



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 06:11 AM EDT

PDB ID : 3N6V  
Title : Structure of the GluA2 NTD-dimer interface mutant, T78A  
Authors : Rossmann, M.; Sukumaran, M.; Greger, I.H.  
Deposited on : 2010-05-26  
Resolution : 3.20 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

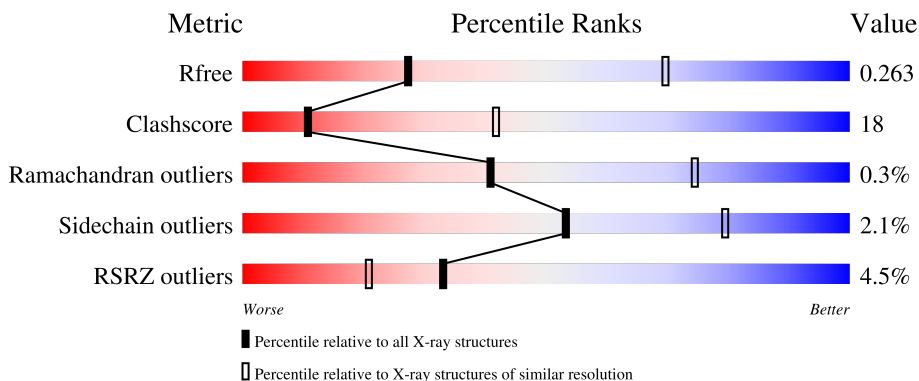
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.



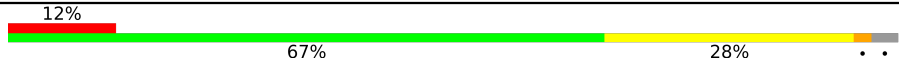
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	374	 73% 25% ..
1	B	374	 72% 26% ..
1	C	374	 2% 70% 28% ..
1	D	374	 2% 70% 27% ..
1	E	374	 8% 74% 21% ..

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Mol	Chain	Length	Quality of chain
1	F	374	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a red segment on the left labeled '12%', a green segment in the middle labeled '67%', and a yellow segment on the right labeled '28%'. At the far right end of the bar, there are two small black dots.</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17102 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	Total 2892	C 1846	N 487	O 551	S 8	0	0	0
1	B	372	Total 2923	C 1865	N 493	O 557	S 8	0	0	0
1	C	369	Total 2826	C 1810	N 461	O 547	S 8	0	0	0
1	D	368	Total 2854	C 1822	N 476	O 548	S 8	0	0	0
1	E	366	Total 2678	C 1713	N 429	O 527	S 9	0	0	1
1	F	364	Total 2791	C 1779	N 467	O 537	S 8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ALA	THR	engineered mutation	UNP P19491
B	78	ALA	THR	engineered mutation	UNP P19491
C	78	ALA	THR	engineered mutation	UNP P19491
D	78	ALA	THR	engineered mutation	UNP P19491
E	78	ALA	THR	engineered mutation	UNP P19491
F	78	ALA	THR	engineered mutation	UNP P19491

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	O 23	0	0
2	B	41	Total 41	O 41	0	0
2	C	26	Total 26	O 26	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	D	26	Total 26	O 26	0	0
2	E	11	Total 11	O 11	0	0
2	F	11	Total 11	O 11	0	0

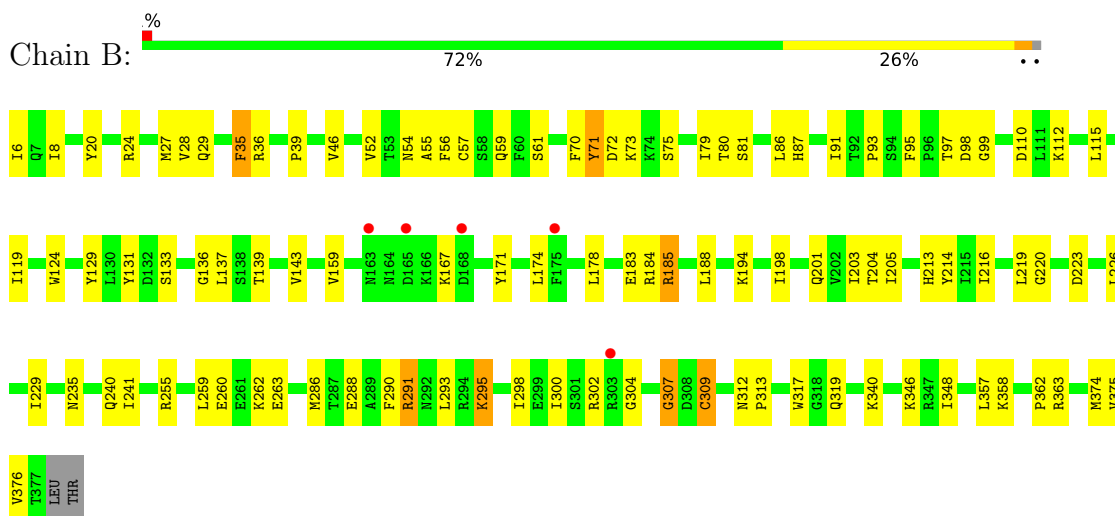
### 3 Residue-property plots [i](#)

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.

