



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2024 – 09:39 AM EST

PDB ID : 2HXY  
Title : Crystal structure of human apo-eIF4AIII  
Authors : Johansen, J.S.; Andersen, G.R.  
Deposited on : 2006-08-04  
Resolution : 3.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

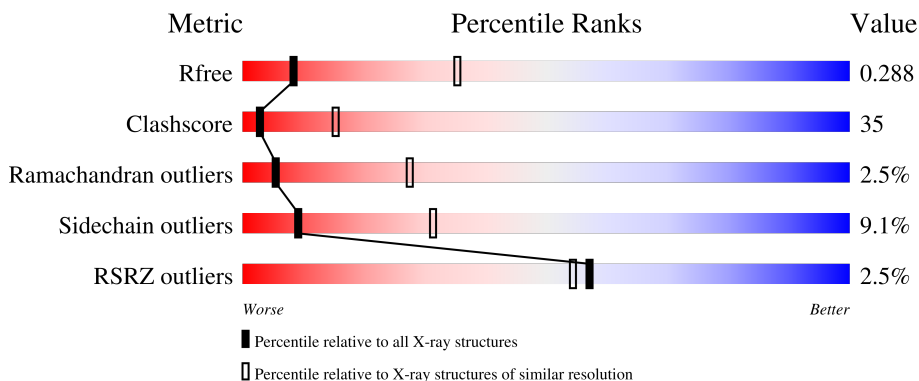
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of 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	391	 2% 47% 41% 8% . .
1	B	391	 2% 45% 44% 7% .
1	C	391	 2% 46% 43% 7% .
1	D	391	 3% 45% 44% 7% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12080 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 Probable ATP-dependent RNA helicase DDX48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	3020	1909	531	562	18	0	0	0
1	B	376	3020	1909	531	562	18	0	0	0
1	C	376	3020	1909	531	562	18	0	0	0
1	D	376	3020	1909	531	562	18	0	0	0

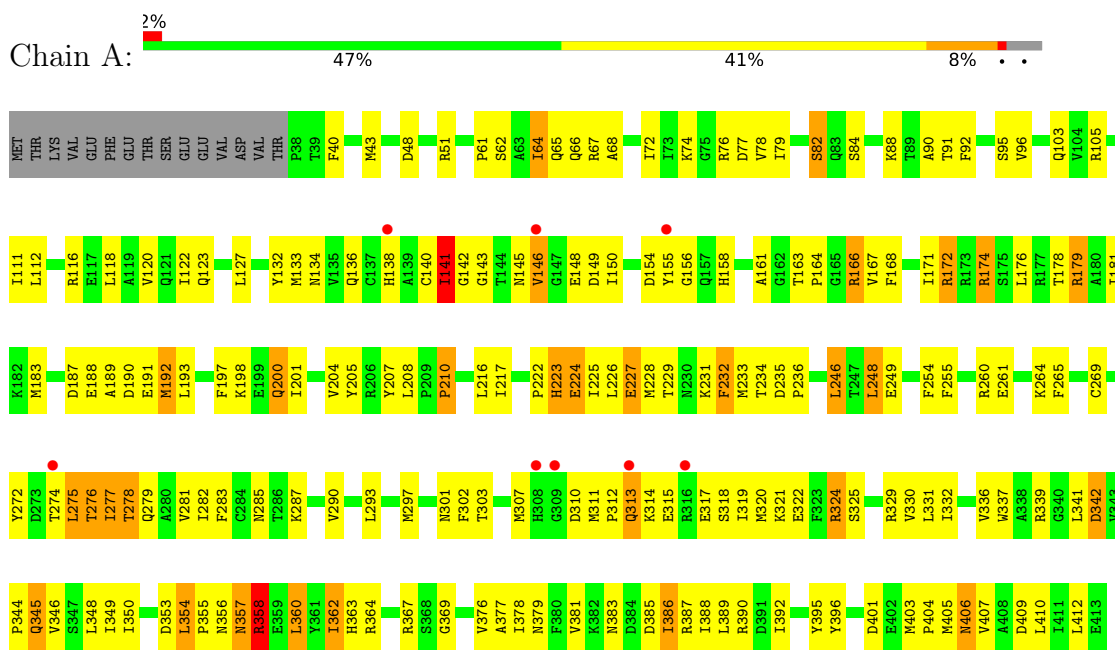
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	LEU	-	cloning artifact	UNP P38919
A	413	GLU	-	cloning artifact	UNP P38919
B	412	LEU	-	cloning artifact	UNP P38919
B	413	GLU	-	cloning artifact	UNP P38919
C	412	LEU	-	cloning artifact	UNP P38919
C	413	GLU	-	cloning artifact	UNP P38919
D	412	LEU	-	cloning artifact	UNP P38919
D	413	GLU	-	cloning artifact	UNP P38919

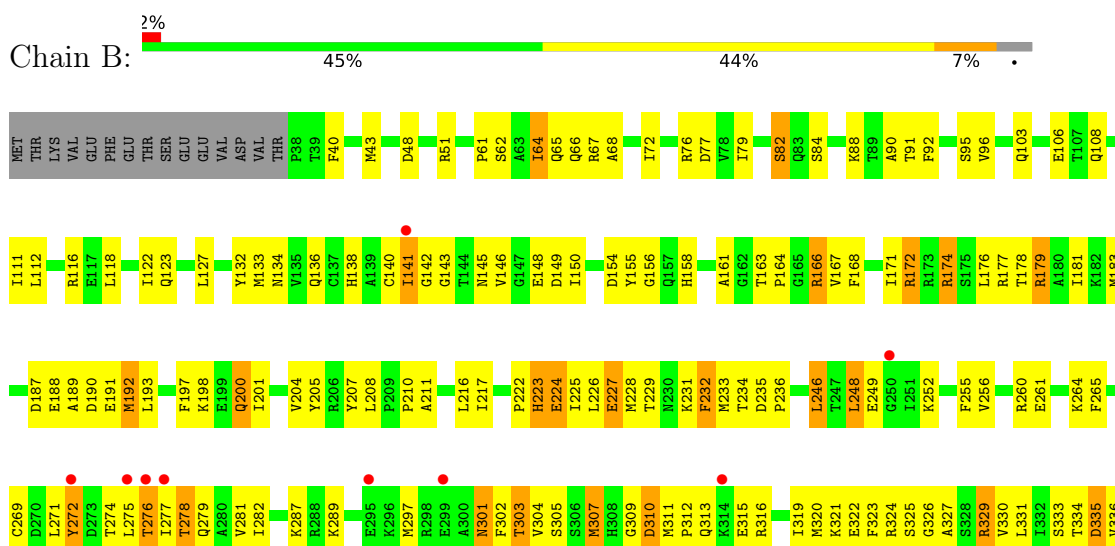
### 3 Residue-property plots

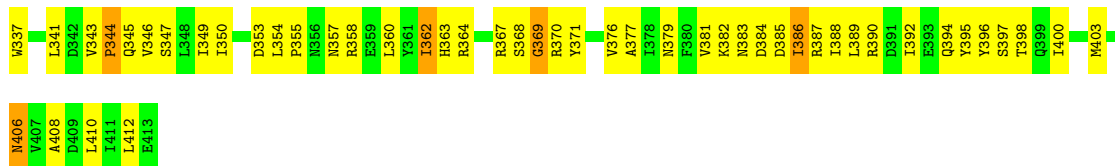
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable ATP-dependent RNA helicase DDX48

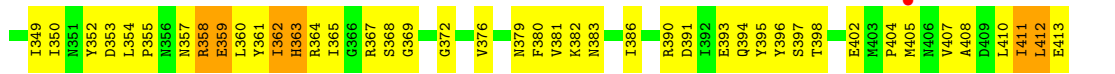
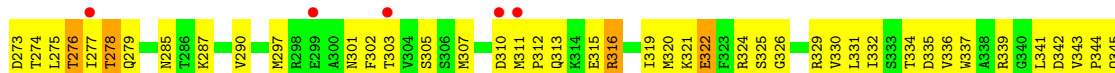
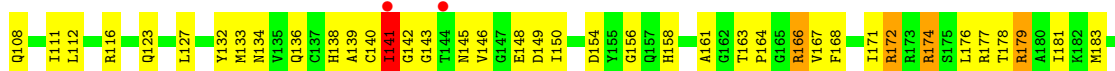
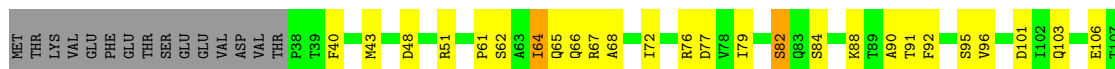


- Molecule 1: Probable ATP-dependent RNA helicase DDX48

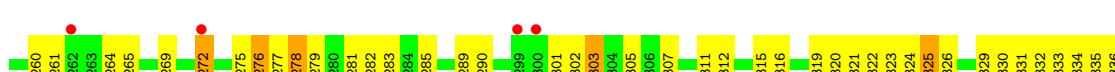
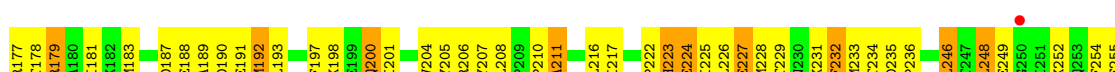
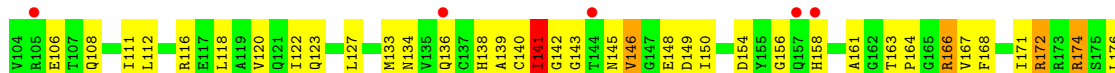
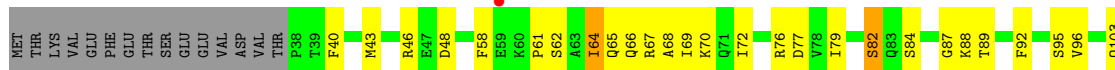




• Molecule 1: Probable ATP-dependent RNA helicase DDX48



• Molecule 1: Probable ATP-dependent RNA helicase DDX48



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.22Å 238.05Å 79.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 99.7 (49.00-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 3.33Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.275 , 0.308 0.262 , 0.288	Depositor DCC
$R_{free}$ test set	1335 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtrriage
Anisotropy	0.435	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 69.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.20% 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](#)

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	0.54	0/3068	0.82	0/4138
1	B	0.53	0/3068	0.83	2/4138 (0.0%)
1	C	0.51	0/3068	0.81	0/4138
1	D	0.51	0/3068	0.80	1/4138 (0.0%)
All	All	0.52	0/12272	0.81	3/16552 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	TYR	CB-CG-CD1	-8.62	115.83	121.00
1	D	272	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	B	272	TYR	CB-CG-CD2	6.06	124.64	121.00

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	3020	0	3075	213	0
1	B	3020	0	3075	199	1
1	C	3020	0	3075	217	0
1	D	3020	0	3075	237	0
All	All	12080	0	12300	857	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 35.

