



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

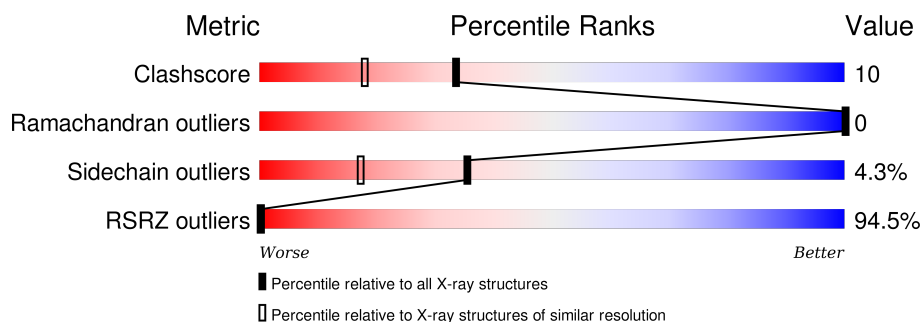
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	222	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1833 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 TRYPSIN.

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

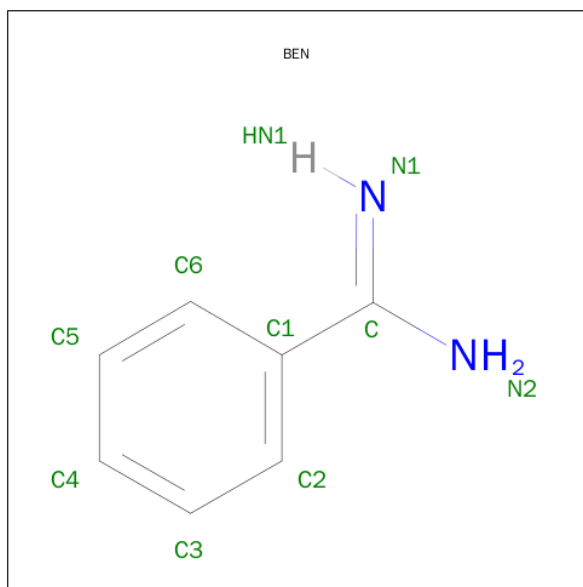
There are 4 discrepancies between the modelled and reference sequences:

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: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



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

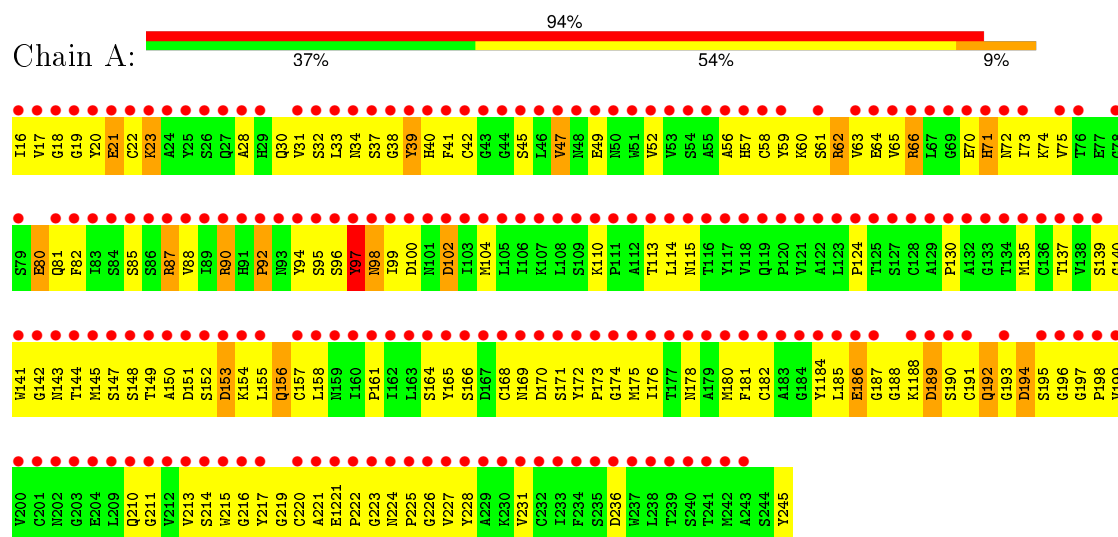
- Molecule 4 is water.

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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.83Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.495 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	12.0	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18298 reflections	Xtriage
$F_o, F_c$ correlation	0.54	EDS
Total number of atoms	1833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1659	0	1562	32	699

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 10.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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:165:TYR:CD2	4:A:339:HOH:O[3_556]	0.34	1.86
1:A:141:TRP:CD1	1:A:220:CYS:C[2_665]	0.34	1.86
1:A:145:MET:SD	1:A:156:GLN:O[2_665]	0.38	1.82
1:A:74:LYS:O	1:A:185:LEU:O[2_665]	0.42	1.78
1:A:40:HIS:C	1:A:215:TRP: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:192:GLN:NE2	1:A:197:GLY:N[2_665]	0.50	1.70
1:A:153:ASP:O	1:A:221:ALA:C[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:192:GLN:CA	1:A:194:ASP:CA[2_665]	0.53	1.67
1:A:187:GLY:O	4:A:375:HOH:O[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
4:A:364:HOH:O	4:A:453:HOH:O[2_665]	0.71	1.49
1:A:141:TRP:O	1:A:190:SER:O[2_665]	0.71	1.49
1:A:32:SER:OG	1:A:217:TYR:N[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:TRP:CE3	1:A:219:GLY:C[2_665]	0.82	1.38
1:A:70:GLU:OE2	1:A:224:ASN:OD1[2_665]	0.82	1.38
1:A:224:ASN:CB	4:A:330:HOH:O[2_665]	0.83	1.37
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
1:A:141:TRP:CZ3	1:A:219:GLY:CA[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:72:ASN:C	1:A:1221:GLU:C[2_665]	0.93	1.27
1:A:18:GLY:C	1:A:150:ALA:O[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:59:TYR:CE1	1:A:96:SER:OG[2_665]	0.95	1.25
1:A:39:TYR:CD2	1:A:227:VAL:CA[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:73:ILE:N	1:A:1221:GLU:CA[2_665]	0.98	1.22
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: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: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:CB	1:A:143:ASN:C[2_665]	1.01	1.19
1:A:41:PHE:N	1:A:215:TRP:O[2_665]	1.02	1.18
1:A:16:ILE:CD1	1:A:143:ASN:CB[2_665]	1.02	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:329:HOH:O	4:A:329:HOH:O[2_665]	1.02	1.18
1:A:62:ARG:N	1:A:98:ASN:N[2_665]	1.02	1.18
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:39:TYR:CE2	1:A:227:VAL:C[2_665]	1.04	1.16
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:74:LYS:C	1:A:185:LEU:O[2_665]	1.05	1.15
1:A:38:GLY:O	1:A:182:CYS:SG[2_665]	1.05	1.15
1:A:19:GLY:C	1:A:147:SER:O[2_665]	1.05	1.15
1:A:72:ASN:C	1:A:1221:GLU:CA[2_665]	1.05	1.15
1:A:151:ASP:CG	1:A:188:GLY:C[2_665]	1.05	1.15
1:A:32:SER:CB	1:A:217:TYR:C[2_665]	1.05	1.15
1:A:16:ILE:CG1	1:A:143:ASN:CB[2_665]	1.05	1.15
1:A:153:ASP:C	1:A:221:ALA:CB[2_665]	1.05	1.15
1:A:73:ILE:C	1:A:1221:GLU:O[2_665]	1.06	1.14
1:A:32:SER:CB	1:A:217:TYR:CA[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
4:A:342:HOH:O	4:A:436:HOH:O[2_665]	1.08	1.12
1:A:16:ILE:CA	1:A:143:ASN:C[2_665]	1.08	1.12
1:A:37:SER:CA	1:A:215:TRP:CZ2[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:C	1:A:145:MET:O[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: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:145:MET:CG	1:A:156:GLN:N[2_665]	1.09	1.11
1:A:192:GLN:C	1:A:194:ASP:CB[2_665]	1.10	1.10
