



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:08 PM GMT

PDB ID : 1BIM  
Title : CRYSTALLOGRAPHIC STUDIES ON THE BINDING MODES OF P2-P3  
BUTANEDIAMIDE RENIN INHIBITORS  
Authors : Tong, L.  
Deposited on : 1995-09-27  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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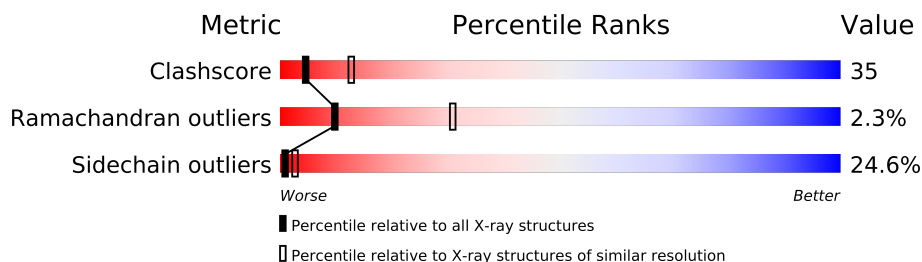
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.80 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	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	

## 2 Entry composition i

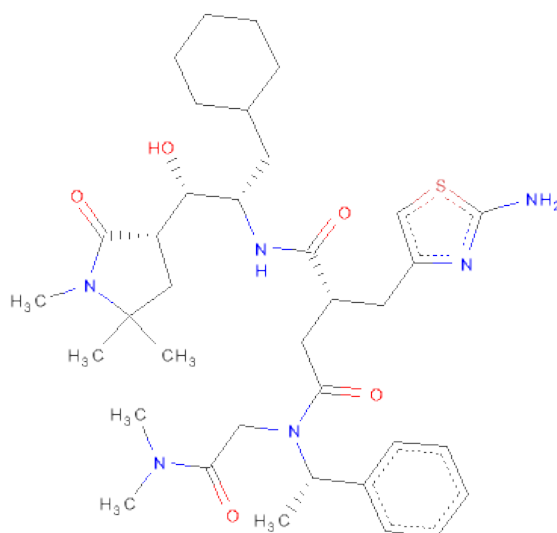
There are 2 unique types of molecules in this entry. The entry contains 5221 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2575	1644	416	501	14			
1	B	333	Total	C	N	O	S	0	0	0
			2550	1630	408	498	14			

- Molecule 2 is (2S)-2-[(2-AMINO-1,3-THIAZOL-4-YL)METHYL]-N 1 -{(1S,2S)-1-(CYCLOHEXYLMETHYL)-2-HYDROXY-2-[(3R)-1,5,5-TRIMETHYL-2-OXOPYRROLIDIN-3-YL]ETHYL}-N 4 -[2-(DIMETHYLAMINO)-2-OXOETHYL]-N 4 -[(1S)-1-PHENYLETHYL]BUTANEDIAMIDE (three-letter code: 0QB) (formula: C<sub>36</sub>H<sub>54</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			48	36	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			48	36	6	5	1		

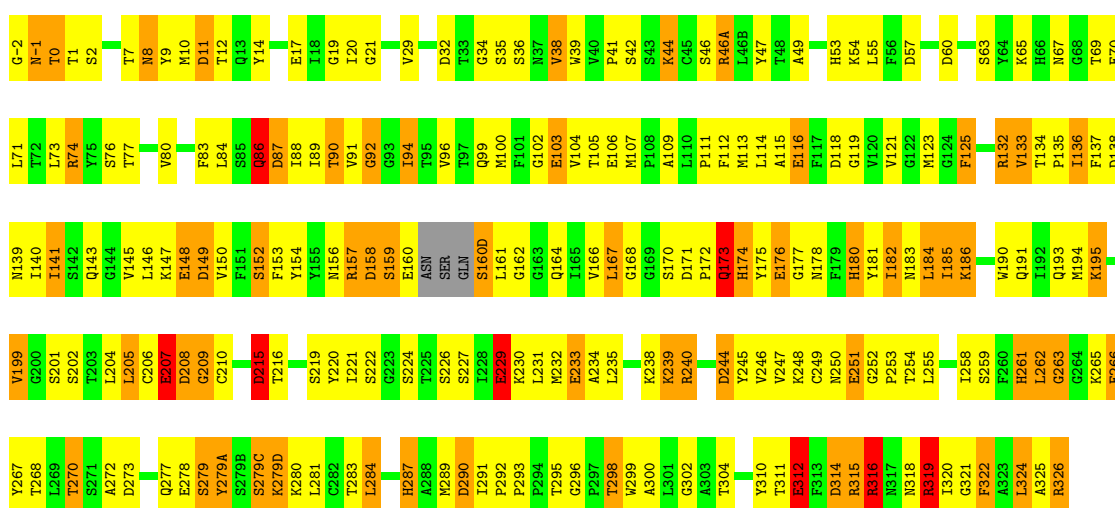
### 3 Residue-property plots

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.

Note EDS was not executed.

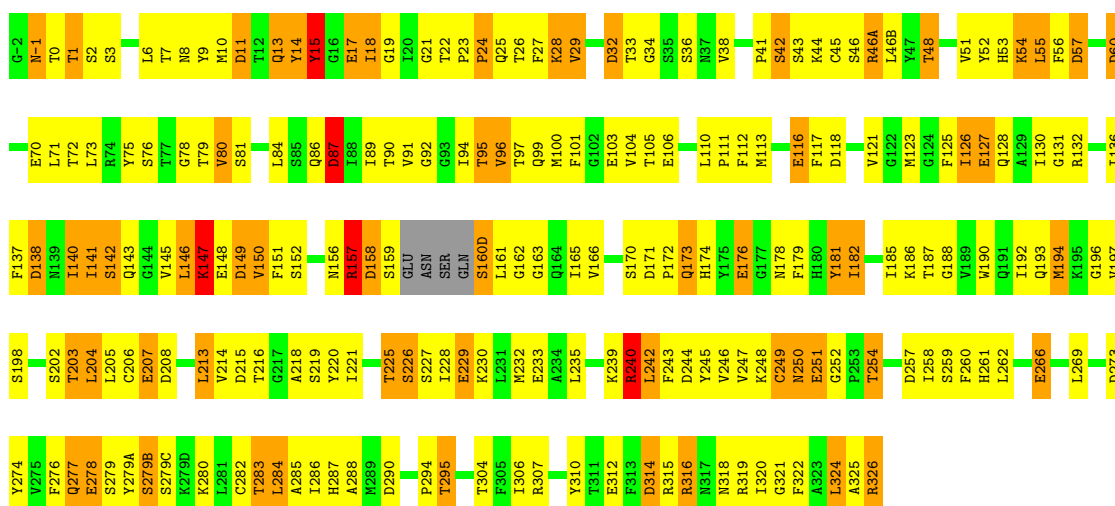
#### • Molecule 1: Renin

Chain A:



#### • Molecule 1: Renin

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.90Å 142.90Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0QB

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	1.12	15/2634 (0.6%)	1.59	42/3570 (1.2%)
1	B	1.12	14/2609 (0.5%)	1.56	39/3540 (1.1%)
All	All	1.12	29/5243 (0.6%)	1.57	81/7110 (1.1%)

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	1	0
1	B	1	0
All	All	2	0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	GLU	CD-OE1	10.04	1.36	1.25
1	B	229	GLU	CD-OE1	9.12	1.35	1.25
1	A	148	GLU	CD-OE2	9.06	1.35	1.25
1	B	278	GLU	CD-OE2	9.00	1.35	1.25
1	A	251	GLU	CD-OE2	8.86	1.35	1.25
1	B	70	GLU	CD-OE2	8.66	1.35	1.25
1	A	207	GLU	CD-OE1	8.46	1.34	1.25
1	B	233	GLU	CD-OE1	8.39	1.34	1.25
1	A	160	GLU	CD-OE1	8.35	1.34	1.25
1	B	207	GLU	CD-OE2	8.25	1.34	1.25
1	A	17	GLU	CD-OE1	8.07	1.34	1.25
1	B	17	GLU	CD-OE2	8.02	1.34	1.25
1	B	127	GLU	CD-OE1	7.71	1.34	1.25
1	A	229	GLU	CD-OE1	7.65	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	GLU	CD-OE2	7.60	1.34	1.25
1	B	176	GLU	CD-OE1	7.45	1.33	1.25
1	B	106	GLU	CD-OE1	7.23	1.33	1.25
1	B	251	GLU	CD-OE1	7.15	1.33	1.25
1	B	103	GLU	CD-OE1	6.96	1.33	1.25
1	B	266	GLU	CD-OE2	6.81	1.33	1.25
1	A	278	GLU	CD-OE1	6.76	1.33	1.25
1	A	116	GLU	CD-OE2	6.60	1.32	1.25
1	A	266	GLU	CD-OE2	6.35	1.32	1.25
1	A	106	GLU	CD-OE2	6.26	1.32	1.25
1	A	233	GLU	CD-OE2	6.12	1.32	1.25
1	A	312	GLU	CD-OE1	5.94	1.32	1.25
1	A	103	GLU	CD-OE1	5.47	1.31	1.25
1	B	312	GLU	CD-OE1	5.34	1.31	1.25
1	A	176	GLU	CD-OE1	5.12	1.31	1.25

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASP	CB-CG-OD2	-11.55	107.90	118.30
1	A	314	ASP	CB-CG-OD1	11.41	128.57	118.30
1	A	60	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	B	149	ASP	CB-CG-OD1	-9.60	109.66	118.30
1	A	132	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	149	ASP	CB-CG-OD2	9.14	126.53	118.30
1	B	60	ASP	CB-CG-OD2	-8.93	110.27	118.30
1	A	273	ASP	CB-CG-OD1	-8.90	110.29	118.30
1	A	319	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	171	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	B	208	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	A	149	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	A	60	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	138	ASP	CB-CG-OD2	8.26	125.73	118.30
1	B	326	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	307	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	87	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	132	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	149	ASP	CB-CG-OD1	7.71	125.24	118.30
1	B	32	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	74	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	138	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	158	ASP	CB-CG-OD2	-7.14	111.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	THR	N-CA-CB	7.11	123.81	110.30
1	B	290	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	171	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	B	57	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	174	HIS	CA-CB-CG	-6.77	102.09	113.60
1	B	273	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	74	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	208	ASP	CB-CG-OD2	6.65	124.28	118.30
1	B	87	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	32	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	208	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	240	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	11	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	319	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	57	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	15	TYR	CB-CG-CD1	6.26	124.76	121.00
1	B	273	ASP	CB-CG-OD1	6.22	123.89	118.30
1	B	157	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	215	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	B	249	CYS	N-CA-CB	6.17	121.70	110.60
1	B	314	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	86	GLN	N-CA-CB	6.06	121.51	110.60
1	B	240	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	290	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	273	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	14	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	240	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	32	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	87	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	B	171	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	181	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	B	290	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	A	290	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	118	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	199	VAL	N-CA-C	-5.80	95.33	111.00
1	B	138	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	279(B)	SER	N-CA-CB	5.66	118.98	110.50
1	A	46(A)	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	257	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	180	HIS	CA-CB-CG	-5.55	104.16	113.60
1	B	316	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	11	ASP	CB-CG-OD1	5.44	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	VAL	CA-CB-CG1	-5.38	102.84	110.90
1	B	11	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	213	LEU	CB-CA-C	-5.37	100.00	110.20
1	B	274	TYR	N-CA-CB	5.34	120.21	110.60
1	B	257	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	B	181	TYR	CB-CG-CD2	5.29	124.17	121.00
1	A	295	THR	N-CA-CB	5.27	120.32	110.30
1	A	244	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	B	14	TYR	CB-CG-CD1	5.21	124.13	121.00
1	A	240	ARG	N-CA-CB	5.18	119.93	110.60
1	A	208	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	259	SER	N-CA-C	5.12	124.82	111.00
1	A	173	GLN	N-CA-CB	5.06	119.71	110.60
1	A	261	HIS	N-CA-CB	5.06	119.71	110.60
1	A	138	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	87	ASP	CB-CG-OD1	5.01	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	215	ASP	CA
1	B	112	PHE	CA

There are no planarity outliers.

## 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	2575	0	2507	174	0
1	B	2550	0	2468	168	0
2	A	48	0	54	18	0
2	B	48	0	54	17	0
All	All	5221	0	5083	363	0

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 35.

