Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 12:49 AM EDT

PDB ID	:	1AHW
Title	:	A COMPLEX OF EXTRACELLULAR DOMAIN OF TISSUE FACTOR WITH AN INHIBITORY FAB (5G9)
Authors	:	Huang, M.; Syed, R.; Stura, E.A.; Stone, M.J.; Stefanko, R.S.; Ruf, W.; Edgington, T.S.; Wilson, I.A.
Deposited on	:	1997-04-10
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

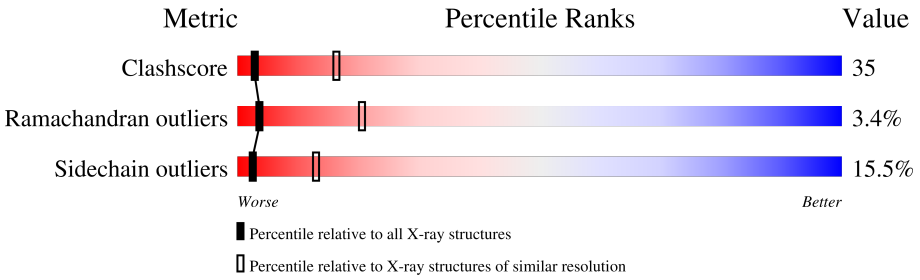
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	39% 46% 13% .
1	D	214	37% 49% 13% .
2	B	214	42% 45% 12% .
2	E	214	44% 49% 7%
3	C	219	34% 47% 10% 9%
3	F	219	37% 47% 7% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9830 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 IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1672	1040	278	346	8			
1	D	214	Total	C	N	O	S	0	0	0
			1672	1040	278	346	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	TYR	conflict	UNP P01837
A	31	LYS	SER	conflict	UNP P01837
A	34	ASN	SER	conflict	UNP P01837
A	36	TYR	PHE	conflict	UNP P01837
A	41	TRP	GLY	conflict	UNP P01837
A	50	TYR	ARG	conflict	UNP P01837
A	52	THR	ASN	conflict	UNP P01837
A	53	SER	ARG	conflict	UNP P01837
A	55	ALA	VAL	conflict	UNP P01837
A	80	SER	TYR	conflict	UNP P01837
A	81	ASP	GLU	conflict	UNP P01837
A	83	THR	LEU	conflict	UNP P01837
A	84	ALA	GLY	conflict	UNP P01837
A	85	THR	ILE	conflict	UNP P01837
A	91	HIS	PHE	conflict	UNP P01837
A	92	GLY	ASP	conflict	UNP P01837
A	94	SER	PHE	conflict	UNP P01837
A	107	ASN	LYS	conflict	UNP P01837
D	30	ARG	TYR	conflict	UNP P01837
D	31	LYS	SER	conflict	UNP P01837
D	34	ASN	SER	conflict	UNP P01837
D	36	TYR	PHE	conflict	UNP P01837
D	41	TRP	GLY	conflict	UNP P01837
D	50	TYR	ARG	conflict	UNP P01837
D	52	THR	ASN	conflict	UNP P01837

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Chain	Residue	Modelled	Actual	Comment	Reference
D	53	SER	ARG	conflict	UNP P01837
D	55	ALA	VAL	conflict	UNP P01837
D	80	SER	TYR	conflict	UNP P01837
D	81	ASP	GLU	conflict	UNP P01837
D	83	THR	LEU	conflict	UNP P01837
D	84	ALA	GLY	conflict	UNP P01837
D	85	THR	ILE	conflict	UNP P01837
D	91	HIS	PHE	conflict	UNP P01837
D	92	GLY	ASP	conflict	UNP P01837
D	94	SER	PHE	conflict	UNP P01837
D	107	ASN	LYS	conflict	UNP P01837

