



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:48 AM GMT

PDB ID : 3Q2V  
Title : Crystal structure of mouse E-cadherin ectodomain  
Authors : Jin,X.; Harrison, O.J.; Shapiro, L.  
Deposited on : 2010-12-20  
Resolution : 3.40 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

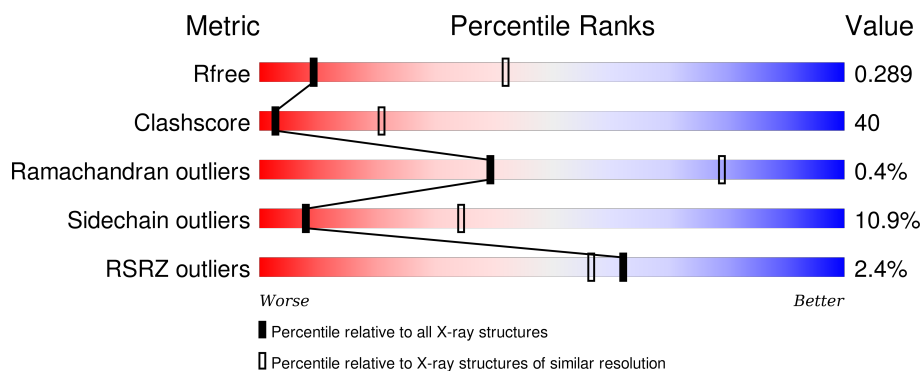
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	550	 2% 41% 48% 8% .
1	B	550	 2% 33% 41% 5% 20%

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
2	CA	A	601	-	-	-	X
2	CA	B	601	-	-	-	X
4	MAN	A	802	X	-	-	X
4	MAN	A	804	X	-	-	-
4	MAN	A	805	X	-	-	X
4	MAN	A	806	X	-	-	-
4	MAN	A	807	X	-	-	-
4	MAN	A	809	-	-	-	X
4	MAN	B	801	X	-	-	-
4	MAN	B	803	X	-	-	-
4	MAN	B	804	X	-	-	X
4	MAN	B	805	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7871 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 Cadherin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	1	0
			4113	2581	683	838	11			
1	B	440	Total	C	N	O	S	0	0	0
			3399	2138	553	701	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	HIS	-	EXPRESSION TAG	UNP P09803
A	546	HIS	-	EXPRESSION TAG	UNP P09803
A	547	HIS	-	EXPRESSION TAG	UNP P09803
A	548	HIS	-	EXPRESSION TAG	UNP P09803
A	549	HIS	-	EXPRESSION TAG	UNP P09803
A	550	HIS	-	EXPRESSION TAG	UNP P09803
B	545	HIS	-	EXPRESSION TAG	UNP P09803
B	546	HIS	-	EXPRESSION TAG	UNP P09803
B	547	HIS	-	EXPRESSION TAG	UNP P09803
B	548	HIS	-	EXPRESSION TAG	UNP P09803
B	549	HIS	-	EXPRESSION TAG	UNP P09803
B	550	HIS	-	EXPRESSION TAG	UNP P09803

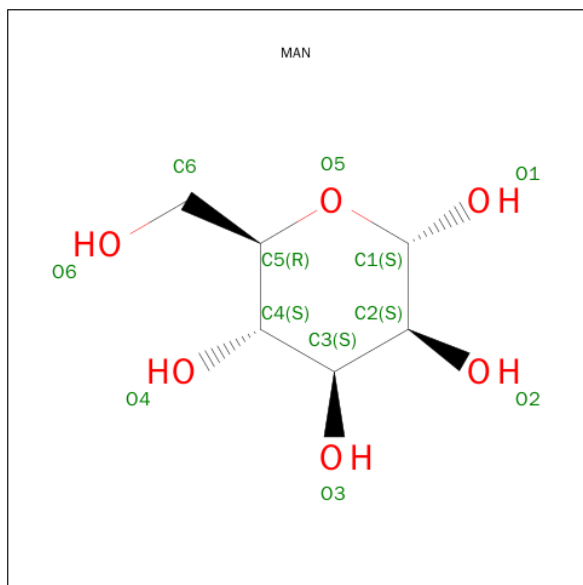
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	12	Total	Ca	0	0
			12	12		
2	A	12	Total	Ca	0	0
			12	12		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

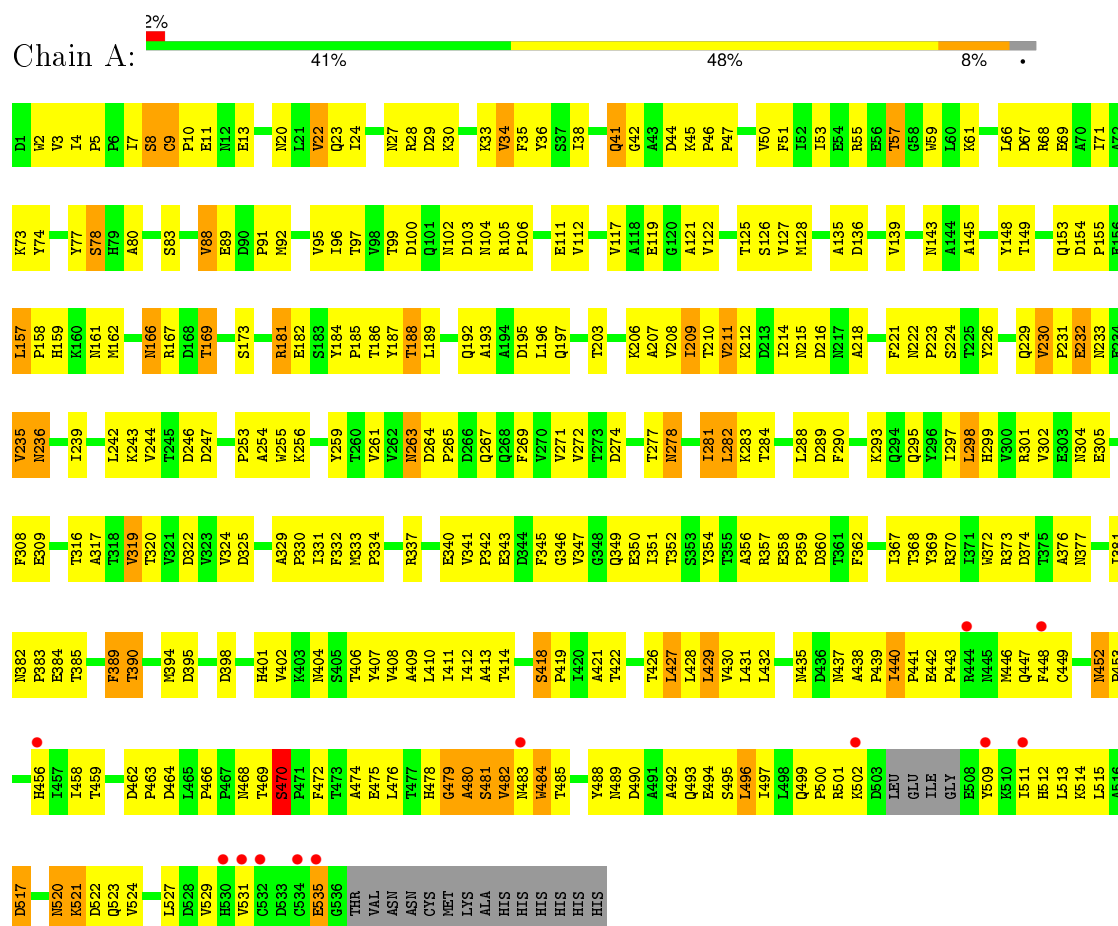
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	B	80	Total	O	0	0
			80	80		