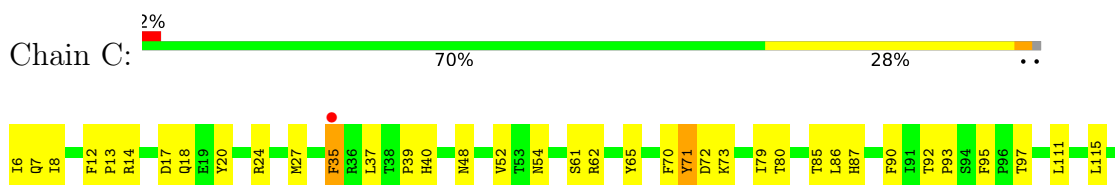
- Molecule 1: Glutamate receptor 2

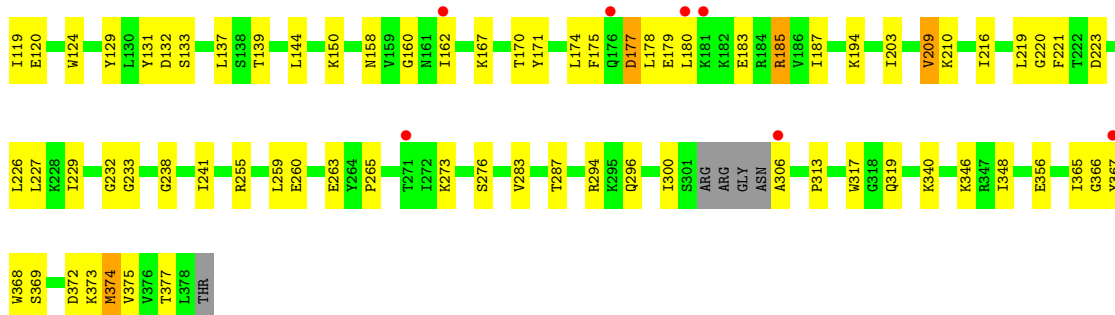


- Molecule 1: Glutamate receptor 2

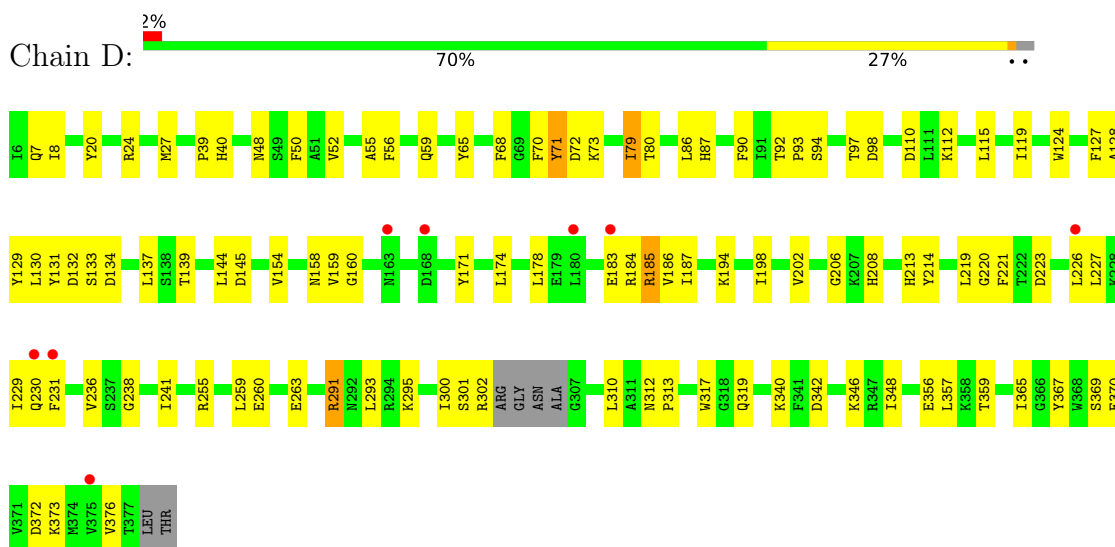


- Molecule 1: Glutamate receptor 2

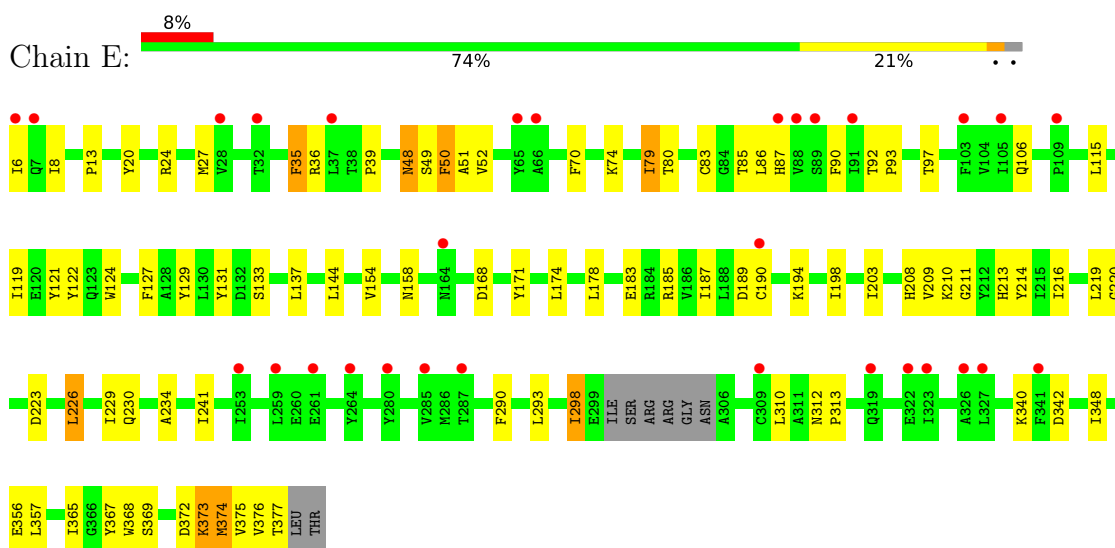




- Molecule 1: Glutamate receptor 2

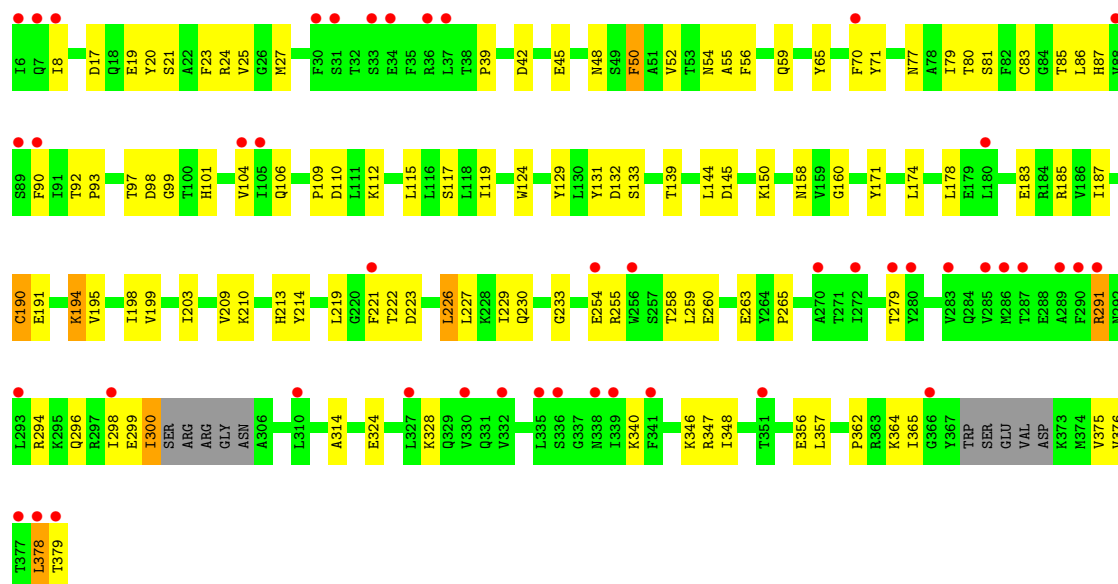


- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.21Å 120.15Å 360.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.78 – 3.20 53.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.78-3.20) 99.9 (53.78-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, $R_{free}$	0.235 , 0.265 0.231 , 0.263	Depositor DCC
$R_{free}$ test set	1890 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.53	0/2953	0.63	1/4009 (0.0%)
1	B	0.56	0/2985	0.67	2/4047 (0.0%)
1	C	0.57	0/2887	0.62	0/3931
1	D	0.52	0/2914	0.62	0/3960
1	E	0.54	0/2734	0.58	0/3745
1	F	0.56	0/2843	0.62	1/3856 (0.0%)
All	All	0.55	0/17316	0.62	4/23548 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	GLY	N-CA-C	7.82	132.64	113.10
1	F	222	THR	N-CA-C	7.14	130.28	111.00
1	B	309	CYS	N-CA-CB	-6.83	98.31	110.60
1	A	305	ASN	CB-CA-C	6.08	122.56	110.40

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	2892	0	2783	97	0
1	B	2923	0	2836	92	3
1	C	2826	0	2657	97	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2854	0	2720	96	0
1	E	2678	0	2401	130	0
1	F	2791	0	2666	118	0
2	A	23	0	0	3	0
2	B	41	0	0	4	0
2	C	26	0	0	3	0
2	D	26	0	0	4	0
2	E	11	0	0	7	0
2	F	11	0	0	3	0
All	All	17102	0	16063	603	3

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 18.