All (363) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:391:0QB:HD21	2:A:391:0QB:CD21	0.97	1.09
1:A:195:LYS:HB2	1:A:261:HIS:HD2	1.11	1.06
2:B:391:0QB:CD21	2:B:391:0QB:HD21	0.97	1.05
2:B:391:0QB:SE2	2:B:391:0QB:CG1	2.55	1.04
2:B:391:0QB:CD21	2:B:391:0QB:SE2	1.78	1.03
2:A:391:0QB:SE2	2:A:391:0QB:CG1	2.58	1.02
2:B:391:0QB:SE2	2:B:391:0QB:CE11	1.74	1.01
1:A:41:PRO:HB2	1:A:55:LEU:HD23	1.41	1.00
2:A:391:0QB:SE2	2:A:391:0QB:CD21	1.80	0.99
2:A:391:0QB:CE11	2:A:391:0QB:SE2	1.76	0.98
1:A:77:THR:HG22	1:A:111:PRO:HG3	1.46	0.97
1:B:48:THR:HG22	1:B:52:TYR:CE2	2.03	0.94
1:A:195:LYS:HB2	1:A:261:HIS:CD2	2.03	0.94
1:B:46(A):ARG:HA	1:B:46(A):ARG:HH11	1.34	0.92
1:A:8:ASN:ND2	1:A:11:ASP:H	1.68	0.91
2:B:391:0QB:SE2	2:B:391:0QB:ND1	2.55	0.90
1:B:41:PRO:HB2	1:B:55:LEU:HD23	1.54	0.90
1:B:25:GLN:HE21	1:B:54:LYS:HZ2	0.92	0.89
1:A:8:ASN:HD21	1:A:11:ASP:H	0.89	0.88
1:A:8:ASN:HD21	1:A:11:ASP:N	1.70	0.87
2:A:391:0QB:SE2	2:A:391:0QB:ND1	2.58	0.87
2:B:391:0QB:HD21	2:B:391:0QB:CG1	2.02	0.87
1:B:205:LEU:HD13	1:B:227:SER:HB2	1.58	0.86
1:B:213:LEU:HD11	2:B:391:0QB:HM21	1.58	0.86
1:B:25:GLN:NE2	1:B:54:LYS:HZ2	1.74	0.85
1:B:204:LEU:HD13	1:B:205:LEU:HG	1.59	0.85
2:A:391:0QB:HD21	2:A:391:0QB:CG1	2.05	0.85
1:B:110:LEU:HD12	1:B:111:PRO:HA	1.61	0.82
1:B:48:THR:HG22	1:B:52:TYR:HE2	1.42	0.82
1:B:-1:ASN:ND2	1:B:147:LYS:HG3	1.96	0.79
2:B:391:0QB:NZ	2:B:391:0QB:SE2	2.66	0.79
2:A:391:0QB:SE2	2:A:391:0QB:NZ	2.65	0.79
1:B:204:LEU:CD1	1:B:205:LEU:HG	2.14	0.78
1:A:195:LYS:HE2	1:A:261:HIS:CD2	2.18	0.78
1:A:-2:GLY:O	1:A:147:LYS:HA	1.84	0.77
1:B:185:ILE:HD11	1:B:193:GLN:HB3	1.65	0.77
2:B:391:0QB:NZ	2:B:391:0QB:ND1	2.26	0.77
1:B:2:SER:OG	1:B:92:GLY:HA3	1.85	0.76
2:A:391:0QB:ND1	2:A:391:0QB:NZ	2.30	0.76
1:A:252:GLY:HA3	1:A:277:GLN:OE1	1.86	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:32:ASP:OD2	2:B:391:0QB:H32	1.85	0.76
1:B:7:THR:O	1:B:14:TYR:HA	1.87	0.76
1:A:156:ASN:ND2	1:A:157:ARG:H	1.84	0.75
1:A:204:LEU:O	1:A:205:LEU:HG	1.87	0.75
1:B:150:VAL:HG22	1:B:314:ASP:HA	1.67	0.74
1:B:18:ILE:HG22	1:B:90:THR:O	1.87	0.74
1:B:46(A):ARG:CA	1:B:46(A):ARG:HH11	1.99	0.74
1:B:21:GLY:HA2	1:B:87:ASP:OD1	1.86	0.74
1:A:109:ALA:O	1:A:113:MET:HB2	1.86	0.74
1:B:170:SER:O	1:B:172:PRO:HD3	1.87	0.74
1:B:204:LEU:HD12	1:B:205:LEU:H	1.54	0.73
1:A:89:ILE:CD1	1:A:99:GLN:HB3	2.20	0.72
1:B:41:PRO:HG2	1:B:54:LYS:O	1.89	0.72
1:B:181:TYR:O	1:B:182:ILE:HG13	1.89	0.72
1:B:73:LEU:HD22	1:B:130:ILE:HD13	1.73	0.71
1:B:25:GLN:HE21	1:B:54:LYS:NZ	1.80	0.71
1:A:232:MET:HG3	1:A:245:TYR:CE2	2.26	0.71
1:B:125:PHE:HB2	1:B:188:GLY:O	1.91	0.70
1:A:181:TYR:CD1	1:A:319:ARG:HD3	2.27	0.70
1:B:196:GLY:HA2	1:B:206:CYS:HB3	1.71	0.70
1:A:199:VAL:O	1:A:204:LEU:HD12	1.92	0.69
1:A:65:LYS:HG3	1:A:86:GLN:HE21	1.57	0.69
1:B:240:ARG:O	1:B:243:PHE:N	2.24	0.69
1:B:226:SER:O	1:B:230:LYS:HD2	1.92	0.69
1:B:225:THR:O	1:B:229:GLU:HG3	1.93	0.69
1:B:279(B):SER:OG	1:B:280:LYS:HB2	1.92	0.69
1:B:252:GLY:HA3	1:B:277:GLN:HE22	1.57	0.68
1:A:39:TRP:CE3	1:A:104:VAL:HG21	2.29	0.68
1:A:42:SER:HB2	1:A:103:GLU:HB3	1.76	0.68
1:A:239:LYS:HB2	1:A:245:TYR:CZ	2.28	0.68
1:B:276:PHE:CZ	1:B:285:ALA:HB2	2.29	0.67
1:B:19:GLY:HA2	1:B:25:GLN:O	1.94	0.67
1:B:218:ALA:HA	2:B:391:0QB:HA	1.77	0.67
1:B:3:SER:HA	1:B:165:ILE:O	1.94	0.67
1:B:197:VAL:HB	1:B:205:LEU:HB2	1.77	0.66
1:A:38:VAL:HG13	1:A:121:VAL:HG22	1.78	0.66
1:B:0:THR:OG1	1:B:145:VAL:HG22	1.96	0.66
2:B:391:0QB:SE2	2:B:391:0QB:HD21	2.46	0.66
1:A:195:LYS:NZ	1:A:263:GLY:N	2.44	0.66
1:A:220:TYR:CE2	2:A:391:0QB:H23	2.30	0.65
1:A:195:LYS:HZ1	1:A:263:GLY:N	1.93	0.65
1:A:204:LEU:C	1:A:205:LEU:HG	2.16	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:291:ILE:O	1:A:296:GLY:HA3	1.96	0.65
1:A:173:GLN:HE22	1:A:326:ARG:HD3	1.62	0.64
1:B:111:PRO:O	1:B:113:MET:N	2.30	0.64
1:A:246:VAL:HG21	1:A:281:LEU:HD13	1.79	0.64
1:B:94:ILE:HG21	1:B:140:ILE:CD1	2.27	0.64
1:B:18:ILE:HG22	1:B:91:VAL:HG22	1.80	0.64
1:A:46:SER:HB2	1:A:47:TYR:CD2	2.33	0.64