1:A:20:TYR:O	1:A:145:MET: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:60:LYS:CD	1:A:99:ILE:O[2_665]	1.10	1.10
1:A:73:ILE:CA	1:A:1221:GLU:O[2_665]	1.11	1.09
1:A:42:CYS:CB	4:A:324:HOH:O[2_665]	1.11	1.09
1:A:19:GLY:O	1:A:147:SER:C[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:CYS:O	1:A:194:ASP:N[2_665]	1.15	1.05
1:A:151:ASP:OD1	1:A:188:GLY:C[2_665]	1.15	1.05
1:A:60:LYS:CG	1:A:99:ILE:CA[2_665]	1.15	1.05
1:A:192:GLN:CA	1:A:194:ASP:C[2_665]	1.15	1.05
1:A:141:TRP:CZ2	4:A:407:HOH:O[2_665]	1.16	1.04
1:A:71:HIS:CA	1:A:1221:GLU:OE1[2_665]	1.16	1.04
1:A:152:SER:OG	1:A:189:ASP:N[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:195:SER:CA	4:A:415:HOH:O[2_665]	1.17	1.03
1:A:60:LYS:CB	1:A:99:ILE:N[2_665]	1.17	1.03
1:A:32:SER:OG	1:A:216:GLY:C[2_665]	1.17	1.03
1:A:66:ARG:CB	1:A:217:TYR:CD2[2_665]	1.18	1.02
1:A:57:HIS:CA	1:A:57:HIS:C[2_665]	1.18	1.02
1:A:64:GLU:OE1	4:A:336:HOH:O[2_665]	1.18	1.02
1:A:57:HIS:CB	1:A:58:CYS:CA[2_665]	1.18	1.02
1:A:172:TYR:OH	4:A:315:HOH:O[2_665]	1.19	1.01
1:A:165:TYR:CG	4:A:339:HOH:O[3_556]	1.19	1.01
1:A:141:TRP:N	1:A:191:CYS:SG[2_665]	1.19	1.01
1:A:34:ASN:ND2	1:A:172:TYR:CE2[2_665]	1.19	1.01
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:39:TYR:CE2	1:A:228:TYR:N[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:153:ASP:O	1:A:221:ALA: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:31:VAL:C	4:A:340:HOH:O[2_665]	1.22	0.98
1:A:64:GLU:CB	1:A:175:MET:SD[2_665]	1.22	0.98
1:A:152:SER:CB	1:A:189:ASP:O[2_665]	1.23	0.97
2:A:247:CA:CA	4:A:351:HOH:O[2_665]	1.24	0.96
1:A:192:GLN:C	1:A:194:ASP:CA[2_665]	1.24	0.96
1:A:140:GLY:C	1:A:191:CYS:SG[2_665]	1.25	0.95
1:A:153:ASP:O	1:A:221:ALA:CA[2_665]	1.25	0.95
1:A:64:GLU:OE2	4:A:336:HOH:O[2_665]	1.25	0.95
1:A:145:MET:SD	1:A:156:GLN:C[2_665]	1.25	0.95
1:A:74:LYS:CE	1:A:225:PRO:CB[2_665]	1.25	0.95
1:A:39:TYR:C	1:A:227:VAL:CG2[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:152:SER:OG	1:A:189:ASP:CA[2_665]	1.27	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:C	4:A:301:HOH:O[2_665]	1.27	0.93
1:A:39:TYR:N	1:A:227:VAL:CG2[2_665]	1.27	0.93
1:A:192:GLN:CD	1:A:197:GLY:N[2_665]	1.27	0.93
1:A:59:TYR:CD1	1:A:96:SER:OG[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: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:60:LYS:CA	1:A:95:SER:O[2_665]	1.29	0.91
1:A:20:TYR:N	1:A:147:SER:N[2_665]	1.29	0.91
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:142:GLY:N	1:A:191:CYS:CA[2_665]	1.31	0.89
1:A:92:PRO:CA	1:A:148:SER:CB[2_664]	1.31	0.89
1:A:173:PRO:CD	4:A:363:HOH:O[2_665]	1.31	0.89
1:A:34:ASN:N	1:A:215:TRP:CE3[2_665]	1.31	0.89
1:A:192:GLN:O	1:A:194:ASP:CG[2_665]	1.31	0.89
1:A:192:GLN:NE2	1:A:197:GLY:CA[2_665]	1.32	0.88
1:A:189:ASP:CG	4:A:458:HOH:O[2_665]	1.32	0.88
1:A:141:TRP:N	1:A:220:CYS:SG[2_665]	1.32	0.88
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:114:LEU:O	1:A:166:SER:OG[3_546]	1.33	0.87
1:A:57:HIS:CG	1:A:58:CYS:CA[2_665]	1.34	0.86
1:A:41:PHE:CB	1:A:214:SER:C[2_665]	1.34	0.86
1:A:153:ASP:C	1:A:221:ALA:CA[2_665]	1.34	0.86
1:A:75:VAL:N	1:A:222:PRO: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:154:LYS:N	1:A:221:ALA:CB[2_665]	1.34	0.86
1:A:143:ASN:N	1:A:194:ASP:OD2[2_665]	1.34	0.86
1:A:141:TRP:CE2	1:A:220:CYS:N[2_665]	1.35	0.85
1:A:70:GLU:OE2	1:A:224:ASN:CG[2_665]	1.35	0.85
1:A:222:PRO:O	4:A:327:HOH:O[2_665]	1.35	0.85
1:A:187:GLY:C	4:A:375:HOH:O[2_665]	1.36	0.84
1:A:39:TYR:O	1:A:227:VAL:CG2[2_665]	1.36	0.84
1:A:34:ASN:C	1:A:215:TRP:CZ2[2_665]	1.36	0.84
1:A:141:TRP:CB	1:A:220:CYS:CB[2_665]	1.37	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TRP:CG	1:A:220:CYS:CB[2_665]	1.37	0.83
1:A:85:SER:OG	1:A:97:TYR:CE1[2_665]	1.37	0.83
1:A:73:ILE:CB	4:A:305:HOH:O[2_665]	1.38	0.82
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: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
1:A:141:TRP:CG	1:A:220:CYS:C[2_665]	1.41	0.79
1:A:74:LYS:N	1:A:1221:GLU: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:19:GLY:CA	1:A:147:SER: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:33:LEU:O	1:A:216:GLY:N[2_665]	1.42	0.78
