



Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2024 – 04:09 PM EDT

PDB ID : 8UAI
Title : Crystal structure of hetero hexameric hazelnut allergen Cor a 9
Authors : Zhang, Y.Z.; Guo, F.
Deposited on : 2023-09-21
Resolution : 1.92 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

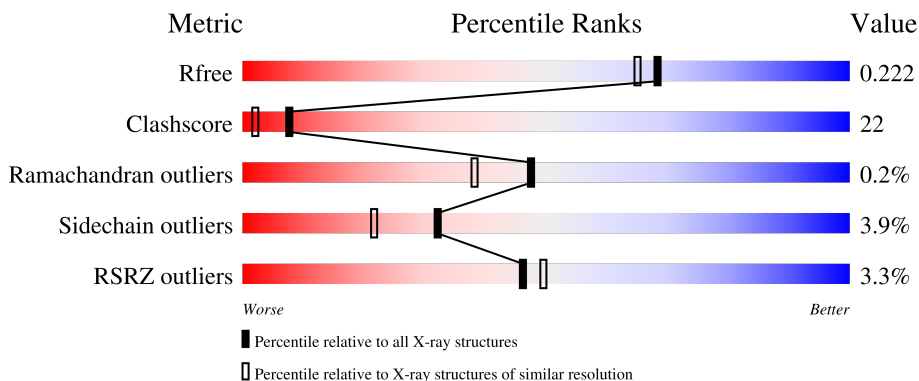
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 ≥ 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	493	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">63% 18% • 17%</p>
1	D	493	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">60% 22% • 16%</p>
2	B	494	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">51% 25% • 22%</p>
2	E	494	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">54% 21% • 23%</p>
3	C	493	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">53% 29% • 16%</p>

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Mol	Chain	Length	Quality of chain
3	F	493	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	502	-	-	X	-
4	GOL	E	505	-	-	X	-
5	CL	B	504	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20351 atoms, of which 96 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 11S globulin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	Total 3289	C 2024	N 628	O 633	S 4	0	4	0
1	D	413	Total 3397	C 2087	N 657	O 649	S 4	0	10	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	ASN	conflict	UNP Q8W1C2
A	12	HIS	TYR	conflict	UNP Q8W1C2
A	35	GLY	CYS	conflict	UNP Q8W1C2
A	74	LYS	GLU	conflict	UNP Q8W1C2
A	144	ILE	CYS	conflict	UNP Q8W1C2
A	260	GLN	VAL	conflict	UNP Q8W1C2
A	314	GLY	CYS	conflict	UNP Q8W1C2
A	457	SER	GLU	conflict	UNP Q8W1C2
D	2	ASP	ASN	conflict	UNP Q8W1C2
D	12	HIS	TYR	conflict	UNP Q8W1C2
D	35	GLY	CYS	conflict	UNP Q8W1C2
D	74	LYS	GLU	conflict	UNP Q8W1C2
D	144	ILE	CYS	conflict	UNP Q8W1C2
D	260	GLN	VAL	conflict	UNP Q8W1C2
D	314	GLY	CYS	conflict	UNP Q8W1C2
D	457	SER	GLU	conflict	UNP Q8W1C2

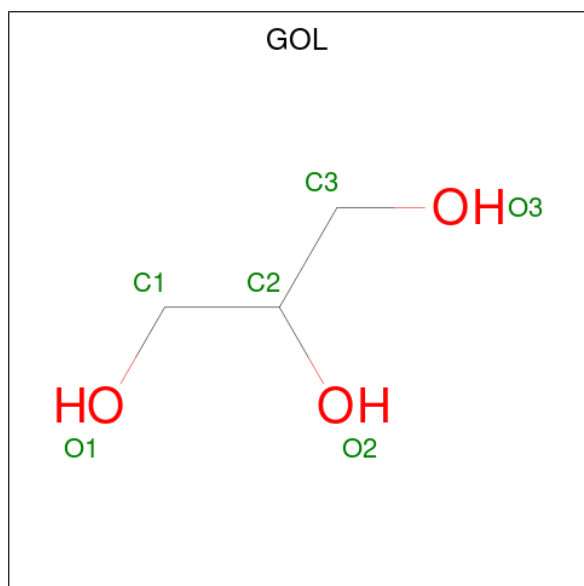
- Molecule 2 is a protein called 11S globulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	387	Total 3146	C 1962	N 596	O 583	S 5	0	12	0
2	E	382	Total 3085	C 1926	N 576	O 578	S 5	0	10	0

- Molecule 3 is a protein called 11S globulin 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	414	Total 3375	C 2094	N 643	O 630	S 8	0	18	0
3	F	402	Total 3248	C 2018	N 610	O 612	S 8	0	13	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	Total 6	C 3	O 3	0	0	
4	A	1	Total 14	C 3	H 8	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0	
4	B	1	Total 6	C 3	O 3	0	0	
4	B	1	Total 14	C 3	H 8	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0	
4	C	1	Total 14	C 3	H 8	O 3	0	0
4	D	1	Total 14	C 3	H 8	O 3	0	0
4	E	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		
6	B	95	Total	O	0	0
			95	95		
6	C	110	Total	O	0	0
			110	110		
6	D	125	Total	O	0	0
			125	125		
6	E	97	Total	O	0	0
			97	97		
6	F	99	Total	O	0	0
			99	99		

R436	T437	S438	R441	M465	R466	T470	L471	S479	E480	ARG	LYS	ARG	ARG	SER	GLU	SER	GLU	GLY	GLY	ARG	ALA	GLU	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	149.17Å 91.09Å 74.85Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	45.80 – 1.92 45.80 – 1.92	Depositor EDS
% Data completeness (in resolution range)	92.6 (45.80-1.92) 92.6 (45.80-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.92Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.174 , 0.221 0.174 , 0.222	Depositor DCC
R_{free} test set	7119 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20351	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

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	0.41	0/3360	0.67	0/4550
1	D	0.42	0/3485	0.70	0/4712
2	B	0.43	0/3231	0.68	0/4355
2	E	0.40	0/3161	0.66	0/4266
3	C	0.43	0/3475	0.67	0/4690
3	F	0.44	0/3337	0.69	0/4509
All	All	0.42	0/20049	0.68	0/27082

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	374	ARG	Sidechain

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	3289	0	3158	90	0
1	D	3397	0	3302	138	0
2	B	3146	0	3151	189	0
2	E	3085	0	3072	144	1
3	C	3375	0	3385	205	0
3	F	3248	0	3223	193	0
4	A	12	8	16	2	0
4	B	18	8	24	1	0
4	C	12	8	16	7	0
4	D	6	8	8	1	0
4	E	30	40	40	7	0
4	F	18	24	24	0	0
5	B	1	0	0	3	0
5	D	1	0	0	0	0
6	A	91	0	0	1	0
6	B	95	0	0	9	0
6	C	110	0	0	10	0
6	D	125	0	0	8	0
6	E	97	0	0	3	0
6	F	99	0	0	5	0
All	All	20255	96	19419	856	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 22.