All (857) 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:D:272:TYR:CD1	1:D:275:LEU:HD13	1.81	1.14
1:C:207:TYR:HA	1:D:210:PRO:HG3	1.32	1.10
1:A:312:PRO:HG2	1:A:315:GLU:HB3	1.30	1.09
1:D:276:THR:HG22	1:D:329:ARG:HB3	1.10	1.09
1:D:346:VAL:HG22	1:D:347:SER:H	1.18	1.09
1:C:116:ARG:HG2	1:C:141:ILE:HD13	1.38	1.05
1:D:116:ARG:HG2	1:D:141:ILE:HD13	1.37	1.04
1:B:116:ARG:HG2	1:B:141:ILE:HD13	1.38	1.04
1:B:383:ASN:O	1:B:386:ILE:HG22	1.61	1.00
1:A:116:ARG:HG2	1:A:141:ILE:HD13	1.39	1.00
1:D:222:PRO:HD2	1:D:225:ILE:HG13	1.44	0.99
1:B:222:PRO:HD2	1:B:225:ILE:HG13	1.44	0.98
1:A:222:PRO:HD2	1:A:225:ILE:HG13	1.44	0.98
1:D:272:TYR:HD1	1:D:275:LEU:HD13	1.14	0.97
1:C:222:PRO:HD2	1:C:225:ILE:HG13	1.44	0.95
1:D:276:THR:CG2	1:D:329:ARG:HB3	1.95	0.95
1:C:383:ASN:O	1:C:386:ILE:HG22	1.68	0.94
1:B:200:GLN:H	1:B:200:GLN:HE21	1.16	0.94
1:C:200:GLN:H	1:C:200:GLN:HE21	1.15	0.93
1:A:355:PRO:HB2	1:A:360:LEU:HD11	1.51	0.93
1:D:276:THR:HG22	1:D:329:ARG:CB	1.97	0.92
1:D:200:GLN:H	1:D:200:GLN:HE21	1.16	0.92
1:C:200:GLN:O	1:C:204:VAL:HG23	1.72	0.90
1:A:200:GLN:H	1:A:200:GLN:HE21	1.16	0.90
1:B:200:GLN:O	1:B:204:VAL:HG23	1.72	0.89
1:D:200:GLN:O	1:D:204:VAL:HG23	1.72	0.89
1:A:290:VAL:HG13	1:A:332:ILE:HG22	1.53	0.89
1:A:200:GLN:O	1:A:204:VAL:HG23	1.72	0.88
1:A:275:LEU:HD21	1:A:330:VAL:CG2	2.05	0.86
1:C:261:GLU:HG2	1:C:382:LYS:HZ2	1.39	0.86
1:C:246:LEU:CD1	1:C:341:LEU:HG	2.05	0.86
1:D:355:PRO:CB	1:D:360:LEU:HD11	2.05	0.85
1:D:235:ASP:OD2	1:D:344:PRO:HA	1.77	0.85
1:D:252:LYS:HB2	1:D:376:VAL:HG22	1.59	0.84
1:C:290:VAL:HG13	1:C:332:ILE:HG22	1.57	0.83
1:A:410:LEU:HD23	1:A:410:LEU:O	1.78	0.83
1:C:200:GLN:H	1:C:200:GLN:NE2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLN:H	1:B:200:GLN:NE2	1.78	0.80
1:C:246:LEU:HD13	1:C:341:LEU:HG	1.63	0.80
1:D:200:GLN:H	1:D:200:GLN:NE2	1.79	0.80
1:A:200:GLN:H	1:A:200:GLN:NE2	1.79	0.79
1:B:381:VAL:HG11	1:B:389:LEU:HD22	1.64	0.79
1:D:272:TYR:HA	1:D:275:LEU:HB2	1.65	0.79
1:D:346:VAL:HG22	1:D:347:SER:N	1.98	0.79
1:D:334:THR:OG1	1:D:336:VAL:HG13	1.84	0.78
1:D:272:TYR:HA	1:D:275:LEU:CB	2.14	0.77
1:A:355:PRO:CB	1:A:360:LEU:HD11	2.15	0.77
1:B:367:ARG:NH1	1:B:369:GLY:HA2	1.99	0.77
1:C:362:ILE:HB	1:C:396:TYR:CE2	2.20	0.76
1:C:341:LEU:HD12	1:C:341:LEU:H	1.51	0.76
1:A:341:LEU:HD12	1:A:341:LEU:H	1.50	0.76
1:A:277:ILE:HG21	1:A:410:LEU:HD22	1.67	0.76
1:A:317:GLU:O	1:A:321:LYS:HG3	1.85	0.76
1:A:383:ASN:O	1:A:386:ILE:HG22	1.86	0.76
1:C:189:ALA:HA	1:C:192:MET:HG3	1.67	0.76
1:A:116:ARG:CG	1:A:141:ILE:HD13	2.16	0.75
1:B:116:ARG:CG	1:B:141:ILE:HD13	2.17	0.75
1:C:312:PRO:O	1:C:316:ARG:HG2	1.87	0.75
1:A:123:GLN:HE21	1:A:138:HIS:HA	1.51	0.74
1:B:276:THR:HG22	1:B:329:ARG:HB3	1.69	0.74
1:C:123:GLN:NE2	1:C:138:HIS:HA	2.03	0.74
1:D:116:ARG:CG	1:D:141:ILE:HD13	2.17	0.74
1:D:285:ASN:HD21	1:D:355:PRO:HA	1.51	0.74
1:A:123:GLN:NE2	1:A:138:HIS:HA	2.03	0.74
1:B:62:SER:HB3	1:B:65:GLN:HG3	1.68	0.74
1:C:123:GLN:HE21	1:C:138:HIS:HA	1.52	0.73
1:A:200:GLN:HE21	1:A:200:GLN:N	1.87	0.73
1:C:200:GLN:HE21	1:C:200:GLN:N	1.87	0.73
1:C:181:ILE:HG21	1:C:208:LEU:HD22	1.69	0.73
1:C:62:SER:HB3	1:C:65:GLN:HG3	1.70	0.72
1:B:304:VAL:HG12	1:B:330:VAL:HB	1.71	0.72
1:A:62:SER:HB3	1:A:65:GLN:HG3	1.71	0.72
1:A:312:PRO:CG	1:A:315:GLU:HB3	2.16	0.72
1:B:62:SER:HB3	1:B:65:GLN:CG	2.19	0.72
1:D:355:PRO:HB3	1:D:360:LEU:HD11	1.69	0.72
1:C:276:THR:HG22	1:C:329:ARG:HB3	1.71	0.72
1:A:287:LYS:HD3	1:A:310:ASP:OD2	1.90	0.72
1:D:62:SER:HB3	1:D:65:GLN:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:SER:HB3	1:C:65:GLN:CG	2.19	0.72
1:A:189:ALA:HA	1:A:192:MET:HG3	1.70	0.72
1:B:123:GLN:HE21	1:B:138:HIS:HA	1.55	0.72
1:A:322:GLU:O	1:A:325:SER:HB3	1.89	0.72
1:B:116:ARG:HG2	1:B:141:ILE:HG21	1.72	0.71
1:D:189:ALA:HA	1:D:192:MET:HG3	1.72	0.71
1:D:123:GLN:HE21	1:D:138:HIS:HA	1.56	0.71
1:D:200:GLN:HE21	1:D:200:GLN:N	1.87	0.71
1:D:316:ARG:HH11	1:D:316:ARG:HG3	1.55	0.71
1:D:255:PHE:CE1	1:D:402:GLU:HG3	2.26	0.71
1:A:275:LEU:HD21	1:A:330:VAL:HG22	1.72	0.71
1:C:337:TRP:CZ2	1:C:344:PRO:HD3	2.26	0.71
1:C:116:ARG:CG	1:C:141:ILE:HD13	2.18	0.70
1:B:189:ALA:HA	1:B:192:MET:HG3	1.73	0.70
1:B:315:GLU:O	1:B:319:ILE:HG12	1.90	0.70
1:D:141:ILE:HA	1:D:166:ARG:HD2	1.72	0.70
1:B:269:CYS:O	1:B:272:TYR:HB3	1.91	0.70
1:B:272:TYR:CE1	1:B:302:PHE:HD1	2.10	0.70
1:D:123:GLN:NE2	1:D:138:HIS:HA	2.06	0.70
1:B:200:GLN:HE21	1:B:200:GLN:N	1.87	0.70
1:B:297:MET:O	1:B:302:PHE:HD2	1.74	0.70
1:C:276:THR:HG22	1:C:329:ARG:CB	2.22	0.70
1:A:362:ILE:HB	1:A:396:TYR:CE2	2.27	0.70
1:B:246:LEU:HB3	1:B:362:ILE:CD1	2.22	0.70
1:B:123:GLN:NE2	1:B:138:HIS:HA	2.07	0.69
1:A:358:ARG:O	1:A:358:ARG:HG2	1.91	0.69
1:D:410:LEU:HD23	1:D:410:LEU:O	1.93	0.69
1:A:272:TYR:CD1	1:A:275:LEU:HD13	2.27	0.69
1:D:311:MET:HB2	1:D:316:ARG:HD2	1.75	0.69
1:C:360:LEU:HD12	1:C:360:LEU:C	2.12	0.69
1:A:311:MET:HB3	1:A:312:PRO:HD2	1.75	0.68
1:D:303:THR:HG23	1:D:329:ARG:HB2	1.75	0.68
1:C:413:GLU:CB	1:D:174:ARG:HH22	2.06	0.68
1:D:62:SER:HB3	1:D:65:GLN:CG	2.23	0.68
1:D:281:VAL:HB	1:D:349:ILE:HD13	1.74	0.68
1:D:346:VAL:CG2	1:D:347:SER:H	2.03	0.68
1:A:181:ILE:HG21	1:A:208:LEU:HD22	1.77	0.67
1:D:360:LEU:C	1:D:360:LEU:HD12	2.15	0.67
1:A:228:MET:HG2	1:A:232:PHE:CE2	2.29	0.67
1:A:62:SER:HB3	1:A:65:GLN:CG	2.24	0.67
1:D:228:MET:HG2	1:D:232:PHE:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:THR:HG21	1:C:407:VAL:HG21	1.77	0.67
1:B:228:MET:HG2	1:B:232:PHE:CE2	2.29	0.67
1:D:355:PRO:HB2	1:D:360:LEU:HD11	1.76	0.67
1:A:248:LEU:H	1:A:248:LEU:HD12	1.60	0.67
1:C:228:MET:HG2	1:C:232:PHE:CE2	2.29	0.66
1:C:315:GLU:O	1:C:319:ILE:HG12	1.95	0.66
1:A:143:GLY:HA2	1:A:146:VAL:HG13	1.78	0.66
1:C:279:GLN:HA	1:C:329:ARG:O	1.96	0.66
1:D:272:TYR:O	1:D:275:LEU:HB3	1.95	0.66
1:C:248:LEU:HD12	1:C:248:LEU:H	1.60	0.66
1:C:255:PHE:CE1	1:C:402:GLU:HG3	2.30	0.66
1:C:402:GLU:O	1:C:404:PRO:HD3	1.94	0.66
1:A:140:CYS:O	1:A:141:ILE:HB	1.93	0.66
1:C:331:LEU:HD12	1:C:332:ILE:N	2.10	0.66
1:B:255:PHE:HA	1:B:379:ASN:O	1.96	0.66
1:D:141:ILE:HG23	1:D:142:GLY:N	2.11	0.66
1:D:143:GLY:HA2	1:D:146:VAL:HG13	1.78	0.66
1:A:141:ILE:HG23	1:A:142:GLY:N	2.11	0.66
1:B:272:TYR:O	1:B:275:LEU:HB3	1.94	0.66
1:B:248:LEU:HD12	1:B:248:LEU:H	1.61	0.66
1:C:285:ASN:HD21	1:C:355:PRO:HA	1.60	0.66
1:D:370:ARG:HG2	1:D:371:TYR:CE1	2.31	0.66
1:B:141:ILE:HG23	1:B:142:GLY:N	2.10	0.66
1:D:140:CYS:O	1:D:141:ILE:HB	1.95	0.65
1:C:141:ILE:HG23	1:C:142:GLY:N	2.12	0.65
1:C:272:TYR:CZ	1:C:302:PHE:HD1	2.13	0.65
1:A:339:ARG:HD2	1:A:342:ASP:OD2	1.96	0.65
1:A:360:LEU:C	1:A:360:LEU:HD12	2.17	0.65
1:C:166:ARG:HB2	1:C:166:ARG:HH11	1.60	0.65
1:B:410:LEU:HD23	1:B:410:LEU:O	1.97	0.65
1:A:141:ILE:HA	1:A:166:ARG:HD2	1.78	0.65
1:D:248:LEU:H	1:D:248:LEU:HD12	1.61	0.65
1:B:276:THR:HG22	1:B:329:ARG:CB	2.26	0.65
1:B:181:ILE:HG21	1:B:208:LEU:HD22	1.78	0.65
1:C:140:CYS:O	1:C:141:ILE:HB	1.97	0.65
1:A:272:TYR:HD1	1:A:275:LEU:HD13	1.61	0.64
1:B:172:ARG:O	1:B:174:ARG:HD3	1.98	0.64
1:C:203:ASP:O	1:C:206:ARG:CB	2.45	0.64
1:D:167:VAL:O	1:D:171:ILE:HG13	1.97	0.64
1:D:181:ILE:HG21	1:D:208:LEU:HD22	1.78	0.64
1:B:205:TYR:HA	1:B:208:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:LEU:HD12	1:D:412:LEU:O	1.98	0.64
1:B:316:ARG:HG3	1:B:316:ARG:HH11	1.61	0.64
1:C:368:SER:HB3	1:C:372:GLY:N	2.12	0.64
1:B:167:VAL:O	1:B:171:ILE:HG13	1.97	0.64
1:A:274:THR:O	1:A:277:ILE:HB	1.98	0.64
1:B:222:PRO:HD2	1:B:225:ILE:CG1	2.26	0.64
1:C:207:TYR:HA	1:D:210:PRO:CG	2.21	0.64
1:B:319:ILE:O	1:B:322:GLU:HB2	1.98	0.64
1:A:172:ARG:O	1:A:174:ARG:HD3	1.98	0.63
1:C:77:ASP:HB3	1:C:233:MET:CG	2.28	0.63
1:C:172:ARG:O	1:C:174:ARG:HD3	1.98	0.63
1:C:275:LEU:C	1:C:275:LEU:HD23	2.17	0.63
1:B:163:THR:O	1:B:167:VAL:HG23	1.98	0.63
1:C:275:LEU:HD23	1:C:276:THR:N	2.13	0.63
1:B:272:TYR:CE1	1:B:302:PHE:CD1	2.87	0.63
1:D:82:SER:HA	1:D:88:LYS:HE2	1.81	0.63
1:A:77:ASP:HB3	1:A:233:MET:CG	2.29	0.63
1:B:82:SER:HA	1:B:88:LYS:HE2	1.81	0.63
1:B:143:GLY:HA2	1:B:146:VAL:HG13	1.80	0.63
1:A:116:ARG:HG2	1:A:141:ILE:HG21	1.81	0.63
1:B:141:ILE:HA	1:B:166:ARG:HD2	1.79	0.63
1:D:163:THR:O	1:D:167:VAL:HG23	1.99	0.63
1:A:275:LEU:C	1:A:275:LEU:HD23	2.18	0.63
1:C:141:ILE:HA	1:C:166:ARG:HD2	1.81	0.62
1:A:275:LEU:HD23	1:A:276:THR:N	2.14	0.62
1:B:166:ARG:HH11	1:B:166:ARG:HB2	1.64	0.62
1:C:167:VAL:O	1:C:171:ILE:HG13	1.98	0.62
1:C:312:PRO:HG2	1:C:315:GLU:HB3	1.82	0.62
1:D:77:ASP:HB3	1:D:233:MET:CG	2.30	0.62
1:D:275:LEU:HD21	1:D:330:VAL:CG2	2.29	0.62
1:C:319:ILE:O	1:C:322:GLU:HB2	1.99	0.62
1:A:167:VAL:O	1:A:171:ILE:HG13	1.99	0.62
1:C:362:ILE:HG23	1:C:363:HIS:N	2.14	0.62
1:A:283:PHE:CE1	1:A:364:ARG:HG2	2.35	0.62
1:D:172:ARG:O	1:D:174:ARG:HD3	1.99	0.62
1:C:274:THR:HA	1:C:277:ILE:HG13	1.80	0.62
1:C:205:TYR:HA	1:C:208:LEU:HD12	1.82	0.61
1:A:82:SER:HA	1:A:88:LYS:HE2	1.81	0.61
1:C:316:ARG:HG3	1:C:316:ARG:HH11	1.63	0.61
1:B:276:THR:HG22	1:B:329:ARG:CG	2.30	0.61
1:C:166:ARG:HB2	1:C:166:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:HB3	1:C:362:ILE:CD1	2.29	0.61
1:C:290:VAL:HG13	1:C:332:ILE:CG2	2.28	0.61
1:A:412:LEU:HD12	1:A:412:LEU:O	2.01	0.61
1:B:141:ILE:CG2	1:B:142:GLY:N	2.63	0.61
1:C:143:GLY:HA2	1:C:146:VAL:HG13	1.81	0.61
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.66	0.61
1:D:116:ARG:HG3	1:D:116:ARG:HH11	1.66	0.61
1:C:163:THR:O	1:C:167:VAL:HG23	1.99	0.61
1:C:307:MET:HE3	1:C:319:ILE:HB	1.82	0.61