1:A:114:LEU:CB	4:A:401:HOH:O[3_546]	1.42	0.78
1:A:189:ASP:OD1	4:A:458:HOH:O[2_665]	1.43	0.77
1:A:144:THR:O	1:A:156:GLN:OE1[2_665]	1.43	0.77
1:A:141:TRP:O	1:A:190:SER:C[2_665]	1.43	0.77
1:A:66:ARG:CG	1:A:217:TYR:CE2[2_665]	1.43	0.77
1:A:144:THR:CB	4:A:392:HOH:O[2_665]	1.43	0.77
1:A:141:TRP:CH2	1:A:219:GLY:CA[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:192:GLN:CB	1:A:194:ASP:C[2_665]	1.46	0.74
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:141:TRP:NE1	1:A:220:CYS:C[2_665]	1.47	0.73
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:155:LEU:CB	4:A:359:HOH:O[2_665]	1.47	0.73
1:A:152:SER:OG	1:A:189:ASP:C[2_665]	1.47	0.73
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:41:PHE:CD1	1:A:215:TRP:CD1[2_665]	1.48	0.72
1:A:20:TYR:O	1:A:145:MET:C[2_665]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:ARG:O	1:A:98:ASN:C[2_665]	1.49	0.71
1:A:59:TYR:CG	1:A:96:SER:CB[2_665]	1.49	0.71
1:A:57:HIS:N	1:A:57:HIS:O[2_665]	1.49	0.71
1:A:19:GLY:N	1:A:150:ALA:O[2_665]	1.49	0.71
1:A:75:VAL:CB	1:A:222:PRO:CB[2_665]	1.50	0.70
1:A:59:TYR:C	1:A:94:TYR:OH[2_665]	1.50	0.70
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:57:HIS:CB	1:A:58:CYS:N[2_665]	1.51	0.69
1:A:141:TRP:CD2	1:A:219:GLY:C[2_665]	1.51	0.69
1:A:74:LYS:CG	4:A:304:HOH:O[2_665]	1.51	0.69
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:59:TYR:CZ	1:A:96:SER:N[2_665]	1.53	0.67
1:A:16:ILE:O	1:A:144:THR:CB[2_665]	1.53	0.67
1:A:141:TRP:CD1	1:A:220:CYS:CA[2_665]	1.53	0.67
1:A:59:TYR:O	1:A:94:TYR:CZ[2_665]	1.53	0.67
1:A:16:ILE:CG2	4:A:319:HOH:O[2_665]	1.53	0.67
1:A:151:ASP:OD1	1:A:1188:LYS:CA[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:19:GLY:O	1:A:147:SER:O[2_665]	1.54	0.66
1:A:41:PHE:CE1	1:A:215:TRP:CG[2_665]	1.54	0.66
1:A:141:TRP:CA	1:A:220:CYS:CB[2_665]	1.54	0.66
1:A:59:TYR:CE2	1:A:96:SER:N[2_665]	1.54	0.66
1:A:22:CYS:SG	1:A:145:MET:CE[2_665]	1.54	0.66
1:A:66:ARG:CG	1:A:217:TYR:CG[2_665]	1.55	0.65
1:A:16:ILE:CA	1:A:144:THR:N[2_665]	1.55	0.65
1:A:82:PHE:CE1	4:A:344:HOH:O[2_665]	1.55	0.65
1:A:16:ILE:CG2	1:A:144:THR:N[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: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:73:ILE:N	1:A:1221:GLU:O[2_665]	1.55	0.65
1:A:60:LYS:O	1:A:96:SER:O[2_665]	1.55	0.65
1:A:40:HIS:C	1:A:215:TRP:C[2_665]	1.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:CG	1:A:215:TRP: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:17:VAL:CA	1:A:144:THR:CG2[2_665]	1.56	0.64
1:A:165:TYR:CB	4:A:455:HOH:O[3_556]	1.56	0.64
1:A:59:TYR:CE1	1:A:96:SER:CB[2_665]	1.56	0.64
1:A:16:ILE:C	1:A:144:THR:CG2[2_665]	1.57	0.63
1:A:141:TRP:CB	1:A:220:CYS:CA[2_665]	1.57	0.63
1:A:97:TYR:CZ	4:A:437:HOH:O[2_665]	1.57	0.63
1:A:40:HIS:O	1:A:215:TRP:O[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:213:VAL:CG2	4:A:460:HOH:O[2_665]	1.59	0.61
1:A:17:VAL:N	1:A:144:THR:CG2[2_665]	1.59	0.61
1:A:141:TRP:CD1	1:A:221:ALA:N[2_665]	1.59	0.61
1:A:16:ILE:N	1:A:143:ASN:C[2_665]	1.59	0.61
1:A:71:HIS:N	1:A:1221:GLU:OE1[2_665]	1.59	0.61
1:A:62:ARG:O	1:A:98:ASN:O[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:CB[2_665]	1.60	0.60
1:A:72:ASN:N	1:A:1221:GLU:OE1[2_665]	1.60	0.60
1:A:64:GLU:O	1:A:217:TYR:CE1[2_665]	1.60	0.60
1:A:182:CYS:SG	4:A:368:HOH:O[2_665]	1.60	0.60
1:A:37:SER:CB	1:A:215:TRP:NE1[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:59:TYR:CB	1:A:94:TYR:OH[2_665]	1.61	0.59
1:A:33:LEU:CB	4:A:384:HOH:O[2_665]	1.61	0.59
1:A:18:GLY:N	1:A:150:ALA:O[2_665]	1.62	0.58
4:A:364:HOH:O	4:A:364:HOH:O[2_665]	1.63	0.57
1:A:224:ASN:CG	4:A:330: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:82:PHE:CE2	4:A:344:HOH: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:39:TYR:O	1:A:227:VAL:CB[2_665]	1.64	0.56
1:A:75:VAL:CA	1:A:222:PRO:CB[2_665]	1.64	0.56
1:A:192:GLN:NE2	1:A:196:GLY:C[2_665]	1.64	0.56
1:A:192:GLN:CG	1:A:194:ASP:C[2_665]	1.64	0.56
1:A:145:MET:CB	1:A:156:GLN:CB[2_665]	1.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TYR:OH	4:A:388:HOH:O[1_554]	1.64	0.56
1:A:57:HIS:CD2	1:A:58:CYS:SG[2_665]	1.64	0.56