1:A:77:THR:HG21	2:A:391:0QB:HB	1.79	0.64
1:A:46(A):ARG:HH11	1:A:46(A):ARG:HG2	1.62	0.63
1:A:153:PHE:CD2	1:A:216:THR:HG21	2.33	0.63
1:A:177:GLY:O	1:A:178:ASN:ND2	2.29	0.63
1:A:176:GLU:HG3	1:A:326:ARG:NE	2.14	0.63
1:A:94:ILE:HD13	1:A:94:ILE:N	2.13	0.63
2:A:391:0QB:SE2	2:A:391:0QB:HD21	2.48	0.63
1:B:176:GLU:HB3	1:B:324:LEU:HB3	1.80	0.63
1:A:156:ASN:OD1	1:A:160(D):SER:HB2	1.97	0.63
1:B:18:ILE:CG2	1:B:91:VAL:HG22	2.29	0.63
1:B:261:HIS:ND1	1:B:266:GLU:OE1	2.33	0.62
1:A:134:THR:HG22	1:A:139:ASN:OD1	1.99	0.62
1:B:277:GLN:HA	1:B:282:CYS:SG	2.38	0.62
1:B:127:GLU:HB2	1:B:188:GLY:HA2	1.80	0.62
1:A:221:ILE:HG13	1:A:304:THR:HB	1.79	0.62
1:B:213:LEU:CD1	2:B:391:0QB:HM21	2.29	0.62
1:A:148:GLU:HB3	1:A:168:GLY:O	2.00	0.62
1:A:311:THR:HG1	1:A:322:PHE:HD1	1.48	0.61
1:A:190:TRP:HH2	1:A:315:ARG:HG3	1.65	0.61
1:B:149:ASP:OD1	1:B:316:ARG:HB2	2.00	0.61
1:B:32:ASP:OD1	1:B:34:GLY:N	2.34	0.61
1:A:8:ASN:HD22	1:A:9:TYR:N	1.98	0.60
1:B:28:LYS:O	1:B:117:PHE:HB2	2.01	0.60
1:A:159:SER:HG	1:A:160(D):SER:N	1.98	0.60
1:A:262:LEU:HB2	1:A:267:TYR:HD2	1.66	0.60
1:B:239:LYS:HG2	1:B:245:TYR:CE2	2.36	0.60
1:B:140:ILE:O	1:B:143:GLN:HB2	2.02	0.60
1:B:204:LEU:HD12	1:B:205:LEU:N	2.15	0.59
1:A:-1:ASN:HD21	1:A:147:LYS:HZ3	1.48	0.59
1:B:216:THR:HG22	1:B:306:ILE:CD1	2.31	0.59
1:B:239:LYS:HG2	1:B:245:TYR:CZ	2.37	0.59
1:A:-1:ASN:HD21	1:A:147:LYS:NZ	2.00	0.59
1:A:283:THR:HG22	1:A:284:LEU:O	2.02	0.59
1:A:195:LYS:NZ	1:A:263:GLY:H	2.00	0.58
1:B:232:MET:HE2	1:B:245:TYR:HB2	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:HIS:HB2	1:A:266:GLU:OE2	2.03	0.58
1:A:298:THR:HG22	1:A:299:TRP:O	2.02	0.58
1:A:156:ASN:HB3	1:A:162:GLY:O	2.03	0.58
1:A:199:VAL:HG22	1:A:258:ILE:HG12	1.86	0.58
1:A:67:ASN:HB3	1:A:84:LEU:O	2.04	0.58
1:B:94:ILE:HD11	1:B:146:LEU:HD23	1.85	0.58
1:A:280:LYS:HG3	1:A:281:LEU:O	2.03	0.57
1:B:192:ILE:HD11	1:B:262:LEU:HD22	1.85	0.57
1:A:89:ILE:HG13	1:A:99:GLN:HB3	1.85	0.57
1:A:262:LEU:HB2	1:A:267:TYR:CD2	2.40	0.57
1:A:174:HIS:HD2	1:A:326:ARG:OXT	1.88	0.57
1:B:220:TYR:HH	1:B:276:PHE:HE2	1.53	0.57
1:B:190:TRP:HE3	1:B:320:ILE:HD11	1.69	0.57
1:B:27:PHE:CD1	1:B:54:LYS:HB3	2.39	0.57
1:B:284:LEU:N	1:B:284:LEU:HD23	2.19	0.57
1:B:56:PHE:CE2	1:B:101:PHE:HZ	2.23	0.56
1:A:34:GLY:O	2:A:391:OQB:HM22	2.05	0.56
1:A:222:SER:OG	1:A:300:ALA:HB3	2.06	0.56
1:B:156:ASN:ND2	1:B:161:LEU:O	2.39	0.56
1:B:116:GLU:HA	1:B:116:GLU:OE1	2.06	0.56
1:A:239:LYS:HG3	1:A:239:LYS:O	2.06	0.56
1:B:204:LEU:HD13	1:B:205:LEU:CG	2.33	0.55
1:A:41:PRO:CB	1:A:55:LEU:HD23	2.26	0.55
1:A:180:HIS:O	1:A:321:GLY:HA2	2.05	0.55
1:B:194:MET:SD	1:B:260:PHE:HD2	2.29	0.55
1:A:222:SER:HA	1:A:287:HIS:O	2.07	0.55
1:A:42:SER:OG	1:A:44:LYS:HG2	2.06	0.55
1:A:252:GLY:HA2	1:A:255:LEU:HD13	1.88	0.55
1:A:150:VAL:HB	1:A:312:GLU:OE1	2.07	0.55
1:B:246:VAL:HG12	1:B:283:THR:HA	1.88	0.55
1:A:184:LEU:HB3	1:A:191:GLN:O	2.06	0.55
1:B:196:GLY:O	1:B:261:HIS:ND1	2.39	0.55
1:A:77:THR:CG2	1:A:111:PRO:HG3	2.30	0.54
1:A:29:VAL:HG21	1:A:121:VAL:HG23	1.89	0.54
1:A:224:SER:OG	1:A:227:SER:HB2	2.07	0.54
1:A:230:LYS:O	1:A:233:GLU:HG2	2.07	0.54
1:B:26:THR:O	1:B:54:LYS:HE3	2.07	0.54
1:A:19:GLY:O	1:A:89:ILE:HA	2.08	0.54
1:A:21:GLY:HA2	1:A:87:ASP:OD1	2.08	0.54
1:B:192:ILE:CD1	1:B:262:LEU:HD22	2.38	0.54
1:B:198:SER:OG	1:B:261:HIS:HE1	1.90	0.53
1:A:248:LYS:O	1:A:251:GLU:HB3	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:126:ILE:HG23	1:B:127:GLU:N	2.23	0.53
1:B:151:PHE:HA	1:B:166:VAL:O	2.08	0.53
1:B:9:TYR:CE1	1:B:10:MET:HG3	2.44	0.53
1:B:34:GLY:HA3	1:B:215:ASP:OD1	2.09	0.53
1:B:-1:ASN:HD22	1:B:147:LYS:HG3	1.69	0.53
1:A:215:ASP:O	1:A:302:GLY:HA2	2.09	0.53
1:B:38:VAL:HG13	1:B:121:VAL:HG22	1.92	0.52
1:A:77:THR:HG21	2:A:391:0QB:CB	2.39	0.52
1:B:249:CYS:O	1:B:251:GLU:N	2.42	0.52
1:A:259:SER:HB3	1:A:266:GLU:HG3	1.92	0.52
1:A:67:ASN:CB	1:A:100:MET:HE1	2.40	0.52
1:B:251:GLU:O	1:B:254:THR:HG22	2.09	0.52
1:A:220:TYR:CZ	2:A:391:0QB:H23	2.45	0.51