All (603) 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:E:124:TRP:CZ3	1:E:185:ARG:HB3	1.53	1.41
1:C:62:ARG:HD2	2:C:401:HOH:O	1.37	1.23
1:F:112:LYS:HG2	1:F:139:THR:HG22	1.27	1.14
1:B:57:CYS:CB	1:B:309:CYS:SG	2.38	1.10
1:F:50:PHE:O	1:F:54:ASN:ND2	1.83	1.10
1:C:367:TYR:CZ	1:C:375:VAL:HG21	1.88	1.08
1:D:227:LEU:O	1:D:227:LEU:HD23	1.54	1.07
1:D:160:GLY:HA2	1:D:194:LYS:HE2	1.36	1.07
1:E:369:SER:HB3	1:E:372:ASP:HB2	1.40	1.03
1:C:72:ASP:OD1	1:C:73:LYS:N	1.90	1.03
1:E:85:THR:HG21	1:F:50:PHE:CE1	1.94	1.01
1:E:124:TRP:CH2	1:E:185:ARG:HB3	1.94	1.00
1:F:50:PHE:CD2	1:F:54:ASN:ND2	2.30	0.99
1:E:293:LEU:HB3	1:E:298:ILE:CG1	1.93	0.98
1:D:40:HIS:HB2	2:D:394:HOH:O	1.63	0.98
1:E:368:TRP:CD1	1:E:374:MET:HB2	1.98	0.98
1:E:293:LEU:HB3	1:E:298:ILE:HG12	1.45	0.95
1:E:124:TRP:CZ3	1:E:185:ARG:CB	2.49	0.95
1:B:72:ASP:OD1	1:B:73:LYS:N	1.99	0.95
1:B:57:CYS:SG	1:B:309:CYS:CB	2.58	0.91
1:E:368:TRP:HA	1:E:374:MET:HA	1.54	0.88
1:A:371:VAL:HG23	2:A:393:HOH:O	1.73	0.87
1:D:194:LYS:O	1:D:198:ILE:HG13	1.73	0.87
1:D:112:LYS:HG3	1:D:139:THR:HG22	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:VAL:O	1:B:194:LYS:HE2	1.74	0.86
1:E:298:ILE:HD12	1:E:298:ILE:O	1.74	0.86
1:F:50:PHE:HD2	1:F:54:ASN:ND2	1.71	0.86
1:B:112:LYS:HG3	1:B:139:THR:HG22	1.57	0.84
1:C:367:TYR:CE2	1:C:375:VAL:HG21	2.13	0.83
1:E:168:ASP:HB3	2:E:390:HOH:O	1.78	0.83
1:F:42:ASP:OD2	1:F:59:GLN:NE2	2.11	0.82
1:E:210:LYS:CA	1:E:211:GLY:N	2.42	0.82
1:C:368:TRP:CD1	1:C:374:MET:HB2	2.14	0.82
1:B:312:ASN:OD1	1:B:313:PRO:HA	1.78	0.82
1:A:194:LYS:O	1:A:198:ILE:HG13	1.79	0.81
1:C:160:GLY:HA2	1:C:194:LYS:HE2	1.62	0.81
1:E:368:TRP:HD1	1:E:374:MET:HB2	1.40	0.81
1:C:373:LYS:O	1:C:374:MET:HB3	1.80	0.81
1:E:312:ASN:OD1	1:E:313:PRO:HA	1.79	0.81
1:E:373:LYS:O	1:E:374:MET:HB3	1.78	0.81
1:D:367:TYR:CZ	1:D:376:VAL:HG21	2.14	0.81
1:C:367:TYR:CZ	1:C:375:VAL:CG2	2.64	0.80
1:A:376:VAL:HG12	1:A:376:VAL:O	1.79	0.80
1:E:312:ASN:OD1	1:E:313:PRO:CA	2.30	0.80
1:D:367:TYR:O	1:D:376:VAL:HG22	1.81	0.80
1:E:298:ILE:O	1:E:298:ILE:CD1	2.30	0.80
1:E:85:THR:CG2	1:F:50:PHE:CE1	2.65	0.79
1:D:367:TYR:CE2	1:D:376:VAL:HG21	2.17	0.79
1:E:377:THR:O	1:E:377:THR:HG22	1.81	0.78
1:A:112:LYS:HG3	1:A:139:THR:HG22	1.64	0.78
1:F:364:LYS:HG2	1:F:378:LEU:HD21	1.62	0.78
1:F:112:LYS:CG	1:F:139:THR:HG22	2.11	0.78
1:C:18:GLN:OE1	1:C:276:SER:OG	2.01	0.77
1:C:366:GLY:HA2	1:C:377:THR:HG23	1.66	0.77
1:A:221:PHE:O	1:A:226:LEU:HD11	1.84	0.77
1:E:293:LEU:O	1:E:298:ILE:HG13	1.86	0.76
1:A:190:CYS:HB3	1:A:194:LYS:HB3	1.66	0.76
1:D:301:SER:O	1:D:302:ARG:HB3	1.85	0.75
1:C:167:LYS:O	1:C:171:TYR:CD2	2.41	0.73
1:E:129:TYR:HE1	1:E:131:TYR:HB3	1.52	0.73
1:A:72:ASP:OD1	1:A:73:LYS:N	2.22	0.73
1:A:195:VAL:O	1:A:199:VAL:HG23	1.90	0.72
1:C:221:PHE:CD1	1:C:238:GLY:HA3	2.24	0.72
1:F:221:PHE:HE2	1:F:362:PRO:HB3	1.54	0.72
1:F:65:TYR:CE2	1:F:300:ILE:HG21	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PHE:HZ	1:A:290:PHE:HB2	1.55	0.71
1:C:373:LYS:O	1:C:374:MET:CB	2.37	0.71
1:A:124:TRP:CE2	1:A:185:ARG:HG2	2.26	0.71
1:D:367:TYR:CE1	1:D:376:VAL:HG21	2.25	0.70
1:C:177:ASP:OD1	1:C:177:ASP:C	2.30	0.70
1:C:129:TYR:HE1	1:C:131:TYR:HB3	1.55	0.70
1:A:367:TYR:CZ	1:A:376:VAL:HG11	2.26	0.70
1:B:171:TYR:OH	1:B:194:LYS:HE3	1.92	0.69
1:E:310:LEU:HD22	1:F:54:ASN:OD1	1.93	0.69
1:E:293:LEU:CB	1:E:298:ILE:HG12	2.20	0.69
1:B:112:LYS:CG	1:B:139:THR:HG22	2.22	0.69
1:E:210:LYS:CA	1:E:210:LYS:O	2.40	0.69
1:A:221:PHE:HE2	1:A:362:PRO:HB3	1.56	0.69
1:C:283:VAL:O	1:C:287:THR:HG23	1.91	0.69
1:C:372:ASP:O	1:C:373:LYS:CB	2.41	0.69
1:B:129:TYR:HE1	1:B:131:TYR:HB3	1.56	0.69
1:B:298:ILE:HG22	1:B:300:ILE:HG23	1.74	0.69
1:C:129:TYR:OH	1:C:139:THR:OG1	2.11	0.68
1:D:129:TYR:HE1	1:D:131:TYR:HB3	1.57	0.68
1:D:198:ILE:O	1:D:202:VAL:HG23	1.93	0.68
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.58	0.68
1:C:124:TRP:CE2	1:C:185:ARG:HG2	2.29	0.68
1:E:210:LYS:O	1:E:211:GLY:N	2.26	0.68
1:C:367:TYR:CE2	1:C:375:VAL:CG2	2.77	0.68
1:B:219:LEU:HD22	1:B:241:ILE:HG23	1.76	0.68
1:D:301:SER:O	1:D:302:ARG:CB	2.41	0.68
1:B:35:PHE:HZ	1:B:290:PHE:HB2	1.58	0.68
1:F:129:TYR:HE1	1:F:131:TYR:HB3	1.58	0.68
1:E:121:TYR:CE2	1:E:376:VAL:HG21	2.29	0.67
1:D:367:TYR:CD2	1:D:376:VAL:HG21	2.30	0.67
1:D:129:TYR:CE1	1:D:131:TYR:HB3	2.30	0.67
1:F:203:ILE:HD11	1:F:229:ILE:CG2	2.24	0.67
1:E:48:ASN:OD1	1:E:51:ALA:N	2.22	0.66
1:E:129:TYR:CE1	1:E:131:TYR:HB3	2.30	0.66
1:E:48:ASN:OD1	1:E:48:ASN:C	2.34	0.66
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.61	0.66
1:E:226:LEU:H	1:E:226:LEU:HD12	1.61	0.66
1:A:129:TYR:HE1	1:A:131:TYR:HB3	1.60	0.66
1:D:112:LYS:CG	1:D:139:THR:HG22	2.24	0.66
1:D:124:TRP:CE2	1:D:185:ARG:HG2	2.32	0.65
1:B:255:ARG:HD3	1:B:255:ARG:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:TYR:HB3	1:E:124:TRP:HE1	1.60	0.65
1:E:376:VAL:O	1:E:377:THR:C	2.35	0.65
1:A:110:ASP:OD1	1:A:112:LYS:HE3	1.94	0.65
1:B:98:ASP:OD1	1:B:99:GLY:N	2.30	0.65
1:E:372:ASP:O	1:E:373:LYS:CB	2.44	0.65
1:E:312:ASN:OD1	1:E:313:PRO:N	2.30	0.65
1:A:198:ILE:O	1:A:202:VAL:HG23	1.96	0.65
1:B:124:TRP:CE2	1:B:185:ARG:HG2	2.32	0.65
1:E:373:LYS:O	1:E:374:MET:CB	2.45	0.65
1:E:122:TYR:HB3	1:E:124:TRP:NE1	2.12	0.65
1:C:124:TRP:CZ3	1:C:185:ARG:HB3	2.32	0.64
1:C:129:TYR:CE1	1:C:131:TYR:HB3	2.31	0.64
1:A:225:ASP:OD1	1:A:225:ASP:C	2.35	0.64
1:A:124:TRP:CZ3	1:A:185:ARG:HB3	2.32	0.64
1:D:158:ASN:OD1	1:D:159:VAL:N	2.30	0.64
1:D:291:ARG:HH11	1:D:291:ARG:HG2	1.61	0.64
1:D:124:TRP:CZ3	1:D:185:ARG:HB3	2.33	0.64
1:B:110:ASP:OD1	1:B:112:LYS:HE3	1.96	0.64
1:B:129:TYR:CE1	1:B:131:TYR:HB3	2.32	0.64
1:E:124:TRP:CE3	1:E:185:ARG:HB3	2.28	0.64
1:E:50:PHE:CZ	1:F:314:ALA:HB2	2.32	0.64
1:F:291:ARG:HG2	1:F:291:ARG:HH11	1.61	0.64
1:C:162:ILE:CG2	1:C:167:LYS:HA	2.28	0.64
1:F:255:ARG:O	1:F:255:ARG:HD3	1.98	0.63
1:C:368:TRP:HD1	1:C:374:MET:HB2	1.62	0.63
1:E:377:THR:O	1:E:377:THR:CG2	2.45	0.63
1:C:368:TRP:HA	1:C:374:MET:HA	1.80	0.63
1:D:312:ASN:OD1	1:D:313:PRO:HA	1.99	0.63
1:A:35:PHE:HZ	1:A:290:PHE:CB	2.12	0.63
1:F:110:ASP:OD1	1:F:112:LYS:HE2	1.99	0.62
1:C:162:ILE:HG21	1:C:167:LYS:HA	1.81	0.62
1:B:70:PHE:CE2	1:B:93:PRO:HG2	2.34	0.62
1:B:71:TYR:OH	1:B:95:PHE:O	2.09	0.62
1:F:144:LEU:CA	1:F:145:ASP:N	2.62	0.62
1:E:293:LEU:CB	1:E:298:ILE:CG1	2.75	0.62
1:E:50:PHE:CD1	1:E:50:PHE:C	2.73	0.62
1:F:117:SER:HB3	1:F:375:VAL:CG1	2.30	0.62
1:C:175:PHE:O	1:C:179:GLU:N	2.31	0.62
1:E:50:PHE:HZ	1:F:314:ALA:HB2	1.63	0.62
1:B:188:LEU:HD12	1:B:216:ILE:CD1	2.30	0.62
1:D:110:ASP:OD1	1:D:112:LYS:HE3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:MET:CG	1:E:375:VAL:N	2.63	0.62
