



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:05 am BST

PDB ID : 3NCZ  
Title : X-Ray Co-structure of Rho-Associated Protein Kinase (ROCK1) with a potent 2H-isoquinolin-1-one inhibitor  
Authors : Li, X.  
Deposited on : 2010-06-06  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

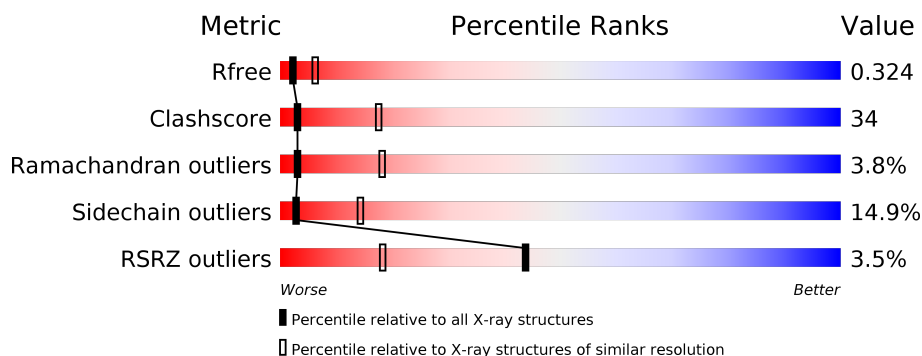
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	415	
1	B	415	
1	C	415	
1	D	415	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12831 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.

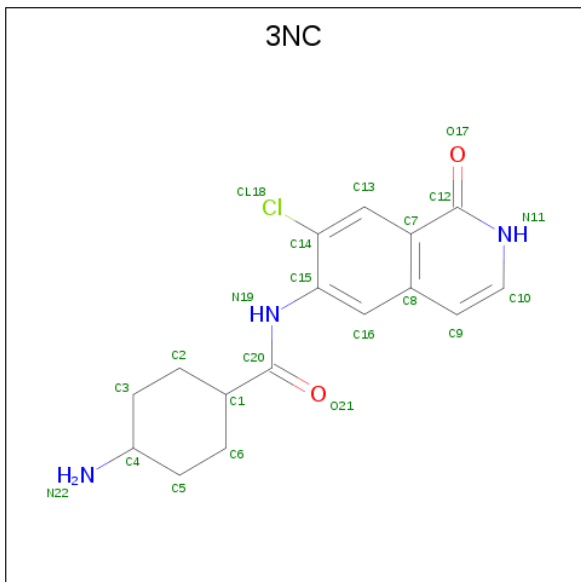
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3221	2057	532	610	22			
1	B	379	Total	C	N	O	S	0	0	0
			3076	1967	510	577	22			
1	C	389	Total	C	N	O	S	0	0	0
			3177	2033	528	594	22			
1	D	397	Total	C	N	O	S	0	0	0
			3206	2047	532	606	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q13464
A	2	SER	-	EXPRESSION TAG	UNP Q13464
A	3	LEU	-	EXPRESSION TAG	UNP Q13464
A	4	HIS	-	EXPRESSION TAG	UNP Q13464
A	5	MET	-	EXPRESSION TAG	UNP Q13464
B	1	GLY	-	EXPRESSION TAG	UNP Q13464
B	2	SER	-	EXPRESSION TAG	UNP Q13464
B	3	LEU	-	EXPRESSION TAG	UNP Q13464
B	4	HIS	-	EXPRESSION TAG	UNP Q13464
B	5	MET	-	EXPRESSION TAG	UNP Q13464
C	1	GLY	-	EXPRESSION TAG	UNP Q13464
C	2	SER	-	EXPRESSION TAG	UNP Q13464
C	3	LEU	-	EXPRESSION TAG	UNP Q13464
C	4	HIS	-	EXPRESSION TAG	UNP Q13464
C	5	MET	-	EXPRESSION TAG	UNP Q13464
D	1	GLY	-	EXPRESSION TAG	UNP Q13464
D	2	SER	-	EXPRESSION TAG	UNP Q13464
D	3	LEU	-	EXPRESSION TAG	UNP Q13464
D	4	HIS	-	EXPRESSION TAG	UNP Q13464
D	5	MET	-	EXPRESSION TAG	UNP Q13464

- Molecule 2 is cis-4-amino-N-(7-chloro-1-oxo-1,2-dihydroisoquinolin-6-yl)cyclohexanecarboxamide (three-letter code: 3NC) (formula: C<sub>16</sub>H<sub>18</sub>ClN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
2	B	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		
2	D	1	Total	C	Cl	N	O	0	0
			22	16	1	3	2		

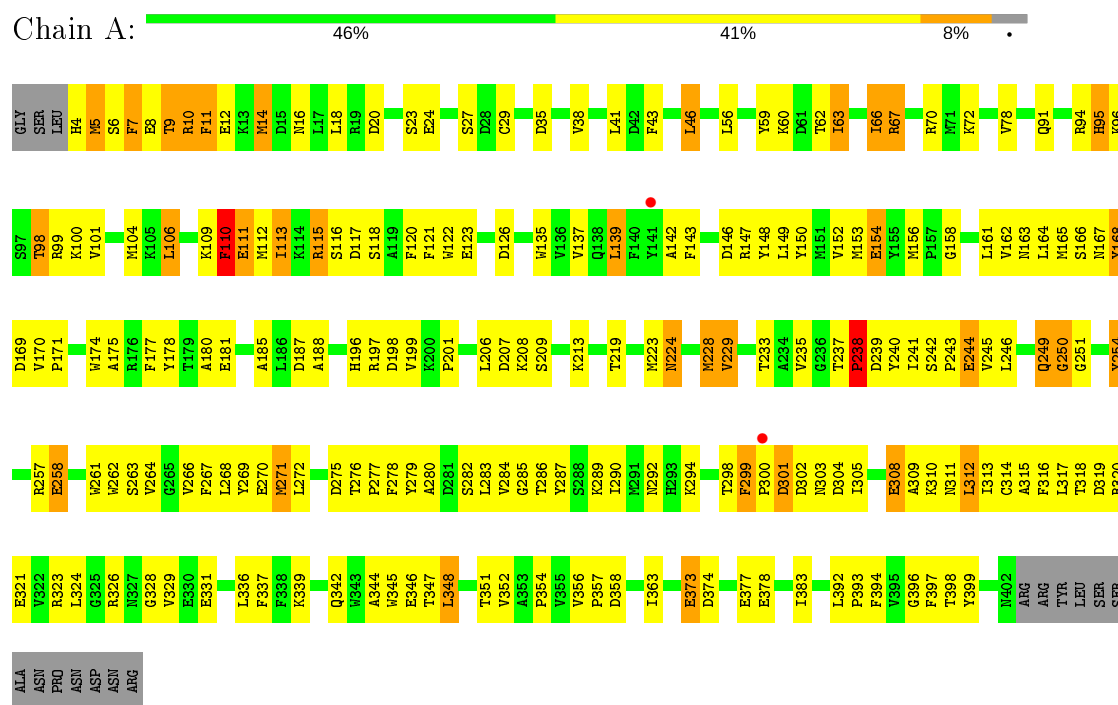
- Molecule 3 is water.

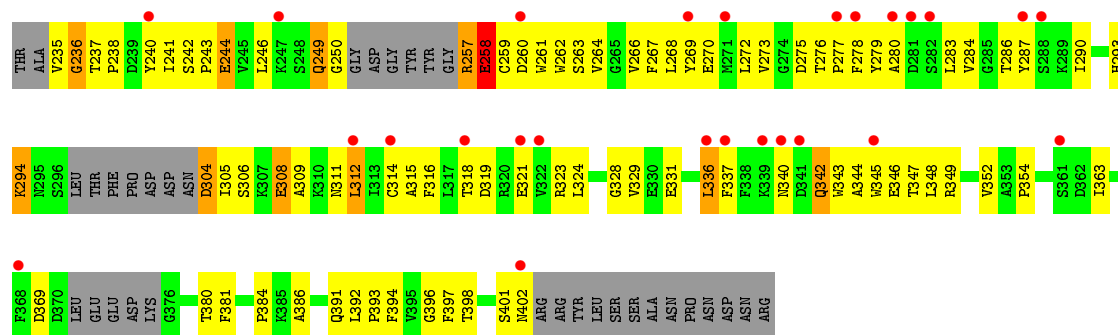
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	13	Total	O	0	0
			13	13		
3	C	15	Total	O	0	0
			15	15		
3	D	15	Total	O	0	0
			15	15		

### 3 Residue-property plots

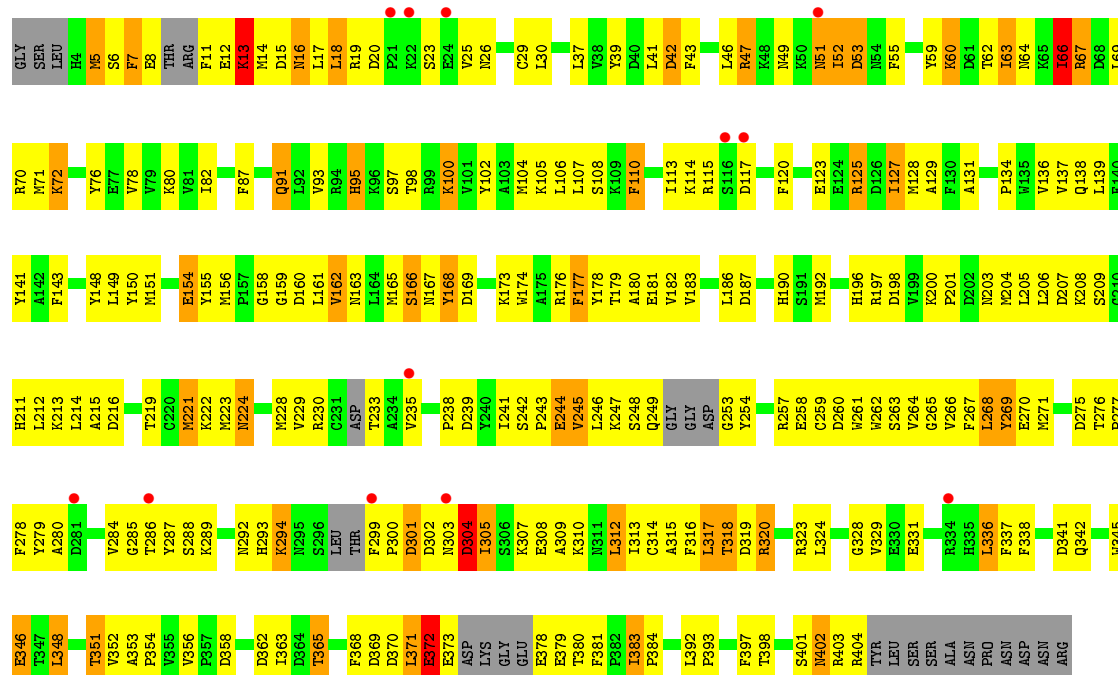
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Rho-associated protein kinase 1

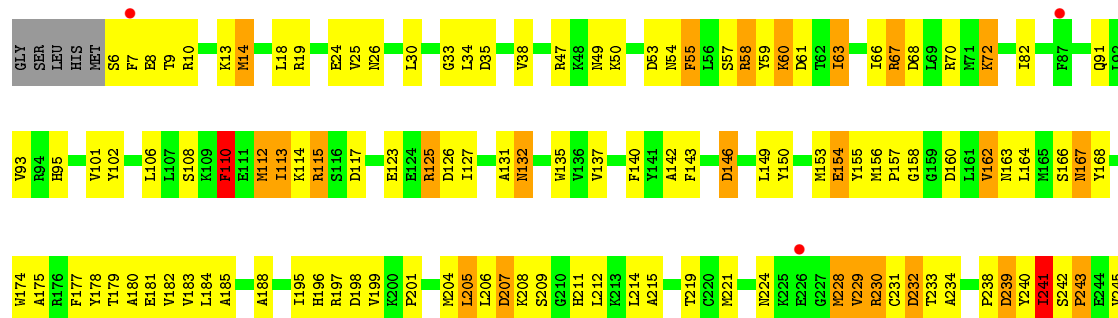
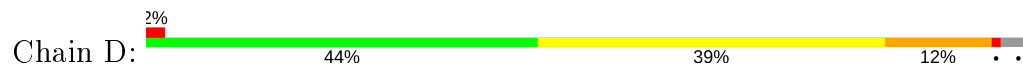


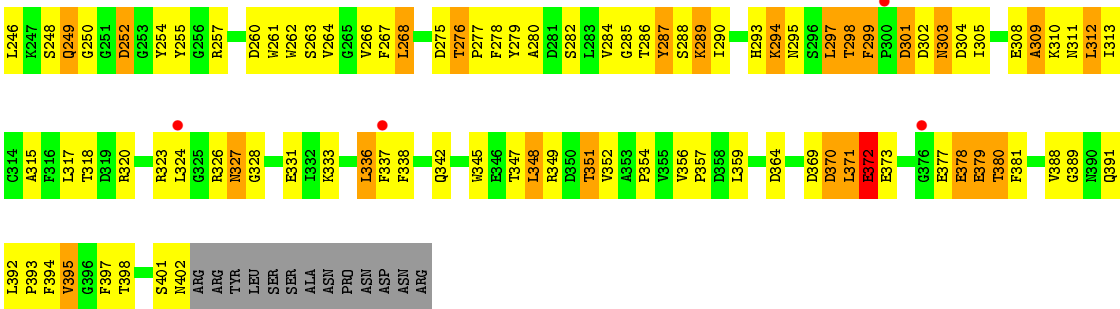


• Molecule 1: Rho-associated protein kinase 1



• Molecule 1: Rho-associated protein kinase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.44 Å   80.86 Å   166.62 Å 90.00°   117.22°   90.00°	Depositor
Resolution (Å)	44.12 – 3.00 44.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.12-3.00) 99.9 (44.12-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357), CNX	Depositor
R, $R_{free}$	0.255   ,   0.328 0.250   ,   0.324	Depositor DCC
$R_{free}$ test set	1926 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 104.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3NC

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	0.48	0/3299	0.63	0/4461
1	B	0.36	0/3146	0.57	0/4245
1	C	0.48	0/3250	0.65	0/4383
1	D	0.46	0/3283	0.64	0/4438
All	All	0.45	0/12978	0.62	0/17527

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3221	0	3091	202	0
1	B	3076	0	2973	194	1
1	C	3177	0	3073	266	1
1	D	3206	0	3084	215	0
2	A	22	0	18	1	0
2	B	22	0	18	5	0
2	C	22	0	18	5	0
2	D	22	0	18	1	0
3	A	20	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	3	0
3	C	15	0	0	8	0
3	D	15	0	0	2	0
All	All	12831	0	12293	849	1

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 34.