### 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: Cadherin-1



LEU	PRO	E380	V313	R238	V171
LYS	GLN	I381	P314	I239	
LEU	PRO	N382	S315	A240	L175
ALA	HIS	F383	T316	T241	T176
ASP	ILE	E384	A317	L242	S177
ASN	ILE	T385		K243	
THR	THR	G386	T320	V244	D180
ASN	ILE	A387	V321	T245	A181
LEU	LEU	I388	D322	D246	E182
D462	D462	F389	V323	D247	S183
P463	P463	T390	V324	D248	V184
D464	D464	R391	D325	A249	P185
I465	I465	A392	V326	P250	T186
P466	P466	E393	N327	N251	Y187
P467	P467	R394	E328	T252	T188
LEU	ASN	D395	A329	P253	L189
ASP	ASP	R396	P330	A254	V190
VAL	THR	E397	I331	W255	V191
HIS	SER	D398	F332	K256	Q192
VAL	PRO				A193
CYS	PHE	T406	R337	T260	A194
ASP	THR		R338	V261	D195
CYS	ALA	L410	V339	V262	L196
GLU	GLU	I411	E340	N263	Q197
GLY	LEU	I412	V341		G198
THR	THR	I413	P342	V271	E199
VAL	HIS	T414	E343		G200
ASN	GLY	D415	D344	D274	L201
ASN	ALA	D416	F345		S202
CYS	SER	D417	G346	T277	T203
MET	VAL	S418	V347	N278	
LYS	ASN	P419	Q348	D279	K206
ALA	TRP	I420	E349	G280	A207
HIS	THR	A421	E350	I281	V208
HIS	ILE	T422	I351	L282	I209
HIS	GLU		T352		T210
HIS	TYR		T353	G287	V211
HIS	ASN	I429	S353	L288	K212
HIS	ASP	V430	V354	D289	D213
	ALA	I431	T355	F290	I214
	ALA	L432	A356		N215
	GLN	D433	R357	K293	D216
	GLU	V434	E358	Q294	N217
	SER	ASN	P359	Q295	A218
	LEU	ASP	D360	Y296	F219
	ILE	ASN	T361	I297	V220
	LEU	ALA	P363	L298	F221
	GLN	PRO	D364	H299	N222
	PRO	ILE	Q365	V300	P223
	ARG	PRO		R301	
	LYS	GLU		V302	V226
	ASP	PRO	T368	E303	Q227
	LEU	ARG	Y369	N304	G228
	GLU	ASN	R370	E305	Q229
	ILE	MET	I371	E306	V230
	GLY	GLN	N372	P307	P231
	GLY	PHE	R373	F308	E232
	TYR	CYS	D374	E309	
	LYS	GLN			V235
	ILE	ARG	N378	L312	
	HIS	ASN	L379		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.14Å 79.70Å 176.00Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	19.92 – 3.40 29.78 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.92-3.40) 99.6 (29.78-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6_289)	Depositor
R, $R_{free}$	0.230 , 0.293 0.229 , 0.289	Depositor DCC
$R_{free}$ test set	1140 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 24685 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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, MN, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/4200	0.71	10/5755 (0.2%)
1	B	0.47	1/3469 (0.0%)	0.67	3/4752 (0.1%)
All	All	0.46	1/7669 (0.0%)	0.69	13/10507 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	PRO	N-CD	5.03	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	ALA	N-CA-CB	-11.52	93.98	110.10
1	A	452	ASN	N-CA-CB	7.71	124.47	110.60
1	A	452	ASN	N-CA-C	-7.34	91.18	111.00
1	B	419	PRO	N-CA-C	-6.72	94.62	112.10
1	B	418	SER	C-N-CD	-5.80	107.84	120.60
1	A	479	GLY	N-CA-C	5.72	127.40	113.10
1	B	419	PRO	CB-CA-C	5.68	126.21	112.00
1	A	232	GLU	N-CA-C	5.56	126.02	111.00
1	A	492	ALA	N-CA-C	5.40	125.59	111.00
1	A	470	SER	N-CA-C	5.18	124.97	111.00
1	A	235	VAL	CB-CA-C	-5.13	101.65	111.40
1	A	233	ASN	N-CA-C	5.08	124.71	111.00
1	A	236	ASN	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	4113	0	3949	353	0
1	B	3399	0	3284	269	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	99	0	90	1	0
4	B	99	0	90	5	0
5	A	55	0	0	1	0
5	B	80	0	0	0	0
All	All	7871	0	7413	612	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (612) 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:483:ASN:CG	1:A:502:LYS:HB2	1.46	1.33
1:A:483:ASN:OD1	1:A:502:LYS:HB2	1.23	1.31
1:B:418:SER:HB2	1:B:419:PRO:CD	1.61	1.30
1:A:483:ASN:OD1	1:A:502:LYS:CB	1.81	1.29
1:B:418:SER:CB	1:B:419:PRO:HD3	1.76	1.15
1:B:418:SER:HB2	1:B:419:PRO:HD2	1.23	1.15
1:A:483:ASN:ND2	1:A:502:LYS:HB2	1.60	1.13
1:B:232:GLU:O	1:B:288:LEU:O	1.65	1.11
1:B:314:PRO:HB2	4:B:804:MAN:O6	1.52	1.08
1:B:186:THR:HG22	1:B:210:THR:HG22	1.34	1.04
1:B:418:SER:CB	1:B:419:PRO:CD	2.24	1.03
1:A:222:ASN:HB3	1:A:223:PRO:HD3	1.39	1.02
1:A:483:ASN:ND2	1:A:502:LYS:CB	2.23	1.01
1:A:483:ASN:HD21	1:A:502:LYS:CB	1.74	0.99
1:B:186:THR:CG2	1:B:210:THR:HG22	1.94	0.97
1:A:27:ASN:HD21	1:B:1:ASP:N	1.60	0.97
1:A:28:ARG:HD3	1:A:88:VAL:HG13	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:THR:OG1	1:B:422:THR:HG23	1.64	0.97
1:A:483:ASN:HA	1:A:501:ARG:HB3	1.44	0.97
1:A:483:ASN:CG	1:A:502:LYS:CB	2.28	0.96
1:A:490:ASP:CB	1:A:494:GLU:HG2	1.96	0.96
1:A:435:ASN:OD1	1:A:468:ASN:HB3	1.69	0.93
1:A:36:TYR:O	1:A:55:ARG:HD2	1.68	0.92
1:B:358:GLU:OE2	1:B:365:GLN:OE1	1.88	0.92
1:A:414:THR:HG22	1:A:422:THR:CG2	1.99	0.91
1:A:340:GLU:HA	1:A:430:VAL:HG13	1.52	0.91
1:A:442:GLU:HB2	1:A:459:THR:HB	1.51	0.91
1:A:442:GLU:HB3	1:A:443:PRO:HD3	1.53	0.91
1:A:27:ASN:HD21	1:B:1:ASP:H2	1.03	0.91
1:B:418:SER:HB3	1:B:419:PRO:HD3	1.51	0.90
1:B:256:LYS:HB2	1:B:305:GLU:OE2	1.73	0.89
1:A:483:ASN:OD1	1:A:502:LYS:CG	2.19	0.88
1:A:484:TRP:CZ2	1:A:511:ILE:HD11	2.08	0.88
1:A:452:ASN:HB3	1:A:535:GLU:O	1.75	0.87
1:A:154:ASP:HB3	1:A:188:THR:HG22	1.55	0.86
1:A:189:LEU:HB2	1:A:207:ALA:HB3	1.56	0.86
1:B:120:GLY:H	1:B:214:ILE:HD12	1.40	0.85
1:B:68:ARG:HD3	1:B:100:ASP:OD1	1.75	0.85
1:A:509:TYR:CZ	1:A:529:VAL:HB	2.12	0.84
1:A:414:THR:HG22	1:A:422:THR:HG21	1.58	0.84
1:B:220:VAL:O	1:B:244:VAL:HA	1.79	0.83
1:A:301:ARG:HD3	4:A:804:MAN:H3	1.60	0.83
1:B:221:PHE:CZ	1:B:302:VAL:HG13	2.13	0.83
1:A:483:ASN:CG	1:A:502:LYS:H	1.82	0.83
1:A:232:GLU:O	1:A:288:LEU:O	1.97	0.82
1:B:119:GLU:HG3	1:B:181:ARG:H	1.42	0.82
1:B:406:THR:HG22	1:B:430:VAL:HG22	1.61	0.81
1:A:483:ASN:CG	1:A:502:LYS:N	2.34	0.81
1:A:360:ASP:HB3	1:A:362:PHE:CE2	2.15	0.81
1:A:119:GLU:HG3	1:A:181:ARG:H	1.46	0.80
1:B:137:ASP:HB2	1:B:139:VAL:HG12	1.64	0.80
1:B:263:ASN:H	1:B:263:ASN:HD22	1.26	0.80
1:A:46:PRO:HA	1:A:47:PRO:C	2.02	0.80
1:B:378:TRP:CE3	1:B:394:MET:HG2	2.17	0.80
1:A:478:HIS:HB2	1:A:512:HIS:HB2	1.64	0.80
1:A:3:VAL:HG22	1:A:4:ILE:H	1.47	0.79
1:A:480:ALA:O	1:A:484:TRP:HB2	1.81	0.79
1:B:158:PRO:HG2	1:B:162:MET:HE1	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:THR:HA	1:A:422:THR:HG22	1.65	0.79
1:B:21:LEU:HD12	1:B:60:LEU:HD22	1.65	0.78
1:A:483:ASN:ND2	1:A:502:LYS:CA	2.45	0.78