1:C:61:SER:O	1:C:306:ALA:N	2.33	0.61
1:C:177:ASP:O	1:C:180:LEU:HB2	2.01	0.61
1:F:50:PHE:CE2	1:F:54:ASN:ND2	2.62	0.61
1:E:115:LEU:HD11	1:E:187:ILE:HD13	1.82	0.60
1:C:70:PHE:CE2	1:C:93:PRO:HG2	2.36	0.60
1:F:226:LEU:HD12	1:F:226:LEU:H	1.65	0.60
1:A:133:SER:OG	1:A:158:ASN:ND2	2.35	0.60
1:D:219:LEU:HD22	1:D:241:ILE:HG23	1.82	0.60
1:E:124:TRP:CH2	1:E:185:ARG:CB	2.78	0.60
1:D:48:ASN:O	1:D:52:VAL:HG23	2.02	0.60
1:D:255:ARG:O	1:D:255:ARG:HD3	2.01	0.60
1:B:124:TRP:CZ3	1:B:185:ARG:HB3	2.37	0.60
1:A:73:LYS:HE2	1:A:133:SER:O	2.01	0.59
1:D:79:ILE:HG22	1:D:80:THR:N	2.16	0.59
1:E:48:ASN:O	1:E:52:VAL:HG23	2.02	0.59
1:E:85:THR:CB	1:F:50:PHE:CE1	2.85	0.59
1:F:97:THR:O	1:F:346:LYS:HE3	2.02	0.59
1:F:99:GLY:HA3	1:F:101:HIS:CE1	2.37	0.59
1:E:310:LEU:CD2	1:F:54:ASN:OD1	2.50	0.59
1:A:35:PHE:CZ	1:A:290:PHE:HB2	2.35	0.59
1:C:255:ARG:O	1:C:255:ARG:HD3	2.02	0.59
1:A:112:LYS:CG	1:A:139:THR:HG22	2.30	0.59
1:B:35:PHE:HZ	1:B:290:PHE:CB	2.15	0.59
1:D:367:TYR:CD1	1:D:376:VAL:HG21	2.38	0.59
1:D:227:LEU:HD23	1:D:227:LEU:C	2.19	0.59
1:E:312:ASN:HA	1:E:313:PRO:C	2.23	0.59
1:F:376:VAL:HG23	1:F:376:VAL:O	2.02	0.59
1:A:300:ILE:HG13	1:A:300:ILE:O	2.03	0.58
1:F:255:ARG:HD2	1:F:259:LEU:HD21	1.85	0.58
1:E:35:PHE:HZ	1:E:290:PHE:CB	2.16	0.58
1:E:122:TYR:CB	1:E:124:TRP:CD1	2.87	0.58
1:A:317:TRP:NE1	1:A:319:GLN:OE1	2.34	0.58
1:A:35:PHE:HD1	1:A:36:ARG:N	2.01	0.58
1:F:117:SER:HB3	1:F:375:VAL:HG13	1.85	0.58
1:B:97:THR:O	1:B:346:LYS:HE3	2.04	0.58
1:F:27:MET:HE1	1:F:39:PRO:HD3	1.86	0.58
1:B:35:PHE:CZ	1:B:290:PHE:HB2	2.39	0.58
1:D:65:TYR:CD2	1:D:300:ILE:HD12	2.39	0.57
1:B:302:ARG:HB3	1:B:304:GLY:O	2.04	0.57
1:F:48:ASN:O	1:F:52:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:VAL:O	1:F:199:VAL:HG23	2.04	0.57
1:A:367:TYR:CE2	1:A:376:VAL:HG11	2.40	0.57
1:C:367:TYR:CE1	1:C:375:VAL:CG2	2.88	0.57
1:E:293:LEU:C	1:E:298:ILE:HG13	2.24	0.57
1:F:194:LYS:O	1:F:198:ILE:HG13	2.05	0.57
1:E:190:CYS:HB3	1:E:194:LYS:CB	2.35	0.57
1:D:71:TYR:CE1	1:D:94:SER:HB2	2.41	0.56
1:F:65:TYR:HE2	1:F:300:ILE:HG21	1.69	0.56
1:C:367:TYR:CE1	1:C:375:VAL:HG22	2.41	0.56
1:B:133:SER:HA	1:B:137:LEU:HD11	1.88	0.56
1:C:97:THR:O	1:C:346:LYS:HE3	2.05	0.56
1:F:79:ILE:HG22	1:F:80:THR:N	2.21	0.56
1:A:97:THR:O	1:A:346:LYS:HE3	2.05	0.56
1:E:174:LEU:O	1:E:178:LEU:HB2	2.05	0.56
1:D:367:TYR:CG	1:D:376:VAL:HG21	2.41	0.56
1:D:70:PHE:CE2	1:D:93:PRO:HG2	2.41	0.56
1:B:28:VAL:HG12	1:B:29:GLN:N	2.21	0.56
1:B:188:LEU:HD12	1:B:216:ILE:HD11	1.88	0.56
1:A:129:TYR:CE1	1:A:131:TYR:HB3	2.41	0.55
1:A:178:LEU:HD23	1:A:183:GLU:HB3	1.88	0.55
1:C:167:LYS:HA	1:C:170:THR:OG1	2.05	0.55
1:F:203:ILE:HD11	1:F:229:ILE:HG23	1.88	0.55
1:B:260:GLU:OE2	1:B:262:LYS:HG2	2.06	0.55
1:F:129:TYR:CE1	1:F:131:TYR:HB3	2.40	0.55
1:B:35:PHE:HD1	1:B:36:ARG:N	2.04	0.55
1:C:72:ASP:OD1	1:C:72:ASP:C	2.40	0.55
1:F:133:SER:OG	1:F:158:ASN:ND2	2.40	0.55
1:E:144:LEU:HD11	1:F:144:LEU:HD11	1.87	0.55
1:B:61:SER:OG	1:B:307:GLY:O	2.23	0.55
1:C:124:TRP:CH2	1:C:185:ARG:HB3	2.42	0.55
1:F:190:CYS:CB	1:F:194:LYS:HB3	2.36	0.55
1:C:178:LEU:HD23	1:C:183:GLU:HB3	1.89	0.55
1:D:115:LEU:O	1:D:119:ILE:HG13	2.07	0.55
1:D:174:LEU:O	1:D:178:LEU:HB2	2.07	0.55
1:A:53:THR:HG22	1:A:53:THR:O	2.07	0.54
1:A:213:HIS:CD2	1:A:235:ASN:HB3	2.42	0.54
1:B:174:LEU:O	1:B:178:LEU:HB2	2.07	0.54
1:D:132:ASP:OD1	1:D:160:GLY:HA2	2.07	0.54
1:C:8:ILE:O	1:C:39:PRO:HA	2.07	0.54
1:F:132:ASP:OD1	1:F:160:GLY:HA3	2.07	0.54
1:F:178:LEU:HD23	1:F:183:GLU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD13	1:A:219:LEU:CD2	2.37	0.54
1:A:174:LEU:O	1:A:178:LEU:HB2	2.07	0.54
1:F:144:LEU:CA	1:F:144:LEU:O	2.56	0.54
1:D:367:TYR:CG	1:D:376:VAL:CG2	2.90	0.54
1:E:293:LEU:CA	1:E:298:ILE:HG13	2.38	0.54
1:F:298:ILE:HG22	1:F:299:GLU:N	2.23	0.54
1:F:115:LEU:HD11	1:F:187:ILE:HD13	1.90	0.54
1:D:367:TYR:CD2	1:D:376:VAL:CG2	2.91	0.53
1:E:122:TYR:HB3	1:E:124:TRP:CD1	2.43	0.53
1:B:115:LEU:O	1:B:119:ILE:HG13	2.07	0.53
1:B:226:LEU:HD12	1:B:362:PRO:HG3	1.91	0.53
1:C:255:ARG:HD2	1:C:259:LEU:HD21	1.90	0.53
1:B:72:ASP:OD1	1:B:72:ASP:C	2.47	0.53
1:C:174:LEU:O	1:C:178:LEU:HB2	2.09	0.53
1:F:70:PHE:CE2	1:F:93:PRO:HG2	2.44	0.53
1:F:45:GLU:HG3	2:F:380:HOH:O	2.08	0.53
1:B:36:ARG:HG2	2:B:417:HOH:O	2.07	0.53
1:B:240:GLN:NE2	2:B:418:HOH:O	2.41	0.53
1:A:178:LEU:HD23	1:A:178:LEU:O	2.09	0.53
1:A:229:ILE:HA	2:E:385:HOH:O	2.08	0.53
1:E:122:TYR:HB2	1:E:124:TRP:CD1	2.43	0.53
1:E:203:ILE:HD11	1:E:229:ILE:CG2	2.38	0.53
1:D:8:ILE:O	1:D:39:PRO:HA	2.08	0.53
1:E:374:MET:HG2	2:E:389:HOH:O	2.07	0.53
1:B:291:ARG:HH11	1:B:291:ARG:CG	2.20	0.53
1:B:374:MET:O	1:B:375:VAL:C	2.47	0.53
1:D:291:ARG:NH2	2:D:395:HOH:O	2.42	0.53
1:C:17:ASP:HB3	1:C:265:PRO:HB2	1.91	0.53
1:E:27:MET:HE1	1:E:39:PRO:HD3	1.90	0.53
1:E:35:PHE:HD1	1:E:36:ARG:N	2.07	0.53
1:A:340:LYS:O	1:A:348:ILE:HG12	2.09	0.53
1:E:178:LEU:HD23	1:E:183:GLU:HB3	1.91	0.53
1:F:144:LEU:O	1:F:145:ASP:N	2.42	0.53
1:A:111:LEU:HD13	1:A:219:LEU:HD21	1.91	0.52
1:A:203:ILE:HD11	1:A:229:ILE:CG2	2.39	0.52
1:A:295:LYS:O	1:A:295:LYS:HG2	2.09	0.52
1:B:203:ILE:HD11	1:B:229:ILE:CG2	2.39	0.52
1:B:255:ARG:HD3	1:B:255:ARG:C	2.28	0.52
1:D:178:LEU:HD23	1:D:183:GLU:HB3	1.90	0.52
1:F:65:TYR:HE2	1:F:300:ILE:CG2	2.22	0.52
1:F:174:LEU:O	1:F:178:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LYS:O	1:D:295:LYS:HG2	2.10	0.52
1:F:178:LEU:HD23	1:F:178:LEU:O	2.10	0.52
1:E:85:THR:CB	1:F:50:PHE:CD1	2.93	0.52
1:D:291:ARG:HH11	1:D:291:ARG:CG	2.23	0.52
1:A:27:MET:HE1	1:A:39:PRO:HD3	1.92	0.52
1:A:79:ILE:HG22	1:A:80:THR:N	2.25	0.52
1:B:178:LEU:HD23	1:B:183:GLU:HB3	1.92	0.52
1:D:7:GLN:NE2	2:D:394:HOH:O	2.40	0.52
1:D:97:THR:O	1:D:346:LYS:HE3	2.10	0.52
1:E:85:THR:HG21	1:F:50:PHE:CZ	2.44	0.52
1:E:85:THR:OG1	1:F:50:PHE:CD1	2.62	0.52
1:E:122:TYR:CB	1:E:124:TRP:NE1	2.73	0.52
1:E:356:GLU:HG3	1:E:365:ILE:HD13	1.91	0.52
1:E:20:TYR:CE2	1:E:24:ARG:HD2	2.45	0.51
1:F:340:LYS:O	1:F:348:ILE:HG12	2.10	0.51
1:C:356:GLU:HG3	1:C:365:ILE:HD13	1.91	0.51
1:D:86:LEU:O	1:D:87:HIS:HB2	2.10	0.51
1:F:255:ARG:HD3	1:F:255:ARG:C	2.30	0.51
1:B:8:ILE:O	1:B:39:PRO:HA	2.10	0.51
1:B:235:ASN:ND2	2:B:391:HOH:O	2.43	0.51
1:C:115:LEU:O	1:C:119:ILE:HG13	2.10	0.51
1:D:221:PHE:O	1:D:226:LEU:HD13	2.11	0.51
1:F:80:THR:HG22	1:F:104:VAL:HG21	1.92	0.51
1:A:191:GLU:O	1:A:195:VAL:HG23	2.11	0.51
1:C:115:LEU:HD11	1:C:187:ILE:HD13	1.91	0.51
1:E:144:LEU:HD11	1:F:144:LEU:CD1	2.41	0.51
1:F:376:VAL:O	1:F:376:VAL:CG2	2.59	0.51
1:F:213:HIS:HD2	1:F:214:TYR:N	2.09	0.51
1:C:79:ILE:HG22	1:C:80:THR:N	2.25	0.51
1:A:190:CYS:CB	1:A:194:LYS:HB3	2.37	0.51