All (849) 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:C:14:MET:SD	1:C:18:LEU:HD13	1.94	1.06
1:C:30:LEU:HD13	1:D:30:LEU:HB2	1.38	1.05
1:B:19:ARG:O	1:B:21:PRO:HD3	1.60	1.00
1:D:276:THR:HG22	1:D:278:PHE:H	1.23	0.98
1:A:278:PHE:O	1:A:286:THR:HG22	1.67	0.95
1:C:221:MET:HG2	1:C:229:VAL:HG21	1.45	0.95
1:B:257:ARG:N	1:B:259:CYS:HG	1.67	0.92
1:B:111:GLU:HB3	1:B:115:ARG:NH1	1.85	0.91
1:C:244:GLU:HG2	1:C:320:ARG:HB2	1.52	0.90
1:C:223:MET:HA	3:C:427:HOH:O	1.72	0.90
1:C:230:ARG:HB2	1:C:254:TYR:CD1	2.07	0.88
1:D:377:GLU:O	1:D:378:GLU:HG2	1.74	0.87
1:B:258:GLU:HA	1:B:261:TRP:CD1	2.08	0.87
1:D:50:LYS:HE3	1:D:54:ASN:HD21	1.39	0.86
1:C:276:THR:HG22	1:C:278:PHE:H	1.40	0.85
1:B:147:ARG:HD3	3:B:417:HOH:O	1.74	0.85
1:C:72:LYS:HE2	1:D:10:ARG:NH2	1.93	0.84
1:A:162:VAL:HG23	1:A:201:PRO:HB2	1.59	0.84
1:A:14:MET:HE3	1:B:70:ARG:HG3	1.59	0.84
1:B:13:LYS:O	1:B:16:ASN:HB2	1.78	0.83
1:D:240:TYR:HA	1:D:266:VAL:HG11	1.60	0.83
1:A:269:TYR:CE1	1:A:277:PRO:HA	2.15	0.82
1:D:35:ASP:OD1	1:D:67:ARG:NH1	2.13	0.82
1:A:239:ASP:HB3	3:A:416:HOH:O	1.79	0.81
1:B:258:GLU:HA	1:B:261:TRP:HD1	1.45	0.81
1:C:52:ILE:HG22	1:C:53:ASP:N	1.95	0.81
1:A:62:THR:HG21	1:B:25:VAL:HG13	1.63	0.80
1:B:29:CYS:SG	1:B:396:GLY:HA2	2.23	0.79
1:C:294:LYS:HB2	3:C:418:HOH:O	1.82	0.79
1:A:258:GLU:HA	1:A:261:TRP:CD1	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ALA:HB2	1:C:139:LEU:HD23	1.65	0.78
1:C:43:PHE:CD2	1:C:384:PRO:HD2	2.19	0.78
1:C:158:GLY:HA3	1:C:206:LEU:HB2	1.64	0.78
1:C:372:GLU:CB	1:C:373:GLU:HA	2.12	0.78
1:C:262:TRP:HB2	1:C:323:ARG:NH1	1.98	0.77
1:A:308:GLU:HB3	1:A:337:PHE:HB2	1.65	0.77
1:D:123:GLU:O	1:D:127:ILE:HG13	1.83	0.77
1:A:171:PRO:HD2	1:A:174:TRP:HB2	1.67	0.77
1:A:276:THR:HG22	1:A:278:PHE:H	1.51	0.76
1:C:336:LEU:H	1:C:336:LEU:HD22	1.51	0.76
1:B:14:MET:O	1:B:18:LEU:HD23	1.85	0.76
1:C:248:SER:HA	1:C:249:GLN:C	2.05	0.76
1:C:301:ASP:N	1:C:302:ASP:HA	2.00	0.76
1:A:258:GLU:HA	1:A:261:TRP:HD1	1.52	0.75
1:C:25:VAL:HG23	1:C:25:VAL:O	1.86	0.75
1:D:140:PHE:O	1:D:401:SER:HB2	1.87	0.75
1:D:278:PHE:O	1:D:286:THR:HG22	1.87	0.75
1:D:359:LEU:HD22	1:D:364:ASP:HB3	1.67	0.75
1:C:162:VAL:HG12	1:C:163:ASN:N	2.02	0.74
1:C:14:MET:SD	1:C:18:LEU:CD1	2.73	0.74
1:C:299:PHE:HB3	1:C:300:PRO:HD2	1.69	0.74
1:D:211:HIS:HB3	1:D:349:ARG:NH1	2.03	0.74
1:C:47:ARG:HG2	1:C:47:ARG:HH11	1.51	0.73
1:B:167:ASN:C	1:B:168:TYR:HD1	1.91	0.73
1:B:269:TYR:CE1	1:B:273:VAL:HG21	2.24	0.73
1:C:372:GLU:HB3	1:C:373:GLU:HA	1.70	0.73
1:A:106:LEU:HD23	1:A:106:LEU:N	2.04	0.73
1:B:276:THR:HB	1:B:279:TYR:HB2	1.70	0.73
1:C:72:LYS:HE2	1:D:10:ARG:HH22	1.51	0.73
1:D:231:CYS:HB3	1:D:255:TYR:HE1	1.54	0.73
1:A:163:ASN:O	1:A:166:SER:HB3	1.89	0.73
1:C:49:ASN:HB3	1:C:52:ILE:HB	1.69	0.73
1:C:300:PRO:HB2	1:C:303:ASN:H	1.52	0.73
1:D:113:ILE:HG21	1:D:381:PHE:HE1	1.53	0.72
1:C:372:GLU:HB3	1:C:373:GLU:CA	2.20	0.72
1:D:276:THR:HG22	1:D:278:PHE:N	2.02	0.72
1:A:175:ALA:HB2	1:A:272:LEU:HD21	1.72	0.72
1:B:124:GLU:HG3	1:B:217:PHE:HB2	1.72	0.72
1:D:234:ALA:HB2	1:D:245:VAL:O	1.90	0.72
1:A:224:ASN:HD21	1:A:228:MET:H	1.38	0.71
1:A:98:THR:HB	1:A:100:LYS:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HG13	2:C:900:3NC:CL18	2.28	0.71
1:C:51:ASN:HB3	1:D:393:PRO:HD3	1.72	0.71
1:B:304:ASP:HB2	1:B:305:ILE:HD12	1.73	0.71
1:C:154:GLU:OE2	1:C:213:LYS:HE3	1.90	0.71
1:C:267:PHE:O	1:C:270:GLU:HB3	1.90	0.70
1:A:165:MET:SD	1:A:271:MET:HG3	2.32	0.70
1:B:124:GLU:HG2	1:B:128:MET:CE	2.22	0.70
1:C:303:ASN:O	1:C:304:ASP:HB2	1.90	0.70
1:B:66:ILE:HG22	1:B:67:ARG:N	2.05	0.70
1:A:10:ARG:HD2	1:B:69:LEU:HA	1.72	0.69
1:D:234:ALA:H	1:D:249:GLN:HE22	1.40	0.69
1:A:264:VAL:O	1:A:267:PHE:HB3	1.93	0.69
1:B:269:TYR:CZ	1:B:273:VAL:HG21	2.28	0.69
1:C:11:PHE:HD2	1:C:12:GLU:N	1.91	0.69
1:A:14:MET:CE	1:B:70:ARG:HG3	2.22	0.69
1:D:198:ASP:HB2	1:D:219:THR:HG21	1.74	0.69
1:B:168:TYR:HD2	1:B:174:TRP:CZ3	2.12	0.68
1:B:179:THR:O	1:B:183:VAL:HG23	1.93	0.68
1:C:179:THR:O	1:C:183:VAL:HG23	1.93	0.68
1:C:131:ALA:HA	1:C:192:MET:CE	2.24	0.68
1:C:198:ASP:HB2	1:C:219:THR:HG21	1.75	0.68
1:C:51:ASN:HB2	1:D:389:GLY:O	1.94	0.68
1:B:105:LYS:HE2	1:B:151:MET:CE	2.23	0.68
1:C:69:LEU:HD12	1:D:14:MET:HG2	1.75	0.68
1:A:276:THR:HG23	3:A:416:HOH:O	1.93	0.68
1:C:154:GLU:OE2	1:C:156:MET:HE1	1.94	0.67
1:C:149:LEU:HD22	1:C:397:PHE:CD1	2.29	0.67
1:D:280:ALA:HB3	1:D:286:THR:HG23	1.76	0.67
1:A:4:HIS:N	1:A:6:SER:HA	2.09	0.67
1:C:72:LYS:CE	1:D:10:ARG:HH22	2.07	0.67
1:D:18:LEU:HD12	1:D:18:LEU:H	1.59	0.67
1:D:276:THR:CG2	1:D:278:PHE:H	2.04	0.67
1:D:313:ILE:HG22	1:D:317:LEU:HD22	1.77	0.67
1:A:224:ASN:ND2	1:A:228:MET:H	1.92	0.67
1:B:124:GLU:HG2	1:B:128:MET:HE2	1.76	0.67
1:D:178:TYR:O	1:D:182:VAL:HG23	1.93	0.67
1:B:294:LYS:NZ	1:B:294:LYS:HB2	2.09	0.66
1:D:312:LEU:HD12	1:D:337:PHE:CD1	2.30	0.66
1:B:19:ARG:O	1:B:21:PRO:CD	2.40	0.66
1:C:204:MET:C	1:C:205:LEU:HD23	2.16	0.66
1:D:293:HIS:N	3:D:419:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:HA	1:A:12:GLU:HG3	1.78	0.66
1:A:228:MET:HG2	1:A:254:TYR:CE1	2.31	0.66
1:A:41:LEU:HB3	1:A:56:LEU:HD11	1.78	0.66
1:A:266:VAL:HG13	1:A:277:PRO:CG	2.26	0.66
1:A:286:THR:O	1:A:290:ILE:HG13	1.96	0.66
1:C:125:ARG:NH1	1:C:397:PHE:O	2.29	0.66
1:B:240:TYR:HA	1:B:266:VAL:HG11	1.77	0.66
1:C:110:PHE:HE1	1:C:114:LYS:HB2	1.60	0.66
1:D:261:TRP:O	1:D:264:VAL:HB	1.96	0.66
1:C:269:TYR:HE1	1:C:275:ASP:O	1.77	0.66
1:C:123:GLU:O	1:C:127:ILE:HG13	1.96	0.65
1:B:158:GLY:HA3	1:B:206:LEU:HB2	1.77	0.65
1:B:340:ASN:ND2	1:B:342:GLN:HG2	2.12	0.65
1:A:158:GLY:HA3	1:A:206:LEU:HB2	1.78	0.65
1:C:106:LEU:HD22	1:C:150:TYR:CD1	2.32	0.65
1:A:8:GLU:O	1:A:12:GLU:HG2	1.96	0.65
1:B:195:ILE:HG23	1:B:260:ASP:OD1	1.96	0.65
1:C:156:MET:SD	3:C:419:HOH:O	2.55	0.65
1:C:47:ARG:HG2	1:C:47:ARG:NH1	2.11	0.65
1:C:62:THR:HG21	1:D:25:VAL:HG13	1.79	0.65
1:D:268:LEU:HD13	1:D:313:ILE:HG12	1.79	0.64
1:C:143:PHE:CE2	1:C:150:TYR:CD2	2.86	0.64
1:C:131:ALA:HA	1:C:192:MET:HE3	1.79	0.64
1:C:7:PHE:O	1:C:8:GLU:HG3	1.97	0.64
1:D:262:TRP:CZ3	1:D:317:LEU:HA	2.32	0.64
1:A:276:THR:CG2	3:A:416:HOH:O	2.45	0.64
1:D:327:ASN:HB2	1:D:331:GLU:OE2	1.98	0.64
1:D:195:ILE:HD13	1:D:257:ARG:HA	1.80	0.64
1:B:47:ARG:O	1:B:53:ASP:HB2	1.97	0.64
1:C:279:TYR:CD1	1:C:280:ALA:N	2.66	0.64
1:D:241:ILE:CD1	1:D:242:SER:H	2.11	0.64
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.80	0.64
1:B:336:LEU:HD22	1:B:336:LEU:H	1.63	0.64
1:C:244:GLU:HB3	1:C:320:ARG:CZ	2.28	0.63
1:C:242:SER:OG	1:C:245:VAL:HB	1.98	0.63
1:B:111:GLU:HB3	1:B:115:ARG:HH11	1.60	0.63
1:B:35:ASP:OD1	1:B:67:ARG:NH1	2.32	0.63
1:D:261:TRP:HE3	1:D:264:VAL:HG21	1.64	0.63
1:A:287:TYR:O	1:A:290:ILE:HB	1.97	0.62
1:D:163:ASN:O	1:D:166:SER:HB3	1.98	0.62
1:B:261:TRP:O	1:B:264:VAL:HB	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ARG:HB2	1:C:254:TYR:HD1	1.60	0.62
1:C:108:SER:HA	1:C:148:TYR:HD2	1.63	0.62
1:C:167:ASN:C	1:C:168:TYR:HD1	2.03	0.62
1:D:110:PHE:C	1:D:110:PHE:HD1	2.03	0.62
1:A:373:GLU:HG2	1:A:374:ASP:H	1.64	0.62
1:B:244:GLU:OE1	1:B:258:GLU:HG2	2.00	0.62
1:D:234:ALA:HB1	1:D:245:VAL:HG12	1.82	0.62
1:D:58:ARG:HG2	1:D:59:TYR:CD1	2.35	0.62
1:A:175:ALA:CB	1:A:272:LEU:HD21	2.29	0.61
1:B:66:ILE:O	1:B:67:ARG:C	2.35	0.61
1:D:177:PHE:CZ	1:D:354:PRO:HD3	2.35	0.61
1:C:55:PHE:HB2	1:D:392:LEU:HB3	1.82	0.61
1:D:110:PHE:C	1:D:110:PHE:CD1	2.72	0.61
1:D:228:MET:O	1:D:229:VAL:HB	1.99	0.61
1:B:135:TRP:HH2	1:B:181:GLU:HG2	1.64	0.61
1:C:108:SER:HA	1:C:148:TYR:CD2	2.36	0.61
1:D:113:ILE:HG22	1:D:114:LYS:N	2.15	0.61
1:D:263:SER:O	1:D:266:VAL:HB	2.01	0.61
1:B:229:VAL:HG13	1:B:231:CYS:SG	2.41	0.61
1:B:246:LEU:HD21	1:B:287:TYR:CE1	2.35	0.61
1:C:110:PHE:CE1	1:C:114:LYS:HB2	2.35	0.61
1:C:39:TYR:CE1	1:C:67:ARG:NH2	2.69	0.61
1:D:146:ASP:OD2	1:D:146:ASP:N	2.33	0.61
1:C:51:ASN:CB	1:D:389:GLY:O	2.49	0.60
1:A:66:ILE:HG23	1:A:70:ARG:HD2	1.83	0.60
1:D:162:VAL:HG23	1:D:201:PRO:HB2	1.83	0.60
1:A:4:HIS:CA	1:A:6:SER:HA	2.31	0.60
1:C:187:ASP:OD1	1:C:329:VAL:HG21	2.00	0.60
1:B:110:PHE:HA	1:B:381:PHE:CZ	2.37	0.60
1:C:362:ASP:OD2	1:C:363:ILE:HG23	2.02	0.60
1:C:371:LEU:HD23	1:C:371:LEU:N	2.16	0.60
1:C:305:ILE:HD11	1:C:310:LYS:CB	2.31	0.60
1:D:336:LEU:N	1:D:336:LEU:HD13	2.16	0.60
1:D:149:LEU:HB3	1:D:397:PHE:CE1	2.36	0.60
1:A:181:GLU:HG2	1:A:348:LEU:HD13	1.84	0.60
1:D:68:ASP:O	1:D:72:LYS:HE2	2.02	0.60
1:A:62:THR:CG2	1:B:25:VAL:HG13	2.30	0.60
1:A:156:MET:CE	1:A:213:LYS:HD2	2.32	0.59
1:C:11:PHE:CD2	1:C:12:GLU:N	2.70	0.59
1:D:66:ILE:HG22	1:D:67:ARG:N	2.16	0.59
1:A:98:THR:HG22	1:A:100:LYS:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:HIS:HD2	1:B:220:CYS:SG	2.25	0.59
1:D:305:ILE:HG21	1:D:310:LYS:HG3	1.83	0.59
1:B:328:GLY:O	1:B:331:GLU:HB3	2.02	0.59
1:C:26:ASN:ND2	3:C:424:HOH:O	2.29	0.59
1:C:107:LEU:HB2	1:C:149:LEU:HB2	1.85	0.59
1:A:284:VAL:O	1:A:287:TYR:HB3	2.03	0.59
1:C:372:GLU:HB3	1:C:373:GLU:HG2	1.84	0.59
1:D:239:ASP:HB3	1:D:276:THR:OG1	2.02	0.59
1:C:262:TRP:CZ3	1:C:317:LEU:HA	2.37	0.59
1:C:5:MET:N	1:C:5:MET:SD	2.76	0.59
1:A:243:PRO:O	1:A:246:LEU:HB3	2.02	0.59
1:C:70:ARG:NH2	1:C:398:THR:HG21	2.17	0.59
1:B:204:MET:O	1:B:205:LEU:HD23	2.03	0.58
1:B:106:LEU:O	1:B:107:LEU:HD23	2.02	0.58
1:C:11:PHE:O	1:C:15:ASP:HB2	2.04	0.58
1:C:167:ASN:C	1:C:168:TYR:CD1	2.77	0.58
1:D:160:ASP:OD1	1:D:162:VAL:HB	2.03	0.58
1:D:58:ARG:HG3	1:D:58:ARG:O	1.97	0.58
1:A:224:ASN:ND2	1:A:224:ASN:C	2.57	0.58
1:A:356:VAL:HG13	1:A:357:PRO:HD2	1.86	0.58
1:B:340:ASN:HD22	1:B:342:GLN:HG2	1.68	0.58
1:D:115:ARG:C	1:D:117:ASP:H	2.07	0.58
1:C:392:LEU:HD13	1:D:55:PHE:CD1	2.39	0.58
1:C:139:LEU:HD11	1:C:141:TYR:O	2.03	0.58
1:C:315:ALA:HB1	1:C:324:LEU:HB2	1.86	0.58
1:D:167:ASN:C	1:D:168:TYR:HD1	2.07	0.58
1:D:241:ILE:HD12	1:D:242:SER:H	1.69	0.58
1:D:34:LEU:O	1:D:38:VAL:HG23	2.04	0.58
1:A:11:PHE:HA	1:A:14:MET:HB2	1.86	0.57
1:D:260:ASP:O	1:D:264:VAL:HG23	2.04	0.57
1:D:336:LEU:HD22	1:D:336:LEU:H	1.69	0.57
1:A:137:VAL:HG11	2:A:900:3NC:H10	1.86	0.57
1:C:299:PHE:HB3	1:C:300:PRO:CD	2.34	0.57
1:A:337:PHE:CD1	1:A:337:PHE:O	2.58	0.57
1:B:199:VAL:HB	1:B:263:SER:CB	2.34	0.57
1:D:168:TYR:HD2	1:D:174:TRP:HZ3	1.52	0.57
1:B:204:MET:C	1:B:205:LEU:HD23	2.24	0.57
1:A:249:GLN:O	1:A:251:GLY:N	2.37	0.57
1:D:143:PHE:CE2	1:D:150:TYR:CD2	2.93	0.57
1:D:303:ASN:ND2	1:D:303:ASN:H	2.01	0.57
1:B:260:ASP:O	1:B:264:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TRP:CE3	1:B:323:ARG:NH2	2.73	0.57
1:B:66:ILE:HG23	1:B:70:ARG:HD2	1.86	0.57
1:C:66:ILE:HG13	1:D:14:MET:HE1	1.85	0.57
1:D:47:ARG:O	1:D:53:ASP:HB2	2.05	0.57
1:C:371:LEU:CD2	1:C:371:LEU:N	2.68	0.57
1:D:34:LEU:HD21	1:D:59:TYR:CD2	2.40	0.57
1:B:140:PHE:O	1:B:401:SER:HB2	2.04	0.56
1:B:279:TYR:CD1	1:B:280:ALA:N	2.73	0.56
1:C:98:THR:HG22	1:C:100:LYS:HG2	1.87	0.56
1:C:110:PHE:HD1	1:C:110:PHE:C	2.09	0.56
1:C:204:MET:O	1:C:205:LEU:HD23	2.05	0.56
1:D:174:TRP:N	1:D:174:TRP:CD1	2.70	0.56
1:B:46:LEU:HD21	1:B:386:ALA:HA	1.87	0.56
1:C:110:PHE:CD1	1:C:110:PHE:C	2.79	0.56
1:C:154:GLU:HG2	1:C:156:MET:HE3	1.86	0.56
1:C:269:TYR:CD1	1:C:269:TYR:C	2.77	0.56
1:C:353:ALA:HB3	1:C:356:VAL:HG22	1.86	0.56
1:A:268:LEU:HD23	1:A:268:LEU:O	2.05	0.56
1:B:135:TRP:CH2	1:B:181:GLU:HG2	2.40	0.56
1:B:47:ARG:NH1	1:B:53:ASP:OD1	2.38	0.56
1:C:160:ASP:OD1	1:C:162:VAL:HB	2.06	0.56
1:A:18:LEU:HD12	1:A:18:LEU:N	2.20	0.56
1:A:239:ASP:C	3:A:416:HOH:O	2.44	0.56
1:C:47:ARG:HA	1:C:52:ILE:HG21	1.88	0.56
1:D:9:THR:O	1:D:13:LYS:HB2	2.05	0.56
1:C:37:LEU:HD23	1:C:55:PHE:CZ	2.40	0.56
1:D:279:TYR:CD1	1:D:280:ALA:N	2.73	0.56
1:D:370:ASP:O	1:D:371:LEU:HD13	2.05	0.56
1:A:305:ILE:HD12	1:A:305:ILE:N	2.20	0.56
1:A:269:TYR:HD1	1:A:277:PRO:HD3	1.70	0.56
1:C:316:PHE:CE2	1:C:324:LEU:HD23	2.40	0.56
1:D:199:VAL:HB	1:D:263:SER:HB2	1.86	0.56
1:D:49:ASN:OD1	1:D:49:ASN:C	2.45	0.56
1:B:308:GLU:HB3	1:B:337:PHE:HB2	1.87	0.56
1:C:269:TYR:CZ	1:C:277:PRO:HA	2.40	0.56
1:D:195:ILE:CD1	1:D:257:ARG:HA	2.35	0.56
1:C:177:PHE:CZ	1:C:354:PRO:HD3	2.41	0.55
1:A:373:GLU:CG	1:A:374:ASP:H	2.19	0.55
1:A:373:GLU:HG2	1:A:374:ASP:N	2.21	0.55
1:A:43:PHE:HB2	1:A:46:LEU:HG	1.88	0.55
1:C:275:ASP:OD1	1:C:279:TYR:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:VAL:HB	1:D:263:SER:CB	2.36	0.55
1:A:10:ARG:NH2	1:B:75:ASP:OD1	2.38	0.55
1:A:177:PHE:CE2	1:A:354:PRO:HD3	2.42	0.55
1:A:177:PHE:CE1	1:A:348:LEU:HD21	2.41	0.55
1:C:156:MET:HA	1:C:156:MET:HE2	1.88	0.55