1:C:64:ILE:HG13	1:C:65:GLN:N	2.16	0.61
1:B:210:PRO:O	1:B:211:ALA:HB3	2.00	0.61
1:D:279:GLN:HG2	1:D:329:ARG:NH2	2.16	0.61
1:A:303:THR:HG23	1:A:303:THR:O	2.01	0.60
1:D:246:LEU:HB3	1:D:362:ILE:CD1	2.31	0.60
1:A:279:GLN:HA	1:A:329:ARG:O	2.01	0.60
1:A:346:VAL:HG22	1:A:348:LEU:H	1.67	0.60
1:C:82:SER:HA	1:C:88:LYS:HE2	1.81	0.60
1:B:141:ILE:HG23	1:B:142:GLY:H	1.67	0.60
1:C:362:ILE:CG2	1:C:363:HIS:N	2.64	0.60
1:D:391:ASP:O	1:D:395:TYR:HB2	2.01	0.60
1:B:164:PRO:HB2	1:B:197:PHE:HD2	1.66	0.60
1:C:360:LEU:HD12	1:C:361:TYR:N	2.16	0.60
1:C:261:GLU:HG2	1:C:382:LYS:NZ	2.13	0.60
1:A:64:ILE:HG13	1:A:65:GLN:N	2.16	0.60
1:C:216:LEU:HD23	1:C:216:LEU:C	2.23	0.60
1:A:222:PRO:HD2	1:A:225:ILE:CG1	2.26	0.59
1:B:355:PRO:HB3	1:B:360:LEU:HD11	1.84	0.59
1:A:216:LEU:HD23	1:A:216:LEU:C	2.23	0.59
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.68	0.59
1:D:222:PRO:HD2	1:D:225:ILE:CG1	2.26	0.59
1:B:64:ILE:HG13	1:B:65:GLN:N	2.17	0.59
1:B:77:ASP:HB3	1:B:233:MET:CG	2.31	0.59
1:B:367:ARG:CZ	1:B:369:GLY:HA2	2.32	0.59
1:C:354:LEU:HD21	1:C:379:ASN:HB3	1.84	0.59
1:D:367:ARG:NH1	1:D:369:GLY:HA2	2.17	0.59
1:A:246:LEU:HA	1:A:367:ARG:O	2.03	0.59
1:A:166:ARG:HH11	1:A:166:ARG:HB2	1.67	0.59
1:A:320:MET:HE1	1:A:331:LEU:HD22	1.83	0.59
1:B:116:ARG:HG2	1:B:141:ILE:CD1	2.25	0.59
1:D:166:ARG:HB2	1:D:166:ARG:HH11	1.68	0.59
1:D:336:VAL:HG23	1:D:336:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:HG3	1:A:116:ARG:HH11	1.68	0.59
1:D:381:VAL:O	1:D:381:VAL:HG23	2.03	0.59
1:B:279:GLN:HB3	1:B:323:PHE:CE1	2.38	0.58
1:B:362:ILE:HB	1:B:396:TYR:CE2	2.38	0.58
1:A:67:ARG:HG3	1:A:67:ARG:HH11	1.68	0.58
1:C:246:LEU:HB3	1:C:362:ILE:HD11	1.84	0.58
1:C:311:MET:HB3	1:C:312:PRO:HD2	1.85	0.58
1:D:116:ARG:HG2	1:D:141:ILE:HG21	1.85	0.58
1:D:255:PHE:HA	1:D:379:ASN:O	2.03	0.58
1:A:68:ALA:O	1:A:72:ILE:HG13	2.04	0.58
1:D:362:ILE:HD13	1:D:362:ILE:O	2.04	0.58
1:D:216:LEU:C	1:D:216:LEU:HD23	2.23	0.58
1:D:272:TYR:HA	1:D:275:LEU:HB3	1.86	0.58
1:B:216:LEU:C	1:B:216:LEU:HD23	2.23	0.58
1:C:362:ILE:HB	1:C:396:TYR:CZ	2.39	0.58
1:C:77:ASP:HB3	1:C:233:MET:HG2	1.86	0.58
1:B:140:CYS:O	1:B:141:ILE:HB	2.04	0.57
1:B:289:LYS:HD3	1:B:353:ASP:OD1	2.02	0.57
1:D:275:LEU:C	1:D:275:LEU:HD23	2.25	0.57
1:D:283:PHE:CE1	1:D:364:ARG:HG3	2.39	0.57
1:B:412:LEU:O	1:B:412:LEU:HD12	2.04	0.57
1:B:275:LEU:C	1:B:275:LEU:HD23	2.25	0.57
1:A:277:ILE:HG22	1:A:278:THR:HG22	1.86	0.57
1:A:348:LEU:HD22	1:A:410:LEU:HD11	1.87	0.57
1:B:388:ILE:O	1:B:392:ILE:HG13	2.03	0.57
1:D:141:ILE:CG2	1:D:142:GLY:N	2.67	0.57
1:A:282:ILE:HG12	1:A:350:ILE:HB	1.85	0.57
1:C:116:ARG:HG2	1:C:141:ILE:HG21	1.85	0.57
1:C:255:PHE:HA	1:C:379:ASN:O	2.04	0.57
1:D:275:LEU:HD23	1:D:276:THR:N	2.19	0.57
1:A:406:ASN:HB3	1:A:409:ASP:OD2	2.05	0.57
1:B:275:LEU:HD23	1:B:276:THR:N	2.19	0.57
1:D:311:MET:HB2	1:D:316:ARG:CD	2.35	0.57
1:B:166:ARG:HB2	1:B:166:ARG:NH1	2.19	0.57
1:A:254:PHE:HA	1:A:401:ASP:O	2.05	0.57
1:A:255:PHE:HA	1:A:379:ASN:O	2.04	0.57
1:A:274:THR:O	1:A:274:THR:HG22	2.03	0.57
1:B:390:ARG:O	1:B:394:GLN:HG2	2.05	0.57
1:B:255:PHE:HD2	1:B:400:ILE:HG22	1.69	0.56
1:D:246:LEU:HB3	1:D:362:ILE:HD11	1.87	0.56
1:B:246:LEU:HB3	1:B:362:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:THR:O	1:B:336:VAL:N	2.39	0.56
1:B:358:ARG:HD2	1:B:395:TYR:CD1	2.40	0.56
1:D:334:THR:O	1:D:336:VAL:N	2.38	0.56
1:B:96:VAL:HA	1:B:183:MET:HE1	1.88	0.56
1:D:316:ARG:HG3	1:D:316:ARG:NH1	2.21	0.56
1:D:349:ILE:HG21	1:D:365:ILE:HG22	1.87	0.56
1:A:297:MET:O	1:A:302:PHE:HB2	2.05	0.56
1:B:305:SER:O	1:B:331:LEU:HD12	2.04	0.56
1:A:272:TYR:HE1	1:A:330:VAL:HG21	1.70	0.56
1:B:362:ILE:CG2	1:B:363:HIS:N	2.69	0.56
1:D:282:ILE:HG12	1:D:350:ILE:HB	1.88	0.56
1:A:355:PRO:HB2	1:A:360:LEU:CD1	2.33	0.56
1:B:281:VAL:HB	1:B:349:ILE:HD13	1.86	0.56
1:C:275:LEU:HD21	1:C:330:VAL:HG22	1.87	0.56
1:C:412:LEU:HD12	1:C:412:LEU:O	2.05	0.56
1:B:304:VAL:HG12	1:B:330:VAL:CB	2.35	0.56
1:D:164:PRO:HB2	1:D:197:PHE:HD2	1.71	0.56
1:C:355:PRO:HB3	1:C:360:LEU:HD11	1.87	0.56
1:D:166:ARG:HB2	1:D:166:ARG:NH1	2.21	0.56
1:A:246:LEU:HD13	1:A:341:LEU:HG	1.88	0.55
1:B:346:VAL:HG22	1:B:347:SER:H	1.70	0.55
1:C:272:TYR:CZ	1:C:302:PHE:CD1	2.93	0.55
1:D:381:VAL:HG11	1:D:389:LEU:HD22	1.87	0.55
1:C:222:PRO:HD2	1:C:225:ILE:CG1	2.26	0.55
1:C:391:ASP:O	1:C:395:TYR:HB2	2.05	0.55
1:C:408:ALA:O	1:C:411:ILE:HG13	2.06	0.55
1:D:64:ILE:HG13	1:D:65:GLN:N	2.21	0.55
1:A:96:VAL:HA	1:A:183:MET:HE1	1.88	0.55
1:D:96:VAL:HA	1:D:183:MET:HE1	1.88	0.55
1:D:223:HIS:ND1	1:D:223:HIS:N	2.53	0.55
1:D:272:TYR:HD1	1:D:275:LEU:CD1	2.03	0.55
1:A:276:THR:HG22	1:A:329:ARG:HB3	1.88	0.55
1:B:96:VAL:HA	1:B:183:MET:CE	2.37	0.55
1:D:312:PRO:O	1:D:316:ARG:HG2	2.07	0.55
1:A:362:ILE:HD13	1:A:362:ILE:O	2.07	0.55
1:C:207:TYR:CA	1:D:210:PRO:HG3	2.22	0.55
1:A:112:LEU:HB2	1:A:192:MET:HE1	1.88	0.55
1:A:141:ILE:CG2	1:A:142:GLY:N	2.70	0.55
1:C:187:ASP:OD1	1:C:188:GLU:HG3	2.07	0.55
1:B:40:PHE:CZ	1:B:61:PRO:HB3	2.42	0.54
1:C:357:ASN:C	1:C:359:GLU:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASN:O	1:A:357:ASN:HB3	2.07	0.54
1:B:287:LYS:HD3	1:B:310:ASP:OD2	2.08	0.54
1:C:141:ILE:CG2	1:C:142:GLY:N	2.71	0.54
1:B:223:HIS:ND1	1:B:223:HIS:N	2.54	0.54
1:A:77:ASP:HB3	1:A:233:MET:HG2	1.88	0.54
1:C:164:PRO:HB2	1:C:197:PHE:HD2	1.72	0.54
1:A:187:ASP:OD1	1:A:188:GLU:HG3	2.07	0.54
1:D:345:GLN:O	1:D:345:GLN:HG3	2.08	0.54
1:A:275:LEU:CD2	1:A:276:THR:N	2.71	0.54
1:A:360:LEU:HA	1:A:363:HIS:HB3	1.89	0.54
1:B:111:ILE:O	1:B:161:ALA:HA	2.08	0.54
1:B:368:SER:O	1:B:370:ARG:N	2.39	0.54
1:D:367:ARG:CZ	1:D:369:GLY:HA2	2.37	0.54
1:D:123:GLN:HG2	1:D:127:LEU:HD12	1.89	0.54
1:B:168:PHE:HE1	1:B:207:TYR:CE2	2.26	0.53
1:C:331:LEU:HD12	1:C:332:ILE:H	1.73	0.53
1:D:187:ASP:OD1	1:D:188:GLU:HG3	2.09	0.53
1:D:168:PHE:HE1	1:D:207:TYR:CE2	2.27	0.53
1:C:96:VAL:HA	1:C:183:MET:CE	2.39	0.53
1:C:275:LEU:CD2	1:C:276:THR:N	2.71	0.53
1:D:92:PHE:O	1:D:95:SER:HB2	2.08	0.53
1:A:96:VAL:HA	1:A:183:MET:CE	2.39	0.53
1:A:163:THR:O	1:A:167:VAL:HG23	2.08	0.53
1:B:360:LEU:HA	1:B:363:HIS:HB3	1.90	0.53
1:A:123:GLN:HG2	1:A:127:LEU:HD12	1.91	0.53
1:A:360:LEU:C	1:A:360:LEU:CD1	2.77	0.53
1:B:146:VAL:HA	1:B:149:ASP:HB2	1.91	0.53
1:B:360:LEU:C	1:B:360:LEU:HD12	2.29	0.53
1:C:320:MET:O	1:C:321:LYS:C	2.47	0.53
1:D:290:VAL:HG13	1:D:332:ILE:HG22	1.91	0.53
1:A:272:TYR:CE2	1:A:302:PHE:HD1	2.27	0.53
1:D:396:TYR:O	1:D:397:SER:HB2	2.08	0.53
1:D:405:MET:SD	1:D:405:MET:N	2.82	0.53
1:A:349:ILE:O	1:A:377:ALA:HA	2.08	0.52
1:B:320:MET:CE	1:B:320:MET:HA	2.39	0.52
1:C:313:GLN:HA	1:C:316:ARG:HG3	1.91	0.52
1:D:255:PHE:HD2	1:D:400:ILE:HG22	1.74	0.52
1:C:77:ASP:OD2	1:C:233:MET:HA	2.08	0.52
1:C:249:GLU:O	1:C:367:ARG:HD3	2.10	0.52
1:D:329:ARG:O	1:D:330:VAL:HG23	2.10	0.52
1:D:395:TYR:HD2	1:D:396:TYR:CE1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HB2	1:A:166:ARG:NH1	2.24	0.52
1:A:283:PHE:CD1	1:A:364:ARG:HG2	2.45	0.52
1:C:367:ARG:NH1	1:C:369:GLY:HA2	2.24	0.52
1:A:276:THR:HG22	1:A:329:ARG:CB	2.40	0.52
1:B:346:VAL:HG22	1:B:347:SER:N	2.24	0.52
1:A:341:LEU:H	1:A:341:LEU:CD1	2.22	0.52
1:B:123:GLN:HG2	1:B:127:LEU:HD12	1.90	0.52
1:B:309:GLY:C	1:B:311:MET:H	2.13	0.52
1:B:349:ILE:O	1:B:377:ALA:HA	2.09	0.52
1:C:223:HIS:ND1	1:C:223:HIS:N	2.53	0.52
1:C:352:TYR:HA	1:C:380:PHE:CD2	2.45	0.52
1:C:413:GLU:HB3	1:D:174:ARG:HH22	1.73	0.52
1:D:96:VAL:HA	1:D:183:MET:CE	2.39	0.52
1:D:315:GLU:O	1:D:319:ILE:HG12	2.08	0.52
1:B:341:LEU:HD12	1:B:341:LEU:H	1.74	0.52
1:C:275:LEU:HD21	1:C:330:VAL:CG2	2.38	0.52
1:D:337:TRP:CD1	1:D:342:ASP:O	2.63	0.52
1:C:316:ARG:HG3	1:C:316:ARG:NH1	2.25	0.52
1:D:285:ASN:OD1	1:D:353:ASP:HB3	2.10	0.52
1:D:320:MET:HA	1:D:320:MET:HE2	1.92	0.52
1:A:168:PHE:HE1	1:A:207:TYR:CE2	2.27	0.52
1:A:174:ARG:HG2	1:A:174:ARG:HH11	1.74	0.52
1:A:272:TYR:O	1:A:275:LEU:HB3	2.10	0.52
1:D:77:ASP:HB3	1:D:233:MET:HG2	1.91	0.52
1:C:123:GLN:HG2	1:C:127:LEU:HD12	1.93	0.51
1:A:77:ASP:OD2	1:A:233:MET:HA	2.10	0.51
1:B:316:ARG:HG3	1:B:316:ARG:NH1	2.25	0.51
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.74	0.51
1:A:140:CYS:O	1:A:141:ILE:CB	2.59	0.51
1:A:320:MET:O	1:A:324:ARG:HG3	2.09	0.51
1:B:276:THR:C	1:B:278:THR:N	2.63	0.51
1:C:336:VAL:HG13	1:C:337:TRP:N	2.25	0.51
1:D:146:VAL:HA	1:D:149:ASP:HB2	1.92	0.51
1:C:111:ILE:O	1:C:161:ALA:HA	2.11	0.51
1:C:272:TYR:O	1:C:275:LEU:HB3	2.10	0.51
1:C:413:GLU:HA	1:D:174:ARG:NH2	2.25	0.51
1:A:40:PHE:CZ	1:A:61:PRO:HB3	2.45	0.51
1:A:385:ASP:C	1:A:387:ARG:N	2.62	0.51
1:D:77:ASP:OD2	1:D:233:MET:HA	2.11	0.51
1:A:276:THR:C	1:A:278:THR:N	2.63	0.51
1:B:312:PRO:O	1:B:316:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:THR:C	1:C:278:THR:N	2.63	0.51
1:A:285:ASN:OD1	1:A:353:ASP:CB	2.59	0.51
1:B:48:ASP:OD2	1:B:133:MET:HG2	2.10	0.51
1:B:77:ASP:HB3	1:B:233:MET:HG2	1.93	0.51
1:C:246:LEU:HD11	1:C:341:LEU:HG	1.92	0.51
1:C:255:PHE:CZ	1:C:402:GLU:HG3	2.46	0.51
1:D:76:ARG:HG3	1:D:76:ARG:HH11	1.76	0.51
1:D:320:MET:HB3	1:D:324:ARG:NH1	2.26	0.51
1:A:223:HIS:ND1	1:A:223:HIS:N	2.54	0.51
1:A:261:GLU:OE2	1:A:264:LYS:HD2	2.11	0.51
1:D:261:GLU:OE2	1:D:264:LYS:HD2	2.11	0.51
1:D:362:ILE:CG2	1:D:363:HIS:N	2.74	0.51
1:A:146:VAL:HA	1:A:149:ASP:HB2	1.93	0.50
1:A:205:TYR:HA	1:A:208:LEU:HD12	1.93	0.50
1:B:112:LEU:HB2	1:B:192:MET:HE1	1.93	0.50
1:D:272:TYR:CD1	1:D:275:LEU:CD1	2.75	0.50
1:D:333:SER:OG	1:D:334:THR:N	2.45	0.50
1:B:362:ILE:HG23	1:B:363:HIS:N	2.25	0.50