- Molecule 2 is a protein called IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1632	1034	263	329	6			
2	E	214	Total	C	N	O	S	0	0	0
			1632	1034	263	329	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	insertion	PIR S49220
B	2	ILE	-	insertion	PIR S49220
B	?	-	VAL	deletion	PIR S49220
B	?	-	LYS	deletion	PIR S49220
B	5	GLN	LEU	conflict	PIR S49220
B	6	GLN	GLU	conflict	PIR S49220
B	13	ARG	LYS	conflict	PIR S49220
B	14	PRO	SER	conflict	PIR S49220
B	17	LEU	SER	conflict	PIR S49220
B	23	LYS	THR	conflict	PIR S49220
B	32	TYR	THR	conflict	PIR S49220
B	50	LEU	ARG	conflict	PIR S49220
B	54	GLU	ALA	conflict	PIR S49220
B	57	ASN	GLU	conflict	PIR S49220
B	58	THR	ILE	conflict	PIR S49220
B	59	ILE	LYS	conflict	PIR S49220
B	67	LYS	THR	conflict	PIR S49220
B	69	SER	THR	conflict	PIR S49220
B	76	SER	THR	conflict	PIR S49220

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	ALA	VAL	conflict	PIR S49220
B	?	-	ARG	deletion	PIR S49220
B	?	-	GLY	deletion	PIR S49220
B	99	ASP	TYR	conflict	PIR S49220
B	100	ASN	GLY	conflict	PIR S49220
B	102	TYR	SER	conflict	PIR S49220
B	103	TYR	GLN	conflict	PIR S49220
B	104	PHE	GLU	conflict	PIR S49220
B	105	ASP	PRO	conflict	PIR S49220
E	1	GLU	-	insertion	PIR S49220
E	2	ILE	-	insertion	PIR S49220
E	?	-	VAL	deletion	PIR S49220
E	?	-	LYS	deletion	PIR S49220
E	5	GLN	LEU	conflict	PIR S49220
E	6	GLN	GLU	conflict	PIR S49220
E	13	ARG	LYS	conflict	PIR S49220
E	14	PRO	SER	conflict	PIR S49220
E	17	LEU	SER	conflict	PIR S49220
E	23	LYS	THR	conflict	PIR S49220
E	32	TYR	THR	conflict	PIR S49220
E	50	LEU	ARG	conflict	PIR S49220
E	54	GLU	ALA	conflict	PIR S49220
E	57	ASN	GLU	conflict	PIR S49220
E	58	THR	ILE	conflict	PIR S49220
E	59	ILE	LYS	conflict	PIR S49220
E	67	LYS	THR	conflict	PIR S49220
E	69	SER	THR	conflict	PIR S49220
E	76	SER	THR	conflict	PIR S49220
E	97	ALA	VAL	conflict	PIR S49220
E	?	-	ARG	deletion	PIR S49220
E	?	-	GLY	deletion	PIR S49220
E	99	ASP	TYR	conflict	PIR S49220
E	100	ASN	GLY	conflict	PIR S49220
E	102	TYR	SER	conflict	PIR S49220
E	103	TYR	GLN	conflict	PIR S49220
E	104	PHE	GLU	conflict	PIR S49220
E	105	ASP	PRO	conflict	PIR S49220

- Molecule 3 is a protein called TISSUE FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	200	Total	C	N	O	S	0	0	0
			1611	1021	262	323	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	200	Total	C	N	O	S	0	0	0
			1611	1021	262	323	5			

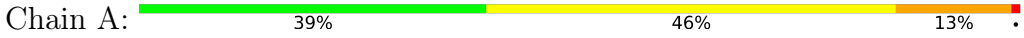
3 Residue-property plots (i)