1:A:153:ASP:CA	1:A:221:ALA:CB[2_665]	1.65	0.55
1:A:145:MET:CG	1:A:156:GLN:C[2_665]	1.65	0.55
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: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:41:PHE:CG	1:A:215:TRP: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:64:GLU:CG	1:A:217:TYR:OH[2_665]	1.66	0.54
1:A:40:HIS:CA	1:A:215:TRP:O[2_665]	1.67	0.53
1:A:66:ARG:NE	1:A:172:TYR:CD1[2_665]	1.67	0.53
1:A:64:GLU:CD	1:A:175:MET:CE[2_665]	1.67	0.53
1:A:59:TYR:O	1:A:94:TYR:OH[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:62:ARG:C	1:A:98:ASN:CB[2_665]	1.68	0.52
1:A:145:MET:N	1:A:156:GLN: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:150:ALA:CA	4:A:452:HOH:O[2_665]	1.69	0.51
1:A:62:ARG:CA	1:A:98:ASN:CB[2_665]	1.69	0.51
1:A:60:LYS:CD	1:A:99:ILE:CB[2_665]	1.69	0.51
1:A:57:HIS:ND1	4:A:328:HOH:O[2_665]	1.69	0.51
1:A:39:TYR:CD1	1:A:227:VAL:CG1[2_665]	1.69	0.51
1:A:144:THR:OG1	4:A:392:HOH:O[2_665]	1.70	0.50
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: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: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:153:ASP:C	1:A:221:ALA:C[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:OD1	1:A:1188:LYS:O[2_665]	1.72	0.48
1:A:73:ILE:CD1	1:A:189:ASP:OD2[2_665]	1.72	0.48
1:A:19:GLY:O	1:A:147:SER:CA[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:144:THR:O	1:A:156:GLN:CD[2_665]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:CA	1:A:188:GLY:O[2_665]	1.72	0.48
1:A:57:HIS:CB	1:A:58:CYS:C[2_665]	1.72	0.48
1:A:192:GLN:CD	1:A:197:GLY:CA[2_665]	1.72	0.48
1:A:71:HIS:N	1:A:1221:GLU:CD[2_665]	1.73	0.47
1:A:61:SER:C	1:A:98:ASN:N[2_665]	1.73	0.47
1:A:80:GLU:OE2	4:A:351:HOH:O[2_665]	1.73	0.47
1:A:34:ASN:OD1	1:A:172:TYR:CG[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:34:ASN:ND2	1:A:172:TYR:CE1[2_665]	1.75	0.45
1:A:17:VAL:C	1:A:152:SER:N[2_665]	1.75	0.45
1:A:16:ILE:CA	1:A:143:ASN: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:30:GLN:NE2	4:A:431:HOH:O[2_665]	1.75	0.45
1:A:95:SER:N	4:A:398:HOH:O[2_665]	1.75	0.45
1:A:85:SER:OG	1:A:97:TYR:CD1[2_665]	1.75	0.45
1:A:150:ALA:CB	4:A:347:HOH:O[2_665]	1.76	0.44
1:A:102:ASP:CG	4:A:328:HOH:O[2_665]	1.76	0.44
1:A:60:LYS:CB	1:A:99:ILE:C[2_665]	1.76	0.44
1:A:151:ASP:CG	1:A:1188:LYS:N[2_665]	1.76	0.44
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:72:ASN:CB	1:A:222:PRO:CD[2_665]	1.76	0.44
1:A:39:TYR:CE1	1:A:227:VAL:CG1[2_665]	1.77	0.43
1:A:38:GLY:O	1:A:168:CYS:SG[2_665]	1.77	0.43
1:A:189:ASP:CA	4:A:458:HOH:O[2_665]	1.77	0.43
1:A:73:ILE:CA	1:A:1221:GLU:C[2_665]	1.77	0.43
1:A:173:PRO:N	4:A:363:HOH:O[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:153:ASP:C	1:A:221:ALA:O[2_665]	1.78	0.42
1:A:16:ILE:CB	1:A:143:ASN:CA[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:39:TYR:CB	1:A:226: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:153:ASP:OD1	4:A:311: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:97:TYR:CE2	4:A:437:HOH:O[2_665]	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:N	1:A:215:TRP:CZ3[2_665]	1.78	0.42
4:A:345:HOH:O	4:A:385:HOH:O[3_556]	1.78	0.42
1:A:17:VAL:CG2	4:A:325:HOH:O[2_665]	1.78	0.42
1:A:21:GLU:N	1:A:145:MET:O[2_665]	1.79	0.41
1:A:64:GLU:C	1:A:217:TYR:OH[2_665]	1.79	0.41
1:A:193:GLY:N	1:A:195:SER:N[2_665]	1.79	0.41
1:A:153:ASP:O	1:A:1221:GLU:N[2_665]	1.79	0.41
1:A:142:GLY:C	1:A:194:ASP:OD2[2_665]	1.79	0.41
1:A:73:ILE:O	1:A:224:ASN:CA[2_665]	1.79	0.41
1:A:155:LEU:CG	4:A:359:HOH: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:32:SER:N	4:A:340:HOH:O[2_665]	1.80	0.40
1:A:141:TRP:CH2	4:A:407: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:153:ASP:CA	1:A:221:ALA:CA[2_665]	1.80	0.40
1:A:17:VAL:O	1:A:152:SER:CA[2_665]	1.80	0.40
1:A:149:THR:CA	4:A:301:HOH:O[2_665]	1.80	0.40
1:A:192:GLN:N	1:A:194:ASP:N[2_665]	1.81	0.39
1:A:142:GLY:CA	1:A:191:CYS:CA[2_665]	1.81	0.39
1:A:30:GLN:CD	4:A:431:HOH:O[2_665]	1.82	0.38
1:A:141:TRP:CE3	1:A:219:GLY:CA[2_665]	1.82	0.38
1:A:59:TYR:CB	4:A:426:HOH:O[2_665]	1.82	0.38
1:A:39:TYR:CD2	1:A:227:VAL:O[2_665]	1.82	0.38
1:A:92:PRO:CA	1:A:148:SER:OG[2_664]	1.82	0.38