1:E:49:SER:HB2	1:F:81:SER:CB	2.41	0.51
1:E:115:LEU:O	1:E:119:ILE:HG13	2.10	0.51
1:A:201:GLN:HA	1:A:201:GLN:OE1	2.10	0.51
1:B:57:CYS:CA	1:B:309:CYS:SG	2.97	0.51
1:B:295:LYS:O	1:B:295:LYS:HG2	2.10	0.51
1:D:227:LEU:O	1:D:227:LEU:CD2	2.44	0.51
1:E:85:THR:HB	1:F:50:PHE:CE1	2.46	0.51
1:F:291:ARG:HH11	1:F:291:ARG:CG	2.24	0.50
1:F:8:ILE:O	1:F:39:PRO:HA	2.11	0.50
1:C:132:ASP:OD1	1:C:160:GLY:HA3	2.10	0.50
1:C:177:ASP:OD1	1:C:177:ASP:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:LEU:HD22	1:E:298:ILE:HG12	1.93	0.50
1:F:50:PHE:O	1:F:50:PHE:HD2	1.95	0.50
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.24	0.50
1:C:178:LEU:HD23	1:C:178:LEU:O	2.11	0.50
1:C:340:LYS:O	1:C:348:ILE:HG12	2.11	0.50
1:A:35:PHE:HD1	1:A:35:PHE:C	2.15	0.50
1:A:115:LEU:HD11	1:A:187:ILE:HD13	1.94	0.50
1:B:136:GLY:O	1:B:137:LEU:HB2	2.11	0.50
1:A:47:ALA:HB2	1:A:72:ASP:OD2	2.12	0.50
1:A:115:LEU:O	1:A:119:ILE:HG13	2.12	0.50
1:B:71:TYR:CD1	1:B:71:TYR:C	2.85	0.50
1:C:111:LEU:HD13	1:C:219:LEU:HD21	1.93	0.50
1:E:189:ASP:OD1	1:E:189:ASP:O	2.30	0.50
1:A:255:ARG:O	1:A:255:ARG:HD3	2.12	0.50
1:D:221:PHE:CD1	1:D:238:GLY:HA3	2.47	0.50
1:D:255:ARG:HD2	1:D:259:LEU:HD21	1.94	0.50
1:E:374:MET:HG2	1:E:375:VAL:N	2.26	0.50
1:F:191:GLU:O	1:F:195:VAL:HG23	2.12	0.50
1:A:376:VAL:O	1:A:376:VAL:CG1	2.52	0.50
1:B:35:PHE:HD1	1:B:35:PHE:C	2.15	0.50
1:E:8:ILE:O	1:E:39:PRO:HA	2.11	0.50
1:A:35:PHE:CZ	1:A:290:PHE:CB	2.95	0.49
1:C:20:TYR:CE2	1:C:24:ARG:HD2	2.47	0.49
1:C:175:PHE:O	1:C:179:GLU:HB2	2.12	0.49
1:E:70:PHE:CE2	1:E:93:PRO:HG2	2.46	0.49
1:F:115:LEU:O	1:F:119:ILE:HG13	2.11	0.49
1:D:55:ALA:O	1:D:59:GLN:HG2	2.12	0.49
1:E:230:GLN:HA	1:E:357:LEU:HD21	1.93	0.49
1:E:298:ILE:O	1:E:298:ILE:HD13	2.12	0.49
1:F:190:CYS:HB3	1:F:194:LYS:HB3	1.93	0.49
1:D:132:ASP:OD2	1:D:134:ASP:HB2	2.12	0.49
1:D:255:ARG:HD3	1:D:255:ARG:C	2.33	0.49
1:C:129:TYR:HH	1:C:139:THR:HG1	1.53	0.49
1:C:133:SER:HA	1:C:137:LEU:HD11	1.94	0.49
1:F:375:VAL:O	1:F:375:VAL:HG23	2.12	0.49
1:A:310:LEU:CD2	1:B:54:ASN:OD1	2.61	0.49
1:B:52:VAL:CG1	1:B:79:ILE:HD13	2.42	0.49
1:D:340:LYS:O	1:D:348:ILE:HG12	2.13	0.49
1:F:199:VAL:O	1:F:203:ILE:HG13	2.13	0.49
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.47	0.49
1:F:260:GLU:HB3	1:F:263:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:HB3	2:A:393:HOH:O	2.12	0.49
1:B:35:PHE:C	1:B:35:PHE:CD1	2.86	0.49
1:B:124:TRP:CH2	1:B:185:ARG:HB3	2.48	0.49
1:D:132:ASP:OD1	1:D:160:GLY:CA	2.60	0.49
1:E:79:ILE:HG22	1:E:80:THR:N	2.28	0.49
1:F:65:TYR:CE2	1:F:300:ILE:CG2	2.95	0.49
1:F:178:LEU:CD2	1:F:183:GLU:HB3	2.43	0.49
1:A:35:PHE:C	1:A:35:PHE:CD1	2.85	0.48
1:A:133:SER:OG	1:A:158:ASN:OD1	2.30	0.48
1:B:79:ILE:CG2	1:B:80:THR:N	2.76	0.48
1:B:129:TYR:CE2	1:B:143:VAL:HG21	2.48	0.48
1:C:317:TRP:NE1	1:C:319:GLN:OE1	2.42	0.48
1:E:213:HIS:HD2	1:E:214:TYR:N	2.11	0.48
1:C:178:LEU:CD2	1:C:183:GLU:HB3	2.44	0.48
1:E:178:LEU:HD23	1:E:178:LEU:O	2.13	0.48
1:E:220:GLY:O	1:E:223:ASP:HB2	2.13	0.48
1:B:358:LYS:HG3	1:B:363:ARG:HD2	1.95	0.48
1:B:291:ARG:NH2	2:B:409:HOH:O	2.47	0.48
1:F:131:TYR:CZ	1:F:158:ASN:HB2	2.48	0.48
1:C:40:HIS:HB3	2:C:401:HOH:O	2.13	0.48
1:F:55:ALA:O	1:F:59:GLN:HG2	2.14	0.48
1:B:71:TYR:C	1:B:71:TYR:HD1	2.17	0.47
1:D:133:SER:HA	1:D:137:LEU:HD11	1.96	0.47
1:A:6:ILE:HD12	1:A:35:PHE:CZ	2.48	0.47
1:C:220:GLY:O	1:C:223:ASP:HB2	2.14	0.47
1:D:131:TYR:CZ	1:D:158:ASN:HB2	2.49	0.47
1:F:124:TRP:CZ2	1:F:185:ARG:CB	2.97	0.47
1:A:8:ILE:O	1:A:39:PRO:HA	2.14	0.47
1:B:255:ARG:HD2	1:B:259:LEU:HD21	1.97	0.47
1:E:50:PHE:CE1	1:F:85:THR:HG21	2.50	0.47
1:E:219:LEU:HD22	1:E:241:ILE:HG23	1.96	0.47
1:E:367:TYR:O	1:E:374:MET:HG3	2.15	0.47
1:A:124:TRP:CH2	1:A:185:ARG:HB3	2.50	0.47
1:E:35:PHE:HD1	1:E:35:PHE:C	2.17	0.47
1:A:50:PHE:HB2	1:B:81:SER:OG	2.14	0.47
1:A:255:ARG:HD2	1:A:259:LEU:HD21	1.95	0.47
1:C:255:ARG:HD3	1:C:255:ARG:C	2.34	0.47
1:E:375:VAL:HA	2:E:389:HOH:O	2.14	0.47
1:A:178:LEU:CD2	1:A:183:GLU:HB3	2.44	0.47
1:D:158:ASN:OD1	1:D:158:ASN:C	2.53	0.47
1:E:293:LEU:HB3	1:E:298:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:HIS:HD2	1:A:214:TYR:N	2.13	0.47
1:C:203:ILE:HD11	1:C:229:ILE:CG2	2.45	0.47
1:D:56:PHE:CD1	1:D:56:PHE:C	2.87	0.47
1:E:121:TYR:HE2	1:E:376:VAL:HG21	1.77	0.47
1:E:298:ILE:CD1	1:E:298:ILE:C	2.80	0.47
1:F:230:GLN:HA	1:F:357:LEU:HD21	1.96	0.47
1:A:232:GLY:N	2:E:385:HOH:O	2.47	0.47
1:B:312:ASN:HA	1:B:313:PRO:C	2.35	0.47
1:C:167:LYS:O	1:C:171:TYR:HD2	1.93	0.47
1:D:219:LEU:HD22	1:D:241:ILE:CG2	2.45	0.47
1:D:227:LEU:C	1:D:227:LEU:CD2	2.84	0.47
1:C:171:TYR:O	1:C:175:PHE:CD1	2.68	0.47
1:B:293:LEU:HD13	1:B:300:ILE:HG21	1.98	0.46
1:E:48:ASN:OD1	1:E:50:PHE:N	2.48	0.46
1:F:150:LYS:CB	2:F:385:HOH:O	2.63	0.46
1:B:27:MET:HE1	1:B:39:PRO:HD3	1.96	0.46
1:E:13:PRO:HD3	1:E:70:PHE:CD1	2.51	0.46
1:F:98:ASP:N	1:F:98:ASP:OD1	2.49	0.46
1:E:375:VAL:HG12	1:E:376:VAL:N	2.30	0.46
1:C:6:ILE:HB	1:C:37:LEU:HD23	1.96	0.46
1:E:185:ARG:HD2	2:E:384:HOH:O	2.15	0.46
1:F:19:GLU:O	1:F:279:THR:HG21	2.16	0.46
1:E:50:PHE:CZ	1:F:85:THR:HG21	2.50	0.46
1:E:90:PHE:CE2	1:E:92:THR:HB	2.51	0.46
1:F:203:ILE:CD1	1:F:229:ILE:HG22	2.46	0.46
1:A:13:PRO:HD3	1:A:70:PHE:CD1	2.51	0.46
1:A:208:HIS:HE1	1:E:208:HIS:HE1	1.64	0.46
1:D:71:TYR:C	1:D:71:TYR:HD1	2.20	0.46
1:E:35:PHE:C	1:E:35:PHE:CD1	2.88	0.46
1:E:340:LYS:O	1:E:348:ILE:HG12	2.16	0.46
1:A:230:GLN:HA	1:A:357:LEU:HD21	1.98	0.46
1:B:35:PHE:CZ	1:B:290:PHE:CB	2.98	0.46
1:B:178:LEU:HD23	1:B:178:LEU:O	2.15	0.46
1:B:226:LEU:CD1	1:B:362:PRO:HG3	2.45	0.46
1:E:178:LEU:CD2	1:E:183:GLU:HB3	2.46	0.46
1:A:174:LEU:O	1:A:174:LEU:HG	2.16	0.45
1:B:55:ALA:O	1:B:59:GLN:HG2	2.16	0.45
1:D:20:TYR:CE2	1:D:24:ARG:HD2	2.51	0.45
1:F:20:TYR:CE2	1:F:24:ARG:HD2	2.51	0.45
1:F:190:CYS:HB2	1:F:194:LYS:HB3	1.98	0.45
1:D:178:LEU:HD23	1:D:178:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:VAL:CA	2:E:389:HOH:O	2.64	0.45
1:A:358:LYS:HG3	1:A:363:ARG:HD2	1.99	0.45
1:C:13:PRO:HB3	2:C:404:HOH:O	2.16	0.45
1:D:130:LEU:N	1:D:130:LEU:HD12	2.30	0.45
1:E:133:SER:HA	1:E:137:LEU:CD1	2.47	0.45
1:F:45:GLU:CG	2:F:380:HOH:O	2.63	0.45
1:B:86:LEU:O	1:B:87:HIS:HB2	2.15	0.45
1:D:220:GLY:O	1:D:223:ASP:HB2	2.15	0.45
1:C:71:TYR:CD1	1:C:71:TYR:C	2.89	0.45
1:C:369:SER:HB3	1:C:372:ASP:HB2	1.99	0.45
1:D:127:PHE:CE1	1:D:154:VAL:HG22	2.51	0.45
1:F:210:LYS:HA	1:F:233:GLY:O	2.17	0.45
1:F:356:GLU:O	1:F:362:PRO:HA	2.17	0.45
1:B:91:ILE:HD13	1:B:286:MET:SD	2.57	0.45
1:F:50:PHE:HD2	1:F:54:ASN:HD22	1.58	0.45
1:F:203:ILE:HD11	1:F:229:ILE:HG22	1.99	0.45
1:A:131:TYR:CZ	1:A:158:ASN:HB2	2.52	0.45
1:C:7:GLN:OE1	1:C:62:ARG:CD	2.65	0.45