1:A:112:PHE:O	1:A:115:ALA:HB3	2.10	0.51
1:B:279(B):SER:OG	1:B:280:LYS:HD3	2.10	0.51
1:A:69:THR:O	1:A:83:PHE:HA	2.11	0.51
1:B:73:LEU:CD2	1:B:130:ILE:HD13	2.39	0.51
1:B:46(A):ARG:NH1	1:B:46(A):ARG:HA	2.14	0.51
1:B:141:ILE:HG22	1:B:142:SER:N	2.24	0.51
1:A:222:SER:HG	2:A:391:0QB:SE2	2.43	0.51
1:A:89:ILE:CG1	1:A:99:GLN:HB3	2.41	0.51
1:A:270:THR:HG22	1:A:272:ALA:H	1.76	0.51
1:A:91:VAL:O	1:A:92:GLY:C	2.48	0.51
1:A:156:ASN:ND2	1:A:157:ARG:N	2.57	0.50
1:A:183:ASN:HB3	1:A:319:ARG:HB3	1.93	0.50
1:B:152:SER:HB3	1:B:310:TYR:CE1	2.46	0.50
1:B:244:ASP:HB3	1:B:287:HIS:NE2	2.25	0.50
1:A:181:TYR:C	1:A:182:ILE:HG13	2.31	0.50
1:B:94:ILE:HG21	1:B:140:ILE:HD13	1.92	0.50
1:B:99:GLN:NE2	1:B:136:ILE:HA	2.27	0.50
1:B:276:PHE:O	1:B:278:GLU:N	2.44	0.50
1:B:235:LEU:HD11	1:B:258:ILE:HD11	1.93	0.50
1:A:103:GLU:O	1:A:105:THR:HG23	2.12	0.50
1:A:248:LYS:HB2	1:A:251:GLU:HB2	1.93	0.50
1:A:175:TYR:HA	1:A:325:ALA:HA	1.94	0.50
1:B:203:THR:CG2	1:B:207:GLU:HG2	2.41	0.50
1:A:53:HIS:HB3	1:A:118:ASP:OD1	2.11	0.50
1:A:39:TRP:CD1	1:A:73:LEU:HD13	2.47	0.49
1:A:238:LYS:HE2	1:A:281:LEU:HD21	1.94	0.49
1:B:173:GLN:OE1	1:B:173:GLN:HA	2.09	0.49
1:B:136:ILE:HG23	1:B:137:PHE:N	2.27	0.49
1:A:233:GLU:HG2	1:A:234:ALA:N	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:ASP:OD1	1:A:149:ASP:O	2.30	0.49
1:B:174:HIS:O	1:B:325:ALA:HA	2.12	0.49
1:B:286:ILE:O	1:B:287:HIS:HD2	1.95	0.49
1:A:195:LYS:HE2	1:A:261:HIS:HD2	1.76	0.49
1:A:152:SER:HB3	1:A:312:GLU:HA	1.93	0.49
1:B:27:PHE:CE1	1:B:54:LYS:HD2	2.48	0.49
1:A:159:SER:HB3	1:A:160(D):SER:N	2.28	0.49
1:B:248:LYS:O	1:B:249:CYS:C	2.51	0.49
1:B:27:PHE:CE1	1:B:54:LYS:HB3	2.48	0.48
1:B:42:SER:O	1:B:55:LEU:HD22	2.13	0.48
1:A:141:ILE:HA	1:A:141:ILE:HD13	1.67	0.48
1:A:244:ASP:N	1:A:244:ASP:OD1	2.46	0.48
1:A:99:GLN:NE2	1:A:136:ILE:HA	2.28	0.48
2:B:391:0QB:H5'2	2:B:391:0QB:CD1	2.43	0.48
1:A:10:MET:O	1:A:11:ASP:HB2	2.13	0.48
1:A:262:LEU:O	1:A:265:LYS:N	2.45	0.48
1:A:133:VAL:O	1:A:135:PRO:HD3	2.14	0.48
1:B:75:TYR:N	1:B:78:GLY:O	2.42	0.48
1:B:11:ASP:OD1	1:B:158:ASP:N	2.43	0.48
1:A:8:ASN:C	1:A:8:ASN:HD22	2.16	0.48
1:B:240:ARG:C	1:B:243:PHE:H	2.13	0.48
1:B:96:VAL:HG11	1:B:140:ILE:HG13	1.96	0.48
1:A:233:GLU:CG	1:A:234:ALA:N	2.77	0.48
1:B:225:THR:HA	1:B:288:ALA:HB1	1.96	0.47
1:A:186:LYS:HA	1:A:186:LYS:HD2	1.68	0.47
1:A:159:SER:HB3	1:A:160(D):SER:OG	2.14	0.47
1:B:232:MET:HG3	1:B:245:TYR:CG	2.50	0.47
1:A:77:THR:HG21	2:A:391:0QB:CG2	2.45	0.47
1:B:110:LEU:HA	1:B:111:PRO:HA	1.63	0.47
1:A:185:ILE:HD11	1:A:193:GLN:HG2	1.97	0.47
1:B:204:LEU:CD1	1:B:205:LEU:N	2.78	0.47
1:A:157:ARG:HG3	1:B:160(D):SER:O	2.15	0.47
1:A:77:THR:HG21	2:A:391:0QB:HG21	1.97	0.47
1:A:89:ILE:HG13	1:A:99:GLN:CB	2.44	0.47
1:A:316:ARG:C	1:A:316:ARG:HD2	2.36	0.47
1:A:67:ASN:HB2	1:A:100:MET:HE1	1.96	0.47
1:B:294:PRO:HD2	1:B:295:THR:H	1.80	0.47
1:A:277:GLN:NE2	1:A:279:SER:O	2.48	0.46
1:B:248:LYS:HE3	1:B:279(C):SER:O	2.14	0.46
1:B:225:THR:HG22	1:B:226:SER:N	2.31	0.46
1:A:154:TYR:HB2	1:A:310:TYR:CE1	2.51	0.46
1:B:41:PRO:CB	1:B:55:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:PRO:HA	1:A:293:PRO:HD2	1.66	0.46
2:B:391:0QB:HN3	2:B:391:0QB:HB	1.67	0.46
1:B:18:ILE:HD13	1:B:29:VAL:HG21	1.98	0.46
1:A:194:MET:O	1:A:209:GLY:HA2	2.16	0.46
1:B:315:ARG:HA	1:B:315:ARG:HD2	1.56	0.46
1:B:53:HIS:O	1:B:55:LEU:HG	2.16	0.46
1:B:7:THR:HG22	1:B:15:TYR:CE1	2.51	0.46
1:A:181:TYR:CD1	1:A:319:ARG:CD	2.98	0.46
1:B:42:SER:HB2	1:B:104:VAL:O	2.16	0.46
1:B:150:VAL:CG2	1:B:314:ASP:HA	2.43	0.46
1:A:2:SER:O	1:A:166:VAL:HA	2.16	0.46
1:B:89:ILE:O	1:B:95:THR:HA	2.16	0.46
2:A:391:0QB:HN3	2:A:391:0QB:HB	1.62	0.45
1:B:239:LYS:HD2	1:B:243:PHE:O	2.16	0.45
1:A:125:PHE:HD1	1:A:125:PHE:H	1.64	0.45
1:A:279(D):LYS:HD2	1:A:279(D):LYS:N	2.31	0.45
1:A:232:MET:HG3	1:A:245:TYR:CZ	2.52	0.45
1:A:280:LYS:HG3	1:A:281:LEU:N	2.30	0.45
2:B:391:0QB:HG22	2:B:391:0QB:HD2	1.76	0.45
1:B:244:ASP:CB	1:B:287:HIS:NE2	2.80	0.45
1:A:235:LEU:HD21	1:A:255:LEU:HD23	1.99	0.45