1:A:71:HIS:O	1:A:1221:GLU:OE1[2_665]	1.82	0.38
1:A:34:ASN:CA	1:A:215:TRP:CH2[2_665]	1.82	0.38
1:A:66:ARG:NE	1:A:172:TYR:CE1[2_665]	1.83	0.37
1:A:141:TRP:N	1:A:220:CYS:CB[2_665]	1.83	0.37
1:A:74:LYS:C	1:A:223:GLY:N[2_665]	1.83	0.37
1:A:41:PHE:O	1:A:214:SER:O[2_665]	1.83	0.37
1:A:60:LYS:CG	1:A:99:ILE: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: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:151:ASP:OD2	1:A:188:GLY:C[2_665]	1.84	0.36
1:A:73:ILE:CG1	4:A:305:HOH:O[2_665]	1.84	0.36
1:A:70:GLU:O	1:A:1221:GLU:OE2[2_665]	1.85	0.35
1:A:61:SER:C	1:A:97:TYR:CB[2_665]	1.85	0.35
1:A:73:ILE:CG1	4:A:302:HOH:O[2_665]	1.85	0.35
1:A:17:VAL:CG1	1:A:151:ASP:O[2_665]	1.85	0.35
1:A:144:THR:O	1:A:156:GLN:CG[2_665]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:C	1:A:215:TRP:CE2[2_665]	1.85	0.35
1:A:19:GLY:N	1:A:144:THR:OG1[2_665]	1.86	0.34
1:A:41:PHE:CG	1:A:214:SER:C[2_665]	1.86	0.34
1:A:39:TYR:CZ	1:A:228:TYR:N[2_665]	1.86	0.34
1:A:192:GLN:C	1:A:194:ASP:C[2_665]	1.86	0.34
1:A:75:VAL:O	1:A:222:PRO:CB[2_665]	1.87	0.33
1:A:57:HIS:O	1:A:57:HIS:CB[2_665]	1.87	0.33
1:A:40:HIS:O	4:A:341:HOH:O[2_665]	1.87	0.33
1:A:192:GLN:C	1:A:194:ASP:N[2_665]	1.87	0.33
1:A:190:SER:CB	4:A:416:HOH:O[2_665]	1.87	0.33
1:A:61:SER:OG	1:A:95:SER:CB[2_665]	1.87	0.33
1:A:41:PHE:CB	1:A:215:TRP:CA[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:19:GLY:O	1:A:147:SER:CB[2_665]	1.87	0.33
1:A:191:CYS:C	1:A:193:GLY:O[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:151:ASP:OD1	1:A:188:GLY:O[2_665]	1.88	0.32
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: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:42:CYS:SG	4:A:324:HOH:O[2_665]	1.89	0.31
1:A:20:TYR:C	1:A:145:MET:C[2_665]	1.89	0.31
1:A:19:GLY:C	1:A:147:SER:N[2_665]	1.89	0.31
1:A:192:GLN:CA	1:A:194:ASP:CB[2_665]	1.89	0.31
1:A:60:LYS:CD	1:A:99:ILE:CA[2_665]	1.89	0.31
1:A:144:THR:C	1:A:156:GLN: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:41:PHE:CE1	1:A:215:TRP:CB[2_665]	1.90	0.30
1:A:39:TYR:CG	1:A:227:VAL:CB[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:71:HIS:O	1:A:1221:GLU:CD[2_665]	1.90	0.30
1:A:16:ILE:CA	1:A:143:ASN:CA[2_665]	1.90	0.30
1:A:145:MET:CA	1:A:156:GLN:CB[2_665]	1.90	0.30
1:A:141:TRP:C	1:A:191:CYS:CB[2_665]	1.90	0.30
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:60:LYS:CG	1:A:99:ILE:CB[2_665]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:412:HOH:O	4:A:433:HOH:O[2_665]	1.91	0.29
1:A:139:SER:CB	4:A:459:HOH:O[2_665]	1.91	0.29
1:A:72:ASN:CA	1:A:1221:GLU:CA[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:65:VAL:N	1:A:217:TYR:OH[2_665]	1.91	0.29
1:A:95:SER:CB	4:A:398:HOH:O[2_665]	1.92	0.28
1:A:192:GLN:CB	1:A:194:ASP: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:114:LEU:CG	4:A:401:HOH:O[3_546]	1.92	0.28
1:A:41:PHE:CG	1:A:215:TRP:CA[2_665]	1.92	0.28
1:A:192:GLN:OE1	1:A:197:GLY:O[2_665]	1.93	0.27
1:A:151:ASP:C	1:A:188:GLY: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:59:TYR:CD1	1:A:96:SER:CA[2_665]	1.93	0.27
1:A:190:SER:N	4:A:458:HOH:O[2_665]	1.93	0.27
1:A:34:ASN:ND2	1:A:172:TYR:CD2[2_665]	1.93	0.27
1:A:85:SER:O	1:A:97:TYR:CZ[2_665]	1.93	0.27
1:A:66:ARG:CB	1:A:217:TYR:CB[2_665]	1.93	0.27
1:A:71:HIS:CA	1:A:1221:GLU:OE2[2_665]	1.94	0.26
1:A:60:LYS:CE	1:A:99:ILE:O[2_665]	1.95	0.25
1:A:39:TYR:C	1:A:227:VAL:CB[2_665]	1.95	0.25
1:A:192:GLN:OE1	1:A:197:GLY:N[2_665]	1.95	0.25
1:A:145:MET:CB	1:A:156:GLN:N[2_665]	1.95	0.25
1:A:92:PRO:CB	1:A:148:SER:CB[2_664]	1.96	0.24
1:A:32:SER:OG	1:A:216:GLY:O[2_665]	1.96	0.24
1:A:16:ILE:CA	1:A:142: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:19:GLY:O	1:A:148:SER:N[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:141:TRP:C	1:A:190:SER:C[2_665]	1.97	0.23
1:A:102:ASP:OD1	4:A:328:HOH:O[2_665]	1.97	0.23
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:40:HIS:N	1:A:227:VAL:N[2_665]	1.98	0.22
1:A:30:GLN:OE1	4:A:431:HOH:O[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:40:HIS:CA	1:A:216:GLY:CA[2_665]	1.98	0.22