1:C:146:VAL:HA	1:C:149:ASP:HB2	1.92	0.50
1:C:261:GLU:OE2	1:C:264:LYS:HD2	2.11	0.50
1:C:272:TYR:CE2	1:C:302:PHE:HD1	2.29	0.50
1:A:111:ILE:O	1:A:161:ALA:HA	2.11	0.50
1:C:92:PHE:O	1:C:95:SER:HB2	2.12	0.50
1:C:322:GLU:O	1:C:325:SER:HB3	2.11	0.50
1:C:76:ARG:HH11	1:C:76:ARG:HG3	1.76	0.50
1:A:164:PRO:HB2	1:A:197:PHE:HD2	1.76	0.50
1:B:246:LEU:HD13	1:B:341:LEU:HG	1.94	0.50
1:D:140:CYS:O	1:D:141:ILE:CB	2.59	0.50
1:A:275:LEU:CD2	1:A:330:VAL:CG2	2.86	0.50
1:B:256:VAL:HG22	1:B:403:MET:SD	2.52	0.50
1:B:309:GLY:O	1:B:311:MET:N	2.44	0.50
1:B:385:ASP:C	1:B:387:ARG:N	2.62	0.50
1:A:307:MET:HE1	1:A:320:MET:HG2	1.93	0.50
1:C:40:PHE:CZ	1:C:61:PRO:HB3	2.47	0.50
1:D:321:LYS:O	1:D:325:SER:HB3	2.12	0.50
1:D:387:ARG:O	1:D:390:ARG:N	2.39	0.50
1:B:261:GLU:OE2	1:B:264:LYS:HD2	2.11	0.50
1:D:362:ILE:HB	1:D:396:TYR:CE2	2.46	0.50
1:C:96:VAL:HA	1:C:183:MET:HE1	1.93	0.49
1:C:178:THR:O	1:C:179:ARG:C	2.50	0.49
1:C:203:ASP:O	1:C:206:ARG:HB2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:PRO:CB	1:C:360:LEU:HD11	2.41	0.49
1:D:48:ASP:OD2	1:D:133:MET:HG2	2.12	0.49
1:D:320:MET:O	1:D:324:ARG:N	2.40	0.49
1:A:92:PHE:O	1:A:95:SER:HB2	2.11	0.49
1:A:190:ASP:HA	1:A:225:ILE:HD11	1.94	0.49
1:A:272:TYR:CE1	1:A:330:VAL:HG21	2.47	0.49
1:D:76:ARG:HG3	1:D:76:ARG:NH1	2.27	0.49
1:D:164:PRO:HD2	1:D:197:PHE:CD2	2.46	0.49
1:A:285:ASN:OD1	1:A:353:ASP:HB2	2.12	0.49
1:C:206:ARG:NH1	1:D:206:ARG:HD2	2.27	0.49
1:C:272:TYR:CE2	1:C:302:PHE:CD1	3.00	0.49
1:B:164:PRO:HD2	1:B:197:PHE:CD2	2.47	0.49
1:A:290:VAL:HG13	1:A:332:ILE:CG2	2.34	0.49
1:B:140:CYS:O	1:B:141:ILE:CB	2.61	0.49
1:B:181:ILE:HG21	1:B:208:LEU:CD2	2.42	0.49
1:A:388:ILE:O	1:A:392:ILE:HG13	2.12	0.49
1:D:275:LEU:CD2	1:D:276:THR:N	2.76	0.49
1:A:76:ARG:HG3	1:A:76:ARG:NH1	2.28	0.49
1:C:357:ASN:C	1:C:359:GLU:N	2.66	0.49
1:A:381:VAL:HG23	1:A:381:VAL:O	2.12	0.49
1:C:278:THR:OG1	1:C:279:GLN:N	2.46	0.49
1:A:40:PHE:CE1	1:A:61:PRO:HB3	2.48	0.49
1:A:197:PHE:O	1:A:201:ILE:HG12	2.13	0.49
1:C:394:GLN:HE21	1:C:394:GLN:HA	1.78	0.49
1:A:189:ALA:O	1:A:190:ASP:C	2.51	0.48
1:A:376:VAL:HG12	1:A:377:ALA:N	2.28	0.48
1:B:164:PRO:HB2	1:B:197:PHE:CD2	2.47	0.48
1:B:406:ASN:C	1:B:408:ALA:H	2.16	0.48
1:C:274:THR:HA	1:C:277:ILE:CD1	2.44	0.48
1:C:381:VAL:HG23	1:C:381:VAL:O	2.12	0.48
1:D:205:TYR:HA	1:D:208:LEU:HD12	1.94	0.48
1:D:276:THR:C	1:D:278:THR:N	2.63	0.48
1:D:278:THR:OG1	1:D:279:GLN:N	2.46	0.48
1:A:278:THR:OG1	1:A:279:GLN:N	2.46	0.48
1:B:112:LEU:O	1:B:192:MET:HE2	2.12	0.48
1:C:193:LEU:HD13	1:C:224:GLU:OE2	2.13	0.48
1:B:40:PHE:CE1	1:B:61:PRO:HB3	2.48	0.48
1:D:111:ILE:O	1:D:161:ALA:HA	2.13	0.48
1:D:404:PRO:O	1:D:406:ASN:N	2.46	0.48
1:A:279:GLN:CA	1:A:329:ARG:O	2.62	0.48
1:B:228:MET:HG2	1:B:232:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:THR:OG1	1:B:279:GLN:N	2.46	0.48
1:D:112:LEU:O	1:D:192:MET:HE2	2.12	0.48
1:A:228:MET:HG2	1:A:232:PHE:CZ	2.49	0.48
1:A:277:ILE:HG21	1:A:410:LEU:CD2	2.39	0.48
1:B:326:GLY:O	1:B:327:ALA:C	2.52	0.48
1:C:274:THR:HA	1:C:277:ILE:CG1	2.44	0.48
1:D:368:SER:O	1:D:370:ARG:N	2.46	0.48
1:C:413:GLU:CG	1:D:174:ARG:HH22	2.26	0.48
1:D:190:ASP:HA	1:D:225:ILE:HD11	1.96	0.48
1:B:133:MET:O	1:B:134:ASN:C	2.52	0.48
1:D:228:MET:HG2	1:D:232:PHE:CZ	2.49	0.48
1:B:146:VAL:O	1:B:150:ILE:HG13	2.14	0.48
1:B:252:LYS:HB2	1:B:376:VAL:HG22	1.95	0.48
1:B:275:LEU:CD2	1:B:276:THR:N	2.76	0.48
1:C:67:ARG:HG3	1:C:67:ARG:HH11	1.79	0.48
1:C:205:TYR:CZ	1:C:232:PHE:HB2	2.49	0.48
1:D:40:PHE:CZ	1:D:61:PRO:HB3	2.49	0.48
1:D:118:LEU:O	1:D:122:ILE:HG13	2.13	0.48
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.79	0.48
1:B:343:VAL:HG23	1:B:345:GLN:HE21	1.79	0.48
1:C:112:LEU:HB2	1:C:192:MET:HE3	1.96	0.48
1:D:146:VAL:O	1:D:150:ILE:HG13	2.14	0.48
1:A:178:THR:O	1:A:179:ARG:C	2.51	0.47
1:C:228:MET:HG2	1:C:232:PHE:CZ	2.49	0.47
1:D:279:GLN:CG	1:D:329:ARG:NH2	2.76	0.47
1:A:246:LEU:CD1	1:A:341:LEU:HG	2.44	0.47
1:C:48:ASP:OD2	1:C:133:MET:HG2	2.14	0.47
1:C:357:ASN:O	1:C:359:GLU:N	2.48	0.47
1:A:235:ASP:OD2	1:A:345:GLN:HG3	2.14	0.47
1:B:177:ARG:HG3	1:B:177:ARG:HH11	1.80	0.47
1:C:76:ARG:HG3	1:C:76:ARG:NH1	2.28	0.47
1:C:140:CYS:O	1:C:141:ILE:CB	2.61	0.47
1:D:205:TYR:CG	1:D:232:PHE:HD1	2.32	0.47
1:B:76:ARG:HG3	1:B:76:ARG:HH11	1.79	0.47
1:B:205:TYR:CZ	1:B:232:PHE:HB2	2.49	0.47
1:B:337:TRP:CZ2	1:B:344:PRO:HD3	2.50	0.47
1:C:360:LEU:O	1:C:363:HIS:N	2.47	0.47
1:A:297:MET:O	1:A:302:PHE:HD2	1.97	0.47
1:A:383:ASN:O	1:A:386:ILE:CG2	2.60	0.47
1:B:187:ASP:OD1	1:B:188:GLU:HG3	2.14	0.47
1:D:210:PRO:O	1:D:211:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:GLU:CG	1:C:382:LYS:NZ	2.77	0.47
1:D:77:ASP:HB3	1:D:233:MET:HG3	1.95	0.47
1:D:276:THR:O	1:D:329:ARG:NH1	2.48	0.47
1:A:146:VAL:O	1:A:150:ILE:HG13	2.15	0.47
1:A:205:TYR:CZ	1:A:232:PHE:HB2	2.49	0.47
1:D:112:LEU:HB2	1:D:192:MET:HE1	1.95	0.47
1:D:319:ILE:O	1:D:322:GLU:HB2	2.14	0.47
1:D:320:MET:HA	1:D:320:MET:CE	2.45	0.47
1:D:360:LEU:C	1:D:360:LEU:CD1	2.83	0.47
1:D:388:ILE:O	1:D:391:ASP:N	2.47	0.47
1:A:315:GLU:O	1:A:319:ILE:HG12	2.15	0.47
1:B:77:ASP:OD2	1:B:233:MET:HA	2.14	0.47
1:B:190:ASP:HA	1:B:225:ILE:HD11	1.95	0.47
1:C:77:ASP:HB3	1:C:233:MET:HG3	1.96	0.47
1:C:190:ASP:HA	1:C:225:ILE:HD11	1.97	0.47
1:D:205:TYR:CZ	1:D:232:PHE:HB2	2.49	0.47
1:A:341:LEU:HD12	1:A:341:LEU:N	2.26	0.47
1:C:390:ARG:HA	1:C:390:ARG:HD2	1.54	0.47
1:B:164:PRO:HD2	1:B:197:PHE:CE2	2.50	0.47
1:B:370:ARG:HG2	1:B:371:TYR:CE1	2.50	0.47
1:A:193:LEU:HD13	1:A:224:GLU:OE2	2.15	0.46
1:C:168:PHE:HE1	1:C:207:TYR:CE2	2.33	0.46
1:D:272:TYR:CZ	1:D:302:PHE:HD1	2.33	0.46
1:D:272:TYR:CA	1:D:275:LEU:HB3	2.45	0.46
1:A:227:GLU:O	1:A:231:LYS:HB2	2.16	0.46
1:B:197:PHE:O	1:B:201:ILE:HG12	2.14	0.46
1:B:275:LEU:HD21	1:B:330:VAL:CG2	2.45	0.46
1:B:77:ASP:HB3	1:B:233:MET:HG3	1.97	0.46
1:C:336:VAL:HG13	1:C:337:TRP:H	1.80	0.46
1:D:171:ILE:HG12	1:D:176:LEU:HD23	1.98	0.46
1:C:68:ALA:O	1:C:72:ILE:HG13	2.16	0.46
1:C:139:ALA:HA	1:C:161:ALA:O	2.15	0.46
1:C:269:CYS:O	1:C:272:TYR:HB3	2.16	0.46
1:C:360:LEU:C	1:C:360:LEU:CD1	2.84	0.46
1:D:178:THR:O	1:D:179:ARG:C	2.54	0.46
1:D:367:ARG:NH2	1:D:369:GLY:HA2	2.31	0.46
1:B:205:TYR:CG	1:B:232:PHE:HD1	2.32	0.46
1:B:355:PRO:CB	1:B:360:LEU:HD11	2.45	0.46
1:C:227:GLU:O	1:C:231:LYS:HB2	2.16	0.46
1:C:248:LEU:HD12	1:C:248:LEU:N	2.29	0.46
1:C:275:LEU:C	1:C:277:ILE:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:HG3	1:A:313:GLN:O	2.15	0.46
1:B:92:PHE:O	1:B:95:SER:HB2	2.15	0.46
1:B:116:ARG:CG	1:B:141:ILE:HG21	2.41	0.46
1:D:399:GLN:NE2	1:D:401:ASP:OD1	2.44	0.46
1:A:112:LEU:O	1:A:192:MET:HE2	2.15	0.46
1:C:349:ILE:HG22	1:C:350:ILE:N	2.30	0.46
1:C:360:LEU:O	1:C:361:TYR:C	2.53	0.46
1:D:197:PHE:O	1:D:198:LYS:C	2.54	0.46
1:D:197:PHE:O	1:D:201:ILE:HG12	2.15	0.46
1:A:79:ILE:HD13	1:A:229:THR:HG21	1.98	0.46
1:A:145:ASN:OD1	1:A:148:GLU:HB3	2.16	0.46
1:A:337:TRP:CD1	1:A:342:ASP:O	2.68	0.46
1:B:76:ARG:HG3	1:B:76:ARG:NH1	2.31	0.46
1:C:177:ARG:HG3	1:C:177:ARG:HH11	1.80	0.46
1:D:43:MET:CE	1:D:66:GLN:HG3	2.45	0.46
1:D:227:GLU:O	1:D:231:LYS:HB2	2.16	0.46
1:A:205:TYR:CG	1:A:232:PHE:HD1	2.32	0.46
1:A:275:LEU:C	1:A:277:ILE:N	2.70	0.46
1:A:320:MET:HA	1:A:320:MET:CE	2.46	0.46
1:B:320:MET:O	1:B:321:LYS:C	2.55	0.46
1:C:334:THR:O	1:C:336:VAL:N	2.49	0.46
1:C:339:ARG:HB2	1:C:342:ASP:OD2	2.16	0.46
1:C:341:LEU:H	1:C:341:LEU:CD1	2.26	0.46
1:D:136:GLN:O	1:D:158:HIS:HB2	2.16	0.46
1:D:275:LEU:C	1:D:277:ILE:N	2.70	0.45
1:D:345:GLN:O	1:D:345:GLN:CG	2.64	0.45
1:A:272:TYR:HA	1:A:275:LEU:HB3	1.97	0.45
1:B:307:MET:HG3	1:B:333:SER:HB2	1.97	0.45
1:C:307:MET:CE	1:C:319:ILE:HB	2.44	0.45
1:D:68:ALA:O	1:D:72:ILE:HG13	2.15	0.45
1:A:48:ASP:OD1	1:A:48:ASP:N	2.50	0.45
1:B:275:LEU:C	1:B:277:ILE:N	2.70	0.45
1:C:79:ILE:HD13	1:C:229:THR:HG21	1.98	0.45
1:D:174:ARG:HH11	1:D:174:ARG:HG2	1.81	0.45
1:D:248:LEU:HD12	1:D:248:LEU:N	2.29	0.45
1:B:227:GLU:O	1:B:231:LYS:HB2	2.16	0.45
1:C:164:PRO:HD2	1:C:197:PHE:CD2	2.52	0.45
1:D:106:GLU:O	1:D:108:GLN:HG3	2.17	0.45
1:A:311:MET:CB	1:A:312:PRO:HD2	2.43	0.45
1:A:355:PRO:CB	1:A:360:LEU:CD1	2.91	0.45
1:C:146:VAL:O	1:C:150:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ASN:OD1	1:C:353:ASP:HB2	2.15	0.45
1:A:77:ASP:HB3	1:A:233:MET:HG3	1.96	0.45
1:A:248:LEU:HD12	1:A:248:LEU:N	2.29	0.45
1:B:248:LEU:HD12	1:B:248:LEU:N	2.29	0.45
1:D:48:ASP:OD1	1:D:48:ASP:N	2.49	0.45
1:D:79:ILE:HD13	1:D:229:THR:HG21	1.99	0.45
1:D:210:PRO:O	1:D:211:ALA:CB	2.65	0.45
1:B:234:THR:O	1:B:235:ASP:C	2.55	0.45
1:B:362:ILE:C	1:B:364:ARG:N	2.68	0.45
1:D:40:PHE:CE1	1:D:61:PRO:HB3	2.51	0.45
1:D:234:THR:O	1:D:235:ASP:C	2.55	0.45
1:D:325:SER:OG	1:D:326:GLY:N	2.49	0.45
1:D:346:VAL:HG13	1:D:348:LEU:H	1.80	0.45
1:A:320:MET:O	1:A:321:LYS:C	2.53	0.45
1:A:358:ARG:O	1:A:395:TYR:CE2	2.70	0.45
1:B:191:GLU:OE1	1:B:191:GLU:HA	2.16	0.45
1:C:205:TYR:CG	1:C:232:PHE:HD1	2.34	0.45
1:D:164:PRO:HD2	1:D:197:PHE:CE2	2.51	0.45
1:D:193:LEU:HD13	1:D:224:GLU:OE2	2.17	0.45
1:B:106:GLU:O	1:B:108:GLN:HG3	2.17	0.45
1:B:136:GLN:O	1:B:158:HIS:HB2	2.17	0.45
1:C:112:LEU:O	1:C:192:MET:HE1	2.17	0.45
1:C:154:ASP:OD1	1:D:329:ARG:HG3	2.17	0.45
1:A:133:MET:O	1:A:134:ASN:C	2.55	0.45
1:B:189:ALA:O	1:B:190:ASP:C	2.55	0.45
1:D:133:MET:O	1:D:134:ASN:C	2.56	0.45
1:A:367:ARG:NH2	1:A:369:GLY:O	2.51	0.44
1:A:405:MET:O	1:A:407:VAL:HG13	2.17	0.44
1:B:178:THR:O	1:B:179:ARG:C	2.55	0.44
1:C:393:GLU:HG2	1:C:398:THR:O	2.17	0.44