All (856) 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)
3:C:436[B]:ARG:HB3	3:C:470:THR:HG22	1.32	1.09
1:D:466:ARG:CZ	1:D:472:VAL:HG21	1.86	1.05
3:C:304:ILE:HG13	3:C:307[B]:LEU:HD11	1.43	1.01
2:B:99:ASN:HD21	1:D:473:ARG:HE	1.07	0.98
3:C:65:VAL:HG22	3:C:144:ILE:H	1.29	0.97
1:D:57[B]:ARG:HH22	1:D:74:LYS:HE3	1.29	0.96
3:C:65:VAL:HG12	3:C:250:LEU:CD2	1.98	0.93
1:A:473:ARG:HD2	2:E:101:ASN:HD21	1.32	0.93
2:B:302:GLU:HB3	2:E:302:GLU:HB3	1.49	0.92
2:E:354:ARG:HG2	2:E:414:SER:O	1.70	0.92
3:C:360:PRO:HD3	3:C:409:ILE:HD13	1.50	0.91
3:F:145:TYR:CE1	3:F:253:LEU:HD12	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:372:VAL:HG21	3:C:394:ILE:CG2	2.00	0.91
3:F:30:ILE:HG23	3:F:181:PRO:HG3	1.53	0.90
1:A:466:ARG:HD2	1:A:472:VAL:HG11	1.55	0.89
3:C:349:ARG:HD3	3:C:420[B]:VAL:HG22	1.53	0.89
3:C:65:VAL:CG2	3:C:144:ILE:H	1.85	0.88
2:E:300:PHE:HD2	2:E:302:GLU:HG3	1.37	0.88
3:F:65:VAL:HG12	3:F:144:ILE:H	1.38	0.88
2:E:39:LYS:HG3	2:E:55:ILE:CD1	2.04	0.88
3:C:307[A]:LEU:HD21	3:C:339:VAL:CG2	2.04	0.88
1:D:74:LYS:HE2	1:D:158:LEU:HD11	1.56	0.88
3:C:85:LEU:CD2	3:C:309[A]:LEU:HD11	2.04	0.87
2:E:262:ILE:HG13	2:E:263:PRO:HD2	1.56	0.87
1:A:46:GLN:HB3	1:A:401[A]:THR:HG21	1.57	0.86
3:C:304:ILE:HG13	3:C:307[B]:LEU:CD1	2.06	0.86
2:E:348:GLU:HG2	2:E:421:ALA:HB3	1.55	0.86
3:F:84:LEU:HD13	3:F:125[A]:VAL:HG11	1.58	0.86
1:D:313:ILE:HD12	1:D:349:ARG:HB2	1.58	0.85
3:F:436[A]:ARG:HB3	3:F:470:THR:HG22	1.59	0.85
2:B:39:LYS:HD3	2:B:55[A]:ILE:HD12	1.59	0.85
3:F:349:ARG:HD3	3:F:420[B]:VAL:HG22	1.59	0.85
3:C:304:ILE:CG1	3:C:307[B]:LEU:HD11	2.07	0.84
2:B:321:ILE:HD12	1:D:95:THR:HB	1.57	0.84
3:C:224:VAL:HG22	3:C:242:GLN:OE1	1.76	0.84
1:A:55:ILE:HD11	1:A:184:HIS:CE1	2.13	0.84
3:F:307:LEU:HD21	3:F:339:VAL:CG2	2.09	0.83
2:E:300:PHE:CD2	2:E:302:GLU:HG3	2.14	0.83
3:F:308:ARG:HH12	3:F:311:GLU:HG2	1.44	0.82
2:E:37:VAL:HG23	6:E:654:HOH:O	1.78	0.82
2:E:119:GLN:HG2	2:E:120:ASP:H	1.45	0.82
3:F:314:THR:HG23	3:F:317:SER:OG	1.78	0.82
2:B:431:LEU:HD13	3:C:90:PRO:HB3	1.61	0.82
1:A:29:ARG:HD2	1:A:31:GLU:OE2	1.80	0.81
2:B:150:SER:HA	4:B:502:GOL:H12	1.62	0.81
3:C:37:VAL:HG22	3:C:57[A]:ARG:HD3	1.59	0.81
3:C:372:VAL:HG21	3:C:394:ILE:HG22	1.62	0.81
3:C:460:GLN:HB3	3:F:114:SER:HB3	1.60	0.81
1:D:74:LYS:HG2	1:D:158:LEU:HD12	1.63	0.81
3:F:394:ILE:O	3:F:394:ILE:HD12	1.80	0.81
3:C:360:PRO:HD3	3:C:409:ILE:CD1	2.11	0.81
2:B:262:ILE:HG23	2:B:265:ARG:HB3	1.62	0.81
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:430:LYS:HE3	6:C:680:HOH:O	1.80	0.80
2:B:320:ASP:O	2:B:321:ILE:HD13	1.82	0.80
3:F:359:VAL:HG21	3:F:434:ALA:O	1.82	0.80
1:A:28:ASN:HB3	1:A:185:GLN:O	1.81	0.80
2:B:77:TYR:CD2	2:B:79:ILE:HD13	2.17	0.80
3:C:254:GLU:HG3	3:C:255:GLN:H	1.46	0.80
2:B:77:TYR:HD2	2:B:79:ILE:HD13	1.45	0.79
2:B:465:ILE:HG21	3:C:232:ASN:O	1.83	0.79
2:E:126:ARG:HD3	2:E:310:MET:HE3	1.64	0.79
3:F:27:THR:HG21	3:F:41:ASP:H	1.47	0.79
1:A:84:ILE:HD12	1:A:260:GLN:HE22	1.48	0.79
3:C:11:ARG:HG3	3:C:13:PHE:H	1.46	0.78
3:C:257:GLN:O	3:C:262:ARG:NH2	2.16	0.78
1:A:20:ARG:NH1	1:A:22:ASN:OD1	2.17	0.78
1:D:55[B]:ILE:HD12	1:D:158:LEU:HD21	1.66	0.78
3:F:71:PRO:HG3	3:F:167:LEU:HD12	1.66	0.78
1:D:289:ARG:HE	1:D:289:ARG:HA	1.48	0.78
3:F:224:VAL:HG22	3:F:242:GLN:OE1	1.84	0.78
3:F:30:ILE:HG23	3:F:181:PRO:CG	2.15	0.78
3:C:305:CYS:HB2	4:C:502:GOL:H11	1.66	0.77
2:B:62:ARG:HH21	2:B:257[B]:ARG:HH11	1.30	0.77
3:C:87[B]:VAL:HG13	3:C:140:VAL:HG11	1.67	0.77
3:C:37:VAL:HG23	6:C:613:HOH:O	1.83	0.77
1:D:364:LEU:HD21	6:D:666:HOH:O	1.82	0.77
2:E:39:LYS:HG3	2:E:55:ILE:HD12	1.67	0.77
1:A:301:GLU:HA	1:A:305:CYS:HB2	1.65	0.76
2:B:33:GLU:HG2	2:B:248:ARG:HB3	1.67	0.76
3:C:307[A]:LEU:HD21	3:C:339:VAL:HG23	1.66	0.76
2:B:299:GLY:HA2	2:B:342:TYR:HB3	1.66	0.76
3:C:349:ARG:HH21	3:C:373:ILE:CD1	1.98	0.76
3:C:359:VAL:HG21	3:C:434:ALA:O	1.85	0.76
2:E:355:GLU:OE2	2:E:414:SER:HA	1.83	0.76
3:F:126:HIS:NE2	3:F:309[B]:LEU:HD21	2.00	0.76
1:A:473:ARG:HD2	2:E:101:ASN:ND2	2.00	0.76
2:B:80[B]:LYS:HA	2:B:130:GLU:CG	2.15	0.76
2:B:362:TYR:CE2	2:B:364:LEU:HD23	2.20	0.76
3:F:436[B]:ARG:HB3	3:F:470:THR:HG22	1.68	0.76
3:F:76:ILE:HD13	3:F:156:ALA:CB	2.16	0.75
2:B:77:TYR:HD2	2:B:79:ILE:CD1	2.00	0.75
3:F:307:LEU:HD21	3:F:339:VAL:HG23	1.68	0.75
2:B:37:VAL:HG13	2:B:55[B]:ILE:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:465:ILE:HG21	3:F:232:ASN:O	1.86	0.74
3:F:27:THR:CG2	3:F:41:ASP:H	2.01	0.74
3:C:349:ARG:CD	3:C:420[B]:VAL:HG22	2.18	0.74
2:B:300:PHE:HB2	2:B:342:TYR:CD2	2.22	0.74
3:F:436[A]:ARG:HB3	3:F:470:THR:CG2	2.18	0.74
3:C:65:VAL:HG22	3:C:144:ILE:N	2.03	0.73
1:D:185:GLN:O	1:D:186:ARG:HB2	1.89	0.73
3:F:359:VAL:HG23	3:F:434:ALA:HB3	1.70	0.73
3:F:74:MET:SD	3:F:76:ILE:HD11	2.28	0.73
1:A:325:GLN:HE22	2:E:102:ARG:HG3	1.52	0.73
3:C:436[B]:ARG:CB	3:C:470:THR:HG22	2.15	0.73
1:A:168:ASP:HA	3:C:15:GLU:OE1	1.88	0.73
1:A:84:ILE:CD1	1:A:260:GLN:HE22	2.01	0.73
2:B:126[A]:ARG:HH11	2:B:310:MET:HE3	1.53	0.72
2:B:329[B]:ILE:HD11	2:B:471:ILE:HD11	1.71	0.72
3:F:30:ILE:HB	3:F:37[A]:VAL:CG2	2.19	0.72
2:B:362:TYR:OH	2:B:431:LEU:HD23	1.89	0.72
2:E:329[A]:ILE:HD11	2:E:471:ILE:HD11	1.70	0.72
2:B:303:THR:HB	2:B:307:LEU:HD21	1.72	0.72
2:B:462:LEU:HD13	3:C:241:GLN:HE22	1.55	0.71
3:C:312:ASN:OD1	3:C:314:THR:HG22	1.91	0.71
3:C:87[B]:VAL:HG13	3:C:140:VAL:CG1	2.19	0.71
2:B:62:ARG:NE	2:B:257[B]:ARG:HG3	2.05	0.71
2:E:181:ASP:HB2	2:E:216:THR:HG21	1.73	0.71
3:F:34:GLY:O	3:F:60:GLU:HG3	1.91	0.71
2:E:461:ARG:HE	2:E:465:ILE:HG13	1.54	0.70
2:B:320:ASP:C	2:B:321:ILE:HD13	2.11	0.70
2:E:315:ASN:HD21	2:E:317:ARG:HH21	1.39	0.70
3:C:11:ARG:HG3	3:C:13:PHE:N	2.06	0.70
3:C:85:LEU:HD21	3:C:309[A]:LEU:HD11	1.74	0.70
3:C:352:LEU:CD2	3:C:472[B]:VAL:HG13	2.21	0.70
3:F:30:ILE:HB	3:F:37[A]:VAL:HG22	1.72	0.70
1:D:319:ALA:HA	1:D:330:ASN:ND2	2.06	0.70
3:C:349:ARG:HH21	3:C:373:ILE:HD13	1.57	0.69
3:F:349:ARG:CD	3:F:420[B]:VAL:HG22	2.21	0.69
1:A:344:GLN:HA	1:A:426:ASP:HB3	1.74	0.69
3:C:182:ASP:OD1	3:C:246:LYS:NZ	2.24	0.69
1:D:334:SER:HB2	1:D:341[B]:ARG:HG2	1.74	0.69
3:F:349:ARG:HH21	3:F:373:ILE:CD1	2.05	0.69
3:F:349:ARG:HH21	3:F:373:ILE:HD11	1.58	0.69
1:D:124:LYS:HE2	1:D:126:ARG:HH22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:CYS:O	4:C:501:GOL:H2	1.93	0.69
3:C:59:ILE:HD12	3:C:250:LEU:HD22	1.74	0.69
3:F:76:ILE:HD13	3:F:156:ALA:HB2	1.73	0.69
2:B:301:GLU:H	2:B:301:GLU:CD	1.96	0.69
3:F:84:LEU:HD11	3:F:262:ARG:HD2	1.74	0.69
2:E:362:TYR:OH	2:E:431:LEU:HD23	1.93	0.69
2:B:303:THR:CB	2:B:307:LEU:HD21	2.23	0.69
3:C:53:ALA:HB3	3:C:158:VAL:CG1	2.23	0.69
3:C:71:PRO:HG3	3:C:167:LEU:HD12	1.74	0.69
3:C:88:VAL:HG22	3:C:141:VAL:HB	1.75	0.69
3:F:436[B]:ARG:HH11	3:F:436[B]:ARG:HG2	1.57	0.69
2:B:461:ARG:HB3	2:B:465:ILE:HG13	1.74	0.68
2:E:320:ASP:C	2:E:321:ILE:HD12	2.14	0.68
2:E:461:ARG:HA	2:E:465:ILE:HG12	1.75	0.68
3:C:307[B]:LEU:HD23	3:F:335:GLN:HG2	1.76	0.68
3:C:461[B]:ARG:NH2	3:F:110:SER:OG	2.27	0.68
1:D:288:ARG:O	1:D:289:ARG:HG2	1.92	0.68
2:B:80[A]:LYS:HA	2:B:130:GLU:CG	2.22	0.68
2:B:99:ASN:ND2	1:D:473:ARG:HE	1.89	0.68
2:B:467:ASN:ND2	1:D:121:ARG:HH22	1.92	0.68
3:C:265:GLN:HE22	3:F:324:ARG:HE	1.39	0.68
2:E:33:GLU:HG2	2:E:253[B]:LYS:HD2	1.76	0.68
3:C:85:LEU:HD23	3:C:309[A]:LEU:HD11	1.76	0.68
2:E:84:PHE:HE2	2:E:262:ILE:CD1	2.06	0.67
3:C:65:VAL:HG21	6:C:704:HOH:O	1.92	0.67
1:D:264:GLU:OE2	1:D:268:GLN:NE2	2.27	0.67
2:E:79:ILE:CD1	2:E:155:VAL:HG23	2.23	0.67
3:F:65:VAL:HG11	6:F:696:HOH:O	1.93	0.67
2:B:170:ASN:HD22	2:B:171:PRO:HD2	1.60	0.67
3:C:15:GLU:OE1	3:C:15:GLU:HA	1.94	0.67
3:F:27:THR:HG22	3:F:44:GLN:OE1	1.94	0.67
2:B:262:ILE:CG2	2:B:265:ARG:HB3	2.24	0.67
2:B:300:PHE:HB2	2:B:342:TYR:CE2	2.29	0.67
1:D:74:LYS:HE2	1:D:158:LEU:CD1	2.25	0.67
3:F:240:ARG:HA	3:F:243:GLN:HG3	1.76	0.67
2:E:126:ARG:HH22	2:E:308:ARG:HA	1.57	0.67
2:B:129:ARG:HG3	2:B:129:ARG:HH11	1.60	0.67
3:F:302:GLU:CG	3:F:305:CYS:HB2	2.25	0.66
1:A:57:ARG:HH22	1:A:74:LYS:HE2	1.59	0.66
2:B:257[A]:ARG:CZ	1:D:288:ARG:HE	2.09	0.66
1:D:124:LYS:HE2	1:D:126:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:304:ILE:O	2:E:304:ILE:HG13	1.96	0.66
3:C:304:ILE:HG21	1:D:300:PHE:CZ	2.30	0.65
2:E:174:PHE:HB3	2:E:218[A]:ILE:HD11	1.77	0.65
3:C:65:VAL:HG12	3:C:250:LEU:HD23	1.77	0.65
1:D:46:GLN:HB3	1:D:401[B]:THR:HG21	1.77	0.65
2:E:98:SER:OG	2:E:119:GLN:HG2	1.96	0.65
3:F:59:ILE:N	3:F:59:ILE:HD12	2.12	0.65
1:D:57[B]:ARG:HH22	1:D:74:LYS:CE	2.06	0.65
3:C:65:VAL:HG12	3:C:250:LEU:HD21	1.79	0.65
3:C:145:TYR:CE1	3:C:253:LEU:HD12	2.32	0.65
3:C:460:GLN:HB3	3:F:114:SER:CB	2.26	0.65
2:E:39:LYS:HG3	2:E:55:ILE:HD11	1.77	0.65
1:A:314:GLY:O	1:A:328:ARG:NH2	2.29	0.65
2:B:302:GLU:O	2:E:302:GLU:HA	1.97	0.65
2:B:39:LYS:CD	2:B:55[A]:ILE:HD12	2.25	0.65
2:E:368:SER:OG	4:E:505:GOL:H32	1.97	0.65
3:C:103:GLN:HA	3:C:103:GLN:OE1	1.97	0.64
3:F:76:ILE:CD1	3:F:156:ALA:HB2	2.27	0.64
2:B:10:GLN:HB2	3:C:163:LYS:HB2	1.80	0.64
2:B:37:VAL:HG12	2:B:39:LYS:HE2	1.79	0.64
2:B:402:ILE:CD1	2:B:408:VAL:HG21	2.28	0.64
3:C:303:THR:HG23	4:C:502:GOL:C3	2.28	0.64
3:C:237:ILE:HG22	3:C:241:GLN:HE21	1.61	0.64
1:D:74:LYS:HG2	1:D:158:LEU:CD1	2.26	0.64
2:E:84:PHE:HE2	2:E:262:ILE:HD12	1.61	0.64
1:D:307:LEU:HD21	1:D:339:VAL:HB	1.78	0.64
3:C:304:ILE:HD12	3:C:307[B]:LEU:HD21	1.78	0.64
2:B:402:ILE:HD13	2:B:408:VAL:HG21	1.80	0.64
3:C:436[B]:ARG:HB3	3:C:470:THR:CG2	2.18	0.64
3:C:37:VAL:HG22	3:C:57[A]:ARG:CD	2.28	0.64
1:D:181:ASP:OD2	1:D:186:ARG:NH2	2.29	0.64
3:F:436[B]:ARG:HB3	3:F:470:THR:CG2	2.28	0.64
2:B:181:ASP:CB	2:B:216:THR:HG21	2.28	0.63
2:E:126:ARG:NH2	2:E:308:ARG:HA	2.14	0.63
3:C:303:THR:HG23	4:C:502:GOL:H31	1.79	0.63
2:E:461:ARG:HH21	2:E:465:ILE:HG21	1.63	0.63