1:A:41:PHE:CE1	1:A:215:TRP:CD1[2_665]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:N	1:A:215:TRP:CD2[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:192:GLN:CA	1:A:194:ASP: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:141:TRP:CE2	4:A:407:HOH:O[2_665]	2.00	0.20
1:A:75:VAL:O	1:A:222:PRO: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:113:THR:CG2	4:A:463:HOH:O[3_546]	2.00	0.20
1:A:153:ASP:O	1:A:221:ALA:CB[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: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:191:CYS:CB	1:A:194:ASP:OD1[2_665]	2.01	0.19
1:A:34:ASN:CG	1:A:172:TYR:CD1[2_665]	2.01	0.19
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:61:SER:N	1:A:95:SER:OG[2_665]	2.02	0.18
1:A:60:LYS:C	1:A:96:SER:C[2_665]	2.02	0.18
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:18:GLY:CA	1:A:151:ASP:CA[2_665]	2.03	0.17
1:A:34:ASN:OD1	1:A:172:TYR:CD2[2_665]	2.03	0.17
1:A:152:SER:CB	1:A:189:ASP:N[2_665]	2.03	0.17
1:A:37:SER:O	1:A:180:MET:SD[2_665]	2.03	0.17
1:A:34:ASN:CG	1:A:172:TYR:CE1[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:151:ASP:CB	1:A:188:GLY:C[2_665]	2.04	0.16
1:A:95:SER:CA	4:A:398:HOH:O[2_665]	2.04	0.16
1:A:64:GLU:OE2	1:A:175:MET:CE[2_665]	2.04	0.16
1:A:16:ILE:CD1	1:A:143:ASN:ND2[2_665]	2.04	0.16
1:A:66:ARG:CA	1:A:217:TYR:CD2[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:150:ALA:N	4:A:452:HOH:O[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:62:ARG:N	1:A:98:ASN:CB[2_665]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLY:O	1:A:147:SER:OG[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:39:TYR:CG	1:A:227:VAL:C[2_665]	2.05	0.15
1:A:32:SER:CA	1:A:219:GLY:N[2_665]	2.05	0.15
1:A:192:GLN:CD	1:A:194:ASP: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:41:PHE:O	1:A:214:SER:C[2_665]	2.06	0.14
1:A:34:ASN:C	1:A:215:TRP:CD2[2_665]	2.06	0.14
1:A:149:THR:OG1	4:A:369:HOH:O[2_666]	2.06	0.14
1:A:42:CYS:N	3:A:246:BEN:C4[2_665]	2.06	0.14
1:A:113:THR:OG1	1:A:164:SER:CB[3_546]	2.06	0.14
1:A:42:CYS:O	4:A:384:HOH:O[2_665]	2.06	0.14
1:A:60:LYS:CE	1:A:99:ILE:CG2[2_665]	2.07	0.13
1:A:41:PHE:N	1:A:215:TRP:N[2_665]	2.07	0.13
4:A:327:HOH:O	4:A:351:HOH:O[2_665]	2.07	0.13
1:A:191:CYS:O	1:A:193:GLY:O[2_665]	2.07	0.13
1:A:62:ARG:CB	1:A:98:ASN: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:73:ILE:N	1:A:1221:GLU:CB[2_665]	2.07	0.13
1:A:40:HIS:ND1	3:A:246:BEN:C2[2_665]	2.07	0.13
1:A:75:VAL:N	1:A:185:LEU:O[2_665]	2.08	0.12
1:A:32:SER:OG	1:A:217:TYR:C[2_665]	2.08	0.12
1:A:37:SER:CB	1:A:215:TRP:CE2[2_665]	2.08	0.12
1:A:114:LEU:CD1	4:A:401:HOH:O[3_546]	2.08	0.12
1:A:75:VAL:O	1:A:222:PRO:C[2_665]	2.08	0.12
1:A:224:ASN:ND2	4:A:330:HOH:O[2_665]	2.08	0.12
1:A:72:ASN:O	1:A:1221:GLU:CA[2_665]	2.08	0.12
1:A:60:LYS:N	1:A:96:SER: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:42:CYS:SG	1:A:57:HIS:CE1[2_665]	2.08	0.12
1:A:34:ASN:ND2	1:A:172:TYR:OH[2_665]	2.08	0.12
1:A:151:ASP:O	1:A:188:GLY:O[2_665]	2.08	0.12
1:A:42:CYS:CA	3:A:246:BEN:C3[2_665]	2.09	0.11
1:A:74:LYS:NZ	1:A:225:PRO:CG[2_665]	2.09	0.11
1:A:66:ARG:NH2	1:A:171:SER:C[2_665]	2.09	0.11
1:A:40:HIS:ND1	3:A:246:BEN:N2[2_665]	2.09	0.11
1:A:113:THR:CG2	1:A:164:SER:CB[3_546]	2.09	0.11
1:A:245:TYR:CZ	4:A:388:HOH:O[1_554]	2.09	0.11
1:A:141:TRP:CE2	1:A:220:CYS:O[2_665]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:CG2	1:A:97:TYR:CA[2_665]	2.09	0.11
1:A:149:THR:CG2	4:A:369:HOH:O[2_666]	2.09	0.11
1:A:41:PHE:C	1:A:214:SER:C[2_665]	2.09	0.11
1:A:17:VAL:CB	1:A:152:SER:CA[2_665]	2.09	0.11
1:A:39:TYR:C	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:39:TYR:CD2	1:A:227:VAL:N[2_665]	2.10	0.10
1:A:141:TRP:C	1:A:191:CYS:CA[2_665]	2.10	0.10
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: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:32:SER:CA	1:A:217:TYR:CA[2_665]	2.11	0.09
1:A:59:TYR:CE1	1:A:96:SER:CA[2_665]	2.12	0.08
1:A:155:LEU:CD1	4:A:359:HOH:O[2_665]	2.12	0.08
1:A:40:HIS:CD2	3:A:246:BEN:C2[2_665]	2.12	0.08
1:A:39:TYR:CE2	1:A:228:TYR:CA[2_665]	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
1:A:165:TYR:CD2	4:A:374:HOH:O[3_556]	2.12	0.08