1:B:152:SER:HB3	1:B:190:VAL:HG12	1.65	0.78
1:A:483:ASN:HA	1:A:501:ARG:CB	2.14	0.77
1:B:277:THR:O	1:B:278:ASN:ND2	2.17	0.77
1:B:314:PRO:CB	4:B:804:MAN:O6	2.33	0.77
1:B:72:ALA:HA	1:B:98:VAL:HG13	1.67	0.77
1:A:112:VAL:HG22	1:A:206:LYS:HB2	1.65	0.77
1:A:27:ASN:ND2	1:B:1:ASP:N	2.32	0.76
1:A:483:ASN:OD1	1:A:502:LYS:HG3	1.86	0.76
1:A:340:GLU:HB3	1:A:432:LEU:HD11	1.66	0.76
1:A:347:VAL:O	1:A:390:THR:HB	1.85	0.76
1:A:489:ASN:HB2	1:A:497:ILE:HG13	1.66	0.76
1:A:484:TRP:CE3	1:A:484:TRP:HA	2.22	0.74
1:B:263:ASN:HD21	1:B:298:LEU:HB2	1.52	0.74
1:B:194:ALA:HB3	1:B:198:GLY:HA2	1.68	0.74
1:B:351:ILE:HD12	1:B:388:ILE:HG22	1.69	0.74
1:B:113:PHE:O	1:B:207:ALA:HA	1.88	0.74
1:B:215:ASN:O	1:B:309:GLU:HG3	1.87	0.74
1:A:483:ASN:O	1:A:484:TRP:CE3	2.40	0.74
1:B:242:LEU:HD12	1:B:280:GLY:HA3	1.70	0.73
1:A:474:ALA:HB2	1:A:515:LEU:HD23	1.70	0.73
1:A:232:GLU:CD	1:A:290:PHE:H	1.91	0.73
1:B:195:ASP:OD1	1:B:201:LEU:HB2	1.88	0.73
1:A:443:PRO:HD2	1:A:458:ILE:HG23	1.69	0.72
1:A:414:THR:HG22	1:A:422:THR:HG22	1.70	0.72
1:A:239:ILE:HD11	1:A:282:LEU:HD13	1.71	0.72
1:A:480:ALA:C	1:A:484:TRP:HB2	2.10	0.72
1:A:263:ASN:HD22	1:A:263:ASN:N	1.83	0.72
1:A:41[B]:GLN:H	1:A:41[B]:GLN:CD	1.91	0.72
1:B:263:ASN:H	1:B:263:ASN:ND2	1.88	0.72
1:A:128:MET:HE3	1:A:207:ALA:HB1	1.71	0.72
1:A:462:ASP:HB3	1:A:469:THR:HG23	1.72	0.71
1:A:480:ALA:HA	1:A:484:TRP:CD1	2.26	0.70
1:A:224:SER:O	1:A:317:ALA:HB1	1.91	0.70
1:B:217:ASN:HB2	1:B:248:ASP:OD1	1.91	0.70
1:B:232:GLU:O	1:B:288:LEU:C	2.29	0.70
1:B:185:PRO:HA	1:B:211:VAL:HG13	1.72	0.70
1:A:117:VAL:HB	1:A:127:VAL:HG13	1.73	0.70
1:A:341:VAL:HG13	1:A:342:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:MET:C	1:A:529:VAL:HG13	2.13	0.69
1:B:242:LEU:CD1	1:B:280:GLY:HA3	2.22	0.69
1:A:230:VAL:CG1	1:A:239:ILE:HG22	2.23	0.69
1:A:484:TRP:HA	1:A:484:TRP:HE3	1.54	0.69
1:B:117:VAL:O	1:B:212:LYS:HG2	1.93	0.69
1:B:176:THR:HG22	1:B:177:SER:H	1.57	0.69
1:A:155:PRO:HD2	1:A:187:TYR:CE1	2.28	0.69
1:A:372:TRP:HB2	1:A:412:ILE:HG23	1.74	0.69
1:B:72:ALA:HA	1:B:98:VAL:CG1	2.23	0.68
1:B:145:ALA:O	1:B:195:ASP:HA	1.92	0.68
1:B:186:THR:HG22	1:B:210:THR:CG2	2.18	0.68
1:A:476:LEU:HD22	1:A:511:ILE:HG22	1.74	0.68
1:A:483:ASN:ND2	1:A:502:LYS:C	2.46	0.68
1:A:442:GLU:CB	1:A:459:THR:HB	2.23	0.68
1:B:138:ASP:HB3	1:B:144:ALA:HB3	1.74	0.67
1:A:127:VAL:HG23	1:A:173:SER:HA	1.75	0.67
1:A:264:ASP:N	1:A:265:PRO:HD3	2.10	0.67
1:B:263:ASN:N	1:B:263:ASN:HD22	1.89	0.67
1:A:483:ASN:CG	1:A:502:LYS:CA	2.63	0.66
1:B:114:GLU:HB3	1:B:208:VAL:HG23	1.77	0.66
1:B:111:GLU:CD	1:B:111:GLU:H	2.00	0.65
1:A:57:THR:HB	1:A:59:TRP:CD1	2.31	0.65
1:A:214:ILE:HG12	1:A:309:GLU:HG3	1.78	0.65
1:A:446:MET:O	1:A:529:VAL:HG13	1.96	0.65
1:A:3:VAL:HG22	1:A:4:ILE:N	2.12	0.65
1:A:74:TYR:HB2	1:A:96:ILE:HB	1.78	0.65
1:A:246:ASP:OD2	1:A:255:TRP:HA	1.95	0.65
1:A:57:THR:HB	1:A:59:TRP:HD1	1.62	0.65
1:A:7:ILE:H	1:A:7:ILE:HD12	1.61	0.65
1:A:448:PHE:CE1	1:A:500:PRO:HD3	2.31	0.64
1:B:152:SER:HB3	1:B:190:VAL:CG1	2.27	0.64
1:A:474:ALA:CB	1:A:515:LEU:HD23	2.27	0.64
1:A:298:LEU:CD1	1:A:319:VAL:HG13	2.27	0.64
1:A:480:ALA:HA	1:A:484:TRP:HB2	1.79	0.64
1:A:121:ALA:HB1	1:A:125:THR:HG21	1.79	0.64
1:A:239:ILE:HG12	1:A:282:LEU:HB3	1.80	0.64
1:B:290:PHE:CD2	1:B:325:ASP:CA	2.80	0.64
1:B:290:PHE:CE2	1:B:325:ASP:N	2.67	0.63
1:A:480:ALA:CA	1:A:484:TRP:HB2	2.28	0.63
1:A:274:ASP:CG	1:A:277:THR:HG22	2.18	0.63
1:A:459:THR:HA	1:A:495:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:CD	1:A:111:GLU:H	1.99	0.63
1:B:290:PHE:CD2	1:B:325:ASP:N	2.66	0.63
1:B:263:ASN:ND2	1:B:298:LEU:HB2	2.13	0.63
1:A:185:PRO:HA	1:A:211:VAL:HG23	1.79	0.63
1:A:10:PRO:HA	1:A:99:THR:OG1	1.99	0.63
1:A:236:ASN:HA	1:A:284:THR:H	1.63	0.63
1:A:119:GLU:HB2	1:A:212:LYS:O	1.99	0.63
1:B:342:PRO:HB3	1:B:434:VAL:HG21	1.81	0.63
1:B:166:ASN:C	1:B:166:ASN:HD22	2.02	0.63
1:B:232:GLU:C	1:B:288:LEU:O	2.37	0.62
1:A:458:ILE:O	1:A:495:SER:HB2	1.99	0.62
1:A:231:PRO:HA	1:A:324:VAL:HB	1.80	0.62
1:B:148:TYR:HA	1:B:192:GLN:O	2.00	0.62
1:A:78:SER:O	1:A:91:PRO:HA	2.00	0.62
1:A:329:ALA:HA	1:A:421:ALA:HB1	1.82	0.62
1:A:483:ASN:HD21	1:A:502:LYS:C	2.04	0.62
1:B:10:PRO:HA	1:B:99:THR:OG1	2.00	0.61
1:A:483:ASN:HD21	1:A:502:LYS:CA	2.12	0.61
1:A:483:ASN:OD1	1:A:502:LYS:N	2.32	0.61
1:B:369:TYR:O	1:B:383:PRO:HA	1.99	0.61
1:B:11:GLU:HG3	1:B:68:ARG:H	1.64	0.61
1:B:395:ASP:HB3	1:B:398:ASP:HB2	1.83	0.61
1:A:230:VAL:HG11	1:A:239:ILE:HG22	1.83	0.61
1:B:290:PHE:CE2	1:B:325:ASP:HB2	2.36	0.61
1:A:159:HIS:HB3	5:A:586:HOH:O	2.00	0.61
1:A:480:ALA:HA	1:A:484:TRP:CB	2.30	0.60
1:A:38:ILE:HA	1:A:77:TYR:O	2.01	0.60
1:A:474:ALA:HA	1:A:514:LYS:O	2.01	0.60
1:B:290:PHE:HE1	1:B:294:GLN:HG3	1.66	0.60
1:A:143:ASN:HD22	1:A:196:LEU:HD21	1.64	0.60
1:B:128:MET:HE2	1:B:207:ALA:HB1	1.84	0.60
1:A:119:GLU:OE1	1:A:214:ILE:HG22	2.01	0.60
1:A:343:GLU:OE1	1:A:395:ASP:OD1	2.20	0.60
1:B:108:PHE:HA	1:B:132:ALA:HA	1.84	0.60
1:A:374:ASP:HB2	1:A:407:TYR:OH	2.01	0.60
1:A:73:LYS:HD2	1:A:95:VAL:HG13	1.83	0.60
1:A:221:PHE:CE2	1:A:302:VAL:HG12	2.37	0.60
1:A:448:PHE:HE1	1:A:500:PRO:HD3	1.67	0.60
1:A:480:ALA:HA	1:A:484:TRP:HD1	1.67	0.60
1:A:298:LEU:HD12	1:A:319:VAL:O	2.02	0.60
1:A:122:VAL:HG23	1:A:125:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:CD	1:A:243:LYS:HB2	2.32	0.60
1:B:344:ASP:OD1	1:B:434:VAL:HG11	2.02	0.60
1:A:483:ASN:OD1	1:A:502:LYS:CA	2.50	0.60
1:A:119:GLU:OE2	1:A:182:GLU:OE2	2.21	0.59
1:A:145:ALA:O	1:A:195:ASP:HA	2.03	0.59
1:A:222:ASN:HB3	1:A:223:PRO:CD	2.23	0.59
1:B:249:ALA:O	1:B:255:TRP:HB2	2.03	0.59
1:A:345:PHE:CE2	1:A:349:GLN:HB2	2.37	0.59
1:B:337:ARG:HB2	1:B:354:TYR:CE1	2.37	0.59
1:A:105:ARG:HD3	1:A:203:THR:HG22	1.84	0.59
1:B:378:TRP:HA	1:B:392:ALA:HB3	1.84	0.59
1:A:429:LEU:HD21	1:A:431:LEU:HD21	1.84	0.59
1:B:226:TYR:CE1	1:B:242:LEU:HA	2.37	0.59
1:B:241:THR:HA	1:B:280:GLY:O	2.03	0.59
1:B:100:ASP:OD2	1:B:136:ASP:HB3	2.02	0.59
1:A:340:GLU:HA	1:A:430:VAL:CG1	2.31	0.58
1:B:218:ALA:HB2	1:B:308:PHE:HE2	1.68	0.58
1:A:376:ALA:HB2	1:A:401:HIS:CD2	2.39	0.58
1:A:382:ASN:ND2	1:A:385:THR:H	2.01	0.58
1:A:489:ASN:CG	1:A:497:ILE:HD11	2.23	0.58