1:D:124:TRP:CH2	1:D:185:ARG:HB3	2.52	0.45
1:B:340:LYS:O	1:B:348:ILE:HG12	2.16	0.45
1:D:342:ASP:HB3	1:D:348:ILE:HD13	1.99	0.45
1:E:293:LEU:HD22	1:E:298:ILE:HG21	1.99	0.45
1:A:56:PHE:CD1	1:A:56:PHE:C	2.90	0.44
1:B:46:VAL:O	1:B:75:SER:OG	2.18	0.44
1:C:221:PHE:O	1:C:226:LEU:HD21	2.17	0.44
1:D:71:TYR:C	1:D:71:TYR:CD1	2.90	0.44
1:D:98:ASP:OD1	1:D:98:ASP:N	2.50	0.44
1:A:184:ARG:HD3	1:A:184:ARG:HA	1.74	0.44
1:A:300:ILE:O	1:A:300:ILE:CG1	2.64	0.44
1:C:120:GLU:OE2	1:C:150:LYS:HE3	2.17	0.44
1:A:135:ARG:NE	1:A:189:ASP:OD1	2.50	0.44
1:A:370:GLU:O	1:A:373:LYS:CG	2.66	0.44
1:B:213:HIS:HD2	1:B:214:TYR:N	2.16	0.44
1:D:367:TYR:CD1	1:D:376:VAL:CG2	3.00	0.44
1:E:226:LEU:HD12	1:E:226:LEU:N	2.30	0.44
1:A:342:ASP:HB3	1:A:348:ILE:HD13	1.99	0.44
1:B:167:LYS:O	1:B:171:TYR:CD2	2.71	0.44
1:B:219:LEU:HB3	1:B:241:ILE:HG12	1.99	0.44
1:F:99:GLY:HA3	1:F:101:HIS:HE1	1.83	0.44
1:F:356:GLU:HG3	1:F:365:ILE:HD13	1.98	0.44
1:B:194:LYS:O	1:B:198:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HA	1:D:184:ARG:HD3	1.77	0.44
1:E:131:TYR:CZ	1:E:158:ASN:HB2	2.53	0.44
1:F:56:PHE:CD1	1:F:56:PHE:C	2.91	0.44
1:A:378:LEU:C	1:A:378:LEU:HD12	2.38	0.44
1:B:374:MET:O	1:B:376:VAL:HG23	2.18	0.44
1:C:71:TYR:OH	1:C:95:PHE:O	2.27	0.44
1:E:6:ILE:HD12	1:E:35:PHE:CZ	2.51	0.44
1:A:6:ILE:HD12	1:A:35:PHE:CE1	2.53	0.44
1:B:300:ILE:HA	1:B:319:GLN:HG2	1.99	0.44
1:D:115:LEU:HD11	1:D:187:ILE:HD13	2.00	0.44
1:E:144:LEU:CD1	1:F:144:LEU:HD11	2.47	0.44
1:B:20:TYR:CE2	1:B:24:ARG:HD2	2.52	0.44
1:C:35:PHE:CD1	1:C:35:PHE:C	2.91	0.44
1:C:90:PHE:CE2	1:C:92:THR:HB	2.53	0.44
1:C:219:LEU:HB3	1:C:241:ILE:HG12	2.00	0.44
1:D:145:ASP:HB3	2:D:382:HOH:O	2.17	0.44
1:D:178:LEU:CD2	1:D:183:GLU:HB3	2.48	0.44
1:D:213:HIS:HD2	1:D:214:TYR:N	2.15	0.44
1:E:50:PHE:CD1	1:F:85:THR:HG21	2.53	0.44
1:C:12:PHE:HA	1:C:13:PRO:HD3	1.91	0.43
1:C:132:ASP:OD1	1:C:160:GLY:CA	2.66	0.43
1:D:260:GLU:HB3	1:D:263:GLU:HB3	1.99	0.43
1:B:178:LEU:CD2	1:B:183:GLU:HB3	2.48	0.43
1:C:209:VAL:HA	1:C:232:GLY:O	2.17	0.43
1:D:229:ILE:HD12	1:D:236:VAL:HG21	1.99	0.43
1:F:298:ILE:CG2	1:F:299:GLU:N	2.82	0.43
1:A:255:ARG:HD3	1:A:255:ARG:C	2.38	0.43
1:C:111:LEU:HD13	1:C:219:LEU:CD2	2.47	0.43
1:D:68:PHE:CE1	1:D:93:PRO:HD3	2.53	0.43
1:B:184:ARG:HD3	1:B:184:ARG:HA	1.75	0.43
1:A:68:PHE:CE1	1:A:93:PRO:HD3	2.53	0.43
1:E:6:ILE:HD12	1:E:35:PHE:CE1	2.54	0.43
1:A:20:TYR:HB3	2:A:395:HOH:O	2.18	0.43
1:A:72:ASP:O	1:A:73:LYS:C	2.57	0.43
1:A:203:ILE:HD11	1:A:229:ILE:HG23	2.01	0.43
1:C:223:ASP:OD2	1:C:273:LYS:HA	2.19	0.43
1:D:27:MET:HE1	1:D:39:PRO:HD3	2.01	0.43
1:D:370:GLU:O	1:D:373:LYS:CG	2.67	0.43
1:C:65:TYR:CE2	1:C:300:ILE:HD12	2.54	0.43
1:D:317:TRP:NE1	1:D:319:GLN:OE1	2.46	0.43
1:E:50:PHE:CE2	1:F:85:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLN:O	1:B:205:ILE:HG12	2.18	0.43
1:B:226:LEU:HD13	1:B:357:LEU:HD13	2.00	0.43
1:D:206:GLY:HA2	1:D:208:HIS:CE1	2.54	0.42
1:D:230:GLN:HA	1:D:357:LEU:HD21	2.00	0.42
1:A:312:ASN:OD1	1:A:313:PRO:HA	2.19	0.42
1:C:86:LEU:O	1:C:87:HIS:HB2	2.19	0.42
1:C:131:TYR:CZ	1:C:158:ASN:HB2	2.54	0.42
1:C:367:TYR:CD1	1:C:375:VAL:HG22	2.55	0.42
1:E:312:ASN:OD1	1:E:312:ASN:C	2.57	0.42
1:C:71:TYR:C	1:C:71:TYR:HD1	2.23	0.42
1:A:70:PHE:CE2	1:A:93:PRO:HG2	2.54	0.42
1:A:260:GLU:HB3	1:A:263:GLU:HB3	2.02	0.42
1:C:366:GLY:CA	1:C:377:THR:HG23	2.41	0.42
1:F:375:VAL:O	1:F:375:VAL:CG2	2.67	0.42
1:A:27:MET:HE1	1:A:37:LEU:O	2.19	0.42
1:B:317:TRP:NE1	1:B:319:GLN:OE1	2.43	0.42
1:D:71:TYR:HD1	1:D:71:TYR:O	2.02	0.42
1:E:174:LEU:O	1:E:174:LEU:HG	2.19	0.42
1:E:219:LEU:HB3	1:E:241:ILE:HG12	2.02	0.42
1:A:117:SER:HB3	1:A:375:VAL:HG22	2.02	0.42
1:B:52:VAL:HG12	1:B:79:ILE:HD13	2.02	0.42
1:E:35:PHE:CZ	1:E:290:PHE:CB	3.00	0.42
1:F:90:PHE:CE2	1:F:92:THR:HB	2.55	0.42
1:F:203:ILE:HG12	1:F:229:ILE:HG22	2.01	0.42
1:B:220:GLY:O	1:B:223:ASP:HB2	2.20	0.42
1:C:260:GLU:HB3	1:C:263:GLU:HB3	2.01	0.42
1:D:293:LEU:HD23	1:D:293:LEU:HA	1.92	0.42
1:F:226:LEU:HD12	1:F:226:LEU:N	2.34	0.42
1:B:56:PHE:CD1	1:B:56:PHE:C	2.92	0.42
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.87	0.42
1:E:209:VAL:O	1:E:234:ALA:HB2	2.20	0.42
1:D:72:ASP:OD1	1:D:73:LYS:N	2.53	0.41
1:B:6:ILE:HD12	1:B:35:PHE:CZ	2.54	0.41
1:B:291:ARG:CG	1:B:291:ARG:NH1	2.82	0.41
1:F:50:PHE:CD2	1:F:50:PHE:C	2.94	0.41
1:F:86:LEU:O	1:F:87:HIS:HB2	2.20	0.41
1:E:74:LYS:O	1:F:77:ASN:HB3	2.20	0.41
1:B:288:GLU:OE1	1:B:291:ARG:NH1	2.53	0.41
1:D:90:PHE:CE2	1:D:92:THR:HB	2.56	0.41
1:D:356:GLU:HG3	1:D:365:ILE:HD13	2.02	0.41
1:D:369:SER:HB3	1:D:372:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:CYS:SG	1:E:90:PHE:HB2	2.60	0.41
1:E:342:ASP:HB3	1:E:348:ILE:HD13	2.01	0.41
1:E:374:MET:HG3	1:E:375:VAL:H	1.85	0.41
1:F:294:ARG:C	1:F:296:GLN:H	2.22	0.41
1:A:97:THR:HG23	1:A:106:GLN:HE21	1.84	0.41
1:D:231:PHE:CD1	1:D:359:THR:HG23	2.55	0.41
1:E:86:LEU:O	1:E:87:HIS:HB2	2.20	0.41
1:E:203:ILE:HG12	1:E:229:ILE:HG22	2.02	0.41
1:F:17:ASP:HB3	1:F:265:PRO:HB2	2.02	0.41
1:F:254:GLU:O	1:F:258:THR:HG23	2.21	0.41
1:F:364:LYS:HG2	1:F:378:LEU:CD2	2.43	0.41
1:A:121:TYR:HB2	1:A:375:VAL:HG21	2.02	0.41
1:C:120:GLU:OE2	1:C:150:LYS:CE	2.69	0.41
1:A:97:THR:H	1:A:106:GLN:NE2	2.19	0.41
1:D:128:ALA:HB3	1:D:186:VAL:HG22	2.02	0.41
1:E:97:THR:HG23	1:E:106:GLN:HE21	1.85	0.41
1:E:293:LEU:HB3	1:E:298:ILE:HG13	1.93	0.41
1:E:374:MET:HG3	1:E:375:VAL:N	2.35	0.41
1:A:90:PHE:CE2	1:A:92:THR:HB	2.56	0.41
1:C:174:LEU:O	1:C:174:LEU:HG	2.20	0.41
1:C:210:LYS:HA	1:C:233:GLY:O	2.21	0.41
1:D:219:LEU:HB3	1:D:241:ILE:HG12	2.02	0.41
1:F:104:VAL:HG12	1:F:106:GLN:HG3	2.03	0.41
1:F:109:PRO:HG3	1:F:347:ARG:HD3	2.03	0.41
1:E:194:LYS:O	1:E:198:ILE:HG13	2.21	0.41
1:F:52:VAL:HG11	1:F:79:ILE:HG12	2.03	0.41
1:F:131:TYR:CE2	1:F:158:ASN:HB2	2.56	0.41
1:A:223:ASP:OD2	1:A:273:LYS:HA	2.20	0.40
1:C:216:ILE:HD13	1:C:216:ILE:HA	1.90	0.40
1:F:21:SER:O	1:F:25:VAL:HG23	2.21	0.40
1:A:133:SER:OG	1:A:158:ASN:CG	2.60	0.40
1:C:27:MET:HE1	1:C:39:PRO:HD3	2.03	0.40
1:C:54:ASN:OD1	1:D:310:LEU:CD2	2.69	0.40
1:B:260:GLU:HB3	1:B:263:GLU:HB3	2.03	0.40
1:C:85:THR:HG21	1:D:50:PHE:CE1	2.55	0.40
1:E:216:ILE:HD13	1:E:216:ILE:HA	1.88	0.40
1:F:324:GLU:HG2	1:F:328:LYS:HE3	2.03	0.40
1:A:203:ILE:HG12	1:A:229:ILE:HG22	2.03	0.40
1:F:83:CYS:SG	1:F:90:PHE:HB2	2.60	0.40
1:B:72:ASP:O	1:B:73:LYS:C	2.59	0.40
1:C:48:ASN:O	1:C:52:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD11	1:D:144:LEU:HD11	2.04	0.40
1:C:294:ARG:C	1:C:296:GLN:H	2.25	0.40
1:E:50:PHE:CD2	1:F:85:THR:HG21	2.57	0.40
1:E:127:PHE:CE1	1:E:154:VAL:HG22	2.56	0.40
1:F:23:PHE:HB2	1:F:279:THR:CG2	2.52	0.40