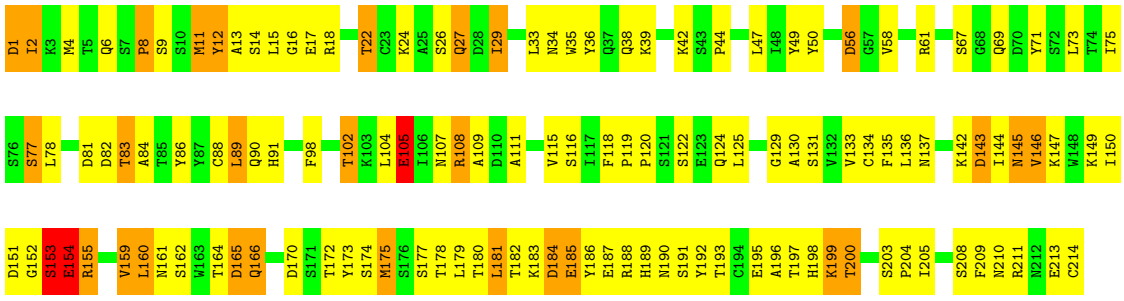
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN)

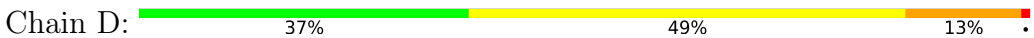
Chain A:

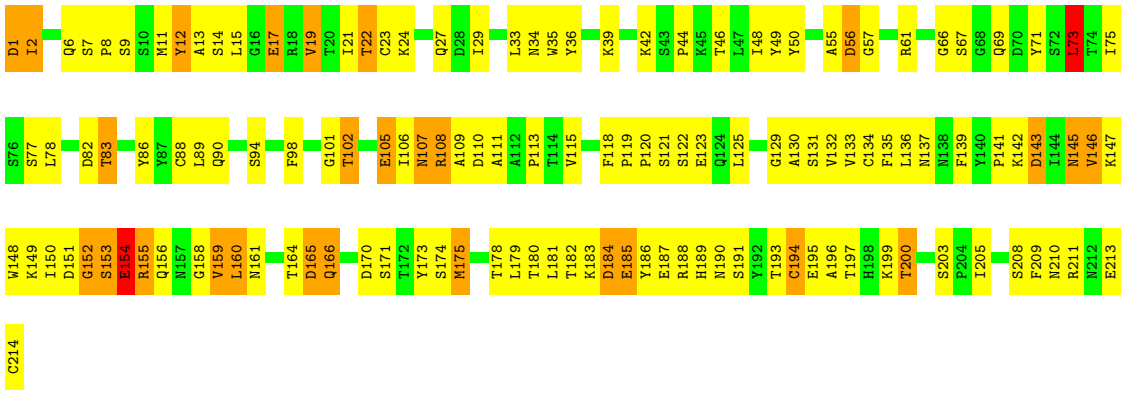




• Molecule 1: IMMUNOGLOBULIN FAB 5G9 (LIGHT CHAIN)

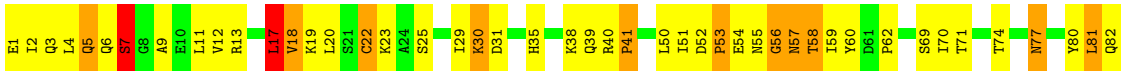
Chain D:

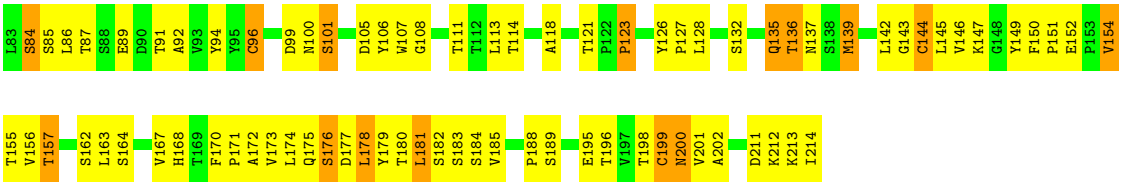




• Molecule 2: IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN)