1:B:43:SER:OG	1:B:57:ASP:HA	2.16	0.45
1:A:235:LEU:HD23	1:A:284:LEU:HD21	1.99	0.45
1:A:39:TRP:HA	1:A:102:GLY:O	2.17	0.45
1:A:10:MET:C	1:A:12:THR:H	2.19	0.45
1:B:-1:ASN:ND2	1:B:147:LYS:CG	2.75	0.45
1:B:248:LYS:HB3	1:B:250:ASN:OD1	2.17	0.45
1:A:7:THR:O	1:A:14:TYR:HA	2.17	0.45
1:B:232:MET:CE	1:B:245:TYR:HB2	2.46	0.44
1:A:104:VAL:HG12	1:A:104:VAL:O	2.16	0.44
1:A:46(A):ARG:HG2	1:A:46(A):ARG:NH1	2.30	0.44
1:B:235:LEU:CD1	1:B:235:LEU:N	2.78	0.44
1:B:156:ASN:HB3	1:B:162:GLY:HA2	1.99	0.44
1:B:221:ILE:HG13	1:B:304:THR:HB	1.99	0.44
1:A:249:CYS:HB3	1:A:279:SER:O	2.17	0.44
1:B:21:GLY:O	1:B:24:PRO:HA	2.17	0.44
1:B:126:ILE:CG2	1:B:127:GLU:N	2.80	0.44
1:B:15:TYR:CD1	1:B:15:TYR:N	2.85	0.44
1:B:94:ILE:HG21	1:B:140:ILE:HD11	1.97	0.44
1:A:190:TRP:CH2	1:A:315:ARG:HG3	2.49	0.44
1:A:150:VAL:HG12	1:A:314:ASP:HA	1.99	0.44
1:A:229:GLU:O	1:A:233:GLU:HB3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:179:PHE:HA	1:B:322:PHE:O	2.17	0.44
1:A:96:VAL:HG21	1:A:136:ILE:HG13	1.99	0.44
1:B:73:LEU:O	1:B:79:THR:HG23	2.17	0.44
1:A:29:VAL:HA	1:A:119:GLY:O	2.18	0.44
1:B:0:THR:HG1	1:B:145:VAL:HG22	1.81	0.44
1:A:279(D):LYS:HD2	1:A:279(D):LYS:H	1.82	0.43
1:B:204:LEU:HD13	1:B:205:LEU:CD2	2.48	0.43
1:B:13:GLN:HB3	1:B:13:GLN:HE21	1.64	0.43
1:A:41:PRO:HG3	1:A:107:MET:SD	2.58	0.43
1:B:232:MET:HG3	1:B:245:TYR:CD2	2.54	0.43
1:A:238:LYS:HB2	1:A:246:VAL:HG23	2.00	0.43
1:A:250:ASN:OD1	1:A:250:ASN:N	2.50	0.43
1:A:233:GLU:HG2	1:A:234:ALA:H	1.84	0.43
1:B:18:ILE:CD1	1:B:29:VAL:HG21	2.48	0.43
2:B:391:0QB:HD1	2:B:391:0QB:H5'2	1.99	0.42
1:A:49:ALA:CB	1:A:107:MET:HG2	2.49	0.42
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.88	0.42
1:A:250:ASN:OD1	1:A:279(C):SER:HA	2.19	0.42
1:B:157:ARG:HG2	1:B:157:ARG:H	1.59	0.42
1:A:279(A):TYR:N	1:A:279(A):TYR:CD1	2.87	0.42
1:B:48:THR:O	1:B:51:VAL:HB	2.18	0.42
1:A:12:THR:O	1:A:219:SER:OG	2.31	0.42
1:A:191:GLN:OE1	1:A:298:THR:HG23	2.19	0.42
1:A:206:CYS:O	1:A:206:CYS:SG	2.77	0.42
1:B:131:GLY:O	1:B:132:ARG:C	2.57	0.42
1:B:6:LEU:HB2	1:B:163:GLY:C	2.39	0.42
1:B:22:THR:HA	1:B:23:PRO:HA	1.92	0.42
1:A:176:GLU:CG	1:A:326:ARG:NE	2.82	0.42
1:B:45:CYS:O	1:B:46(A):ARG:NH1	2.49	0.42
1:A:315:ARG:O	1:A:316:ARG:O	2.38	0.42
1:B:248:LYS:HE2	1:B:250:ASN:OD1	2.20	0.42
1:A:0:THR:OG1	1:A:145:VAL:HB	2.19	0.42
1:A:20:ILE:HA	1:A:88:ILE:O	2.20	0.42
1:B:147:LYS:HB2	1:B:147:LYS:HE2	1.60	0.42
1:B:149:ASP:O	1:B:149:ASP:OD1	2.37	0.42
1:A:326:ARG:HH12	1:B:1:THR:HG22	1.85	0.42
1:A:84:LEU:HB3	1:A:100:MET:HE3	2.02	0.42
1:A:207:GLU:O	1:A:208:ASP:HB2	2.20	0.42
1:B:181:TYR:HA	1:B:321:GLY:HA2	2.02	0.41
1:A:2:SER:HB3	1:A:92:GLY:O	2.19	0.41
1:B:203:THR:HG22	1:B:207:GLU:HG2	2.02	0.41
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:PHE:CE2	1:A:216:THR:HG21	2.56	0.41
1:B:8:ASN:ND2	1:B:156:ASN:O	2.54	0.41
1:B:220:TYR:OH	1:B:276:PHE:HE2	2.04	0.41
1:A:94:ILE:HG13	1:A:140:ILE:HD13	2.01	0.41
1:B:-1:ASN:CG	1:B:147:LYS:HD3	2.40	0.41
1:A:182:ILE:HD13	1:A:322:PHE:CE2	2.55	0.41
1:A:137:PHE:HE1	1:A:167:LEU:HB3	1.86	0.41
1:A:8:ASN:ND2	1:A:8:ASN:C	2.74	0.41
1:A:232:MET:CG	1:A:245:TYR:CE2	2.99	0.41
1:A:153:PHE:CD2	1:A:216:THR:CG2	3.03	0.41
1:A:46:SER:HB2	1:A:47:TYR:CE2	2.55	0.41
1:B:33:THR:HG22	1:B:123:MET:HB2	2.03	0.41
1:B:215:ASP:OD2	1:B:218:ALA:HB2	2.21	0.41
1:B:7:THR:CG2	1:B:8:ASN:N	2.83	0.41
1:A:89:ILE:HD11	1:A:99:GLN:HB3	2.02	0.41
1:B:242:LEU:HB3	1:B:243:PHE:CE2	2.56	0.41
1:A:42:SER:HB3	1:A:105:THR:HG22	2.02	0.41
1:B:33:THR:HG23	1:B:216:THR:OG1	2.21	0.41
1:B:80:VAL:O	1:B:81:SER:HB3	2.20	0.41
1:B:1:THR:O	1:B:1:THR:HG22	2.20	0.41
1:B:8:ASN:HA	1:B:13:GLN:O	2.21	0.40
1:A:148:GLU:O	1:A:168:GLY:HA2	2.21	0.40
1:A:141:ILE:C	1:A:143:GLN:H	2.25	0.40
1:B:-1:ASN:ND2	1:B:147:LYS:HD3	2.35	0.40
1:B:73:LEU:HA	1:B:73:LEU:HD23	1.65	0.40
1:A:194:MET:HB3	1:A:210:CYS:SG	2.60	0.40
1:B:279:SER:O	1:B:279(A):TYR:HD1	2.04	0.40
1:B:190:TRP:CE3	1:B:320:ILE:HD11	2.54	0.40
1:A:174:HIS:O	1:A:325:ALA:HB1	2.21	0.40