1:A:76:ARG:CZ	1:A:324:ARG:NH2	2.80	0.44
1:A:191:GLU:OE1	1:A:191:GLU:HA	2.17	0.44
1:B:118:LEU:O	1:B:122:ILE:HG13	2.17	0.44
1:C:174:ARG:HG2	1:C:174:ARG:HH11	1.81	0.44
1:A:315:GLU:O	1:A:318:SER:HB3	2.18	0.44
1:B:396:TYR:O	1:B:397:SER:C	2.53	0.44
1:C:92:PHE:CD1	1:C:92:PHE:C	2.90	0.44
1:B:187:ASP:HA	1:B:217:ILE:HB	1.99	0.44
1:D:145:ASN:OD1	1:D:148:GLU:HB3	2.17	0.44
1:D:360:LEU:O	1:D:363:HIS:HB3	2.17	0.44
1:D:381:VAL:O	1:D:381:VAL:CG2	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:O	1:A:235:ASP:C	2.55	0.44
1:A:407:VAL:C	1:A:409:ASP:H	2.21	0.44
1:B:67:ARG:HG3	1:B:67:ARG:HH11	1.82	0.44
1:C:363:HIS:ND1	1:C:363:HIS:C	2.70	0.44
1:A:354:LEU:CG	1:A:381:VAL:HG12	2.47	0.44
1:B:281:VAL:HB	1:B:349:ILE:CD1	2.48	0.44
1:C:40:PHE:CE1	1:C:61:PRO:HB3	2.53	0.44
1:B:193:LEU:HD13	1:B:224:GLU:OE2	2.18	0.44
1:C:43:MET:CE	1:C:66:GLN:HG3	2.48	0.44
1:C:171:ILE:HG12	1:C:176:LEU:HD23	2.00	0.44
1:C:234:THR:O	1:C:235:ASP:C	2.55	0.44
1:D:177:ARG:HG3	1:D:177:ARG:HH11	1.81	0.44
1:A:293:LEU:HG	1:A:332:ILE:HD13	2.00	0.44
1:A:312:PRO:C	1:A:314:LYS:H	2.21	0.44
1:B:48:ASP:OD1	1:B:48:ASP:N	2.51	0.44
1:B:303:THR:HG23	1:B:329:ARG:HB2	2.00	0.44
1:A:336:VAL:HG13	1:A:337:TRP:N	2.33	0.44
1:A:116:ARG:CG	1:A:141:ILE:HG21	2.47	0.43
1:B:68:ALA:O	1:B:72:ILE:HG13	2.17	0.43
1:A:48:ASP:OD2	1:A:133:MET:HG2	2.18	0.43
1:A:354:LEU:HG	1:A:381:VAL:HG12	2.00	0.43
1:C:154:ASP:C	1:C:156:GLY:N	2.71	0.43
1:C:191:GLU:HA	1:C:191:GLU:OE1	2.18	0.43
1:B:145:ASN:OD1	1:B:148:GLU:HB3	2.18	0.43
1:D:228:MET:CG	1:D:232:PHE:CZ	3.02	0.43
1:A:164:PRO:HD2	1:A:197:PHE:CD2	2.53	0.43
1:C:197:PHE:O	1:C:198:LYS:C	2.57	0.43
1:C:297:MET:O	1:C:302:PHE:HD2	2.01	0.43
1:D:323:PHE:O	1:D:324:ARG:C	2.56	0.43
1:A:120:VAL:O	1:A:123:GLN:HB3	2.19	0.43
1:B:51:ARG:HD3	1:B:132:TYR:CD2	2.54	0.43
1:C:320:MET:HB3	1:C:324:ARG:NH1	2.33	0.43
1:D:164:PRO:HB2	1:D:197:PHE:CD2	2.53	0.43
1:A:228:MET:CG	1:A:232:PHE:CZ	3.02	0.43
1:B:228:MET:CG	1:B:232:PHE:CZ	3.02	0.43
1:D:172:ARG:C	1:D:174:ARG:H	2.22	0.43
1:A:233:MET:HG2	1:A:236:PRO:HB3	2.01	0.43
1:C:172:ARG:C	1:C:174:ARG:H	2.22	0.43
1:C:228:MET:CG	1:C:232:PHE:CZ	3.02	0.43
1:C:287:LYS:HD3	1:C:310:ASP:OD2	2.17	0.43
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HG12	1:A:176:LEU:HD23	2.00	0.43
1:A:312:PRO:O	1:A:314:LYS:N	2.52	0.43
1:D:67:ARG:HH11	1:D:67:ARG:HG3	1.84	0.43
1:A:354:LEU:HD21	1:A:379:ASN:HB3	2.00	0.43
1:A:387:ARG:O	1:A:390:ARG:N	2.52	0.43
1:B:154:ASP:C	1:B:156:GLY:N	2.71	0.43
1:B:354:LEU:HD11	1:B:381:VAL:HG12	2.01	0.43
1:C:197:PHE:O	1:C:201:ILE:HG12	2.17	0.43
1:D:282:ILE:HG23	1:D:352:TYR:HB2	2.01	0.43
1:D:316:ARG:NH1	1:D:316:ARG:CG	2.80	0.43
1:A:187:ASP:HA	1:A:217:ILE:HB	2.00	0.43
1:C:116:ARG:CG	1:C:141:ILE:HG21	2.49	0.43
1:D:264:LYS:HB3	1:D:352:TYR:CE1	2.54	0.43
1:D:360:LEU:HD12	1:D:361:TYR:N	2.32	0.43
1:A:339:ARG:HG3	1:A:339:ARG:HH11	1.83	0.42
1:B:385:ASP:O	1:B:387:ARG:N	2.52	0.42
1:C:145:ASN:OD1	1:C:148:GLU:HB3	2.18	0.42
1:B:43:MET:CE	1:B:66:GLN:HG3	2.48	0.42
1:B:233:MET:HG2	1:B:236:PRO:HB3	2.01	0.42
1:B:275:LEU:C	1:B:277:ILE:H	2.23	0.42
1:C:275:LEU:C	1:C:275:LEU:CD2	2.87	0.42
1:D:390:ARG:O	1:D:394:GLN:HG2	2.19	0.42
1:C:48:ASP:OD1	1:C:48:ASP:N	2.52	0.42
1:C:51:ARG:HD3	1:C:132:TYR:CD2	2.54	0.42
1:C:101:ASP:H	1:C:108:GLN:HE22	1.67	0.42
1:D:120:VAL:O	1:D:123:GLN:HB3	2.20	0.42
1:A:197:PHE:O	1:A:198:LYS:C	2.57	0.42
1:C:187:ASP:HA	1:C:217:ILE:HB	2.00	0.42
1:C:297:MET:O	1:C:302:PHE:HB2	2.19	0.42
1:D:272:TYR:CE2	1:D:302:PHE:CD1	3.07	0.42
1:D:336:VAL:O	1:D:337:TRP:CG	2.72	0.42
1:D:362:ILE:HG23	1:D:363:HIS:N	2.34	0.42
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.92	0.42
1:B:246:LEU:HB3	1:B:362:ILE:HD11	1.99	0.42
1:C:361:TYR:O	1:C:365:ILE:HG12	2.20	0.42
1:D:116:ARG:CG	1:D:141:ILE:HG21	2.49	0.42
1:D:254:PHE:HA	1:D:401:ASP:O	2.19	0.42
1:A:275:LEU:C	1:A:277:ILE:H	2.23	0.42
1:A:385:ASP:O	1:A:386:ILE:C	2.58	0.42
1:B:281:VAL:HG22	1:B:331:LEU:HD23	2.01	0.42
1:B:335:ASP:OD1	1:B:363:HIS:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:CYS:O	1:C:272:TYR:N	2.46	0.42
1:D:360:LEU:HA	1:D:363:HIS:HB3	2.00	0.42
1:D:402:GLU:O	1:D:404:PRO:HD3	2.20	0.42
1:A:92:PHE:CD1	1:A:92:PHE:C	2.93	0.42
1:A:118:LEU:O	1:A:122:ILE:HG13	2.19	0.42
1:A:360:LEU:HA	1:A:363:HIS:CB	2.49	0.42
1:A:360:LEU:CA	1:A:363:HIS:HB3	2.50	0.42
1:B:92:PHE:CD1	1:B:92:PHE:C	2.92	0.42
1:C:133:MET:O	1:C:134:ASN:C	2.56	0.42
1:C:233:MET:HG2	1:C:236:PRO:HB3	2.01	0.42
1:C:274:THR:CA	1:C:277:ILE:HG13	2.48	0.42
1:D:171:ILE:CG1	1:D:176:LEU:HD23	2.49	0.42
1:D:189:ALA:O	1:D:190:ASP:C	2.55	0.42
1:D:334:THR:OG1	1:D:336:VAL:CG1	2.61	0.42
1:A:171:ILE:CD1	1:A:204:VAL:HG13	2.50	0.42
1:B:271:LEU:O	1:B:272:TYR:C	2.57	0.42
1:C:359:GLU:HA	1:C:359:GLU:OE1	2.20	0.42
1:D:336:VAL:O	1:D:337:TRP:CD2	2.73	0.42
1:A:285:ASN:OD1	1:A:353:ASP:HB3	2.20	0.42
1:B:171:ILE:HG12	1:B:176:LEU:HD23	2.02	0.42
1:B:265:PHE:CE1	1:B:269:CYS:SG	3.13	0.42
1:B:301:ASN:C	1:B:301:ASN:HD22	2.23	0.42
1:B:320:MET:HA	1:B:320:MET:HE2	2.02	0.42
1:B:360:LEU:HD12	1:B:360:LEU:O	2.19	0.42
1:B:385:ASP:C	1:B:387:ARG:H	2.23	0.42
1:C:106:GLU:O	1:C:108:GLN:HG3	2.20	0.42
1:C:222:PRO:C	1:C:224:GLU:H	2.23	0.42
1:A:51:ARG:HD3	1:A:132:TYR:CD2	2.54	0.42
1:A:403:MET:HA	1:A:404:PRO:HD3	1.79	0.42
1:B:171:ILE:CD1	1:B:204:VAL:HG13	2.50	0.42
1:B:246:LEU:CD1	1:B:341:LEU:HG	2.50	0.42
1:B:382:LYS:O	1:B:383:ASN:C	2.58	0.42
1:C:410:LEU:O	1:C:410:LEU:HD23	2.20	0.42
1:D:335:ASP:OD2	1:D:364:ARG:HD3	2.20	0.42
1:A:226:LEU:HA	1:A:229:THR:OG1	2.20	0.41
1:C:136:GLN:O	1:C:158:HIS:HB2	2.20	0.41
1:C:226:LEU:HA	1:C:229:THR:OG1	2.20	0.41
1:D:233:MET:HG2	1:D:236:PRO:HB3	2.01	0.41
1:D:382:LYS:O	1:D:383:ASN:C	2.58	0.41
1:B:197:PHE:O	1:B:198:LYS:C	2.58	0.41
1:B:255:PHE:CD2	1:B:400:ILE:HG22	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:VAL:HG23	1:B:343:VAL:O	2.20	0.41
1:D:40:PHE:CZ	1:D:58:PHE:CD2	3.08	0.41
1:A:90:ALA:O	1:A:91:THR:C	2.57	0.41
1:A:274:THR:O	1:A:274:THR:CG2	2.67	0.41
1:B:222:PRO:C	1:B:224:GLU:H	2.23	0.41
1:B:272:TYR:CZ	1:B:302:PHE:HD1	2.38	0.41
1:B:274:THR:HA	1:B:277:ILE:HG13	2.03	0.41
1:D:272:TYR:C	1:D:275:LEU:HB3	2.39	0.41
1:A:154:ASP:C	1:A:156:GLY:N	2.73	0.41
1:A:319:ILE:O	1:A:322:GLU:HB2	2.21	0.41
1:B:282:ILE:HG12	1:B:350:ILE:HB	2.02	0.41
1:C:171:ILE:CD1	1:C:204:VAL:HG13	2.49	0.41
1:C:252:LYS:HB2	1:C:376:VAL:HG22	2.02	0.41
1:C:253:GLN:HE22	1:C:398:THR:HG21	1.85	0.41
1:C:274:THR:C	1:C:277:ILE:HG13	2.41	0.41
1:C:345:GLN:O	1:C:345:GLN:HG2	2.20	0.41
1:D:40:PHE:CZ	1:D:58:PHE:HD2	2.39	0.41
1:D:275:LEU:C	1:D:277:ILE:H	2.23	0.41
1:A:88:LYS:HD2	1:A:88:LYS:HA	1.92	0.41
1:A:265:PHE:CE1	1:A:269:CYS:SG	3.13	0.41
1:B:210:PRO:O	1:B:211:ALA:CB	2.64	0.41
1:D:46:ARG:CZ	1:D:133:MET:HE3	2.50	0.41
1:D:139:ALA:HA	1:D:161:ALA:O	2.20	0.41
1:D:187:ASP:HA	1:D:217:ILE:HB	2.03	0.41
1:D:265:PHE:CE1	1:D:269:CYS:SG	3.13	0.41
1:B:155:TYR:O	1:B:155:TYR:CD1	2.74	0.41
1:C:265:PHE:CE1	1:C:269:CYS:SG	3.13	0.41
1:D:154:ASP:C	1:D:156:GLY:N	2.71	0.41
1:D:226:LEU:HA	1:D:229:THR:OG1	2.20	0.41
1:D:279:GLN:HB3	1:D:323:PHE:CZ	2.55	0.41
1:D:305:SER:O	1:D:331:LEU:HD12	2.21	0.41
1:A:275:LEU:C	1:A:275:LEU:CD2	2.87	0.41
1:B:172:ARG:C	1:B:174:ARG:H	2.22	0.41
1:B:357:ASN:O	1:B:358:ARG:C	2.59	0.41
1:D:275:LEU:HD21	1:D:330:VAL:HG23	1.99	0.41
1:D:386:ILE:HD12	1:D:386:ILE:HA	1.88	0.41
1:C:341:LEU:HD12	1:C:341:LEU:N	2.29	0.41
1:D:227:GLU:OE2	1:D:227:GLU:HA	2.21	0.41
1:D:390:ARG:HD2	1:D:390:ARG:HA	1.79	0.41
1:A:43:MET:CE	1:A:66:GLN:HG3	2.50	0.41
1:A:281:VAL:HG23	1:A:346:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HD13	1:B:229:THR:HG21	2.02	0.41
1:B:226:LEU:HA	1:B:229:THR:OG1	2.20	0.41
1:C:164:PRO:HB2	1:C:197:PHE:CD2	2.53	0.41
1:C:189:ALA:O	1:C:190:ASP:C	2.59	0.41
1:C:275:LEU:C	1:C:277:ILE:H	2.23	0.41
1:C:367:ARG:HH12	1:C:369:GLY:HA2	1.85	0.41
1:D:40:PHE:CE2	1:D:58:PHE:HD2	2.38	0.41
1:D:40:PHE:HZ	1:D:58:PHE:CE2	2.38	0.41
1:D:87:GLY:C	1:D:89:THR:H	2.24	0.41
1:D:337:TRP:CG	1:D:342:ASP:O	2.74	0.41
1:A:74:LYS:HD2	1:A:317:GLU:OE2	2.21	0.41
1:A:367:ARG:CZ	1:A:369:GLY:HA2	2.51	0.41
1:B:64:ILE:CG1	1:B:65:GLN:N	2.84	0.41
1:C:203:ASP:O	1:C:206:ARG:HB3	2.20	0.41
1:C:203:ASP:HA	1:C:206:ARG:HB2	2.01	0.41
1:D:362:ILE:HB	1:D:396:TYR:CZ	2.55	0.41
1:A:362:ILE:HB	1:A:396:TYR:CZ	2.56	0.40
1:B:141:ILE:HD11	1:B:163:THR:OG1	2.21	0.40
1:D:69:ILE:O	1:D:70:LYS:C	2.59	0.40
1:D:92:PHE:CD1	1:D:92:PHE:C	2.94	0.40
1:D:222:PRO:C	1:D:224:GLU:H	2.23	0.40
1:A:136:GLN:O	1:A:158:HIS:HB2	2.21	0.40
1:A:381:VAL:HG11	1:A:389:LEU:HD13	2.02	0.40
1:B:313:GLN:HA	1:B:316:ARG:HG3	2.02	0.40
1:C:116:ARG:HG3	1:C:116:ARG:NH1	2.34	0.40
1:A:174:ARG:HG2	1:A:174:ARG:NH1	2.35	0.40
1:B:90:ALA:O	1:B:91:THR:C	2.59	0.40
1:D:289:LYS:HD3	1:D:353:ASP:OD1	2.22	0.40
1:A:67:ARG:O	1:A:68:ALA:C	2.60	0.40
1:A:78:VAL:HG12	1:A:79:ILE:N	2.36	0.40
1:A:232:PHE:CD2	1:A:232:PHE:N	2.89	0.40
1:B:320:MET:O	1:B:322:GLU:N	2.54	0.40
1:C:335:ASP:OD1	1:C:363:HIS:CE1	2.74	0.40
1:D:87:GLY:C	1:D:89:THR:N	2.75	0.40
1:D:312:PRO:HG2	1:D:315:GLU:HB3	2.02	0.40
1:A:105:ARG:NH1	1:A:155:TYR:CE1	2.90	0.40
1:A:222:PRO:C	1:A:224:GLU:H	2.23	0.40
1:A:314:LYS:O	1:A:318:SER:HB2	2.22	0.40
1:C:90:ALA:O	1:C:91:THR:C	2.59	0.40
1:D:272:TYR:CD2	1:D:302:PHE:HE1	2.40	0.40
1:D:272:TYR:CE1	1:D:275:LEU:HD22	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:NH2	1:B:326:GLY:O[2_555]	2.10	0.10