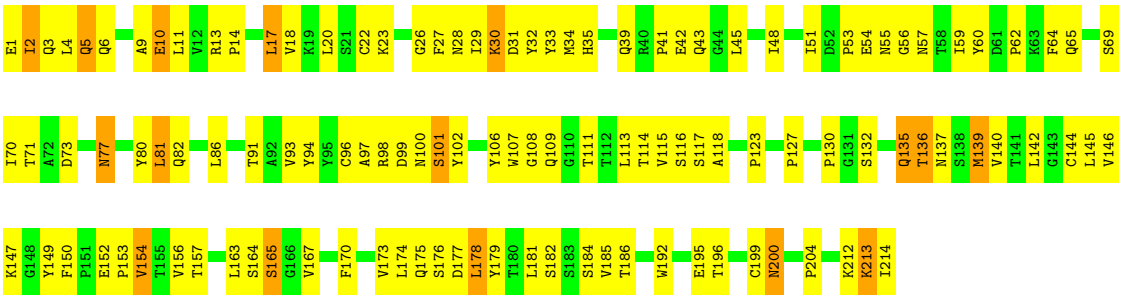
Chain B:





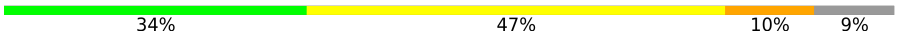
• Molecule 2: IMMUNOGLOBULIN FAB 5G9 (HEAVY CHAIN)

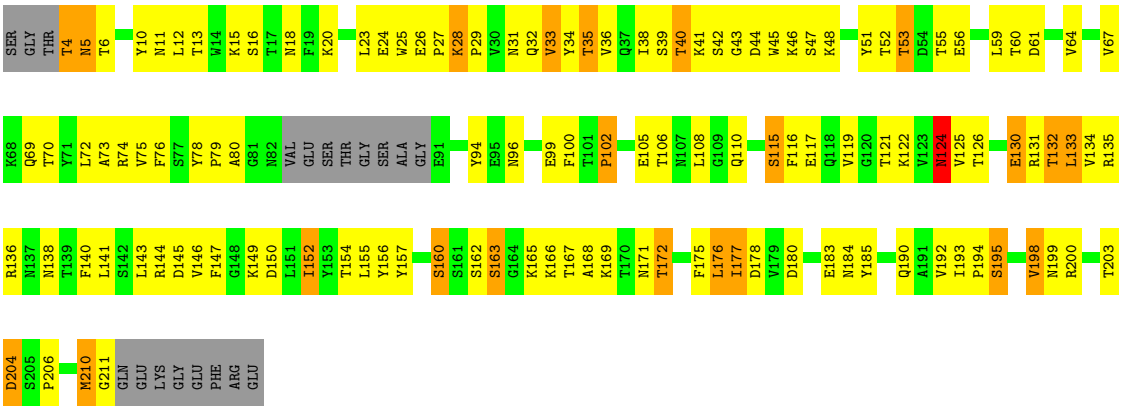
Chain E:



• Molecule 3: TISSUE FACTOR

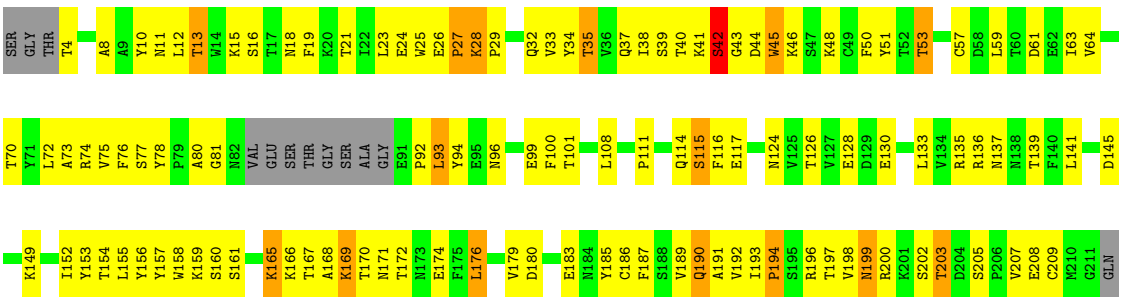
Chain C:





• Molecule 3: TISSUE FACTOR

Chain F:



GLU
LYS
GLY
GLU
PHE
ARG
GLU

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.30Å 73.31Å 115.83Å 90.00° 90.89° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	78.1 (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9830	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