All (3) 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:29:GLN:OE1	1:C:313:PRO:CB[1_455]	1.39	0.81
1:B:29:GLN:OE1	1:C:313:PRO:CA[1_455]	1.57	0.63
1:B:204:THR:O	1:C:14:ARG:NH2[4_455]	1.80	0.40

## 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	366/374 (98%)	337 (92%)	28 (8%)	1 (0%)	41	74
1	B	370/374 (99%)	342 (92%)	27 (7%)	1 (0%)	41	74
1	C	365/374 (98%)	335 (92%)	28 (8%)	2 (0%)	29	67
1	D	364/374 (97%)	333 (92%)	31 (8%)	0	100	100
1	E	360/374 (96%)	332 (92%)	26 (7%)	2 (1%)	25	64
1	F	356/374 (95%)	327 (92%)	28 (8%)	1 (0%)	41	74
All	All	2181/2244 (97%)	2006 (92%)	168 (8%)	7 (0%)	41	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	MET

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Mol	Chain	Res	Type
1	E	374	MET
1	B	295	LYS
1	A	376	VAL
1	E	373	LYS
1	F	209	VAL
1	C	209	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	305/322 (95%)	301 (99%)	4 (1%)	69 87
1	B	310/322 (96%)	306 (99%)	4 (1%)	69 87
1	C	292/322 (91%)	288 (99%)	4 (1%)	67 86
1	D	298/322 (92%)	293 (98%)	5 (2%)	60 83
1	E	263/322 (82%)	256 (97%)	7 (3%)	44 75
1	F	290/322 (90%)	277 (96%)	13 (4%)	27 63
All	All	1758/1932 (91%)	1721 (98%)	37 (2%)	53 79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	PHE
1	A	71	TYR
1	A	185	ARG
1	A	291	ARG
1	B	35	PHE
1	B	71	TYR
1	B	185	ARG
1	B	291	ARG
1	C	35	PHE
1	C	71	TYR
1	C	177	ASP
1	C	185	ARG