There are no symmetry-related clashes.

## 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	330/337 (98%)	288 (87%)	33 (10%)	9 (3%)	8	25
1	B	329/337 (98%)	284 (86%)	39 (12%)	6 (2%)	13	39
All	All	659/674 (98%)	572 (87%)	72 (11%)	15 (2%)	10	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	316	ARG
1	B	112	PHE
1	B	242	LEU
1	A	92	GLY
1	B	250	ASN
1	B	277	GLN
1	A	209	GLY
1	A	279	SER
1	A	253	PRO
1	B	147	LYS
1	B	182	ILE
1	A	263	GLY
1	A	172	PRO
1	A	136	ILE

### 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	284/287 (99%)	213 (75%)	71 (25%)	1	2
1	B	280/287 (98%)	212 (76%)	68 (24%)	1	3
All	All	564/574 (98%)	425 (75%)	139 (25%)	1	3

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	0	THR

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Mol	Chain	Res	Type
1	A	1	THR
1	A	8	ASN
1	A	35	SER
1	A	36	SER
1	A	38	VAL
1	A	44	LYS
1	A	54	LYS
1	A	63	SER
1	A	71	LEU
1	A	74	ARG
1	A	76	SER
1	A	80	VAL
1	A	86	GLN
1	A	90	THR
1	A	94	ILE
1	A	114	LEU
1	A	116	GLU
1	A	123	MET
1	A	125	PHE
1	A	132	ARG
1	A	133	VAL
1	A	141	ILE
1	A	146	LEU
1	A	152	SER
1	A	157	ARG
1	A	158	ASP
1	A	159	SER
1	A	160(D)	SER
1	A	161	LEU
1	A	164	GLN
1	A	167	LEU
1	A	170	SER
1	A	173	GLN
1	A	182	ILE
1	A	184	LEU
1	A	186	LYS
1	A	195	LYS
1	A	201	SER
1	A	202	SER
1	A	205	LEU
1	A	207	GLU
1	A	215	ASP

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Mol	Chain	Res	Type
1	A	226	SER
1	A	229	GLU
1	A	231	LEU
1	A	239	LYS
1	A	240	ARG
1	A	247	VAL
1	A	254	THR
1	A	262	LEU
1	A	268	THR
1	A	270	THR
1	A	279(A)	TYR
1	A	279(C)	SER
1	A	279(D)	LYS
1	A	284	LEU
1	A	287	HIS
1	A	289	MET
1	A	290	ASP
1	A	298	THR
1	A	312	GLU
1	A	315	ARG
1	A	316	ARG
1	A	318	ASN
1	A	319	ARG
1	A	320	ILE
1	A	322	PHE
1	A	324	LEU
1	A	326	ARG
1	B	-1	ASN
1	B	1	THR
1	B	13	GLN
1	B	15	TYR
1	B	17	GLU
1	B	18	ILE
1	B	24	PRO
1	B	28	LYS
1	B	36	SER
1	B	42	SER
1	B	44	LYS
1	B	46	SER
1	B	46(A)	ARG
1	B	46(B)	LEU
1	B	48	THR