1:D:63:ILE:HG23	1:D:67:ARG:NH1	2.21	0.55
1:A:224:ASN:HD22	1:A:224:ASN:C	2.09	0.55
1:B:276:THR:HG22	1:B:278:PHE:H	1.71	0.55
1:C:280:ALA:N	1:C:286:THR:HG22	2.20	0.55
1:C:42:ASP:O	1:C:43:PHE:CD1	2.59	0.55
1:A:328:GLY:O	1:A:331:GLU:HB3	2.07	0.55
1:B:201:PRO:HG3	1:B:267:PHE:CD1	2.41	0.55
1:C:178:TYR:O	1:C:182:VAL:HG23	2.07	0.55
1:D:33:GLY:HA2	1:D:395:VAL:HG21	1.89	0.55
1:B:135:TRP:HZ3	1:B:181:GLU:OE1	1.90	0.55
1:D:156:MET:HA	1:D:156:MET:CE	2.37	0.55
1:D:212:LEU:C	1:D:212:LEU:HD23	2.27	0.55
1:B:258:GLU:N	1:B:258:GLU:CD	2.61	0.54
1:D:14:MET:O	1:D:18:LEU:HD12	2.07	0.54
1:B:20:ASP:O	1:B:23:SER:HB3	2.07	0.54
1:B:278:PHE:O	1:B:286:THR:HG22	2.07	0.54
1:D:181:GLU:OE1	1:D:212:LEU:HB3	2.07	0.54
1:C:284:VAL:O	1:C:287:TYR:HB3	2.08	0.54
1:C:95:HIS:CE1	1:C:97:SER:OG	2.61	0.54
1:D:248:SER:HA	1:D:252:ASP:HB2	1.89	0.54
1:A:6:SER:O	1:A:9:THR:HG23	2.07	0.54
1:C:229:VAL:HB	3:C:427:HOH:O	2.07	0.54
1:B:199:VAL:HB	1:B:263:SER:HB2	1.89	0.54
1:D:392:LEU:N	1:D:393:PRO:CD	2.71	0.54
1:A:187:ASP:OD1	1:A:329:VAL:HG21	2.07	0.54
1:B:95:HIS:CD2	1:B:98:THR:OG1	2.60	0.54
1:C:25:VAL:CG2	1:C:25:VAL:O	2.56	0.54
1:C:268:LEU:HD12	1:C:312:LEU:HD13	1.89	0.54
1:A:147:ARG:C	1:A:148:TYR:HD2	2.11	0.54
1:A:168:TYR:CD2	1:A:174:TRP:HZ3	2.25	0.54
1:A:198:ASP:CB	1:A:219:THR:HG21	2.37	0.54
1:B:305:ILE:N	1:B:305:ILE:HD12	2.23	0.54
1:C:308:GLU:HB2	1:C:337:PHE:HD2	1.72	0.54
1:C:7:PHE:HB3	1:C:8:GLU:OE1	2.07	0.54
1:D:177:PHE:CE1	1:D:354:PRO:HD3	2.43	0.54
1:A:106:LEU:CD2	1:A:106:LEU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:VAL:HG23	1:D:285:GLY:N	2.23	0.53
1:C:269:TYR:CE1	1:C:275:ASP:O	2.61	0.53
1:A:38:VAL:HG21	1:A:63:ILE:HG13	1.89	0.53
1:B:129:ALA:O	1:B:130:PHE:CD2	2.61	0.53
1:C:115:ARG:C	1:C:117:ASP:H	2.11	0.53
1:A:143:PHE:HE1	1:A:152:VAL:CG2	2.21	0.53
1:B:168:TYR:HD2	1:B:174:TRP:CH2	2.26	0.53
1:C:60:LYS:C	1:C:60:LYS:HD3	2.29	0.53
1:A:9:THR:HA	1:A:12:GLU:CG	2.38	0.53
1:B:293:HIS:HE2	1:B:319:ASP:CG	2.12	0.53
1:B:343:TRP:HE3	1:B:344:ALA:C	2.10	0.53
1:A:223:MET:HA	1:A:229:VAL:HG12	1.89	0.53
1:A:110:PHE:CD1	1:A:110:PHE:C	2.80	0.53
1:B:115:ARG:C	1:B:117:ASP:H	2.11	0.53
1:B:314:CYS:O	1:B:318:THR:HG23	2.09	0.53
1:C:380:THR:HA	3:C:417:HOH:O	2.09	0.53
1:D:207:ASP:O	1:D:209:SER:N	2.42	0.53
1:D:239:ASP:HB3	1:D:276:THR:HG21	1.90	0.53
1:A:180:ALA:HB1	1:A:345:TRP:CZ3	2.44	0.52
1:B:284:VAL:O	1:B:287:TYR:HB3	2.09	0.52
1:C:156:MET:SD	1:C:213:LYS:HD2	2.49	0.52
1:B:41:LEU:HD13	1:B:52:ILE:HG23	1.91	0.52
1:D:352:VAL:O	1:D:352:VAL:HG13	2.10	0.52
1:B:181:GLU:OE1	1:B:212:LEU:HB3	2.10	0.52
1:D:179:THR:O	1:D:183:VAL:HG23	2.09	0.52
1:D:38:VAL:HG21	1:D:63:ILE:HG13	1.90	0.52
1:B:174:TRP:CD1	1:B:354:PRO:HB3	2.45	0.52
1:A:149:LEU:HB3	1:A:397:PHE:CE1	2.43	0.52
1:A:269:TYR:CE1	1:A:277:PRO:CA	2.90	0.52
1:B:340:ASN:ND2	1:B:343:TRP:CD1	2.76	0.52
1:B:5:MET:HG3	1:B:10:ARG:HG3	1.91	0.52
1:A:317:LEU:N	1:A:317:LEU:HD12	2.25	0.52
1:A:198:ASP:HB2	1:A:219:THR:HG21	1.90	0.52
1:C:131:ALA:HA	1:C:192:MET:HE1	1.92	0.52
1:C:233:THR:HG23	1:C:235:VAL:HG23	1.92	0.52
1:D:180:ALA:HB2	1:D:338:PHE:HE2	1.73	0.52
1:B:86:ALA:HB3	1:B:87:PHE:CD2	2.44	0.52
1:C:244:GLU:CG	1:C:320:ARG:HB2	2.34	0.52
1:A:110:PHE:O	1:A:113:ILE:N	2.40	0.51
1:A:240:TYR:OH	1:A:270:GLU:OE1	2.08	0.51
1:B:146:ASP:N	1:B:146:ASP:OD2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:THR:OG1	1:C:323:ARG:HA	2.10	0.51
1:D:177:PHE:CZ	1:D:181:GLU:OE2	2.62	0.51
1:D:392:LEU:N	1:D:393:PRO:HD2	2.25	0.51
1:A:285:GLY:O	1:A:289:LYS:HB2	2.10	0.51
1:A:308:GLU:O	1:A:309:ALA:C	2.48	0.51
1:B:283:LEU:O	1:B:286:THR:OG1	2.23	0.51
1:B:318:THR:OG1	1:B:323:ARG:HA	2.11	0.51
1:D:207:ASP:OD2	1:D:207:ASP:N	2.41	0.51
1:D:298:THR:C	1:D:299:PHE:CG	2.82	0.51
1:A:5:MET:HA	1:A:6:SER:OG	2.10	0.51
1:B:178:TYR:O	1:B:182:VAL:HG23	2.10	0.51
1:B:241:ILE:HD12	1:B:242:SER:H	1.76	0.51
1:B:4:HIS:N	1:B:4:HIS:ND1	2.58	0.51
1:C:190:HIS:CG	1:C:257:ARG:HD3	2.45	0.51
1:D:268:LEU:HD13	1:D:313:ILE:CG1	2.41	0.51
1:D:125:ARG:NH1	1:D:397:PHE:O	2.44	0.51
1:D:328:GLY:O	1:D:331:GLU:HB3	2.11	0.51
1:B:112:MET:HE3	1:B:149:LEU:HD11	1.91	0.51
1:C:104:MET:HE2	1:C:106:LEU:HD21	1.92	0.51
1:C:105:LYS:C	1:C:106:LEU:HD23	2.31	0.51
1:C:137:VAL:HG23	1:C:214:LEU:O	2.11	0.51
1:C:7:PHE:C	1:C:8:GLU:OE1	2.48	0.51
1:A:344:ALA:HA	3:A:425:HOH:O	2.09	0.51
1:C:181:GLU:OE2	1:C:211:HIS:ND1	2.44	0.51
1:C:105:LYS:HE2	1:C:151:MET:CE	2.40	0.51
1:A:14:MET:HE1	1:B:69:LEU:HB2	1.91	0.51
1:A:315:ALA:HB1	1:A:324:LEU:HB2	1.92	0.51
1:A:392:LEU:N	1:A:393:PRO:HD2	2.26	0.51
1:B:216:ASP:CB	2:B:900:3NC:HN22	2.23	0.51
1:D:241:ILE:HD11	1:D:245:VAL:HB	1.92	0.51
1:D:264:VAL:O	1:D:267:PHE:HB3	2.11	0.51
1:D:184:LEU:HD21	1:D:345:TRP:HE3	1.76	0.51
1:B:87:PHE:CD2	1:B:87:PHE:N	2.78	0.51
1:C:166:SER:OG	1:C:167:ASN:ND2	2.42	0.51
1:B:343:TRP:HE3	1:B:344:ALA:O	1.95	0.50
1:C:300:PRO:HA	1:C:301:ASP:HB2	1.94	0.50
1:D:167:ASN:C	1:D:168:TYR:CD1	2.84	0.50
1:C:43:PHE:CE2	1:C:384:PRO:HD2	2.46	0.50
1:A:393:PRO:HG2	1:A:394:PHE:CE1	2.47	0.50
1:B:168:TYR:HD2	1:B:174:TRP:HZ3	1.58	0.50
1:C:221:MET:HG2	1:C:229:VAL:CG2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PHE:CE1	1:C:348:LEU:HD21	2.46	0.50
1:B:182:VAL:O	1:B:186:LEU:HG	2.12	0.50
1:C:66:ILE:O	1:C:67:ARG:C	2.50	0.50
1:D:230:ARG:NH1	1:D:230:ARG:HB2	2.26	0.50
1:D:276:THR:HG22	1:D:279:TYR:N	2.27	0.50
1:D:379:GLU:C	1:D:380:THR:HG22	2.32	0.50
1:D:33:GLY:HA2	1:D:395:VAL:CG2	2.42	0.50
1:B:257:ARG:N	1:B:259:CYS:SG	2.80	0.50
1:C:180:ALA:HB1	1:C:345:TRP:CZ3	2.47	0.50
1:C:314:CYS:O	1:C:318:THR:HG23	2.12	0.50
1:D:158:GLY:HA3	1:D:206:LEU:HB2	1.92	0.50
1:C:243:PRO:O	1:C:247:LYS:HG2	2.12	0.50
1:C:244:GLU:HB3	1:C:320:ARG:NH2	2.26	0.50
1:C:59:TYR:O	1:C:63:ILE:HB	2.12	0.50
1:B:315:ALA:HB1	1:B:324:LEU:HB2	1.94	0.49
1:D:142:ALA:O	1:D:398:THR:HA	2.11	0.49
1:A:266:VAL:HG13	1:A:277:PRO:HG2	1.94	0.49
1:B:278:PHE:CD2	1:B:290:ILE:HG12	2.47	0.49
1:B:43:PHE:CD2	1:B:384:PRO:HD2	2.48	0.49
1:C:242:SER:HB2	1:C:244:GLU:OE1	2.10	0.49
1:C:7:PHE:HE1	1:D:95:HIS:NE2	2.10	0.49
1:A:258:GLU:HG2	1:A:323:ARG:HD2	1.93	0.49
1:B:34:LEU:HD23	1:B:63:ILE:HD11	1.94	0.49
1:A:168:TYR:CD2	1:A:174:TRP:CZ3	3.00	0.49
1:A:314:CYS:O	1:A:318:THR:HG23	2.12	0.49
1:C:106:LEU:CD2	1:C:150:TYR:HD1	2.24	0.49
1:C:137:VAL:HG11	2:C:900:3NC:H10	1.94	0.49
1:C:160:ASP:HB3	1:C:205:LEU:HD22	1.94	0.49
1:A:29:CYS:SG	1:A:396:GLY:HA2	2.53	0.49
1:A:5:MET:N	1:A:9:THR:HG21	2.27	0.49
1:B:124:GLU:HG2	1:B:128:MET:HE1	1.93	0.49
1:B:345:TRP:HB2	1:B:346:GLU:OE2	2.12	0.49
1:A:143:PHE:HE1	1:A:152:VAL:HG21	1.77	0.49
1:B:163:ASN:O	1:B:166:SER:HB3	2.12	0.49
1:B:82:ILE:HD11	2:B:900:3NC:H13	1.94	0.49
1:D:239:ASP:HB3	1:D:276:THR:CG2	2.43	0.49
1:A:135:TRP:CZ3	1:A:181:GLU:HB3	2.47	0.49
1:A:207:ASP:O	1:A:209:SER:N	2.45	0.49
1:C:198:ASP:OD1	1:C:200:LYS:HE2	2.13	0.49
1:C:7:PHE:O	1:C:8:GLU:CG	2.61	0.49
1:A:20:ASP:HB3	1:A:23:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TRP:CE3	1:A:317:LEU:HA	2.48	0.49
1:C:244:GLU:HB3	1:C:320:ARG:NH1	2.27	0.49
1:C:293:HIS:CD2	1:C:294:LYS:N	2.81	0.49
1:C:300:PRO:HB2	1:C:303:ASN:N	2.26	0.49
1:D:308:GLU:O	1:D:309:ALA:C	2.50	0.49
1:A:142:ALA:O	1:A:398:THR:HA	2.13	0.48
1:D:162:VAL:HG12	1:D:163:ASN:N	2.27	0.48
1:A:109:LYS:HG2	1:A:394:PHE:CE1	2.48	0.48
1:B:207:ASP:O	1:B:209:SER:N	2.46	0.48
1:B:109:LYS:HB3	1:B:394:PHE:HE1	1.77	0.48
1:C:205:LEU:HG	1:C:215:ALA:CB	2.43	0.48
1:C:43:PHE:HB2	1:C:46:LEU:HG	1.95	0.48
1:D:293:HIS:NE2	1:D:294:LYS:HD3	2.29	0.48
1:A:237:THR:HG23	1:A:238:PRO:HD2	1.95	0.48
1:B:294:LYS:HZ2	1:B:294:LYS:HB2	1.75	0.48
1:D:168:TYR:CD2	1:D:174:TRP:HZ3	2.30	0.48
1:B:216:ASP:C	1:B:217:PHE:CD2	2.86	0.48
1:D:163:ASN:ND2	1:D:369:ASP:OD1	2.47	0.48
1:D:6:SER:C	1:D:8:GLU:H	2.16	0.48
1:B:42:ASP:OD1	1:B:47:ARG:NE	2.31	0.48
1:C:71:MET:HG2	1:C:143:PHE:CD1	2.49	0.48
1:D:297:LEU:O	1:D:298:THR:HG23	2.13	0.48
1:B:211:HIS:CE1	1:B:349:ARG:O	2.67	0.48
1:C:165:MET:HE3	1:C:165:MET:HB2	1.67	0.48
1:C:303:ASN:O	1:C:304:ASP:CB	2.60	0.48
1:C:372:GLU:HB3	1:C:373:GLU:CB	2.43	0.48
1:C:138:GLN:HE21	1:C:403:ARG:NH2	2.10	0.48
1:C:156:MET:HA	1:C:156:MET:CE	2.42	0.48
1:C:205:LEU:HG	1:C:215:ALA:HB2	1.95	0.48
1:C:186:LEU:HD13	1:C:260:ASP:HB3	1.96	0.48
1:C:98:THR:HG22	1:C:100:LYS:CG	2.43	0.48
1:C:43:PHE:CE2	1:C:384:PRO:CD	2.97	0.48
1:A:24:GLU:O	1:A:29:CYS:SG	2.71	0.48
1:A:66:ILE:HD12	1:A:66:ILE:H	1.78	0.48
1:C:265:GLY:HA2	1:C:316:PHE:HD1	1.79	0.48
1:C:383:ILE:HG12	1:C:383:ILE:H	1.44	0.48
1:A:168:TYR:CD1	1:A:168:TYR:N	2.82	0.47
1:B:106:LEU:HD21	1:B:150:TYR:CD1	2.49	0.47
1:C:293:HIS:NE2	1:C:294:LYS:HD3	2.29	0.47
1:D:228:MET:HA	1:D:255:TYR:O	2.14	0.47
1:D:241:ILE:HD12	1:D:242:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:O	1:A:262:TRP:NE1	2.47	0.47
1:B:268:LEU:O	1:B:268:LEU:HD23	2.15	0.47
1:D:207:ASP:C	1:D:209:SER:H	2.17	0.47
3:C:425:HOH:O	1:D:58:ARG:NH1	2.29	0.47
1:A:78:VAL:HG22	1:A:78:VAL:O	2.14	0.47
1:B:87:PHE:HZ	1:B:117:ASP:OD1	1.97	0.47
1:B:109:LYS:NZ	1:B:391:GLN:OE1	2.42	0.47
1:D:287:TYR:CD2	1:D:288:SER:N	2.82	0.47
1:D:93:VAL:O	1:D:101:VAL:HG13	2.14	0.47
1:B:280:ALA:HB3	1:B:286:THR:HG23	1.96	0.47
1:C:120:PHE:CD1	1:C:120:PHE:C	2.87	0.47
1:C:276:THR:HG22	1:C:278:PHE:N	2.21	0.47
1:A:319:ASP:O	1:A:320:ARG:C	2.53	0.47
1:B:190:HIS:HD2	1:B:194:PHE:O	1.98	0.47
1:D:180:ALA:HB2	1:D:338:PHE:CE2	2.48	0.47
1:A:348:LEU:HD22	1:A:348:LEU:O	2.14	0.47
1:A:348:LEU:CD2	1:A:348:LEU:O	2.62	0.47
1:C:190:HIS:NE2	1:C:257:ARG:HB2	2.30	0.47
1:C:160:ASP:HB3	1:C:205:LEU:CD2	2.44	0.47
1:C:52:ILE:O	1:C:55:PHE:HB3	2.14	0.47
1:A:156:MET:HE1	1:A:207:ASP:HB3	1.97	0.47
1:B:105:LYS:HE2	1:B:151:MET:HE1	1.95	0.47
1:C:162:VAL:CG1	1:C:163:ASN:N	2.69	0.47
1:D:293:HIS:CG	3:D:419:HOH:O	2.68	0.47
1:D:294:LYS:NZ	1:D:294:LYS:HB2	2.30	0.47
1:D:34:LEU:HD21	1:D:59:TYR:CE2	2.49	0.47
1:A:383:ILE:N	1:A:383:ILE:HD13	2.29	0.47
1:B:206:LEU:HA	1:B:211:HIS:O	2.15	0.47
1:B:84:ARG:CZ	1:B:84:ARG:HB2	2.44	0.47
1:C:30:LEU:HD13	1:D:30:LEU:CB	2.27	0.47
1:A:110:PHE:C	1:A:110:PHE:HD1	2.18	0.47
1:A:95:HIS:O	1:A:99:ARG:N	2.48	0.47
1:B:216:ASP:HB2	2:B:900:3NC:HN22	1.80	0.47
1:B:224:ASN:ND2	1:B:228:MET:O	2.48	0.47
1:B:266:VAL:HG13	1:B:277:PRO:CG	2.45	0.47
1:B:29:CYS:SG	1:B:396:GLY:CA	3.00	0.46
1:C:15:ASP:O	1:C:16:ASN:HB2	2.15	0.46
1:C:230:ARG:HG3	1:C:253:GLY:O	2.14	0.46
1:C:265:GLY:CA	1:C:316:PHE:HD1	2.29	0.46
1:A:115:ARG:C	1:A:117:ASP:H	2.18	0.46
1:B:141:TYR:HD2	1:B:152:VAL:HG11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ASP:HB3	1:C:23:SER:HB2	1.97	0.46
1:B:279:TYR:HD1	1:B:280:ALA:H	1.62	0.46
1:A:10:ARG:CD	1:B:69:LEU:HA	2.42	0.46
1:C:222:LYS:HB2	1:C:222:LYS:HE2	1.59	0.46
1:C:371:LEU:HD23	1:C:371:LEU:H	1.78	0.46
1:C:379:GLU:N	1:C:379:GLU:OE1	2.48	0.46
1:D:185:ALA:O	1:D:188:ALA:HB3	2.16	0.46
1:A:167:ASN:C	1:A:168:TYR:CD1	2.89	0.46
1:B:257:ARG:C	1:B:259:CYS:N	2.69	0.46
1:B:305:ILE:HG22	1:B:306:SER:N	2.30	0.46
1:B:392:LEU:C	1:B:394:PHE:H	2.17	0.46
1:B:59:TYR:O	1:B:63:ILE:HB	2.14	0.46
1:C:80:LYS:NZ	1:C:365:THR:HB	2.31	0.46
1:C:293:HIS:CD2	1:C:294:LYS:HD3	2.51	0.46
1:D:6:SER:O	1:D:8:GLU:N	2.49	0.46
1:A:242:SER:HA	1:A:262:TRP:CD1	2.50	0.46
1:A:4:HIS:HA	1:A:6:SER:HA	1.98	0.46
1:A:4:HIS:N	1:A:9:THR:HG1	2.14	0.46
1:C:47:ARG:C	1:C:49:ASN:H	2.19	0.46
1:A:111:GLU:HB3	1:A:115:ARG:NH1	2.31	0.46
1:A:147:ARG:C	1:A:148:TYR:CD2	2.90	0.46
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.61	0.46
1:B:308:GLU:O	1:B:309:ALA:C	2.53	0.46
1:C:261:TRP:O	1:C:264:VAL:HB	2.16	0.46
1:A:147:ARG:O	1:A:148:TYR:HD2	1.98	0.46
1:A:7:PHE:O	1:A:10:ARG:HB2	2.16	0.46
1:D:115:ARG:C	1:D:117:ASP:N	2.69	0.46
1:D:115:ARG:H	1:D:115:ARG:CD	2.29	0.46
1:D:242:SER:HB3	1:D:262:TRP:HB3	1.98	0.46
1:C:11:PHE:C	1:C:11:PHE:CD2	2.90	0.45
1:C:258:GLU:CD	1:C:258:GLU:H	2.19	0.45
1:C:276:THR:HG23	1:C:277:PRO:HD2	1.98	0.45
1:B:120:PHE:CD1	1:B:120:PHE:C	2.88	0.45
1:C:107:LEU:O	1:C:148:TYR:HA	2.16	0.45
1:C:154:GLU:HG2	1:C:156:MET:CE	2.45	0.45
1:C:174:TRP:N	1:C:174:TRP:CD1	2.84	0.45
1:C:262:TRP:CD2	1:C:317:LEU:HD12	2.51	0.45
1:A:139:LEU:HD23	1:A:399:TYR:CE2	2.51	0.45
1:A:244:GLU:OE1	1:A:323:ARG:NH1	2.50	0.45
1:A:6:SER:O	1:A:7:PHE:C	2.54	0.45
1:C:115:ARG:C	1:C:117:ASP:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PHE:O	1:B:323:ARG:HG3	2.16	0.45
1:C:259:CYS:SG	1:C:260:ASP:N	2.90	0.45
1:D:242:SER:OG	1:D:245:VAL:HG23	2.16	0.45
