1
1	A	171	SER	3.1
1	A	122	ALA	3.1
1	A	130	PRO	3.1
1	A	23	LYS	3.0
1	A	197	GLY	3.0
1	A	1221	GLU	3.0
1	A	32	SER	3.0
1	A	86	SER	3.0
1	A	232	CYS	3.0
1	A	177	THR	2.9
1	A	151	ASP	2.9
1	A	58	CYS	2.8
1	A	57	HIS	2.8
1	A	211	GLY	2.8
1	A	187	GLY	2.8
1	A	62	ARG	2.7
1	A	55	ALA	2.7
1	A	180	MET	2.7
1	A	19	GLY	2.6
1	A	73	ILE	2.6
1	A	16	ILE	2.6
1	A	78	GLY	2.6
1	A	166	SER	2.5
1	A	79	SER	2.5
1	A	222	PRO	2.5
1	A	227	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLY	2.4
1	A	201	CYS	2.4
1	A	230	LYS	2.3
1	A	153	ASP	2.3
1	A	219	GLY	2.3
1	A	77	GLU	2.2
1	A	226	GLY	2.1
1	A	64	GLU	2.1
1	A	145	MET	2.1
1	A	173	PRO	2.1
1	A	188	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BEN	A	246	9/9	0.35	0.39	8,19,22,25	0
2	CA	A	247	1/1	0.32	-0.15	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.