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Mol	Chain	Res	Type
1	B	54	LYS
1	B	55	LEU
1	B	60	ASP
1	B	71	LEU
1	B	72	THR
1	B	76	SER
1	B	80	VAL
1	B	84	LEU
1	B	86	GLN
1	B	87	ASP
1	B	95	THR
1	B	96	VAL
1	B	97	THR
1	B	100	MET
1	B	105	THR
1	B	116	GLU
1	B	126	ILE
1	B	128	GLN
1	B	138	ASP
1	B	140	ILE
1	B	141	ILE
1	B	142	SER
1	B	146	LEU
1	B	147	LYS
1	B	150	VAL
1	B	157	ARG
1	B	158	ASP
1	B	159	SER
1	B	160(D)	SER
1	B	173	GLN
1	B	178	ASN
1	B	186	LYS
1	B	187	THR
1	B	194	MET
1	B	202	SER
1	B	203	THR
1	B	204	LEU
1	B	214	VAL
1	B	219	SER
1	B	225	THR
1	B	226	SER
1	B	228	ILE

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Mol	Chain	Res	Type
1	B	240	ARG
1	B	247	VAL
1	B	254	THR
1	B	269	LEU
1	B	283	THR
1	B	284	LEU
1	B	295	THR
1	B	318	ASN
1	B	319	ARG
1	B	324	LEU
1	B	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	8	ASN
1	A	25	GLN
1	A	86	GLN
1	A	99	GLN
1	A	156	ASN
1	A	173	GLN
1	A	174	HIS
1	A	178	ASN
1	A	193	GLN
1	A	261	HIS
1	B	-1	ASN
1	B	25	GLN
1	B	128	GLN
1	B	139	ASN
1	B	143	GLN
1	B	261	HIS
1	B	277	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 ⓘ

2 ligands are modelled in this entry.

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	$\# Z  > 2$
2	0QB	A	391	-	51,51,51	1.95	11 (21%)	71,73,73	2.16	23 (32%)
2	0QB	B	391	-	51,51,51	1.82	11 (21%)	71,73,73	2.18	19 (26%)

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
2	0QB	A	391	-	-	0/47/75/75	0/4/4/4
2	0QB	B	391	-	-	0/47/75/75	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	391	0QB	CD21-SE2	5.74	1.80	1.70
2	A	391	0QB	C5-N11	-5.17	1.42	1.49
2	B	391	0QB	CE11-ND1	-5.13	1.26	1.34
2	B	391	0QB	CD21-SE2	4.60	1.78	1.70
2	B	391	0QB	O21-C22	4.01	1.29	1.22
2	A	391	0QB	CE11-ND1	-3.83	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391	0QB	C5-N11	-3.80	1.44	1.49
2	A	391	0QB	O21-C22	3.36	1.28	1.22
2	B	391	0QB	CD21-CG1	-3.20	1.31	1.37
2	A	391	0QB	CD2-CG	-2.75	1.34	1.39
2	A	391	0QB	CD1-CG	-2.72	1.34	1.39
2	B	391	0QB	CD1-CG	-2.59	1.34	1.39
2	A	391	0QB	C31-C21	2.51	1.57	1.53
2	B	391	0QB	CD2-CG	-2.50	1.34	1.39
2	A	391	0QB	C41-C32	2.41	1.58	1.54
2	A	391	0QB	CB-N1	-2.40	1.45	1.48
2	A	391	0QB	C32-C11	2.40	1.57	1.53
2	B	391	0QB	CE1-CD1	-2.39	1.33	1.39
2	B	391	0QB	C4-N2	2.39	1.39	1.34
2	A	391	0QB	O-C	-2.35	1.17	1.23
2	B	391	0QB	CE2-CD2	-2.33	1.33	1.39
2	B	391	0QB	C-N	2.32	1.37	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	0QB	CG2-CB-CG	-9.78	88.83	113.23
2	A	391	0QB	O2-C4-CA1	-6.30	115.28	121.89
2	A	391	0QB	CM2-C5-N11	-5.93	104.29	111.16
2	B	391	0QB	C32-C11-C21	-4.92	107.22	113.04
2	A	391	0QB	CB1-CG1-CD21	-4.78	121.50	130.18
2	A	391	0QB	C41-C5-N11	4.75	104.40	100.44
2	B	391	0QB	CB1-CG1-CD21	-4.53	121.95	130.18
2	B	391	0QB	O2-C4-CA1	-4.34	117.34	121.89
2	A	391	0QB	C32-C22-N11	4.33	112.64	107.97
2	A	391	0QB	CG2-CB-N1	-4.24	105.61	110.32
2	B	391	0QB	CN-CA1-C4	-4.22	103.54	110.06
2	A	391	0QB	CN-CA1-C4	-4.21	103.55	110.06
2	A	391	0QB	CA1-C4-N2	4.01	122.55	116.19
2	A	391	0QB	O21-C22-C32	-3.92	123.17	127.24
2	B	391	0QB	CA-N1-CB	3.73	125.16	118.14
2	A	391	0QB	C1'-C31-C21	-3.70	110.64	115.66
2	B	391	0QB	CG2-CB-N1	3.67	114.40	110.32
2	A	391	0QB	CA-C-N	3.39	122.25	116.76
2	B	391	0QB	CD21-SE2-CE11	-3.22	85.57	90.49
2	B	391	0QB	CM3-C5-N11	-3.15	107.50	111.16
2	B	391	0QB	C32-C22-N11	2.99	111.19	107.97
2	A	391	0QB	CA1-CN-C3	-2.88	109.28	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	0QB	C1'-C31-C21	-2.79	111.88	115.66
2	B	391	0QB	CB1-CA1-CN	-2.76	107.98	111.39
2	B	391	0QB	O21-C22-C32	-2.73	124.40	127.24
2	A	391	0QB	CD21-SE2-CE11	-2.72	86.34	90.49
2	B	391	0QB	C31-C1'-C6'	-2.66	105.86	111.58
2	A	391	0QB	SE2-CE11-NZ	-2.60	119.09	123.23
2	B	391	0QB	C31-C21-C11	-2.58	107.95	112.31
2	A	391	0QB	CB1-CA1-CN	-2.53	108.27	111.39
2	A	391	0QB	CM3-C5-N11	2.44	113.99	111.16
2	B	391	0QB	CM2-C5-N11	2.41	113.95	111.16
2	A	391	0QB	C31-C1'-C6'	-2.36	106.50	111.58
2	B	391	0QB	CB1-CA1-C4	-2.32	106.47	110.06
2	A	391	0QB	C-CA-N1	-2.19	108.80	112.08
2	A	391	0QB	NZ-CE11-ND1	2.18	126.00	122.98
2	A	391	0QB	CG-CB-N1	-2.17	107.52	110.35
2	A	391	0QB	C31-C21-C11	-2.17	108.64	112.31
2	B	391	0QB	C41-C5-N11	2.14	102.23	100.44
2	A	391	0QB	C32-C11-C21	-2.11	110.55	113.04
2	A	391	0QB	O-C-N	-2.10	117.84	121.67
2	B	391	0QB	CA-N1-C3	-2.01	115.69	121.12

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.