2:E:315:ASN:ND2	2:E:317:ARG:HH21	1.96	0.63
3:C:349:ARG:NH2	3:C:373:ILE:HD13	2.14	0.63
3:F:312:ASN:ND2	3:F:314:THR:HG22	2.13	0.63
1:D:319:ALA:CA	1:D:330:ASN:HD21	2.12	0.63
3:C:65:VAL:CG2	3:C:144:ILE:N	2.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:46[B]:GLN:HG3	2:E:401[B]:THR:HB	1.80	0.62
2:B:80[B]:LYS:HA	2:B:130:GLU:HG3	1.80	0.62
2:B:378:ARG:HG3	2:B:378:ARG:HH11	1.63	0.62
1:D:240:ARG:HG2	6:D:625:HOH:O	1.99	0.62
3:F:253:LEU:HD13	3:F:257:GLN:CD	2.20	0.62
1:D:124:LYS:NZ	1:D:305:CYS:O	2.29	0.62
2:E:54:LEU:O	2:E:55:ILE:HD13	1.99	0.62
1:A:466:ARG:HD2	1:A:472:VAL:CG1	2.28	0.62
1:D:472:VAL:HG23	6:D:612:HOH:O	1.99	0.62
3:F:374[B]:ARG:NE	3:F:418:GLU:OE2	2.31	0.62
1:D:55[A]:ILE:HD13	1:D:158:LEU:HD21	1.81	0.62
2:E:79:ILE:HD11	2:E:155:VAL:CG2	2.29	0.62
2:E:303:THR:OG1	2:E:307:LEU:HD13	1.99	0.62
1:A:278:ARG:O	1:A:282:GLN:HG2	2.00	0.62
6:D:666:HOH:O	2:E:90:PRO:HG3	1.98	0.62
1:D:310:ARG:CZ	1:D:310:ARG:HB2	2.29	0.62
1:A:278:ARG:HH22	1:A:317:SER:HB3	1.63	0.61
3:C:88:VAL:O	3:C:140:VAL:HG13	2.00	0.61
3:C:100:SER:OG	3:C:103:GLN:HG2	2.00	0.61
3:C:436[A]:ARG:HB3	3:C:470:THR:HG22	1.82	0.61
3:C:161:ASN:OD1	4:C:501:GOL:H11	2.01	0.61
3:F:22:ASN:H	3:F:46:GLN:NE2	1.98	0.61
3:C:11:ARG:HD3	3:C:12:HIS:H	1.65	0.61
3:C:22:ASN:H	3:C:46:GLN:HE21	1.47	0.61
1:D:57[B]:ARG:NH2	1:D:74:LYS:HE3	2.10	0.61
3:F:350:GLY:HA3	3:F:419:TYR:CE1	2.35	0.61
1:A:46:GLN:HB3	1:A:401[A]:THR:CG2	2.31	0.61
3:C:46:GLN:HG2	6:C:679:HOH:O	2.01	0.61
3:C:87[B]:VAL:CG1	3:C:140:VAL:HG11	2.30	0.61
1:D:351:ASP:OD1	1:D:418:GLU:HG2	2.00	0.61
3:F:30:ILE:CG2	3:F:181:PRO:HG3	2.28	0.61
3:C:304:ILE:CD1	3:C:307[B]:LEU:HD11	2.31	0.61
3:F:65:VAL:HG12	3:F:144:ILE:N	2.14	0.61
3:F:377:ALA:HB3	3:F:394:ILE:HD11	1.83	0.61
2:B:395[A]:ARG:NH1	6:B:604:HOH:O	2.34	0.61
2:E:61[A]:ARG:HH11	2:E:149:ASP:HA	1.66	0.61
2:E:126:ARG:HD3	2:E:310:MET:CE	2.31	0.60
1:D:299:GLY:N	1:D:302:GLU:OE2	2.34	0.60
2:B:74:GLU:OE1	2:B:156:THR:HG21	2.01	0.60
2:B:77:TYR:CD2	2:B:79:ILE:CD1	2.80	0.60
3:F:163:LYS:HD2	3:F:163:LYS:C	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:244:GLN:HB3	3:F:246:LYS:NZ	2.15	0.60
3:C:470:THR:HG23	6:C:696:HOH:O	2.01	0.60
1:D:307:LEU:HD22	1:D:309:LEU:CD2	2.32	0.60
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.12	0.60
2:B:55[B]:ILE:HG23	2:B:156:THR:HB	1.83	0.60
2:B:395[A]:ARG:HH11	2:B:395[A]:ARG:CG	2.15	0.60
2:E:378:ARG:NH2	6:E:604:HOH:O	2.33	0.60
3:F:359:VAL:CG1	3:F:471:LEU:HA	2.32	0.60
3:C:151:GLN:NE2	6:C:602:HOH:O	2.34	0.60
1:D:253:LYS:HD2	1:D:254:VAL:N	2.16	0.60
2:B:257[A]:ARG:NH2	1:D:288:ARG:HG2	2.17	0.59
2:E:74:GLU:OE1	2:E:156:THR:HG21	2.02	0.59
3:F:41:ASP:HB3	3:F:43:ASN:OD1	2.02	0.59
3:F:214:GLU:CG	3:F:215:SER:H	2.15	0.59
3:C:304:ILE:O	3:C:307[B]:LEU:HG	2.02	0.59
1:A:55:ILE:HD11	1:A:184:HIS:HE1	1.66	0.59
2:B:315:ASN:HD21	2:B:317:ARG:HH21	1.48	0.59
3:C:368:ARG:HG2	3:C:423:LYS:HG2	1.85	0.59
1:D:79:GLU:HG2	1:D:80:ARG:HG2	1.84	0.59
3:F:438:SER:OG	3:F:441:ARG:HG3	2.02	0.59
1:A:76:ILE:HG12	1:A:156:SER:OG	2.03	0.59
3:C:145:TYR:CE1	3:C:253:LEU:CD1	2.86	0.59
1:D:334:SER:CB	1:D:341[B]:ARG:HG2	2.33	0.59
3:F:349:ARG:HD2	3:F:419:TYR:O	2.02	0.59
3:C:224:VAL:HG12	3:C:235:VAL:HG13	1.84	0.59
3:C:325:GLN:HG2	6:F:672:HOH:O	2.03	0.59
1:D:129[B]:ARG:HH22	1:D:310:ARG:HH12	1.51	0.59
1:D:214:GLU:N	1:D:244:ASN:OD1	2.36	0.59
1:D:289:ARG:HA	1:D:289:ARG:NE	2.17	0.59
2:E:321:ILE:HD12	2:E:321:ILE:N	2.18	0.59
3:F:302:GLU:HG2	3:F:305:CYS:HB2	1.82	0.59
3:F:349:ARG:NH2	3:F:373:ILE:HD13	2.18	0.59
3:F:359:VAL:HG12	3:F:471:LEU:HA	1.85	0.59
2:B:255:GLU:O	2:B:255:GLU:HG2	2.01	0.59
3:C:395[B]:ARG:NH2	3:C:398:ASN:OD1	2.36	0.59
1:A:348:GLU:HG2	1:A:421:ALA:HB3	1.84	0.59
2:B:37:VAL:HG22	2:B:57:HIS:ND1	2.17	0.59
3:F:22:ASN:HA	3:F:392:ARG:HH11	1.67	0.59
1:A:325:GLN:NE2	2:E:102:ARG:HG3	2.18	0.58
2:B:119:GLN:N	6:B:605:HOH:O	2.34	0.58
1:D:319:ALA:HA	1:D:330:ASN:HD21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:22:ASN:HA	3:F:392:ARG:NH1	2.18	0.58
3:C:159:ASN:ND2	6:C:603:HOH:O	2.36	0.58
2:B:321:ILE:HD12	1:D:95:THR:CB	2.33	0.58
3:C:314:THR:HG23	3:C:314:THR:O	2.04	0.58
3:C:22:ASN:H	3:C:46:GLN:NE2	2.01	0.58
3:F:163:LYS:HD2	3:F:163:LYS:O	2.04	0.58
3:F:264:GLU:O	3:F:264:GLU:HG2	2.02	0.58
2:B:462:LEU:HD13	3:C:241:GLN:NE2	2.18	0.58
3:C:198:GLN:O	3:C:199:ALA:HB2	2.03	0.58
1:D:472:VAL:CG2	1:D:473:ARG:N	2.67	0.58
3:F:312:ASN:HD21	3:F:314:THR:HG22	1.69	0.58
2:B:62:ARG:NH2	2:B:257[B]:ARG:HD3	2.18	0.58
1:D:267:ARG:O	1:D:271:GLU:HG3	2.04	0.58
2:E:79:ILE:HD12	2:E:155:VAL:HG23	1.84	0.58
2:B:338:PRO:HG3	1:D:338:PRO:HG3	1.86	0.57
1:D:466:ARG:NH2	1:D:472:VAL:HG21	2.18	0.57
2:B:37:VAL:HG23	6:B:652:HOH:O	2.02	0.57
2:E:354:ARG:HG2	2:E:414:SER:C	2.24	0.57
2:E:384:ASP:CB	3:F:172:ARG:HG2	2.34	0.57
2:E:34:ALA:HB2	2:E:253[A]:LYS:HG2	1.86	0.57
1:A:278:ARG:NH2	1:A:317:SER:HB3	2.19	0.57
2:B:304:ILE:O	2:B:305:CYS:HB2	2.04	0.57
1:D:348:GLU:HG2	1:D:421:ALA:HB3	1.86	0.57
2:E:126:ARG:HB3	2:E:310:MET:CE	2.34	0.57
2:E:384:ASP:HB3	3:F:172:ARG:HG2	1.86	0.57
3:F:42:THR:HG22	3:F:53:ALA:HB2	1.87	0.57
2:E:436:ARG:NH2	6:E:602:HOH:O	2.31	0.57
2:B:384:ASP:CB	3:C:172:ARG:HG2	2.34	0.57
1:A:30:ILE:HD12	4:A:501:GOL:H12	1.85	0.57
3:C:170:GLU:HG3	3:C:170:GLU:O	2.03	0.57
2:E:411:ARG:NH1	3:F:229:GLU:OE1	2.38	0.57
3:F:314:THR:CG2	3:F:317:SER:OG	2.52	0.57
2:B:37:VAL:CG1	2:B:55[B]:ILE:HD11	2.33	0.57
1:D:55[A]:ILE:CD1	1:D:158:LEU:HD21	2.35	0.57
2:E:430[A]:ARG:NH1	4:E:505:GOL:O1	2.38	0.57
2:B:378:ARG:NH2	2:B:391:ASP:OD1	2.36	0.56
2:E:99:ASN:ND2	2:E:101:ASN:OD1	2.38	0.56
2:E:181:ASP:CB	2:E:216:THR:HG21	2.33	0.56
2:E:307:LEU:HD23	2:E:307:LEU:H	1.69	0.56
2:E:353:TYR:HB3	2:E:354:ARG:NH2	2.19	0.56
2:B:301:GLU:HA	2:B:304:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:384:ASP:HA	3:F:174:PHE:CD2	2.40	0.56
1:D:334:SER:OG	1:D:426:ASP:OD1	2.20	0.56
2:E:431:LEU:HD12	2:E:432:PRO:HD2	1.86	0.56
3:F:88:VAL:HG22	3:F:141:VAL:HB	1.88	0.56
2:B:336:ILE:HD11	6:D:653:HOH:O	2.05	0.56
3:C:115:GLN:OE1	3:C:115:GLN:HA	2.06	0.56
2:E:24:LEU:HD13	2:E:47:PHE:CE2	2.40	0.56
3:F:302:GLU:HG3	3:F:305:CYS:HB2	1.86	0.56
3:C:253:LEU:HD13	3:C:257:GLN:CD	2.26	0.56
2:E:126:ARG:HB3	2:E:310:MET:HE1	1.87	0.56
2:E:307:LEU:H	2:E:307:LEU:CD2	2.19	0.56
1:A:466:ARG:CD	1:A:472:VAL:HG11	2.33	0.56
3:C:168:ASP:OD1	3:C:172:ARG:NH2	2.39	0.56
3:F:22:ASN:H	3:F:46:GLN:HE21	1.54	0.56
3:C:11:ARG:HD3	3:C:12:HIS:N	2.21	0.56
3:C:307[A]:LEU:HD21	3:C:339:VAL:CB	2.36	0.56
1:D:55[B]:ILE:HD11	1:D:184:HIS:CE1	2.41	0.56
2:E:300:PHE:HD2	2:E:302:GLU:CG	2.14	0.56
1:A:299:GLY:C	2:E:429:GLN:HE21	2.08	0.56
2:B:175:TYR:CG	2:B:180:PRO:HG3	2.40	0.56
2:B:384:ASP:HB3	3:C:172:ARG:HG2	1.88	0.56
3:C:360:PRO:CD	3:C:409:ILE:HD13	2.29	0.56
1:A:277:GLU:O	1:A:281:GLU:HG3	2.06	0.55
1:A:413:GLU:OE2	1:A:413:GLU:HA	2.06	0.55
2:E:461:ARG:O	2:E:465:ILE:HG12	2.06	0.55
3:F:20:ARG:HG3	3:F:20:ARG:HH11	1.71	0.55
1:D:307:LEU:HD22	1:D:309:LEU:HD21	1.88	0.55
1:D:472:VAL:HG22	1:D:473:ARG:N	2.19	0.55
3:F:145:TYR:CE1	3:F:253:LEU:CD1	2.86	0.55
2:B:299:GLY:CA	2:B:342:TYR:HB3	2.35	0.55
1:D:267:ARG:NE	1:D:271:GLU:OE2	2.39	0.55
1:A:39:SER:HB3	1:A:55:ILE:CD1	2.37	0.55
3:C:464:HIS:CD2	3:F:114:SER:HA	2.42	0.55
1:A:12:HIS:CG	2:B:168:ASP:HA	2.42	0.55
3:C:304:ILE:HG21	1:D:300:PHE:CE2	2.42	0.55
3:C:349:ARG:HD2	3:C:419:TYR:O	2.07	0.55
3:C:376:ASN:HD22	3:C:395[A]:ARG:NH1	2.05	0.55
1:D:265:ARG:O	1:D:269:GLU:HG3	2.06	0.55
3:F:23:VAL:HG22	3:F:392:ARG:NH2	2.22	0.55
1:A:308:ARG:HH12	1:A:311:GLU:HG3	1.72	0.55
3:F:308:ARG:NH1	3:F:311:GLU:HG2	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:HG23	1:A:318:ARG:HB2	1.88	0.55
2:B:85:GLN:OE1	2:B:126[A]:ARG:NH1	2.37	0.55
3:C:11:ARG:CG	3:C:13:PHE:H	2.19	0.55
2:B:303:THR:HB	2:B:307:LEU:CD2	2.37	0.54
2:B:325:GLN:HG3	1:D:99:PRO:HG2	1.87	0.54
2:E:363:ASN:HD21	4:E:505:GOL:C1	2.20	0.54
3:C:314:THR:HG23	3:C:317:SER:HB2	1.88	0.54
1:A:74:LYS:HE3	1:A:158:LEU:HD21	1.89	0.54
2:B:362:TYR:CZ	2:B:431:LEU:HD23	2.42	0.54
2:E:84:PHE:CE2	2:E:262:ILE:CD1	2.88	0.54
2:B:313:ILE:HD12	2:B:349:ARG:HB2	1.88	0.54
3:C:303:THR:HG23	4:C:502:GOL:C2	2.37	0.54
2:B:329[B]:ILE:CD1	2:B:471:ILE:HD11	2.37	0.54
2:B:37:VAL:CG1	2:B:39:LYS:HE2	2.37	0.54
2:B:89:ILE:CG2	2:B:304:ILE:HG23	2.36	0.54
1:A:265:ARG:O	1:A:265:ARG:HG3	2.06	0.54
2:B:16:CYS:O	2:B:18:LEU:HD22	2.07	0.54
2:B:126[A]:ARG:HD3	5:B:504:CL:CL	2.45	0.54
2:B:461:ARG:HA	2:B:465:ILE:HG12	1.90	0.54
2:E:119:GLN:CG	2:E:120:ASP:H	2.18	0.54
3:F:34:GLY:C	3:F:60:GLU:HG3	2.27	0.54
2:E:84:PHE:CE2	2:E:262:ILE:HD13	2.42	0.54
3:F:37[B]:VAL:HG23	6:F:603:HOH:O	2.08	0.54
3:F:253:LEU:HD13	3:F:257:GLN:NE2	2.23	0.54
1:A:20:ARG:HD2	1:A:20:ARG:C	2.28	0.54
2:B:80[A]:LYS:HA	2:B:130:GLU:HG3	1.89	0.54
3:C:338:PRO:HD3	3:F:338:PRO:HG3	1.89	0.54
2:E:76:ILE:HG12	2:E:156:THR:HG23	1.89	0.54
1:D:443:LEU:HD12	1:D:448:LEU:HD21	1.90	0.53
3:F:65:VAL:HG23	3:F:250:LEU:HD23	1.90	0.53
3:C:214:GLU:HB2	6:C:689:HOH:O	2.09	0.53
2:B:170:ASN:HD22	2:B:171:PRO:CD	2.20	0.53
3:C:64:GLU:HG2	3:C:253:LEU:HD21	1.89	0.53
1:D:264:GLU:OE1	1:D:264:GLU:HA	2.08	0.53
1:A:453:GLN:HB2	2:B:240:ARG:NH2	2.24	0.53
3:C:76:ILE:HD12	3:C:136[A]:ILE:HG12	1.91	0.53
2:E:79:ILE:CD1	2:E:155:VAL:CG2	2.86	0.53
2:E:135:ALA:O	2:E:136:LEU:HD22	2.09	0.53
3:F:323:SER:HB3	3:F:326:ALA:HB3	1.91	0.53
3:C:302:GLU:HB2	1:D:304:ILE:HD13	1.90	0.53
3:F:373:ILE:HD11	3:F:418:GLU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:CG	1:A:325:GLN:HG3	2.39	0.53
3:C:307[A]:LEU:HD21	3:C:339:VAL:HB	1.91	0.53
3:C:372:VAL:HG21	3:C:394:ILE:HG21	1.89	0.53
1:D:221:GLY:HA3	3:F:382:SER:HB2	1.91	0.53