4:A:342:HOH:O	4:A:365:HOH:O[2_665]	2.12	0.08
1:A:18:GLY:O	1:A:150:ALA:O[2_665]	2.12	0.08
1:A:73:ILE:C	1:A:224:ASN:N[2_665]	2.12	0.08
1:A:156:GLN:OE1	4:A:347:HOH:O[2_665]	2.13	0.07
1:A:20:TYR:N	1:A:147:SER:O[2_665]	2.13	0.07
1:A:40:HIS:NE2	3:A:246:BEN:N2[2_665]	2.13	0.07
1:A:17:VAL:O	1:A:151:ASP:C[2_665]	2.13	0.07
1:A:60:LYS:CA	1:A:99:ILE:CA[2_665]	2.13	0.07
1:A:141:TRP:CA	1:A:220:CYS:SG[2_665]	2.13	0.07
1:A:41:PHE:CE1	1:A:99:ILE:CD1[2_665]	2.13	0.07
1:A:113:THR:OG1	4:A:349:HOH:O[3_546]	2.13	0.07
1:A:34:ASN:CG	1:A:172:TYR:CZ[2_665]	2.13	0.07
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:141:TRP:N	1:A:191:CYS:CB[2_665]	2.14	0.06
1:A:92:PRO:C	1:A:148:SER:CB[2_664]	2.14	0.06
1:A:41:PHE:CG	1:A:215:TRP:CG[2_665]	2.14	0.06
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:74:LYS:C	1:A:185:LEU:C[2_665]	2.14	0.06
1:A:70:GLU:C	1:A:1221:GLU:OE2[2_665]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:C	1:A:98:ASN:N[2_665]	2.14	0.06
1:A:144:THR:C	4:A:392:HOH: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: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: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:155:LEU:C	4:A:359:HOH:O[2_665]	2.15	0.05
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:187:GLY:CA	4:A:375:HOH:O[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:192:GLN:CA	1:A:195: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:245:TYR:CE2	4:A:388:HOH:O[1_554]	2.16	0.04
1:A:41:PHE:CZ	1:A:99:ILE:CG2[2_665]	2.16	0.04
1:A:20:TYR:CA	1:A:147:SER:C[2_665]	2.16	0.04
1:A:144:THR:O	4:A:392:HOH:O[2_665]	2.16	0.04
1:A:142:GLY:N	1:A:190:SER:C[2_665]	2.16	0.04
1:A:61:SER:CB	1:A:95:SER:CB[2_665]	2.16	0.04
1:A:70:GLU:C	1:A:1221:GLU:CD[2_665]	2.16	0.04
1:A:62:ARG:N	1:A:97:TYR:C[2_665]	2.16	0.04
1:A:141:TRP:CZ3	1:A:219:GLY:N[2_665]	2.16	0.04
1:A:72:ASN:C	1:A:1221:GLU:CB[2_665]	2.16	0.04
1:A:20:TYR:CB	1:A:148:SER:N[2_665]	2.16	0.04
1:A:60:LYS:CB	1:A:100:ASP:N[2_665]	2.17	0.03
1:A:73:ILE:O	1:A:223:GLY:C[2_665]	2.17	0.03
1:A:41:PHE:CE2	1:A:99:ILE:CG2[2_665]	2.17	0.03
1:A:61:SER:C	1:A:97:TYR:CA[2_665]	2.17	0.03
1:A:40:HIS:CG	3:A:246:BEN:C1[2_665]	2.17	0.03
1:A:59:TYR:CE1	1:A:96:SER:N[2_665]	2.17	0.03
1:A:72:ASN:O	1:A:222:PRO:CA[2_665]	2.17	0.03
1:A:195:SER:OG	4:A:415:HOH:O[2_665]	2.17	0.03
1:A:59:TYR:CG	1:A:96:SER: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:57:HIS:CB	1:A:59:TYR:N[2_665]	2.17	0.03
1:A:17:VAL:O	1:A:152:SER:CB[2_665]	2.17	0.03
1:A:153:ASP:CB	1:A:188:GLY:N[2_665]	2.18	0.02
1:A:73:ILE:CA	1:A:1221:GLU:CA[2_665]	2.18	0.02
1:A:182:CYS:CA	4:A:368:HOH:O[2_665]	2.18	0.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:CA	1:A:185:LEU:O[2_665]	2.18	0.02
1:A:144:THR:O	1:A:156:GLN:CB[2_665]	2.18	0.02
1:A:33:LEU:O	1:A:215:TRP:CE3[2_665]	2.18	0.02
1:A:32:SER:CB	1:A:217:TYR:O[2_665]	2.18	0.02
1:A:73:ILE:CG2	1:A:217:TYR: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:18:GLY:N	1:A:151:ASP:N[2_665]	2.18	0.02
1:A:41:PHE:CA	1:A:215:TRP:O[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:39:TYR:CB	1:A:226:GLY:C[2_665]	2.18	0.02
1:A:16:ILE:C	1:A:144:THR:CB[2_665]	2.18	0.02
1:A:37:SER:OG	1:A:215:TRP:CE2[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
1:A:20:TYR:CA	1:A:147:SER:N[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

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

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/185 (100%)	177 (96%)	8 (4%)	35 17

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
1	A	169	ASN
1	A	210	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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	3.07	4 (44%)	9,11,11	4.77	8 (88%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	BEN	C1-C	-7.71	1.34	1.47
3	A	246	BEN	C-N1	2.04	1.35	1.28
3	A	246	BEN	C5-C4	2.08	1.43	1.38
3	A	246	BEN	C4-C3	2.59	1.44	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	BEN	C5-C4-C3	-7.90	106.06	119.93
3	A	246	BEN	C6-C1-C	-4.39	115.11	120.67
3	A	246	BEN	C3-C2-C1	-3.83	115.52	120.33
3	A	246	BEN	C5-C6-C1	-2.93	116.65	120.33
3	A	246	BEN	C6-C1-C2	3.11	123.22	118.60