1:B:288:LEU:HD22	1:B:296:TYR:CE2	2.38	0.58
1:B:68:ARG:NH1	1:B:100:ASP:OD1	2.36	0.58
1:B:361:THR:HG22	1:B:361:THR:O	2.03	0.58
1:A:381:ILE:O	1:A:383:PRO:HD3	2.03	0.58
1:A:511:ILE:O	1:A:527:LEU:HD12	2.03	0.57
1:B:68:ARG:NH1	1:B:69:GLU:OE2	2.37	0.57
1:B:344:ASP:OD1	1:B:434:VAL:CG1	2.52	0.57
1:B:235:VAL:HG22	1:B:287:GLY:N	2.19	0.57
1:A:513:LEU:O	1:A:523:GLN:HA	2.04	0.57
1:B:330:PRO:HA	1:B:359:PRO:CD	2.35	0.57
1:B:358:GLU:CD	1:B:365:GLN:OE1	2.43	0.57
1:A:440:ILE:HG22	1:A:441:PRO:HD2	1.87	0.57
1:B:246:ASP:OD2	1:B:304:ASN:ND2	2.35	0.57
1:B:112:VAL:HG22	1:B:206:LYS:HB2	1.87	0.57
1:A:409:ALA:HB3	1:A:427:LEU:HB3	1.86	0.56
1:A:186:THR:HG22	1:A:210:THR:HG22	1.88	0.56
1:A:297:ILE:HG12	1:A:320:THR:HG23	1.87	0.56
1:B:348:GLY:N	1:B:390:THR:O	2.38	0.56
1:B:412:ILE:HG23	1:B:422:THR:HG22	1.87	0.56
1:B:290:PHE:CE1	1:B:294:GLN:HG3	2.40	0.56
1:A:472:PHE:HD2	1:A:493:GLN:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:VAL:HG12	1:A:404:ASN:O	2.06	0.56
1:B:301:ARG:HD3	4:B:804:MAN:H61	1.88	0.56
1:A:350:GLU:HA	1:A:389:PHE:HA	1.87	0.56
1:A:484:TRP:CE2	1:A:511:ILE:CD1	2.89	0.56
1:A:360:ASP:HB3	1:A:362:PHE:HE2	1.69	0.56
1:A:341:VAL:O	1:A:431:LEU:HA	2.04	0.56
1:A:509:TYR:OH	1:A:529:VAL:HB	2.06	0.56
1:A:71:ILE:HG21	1:A:74:TYR:CE2	2.41	0.56
1:A:263:ASN:ND2	1:A:263:ASN:N	2.53	0.56
1:B:368:THR:CG2	1:B:414:THR:HB	2.36	0.56
1:B:215:ASN:HB2	1:B:254:ALA:CB	2.36	0.56
1:B:290:PHE:CD2	1:B:325:ASP:HA	2.41	0.56
1:A:382:ASN:HD22	1:A:385:THR:H	1.52	0.56
1:A:218:ALA:HA	1:A:308:PHE:HE1	1.71	0.56
1:A:489:ASN:HB2	1:A:497:ILE:CG1	2.36	0.55
1:A:478:HIS:CB	1:A:512:HIS:HB2	2.35	0.55
1:A:447:GLN:O	1:A:447:GLN:HG2	2.04	0.55
1:A:236:ASN:N	1:A:284:THR:O	2.39	0.55
1:B:374:ASP:OD2	1:B:379:LEU:HB2	2.05	0.55
1:A:239:ILE:HD11	1:A:282:LEU:HD22	1.89	0.55
1:B:229:GLN:HA	1:B:322:ASP:O	2.06	0.55
1:A:298:LEU:HD13	1:A:319:VAL:HG13	1.89	0.55
1:B:11:GLU:HG2	1:B:67:ASP:HA	1.88	0.55
1:A:230:VAL:HG13	1:A:239:ILE:HG22	1.88	0.55
1:B:122:VAL:HG23	1:B:125:THR:HB	1.89	0.55
1:A:418:SER:CB	1:A:419:PRO:HD3	2.37	0.55
1:A:370:ARG:HD2	1:A:412:ILE:HD11	1.89	0.55
1:A:274:ASP:O	1:A:278:ASN:N	2.34	0.55
1:B:299:HIS:CD2	4:B:805:MAN:H2	2.42	0.55
1:B:119:GLU:OE1	1:B:182:GLU:OE1	2.25	0.55
1:A:441:PRO:HD3	1:A:524:VAL:HG21	1.89	0.55
1:A:104:ASN:HB2	1:A:136:ASP:OD1	2.07	0.54
1:B:41:GLN:HG2	1:B:45:LYS:HB3	1.90	0.54
1:A:341:VAL:HG13	1:A:345:PHE:CD1	2.42	0.54
1:A:299:HIS:HB3	1:A:316:THR:HG21	1.88	0.54
1:A:229:GLN:HA	1:A:322:ASP:O	2.08	0.54
1:B:114:GLU:CB	1:B:208:VAL:HG23	2.38	0.54
1:A:382:ASN:HD21	1:A:384:GLU:HB2	1.72	0.54
1:A:488:TYR:HA	1:A:496:LEU:HB3	1.88	0.54
1:A:332:PHE:HA	1:A:356:ALA:HA	1.89	0.54
1:A:27:ASN:ND2	1:B:1:ASP:H3	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:N	1:B:222:ASN:HD22	2.06	0.54
1:A:517:ASP:N	1:A:517:ASP:OD2	2.41	0.54
1:A:346:GLY:HA3	1:A:349:GLN:HG3	1.89	0.54
1:A:382:ASN:ND2	1:A:384:GLU:HB2	2.22	0.54
1:A:189:LEU:CD1	1:A:209:ILE:HD11	2.37	0.53
1:A:126:SER:HA	1:A:173:SER:HB3	1.89	0.53
1:A:157:LEU:HA	1:A:159:HIS:N	2.22	0.53
1:A:337:ARG:HD3	1:A:352:THR:HG21	1.90	0.53
1:A:269:PHE:CD1	1:A:284:THR:HG22	2.42	0.53
1:A:269:PHE:HA	1:A:284:THR:HA	1.90	0.53
1:A:5:PRO:HG2	1:B:23:GLN:HG3	1.90	0.53
1:A:119:GLU:HG3	1:A:181:ARG:N	2.19	0.53
1:A:489:ASN:H	1:A:496:LEU:HA	1.74	0.53
1:A:329:ALA:CA	1:A:421:ALA:HB1	2.38	0.53
1:B:100:ASP:O	1:B:101:GLN:HG2	2.09	0.53
1:A:470:SER:O	1:A:472:PHE:N	2.41	0.53
1:B:209:ILE:N	1:B:209:ILE:HD12	2.24	0.53
1:B:362:PHE:C	1:B:364:ASP:H	2.09	0.53
1:B:21:LEU:HD12	1:B:60:LEU:CD2	2.36	0.53
1:B:239:ILE:HG21	1:B:321:VAL:HG22	1.89	0.53
1:A:47:PRO:HB2	1:A:50:VAL:HG21	1.90	0.52
1:B:17:PHE:CB	1:B:18:PRO:HA	2.40	0.52
1:B:223:PRO:O	1:B:226:TYR:CE2	2.62	0.52
1:A:274:ASP:HB3	1:A:277:THR:CG2	2.39	0.52
1:A:47:PRO:HB2	1:A:50:VAL:CG2	2.39	0.52
1:B:274:ASP:O	1:B:278:ASN:N	2.41	0.52
1:B:325:ASP:CG	1:B:362:PHE:HE1	2.13	0.52
1:A:369:TYR:O	1:A:383:PRO:HA	2.10	0.52
1:A:68:ARG:HD3	1:A:100:ASP:OD2	2.10	0.52
1:B:380:GLU:OE1	1:B:391:ARG:HG2	2.10	0.52
1:B:11:GLU:HB2	1:B:99:THR:O	2.10	0.52
1:B:153:GLN:NE2	1:B:159:HIS:O	2.43	0.52
1:A:484:TRP:CZ2	1:A:511:ILE:CD1	2.89	0.52
1:A:511:ILE:HB	1:A:527:LEU:HD13	1.91	0.52
1:B:368:THR:O	1:B:368:THR:HG23	2.10	0.52
1:A:44:ASP:OD1	1:A:45:LYS:N	2.42	0.52
1:A:478:HIS:CG	1:A:512:HIS:HB2	2.45	0.52
1:A:479:GLY:O	1:A:480:ALA:HB3	2.10	0.52
1:A:330:PRO:HG3	1:A:358:GLU:OE2	2.10	0.52
1:B:299:HIS:HA	1:B:317:ALA:O	2.10	0.52
1:A:36:TYR:O	1:A:55:ARG:CD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:HG11	1:B:302:VAL:HG11	1.92	0.51
1:A:337:ARG:HH11	1:A:337:ARG:HG3	1.75	0.51
1:B:119:GLU:HB2	1:B:212:LYS:O	2.10	0.51
1:A:345:PHE:CD2	1:A:349:GLN:HB2	2.46	0.51
1:A:264:ASP:O	1:A:264:ASP:CG	2.46	0.51
1:B:238:ARG:NH1	1:B:281:ILE:HD12	2.25	0.51
1:A:254:ALA:C	1:A:304:ASN:OD1	2.49	0.51
1:A:480:ALA:O	1:A:482:VAL:N	2.44	0.51
1:B:232:GLU:HB2	1:B:288:LEU:O	2.10	0.51
1:A:439:PRO:HB2	1:A:515:LEU:HB2	1.92	0.51
1:B:290:PHE:C	1:B:290:PHE:CD1	2.83	0.51
1:B:17:PHE:HB3	1:B:18:PRO:HA	1.91	0.51
1:A:41[A]:GLN:HA	1:A:45:LYS:O	2.10	0.51
1:B:345:PHE:HZ	1:B:350:GLU:O	1.94	0.51
1:A:476:LEU:HD22	1:A:511:ILE:CG2	2.39	0.51
1:A:51:PHE:CZ	1:A:66:LEU:HD11	2.46	0.51
1:A:232:GLU:HG3	1:A:289:ASP:HA	1.91	0.51
1:B:327:ASN:ND2	1:B:415:ASP:OD1	2.43	0.51
1:A:442:GLU:N	1:A:459:THR:O	2.44	0.51
1:B:145:ALA:HB1	1:B:197:GLN:HG3	1.92	0.51
1:A:376:ALA:HB2	1:A:401:HIS:NE2	2.25	0.50
1:A:186:THR:HA	1:A:210:THR:HA	1.92	0.50
1:B:119:GLU:OE1	1:B:216:ASP:OD2	2.30	0.50
1:B:314:PRO:HB2	4:B:804:MAN:HO6	1.73	0.50
1:A:11:GLU:OE1	1:A:103:ASP:OD1	2.29	0.50
1:A:226:TYR:HB2	1:A:319:VAL:HB	1.93	0.50
1:B:414:THR:OG1	1:B:422:THR:CG2	2.50	0.50
1:A:232:GLU:CG	1:A:289:ASP:HA	2.41	0.50
1:B:23:GLN:HB3	1:B:59:TRP:CD2	2.46	0.50
1:B:181:ARG:HD2	1:B:213:ASP:HA	1.94	0.50
1:A:256:LYS:O	1:A:304:ASN:ND2	2.45	0.50
1:A:223:PRO:HD2	1:A:243:LYS:HB2	1.94	0.50
1:A:215:ASN:ND2	1:A:308:PHE:HA	2.27	0.50
1:A:157:LEU:HA	1:A:158:PRO:C	2.32	0.49
1:B:371:ILE:HG13	1:B:410:LEU:O	2.12	0.49
1:B:151:VAL:HG23	1:B:190:VAL:HG13	1.94	0.49
1:A:390:THR:HG23	1:A:394:MET:HE3	1.94	0.49