1:D:285:GLY:O	1:D:289:LYS:HB2	2.16	0.45
1:A:223:MET:HE3	1:A:257:ARG:HH21	1.82	0.45
1:A:262:TRP:CZ3	1:A:317:LEU:HA	2.52	0.45
2:B:900:3NC:H16	2:B:900:3NC:O21	2.16	0.45
1:C:159:GLY:HA2	1:C:368:PHE:CE1	2.51	0.45
1:C:190:HIS:CD2	1:C:257:ARG:HD3	2.52	0.45
1:D:156:MET:HA	1:D:156:MET:HE2	1.97	0.45
1:D:231:CYS:CB	1:D:255:TYR:HE1	2.25	0.45
1:D:303:ASN:HD22	1:D:303:ASN:H	1.62	0.45
1:B:125:ARG:NH1	1:B:396:GLY:O	2.50	0.45
1:B:167:ASN:O	1:B:168:TYR:HD1	1.98	0.45
1:B:16:ASN:O	1:B:20:ASP:N	2.44	0.45
1:B:26:ASN:HB3	3:B:424:HOH:O	2.15	0.45
1:B:172:GLU:OE1	1:B:306:SER:HB2	2.15	0.45
1:B:187:ASP:OD1	1:B:329:VAL:HG21	2.16	0.45
1:C:308:GLU:O	1:C:309:ALA:C	2.54	0.45
1:D:207:ASP:OD2	1:D:211:HIS:O	2.34	0.45
1:A:146:ASP:OD2	1:A:147:ARG:HG3	2.17	0.45
1:B:184:LEU:HD21	1:B:345:TRP:HE3	1.82	0.45
1:B:43:PHE:CE2	1:B:384:PRO:HD2	2.51	0.45
1:C:168:TYR:N	1:C:168:TYR:CD1	2.84	0.45
1:D:174:TRP:CD1	1:D:354:PRO:HB3	2.52	0.45
1:A:70:ARG:NH2	1:A:398:THR:HG21	2.32	0.45
1:B:29:CYS:N	3:B:424:HOH:O	2.50	0.45
1:C:162:VAL:HG12	1:C:163:ASN:H	1.81	0.45
1:C:224:ASN:ND2	1:C:228:MET:O	2.50	0.45
1:C:70:ARG:HH21	1:C:398:THR:HG21	1.81	0.45
1:D:228:MET:H	1:D:228:MET:HG3	1.62	0.45
1:A:59:TYR:O	1:A:63:ILE:HB	2.17	0.45
1:B:25:VAL:HG23	1:B:25:VAL:O	2.17	0.45
1:A:237:THR:O	1:A:238:PRO:C	2.55	0.45
1:C:319:ASP:O	1:C:320:ARG:C	2.55	0.45
1:A:94:ARG:HG3	1:A:101:VAL:HG23	1.99	0.44
1:A:168:TYR:HD2	1:A:174:TRP:CZ3	2.36	0.44
1:A:268:LEU:C	1:A:268:LEU:HD23	2.37	0.44
1:B:115:ARG:C	1:B:117:ASP:N	2.70	0.44
1:C:106:LEU:N	1:C:106:LEU:HD23	2.32	0.44
1:C:372:GLU:HB3	1:C:373:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:PHE:N	1:D:299:PHE:CD1	2.85	0.44
1:A:143:PHE:CE2	1:A:150:TYR:CD2	3.05	0.44
1:C:26:ASN:O	1:C:29:CYS:N	2.49	0.44
1:C:7:PHE:O	1:C:7:PHE:CD2	2.70	0.44
1:A:104:MET:HG3	1:A:152:VAL:HG22	1.99	0.44
1:A:276:THR:HB	1:A:279:TYR:HB2	1.98	0.44
1:B:308:GLU:OE1	1:B:336:LEU:HB2	2.18	0.44
1:D:241:ILE:CD1	1:D:245:VAL:HB	2.47	0.44
1:A:321:GLU:O	1:A:326:ARG:HD2	2.18	0.44
1:B:268:LEU:CD2	1:B:272:LEU:HD12	2.48	0.44
1:B:273:VAL:HG12	1:B:275:ASP:H	1.82	0.44
1:B:343:TRP:CE3	1:B:344:ALA:C	2.89	0.44
1:C:14:MET:CG	1:C:14:MET:O	2.66	0.44
1:C:161:LEU:O	1:C:165:MET:HE2	2.18	0.44
1:C:276:THR:HB	1:C:279:TYR:HB2	1.98	0.44
1:C:279:TYR:HD1	1:C:280:ALA:H	1.62	0.44
1:C:63:ILE:HG22	1:C:64:ASN:N	2.33	0.44
1:A:300:PRO:O	1:A:302:ASP:N	2.46	0.44
1:A:308:GLU:CA	1:A:308:GLU:OE2	2.66	0.44
1:B:343:TRP:HZ3	1:B:345:TRP:HA	1.82	0.44
1:C:128:MET:HE3	1:C:139:LEU:HB2	1.99	0.44
1:C:262:TRP:CE3	1:C:317:LEU:HA	2.53	0.44
1:D:242:SER:HB3	1:D:262:TRP:CG	2.52	0.44
1:D:91:GLN:HE21	1:D:91:GLN:HB3	1.58	0.44
1:A:239:ASP:CA	3:A:416:HOH:O	2.64	0.44
1:A:283:LEU:O	1:A:286:THR:OG1	2.34	0.44
1:B:201:PRO:HG3	1:B:267:PHE:CE1	2.53	0.44
1:C:328:GLY:O	1:C:331:GLU:HB3	2.18	0.44
1:D:196:HIS:O	1:D:197:ARG:HB2	2.16	0.44
1:D:204:MET:C	1:D:205:LEU:HD23	2.38	0.44
1:A:96:LYS:HG2	3:A:430:HOH:O	2.18	0.44
1:D:174:TRP:O	1:D:175:ALA:C	2.56	0.44
1:D:234:ALA:CB	1:D:245:VAL:HG12	2.47	0.44
1:B:199:VAL:HB	1:B:263:SER:HB3	2.00	0.44
1:B:269:TYR:CE1	1:B:277:PRO:HA	2.52	0.44
1:C:213:LYS:HB2	3:C:419:HOH:O	2.18	0.44
1:C:268:LEU:HD12	1:C:312:LEU:CD1	2.47	0.44
1:D:315:ALA:HB1	1:D:324:LEU:HB2	1.99	0.44
1:D:356:VAL:HA	1:D:357:PRO:HD2	1.77	0.44
1:D:60:LYS:HD3	1:D:61:ASP:N	2.32	0.44
1:A:4:HIS:HA	1:A:5:MET:HA	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:CE3	1:C:317:LEU:HD12	2.52	0.44
1:D:255:TYR:HB3	1:D:320:ARG:HH21	1.83	0.44
1:A:167:ASN:C	1:A:168:TYR:HD1	2.21	0.43
1:C:98:THR:CG2	1:C:100:LYS:HG2	2.48	0.43
1:C:224:ASN:N	1:C:224:ASN:HD22	2.16	0.43
1:C:352:VAL:HG13	1:C:352:VAL:O	2.18	0.43
1:D:372:GLU:HB2	1:D:373:GLU:H	1.45	0.43
1:A:14:MET:O	1:A:18:LEU:HD13	2.18	0.43
1:A:177:PHE:HD2	1:A:178:TYR:CD1	2.34	0.43
1:B:42:ASP:HA	1:B:56:LEU:CD1	2.48	0.43
1:C:285:GLY:O	1:C:289:LYS:HB2	2.18	0.43
1:A:254:TYR:CD1	1:C:380:THR:HG21	2.53	0.43
1:D:113:ILE:CG2	1:D:114:LYS:N	2.78	0.43
1:D:155:TYR:O	1:D:157:PRO:HD3	2.17	0.43
1:D:110:PHE:CE2	1:D:380:THR:O	2.70	0.43
1:C:131:ALA:CB	1:C:136:VAL:HG11	2.49	0.43
1:C:176:ARG:NE	1:C:337:PHE:O	2.52	0.43
1:B:111:GLU:O	1:B:115:ARG:HD2	2.18	0.43
1:B:258:GLU:CD	1:B:258:GLU:H	2.21	0.43
1:B:345:TRP:C	1:B:347:THR:H	2.22	0.43
1:C:212:LEU:HG	1:C:213:LYS:N	2.33	0.43
1:B:156:MET:SD	1:B:213:LYS:HD2	2.58	0.43
1:C:215:ALA:HB1	2:C:900:3NC:H16	2.00	0.43
1:D:241:ILE:CD1	1:D:242:SER:N	2.78	0.43
1:D:241:ILE:HD13	1:D:242:SER:H	1.81	0.43
1:A:262:TRP:O	1:A:263:SER:C	2.55	0.43
1:A:269:TYR:CD1	1:A:277:PRO:HD3	2.53	0.43
1:B:142:ALA:HA	1:B:150:TYR:O	2.19	0.43
1:C:269:TYR:CD2	1:C:277:PRO:HB3	2.54	0.43
1:D:137:VAL:HG21	1:D:215:ALA:CB	2.49	0.43
1:A:121:PHE:HE1	1:A:122:TRP:CE2	2.36	0.43
1:C:207:ASP:O	1:C:209:SER:N	2.52	0.43
1:A:178:TYR:CE1	1:A:354:PRO:HG2	2.54	0.43
1:B:121:PHE:HE1	1:B:122:TRP:CE2	2.37	0.43
1:A:14:MET:CE	1:B:69:LEU:HB2	2.49	0.43
1:C:13:LYS:HD2	1:C:14:MET:N	2.34	0.43
1:C:247:LYS:C	1:C:249:GLN:HB3	2.39	0.43
1:C:25:VAL:HA	1:C:29:CYS:HB2	2.01	0.43
1:D:243:PRO:O	1:D:246:LEU:N	2.51	0.43
1:A:284:VAL:HG23	1:A:285:GLY:N	2.34	0.43
1:A:95:HIS:O	1:A:99:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LEU:CD2	1:B:150:TYR:CD1	3.01	0.43
1:C:300:PRO:HA	1:C:301:ASP:C	2.39	0.43
1:D:108:SER:O	1:D:112:MET:HE2	2.19	0.43
1:D:207:ASP:C	1:D:209:SER:N	2.72	0.43
1:D:280:ALA:N	1:D:286:THR:CG2	2.82	0.43
1:A:298:THR:C	1:A:299:PHE:CG	2.91	0.43
1:A:38:VAL:HG21	1:A:63:ILE:CG1	2.48	0.43
1:B:243:PRO:O	1:B:246:LEU:N	2.45	0.43
1:C:137:VAL:CG1	2:C:900:3NC:H10	2.49	0.43
1:C:402:ASN:HD22	1:C:402:ASN:H	1.67	0.43
1:D:164:LEU:C	1:D:164:LEU:HD23	2.39	0.43
1:A:121:PHE:C	1:A:121:PHE:CD1	2.92	0.42
1:A:168:TYR:N	1:A:168:TYR:HD1	2.17	0.42
1:A:196:HIS:O	1:A:197:ARG:HB2	2.19	0.42
1:A:309:ALA:O	1:A:310:LYS:C	2.57	0.42
1:C:392:LEU:N	1:C:393:PRO:HD2	2.34	0.42
1:C:91:GLN:O	1:C:93:VAL:HG13	2.18	0.42
1:D:261:TRP:CE3	1:D:264:VAL:HG21	2.50	0.42
1:C:177:PHE:CD2	1:C:354:PRO:HG2	2.54	0.42
1:D:167:ASN:HD22	1:D:167:ASN:N	2.17	0.42
1:C:168:TYR:N	1:C:168:TYR:HD1	2.17	0.42
1:D:277:PRO:HB2	1:D:278:PHE:CE2	2.55	0.42
1:A:363:ILE:HG13	1:A:363:ILE:O	2.19	0.42
1:B:316:PHE:CD2	1:B:324:LEU:HB3	2.54	0.42
1:B:216:ASP:CB	2:B:900:3NC:N22	2.83	0.42
1:D:110:PHE:HA	1:D:381:PHE:CZ	2.54	0.42
1:D:301:ASP:N	1:D:301:ASP:OD2	2.51	0.42
1:C:49:ASN:HD21	1:D:388:VAL:HA	1.84	0.42
1:D:392:LEU:C	1:D:394:PHE:H	2.21	0.42
1:A:35:ASP:OD1	1:A:67:ARG:NH1	2.53	0.42
1:B:391:GLN:C	1:B:393:PRO:HD2	2.40	0.42
1:C:129:ALA:O	1:C:403:ARG:NH2	2.52	0.42
1:D:106:LEU:HD22	1:D:150:TYR:CD1	2.54	0.42
1:A:98:THR:CB	1:A:100:LYS:HG2	2.45	0.42
1:B:142:ALA:O	1:B:398:THR:HA	2.19	0.42
1:C:165:MET:HE2	1:C:201:PRO:HB3	2.01	0.42
1:A:254:TYR:OH	1:C:381:PHE:O	2.21	0.42
1:D:135:TRP:HB3	1:D:185:ALA:CB	2.50	0.42
1:D:333:LYS:HA	1:D:345:TRP:CZ2	2.54	0.42
1:A:185:ALA:O	1:A:188:ALA:HB3	2.20	0.42
1:A:345:TRP:C	1:A:347:THR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HB	1:B:30:LEU:HD21	2.00	0.42
1:C:106:LEU:HD22	1:C:150:TYR:HD1	1.76	0.42
1:C:46:LEU:O	1:C:52:ILE:HD12	2.19	0.42
1:C:82:ILE:HD11	2:C:900:3NC:H13	2.02	0.42
1:D:206:LEU:HA	1:D:211:HIS:O	2.19	0.42
1:D:286:THR:O	1:D:290:ILE:HG13	2.20	0.42
1:D:372:GLU:H	1:D:372:GLU:CD	2.21	0.42
1:D:58:ARG:HG2	1:D:59:TYR:CE1	2.54	0.42
1:A:110:PHE:O	1:A:111:GLU:C	2.58	0.42
1:A:336:LEU:HD22	1:A:336:LEU:H	1.84	0.42
1:C:87:PHE:HB2	1:C:107:LEU:CD2	2.50	0.42
1:C:30:LEU:HB3	1:D:30:LEU:HB3	2.02	0.42
1:D:401:SER:O	1:D:402:ASN:C	2.58	0.42
1:A:164:LEU:HD23	1:A:164:LEU:C	2.39	0.42
1:A:207:ASP:C	1:A:209:SER:H	2.23	0.42
1:A:245:VAL:HG12	1:A:245:VAL:O	2.19	0.42
1:D:182:VAL:HG22	1:D:212:LEU:HD11	2.02	0.42
1:C:30:LEU:CD1	1:D:30:LEU:HB2	2.27	0.42
1:B:167:ASN:C	1:B:168:TYR:CD1	2.81	0.42
1:B:401:SER:O	1:B:402:ASN:HB2	2.19	0.42
1:B:42:ASP:O	1:B:43:PHE:CD1	2.73	0.42
1:C:203:ASN:OD1	1:C:216:ASP:HB3	2.19	0.42
1:D:277:PRO:C	1:D:278:PHE:CD2	2.93	0.42
1:D:309:ALA:O	1:D:313:ILE:HG13	2.20	0.42
1:D:318:THR:OG1	1:D:323:ARG:HA	2.20	0.42
1:A:177:PHE:CZ	1:A:181:GLU:OE2	2.73	0.41
1:A:156:MET:HE1	1:A:213:LYS:HD2	2.00	0.41
1:A:302:ASP:C	1:A:304:ASP:H	2.23	0.41
1:B:149:LEU:HD22	1:B:397:PHE:CG	2.55	0.41
1:C:183:VAL:HG13	1:C:261:TRP:CZ3	2.54	0.41
1:C:47:ARG:HA	1:C:52:ILE:CG2	2.50	0.41
1:D:137:VAL:HG11	2:D:900:3NC:H10	2.02	0.41
1:A:153:MET:O	1:A:154:GLU:C	2.57	0.41
1:A:135:TRP:HZ3	1:A:181:GLU:HB3	1.84	0.41
1:A:199:VAL:HB	1:A:263:SER:CB	2.50	0.41
1:B:109:LYS:HG3	1:B:147:ARG:O	2.19	0.41
1:B:113:ILE:HG22	1:B:114:LYS:N	2.35	0.41
1:B:198:ASP:CB	1:B:219:THR:HG21	2.50	0.41
1:C:177:PHE:CD2	1:C:354:PRO:CG	3.03	0.41
1:C:63:ILE:CG2	1:C:64:ASN:N	2.82	0.41
1:D:174:TRP:HD1	1:D:174:TRP:N	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ASP:OD2	1:D:239:ASP:N	2.53	0.41
1:A:308:GLU:HA	1:A:308:GLU:OE2	2.17	0.41
1:A:308:GLU:OE1	1:A:336:LEU:HB2	2.20	0.41
1:B:217:PHE:N	1:B:217:PHE:CD2	2.88	0.41
1:C:204:MET:HB3	1:C:212:LEU:HD11	2.02	0.41
1:C:263:SER:O	1:C:266:VAL:HB	2.20	0.41
1:B:205:LEU:N	1:B:205:LEU:HD23	2.34	0.41
1:B:207:ASP:C	1:B:209:SER:H	2.23	0.41
1:B:363:ILE:O	1:B:363:ILE:HG13	2.19	0.41
1:B:392:LEU:C	1:B:394:PHE:N	2.74	0.41
1:B:149:LEU:HD22	1:B:397:PHE:CD1	2.55	0.41
1:D:168:TYR:CD1	1:D:168:TYR:N	2.88	0.41
1:D:137:VAL:HG23	1:D:214:LEU:O	2.20	0.41
1:D:348:LEU:O	1:D:351:THR:HG23	2.20	0.41
1:A:115:ARG:C	1:A:117:ASP:N	2.73	0.41
1:A:170:VAL:HA	1:A:171:PRO:HD3	1.91	0.41
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.78	0.41
1:B:106:LEU:HD13	1:B:148:TYR:CD1	2.55	0.41
1:B:177:PHE:CE1	1:B:354:PRO:HD3	2.55	0.41
1:B:235:VAL:HG23	1:B:236:GLY:H	1.86	0.41
1:C:98:THR:CG2	1:C:100:LYS:CG	2.99	0.41
1:C:205:LEU:HD23	1:C:205:LEU:N	2.36	0.41
1:C:348:LEU:HA	1:C:351:THR:HG23	2.02	0.41
1:C:369:ASP:C	1:C:370:ASP:O	2.58	0.41
1:A:115:ARG:H	1:A:115:ARG:HD2	1.85	0.41
1:A:268:LEU:C	1:A:268:LEU:CD2	2.88	0.41
1:A:317:LEU:N	1:A:317:LEU:CD1	2.84	0.41
1:A:4:HIS:C	1:A:9:THR:HG21	2.40	0.41
1:B:109:LYS:HD2	1:B:146:ASP:O	2.20	0.41
1:C:66:ILE:HD12	1:C:66:ILE:HA	1.84	0.41
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.66	0.41
1:D:391:GLN:C	1:D:393:PRO:HD2	2.40	0.41
1:A:120:PHE:CD1	1:A:120:PHE:C	2.93	0.41
1:A:266:VAL:HG13	1:A:277:PRO:HG3	2.00	0.41
1:A:177:PHE:CG	1:A:354:PRO:HG3	2.55	0.41
1:B:105:LYS:HB2	1:B:153:MET:HE2	2.02	0.41
1:C:242:SER:O	1:C:246:LEU:HB2	2.20	0.41
1:D:380:THR:OG1	1:D:381:PHE:N	2.53	0.41
1:A:279:TYR:CD1	1:A:280:ALA:N	2.88	0.41
1:A:312:LEU:HD21	1:A:316:PHE:CE1	2.56	0.41
1:A:337:PHE:CD1	1:A:337:PHE:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PHE:HD2	1:B:87:PHE:N	2.18	0.41
1:D:198:ASP:CB	1:D:219:THR:HG21	2.47	0.41
1:D:268:LEU:CD1	1:D:313:ILE:HG12	2.49	0.41
1:D:153:MET:O	1:D:154:GLU:C	2.59	0.41
1:D:66:ILE:HG23	1:D:70:ARG:HD2	2.03	0.41
1:A:66:ILE:O	1:A:67:ARG:C	2.59	0.41
1:B:185:ALA:O	1:B:189:ILE:HG12	2.21	0.41
1:B:321:GLU:HA	1:B:321:GLU:OE2	2.21	0.41
1:B:63:ILE:HG23	1:B:67:ARG:NH1	2.36	0.41
1:B:86:ALA:HB3	1:B:87:PHE:HD2	1.85	0.41
1:C:134:PRO:O	1:C:213:LYS:NZ	2.44	0.41
1:C:76:TYR:HD1	1:C:93:VAL:HG21	1.85	0.41
1:D:280:ALA:N	1:D:286:THR:HG22	2.35	0.41
1:D:302:ASP:C	1:D:304:ASP:H	2.24	0.41
1:D:157:PRO:HB2	1:D:359:LEU:HD11	2.01	0.41
1:A:110:PHE:O	1:A:112:MET:N	2.55	0.40
1:A:249:GLN:HG2	1:A:250:GLY:N	2.32	0.40
1:B:312:LEU:HD23	1:B:324:LEU:HD23	2.03	0.40
1:C:41:LEU:O	1:C:43:PHE:N	2.53	0.40
1:D:242:SER:HB3	1:D:262:TRP:CB	2.51	0.40
1:A:336:LEU:O	1:A:339:LYS:HB3	2.21	0.40
1:C:106:LEU:CD2	1:C:150:TYR:CD1	3.00	0.40
1:B:155:TYR:CZ	1:B:157:PRO:HA	2.56	0.40
1:C:125:ARG:HD2	1:C:125:ARG:HH11	1.65	0.40
1:C:269:TYR:HD1	1:C:270:GLU:N	2.18	0.40
1:C:176:ARG:HD3	1:C:338:PHE:HA	2.03	0.40
1:C:177:PHE:CD1	1:C:348:LEU:HD21	2.55	0.40
1:D:131:ALA:O	1:D:132:ASN:C	2.58	0.40
1:D:326:ARG:CG	1:D:327:ASN:N	2.84	0.40
1:D:345:TRP:C	1:D:347:THR:H	2.23	0.40
1:A:146:ASP:OD2	1:A:146:ASP:N	2.54	0.40
1:A:304:ASP:OD2	1:A:305:ILE:HD12	2.21	0.40
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.87	0.40
1:C:196:HIS:O	1:C:197:ARG:HB2	2.20	0.40
1:D:115:ARG:N	1:D:115:ARG:CD	2.84	0.40
1:D:102:TYR:CD1	1:D:140:PHE:HD2	2.40	0.40
1:D:268:LEU:HD13	1:D:313:ILE:CD1	2.52	0.40
1:C:155:TYR:CD1	1:C:156:MET:N	2.90	0.40
1:C:173:LYS:HB3	1:C:173:LYS:HE2	1.79	0.40
1:D:241:ILE:HD12	1:D:242:SER:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLY:O	1:C:249:GLN:OE1[4_445]	2.18	0.02