2:E:313:ILE:HD12	2:E:349:ARG:HB2	1.91	0.53
2:B:344:GLN:OE1	2:B:426:ASP:HB2	2.09	0.53
3:C:371:TYR:HB3	3:C:420[A]:VAL:CG1	2.39	0.53
3:F:390:PHE:CE1	3:F:392:ARG:HD3	2.44	0.53
1:D:212:GLN:HB2	1:D:223:ASP:HA	1.91	0.52
1:D:334:SER:CB	1:D:426:ASP:OD1	2.56	0.52
3:C:13:PHE:HA	3:C:18:LEU:HD21	1.90	0.52
3:C:58:THR:HG22	3:C:153:VAL:HG22	1.91	0.52
3:C:145:TYR:CD1	3:C:253:LEU:HD11	2.44	0.52
2:E:320:ASP:CB	2:E:321:ILE:HD12	2.40	0.52
2:B:22:ASN:O	2:B:24:LEU:HD23	2.10	0.52
2:B:24:LEU:HD12	6:B:644:HOH:O	2.08	0.52
3:F:82:ARG:NH2	3:F:149:ASP:H	2.07	0.52
2:B:11:ARG:HG2	2:B:11:ARG:HH11	1.75	0.52
2:B:311:GLU:HG2	2:B:332:LEU:HD13	1.91	0.52
2:B:74:GLU:HG2	6:B:628:HOH:O	2.09	0.52
2:B:135:ALA:HB1	2:B:343:LEU:CD1	2.40	0.52
3:C:358:TYR:O	3:C:409:ILE:HD12	2.09	0.52
3:F:64:GLU:CG	3:F:253:LEU:HD21	2.39	0.52
3:F:349:ARG:NH2	3:F:373:ILE:CD1	2.71	0.52
2:E:46[A]:GLN:HB3	2:E:401[A]:THR:OG1	2.09	0.52
2:B:329[B]:ILE:CG1	2:B:471:ILE:HD11	2.40	0.52
1:D:307:LEU:HD23	1:D:308:ARG:O	2.09	0.52
2:B:262:ILE:HG13	2:B:263:PRO:HD2	1.92	0.52
2:B:364:LEU:HD22	3:C:139:GLY:O	2.10	0.52
3:C:39:LYS:NZ	3:C:39:LYS:HB3	2.25	0.52
3:C:41:ASP:OD1	3:C:43:ASN:OD1	2.28	0.52
1:D:234:ASP:OD2	1:D:236:ASP:HB3	2.09	0.52
3:F:64:GLU:HG2	3:F:253:LEU:HD21	1.92	0.52
2:B:80[B]:LYS:HA	2:B:130:GLU:HG2	1.91	0.51
2:B:126[A]:ARG:CD	5:B:504:CL:CL	2.96	0.51
2:B:395[A]:ARG:NH1	2:B:395[A]:ARG:HG3	2.25	0.51
1:D:334:SER:HB3	1:D:426:ASP:OD1	2.10	0.51
2:B:411:ARG:HD3	3:C:226:LEU:HD21	1.90	0.51
3:C:265:GLN:NE2	3:F:324:ARG:HE	2.05	0.51
3:C:349:ARG:NH1	3:C:349:ARG:HG2	2.25	0.51
1:D:466:ARG:NH1	1:D:472:VAL:HG21	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:HA	1:A:396:GLN:HB2	1.91	0.51
2:B:315:ASN:ND2	2:B:317:ARG:HH21	2.08	0.51
2:B:362:TYR:HE2	2:B:364:LEU:HD23	1.74	0.51
3:F:27:THR:HG23	3:F:40:TRP:HA	1.92	0.51
2:B:300:PHE:H	2:B:342:TYR:HB3	1.74	0.51
3:C:371:TYR:HB3	3:C:420[A]:VAL:HG12	1.93	0.51
3:F:349:ARG:NH1	3:F:349:ARG:HG2	2.26	0.51
2:B:262:ILE:HG23	2:B:265:ARG:CB	2.37	0.51
2:E:431:LEU:HD13	3:F:90:PRO:HB3	1.91	0.51
3:F:76:ILE:HD13	3:F:156:ALA:HB1	1.91	0.51
3:C:457:GLU:O	3:C:461[B]:ARG:HD2	2.11	0.51
1:D:319:ALA:CA	1:D:330:ASN:ND2	2.71	0.51
3:C:76:ILE:HD12	3:C:136[B]:ILE:HG13	1.93	0.51
1:A:316:ARG:HD3	1:A:316:ARG:N	2.25	0.51
1:A:374:ARG:CG	1:A:418:GLU:HG3	2.40	0.51
2:B:302:GLU:HB3	2:E:302:GLU:CB	2.34	0.51
2:E:348:GLU:OE1	2:E:423:LYS:NZ	2.43	0.51
2:B:308:ARG:HH22	1:D:318[B]:ARG:CZ	2.24	0.51
2:B:325:GLN:HG3	1:D:99:PRO:CG	2.41	0.51
3:F:70:GLN:NE2	3:F:74:MET:HE3	2.26	0.51
2:B:129:ARG:HG3	2:B:129:ARG:NH1	2.25	0.50
3:F:68:ASN:HB3	3:F:175:LEU:HD23	1.94	0.50
1:A:324:GLU:HG2	1:A:325:GLN:HG3	1.91	0.50
3:C:253:LEU:HD13	3:C:257:GLN:NE2	2.25	0.50
1:A:37:ILE:HG21	1:A:183:GLU:HG2	1.94	0.50
2:B:16:CYS:C	2:B:18:LEU:HD22	2.30	0.50
3:F:361:HIS:CD2	3:F:430:LYS:HE2	2.46	0.50
2:B:237:LEU:O	2:B:240:ARG:HB2	2.12	0.50
2:B:262:ILE:HD11	1:D:317:SER:O	2.11	0.50
3:C:86:GLY:O	3:C:142:HIS:HA	2.11	0.50
2:E:46[B]:GLN:HG3	2:E:401[B]:THR:CB	2.42	0.50
3:F:244:GLN:HB3	3:F:246:LYS:HZ3	1.76	0.50
2:B:52:VAL:HG21	2:B:369:VAL:HG21	1.94	0.50
2:B:67:PRO:HA	2:B:142:HIS:O	2.12	0.50
3:C:254:GLU:HG3	3:C:255:GLN:N	2.23	0.50
1:D:168:ASP:HA	3:F:15:GLU:OE2	2.12	0.50
2:E:315:ASN:HD21	2:E:317:ARG:NH2	2.06	0.50
2:B:387:GLN:HB3	3:C:194:LYS:HE3	1.93	0.50
3:F:167:LEU:HD13	3:F:172:ARG:HD2	1.93	0.50
3:F:254[B]:GLU:HG2	3:F:255:GLN:H	1.76	0.50
3:F:307:LEU:HD11	3:F:339:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:HIS:CE1	2:B:12:HIS:ND1	2.79	0.49
3:C:57[A]:ARG:HD2	3:C:250:LEU:HD21	1.94	0.49
3:F:307:LEU:HD11	6:F:615:HOH:O	2.10	0.49
3:F:380:GLN:HA	3:F:390:PHE:O	2.11	0.49
3:F:436[B]:ARG:HH11	3:F:436[B]:ARG:CG	2.22	0.49
2:B:128:ILE:HG22	2:B:310:MET:CE	2.43	0.49
2:B:303:THR:OG1	2:B:307:LEU:HD11	2.12	0.49
1:A:315:THR:HG23	1:A:318:ARG:CB	2.42	0.49
2:B:85:GLN:OE1	2:B:126[A]:ARG:NH2	2.42	0.49
2:E:55:ILE:HG12	2:E:158:LEU:CD1	2.42	0.49
2:E:256:GLN:OE1	2:E:256:GLN:HA	2.11	0.49
2:E:258:LEU:HG	2:E:260:ILE:HG13	1.94	0.49
2:E:354:ARG:CZ	2:E:354:ARG:H	2.26	0.49
3:F:214:GLU:HG3	3:F:215:SER:H	1.77	0.49
3:F:313[A]:MET:SD	3:F:332:VAL:HG21	2.53	0.49
1:A:175:TYR:CG	1:A:180:PRO:HG3	2.47	0.49
1:A:473:ARG:CD	2:E:101:ASN:HD21	2.15	0.49
3:F:37[A]:VAL:HG13	6:F:603:HOH:O	2.12	0.49
1:A:468:GLU:HB2	1:A:472:VAL:HG12	1.93	0.49
2:B:121:GLN:NE2	6:B:610:HOH:O	2.46	0.49
2:B:180:PRO:HB3	2:B:250:LYS:HG2	1.93	0.49
3:C:359:VAL:HG23	3:C:434:ALA:HB3	1.94	0.49
1:D:349:ARG:HG3	1:D:349:ARG:NH1	2.26	0.49
3:C:308:ARG:HH21	3:F:318:GLN:HE22	1.59	0.49
2:E:18:LEU:N	2:E:18:LEU:HD12	2.28	0.49
2:E:360:PRO:HA	2:E:408:VAL:O	2.12	0.49
1:A:310:ARG:HB2	1:A:310:ARG:CZ	2.41	0.49
2:B:257[A]:ARG:HH22	1:D:288:ARG:HG2	1.77	0.49
3:C:64:GLU:CG	3:C:253:LEU:HD21	2.43	0.49
3:F:149:ASP:HB2	3:F:150:GLN:NE2	2.28	0.49
1:A:431[A]:SER:OG	2:B:90:PRO:HB3	2.13	0.48
2:B:411:ARG:NH1	3:C:229:GLU:OE2	2.46	0.48
1:D:46:GLN:HB3	1:D:401[B]:THR:CG2	2.41	0.48
3:F:70:GLN:CD	3:F:74:MET:HE3	2.33	0.48
2:B:44:ASP:OD2	2:B:46:GLN:HG2	2.12	0.48
2:B:374:ARG:HG2	2:B:375:GLY:N	2.27	0.48
2:E:119:GLN:HG2	2:E:120:ASP:N	2.20	0.48
3:F:145:TYR:CD1	3:F:253:LEU:CD1	2.96	0.48
1:A:380:GLN:HA	1:A:390:PHE:O	2.13	0.48
1:D:312:ASN:OD1	1:D:315:THR:N	2.46	0.48
1:D:448:LEU:HD12	1:D:463:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:CD2	2:B:310:MET:HE2	2.42	0.48
2:B:467:ASN:HD21	3:C:115:GLN:HE22	1.61	0.48
2:B:395[B]:ARG:HH11	2:B:395[B]:ARG:HB3	1.78	0.48
1:D:82:ARG:NH2	1:D:148:GLY:HA2	2.29	0.48
2:B:336:ILE:HG23	1:D:308:ARG:HB2	1.95	0.48
2:E:169:GLU:H	2:E:169:GLU:CD	2.16	0.48
1:A:300:PHE:CZ	3:F:304:ILE:HG12	2.49	0.48
2:E:16:CYS:C	2:E:18:LEU:HD12	2.33	0.48
3:C:255:GLN:HG3	3:C:256:GLN:N	2.29	0.47
2:B:465:ILE:CG2	3:C:232:ASN:O	2.58	0.47
1:D:319:ALA:N	1:D:330:ASN:HD21	2.12	0.47
3:F:321:ILE:N	3:F:321:ILE:HD12	2.30	0.47
3:C:70:GLN:OE1	3:C:171:TYR:HE1	1.97	0.47
1:D:128:PHE:CE2	1:D:144:ILE:HG23	2.49	0.47
3:F:65:VAL:CG1	3:F:144:ILE:HG22	2.44	0.47
1:A:90:PRO:HG3	3:C:364:GLN:OE1	2.14	0.47
2:B:388:ASN:O	3:C:194:LYS:HD3	2.15	0.47
3:C:59:ILE:HD12	3:C:250:LEU:CD2	2.44	0.47
3:C:307[A]:LEU:HD12	3:F:335:GLN:O	2.14	0.47
3:F:312:ASN:HD21	3:F:314:THR:CG2	2.26	0.47
3:F:365:ASN:HA	3:F:404:GLN:HE21	1.80	0.47
1:D:364:LEU:HD11	6:D:666:HOH:O	2.15	0.47
2:B:303:THR:OG1	2:B:307:LEU:HD21	2.15	0.47
2:B:307:LEU:HD23	1:D:335:ASN:HB3	1.97	0.47
1:D:128:PHE:HE2	1:D:144:ILE:HG23	1.79	0.47
2:E:89:ILE:CG2	2:E:92:CYS:SG	3.03	0.47
2:E:301:GLU:OE2	2:E:304:ILE:HG22	2.15	0.47
1:A:82:ARG:HH21	1:A:267:ARG:NH1	2.13	0.47
2:B:134:LEU:HD22	2:B:310:MET:HE2	1.97	0.47
3:C:57[A]:ARG:HB3	3:C:59:ILE:HD11	1.97	0.47
1:D:264:GLU:O	1:D:268:GLN:HG2	2.15	0.47
3:F:479:SER:O	3:F:480:GLU:CB	2.63	0.47
2:B:439:ALA:O	2:B:443:ILE:HG13	2.15	0.46
1:D:354:ARG:HG3	1:D:355:GLU:HG3	1.96	0.46
3:F:42:THR:CG2	3:F:53:ALA:HB2	2.45	0.46
2:B:306[A]:SER:OG	4:E:501:GOL:H12	2.15	0.46
3:C:27:THR:CG2	3:C:41:ASP:H	2.29	0.46
3:C:137:PRO:HB2	3:C:140:VAL:CG2	2.44	0.46
2:E:42:LYS:HZ2	2:E:171:PRO:HD2	1.80	0.46
2:E:450:ASN:ND2	3:F:257:GLN:OE1	2.44	0.46
1:D:129[B]:ARG:NH2	1:D:310:ARG:HH12	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:374[A]:ARG:HD2	3:F:418:GLU:OE2	2.15	0.46
3:C:113:GLN:CB	3:F:465:ASN:OD1	2.63	0.46
2:E:320:ASP:HB2	2:E:321:ILE:HD12	1.98	0.46
1:A:436:ARG:NH2	2:E:97:GLU:OE1	2.49	0.46
2:B:395[A]:ARG:NH1	2:B:395[A]:ARG:CG	2.75	0.46
2:E:431:LEU:HD12	2:E:432:PRO:CD	2.45	0.46
3:F:224:VAL:HG13	3:F:238:VAL:HG12	1.98	0.46
3:C:88:VAL:CG2	3:C:141:VAL:HB	2.43	0.46
3:C:436[A]:ARG:NH2	3:F:94:GLU:OE1	2.49	0.46
2:E:300:PHE:HB2	2:E:342:TYR:CD1	2.51	0.46
3:F:349:ARG:HG2	3:F:349:ARG:HH11	1.81	0.46
2:B:240:ARG:HD2	2:B:240:ARG:HA	1.67	0.46
1:D:411:ARG:HD2	1:D:477:SER:OG	2.16	0.46
2:E:461:ARG:HH21	2:E:465:ILE:CG2	2.26	0.46
2:B:33:GLU:HG2	2:B:248:ARG:CB	2.43	0.46
1:D:433:LEU:HD11	2:E:218[B]:ILE:HD12	1.97	0.46
1:A:84:ILE:HD12	1:A:260:GLN:NE2	2.24	0.46
3:F:137:PRO:HB3	3:F:342[A]:TYR:HE2	1.81	0.46
1:A:29:ARG:HG3	1:A:38:GLU:HG2	1.98	0.45
3:C:436[B]:ARG:HH22	2:E:441:ARG:HH21	1.62	0.45
3:F:105:LYS:HD2	3:F:105:LYS:HA	1.80	0.45
1:D:342:TRP:HA	1:D:342:TRP:CE3	2.51	0.45
2:B:431:LEU:CD1	3:C:90:PRO:HB3	2.41	0.45
3:C:157:VAL:HB	3:C:422:ILE:HG21	1.97	0.45
2:B:157:LEU:HD13	2:B:422:PHE:HB2	1.97	0.45
2:B:395[A]:ARG:HH11	2:B:395[A]:ARG:HG3	1.78	0.45
3:C:359:VAL:HG12	3:C:471:LEU:HD12	1.98	0.45
3:F:119:GLN:O	3:F:119:GLN:HG3	2.16	0.45
3:F:145:TYR:CE2	3:F:147:ASP:HB3	2.51	0.45
3:F:430:LYS:HB3	3:F:430:LYS:HE3	1.83	0.45
3:C:380:GLN:HA	3:C:390:PHE:O	2.17	0.45
1:D:342:TRP:HA	1:D:342:TRP:HE3	1.82	0.45
2:E:363:ASN:OD1	4:E:505:GOL:C1	2.65	0.45
3:F:23:VAL:HG22	3:F:392:ARG:CZ	2.47	0.45
3:C:76:ILE:CD1	3:C:136[A]:ILE:HG13	2.47	0.45
2:E:461:ARG:CA	2:E:465:ILE:HG12	2.43	0.45
3:F:308:ARG:HH12	3:F:311:GLU:CG	2.22	0.45
2:B:467:ASN:ND2	3:C:115:GLN:HE22	2.15	0.45
3:C:182:ASP:CG	3:C:246:LYS:NZ	2.70	0.45
1:D:307:LEU:CD2	1:D:309:LEU:HD23	2.47	0.45
3:F:82:ARG:HH22	3:F:149:ASP:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLY:HA2	1:A:244:ASN:OD1	2.17	0.45
2:B:340:LEU:HD23	2:B:343:LEU:HD12	1.99	0.45
2:B:461:ARG:HG2	2:B:465:ILE:HD11	1.99	0.45
3:C:124:ARG:HD2	6:C:687:HOH:O	2.17	0.45
3:F:51:GLY:HA3	3:F:161:ASN:ND2	2.32	0.45
1:A:28:ASN:HB2	1:A:39:SER:OG	2.17	0.45
1:A:30:ILE:HD13	1:A:30:ILE:N	2.32	0.45
3:C:80:LYS:HG2	3:C:81:GLY:N	2.32	0.45
3:C:307[B]:LEU:CD2	3:F:335:GLN:HG2	2.45	0.44
1:D:66:LEU:HD13	1:D:178:GLY:HA3	1.99	0.44
3:F:394:ILE:CD1	3:F:417:PHE:CE1	3.00	0.44
2:B:80[A]:LYS:HA	2:B:130:GLU:HG2	1.97	0.44
2:E:362:TYR:CZ	2:E:431:LEU:HD23	2.52	0.44
1:A:129:ARG:NH2	1:A:274:GLU:OE2	2.50	0.44