### 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	374/391 (96%)	309 (83%)	55 (15%)	10 (3%)	5	26
1	B	374/391 (96%)	297 (79%)	68 (18%)	9 (2%)	6	28
1	C	374/391 (96%)	303 (81%)	62 (17%)	9 (2%)	6	28
1	D	374/391 (96%)	300 (80%)	64 (17%)	10 (3%)	5	26
All	All	1496/1564 (96%)	1209 (81%)	249 (17%)	38 (2%)	5	27

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ILE
1	A	406	ASN
1	B	141	ILE
1	B	310	ASP
1	C	141	ILE
1	D	141	ILE
1	A	179	ARG
1	A	313	GLN
1	A	342	ASP
1	A	357	ASN
1	A	358	ARG
1	B	179	ARG
1	B	335	ASP
1	B	406	ASN
1	C	179	ARG

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Mol	Chain	Res	Type
1	C	316	ARG
1	D	179	ARG
1	D	211	ALA
1	D	345	GLN
1	D	405	MET
1	C	358	ARG
1	C	411	ILE
1	D	103	GLN
1	D	342	ASP
1	A	103	GLN
1	A	210	PRO
1	B	103	GLN
1	B	369	GLY
1	B	384	ASP
1	C	103	GLN
1	B	344	PRO
1	C	322	GLU
1	D	383	ASN
1	C	301	ASN
1	D	369	GLY
1	C	326	GLY
1	A	146	VAL
1	D	146	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	331/346 (96%)	299 (90%)	32 (10%)	8 29
1	B	331/346 (96%)	304 (92%)	27 (8%)	11 36
1	C	331/346 (96%)	298 (90%)	33 (10%)	7 27
1	D	331/346 (96%)	302 (91%)	29 (9%)	10 33
All	All	1324/1384 (96%)	1203 (91%)	121 (9%)	9 31