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	0.86	1/1711 (0.1%)	1.04	1/2321 (0.0%)
1	D	0.84	0/1711	0.98	2/2321 (0.1%)
2	B	0.86	0/1675	1.03	4/2292 (0.2%)
2	E	0.77	0/1675	1.00	2/2292 (0.1%)
3	C	0.78	0/1646	0.96	1/2239 (0.0%)
3	F	0.74	1/1646 (0.1%)	0.92	0/2239
All	All	0.81	2/10064 (0.0%)	0.99	10/13704 (0.1%)

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
1	A	0	1
2	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	45	TRP	CB-CG	-5.79	1.39	1.50
1	A	105	GLU	CG-CD	5.20	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	81	LEU	CA-CB-CG	7.35	132.20	115.30
2	E	213	LYS	N-CA-C	-6.22	94.20	111.00
2	B	56	GLY	N-CA-C	5.98	128.04	113.10
1	A	89	LEU	CA-CB-CG	5.90	128.87	115.30
3	C	133	LEU	CA-CB-CG	-5.84	101.88	115.30
2	B	17	LEU	CB-CG-CD2	-5.75	101.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	144	CYS	CA-CB-SG	-5.57	103.98	114.00
1	D	158	GLY	N-CA-C	-5.43	99.53	113.10
2	B	96	CYS	N-CA-C	-5.42	96.38	111.00
1	D	73	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain
2	E	94	TYR	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	1672	0	1590	125	0
1	D	1672	0	1590	131	0
2	B	1632	0	1580	106	0
2	E	1632	0	1580	110	0
3	C	1611	0	1564	111	0
3	F	1611	0	1564	130	0
All	All	9830	0	9468	679	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (679) 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)
2:E:91:THR:HG23	2:E:114:THR:HA	1.35	1.06
3:F:136:ARG:HB3	3:F:141:LEU:HD11	1.35	1.05
1:D:6:GLN:HE21	1:D:102:THR:HG23	1.29	0.94
1:D:196:ALA:HB3	1:D:205:ILE:HB	1.51	0.92
2:E:4:LEU:HD23	2:E:22:CYS:SG	2.11	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ASN:HD22	1:D:49:TYR:HA	1.39	0.87
1:D:149:LYS:HG2	1:D:155:ARG:HB3	1.56	0.87
1:D:147:LYS:HB2	1:D:195:GLU:HB2	1.56	0.87
3:F:136:ARG:HD2	3:F:141:LEU:HD21	1.55	0.86
1:D:6:GLN:NE2	1:D:102:THR:HG23	1.93	0.83
3:C:135:ARG:NH2	3:C:138:ASN:HA	1.94	0.83
3:C:13:THR:HG21	3:C:15:LYS:HE2	1.60	0.81
3:F:11:ASN:HB2	3:F:26:GLU:HG3	1.62	0.81
1:A:8:PRO:O	1:A:102:THR:HB	1.81	0.81
1:D:149:LYS:HA	1:D:155:ARG:HA	1.61	0.80
3:F:183:GLU:HB2	3:F:185:TYR:HE1	1.46	0.80
2:E:60:TYR:OH	2:E:69:SER:HA	1.82	0.80
1:D:136:LEU:HD11	1:D:146:VAL:HG21	1.64	0.79