1:D:74:LYS:HG3	6:D:669:HOH:O	2.17	0.44
2:E:465:ILE:CG2	3:F:232:ASN:O	2.61	0.44
3:F:21:LEU:HA	3:F:46:GLN:HE21	1.82	0.44
3:C:17:ASN:ND2	6:C:606:HOH:O	2.42	0.44
2:E:175:TYR:CD2	2:E:180:PRO:HG2	2.52	0.44
3:F:76:ILE:CD1	3:F:156:ALA:CB	2.89	0.44
1:A:20:ARG:HD2	1:A:20:ARG:O	2.18	0.44
2:B:402:ILE:HD13	2:B:408:VAL:CG2	2.46	0.44
2:B:434:ALA:HB2	3:C:231:TYR:CZ	2.52	0.44
3:C:307[A]:LEU:HD11	3:C:339:VAL:HB	1.99	0.44
1:D:431[B]:SER:OG	2:E:90:PRO:HB3	2.17	0.44
2:B:334:SER:HB3	2:B:426:ASP:OD1	2.17	0.44
2:B:469:THR:O	2:B:469:THR:HG23	2.18	0.44
3:C:329:ILE:HD11	3:C:472[A]:VAL:CG1	2.48	0.44
1:A:374:ARG:HG3	1:A:418:GLU:HG3	1.99	0.44
2:B:384:ASP:HA	3:C:174:PHE:CD2	2.52	0.44
3:C:87[B]:VAL:HG13	3:C:140:VAL:HG12	1.95	0.44
1:D:334:SER:HB2	1:D:341[B]:ARG:CG	2.46	0.44
2:E:461:ARG:NH2	2:E:465:ILE:HG21	2.31	0.44
3:C:373:ILE:HG13	3:C:418:GLU:HB2	1.99	0.44
3:F:368:ARG:HG2	3:F:423:LYS:HG2	2.00	0.44
2:B:55[B]:ILE:CG2	2:B:156:THR:HB	2.46	0.44
2:B:378:ARG:NH1	2:B:391:ASP:OD1	2.46	0.44
1:D:433:LEU:HD21	2:E:218[B]:ILE:HD11	2.00	0.44
2:E:374:ARG:HD3	2:E:418:GLU:OE2	2.18	0.44
3:F:214:GLU:CG	3:F:215:SER:N	2.80	0.44
2:B:465:ILE:HG22	3:C:232:ASN:HB3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:302:GLU:CG	1:D:304:ILE:HG12	2.48	0.43
3:F:65:VAL:HG12	3:F:144:ILE:HG22	1.99	0.43
2:B:126[A]:ARG:NH1	2:B:310:MET:HE3	2.27	0.43
1:A:31:GLU:O	1:A:249[A]:ARG:HD2	2.17	0.43
3:C:304:ILE:HD11	3:C:307[B]:LEU:HD11	2.00	0.43
2:E:351:THR:HG23	2:E:418:GLU:HG2	2.00	0.43
3:F:22:ASN:HB3	3:F:392:ARG:HH12	1.82	0.43
3:F:84:LEU:HD11	3:F:262:ARG:CD	2.44	0.43
1:A:300:PHE:CE2	3:F:304:ILE:HG12	2.54	0.43
2:B:224:GLN:HE22	2:B:239:ARG:HE	1.66	0.43
2:B:257[A]:ARG:NE	1:D:288:ARG:HE	2.15	0.43
2:B:329[B]:ILE:HD11	2:B:471:ILE:CD1	2.46	0.43
2:E:327:GLY:HA3	2:E:351:THR:O	2.18	0.43
3:F:88:VAL:CG2	3:F:141:VAL:HB	2.48	0.43
2:E:21:LEU:HD23	2:E:46[A]:GLN:HG2	2.00	0.43
2:E:262:ILE:HG13	2:E:263:PRO:CD	2.38	0.43
3:F:82:ARG:NH2	3:F:150:GLN:HE21	2.16	0.43
3:F:89:ILE:HG22	3:F:92:CYS:SG	2.58	0.43
2:B:358:GLN:OE1	2:B:410:LYS:HD2	2.18	0.43
3:C:224:VAL:CG1	3:C:235:VAL:HG13	2.49	0.43
1:D:361:HIS:CE1	1:D:408:VAL:HG13	2.53	0.43
2:E:21:LEU:HG	2:E:389:ILE:HD12	2.01	0.43
2:E:307:LEU:HD23	2:E:307:LEU:N	2.34	0.43
1:A:300:PHE:HD1	3:F:90:PRO:O	2.01	0.43
3:C:76:ILE:HD11	3:C:136[B]:ILE:HD12	1.99	0.43
3:C:182:ASP:HB3	3:C:246:LYS:NZ	2.33	0.43
3:F:33:GLU:OE1	3:F:247:ARG:HD2	2.19	0.43
1:A:181:ASP:OD2	4:A:501:GOL:H11	2.19	0.43
1:D:67:PRO:HA	1:D:142:HIS:O	2.19	0.43
1:D:301[A]:GLU:HA	1:D:305:CYS:HB2	2.00	0.43
2:E:329[A]:ILE:HD11	2:E:471:ILE:CD1	2.45	0.43
1:A:453:GLN:HB2	2:B:240:ARG:HH21	1.82	0.43
2:B:260:ILE:CA	2:B:267:GLN:HE21	2.32	0.43
1:D:31:GLU:H	1:D:186:ARG:HH12	1.67	0.43
1:D:85[A]:THR:OG1	1:D:144:ILE:HG13	2.19	0.43
1:D:282:GLN:HA	1:D:282:GLN:OE1	2.19	0.43
3:F:404:GLN:O	3:F:405:PHE:HB2	2.19	0.43
1:A:20:ARG:HD3	1:A:22:ASN:ND2	2.33	0.42
1:A:307:LEU:HD11	1:A:339:VAL:HB	2.00	0.42
1:D:29:ARG:HD2	1:D:36:GLN:CD	2.38	0.42
1:D:212:GLN:HB3	1:D:242:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:373:ILE:O	2:E:396:GLN:HG3	2.18	0.42
3:C:65:VAL:HG22	3:C:144:ILE:HB	2.00	0.42
3:C:145:TYR:CE2	3:C:147:ASP:HB3	2.54	0.42
3:C:158:VAL:HG22	3:C:160:GLN:OE1	2.20	0.42
2:E:430[B]:ARG:HD3	4:E:505:GOL:O1	2.20	0.42
3:F:258[B]:ILE:H	3:F:258[B]:ILE:HG12	1.61	0.42
2:B:99:ASN:HD21	1:D:473:ARG:NE	1.92	0.42
2:B:126[A]:ARG:HD2	5:B:504:CL:CL	2.56	0.42
3:F:65:VAL:HA	3:F:250:LEU:HD23	2.01	0.42
2:B:39:LYS:HD3	2:B:55[A]:ILE:HG23	2.02	0.42
2:B:89:ILE:HG21	2:B:304:ILE:HG23	2.02	0.42
1:D:124:LYS:HE2	1:D:126:ARG:NH1	2.33	0.42
3:F:64:GLU:HB3	3:F:253:LEU:HD11	2.01	0.42
3:F:128:ILE:C	3:F:129:ARG:HG3	2.40	0.42
1:A:411:ARG:NH1	1:A:474:SER:OG	2.51	0.42
3:C:264:GLU:HB3	3:F:316:ARG:O	2.19	0.42
1:D:349:ARG:HG3	1:D:349:ARG:HH11	1.84	0.42
2:E:329[A]:ILE:CD1	2:E:471:ILE:HD11	2.46	0.42
3:F:84:LEU:HD13	3:F:125[A]:VAL:CG1	2.40	0.42
3:F:358:TYR:CE1	3:F:471:LEU:HD11	2.54	0.42
2:B:80[B]:LYS:NZ	6:B:617:HOH:O	2.53	0.42
2:B:430:ARG:O	1:D:299:GLY:N	2.52	0.42
3:C:58:THR:C	3:C:59:ILE:HD13	2.39	0.42
3:C:461[B]:ARG:NH2	3:F:110:SER:HG	2.18	0.42
1:D:37:ILE:HG21	1:D:183:GLU:HG2	2.01	0.42
3:F:394:ILE:HD11	3:F:417:PHE:CE1	2.55	0.42
3:C:395[A]:ARG:HE	3:C:395[A]:ARG:HB3	1.36	0.42
1:D:29:ARG:HD2	1:D:36:GLN:OE1	2.19	0.42
2:E:384:ASP:HA	3:F:174:PHE:CE2	2.55	0.42
1:D:364:LEU:HD11	1:D:431[A]:SER:HB2	2.02	0.42
1:D:370:VAL:O	1:D:399:VAL:HA	2.20	0.42
2:E:380:GLN:HB2	2:E:409:ILE:HG22	2.01	0.42
2:E:425:ASN:HD21	3:F:163:LYS:NZ	2.18	0.42
3:F:436[B]:ARG:CG	3:F:436[B]:ARG:NH1	2.80	0.42
6:B:604:HOH:O	3:C:188:GLN:HG2	2.20	0.42
3:C:88:VAL:O	3:C:140:VAL:CG1	2.67	0.42
3:F:20:ARG:HG3	3:F:20:ARG:NH1	2.31	0.42
1:A:336:THR:HB	2:E:308:ARG:CD	2.50	0.42
1:A:474:SER:OG	2:B:229:ASP:OD2	2.32	0.42
2:B:329[B]:ILE:HD13	2:B:329[B]:ILE:HG21	1.84	0.42
2:E:42:LYS:HZ2	2:E:171:PRO:CD	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:ILE:HD11	2:E:155:VAL:HG21	2.01	0.42
3:F:30:ILE:HG23	3:F:181:PRO:CD	2.50	0.42
3:F:137:PRO:O	3:F:140:VAL:HG22	2.20	0.42
1:A:318:ARG:HG2	1:A:318:ARG:HH11	1.85	0.41
3:C:59:ILE:HD13	3:C:59:ILE:N	2.34	0.41
2:E:465:ILE:HG22	3:F:232:ASN:HB3	2.01	0.41
3:F:64:GLU:HB3	3:F:253:LEU:HD21	2.02	0.41
3:F:84:LEU:HD11	3:F:262:ARG:CG	2.50	0.41
3:F:86:GLY:HA3	3:F:143:TRP:CE2	2.55	0.41
1:D:307:LEU:HD22	1:D:309:LEU:HD23	2.02	0.41
2:E:363:ASN:OD1	4:E:505:GOL:H12	2.20	0.41
3:F:359:VAL:HG11	3:F:471:LEU:HA	2.01	0.41
1:A:161:ASN:O	1:A:161:ASN:CG	2.58	0.41
1:A:239:ARG:HD3	6:A:609:HOH:O	2.19	0.41
1:A:338:PRO:HG3	2:E:338:PRO:HG3	2.02	0.41
2:B:128:ILE:HG22	2:B:310:MET:HE2	2.03	0.41
2:B:159:ASP:OD1	2:B:162:ASN:HB2	2.20	0.41
3:C:64:GLU:HB3	3:C:253:LEU:HD21	2.03	0.41
3:C:76:ILE:HD12	3:C:136[A]:ILE:CG1	2.49	0.41
3:C:326:ALA:HB1	3:C:472[B]:VAL:HG12	2.03	0.41
3:C:349:ARG:HH21	3:C:373:ILE:HD11	1.81	0.41
1:D:124:LYS:HE2	1:D:126:ARG:CZ	2.50	0.41
3:F:376:ASN:HB3	3:F:395[A]:ARG:HD2	2.03	0.41
1:A:349:ARG:NH1	1:A:351:ASP:OD1	2.37	0.41
1:A:357:LEU:HD22	1:A:474:SER:HB2	2.03	0.41
2:B:370:ILE:HD11	2:B:402:ILE:CD1	2.51	0.41
1:D:74:LYS:HD2	6:D:672:HOH:O	2.20	0.41
1:D:124:LYS:HE2	1:D:126:ARG:HH12	1.85	0.41
1:D:411:ARG:HD2	1:D:477:SER:CB	2.51	0.41
1:D:476:ARG:HB2	2:E:229:ASP:OD1	2.21	0.41
1:A:260:GLN:OE1	1:A:262:ARG:HD3	2.20	0.41
1:A:316:ARG:HA	1:A:328:ARG:HH12	1.86	0.41
3:C:23:VAL:CG1	3:C:394:ILE:CD1	2.99	0.41
3:C:372:VAL:HG12	3:C:396:GLN:HA	2.02	0.41
1:D:166:GLN:O	4:D:502:GOL:H31	2.20	0.41
1:D:352:LEU:HD21	1:D:471:LEU:HD22	2.02	0.41
1:D:476:ARG:HB2	2:E:229:ASP:OD2	2.21	0.41
2:B:11:ARG:HG2	2:B:11:ARG:NH1	2.34	0.41
1:D:382:VAL:HA	1:D:387:ASN:O	2.21	0.41
2:E:55:ILE:HG12	2:E:158:LEU:HD11	2.02	0.41
3:F:466:ARG:HD3	3:F:466:ARG:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:TYR:O	2:B:453:ARG:HB2	2.20	0.41
3:C:349:ARG:HG2	3:C:349:ARG:HH11	1.86	0.41
3:C:373:ILE:HG13	3:C:374:ARG:N	2.35	0.41
3:C:395[B]:ARG:CZ	3:C:398:ASN:OD1	2.68	0.41
1:D:124:LYS:CE	1:D:126:ARG:HH22	2.31	0.41
3:F:70:GLN:NE2	3:F:74:MET:CE	2.84	0.41
2:B:362:TYR:CE2	2:B:364:LEU:CD2	2.97	0.41
1:D:62:ASN:ND2	1:D:256:GLY:O	2.46	0.41
1:A:39:SER:CB	1:A:55:ILE:CD1	2.98	0.41
2:B:135:ALA:HB1	2:B:343:LEU:HD11	2.01	0.41
2:B:402:ILE:HD13	2:B:408:VAL:CB	2.51	0.41
3:C:191:LYS:HE2	3:C:191:LYS:HB2	1.68	0.41
3:C:365:ASN:HA	3:C:404:GLN:HE21	1.85	0.41
2:E:42:LYS:NZ	2:E:171:PRO:HD2	2.36	0.41
2:E:255:GLU:O	2:E:256:GLN:HB2	2.21	0.41
3:F:82:ARG:HH22	3:F:150:GLN:HE21	1.69	0.41
3:F:307:LEU:HA	3:F:307:LEU:HD12	1.83	0.41
3:F:436[A]:ARG:CB	3:F:470:THR:HG22	2.40	0.41
2:B:378:ARG:HH11	2:B:378:ARG:CG	2.30	0.41
2:B:441:ARG:HG2	3:C:94:GLU:OE2	2.21	0.41
3:C:137:PRO:HB2	3:C:140:VAL:HG21	2.03	0.41
3:C:161:ASN:OD1	4:C:501:GOL:C1	2.68	0.41
3:C:457:GLU:OE1	3:C:457:GLU:N	2.54	0.41
3:F:65:VAL:CG1	3:F:144:ILE:H	2.20	0.41
3:F:167:LEU:HD13	3:F:172:ARG:CD	2.50	0.41
3:F:182:ASP:C	3:F:183:GLU:HG3	2.41	0.41
1:A:20:ARG:HD3	1:A:22:ASN:CG	2.41	0.40
2:B:315:ASN:HD21	2:B:317:ARG:NH2	2.17	0.40
3:C:65:VAL:CG1	3:C:250:LEU:CD2	2.85	0.40
1:D:260:GLN:CG	1:D:262:ARG:HD3	2.51	0.40
1:D:476:ARG:HB2	2:E:229:ASP:CG	2.41	0.40
2:E:62:ARG:O	2:E:254:VAL:HG22	2.20	0.40
3:F:373:ILE:HD11	3:F:418:GLU:CB	2.50	0.40
1:A:361:HIS:CE1	1:A:408:VAL:HG13	2.56	0.40
1:A:429:GLN:HE21	2:B:90:PRO:HG2	1.85	0.40
2:B:262:ILE:HG13	2:B:263:PRO:CD	2.50	0.40
2:B:431:LEU:HD12	2:B:432:PRO:HD2	2.02	0.40
3:C:74:MET:HG2	3:C:76:ILE:HD11	2.02	0.40
3:C:347:ALA:HA	3:C:421:SER:O	2.21	0.40
1:D:301[B]:GLU:HA	1:D:305:CYS:HB2	2.03	0.40
3:F:303:THR:O	3:F:306:SER:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HG3	1:A:349:ARG:HH11	1.87	0.40
2:B:46:GLN:HB2	2:B:401:THR:HB	2.02	0.40
2:B:331:THR:HG21	1:D:302:GLU:HB3	2.03	0.40
3:C:76:ILE:CD1	3:C:136[B]:ILE:CD1	3.00	0.40
3:C:329:ILE:HD11	3:C:472[B]:VAL:HG22	2.02	0.40
1:D:226:PHE:CE1	3:F:411[A]:ARG:HB2	2.56	0.40
2:E:236:ASP:O	2:E:240[B]:ARG:HG2	2.21	0.40
3:F:74:MET:HE2	3:F:158:VAL:HG22	2.03	0.40
2:B:133:ILE:O	2:B:310:MET:HA	2.20	0.40
3:C:20:ARG:HD2	3:C:21:LEU:O	2.21	0.40
3:C:179:GLY:O	3:C:248:GLY:HA2	2.22	0.40
1:D:411:ARG:HD2	1:D:477:SER:HB3	2.03	0.40
3:F:145:TYR:CD1	3:F:253:LEU:HD11	2.56	0.40
1:A:132:ASP:HA	1:A:312:ASN:HA	2.03	0.40
2:B:101:ASN:O	2:B:102:ARG:C	2.59	0.40
2:B:124:LYS:HE2	6:B:616:HOH:O	2.20	0.40
2:B:247:LYS:HE2	2:B:247:LYS:HB2	1.85	0.40
2:B:437:ASN:HD22	2:B:437:ASN:HA	1.71	0.40
1:D:100:GLN:HA	1:D:119:GLN:HE22	1.86	0.40
2:E:21:LEU:CD2	2:E:46[A]:GLN:HG2	2.52	0.40
2:E:126:ARG:HB3	2:E:310:MET:HE3	2.04	0.40
3:F:94:GLU:OE1	3:F:94:GLU:N	2.49	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)
2:E:415:GLU:OE2	2:E:456:ARG:NH2[2_655]	2.17	0.03