## 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	397/415 (96%)	332 (84%)	52 (13%)	13 (3%)	4	21
1	B	369/415 (89%)	299 (81%)	59 (16%)	11 (3%)	4	24
1	C	377/415 (91%)	304 (81%)	56 (15%)	17 (4%)	2	14
1	D	395/415 (95%)	330 (84%)	48 (12%)	17 (4%)	2	15
All	All	1538/1660 (93%)	1265 (82%)	215 (14%)	58 (4%)	3	18

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	GLU
1	C	238	PRO
1	C	241	ILE
1	D	229	VAL
1	D	232	ASP
1	D	252	ASP
1	D	372	GLU
1	A	7	PHE
1	A	250	GLY
1	B	70	ARG
1	B	238	PRO
1	B	258	GLU
1	C	16	ASN
1	C	208	LYS
1	D	7	PHE
1	D	208	LYS

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Mol	Chain	Res	Type
1	A	154	GLU
1	A	208	LYS
1	B	110	PHE
1	B	208	LYS
1	C	7	PHE
1	C	304	ASP
1	C	346	GLU
1	D	60	LYS
1	D	110	PHE
1	D	154	GLU
1	D	250	GLY
1	D	327	ASN
1	A	14	MET
1	A	110	PHE
1	A	111	GLU
1	A	301	ASP
1	A	303	ASN
1	A	311	ASN
1	C	13	LYS
1	C	42	ASP
1	C	154	GLU
1	C	177	PHE
1	C	372	GLU
1	B	66	ILE
1	B	67	ARG
1	B	311	ASN
1	C	6	SER
1	D	238	PRO
1	D	243	PRO
1	D	309	ALA
1	D	311	ASN
1	B	249	GLN
1	C	239	ASP
1	C	320	ARG
1	D	26	ASN
1	A	66	ILE
1	B	20	ASP
1	B	236	GLY
1	A	238	PRO
1	C	127	ILE
1	C	66	ILE
1	D	241	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	349/369 (95%)	295 (84%)	54 (16%)	2	13
1	B	336/369 (91%)	301 (90%)	35 (10%)	7	27
1	C	347/369 (94%)	288 (83%)	59 (17%)	2	10
1	D	347/369 (94%)	290 (84%)	57 (16%)	2	11
All	All	1379/1476 (93%)	1174 (85%)	205 (15%)	3	14