1:B:176:THR:HG22	1:B:177:SER:N	2.26	0.49
1:A:236:ASN:HB2	1:A:283:LYS:HD3	1.93	0.49
1:B:230:VAL:O	1:B:323:VAL:HA	2.12	0.49
1:B:411:ILE:HG22	1:B:412:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:O	1:A:167:ARG:C	2.51	0.49
1:B:327:ASN:OD1	1:B:415:ASP:OD1	2.31	0.49
1:A:128:MET:CE	1:A:207:ALA:HB1	2.41	0.49
1:A:242:LEU:HD12	1:A:271:VAL:HG21	1.95	0.49
1:B:214:ILE:O	1:B:216:ASP:N	2.45	0.49
1:B:352:THR:HG22	1:B:353:SER:N	2.27	0.49
1:B:373:ARG:HB3	1:B:410:LEU:H	1.78	0.49
1:A:35:PHE:HE2	1:A:83:SER:HB3	1.78	0.49
1:B:341:VAL:O	1:B:431:LEU:HA	2.12	0.49
1:A:277:THR:O	1:A:278:ASN:ND2	2.32	0.49
1:A:22:VAL:HG12	1:A:23:GLN:H	1.77	0.49
1:B:220:VAL:O	1:B:244:VAL:CA	2.56	0.49
1:A:438:ALA:HB2	1:A:520:ASN:ND2	2.28	0.49
1:B:9:CYS:SG	1:B:13:GLU:OE2	2.71	0.49
1:B:120:GLY:N	1:B:214:ILE:HD12	2.20	0.49
1:A:468:ASN:O	1:A:517:ASP:OD1	2.31	0.49
1:A:489:ASN:ND2	1:A:497:ILE:HD11	2.28	0.49
1:A:484:TRP:CE2	1:A:511:ILE:HD11	2.47	0.48
1:A:346:GLY:CA	1:A:349:GLN:HG3	2.42	0.48
1:B:271:VAL:HA	1:B:281:ILE:O	2.13	0.48
1:A:224:SER:O	1:A:317:ALA:CB	2.60	0.48
1:A:521:LYS:N	1:A:521:LYS:HD3	2.28	0.48
1:A:350:GLU:HA	1:A:389:PHE:HB3	1.96	0.48
1:B:358:GLU:HA	1:B:358:GLU:OE1	2.11	0.48
1:A:3:VAL:CG2	1:A:4:ILE:H	2.22	0.48
1:A:437:ASN:HB2	1:A:464:ASP:OD2	2.13	0.48
1:B:67:ASP:O	1:B:70:ALA:HB3	2.14	0.48
1:B:24:ILE:HD11	1:B:53:ILE:CD1	2.44	0.48
1:B:221:PHE:HA	1:B:243:LYS:O	2.13	0.48
1:A:214:ILE:HG23	1:A:216:ASP:HB3	1.96	0.48
1:B:215:ASN:HB2	1:B:254:ALA:HB1	1.95	0.48
1:A:264:ASP:OD2	1:A:267:GLN:HA	2.13	0.48
1:A:409:ALA:O	1:A:410:LEU:HD23	2.14	0.48
1:A:20:ASN:HA	1:A:61:LYS:HB3	1.95	0.48
1:A:481:SER:O	1:A:483:ASN:N	2.46	0.48
1:A:223:PRO:HD2	1:A:226:TYR:OH	2.14	0.48
1:A:298:LEU:H	1:A:298:LEU:HD12	1.78	0.48
1:A:484:TRP:CE2	1:A:511:ILE:HD13	2.49	0.47
1:A:432:LEU:HD12	1:A:432:LEU:H	1.79	0.47
1:A:121:ALA:CB	1:A:125:THR:HG21	2.45	0.47
1:A:330:PRO:HA	1:A:359:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HA	1:B:77:TYR:O	2.14	0.47
1:B:395:ASP:OD2	1:B:397:GLU:HB2	2.14	0.47
1:B:150:ILE:HG21	1:B:189:LEU:HD22	1.94	0.47
1:B:290:PHE:C	1:B:290:PHE:HD1	2.17	0.47
1:B:300:VAL:CG2	1:B:317:ALA:HB3	2.44	0.47
1:A:474:ALA:HB2	1:A:515:LEU:CD2	2.43	0.47
1:A:239:ILE:CD1	1:A:282:LEU:HD22	2.45	0.47
1:A:453:PRO:CB	1:A:500:PRO:HG2	2.45	0.47
1:A:166:ASN:HB3	1:A:169:THR:HB	1.97	0.47
1:B:263:ASN:OD1	1:B:298:LEU:HA	2.14	0.47
1:B:290:PHE:CD2	1:B:325:ASP:HB2	2.49	0.47
1:A:184:TYR:O	1:A:211:VAL:HG21	2.15	0.47
1:B:62:VAL:HG21	1:B:66:LEU:HD11	1.97	0.47
1:A:8:SER:HA	1:A:97:THR:O	2.15	0.47
1:A:480:ALA:O	1:A:481:SER:C	2.52	0.47
1:A:80:ALA:HB3	1:A:89:GLU:HB2	1.96	0.47
1:B:303:GLU:HA	1:B:308:PHE:HE1	1.80	0.47
1:A:411:ILE:N	1:A:411:ILE:HD12	2.30	0.47
1:A:148:TYR:HA	1:A:192:GLN:O	2.15	0.47
1:A:53:ILE:HG23	1:A:55:ARG:HH11	1.80	0.47
1:B:53:ILE:HA	1:B:59:TRP:O	2.14	0.47
1:A:53:ILE:HA	1:A:59:TRP:O	2.15	0.47
1:A:345:PHE:CE2	1:A:349:GLN:CB	2.98	0.47
1:A:509:TYR:CE2	1:A:511:ILE:HD11	2.49	0.46
1:A:475:GLU:O	1:A:513:LEU:HD12	2.14	0.46
1:B:114:GLU:HB3	1:B:208:VAL:CG2	2.43	0.46
1:B:187:TYR:N	1:B:209:ILE:O	2.39	0.46
1:B:312:LEU:N	1:B:312:LEU:HD12	2.30	0.46
1:A:232:GLU:HG3	1:A:290:PHE:N	2.30	0.46
1:B:122:VAL:O	1:B:125:THR:HB	2.16	0.46
1:B:341:VAL:HG21	1:B:429:LEU:HD11	1.97	0.46
1:B:339:VAL:HG23	1:B:429:LEU:HD12	1.97	0.46
1:B:148:TYR:CD2	1:B:170:GLY:HA2	2.51	0.46
1:A:166:ASN:HD22	1:A:166:ASN:C	2.19	0.46
1:B:414:THR:CG2	1:B:420:ILE:HG23	2.46	0.46
1:B:119:GLU:HA	1:B:211:VAL:HG23	1.98	0.46
1:A:244:VAL:HG11	1:A:302:VAL:HG11	1.96	0.46
1:B:20:ASN:HA	1:B:61:LYS:HG2	1.96	0.46
1:B:122:VAL:O	1:B:123:PRO:C	2.52	0.46
1:B:380:GLU:HB3	1:B:389:PHE:CE1	2.51	0.46
1:B:231:PRO:HA	1:B:324:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PHE:HE2	1:B:325:ASP:H	1.62	0.46
1:B:108:PHE:HE1	1:B:203:THR:O	1.99	0.46
1:B:332:PHE:HD1	1:B:355:THR:O	1.99	0.46
1:A:24:ILE:HD12	1:B:2:TRP:CH2	2.51	0.46
1:A:192:GLN:HG2	1:A:193:ALA:N	2.31	0.46
1:B:325:ASP:OD2	1:B:325:ASP:C	2.54	0.46
1:B:46:PRO:HA	1:B:48:VAL:N	2.31	0.46
1:A:41[B]:GLN:NE2	1:A:41[B]:GLN:H	2.13	0.46
1:A:3:VAL:HG13	1:B:25:LYS:HD3	1.97	0.46
1:A:153:GLN:HE22	1:A:162:MET:HG2	1.81	0.46
1:A:236:ASN:HA	1:A:284:THR:O	2.16	0.45
1:A:350:GLU:HB2	1:A:389:PHE:HD2	1.81	0.45
1:A:274:ASP:HB3	1:A:277:THR:HG22	1.98	0.45
1:A:29:ASP:HA	1:A:34:VAL:HG22	1.97	0.45
1:B:261:VAL:HG12	1:B:300:VAL:HG12	1.98	0.45
1:A:485:THR:HG22	1:A:499:GLN:O	2.17	0.45
1:A:263:ASN:H	1:A:263:ASN:HD22	1.63	0.45
1:B:11:GLU:OE1	1:B:67:ASP:OD2	2.35	0.45
1:B:219:PRO:O	1:B:302:VAL:HG21	2.17	0.45
1:A:102:ASN:HA	1:A:136:ASP:OD2	2.16	0.45
1:A:374:ASP:OD1	1:A:377:ASN:HA	2.16	0.45
1:B:145:ALA:HB3	1:B:197:GLN:H	1.80	0.45
1:A:449:CYS:HB3	1:A:453:PRO:HA	1.97	0.45
1:B:119:GLU:HB3	1:B:214:ILE:HB	1.99	0.44
1:A:67:ASP:OD2	1:A:69:GLU:N	2.50	0.44
1:B:24:ILE:HD11	1:B:53:ILE:HD11	1.98	0.44
1:B:466:PRO:HA	1:B:467:PRO:C	2.37	0.44
1:B:347:VAL:HG12	1:B:392:ALA:O	2.18	0.44
1:A:67:ASP:C	1:A:67:ASP:OD2	2.55	0.44
1:A:480:ALA:HA	1:A:484:TRP:CG	2.53	0.44
1:B:11:GLU:CG	1:B:67:ASP:HA	2.46	0.44
1:B:406:THR:CG2	1:B:430:VAL:HG22	2.38	0.44
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.35	0.44
1:A:45:LYS:O	1:A:47:PRO:O	2.35	0.44
1:B:129:LYS:HD3	1:B:171:VAL:HG22	2.00	0.44
1:A:38:ILE:HG23	1:A:53:ILE:HG21	1.99	0.44
1:A:155:PRO:HD2	1:A:187:TYR:CD1	2.53	0.44
1:A:188:THR:OG1	1:A:208:VAL:HG22	2.18	0.44
1:A:253:PRO:HB3	1:A:305:GLU:HG2	1.99	0.44
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.84	0.44
1:A:447:GLN:N	1:A:529:VAL:HG13	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:THR:HA	1:B:422:THR:HA	1.99	0.44
1:B:11:GLU:CG	1:B:68:ARG:H	2.28	0.44
1:A:143:ASN:ND2	1:A:196:LEU:HD21	2.31	0.44
1:B:332:PHE:CD1	1:B:355:THR:O	2.71	0.44
1:B:232:GLU:O	1:B:288:LEU:N	2.51	0.44
1:B:214:ILE:HG22	1:B:214:ILE:O	2.18	0.44
1:B:150:ILE:HG13	1:B:165:VAL:HG12	2.00	0.44
1:B:166:ASN:HD22	1:B:167:ARG:N	2.14	0.44
1:B:180:ASP:HB3	1:B:183:SER:HB3	2.00	0.44
1:A:274:ASP:CB	1:A:277:THR:HG22	2.48	0.44
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.81	0.44
1:A:331:ILE:CD1	1:A:359:PRO:HG3	2.48	0.44