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	403/493 (82%)	390 (97%)	12 (3%)	1 (0%)	47	38
1	D	415/493 (84%)	402 (97%)	12 (3%)	1 (0%)	47	38
2	B	391/494 (79%)	376 (96%)	14 (4%)	1 (0%)	41	31
2	E	384/494 (78%)	369 (96%)	14 (4%)	1 (0%)	41	31
3	C	422/493 (86%)	406 (96%)	16 (4%)	0	100	100
3	F	405/493 (82%)	391 (96%)	13 (3%)	1 (0%)	47	38
All	All	2420/2960 (82%)	2334 (96%)	81 (3%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	305	CYS
3	F	114	SER
1	A	307	LEU
1	D	307	LEU
2	E	167	LEU

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	350/422 (83%)	336 (96%)	14 (4%)	31	21
1	D	365/422 (86%)	356 (98%)	9 (2%)	47	39
2	B	338/422 (80%)	317 (94%)	21 (6%)	18	8
2	E	332/422 (79%)	319 (96%)	13 (4%)	32	22
3	C	368/420 (88%)	347 (94%)	21 (6%)	20	10
3	F	353/420 (84%)	341 (97%)	12 (3%)	37	27
All	All	2106/2528 (83%)	2016 (96%)	90 (4%)	32	18