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	9	THR
1	A	10	ARG
1	A	11	PHE
1	A	16	ASN
1	A	27	SER
1	A	46	LEU
1	A	60	LYS
1	A	63	ILE
1	A	67	ARG
1	A	72	LYS
1	A	91	GLN
1	A	95	HIS
1	A	98	THR
1	A	106	LEU
1	A	110	PHE
1	A	113	ILE
1	A	115	ARG
1	A	116	SER
1	A	118	SER
1	A	123	GLU
1	A	126	ASP
1	A	139	LEU
1	A	161	LEU

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Mol	Chain	Res	Type
1	A	168	TYR
1	A	169	ASP
1	A	224	ASN
1	A	228	MET
1	A	229	VAL
1	A	233	THR
1	A	235	VAL
1	A	238	PRO
1	A	244	GLU
1	A	249	GLN
1	A	254	TYR
1	A	258	GLU
1	A	271	MET
1	A	275	ASP
1	A	282	SER
1	A	292	ASN
1	A	294	LYS
1	A	299	PHE
1	A	301	ASP
1	A	308	GLU
1	A	312	LEU
1	A	313	ILE
1	A	342	GLN
1	A	346	GLU
1	A	348	LEU
1	A	351	THR
1	A	352	VAL
1	A	358	ASP
1	A	377	GLU
1	A	378	GLU
1	B	4	HIS
1	B	5	MET
1	B	8	GLU
1	B	13	LYS
1	B	18	LEU
1	B	63	ILE
1	B	67	ARG
1	B	72	LYS
1	B	87	PHE
1	B	98	THR
1	B	110	PHE
1	B	113	ILE

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Mol	Chain	Res	Type
1	B	115	ARG
1	B	116	SER
1	B	121	PHE
1	B	166	SER
1	B	169	ASP
1	B	221	MET
1	B	224	ASN
1	B	237	THR
1	B	244	GLU
1	B	249	GLN
1	B	257	ARG
1	B	258	GLU
1	B	270	GLU
1	B	294	LYS
1	B	304	ASP
1	B	308	GLU
1	B	312	LEU
1	B	336	LEU
1	B	342	GLN
1	B	348	LEU
1	B	352	VAL
1	B	369	ASP
1	B	380	THR
1	C	5	MET
1	C	13	LYS
1	C	17	LEU
1	C	18	LEU
1	C	19	ARG
1	C	47	ARG
1	C	51	ASN
1	C	52	ILE
1	C	53	ASP
1	C	60	LYS
1	C	63	ILE
1	C	66	ILE
1	C	67	ARG
1	C	72	LYS
1	C	78	VAL
1	C	91	GLN
1	C	95	HIS
1	C	100	LYS
1	C	102	TYR

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Mol	Chain	Res	Type
1	C	110	PHE
1	C	113	ILE
1	C	125	ARG
1	C	162	VAL
1	C	166	SER
1	C	168	TYR
1	C	169	ASP
1	C	221	MET
1	C	224	ASN
1	C	244	GLU
1	C	245	VAL
1	C	268	LEU
1	C	269	TYR
1	C	271	MET
1	C	288	SER
1	C	292	ASN
1	C	294	LYS
1	C	301	ASP
1	C	304	ASP
1	C	305	ILE
1	C	307	LYS
1	C	312	LEU
1	C	313	ILE
1	C	317	LEU
1	C	318	THR
1	C	336	LEU
1	C	341	ASP
1	C	342	GLN
1	C	346	GLU
1	C	348	LEU
1	C	351	THR
1	C	358	ASP
1	C	365	THR
1	C	371	LEU
1	C	372	GLU
1	C	378	GLU
1	C	383	ILE
1	C	401	SER
1	C	402	ASN
1	C	404	ARG
1	D	14	MET
1	D	19	ARG

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Mol	Chain	Res	Type
1	D	24	GLU
1	D	55	PHE
1	D	57	SER
1	D	58	ARG
1	D	63	ILE
1	D	67	ARG
1	D	72	LYS
1	D	82	ILE
1	D	110	PHE
1	D	112	MET
1	D	113	ILE
1	D	115	ARG
1	D	125	ARG
1	D	126	ASP
1	D	132	ASN
1	D	146	ASP
1	D	162	VAL
1	D	167	ASN
1	D	205	LEU
1	D	207	ASP
1	D	221	MET
1	D	224	ASN
1	D	228	MET
1	D	230	ARG
1	D	232	ASP
1	D	233	THR
1	D	239	ASP
1	D	241	ILE
1	D	249	GLN
1	D	254	TYR
1	D	268	LEU
1	D	275	ASP
1	D	276	THR
1	D	282	SER
1	D	287	TYR
1	D	289	LYS
1	D	294	LYS
1	D	295	ASN
1	D	297	LEU
1	D	298	THR
1	D	299	PHE
1	D	301	ASP

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Mol	Chain	Res	Type
1	D	303	ASN
1	D	312	LEU
1	D	336	LEU
1	D	342	GLN
1	D	348	LEU
1	D	351	THR
1	D	370	ASP
1	D	371	LEU
1	D	372	GLU
1	D	378	GLU
1	D	379	GLU
1	D	380	THR
1	D	395	VAL

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	91	GLN
1	A	163	ASN
1	A	224	ASN
1	B	91	GLN
1	B	95	HIS
1	B	167	ASN
1	B	196	HIS
1	B	211	HIS
1	B	224	ASN
1	B	340	ASN
1	B	402	ASN
1	C	91	GLN
1	C	95	HIS
1	C	138	GLN
1	C	163	ASN
1	C	167	ASN
1	C	224	ASN
1	C	249	GLN
1	C	295	ASN
1	C	402	ASN
1	D	54	ASN
1	D	91	GLN
1	D	163	ASN
1	D	167	ASN
1	D	249	GLN