1:A:263:ASN:OD1	1:A:298:LEU:HA	2.18	0.44
1:B:246:ASP:HB3	1:B:255:TRP:CD1	2.53	0.44
1:A:472:PHE:H	1:A:493:GLN:CB	2.30	0.44
1:B:60:LEU:HD23	1:B:61:LYS:N	2.33	0.43
1:B:105:ARG:HB3	1:B:201:LEU:HD13	2.00	0.43
1:B:357:ARG:O	1:B:359:PRO:HD3	2.17	0.43
1:A:102:ASN:HB2	1:A:143:ASN:ND2	2.34	0.43
1:B:337:ARG:HA	1:B:337:ARG:HD2	1.88	0.43
1:B:379:LEU:HD12	1:B:379:LEU:N	2.32	0.43
1:B:18:PRO:HB3	1:B:63:THR:HA	1.98	0.43
1:B:368:THR:HG23	1:B:414:THR:HB	1.99	0.43
1:A:456:HIS:O	1:A:497:ILE:HA	2.18	0.43
1:A:221:PHE:HA	1:A:243:LYS:O	2.19	0.43
1:A:89:GLU:HG2	1:B:2:TRP:CD1	2.53	0.43
1:A:89:GLU:OE2	1:B:1:ASP:HA	2.18	0.43
1:A:264:ASP:N	1:A:265:PRO:CD	2.78	0.43
1:A:2:TRP:CZ3	1:B:24:ILE:HD12	2.53	0.43
1:B:50:VAL:HG22	1:B:64:GLN:NE2	2.33	0.43
1:B:253:PRO:HB2	1:B:306:GLU:HB2	2.01	0.43
1:A:341:VAL:HG21	1:A:351:ILE:HG23	2.00	0.43
1:B:337:ARG:HH22	1:B:352:THR:HG21	1.83	0.43
1:A:483:ASN:HD21	1:A:502:LYS:HB3	1.74	0.43
1:A:41[B]:GLN:HA	1:A:45:LYS:O	2.18	0.43
1:A:111:GLU:CD	1:A:111:GLU:N	2.69	0.43
1:B:159:HIS:CD2	1:B:162:MET:CE	3.02	0.43
1:B:162:MET:HB3	1:B:163:PHE:CD2	2.54	0.43
1:A:196:LEU:O	1:A:197:GLN:HB2	2.19	0.43
1:A:395:ASP:HB3	1:A:398:ASP:HB2	2.01	0.43
1:A:106:PRO:O	1:A:203:THR:HG21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ASP:HA	1:B:463:PRO:HD3	1.79	0.43
1:B:240:ALA:O	1:B:282:LEU:HB2	2.18	0.43
1:A:77:TYR:HA	1:A:92:MET:O	2.18	0.43
1:A:290:PHE:CG	1:A:325:ASP:HB2	2.54	0.43
1:A:186:THR:CG2	1:A:210:THR:HG22	2.49	0.43
1:B:63:THR:OG1	1:B:64:GLN:HG2	2.19	0.43
1:A:333:MET:HA	1:A:334:PRO:HA	1.85	0.43
1:B:255:TRP:C	1:B:304:ASN:ND2	2.71	0.43
1:B:218:ALA:HA	1:B:219:PRO:HD3	1.77	0.43
1:A:290:PHE:CD1	1:A:290:PHE:C	2.92	0.43
1:A:290:PHE:CD2	1:A:325:ASP:HB2	2.54	0.43
1:A:42:GLY:HA2	1:A:47:PRO:O	2.19	0.43
1:A:253:PRO:C	1:A:255:TRP:H	2.22	0.43
1:B:290:PHE:HD2	1:B:325:ASP:N	2.16	0.43
1:B:327:ASN:HB3	1:B:419:PRO:HD2	2.00	0.42
1:A:154:ASP:HA	1:A:155:PRO:HA	1.71	0.42
1:A:439:PRO:HB2	1:A:515:LEU:CB	2.48	0.42
1:A:370:ARG:HG3	1:A:412:ILE:HG12	2.01	0.42
1:B:229:GLN:CA	1:B:322:ASP:O	2.66	0.42
1:B:239:ILE:HG21	1:B:321:VAL:CG2	2.48	0.42
1:A:148:TYR:N	1:A:167:ARG:O	2.51	0.42
1:B:120:GLY:H	1:B:214:ILE:CD1	2.22	0.42
1:B:152:SER:O	1:B:189:LEU:HD23	2.19	0.42
1:A:438:ALA:HB1	1:A:522:ASP:HB2	2.01	0.42
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.19	0.42
1:B:51:PHE:CE2	1:B:74:TYR:CD2	3.07	0.42
1:B:432:LEU:HD12	1:B:432:LEU:HA	1.77	0.42
1:B:150:ILE:CG2	1:B:189:LEU:HD22	2.50	0.42
1:A:341:VAL:CG1	1:A:345:PHE:CD1	3.02	0.42
1:B:362:PHE:C	1:B:364:ASP:N	2.72	0.42
1:A:104:ASN:ND2	1:A:135:ALA:HB3	2.35	0.42
1:A:332:PHE:CZ	1:A:411:ILE:HG22	2.55	0.42
1:B:55:ARG:HG3	1:B:55:ARG:H	1.52	0.42
1:B:412:ILE:HG23	1:B:422:THR:CG2	2.50	0.42
1:A:351:ILE:HD11	1:A:394:MET:HE1	2.02	0.42
1:B:215:ASN:CB	1:B:254:ALA:HB1	2.49	0.42
1:A:51:PHE:HZ	1:A:66:LEU:HD11	1.83	0.42
1:A:71:ILE:HG21	1:A:74:TYR:CZ	2.55	0.42
1:A:272:VAL:HG23	1:A:281:ILE:HG13	2.01	0.42
1:B:232:GLU:HG3	1:B:326:VAL:HG22	2.01	0.42
1:B:242:LEU:HD12	1:B:280:GLY:CA	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:HB3	1:A:277:THR:HG23	2.01	0.42
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.81	0.42
1:A:9:CYS:SG	1:A:13:GLU:OE1	2.76	0.42
1:A:414:THR:CG2	1:A:422:THR:HG22	2.45	0.41
1:B:45:LYS:N	1:B:45:LYS:HD2	2.35	0.41
1:B:282:LEU:HA	1:B:282:LEU:HD23	1.76	0.41
1:B:382:ASN:HB3	1:B:387:ALA:HB3	2.01	0.41
1:A:244:VAL:HG22	1:A:259:TYR:OH	2.20	0.41
1:B:242:LEU:HD11	1:B:280:GLY:HA3	1.98	0.41
1:B:382:ASN:N	1:B:387:ALA:O	2.43	0.41
1:B:221:PHE:CD2	1:B:244:VAL:HG12	2.55	0.41
1:B:215:ASN:HB2	1:B:254:ALA:HB2	2.02	0.41
1:A:462:ASP:HA	1:A:463:PRO:HD3	1.70	0.41
1:B:33:LYS:HG3	1:B:35:PHE:CE1	2.55	0.41
1:A:367:ILE:HG22	1:A:413:ALA:HB1	2.01	0.41
1:A:38:ILE:HG12	1:A:53:ILE:HG22	2.03	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.84	0.41
1:A:111:GLU:HG2	1:A:112:VAL:N	2.35	0.41
1:A:7:ILE:HD12	1:A:7:ILE:N	2.32	0.41
1:A:406:THR:HG22	1:A:407:TYR:O	2.21	0.41
1:B:196:LEU:HB2	1:B:200:GLY:N	2.36	0.41
1:A:476:LEU:HD23	1:A:513:LEU:HA	2.01	0.41
1:A:466:PRO:HA	1:A:468:ASN:N	2.35	0.41
1:B:304:ASN:O	1:B:305:GLU:C	2.59	0.41
1:A:33:LYS:O	1:A:83:SER:N	2.54	0.41
1:B:301:ARG:HA	1:B:315:SER:O	2.21	0.41
1:B:185:PRO:O	1:B:210:THR:HA	2.20	0.41
1:B:390:THR:HG22	1:B:392:ALA:O	2.21	0.41
1:B:373:ARG:HB3	1:B:410:LEU:HB2	2.01	0.41
1:B:66:LEU:H	1:B:66:LEU:HD12	1.85	0.41
1:B:164:THR:HG23	1:B:175:LEU:HD22	2.03	0.41
1:B:411:ILE:CG2	1:B:412:ILE:N	2.83	0.41
1:B:232:GLU:O	1:B:288:LEU:CA	2.69	0.41
1:A:488:TYR:CD2	1:A:488:TYR:N	2.89	0.41
1:B:166:ASN:C	1:B:166:ASN:ND2	2.72	0.41
1:A:408:VAL:HG22	1:A:428:LEU:HD23	2.03	0.41
1:B:415:ASP:OD2	1:B:416:ASP:N	2.51	0.41
1:B:232:GLU:HG2	1:B:324:VAL:O	2.21	0.41
1:A:494:GLU:HG3	1:A:495:SER:N	2.36	0.41
1:A:442:GLU:HB3	1:A:443:PRO:CD	2.36	0.41
1:A:515:LEU:O	1:A:521:LYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:HB2	1:B:248:ASP:CG	2.41	0.41
1:A:453:PRO:HB3	1:A:500:PRO:HG2	2.03	0.41
1:A:410:LEU:HD23	1:A:426:THR:HG23	2.01	0.41
1:A:295:GLN:OE1	1:A:322:ASP:OD1	2.39	0.41
1:B:298:LEU:H	1:B:298:LEU:HD23	1.86	0.41
1:B:105:ARG:HA	1:B:106:PRO:HD3	1.88	0.41
1:A:372:TRP:HB2	1:A:412:ILE:CG2	2.47	0.41
1:A:441:PRO:CD	1:A:524:VAL:HG21	2.51	0.41
1:A:29:ASP:HA	1:A:34:VAL:CG2	2.51	0.41
1:B:51:PHE:HE2	1:B:74:TYR:CG	2.37	0.41
1:B:382:ASN:ND2	1:B:385:THR:H	2.19	0.41
1:B:152:SER:O	1:B:189:LEU:HA	2.20	0.40
1:B:373:ARG:HD3	1:B:410:LEU:HD13	2.02	0.40
1:A:414:THR:CA	1:A:422:THR:HG22	2.42	0.40
1:B:252:THR:O	1:B:255:TRP:N	2.49	0.40
1:B:157:LEU:HA	1:B:158:PRO:C	2.42	0.40
1:B:128:MET:CE	1:B:207:ALA:HB1	2.51	0.40
1:A:51:PHE:CE2	1:A:96:ILE:HD13	2.56	0.40
1:B:329:ALA:O	1:B:359:PRO:HG2	2.22	0.40
1:A:418:SER:HB2	1:A:419:PRO:HD3	2.04	0.40
1:A:281:ILE:H	1:A:281:ILE:HG12	1.72	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	529/550 (96%)	454 (86%)	72 (14%)	3 (1%)	30	72
1	B	436/550 (79%)	387 (89%)	48 (11%)	1 (0%)	52	87
All	All	965/1100 (88%)	841 (87%)	120 (12%)	4 (0%)	39	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	A	481	SER
1	A	482	VAL
1	B	419	PRO