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	82	SER
1	A	84	SER
1	A	141	ILE
1	A	166	ARG
1	A	172	ARG
1	A	174	ARG
1	A	192	MET
1	A	200	GLN
1	A	210	PRO
1	A	223	HIS
1	A	224	GLU
1	A	227	GLU
1	A	232	PHE
1	A	246	LEU
1	A	248	LEU
1	A	249	GLU
1	A	260	ARG
1	A	275	LEU
1	A	276	THR
1	A	277	ILE
1	A	278	THR
1	A	301	ASN
1	A	324	ARG
1	A	344	PRO
1	A	345	GLN
1	A	354	LEU
1	A	358	ARG
1	A	360	LEU
1	A	362	ILE
1	A	378	ILE
1	A	386	ILE
1	B	64	ILE
1	B	82	SER
1	B	84	SER
1	B	166	ARG
1	B	172	ARG
1	B	174	ARG
1	B	192	MET
1	B	200	GLN
1	B	223	HIS
1	B	224	GLU
1	B	227	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	232	PHE
1	B	246	LEU
1	B	248	LEU
1	B	249	GLU
1	B	260	ARG
1	B	276	THR
1	B	278	THR
1	B	301	ASN
1	B	303	THR
1	B	307	MET
1	B	324	ARG
1	B	325	SER
1	B	329	ARG
1	B	362	ILE
1	B	386	ILE
1	B	398	THR
1	C	64	ILE
1	C	82	SER
1	C	84	SER
1	C	141	ILE
1	C	166	ARG
1	C	172	ARG
1	C	174	ARG
1	C	191	GLU
1	C	192	MET
1	C	200	GLN
1	C	223	HIS
1	C	224	GLU
1	C	227	GLU
1	C	232	PHE
1	C	246	LEU
1	C	248	LEU
1	C	249	GLU
1	C	260	ARG
1	C	271	LEU
1	C	273	ASP
1	C	276	THR
1	C	278	THR
1	C	303	THR
1	C	305	SER
1	C	343	VAL
1	C	358	ARG