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Mol	Chain	Res	Type
1	D	303	ASN

### 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](#)

4 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	3NC	C	900	-	23,24,24	0.81	1 (4%)	29,34,34	1.12	2 (6%)
2	3NC	A	900	-	23,24,24	0.80	1 (4%)	29,34,34	1.47	5 (17%)
2	3NC	D	900	-	23,24,24	0.85	1 (4%)	29,34,34	1.26	3 (10%)
2	3NC	B	900	-	23,24,24	0.77	1 (4%)	29,34,34	1.73	6 (20%)

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	3NC	C	900	-	-	0/8/18/18	0/3/3/3
2	3NC	A	900	-	-	0/8/18/18	0/3/3/3
2	3NC	D	900	-	-	2/8/18/18	0/3/3/3
2	3NC	B	900	-	-	3/8/18/18	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	3NC	C9-C8	2.43	1.47	1.41
2	B	900	3NC	C9-C8	2.30	1.47	1.41
2	A	900	3NC	C9-C8	2.16	1.47	1.41
2	C	900	3NC	C9-C8	2.08	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	3NC	C2-C3-C4	-4.42	106.47	111.53
2	B	900	3NC	C5-C4-C3	-3.46	106.70	110.28
2	B	900	3NC	C1-C20-N19	3.16	119.66	115.02
2	A	900	3NC	C5-C4-C3	-3.11	107.06	110.28
2	C	900	3NC	C16-C15-C14	2.86	121.14	118.17
2	A	900	3NC	C1-C20-N19	2.81	119.15	115.02
2	D	900	3NC	C15-C14-CL18	-2.63	116.55	119.54
2	D	900	3NC	C10-N11-C12	2.62	122.69	116.43
2	B	900	3NC	C10-N11-C12	2.59	122.64	116.43
2	B	900	3NC	O21-C20-C1	-2.33	119.08	122.12
2	A	900	3NC	C12-C7-C8	-2.23	116.90	118.78
2	D	900	3NC	C6-C5-C4	-2.21	109.01	111.53
2	C	900	3NC	C1-C20-N19	2.17	118.21	115.02
2	B	900	3NC	C6-C5-C4	-2.16	109.06	111.53
2	A	900	3NC	C2-C3-C4	-2.10	109.13	111.53
2	A	900	3NC	C10-N11-C12	2.08	121.41	116.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	3NC	C6-C1-C20-O21
2	B	900	3NC	C6-C1-C20-N19
2	D	900	3NC	C6-C1-C20-O21
2	D	900	3NC	C2-C1-C20-O21
2	B	900	3NC	C2-C1-C20-O21



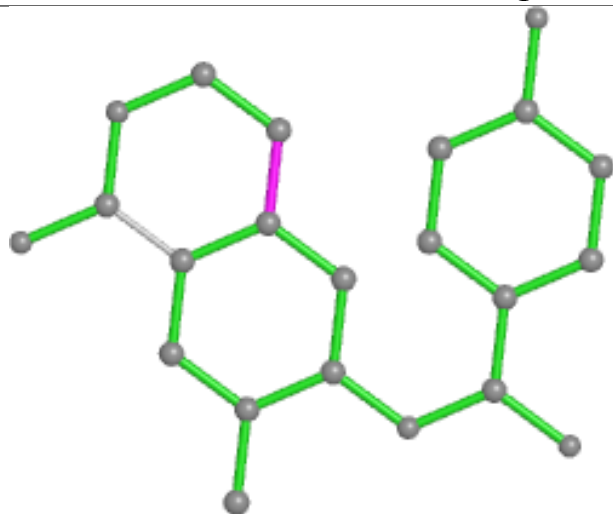
There are no ring outliers.

4 monomers are involved in 12 short contacts:

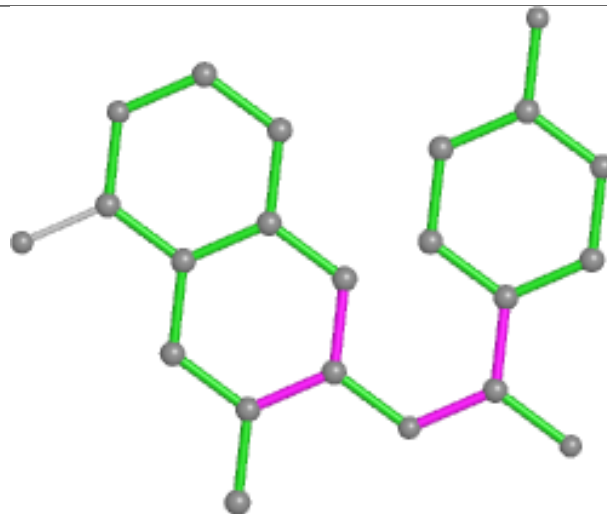
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	3NC	5	0
2	A	900	3NC	1	0
2	D	900	3NC	1	0
2	B	900	3NC	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