### 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	458/482 (95%)	410 (90%)	48 (10%)	8	36
1	B	381/482 (79%)	337 (88%)	44 (12%)	7	31
All	All	839/964 (87%)	747 (89%)	92 (11%)	8	34

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	CYS
1	A	22	VAL
1	A	34	VAL
1	A	41[A]	GLN
1	A	41[B]	GLN
1	A	57	THR
1	A	78	SER
1	A	88	VAL
1	A	139	VAL
1	A	149	THR
1	A	157	LEU
1	A	161	ASN
1	A	166	ASN
1	A	169	THR
1	A	181	ARG
1	A	188	THR
1	A	209	ILE
1	A	211	VAL

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Mol	Chain	Res	Type
1	A	230	VAL
1	A	235	VAL
1	A	247	ASP
1	A	261	VAL
1	A	263	ASN
1	A	278	ASN
1	A	281	ILE
1	A	282	LEU
1	A	293	LYS
1	A	298	LEU
1	A	319	VAL
1	A	354	TYR
1	A	357	ARG
1	A	368	THR
1	A	373	ARG
1	A	389	PHE
1	A	390	THR
1	A	418	SER
1	A	427	LEU
1	A	429	LEU
1	A	440	ILE
1	A	470	SER
1	A	484	TRP
1	A	496	LEU
1	A	517	ASP
1	A	520	ASN
1	A	521	LYS
1	A	531	VAL
1	A	535	GLU
1	B	1	ASP
1	B	9	CYS
1	B	45	LYS
1	B	56	GLU
1	B	98	VAL
1	B	111	GLU
1	B	122	VAL
1	B	140	ASN
1	B	146	ILE
1	B	154	ASP
1	B	162	MET
1	B	166	ASN
1	B	186	THR