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Mol	Chain	Res	Type
1	C	359	GLU
1	C	362	ILE
1	C	363	HIS
1	C	364	ARG
1	C	397	SER
1	C	405	MET
1	C	412	LEU
1	D	64	ILE
1	D	82	SER
1	D	84	SER
1	D	141	ILE
1	D	166	ARG
1	D	172	ARG
1	D	174	ARG
1	D	192	MET
1	D	200	GLN
1	D	223	HIS
1	D	224	GLU
1	D	227	GLU
1	D	232	PHE
1	D	246	LEU
1	D	248	LEU
1	D	249	GLU
1	D	260	ARG
1	D	276	THR
1	D	278	THR
1	D	301	ASN
1	D	303	THR
1	D	307	MET
1	D	325	SER
1	D	343	VAL
1	D	358	ARG
1	D	360	LEU
1	D	362	ILE
1	D	364	ARG
1	D	403	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	121	GLN

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Mol	Chain	Res	Type
1	A	123	GLN
1	A	200	GLN
1	A	253	GLN
1	A	301	ASN
1	A	345	GLN
1	A	394	GLN
1	B	103	GLN
1	B	123	GLN
1	B	200	GLN
1	B	301	ASN
1	B	345	GLN
1	C	103	GLN
1	C	108	GLN
1	C	121	GLN
1	C	123	GLN
1	C	200	GLN
1	C	253	GLN
1	C	285	ASN
1	C	301	ASN
1	C	394	GLN
1	D	103	GLN
1	D	121	GLN
1	D	123	GLN
1	D	200	GLN
1	D	285	ASN
1	D	301	ASN
1	D	394	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	376/391 (96%)	-0.07	8 (2%) 63 62	4, 45, 113, 151	0
1	B	376/391 (96%)	-0.09	9 (2%) 59 56	6, 52, 129, 173	0
1	C	376/391 (96%)	-0.10	8 (2%) 63 62	3, 49, 126, 165	0
1	D	376/391 (96%)	0.06	13 (3%) 44 42	9, 62, 135, 156	0
All	All	1504/1564 (96%)	-0.05	38 (2%) 57 54	3, 51, 127, 173	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	GLU	6.1
1	B	272	TYR	3.9
1	A	313	GLN	3.6
1	C	299	GLU	3.3
1	C	310	ASP	3.3
1	D	250	GLY	3.3
1	A	308	HIS	3.2
1	B	299	GLU	3.2
1	B	314	LYS	3.1
1	D	272	TYR	3.0
1	B	141	ILE	2.9
1	D	157	GLN	2.9
1	A	309	GLY	2.8
1	B	275	LEU	2.6
1	D	300	ALA	2.5
1	A	316	ARG	2.5
1	C	277	ILE	2.5
1	B	295	GLU	2.5
1	D	407	VAL	2.5
1	D	59	GLU	2.5
1	C	303	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	138	HIS	2.4
1	A	155	TYR	2.3
1	D	262	GLU	2.3
1	B	250	GLY	2.3
1	B	276	THR	2.3
1	D	144	THR	2.3
1	D	413	GLU	2.3
1	A	146	VAL	2.3
1	C	144	THR	2.2
1	D	136	GLN	2.2
1	D	158	HIS	2.2
1	A	274	THR	2.1
1	B	277	ILE	2.1
1	D	105	ARG	2.1
1	C	141	ILE	2.1
1	C	311	MET	2.1
1	C	405	MET	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.