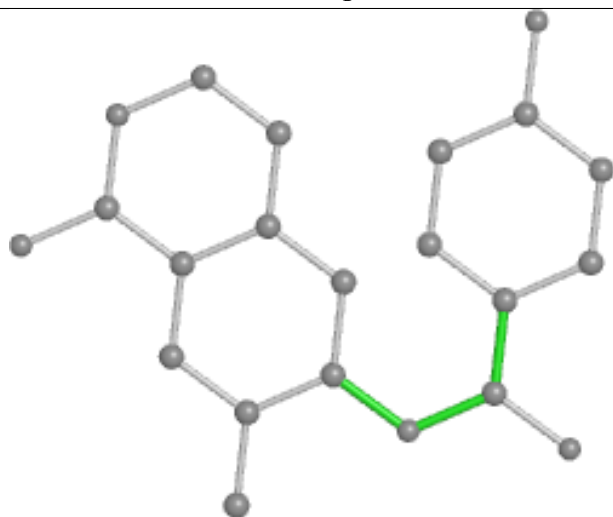
## Ligand 3NC C 900



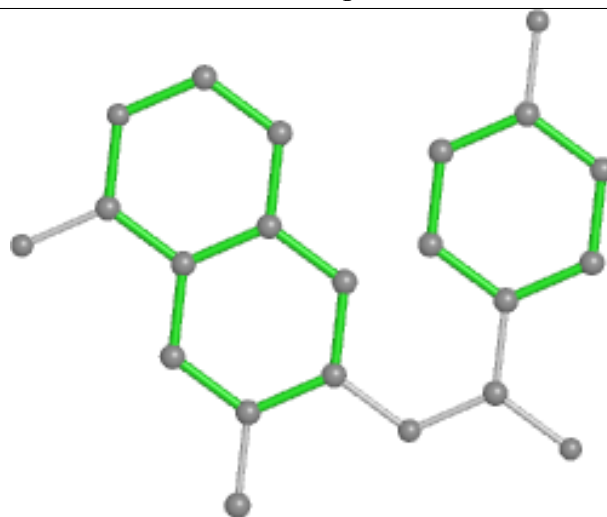
Bond lengths



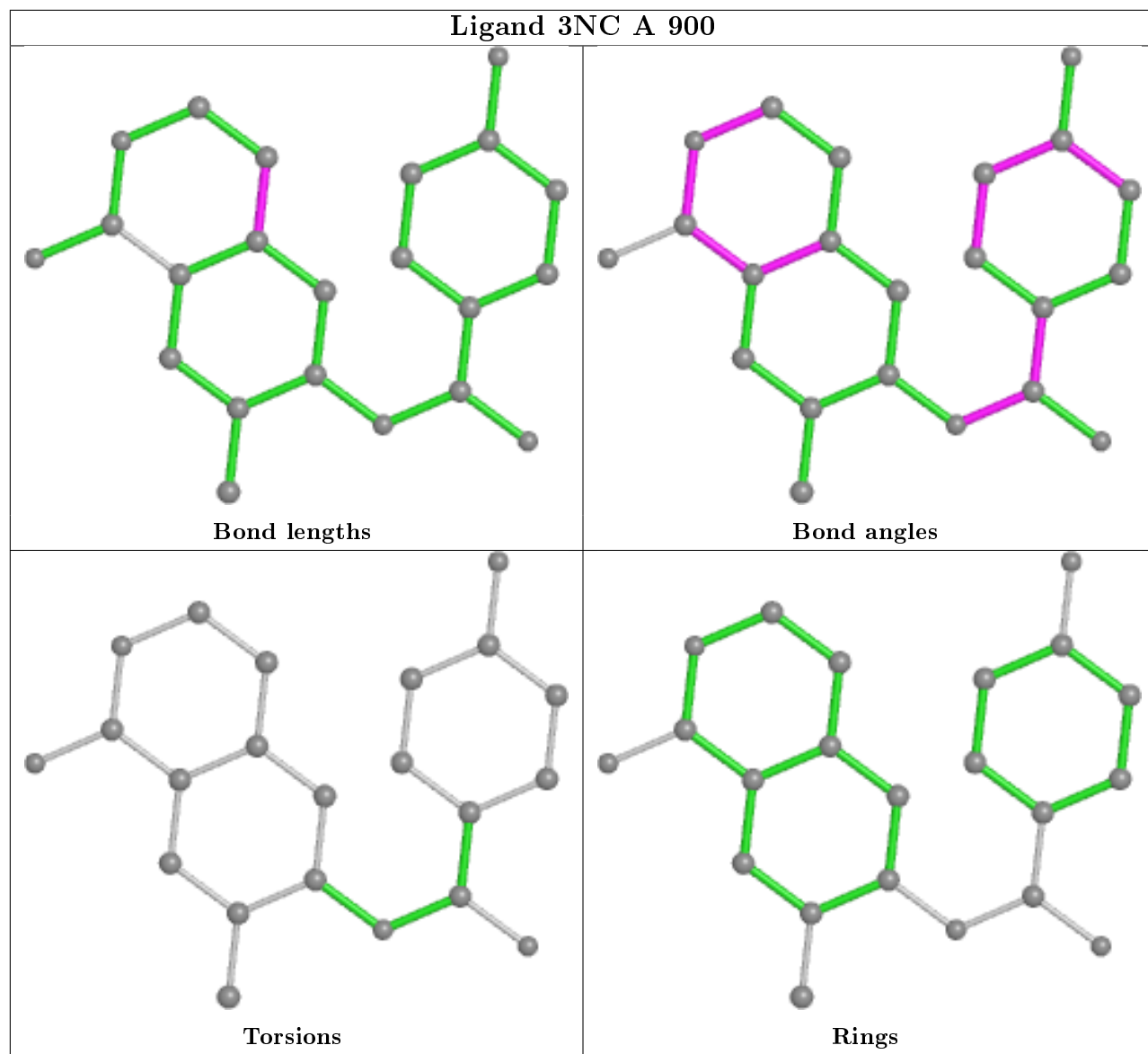
Bond angles

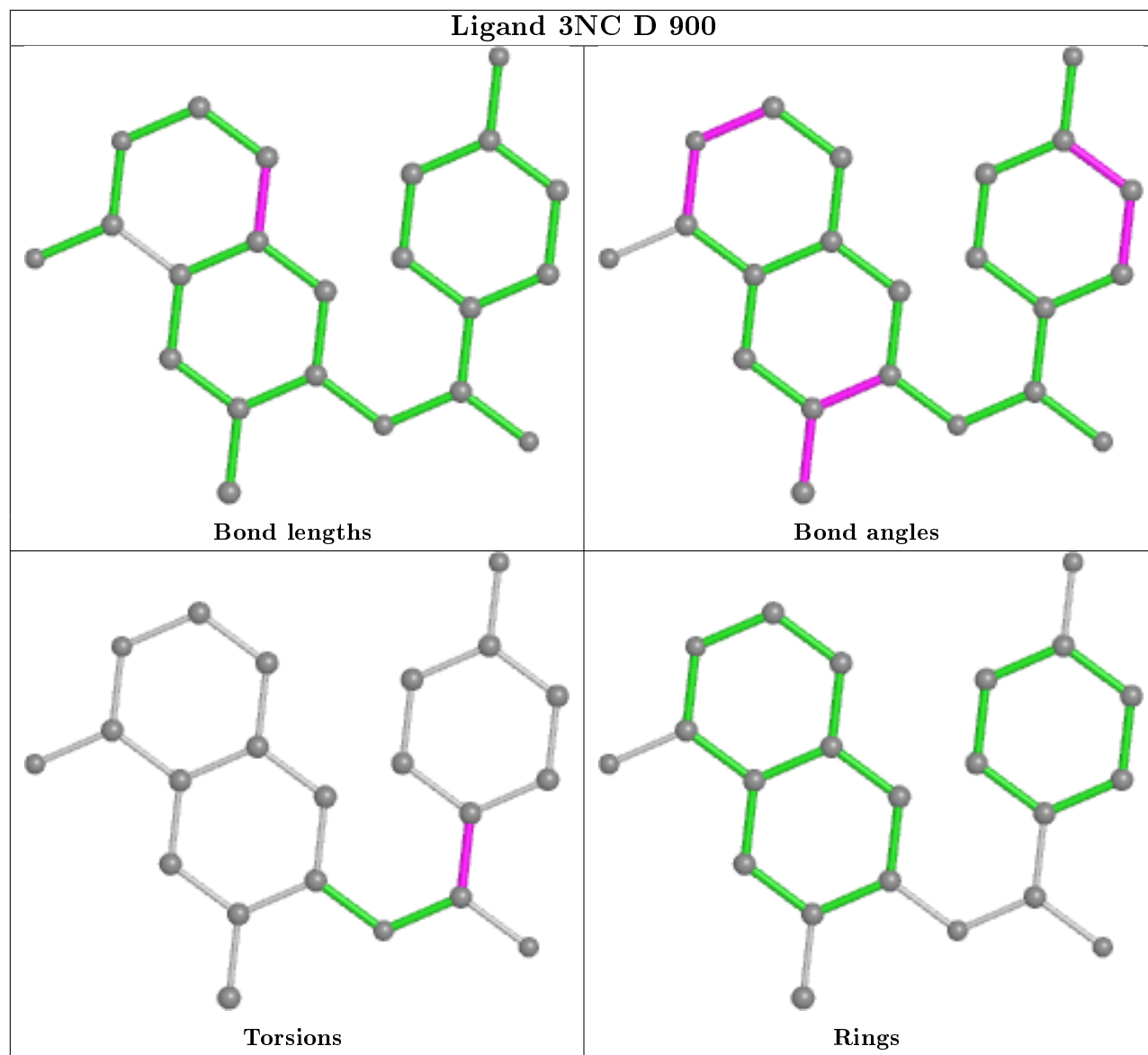


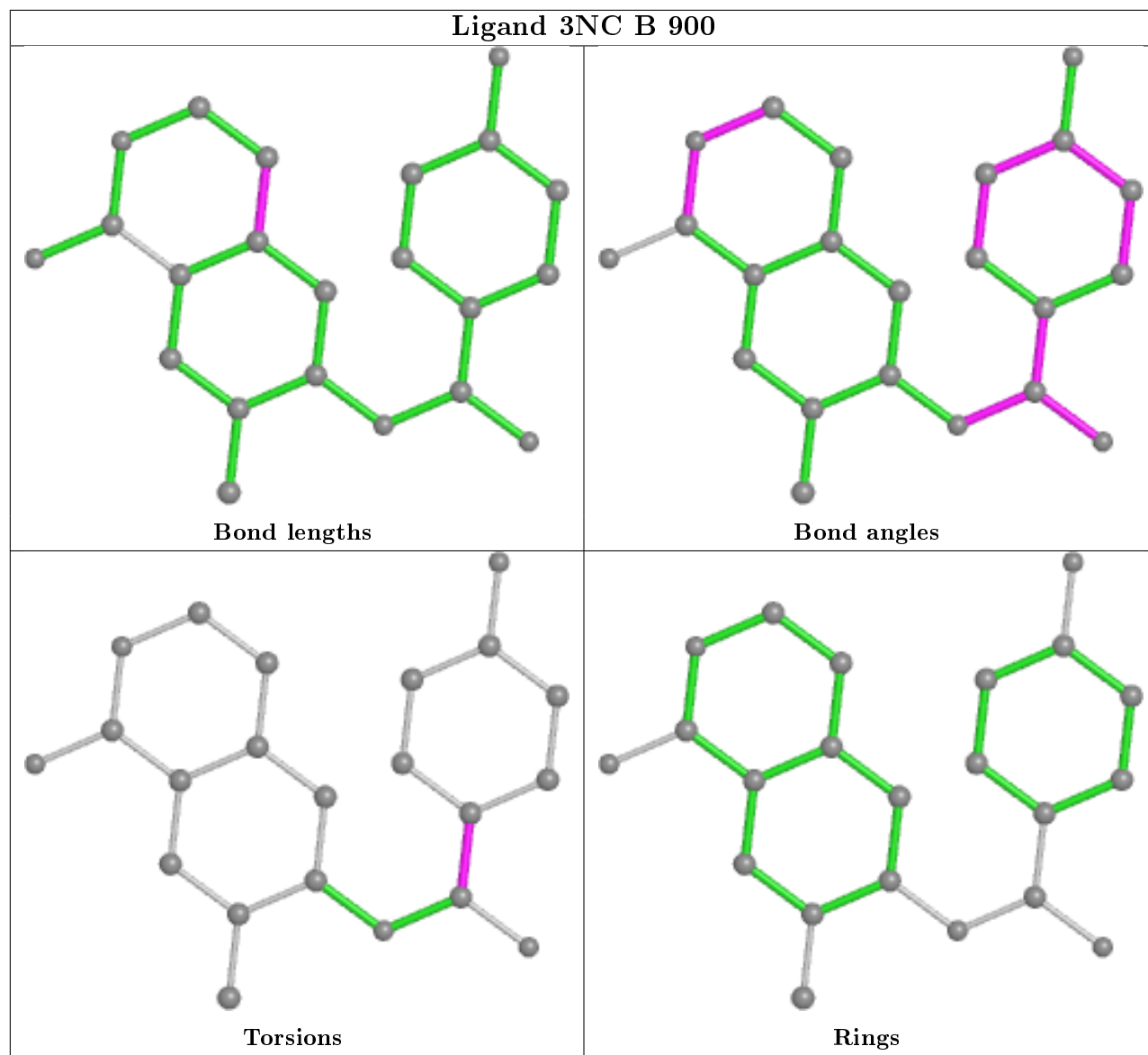
Torsions



Rings







## 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	399/415 (96%)	-0.28	2 (0%) 91 75	54, 102, 170, 238	0
1	B	379/415 (91%)	0.40	34 (8%) 9 3	77, 149, 284, 468	0
1	C	389/415 (93%)	-0.07	12 (3%) 49 21	61, 113, 202, 346	0
1	D	397/415 (95%)	-0.17	7 (1%) 68 40	57, 111, 189, 381	0
All	All	1564/1660 (94%)	-0.04	55 (3%) 44 18	54, 117, 221, 468	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	ASN	9.6
1	B	337	PHE	7.4
1	D	300	PRO	6.0
1	C	117	ASP	6.0
1	B	287	TYR	5.5
1	B	314	CYS	5.3
1	A	300	PRO	5.1
1	B	339	LYS	4.6
1	C	24	GLU	4.6
1	B	341	ASP	4.1
1	B	240	TYR	4.1
1	D	324	LEU	4.0
1	C	281	ASP	4.0
1	B	318	THR	3.7
1	B	229	VAL	3.5
1	B	345	TRP	3.4
1	B	271	MET	3.4
1	B	269	TYR	3.3
1	B	312	LEU	3.3
1	C	303	ASN	3.3
1	B	277	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	170	VAL	3.0
1	B	281	ASP	2.9
1	D	87	PHE	2.9
1	B	282	SER	2.9
1	B	132	ASN	2.9
1	B	336	LEU	2.9
1	D	376	GLY	2.9
1	C	51	ASN	2.8
1	D	7	PHE	2.7
1	B	288	SER	2.6
1	B	361	SER	2.4
1	C	334	ARG	2.4
1	B	89	GLU	2.4
1	A	141	TYR	2.3
1	B	280	ALA	2.3
1	D	226	GLU	2.3
1	B	20	ASP	2.3
1	C	235	VAL	2.3
1	B	232	ASP	2.3
1	C	116	SER	2.3
1	B	107	LEU	2.2
1	C	286	THR	2.2
1	B	322	VAL	2.2
1	C	299	PHE	2.2
1	C	22	LYS	2.1
1	B	321	GLU	2.1
1	C	21	PRO	2.1
1	B	368	PHE	2.1
1	B	247	LYS	2.1
1	B	278	PHE	2.1
1	B	402	ASN	2.1
1	B	226	GLU	2.0
1	B	260	ASP	2.0
1	D	337	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

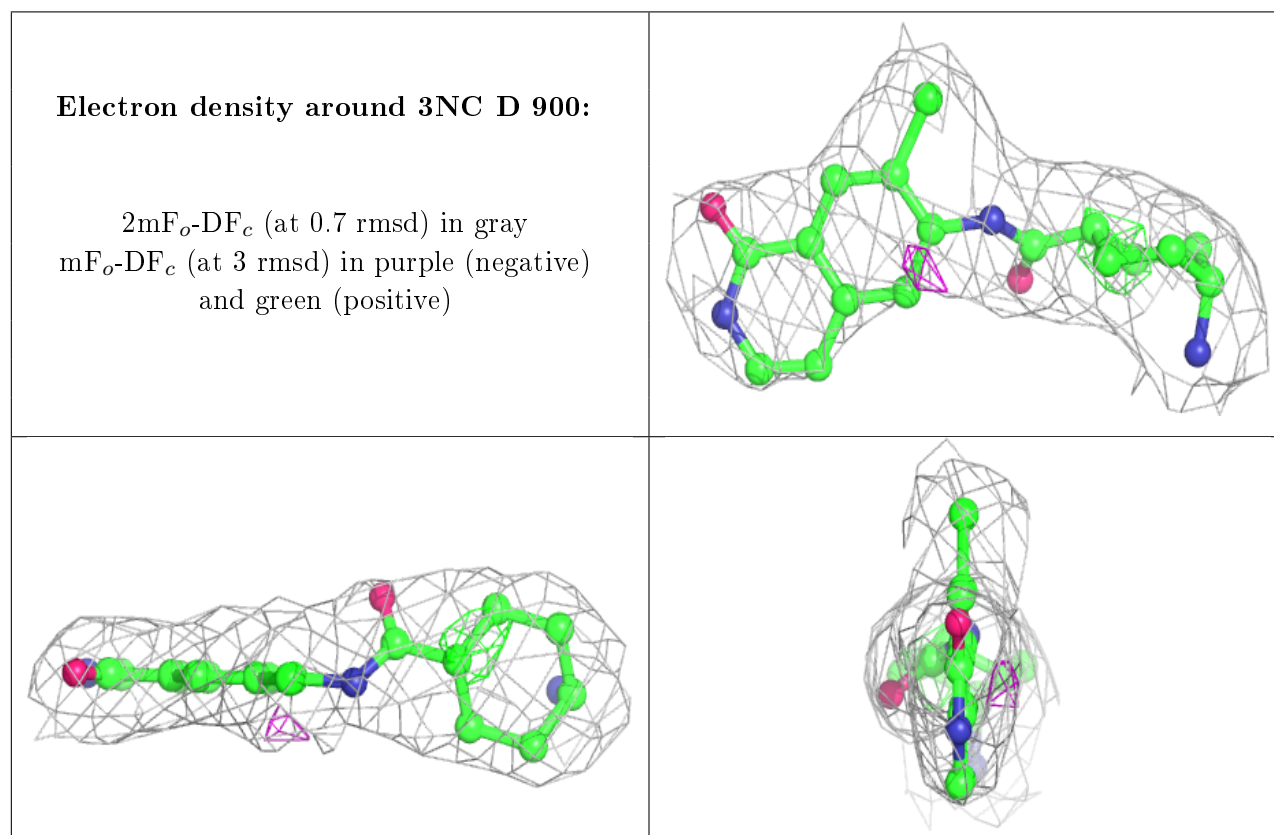
There are no carbohydrates in this entry.

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	3NC	D	900	22/22	0.85	0.25	84,84,84,84	0
2	3NC	B	900	22/22	0.85	0.29	122,122,122,122	0
2	3NC	A	900	22/22	0.86	0.26	93,93,93,93	0
2	3NC	C	900	22/22	0.88	0.33	110,110,110,110	0

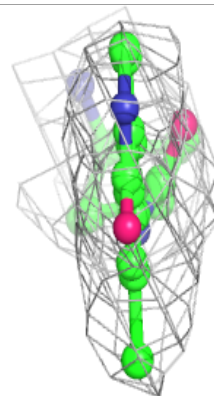
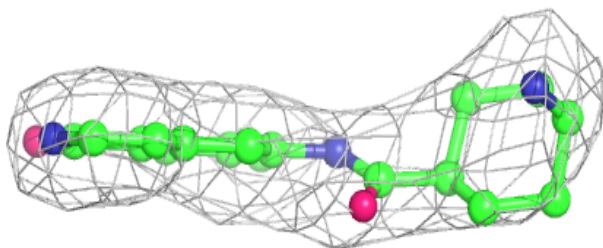
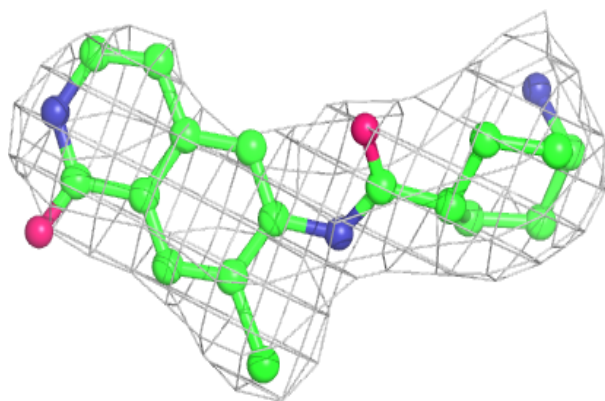
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



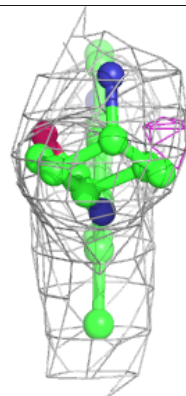
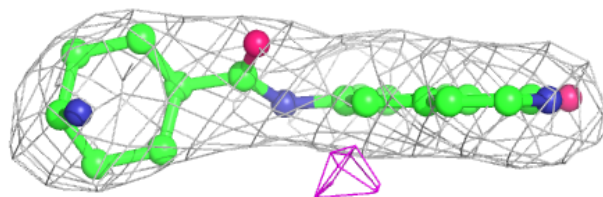
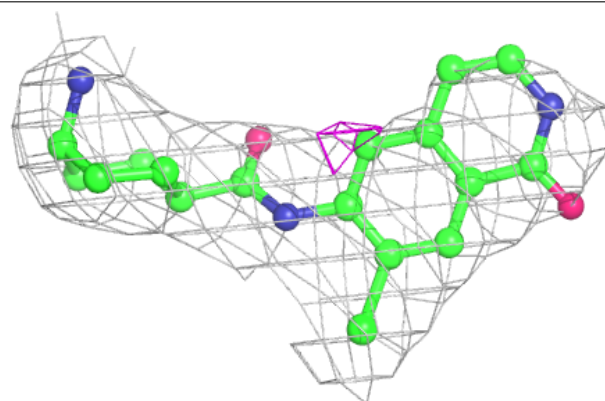


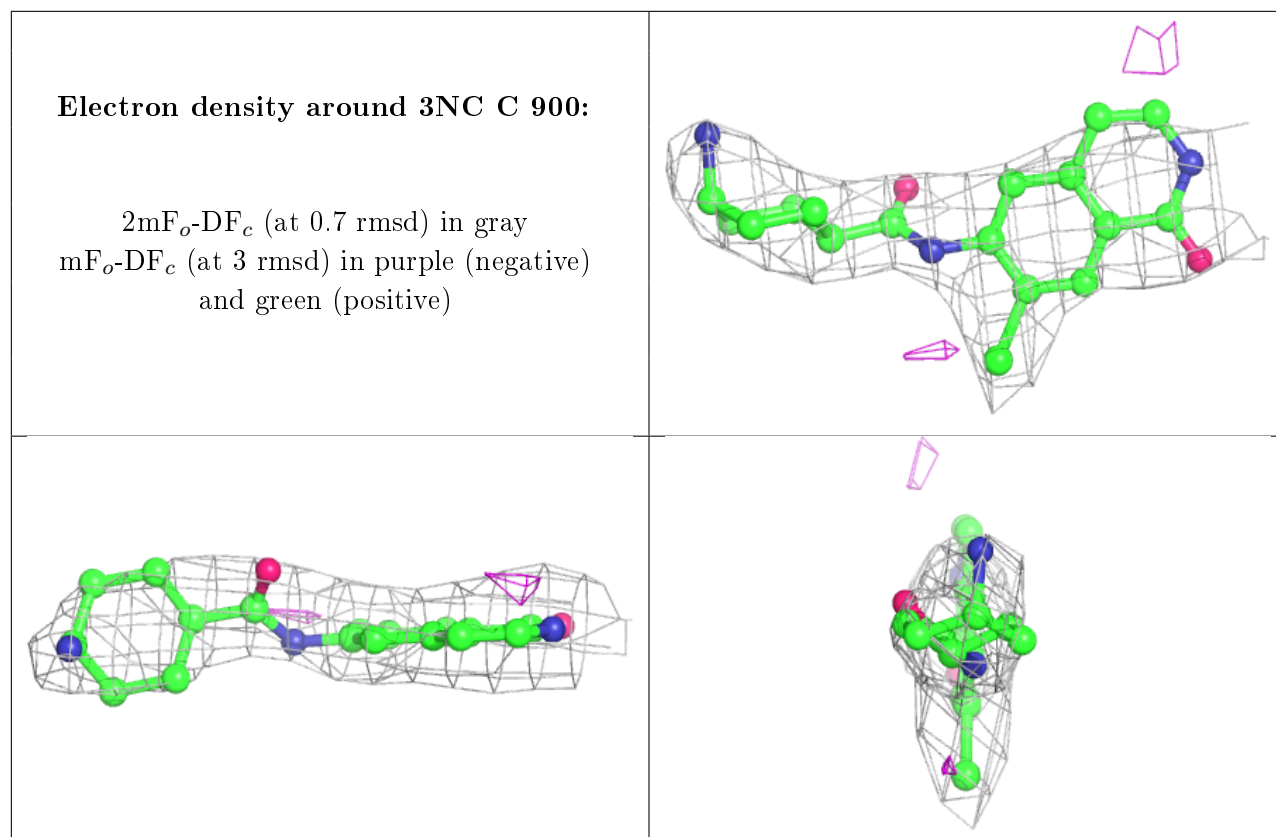
**Electron density around 3NC B 900:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 3NC A 900:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.