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	74	LYS
1	A	80	ARG
1	A	226	PHE
1	A	240	ARG
1	A	260	GLN
1	A	265	ARG
1	A	278	ARG
1	A	324	GLU
1	A	328	ARG
1	A	341[A]	ARG
1	A	341[B]	ARG
1	A	358	TYR
1	A	376	ARG
2	B	19	ASP
2	B	24	LEU
2	B	43	ASN
2	B	97	GLU
2	B	102	ARG
2	B	124	LYS
2	B	142	HIS
2	B	157	LEU
2	B	170	ASN
2	B	236	ASP
2	B	255	GLU
2	B	257[A]	ARG
2	B	257[B]	ARG
2	B	266	GLN
2	B	300	PHE
2	B	301	GLU
2	B	304	ILE
2	B	378	ARG
2	B	395[A]	ARG
2	B	395[B]	ARG
2	B	415	GLU
3	C	17	ASN
3	C	19	ASP
3	C	20	ARG
3	C	22	ASN
3	C	129	ARG
3	C	149	ASP
3	C	163	LYS
3	C	180	GLN

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Mol	Chain	Res	Type
3	C	240[A]	ARG
3	C	240[B]	ARG
3	C	243	GLN
3	C	262	ARG
3	C	264	GLU
3	C	309[A]	LEU
3	C	309[B]	LEU
3	C	392	ARG
3	C	395[A]	ARG
3	C	395[B]	ARG
3	C	436[A]	ARG
3	C	436[B]	ARG
3	C	465	ASN
1	D	129[A]	ARG
1	D	129[B]	ARG
1	D	226	PHE
1	D	257	ARG
1	D	267	ARG
1	D	289	ARG
1	D	354	ARG
1	D	374	ARG
1	D	378	ARG
2	E	11	ARG
2	E	30	LYS
2	E	97	GLU
2	E	99	ASN
2	E	124	LYS
2	E	142	HIS
2	E	181	ASP
2	E	236	ASP
2	E	307	LEU
2	E	308	ARG
2	E	310	MET
2	E	430[A]	ARG
2	E	430[B]	ARG
3	F	20	ARG
3	F	44	GLN
3	F	57	ARG
3	F	82	ARG
3	F	163	LYS
3	F	308	ARG
3	F	313[A]	MET