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Mol	Chain	Res	Type
1	D	71	TYR
1	D	79	ILE
1	D	171	TYR
1	D	185	ARG
1	D	291	ARG
1	E	35	PHE
1	E	48	ASN
1	E	50	PHE
1	E	79	ILE
1	E	171	TYR
1	E	226	LEU
1	E	298	ILE
1	F	50	PHE
1	F	71	TYR
1	F	171	TYR
1	F	190	CYS
1	F	194	LYS
1	F	219	LEU
1	F	223	ASP
1	F	226	LEU
1	F	227	LEU
1	F	291	ARG
1	F	300	ILE
1	F	378	LEU
1	F	379	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	ASN
1	E	331	GLN
1	E	338	ASN
1	F	349	ASN

### 5.3.3 RNA

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	370/374 (98%)	0.00	2 (0%) 91 86	27, 62, 104, 137	0
1	B	372/374 (99%)	-0.02	5 (1%) 77 65	24, 45, 94, 153	0
1	C	369/374 (98%)	0.09	8 (2%) 62 48	26, 65, 102, 129	0
1	D	368/374 (98%)	0.07	8 (2%) 62 48	23, 50, 112, 155	0
1	E	366/374 (97%)	0.61	30 (8%) 11 6	42, 87, 121, 142	0
1	F	364/374 (97%)	0.63	46 (12%) 3 2	47, 99, 126, 160	0
All	All	2209/2244 (98%)	0.23	99 (4%) 33 21	23, 68, 119, 160	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	287	THR	5.3
1	B	168	ASP	5.2
1	E	65	TYR	5.1
1	F	89	SER	4.7
1	F	6	ILE	4.7
1	E	6	ILE	4.5
1	E	91	ILE	4.3
1	E	37	LEU	4.3
1	C	180	LEU	4.3
1	F	341	PHE	4.2
1	F	366	GLY	4.0
1	E	341	PHE	4.0
1	E	319	GLN	3.8
1	F	88	VAL	3.7
1	F	272	ILE	3.6
1	C	306	ALA	3.6
1	F	280	TYR	3.6
1	D	180	LEU	3.6
1	F	289	ALA	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	323	ILE	3.4
1	F	33	SER	3.3
1	F	378	LEU	3.3
1	F	180	LEU	3.2
1	F	34	GLU	3.2
1	D	226	LEU	3.2
1	B	163	ASN	3.2
1	F	293	LEU	3.2
1	E	322	GLU	3.2
1	E	89	SER	3.2
1	A	372	ASP	3.1
1	F	379	THR	3.1
1	D	375	VAL	3.1
1	F	339	ILE	3.1
1	C	271	THR	3.1
1	E	109	PRO	3.0
1	F	338	ASN	3.0
1	E	66	ALA	2.9
1	F	377	THR	2.9
1	E	105	ILE	2.8
1	B	303	ARG	2.8
1	F	286	MET	2.8
1	C	181	LYS	2.8
1	E	326	ALA	2.8
1	F	90	PHE	2.7
1	D	230	GLN	2.7
1	B	165	ASP	2.7
1	D	168	ASP	2.7
1	D	183	GLU	2.6
1	F	256	TRP	2.6
1	E	88	VAL	2.6
1	E	103	PHE	2.6
1	F	290	PHE	2.5
1	F	254	GLU	2.5
1	F	287	THR	2.5
1	C	367	TYR	2.5
1	A	180	LEU	2.5
1	E	309	CYS	2.5
1	E	327	LEU	2.5
1	F	330	VAL	2.5
1	D	163	ASN	2.4
1	F	37	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	270	ALA	2.4
1	F	336	SER	2.4
1	F	105	ILE	2.4
1	E	87	HIS	2.4
1	F	298	ILE	2.4
1	F	285	VAL	2.4
1	E	190	CYS	2.4
1	E	280	TYR	2.3
1	B	175	PHE	2.3
1	E	259	LEU	2.3
1	F	332	VAL	2.3
1	E	7	GLN	2.3
1	C	162	ILE	2.3
1	E	32	THR	2.2
1	D	231	PHE	2.2
1	F	30	PHE	2.2
1	F	36	ARG	2.2
1	E	285	VAL	2.2
1	F	327	LEU	2.2
1	F	104	VAL	2.2
1	E	164	ASN	2.1
1	F	221	PHE	2.1
1	C	35	PHE	2.1
1	F	8	ILE	2.1
1	E	253	ILE	2.1
1	F	335	LEU	2.1
1	F	351	THR	2.1
1	E	261	GLU	2.1
1	F	7	GLN	2.1
1	E	264	TYR	2.1
1	F	283	VAL	2.1
1	F	31	SER	2.0
1	F	70	PHE	2.0
1	F	279	THR	2.0
1	E	28	VAL	2.0
1	F	291	ARG	2.0
1	C	176	GLN	2.0
1	F	310	LEU	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 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.