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Mol	Chain	Res	Type
1	B	188	THR
1	B	208	VAL
1	B	211	VAL
1	B	214	ILE
1	B	222	ASN
1	B	227	GLN
1	B	232	GLU
1	B	238	ARG
1	B	242	LEU
1	B	251	ASN
1	B	260	THR
1	B	263	ASN
1	B	278	ASN
1	B	282	LEU
1	B	290	PHE
1	B	293	LYS
1	B	320	THR
1	B	323	VAL
1	B	338	ARG
1	B	350	GLU
1	B	355	THR
1	B	362	PHE
1	B	363	MET
1	B	384	GLU
1	B	385	THR
1	B	389	PHE
1	B	390	THR
1	B	391	ARG
1	B	422	THR
1	B	433	ASP
1	B	464	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	23	GLN
1	A	27	ASN
1	A	64	GLN
1	A	84	ASN
1	A	104	ASN
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	143	ASN
1	A	161	ASN
1	A	166	ASN
1	A	263	ASN
1	A	299	HIS
1	A	382	ASN
1	A	452	ASN
1	A	489	ASN
1	A	512	HIS
1	A	520	ASN
1	B	64	GLN
1	B	110	GLN
1	B	143	ASN
1	B	166	ASN
1	B	197	GLN
1	B	222	ASN
1	B	227	GLN
1	B	263	ASN
1	B	299	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 26 are monoatomic - leaving 18 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	$\# Z  > 2$
4	MAN	A	801	1	11,11,12	0.53	0	14,15,17	1.25	1 (7%)
4	MAN	A	802	1	11,11,12	0.61	0	14,15,17	0.87	0
4	MAN	A	803	1	11,11,12	0.70	0	14,15,17	0.90	1 (7%)
4	MAN	A	804	1	11,11,12	0.54	0	14,15,17	0.96	1 (7%)
4	MAN	A	805	1	11,11,12	0.58	0	14,15,17	0.77	0
4	MAN	A	806	1	11,11,12	0.54	0	14,15,17	0.89	1 (7%)
4	MAN	A	807	1	11,11,12	0.55	0	14,15,17	1.09	2 (14%)
4	MAN	A	808	1	11,11,12	0.54	0	14,15,17	1.00	1 (7%)
4	MAN	A	809	1	11,11,12	0.56	0	14,15,17	0.96	1 (7%)
4	MAN	B	801	1	11,11,12	0.61	0	14,15,17	0.70	0
4	MAN	B	802	1	11,11,12	0.55	0	14,15,17	0.95	1 (7%)
4	MAN	B	803	1	11,11,12	0.67	0	14,15,17	0.81	1 (7%)
4	MAN	B	804	1	11,11,12	0.71	0	14,15,17	1.34	1 (7%)
4	MAN	B	805	1	11,11,12	0.58	0	14,15,17	0.73	0
4	MAN	B	806	1	11,11,12	0.61	0	14,15,17	0.95	1 (7%)
4	MAN	B	807	1	11,11,12	0.63	0	14,15,17	0.82	0
4	MAN	B	808	1	11,11,12	0.60	0	14,15,17	0.73	0
4	MAN	B	809	1	11,11,12	0.57	0	14,15,17	0.82	0

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
4	MAN	A	801	1	-	0/2/19/22	0/1/1/1
4	MAN	A	802	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	803	1	-	0/2/19/22	0/1/1/1
4	MAN	A	804	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	805	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	806	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	807	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	808	1	-	0/2/19/22	0/1/1/1
4	MAN	A	809	1	-	0/2/19/22	0/1/1/1
4	MAN	B	801	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	802	1	-	0/2/19/22	0/1/1/1
4	MAN	B	803	1	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	804	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	805	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	806	1	-	0/2/19/22	0/1/1/1
4	MAN	B	807	1	-	0/2/19/22	0/1/1/1
4	MAN	B	808	1	-	0/2/19/22	0/1/1/1
4	MAN	B	809	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	807	MAN	C3-C4-C5	2.19	114.02	110.20
4	B	803	MAN	C1-C2-C3	2.30	112.26	109.54
4	B	806	MAN	C1-C2-C3	2.31	112.28	109.54
4	A	804	MAN	C1-O5-C5	2.35	115.23	112.25
4	A	807	MAN	C1-O5-C5	2.38	115.26	112.25
4	A	806	MAN	C1-O5-C5	2.44	115.34	112.25
4	B	802	MAN	C1-O5-C5	2.46	115.37	112.25
4	A	809	MAN	C1-O5-C5	2.62	115.57	112.25
4	A	803	MAN	C1-C2-C3	2.64	112.67	109.54
4	A	808	MAN	C1-O5-C5	2.67	115.63	112.25
4	A	801	MAN	C1-O5-C5	3.93	117.24	112.25
4	B	804	MAN	C1-C2-C3	4.12	114.41	109.54

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	801	MAN	C1
4	B	805	MAN	C1
4	A	805	MAN	C1
4	A	802	MAN	C1
4	B	804	MAN	C1
4	A	806	MAN	C1
4	A	807	MAN	C1
4	A	804	MAN	C1
4	B	803	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	MAN	1	0
4	B	804	MAN	4	0
4	B	805	MAN	1	0

## 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	532/550 (96%)	-0.20	12 (2%) 64 58	25, 59, 123, 157	0
1	B	440/550 (80%)	-0.13	11 (2%) 61 55	32, 61, 112, 131	0
All	All	972/1100 (88%)	-0.17	23 (2%) 62 57	25, 60, 116, 157	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	TYR	5.1
1	A	448	PHE	3.3
1	A	532	CYS	3.2
1	A	534	CYS	3.1
1	B	467	PRO	3.0
1	A	535	GLU	3.0
1	A	531	VAL	2.9
1	B	392	ALA	2.9
1	B	368	THR	2.7
1	B	394	MET	2.6
1	A	530	HIS	2.5
1	A	511	ILE	2.4
1	A	444	ARG	2.4
1	B	391	ARG	2.4
1	B	466	PRO	2.3
1	B	364	ASP	2.3
1	A	502	LYS	2.3
1	B	363	MET	2.2
1	B	362	PHE	2.1
1	B	465	LEU	2.1
1	B	420	ILE	2.0
1	A	456	HIS	2.0
1	A	483	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
4	MAN	A	802	11/12	0.88	0.42	6.42	59,63,79,91	0
4	MAN	B	804	11/12	0.69	0.46	5.97	91,100,120,132	0
2	CA	B	601	1/1	0.93	0.18	4.37	44,44,44,44	0
4	MAN	A	809	11/12	0.89	0.37	2.81	87,91,98,112	0
2	CA	A	601	1/1	0.96	0.22	2.53	41,41,41,41	0
4	MAN	A	805	11/12	0.85	0.28	2.52	66,69,89,95	0
2	CA	A	604	1/1	0.95	0.20	1.49	35,35,35,35	0
4	MAN	A	803	11/12	0.88	0.21	0.98	50,69,77,78	0
4	MAN	B	805	11/12	0.85	0.27	0.89	79,84,96,96	0
4	MAN	A	804	11/12	0.95	0.18	0.61	47,60,76,80	0
4	MAN	B	807	11/12	0.83	0.33	0.46	106,117,122,129	0
3	MN	B	901	1/1	0.98	0.22	0.25	54,54,54,54	0
4	MAN	A	808	11/12	0.81	0.23	0.21	72,85,90,98	0
2	CA	A	612	1/1	0.91	0.16	0.08	74,74,74,74	0
2	CA	A	605	1/1	0.83	0.16	-0.01	31,31,31,31	0
4	MAN	B	801	11/12	0.91	0.19	-0.09	55,60,72,73	0
4	MAN	A	807	11/12	0.83	0.26	-0.11	74,85,90,91	0
2	CA	A	610	1/1	0.82	0.16	-0.18	74,74,74,74	0
4	MAN	B	809	11/12	0.88	0.19	-0.68	95,99,112,113	0
2	CA	A	602	1/1	0.98	0.13	-0.75	35,35,35,35	0
4	MAN	B	802	11/12	0.88	0.18	-0.82	67,71,81,83	0
2	CA	A	607	1/1	0.89	0.10	-0.91	72,72,72,72	0
2	CA	B	605	1/1	0.93	0.14	-0.96	38,38,38,38	0
2	CA	A	611	1/1	0.97	0.09	-1.36	81,81,81,81	0
2	CA	B	602	1/1	0.92	0.12	-1.61	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	603	1/1	0.94	0.11	-1.73	39,39,39,39	0
2	CA	B	609	1/1	0.80	0.12	-1.75	105,105,105,105	0
2	CA	A	606	1/1	0.94	0.09	-1.85	35,35,35,35	0
2	CA	B	606	1/1	0.93	0.07	-1.86	55,55,55,55	0
2	CA	A	608	1/1	0.84	0.10	-1.88	58,58,58,58	0
2	CA	A	609	1/1	0.96	0.04	-1.96	87,87,87,87	0
2	CA	B	603	1/1	0.98	0.09	-2.10	38,38,38,38	0
2	CA	B	607	1/1	0.85	0.07	-3.38	87,87,87,87	0
4	MAN	A	801	11/12	0.94	0.20	-	44,48,59,71	0
2	CA	B	604	1/1	0.97	0.12	-	37,37,37,37	0
4	MAN	B	806	11/12	0.79	0.28	-	99,109,124,129	0
4	MAN	B	808	11/12	0.87	0.21	-	114,123,126,127	0
4	MAN	A	806	11/12	0.80	0.32	-	73,88,105,107	0
4	MAN	B	803	11/12	0.90	0.31	-	72,93,114,121	0
2	CA	B	610	1/1	0.81	0.09	-	93,93,93,93	0
2	CA	B	611	1/1	0.81	0.17	-	104,104,104,104	0
3	MN	A	901	1/1	0.99	0.27	-	59,59,59,59	0
2	CA	B	608	1/1	0.93	0.10	-	81,81,81,81	0
2	CA	B	612	1/1	0.82	0.09	-	89,89,89,89	0

## 6.5 Other polymers

There are no such residues in this entry.