3	A	246	BEN	C1-C-N2	3.73	124.07	118.11
3	A	246	BEN	C4-C5-C6	6.10	129.11	120.19
3	A	246	BEN	C4-C3-C2	6.23	129.30	120.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	246	BEN	0	11

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/222 (99%)	4.97	208 (94%) 0 0	6, 15, 27, 46	9 (4%)

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	13.6
1	A	240	SER	11.6
1	A	191	CYS	10.1
1	A	134	THR	9.7
1	A	25	TYR	9.6
1	A	94	TYR	9.3
1	A	168	CYS	9.1
1	A	56	ALA	9.0
1	A	117	TYR	8.6
1	A	234	PHE	8.3
1	A	65	VAL	8.3
1	A	107	LYS	8.3
1	A	203	GLY	8.3
1	A	105	LEU	8.2
1	A	121	VAL	8.1
1	A	17	VAL	7.9
1	A	89	ILE	7.9
1	A	225	PRO	7.9
1	A	241	THR	7.9
1	A	111	PRO	7.8
1	A	149	THR	7.7
1	A	97	TYR	7.7
1	A	96	SER	7.7
1	A	82	PHE	7.6
1	A	52	VAL	7.6
1	A	213	VAL	7.5
1	A	141	TRP	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	83	ILE	7.5
1	A	233	ILE	7.2
1	A	160	ILE	7.2
1	A	237	TRP	7.2
1	A	49	GLU	7.2
1	A	157	CYS	7.2
1	A	71	HIS	7.2
1	A	204	GLU	7.2
1	A	44	GLY	7.2
1	A	75	VAL	7.1
1	A	1184	TYR	7.1
1	A	125	THR	7.1
1	A	20	TYR	7.0
1	A	142	GLY	6.8
1	A	92	PRO	6.8
1	A	193	GLY	6.7
1	A	176	ILE	6.7
1	A	39	TYR	6.7
1	A	114	LEU	6.7
1	A	88	VAL	6.6
1	A	202	ASN	6.6
1	A	115	ASN	6.6
1	A	63	VAL	6.5
1	A	169	ASN	6.5
1	A	162	ILE	6.5
1	A	59	TYR	6.4
1	A	127	SER	6.4
1	A	18	GLY	6.4
1	A	128	CYS	6.3
1	A	33	LEU	6.3
1	A	42	CYS	6.2
1	A	209	LEU	6.2
1	A	101	ASN	6.2
1	A	163	LEU	6.2
1	A	72	ASN	6.2
1	A	178	ASN	6.2
1	A	150	ALA	6.1
1	A	50	ASN	5.9
1	A	93	ASN	5.9
1	A	103	ILE	5.9
1	A	138	VAL	5.8
1	A	229	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	5.8
1	A	47	VAL	5.7
1	A	133	GLY	5.7
1	A	243	ALA	5.6
1	A	148	SER	5.6
1	A	116	THR	5.6
1	A	46	LEU	5.5
1	A	26	SER	5.5
1	A	223	GLY	5.5
1	A	119	GLN	5.5
1	A	170	ASP	5.5
1	A	181	PHE	5.5
1	A	129	ALA	5.5
1	A	183	ALA	5.4
1	A	236	ASP	5.4
1	A	90	ARG	5.4
1	A	98	ASN	5.4
1	A	118	VAL	5.3
1	A	239	THR	5.3
1	A	165	TYR	5.2
1	A	175	MET	5.2
1	A	24	ALA	5.2
1	A	232	CYS	5.2
1	A	22	CYS	5.2
1	A	152	SER	5.1
1	A	242	MET	5.1
1	A	155	LEU	5.1
1	A	217	TYR	5.1
1	A	214	SER	5.1
1	A	198	PRO	5.0
1	A	84	SER	5.0
1	A	67	LEU	5.0
1	A	231	VAL	5.0
1	A	108	LEU	5.0
1	A	158	LEU	5.0
1	A	174	GLY	4.9
1	A	113	THR	4.9
1	A	1188	LYS	4.9
1	A	212	VAL	4.9
1	A	135	MET	4.8
1	A	69	GLY	4.8
1	A	215	TRP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	37	SER	4.7
1	A	200	VAL	4.7
1	A	87	ARG	4.7
1	A	100	ASP	4.7
1	A	85	SER	4.7
1	A	190	SER	4.7
1	A	110	LYS	4.7
1	A	99	ILE	4.6
1	A	76	THR	4.6
1	A	228	TYR	4.6
1	A	61	SER	4.6
1	A	124	PRO	4.6
1	A	102	ASP	4.5
1	A	106	ILE	4.5
1	A	41	PHE	4.5
1	A	187	GLY	4.4
1	A	136	CYS	4.4
1	A	120	PRO	4.3
1	A	186	GLU	4.3
1	A	224	ASN	4.3
1	A	45	SER	4.3
1	A	144	THR	4.2
1	A	147	SER	4.2
1	A	28	ALA	4.2
1	A	53	VAL	4.1
1	A	23	LYS	4.1
1	A	185	LEU	4.1
1	A	171	SER	4.1
1	A	109	SER	4.1
1	A	38	GLY	4.0
1	A	137	THR	4.0
1	A	132	ALA	4.0
1	A	195	SER	3.9
1	A	91	HIS	3.9
1	A	48	ASN	3.9
1	A	95	SER	3.9
1	A	1221	GLU	3.8
1	A	54	SER	3.8
1	A	27	GLN	3.7
1	A	220	CYS	3.7
1	A	81	GLN	3.7
1	A	73	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	159	ASN	3.7
1	A	104	MET	3.7
1	A	55	ALA	3.7
1	A	196	GLY	3.7
1	A	122	ALA	3.7
1	A	197	GLY	3.6
1	A	216	GLY	3.6
1	A	210	GLN	3.6
1	A	51	TRP	3.6
1	A	58	CYS	3.5
1	A	43	GLY	3.5
1	A	172	TYR	3.5
1	A	31	VAL	3.5
1	A	143	ASN	3.5
1	A	199	VAL	3.4
1	A	21	GLU	3.4
1	A	235	SER	3.4
1	A	151	ASP	3.3
1	A	222	PRO	3.3
1	A	66	ARG	3.3
1	A	86	SER	3.2
1	A	139	SER	3.2
1	A	145	MET	3.2
1	A	16	ILE	3.2
1	A	57	HIS	3.1
1	A	182	CYS	3.1
1	A	154	LYS	3.1
1	A	179	ALA	3.0
1	A	29	HIS	3.0
1	A	177	THR	3.0
1	A	184	GLY	2.9
1	A	166	SER	2.9
1	A	32	SER	2.9
1	A	70	GLU	2.9
1	A	19	GLY	2.9
1	A	40	HIS	2.8
1	A	130	PRO	2.8
1	A	112	ALA	2.8
1	A	78	GLY	2.8
1	A	161	PRO	2.8
1	A	189	ASP	2.7
1	A	180	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	167	ASP	2.7
1	A	211	GLY	2.7
1	A	201	CYS	2.6
1	A	226	GLY	2.6
1	A	79	SER	2.4
1	A	64	GLU	2.3
1	A	34	ASN	2.3
1	A	230	LYS	2.3
1	A	173	PRO	2.2
1	A	164	SER	2.2
1	A	153	ASP	2.1
1	A	227	VAL	2.1
1	A	221	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BEN	A	246	9/9	0.60	0.38	0.77	8,19,22,25	0
2	CA	A	247	1/1	0.87	0.35	-0.08	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.