3:F:33:VAL:HG12	3:F:53:THR:HG23	1.65	0.79
2:B:142:LEU:HD22	2:B:214:ILE:HD12	1.64	0.78
1:D:193:THR:HB	1:D:208:SER:CB	2.13	0.78
1:D:34:ASN:ND2	1:D:49:TYR:HA	1.97	0.78
3:C:149:LYS:HG3	3:C:171:ASN:HD22	1.48	0.78
3:C:136:ARG:HB3	3:C:141:LEU:HD21	1.64	0.77
1:A:29:ILE:HD11	1:A:71:TYR:CE2	2.19	0.77
1:D:188:ARG:HB3	1:D:189:HIS:CD2	2.19	0.77
1:A:147:LYS:HD3	1:A:155:ARG:HH12	1.49	0.77
2:E:86:LEU:HD13	2:E:115:VAL:HG22	1.67	0.76
3:F:152:ILE:HD13	3:F:171:ASN:HB3	1.66	0.76
2:B:4:LEU:HD23	2:B:22:CYS:SG	2.25	0.76
1:D:187:GLU:HA	1:D:211:ARG:CZ	2.16	0.75
1:D:150:ILE:HD12	1:D:156:GLN:OE1	1.87	0.75
2:E:35:HIS:CD2	2:E:99:ASP:HB2	2.22	0.75
1:A:193:THR:HB	1:A:208:SER:HB2	1.68	0.74
3:F:149:LYS:HG3	3:F:171:ASN:HD22	1.52	0.74
1:D:150:ILE:HD13	1:D:181:LEU:HD21	1.68	0.74
3:F:8:ALA:HB2	3:F:93:LEU:HD12	1.69	0.74
1:A:129:GLY:HA2	1:A:182:THR:HA	1.67	0.74
3:F:57:CYS:SG	3:F:59:LEU:HD21	2.27	0.74
3:F:10:TYR:O	3:F:26:GLU:HB2	1.86	0.74
1:D:193:THR:HB	1:D:208:SER:HB2	1.71	0.73
1:A:183:LYS:O	1:A:187:GLU:HG3	1.89	0.73
1:D:75:ILE:HG21	1:D:78:LEU:HD12	1.69	0.73
1:D:190:ASN:O	1:D:210:ASN:HA	1.89	0.73
3:C:194:PRO:HA	3:C:200:ARG:NH2	2.04	0.73
1:A:33:LEU:HD22	1:A:71:TYR:CG	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:HD21	2:B:147:LYS:HD2	1.71	0.72
3:F:32:GLN:HB2	3:F:78:TYR:O	1.90	0.71
1:A:181:LEU:HG	1:A:185:GLU:HG2	1.70	0.71
1:D:111:ALA:C	1:D:200:THR:HG21	2.10	0.71
1:A:108:ARG:HG2	1:A:109:ALA:N	2.06	0.70
1:D:185:GLU:O	1:D:189:HIS:HD2	1.73	0.70
1:D:24:LYS:HA	1:D:69:GLN:O	1.91	0.70
1:A:150:ILE:HD13	1:A:181:LEU:HD21	1.73	0.70
1:A:188:ARG:HB3	1:A:189:HIS:CD2	2.26	0.70
1:D:6:GLN:HB2	1:D:23:CYS:SG	2.32	0.70
2:B:29:ILE:H	2:B:77:ASN:HD21	1.39	0.70
3:F:11:ASN:O	3:F:25:TRP:HA	1.92	0.70
1:D:39:LYS:O	1:D:42:LYS:HB2	1.92	0.70
3:C:149:LYS:HB2	3:C:149:LYS:NZ	2.07	0.69
3:C:38:ILE:HD12	3:C:59:LEU:HD13	1.72	0.69
3:C:135:ARG:CZ	3:C:138:ASN:HA	2.22	0.69
3:F:141:LEU:HB3	3:F:145:ASP:HB2	1.72	0.69
1:A:115:VAL:O	2:B:136:THR:HG21	1.92	0.69
1:A:150:ILE:CD1	1:A:181:LEU:HD21	2.21	0.69
1:A:39:LYS:O	1:A:42:LYS:HB2	1.93	0.69
2:E:6:GLN:HE21	2:E:108:GLY:HA3	1.56	0.68
3:F:78:TYR:HE1	3:F:92:PRO:HG3	1.59	0.68