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Mol	Chain	Res	Type
3	F	313[B]	MET
3	F	382	SER
3	F	430	LYS
3	F	436[A]	ARG
3	F	436[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	260	GLN
1	A	325	GLN
1	A	344	GLN
2	B	45	GLN
2	B	99	ASN
2	B	170	ASN
2	B	224	GLN
2	B	467	ASN
3	C	115	GLN
3	C	193	GLN
3	C	241	GLN
3	C	464	HIS
1	D	325	GLN
1	D	330	ASN
2	E	119	GLN
2	E	429	GLN
3	F	46	GLN
3	F	70	GLN
3	F	150	GLN
3	F	151	GLN
3	F	312	ASN
3	F	318	GLN
3	F	378	GLN

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](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	E	501	-	5,5,5	0.85	0	5,5,5	1.10	1 (20%)
4	GOL	E	505	-	5,5,5	0.91	0	5,5,5	1.17	1 (20%)
4	GOL	B	501	-	5,5,5	0.71	0	5,5,5	1.20	1 (20%)
4	GOL	A	501	-	5,5,5	0.79	0	5,5,5	1.16	0
4	GOL	E	502	-	5,5,5	0.65	0	5,5,5	0.83	0
4	GOL	F	503	-	5,5,5	0.83	0	5,5,5	1.04	0
4	GOL	D	502	-	5,5,5	0.79	0	5,5,5	0.93	0
4	GOL	E	504	-	5,5,5	1.10	0	5,5,5	1.23	1 (20%)
4	GOL	F	501	-	5,5,5	0.86	0	5,5,5	0.93	0
4	GOL	C	501	-	5,5,5	0.70	0	5,5,5	1.09	0
4	GOL	E	503	-	5,5,5	0.52	0	5,5,5	0.63	0
4	GOL	F	502	-	5,5,5	0.95	0	5,5,5	1.03	0
4	GOL	B	503	-	5,5,5	0.92	0	5,5,5	1.22	1 (20%)
4	GOL	B	502	-	5,5,5	1.11	0	5,5,5	1.00	0
4	GOL	A	502	-	5,5,5	0.94	0	5,5,5	1.26	1 (20%)
4	GOL	C	502	-	5,5,5	1.07	0	5,5,5	1.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	501	-	-	2/4/4/4	-
4	GOL	E	505	-	-	0/4/4/4	-
4	GOL	B	501	-	-	2/4/4/4	-
4	GOL	A	501	-	-	3/4/4/4	-
4	GOL	E	502	-	-	2/4/4/4	-
4	GOL	F	503	-	-	0/4/4/4	-
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	E	504	-	-	2/4/4/4	-
4	GOL	F	501	-	-	2/4/4/4	-
4	GOL	C	501	-	-	2/4/4/4	-
4	GOL	E	503	-	-	2/4/4/4	-
4	GOL	F	502	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	B	502	-	-	0/4/4/4	-
4	GOL	A	502	-	-	4/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	GOL	C3-C2-C1	-2.42	102.31	111.70
4	A	502	GOL	C3-C2-C1	-2.42	102.31	111.70
4	E	504	GOL	C3-C2-C1	-2.38	102.46	111.70
4	E	505	GOL	C3-C2-C1	-2.25	102.94	111.70
4	B	501	GOL	C3-C2-C1	-2.06	103.69	111.70
4	E	501	GOL	C3-C2-C1	-2.06	103.70	111.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GOL	O2-C2-C3-O3
4	A	502	GOL	O1-C1-C2-C3
4	A	502	GOL	C1-C2-C3-O3
4	B	501	GOL	C1-C2-C3-O3
4	C	501	GOL	C1-C2-C3-O3
4	C	501	GOL	O2-C2-C3-O3
4	E	501	GOL	C1-C2-C3-O3
4	E	502	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	E	502	GOL	O2-C2-C3-O3
4	E	503	GOL	C1-C2-C3-O3
4	E	504	GOL	O1-C1-C2-C3
4	B	501	GOL	O2-C2-C3-O3
4	E	503	GOL	O2-C2-C3-O3
4	A	501	GOL	C1-C2-C3-O3
4	F	501	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	E	501	GOL	O2-C2-C3-O3
4	E	504	GOL	O1-C1-C2-O2
4	F	501	GOL	O2-C2-C3-O3
4	A	502	GOL	O1-C1-C2-O2
4	D	502	GOL	O2-C2-C3-O3
4	A	501	GOL	O1-C1-C2-O2
4	D	502	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	GOL	1	0
4	E	505	GOL	6	0
4	A	501	GOL	2	0
4	D	502	GOL	1	0
4	C	501	GOL	3	0
4	B	502	GOL	1	0
4	C	502	GOL	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	407/493 (82%)	0.15	15 (3%) 41 44	26, 36, 58, 72	0
1	D	413/493 (83%)	0.08	12 (2%) 51 55	24, 35, 58, 85	0
2	B	387/494 (78%)	0.12	15 (3%) 39 42	25, 34, 55, 76	0
2	E	382/494 (77%)	0.10	12 (3%) 49 52	26, 37, 58, 77	0
3	C	414/493 (83%)	0.14	13 (3%) 49 52	25, 35, 56, 77	0
3	F	402/493 (81%)	0.12	13 (3%) 47 50	24, 34, 55, 82	0
All	All	2405/2960 (81%)	0.12	80 (3%) 46 49	24, 35, 57, 85	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	182	ASP	4.9
2	E	300	PHE	4.8
2	E	13	PHE	4.7
3	C	116	ARG	4.7
1	D	300	PHE	4.7
1	A	300	PHE	4.3
1	A	475	SER	4.2
2	E	304	ILE	4.2
2	B	299	GLY	4.1
3	F	254[A]	GLU	4.0
2	B	300	PHE	3.9
1	D	342	TRP	3.8
2	B	304	ILE	3.6
2	E	12	HIS	3.6
3	F	184	HIS	3.5
1	A	101	GLN	3.4
2	B	303	THR	3.3
3	F	116	ARG	3.2
3	C	189	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	183	GLU	3.1
2	E	303	THR	3.1
1	D	272	ARG	3.1
2	E	102	ARG	3.1
1	D	289	ARG	3.0
3	C	11	ARG	3.0
1	A	13	PHE	2.9
1	A	213	GLY	2.9
3	C	112	GLY	2.8
2	B	257[A]	ARG	2.8
1	D	472	VAL	2.8
2	B	244	ASN	2.7
3	C	188	GLN	2.7
2	B	119	GLN	2.7
3	F	303	THR	2.7
3	F	183	GLU	2.6
3	F	255	GLN	2.6
2	B	29[A]	ARG	2.6
1	D	255	GLU	2.6
2	E	256	GLN	2.6
3	C	341[A]	ARG	2.6
1	A	17	ASN	2.5
3	F	256	GLN	2.5
1	D	316	ARG	2.5
2	E	181	ASP	2.5
1	D	476	ARG	2.4
2	B	10	GLN	2.4
1	A	274	GLU	2.4
1	A	12	HIS	2.4
1	A	277	GLU	2.4
3	F	394	ILE	2.4
2	B	342	TYR	2.3
2	B	255	GLU	2.3
2	B	245	GLN	2.3
1	A	14	GLY	2.3
1	D	18	LEU	2.3
3	C	18	LEU	2.3
3	C	342[A]	TYR	2.3
2	B	216	THR	2.3
3	F	302	GLU	2.3
3	F	382	SER	2.3
1	A	414	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	10	GLN	2.2
3	F	342[A]	TYR	2.2
2	E	182	ASP	2.2
3	F	246	LYS	2.2
2	B	102	ARG	2.2
2	B	101	ASN	2.1
1	D	287	GLN	2.1
3	F	114	SER	2.1
1	A	272	ARG	2.1
2	E	235	VAL	2.1
2	E	245	GLN	2.1
1	D	286	ARG	2.1
3	C	302	GLU	2.1
3	C	20	ARG	2.1
1	D	17	ASN	2.1
1	A	304	ILE	2.1
1	A	325	GLN	2.0
3	C	307[A]	LEU	2.0
1	A	186	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	E	501	6/6	0.62	0.21	60,73,86,86	0
4	GOL	B	503	6/6	0.63	0.25	59,75,86,91	0
4	GOL	F	502	6/6	0.68	0.20	73,88,97,97	0
4	GOL	C	502	6/6	0.71	0.18	54,65,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	501	6/6	0.73	0.24	53,58,61,74	0
4	GOL	A	502	6/6	0.74	0.21	66,80,85,85	0
4	GOL	E	503	6/6	0.76	0.15	57,69,82,82	0
4	GOL	E	504	6/6	0.77	0.28	58,69,84,84	0
4	GOL	D	502	6/6	0.77	0.23	46,58,69,69	0
4	GOL	F	503	6/6	0.78	0.17	74,89,98,100	0
4	GOL	C	501	6/6	0.82	0.23	47,50,53,57	0
4	GOL	B	502	6/6	0.83	0.25	39,45,49,52	0
4	GOL	E	502	6/6	0.83	0.13	44,57,68,71	0
4	GOL	F	501	6/6	0.90	0.12	48,60,72,72	0
4	GOL	B	501	6/6	0.90	0.17	43,47,50,53	0
4	GOL	E	505	6/6	0.90	0.19	42,51,59,62	0
5	CL	B	504	1/1	0.98	0.05	46,46,46,46	0
5	CL	D	501	1/1	0.98	0.07	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.