1:A:160:LEU:HG	2:B:173:VAL:HG11	1.74	0.68
1:A:149:LYS:HG2	1:A:155:ARG:HB3	1.75	0.68
3:F:93:LEU:HD23	3:F:93:LEU:H	1.59	0.67
3:F:167:THR:HG22	3:F:168:ALA:H	1.58	0.67
3:F:37:GLN:HG2	3:F:45:TRP:HB3	1.77	0.67
3:C:180:ASP:HB2	3:C:183:GLU:HG3	1.76	0.67
1:D:14:SER:O	1:D:17:GLU:HB2	1.94	0.67
1:D:136:LEU:CD1	1:D:146:VAL:HG21	2.23	0.67
1:A:185:GLU:O	1:A:189:HIS:HD2	1.78	0.67
2:B:142:LEU:HD13	2:B:214:ILE:HD11	1.77	0.67
2:B:199:CYS:O	2:B:199:CYS:SG	2.52	0.67
1:D:108:ARG:HG3	1:D:108:ARG:HH11	1.59	0.67
2:E:181:LEU:HD23	2:E:182:SER:N	2.10	0.66
3:C:149:LYS:HG3	3:C:171:ASN:ND2	2.09	0.66
1:D:83:THR:HG21	1:D:166:GLN:HB3	1.76	0.66
1:A:6:GLN:HA	1:A:22:THR:O	1.93	0.66
3:C:74:ARG:NE	3:C:94:TYR:CE2	2.63	0.66
1:D:19:VAL:HG23	1:D:75:ILE:HB	1.77	0.66
2:E:157:THR:HG23	2:E:200:ASN:OD1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:PRO:HD2	2:E:192:TRP:CH2	2.30	0.66
2:E:130:PRO:HB2	2:E:132:SER:O	1.97	0.65
3:F:136:ARG:HD2	3:F:141:LEU:CD2	2.26	0.65
2:B:196:THR:HG23	2:B:213:LYS:HE3	1.78	0.65
2:B:175:GLN:O	2:B:176:SER:HB3	1.97	0.65
1:D:8:PRO:O	1:D:102:THR:HB	1.95	0.65
1:D:134:CYS:HB2	1:D:148:TRP:CZ2	2.32	0.65
3:F:152:ILE:CD1	3:F:171:ASN:HB3	2.27	0.65
1:A:149:LYS:HA	1:A:155:ARG:HA	1.78	0.65
3:C:156:TYR:HB3	3:C:165:LYS:NZ	2.11	0.65
2:B:29:ILE:HG12	2:B:77:ASN:ND2	2.11	0.64
1:A:12:TYR:CD1	1:A:12:TYR:N	2.65	0.64
2:B:127:PRO:CB	2:B:214:ILE:HG22	2.28	0.64
3:C:122:LYS:HG2	3:C:178:ASP:OD1	1.97	0.64
1:D:147:LYS:HD3	1:D:155:ARG:HH12	1.63	0.64
2:B:127:PRO:HB2	2:B:214:ILE:HG22	1.79	0.64
2:E:29:ILE:H	2:E:77:ASN:HD21	1.44	0.64
3:F:32:GLN:HA	3:F:80:ALA:N	2.12	0.64
3:C:26:GLU:HB3	3:C:27:PRO:HA	1.80	0.64
3:F:23:LEU:HD12	3:F:24:GLU:N	2.12	0.64
3:F:149:LYS:HG3	3:F:171:ASN:ND2	2.13	0.63
1:A:2:ILE:HD13	1:A:27:GLN:HG2	1.79	0.63
1:D:160:LEU:HG	2:E:173:VAL:HG11	1.79	0.63
2:E:5:GLN:CG	2:E:23:LYS:HB3	2.29	0.63
3:C:13:THR:CG2	3:C:15:LYS:HE2	2.28	0.63
3:F:136:ARG:CD	3:F:141:LEU:HD21	2.28	0.63
1:A:91:HIS:HD2	3:C:169:LYS:NZ	1.97	0.63
3:C:177:ILE:HG13	3:C:177:ILE:O	1.98	0.63
1:A:153:SER:O	1:A:155:ARG:N	2.31	0.63
3:F:39:SER:HB3	3:F:45:TRP:HA	1.81	0.63
1:A:193:THR:HB	1:A:208:SER:CB	2.29	0.62
1:D:12:TYR:N	1:D:12:TYR:CD1	2.67	0.62
1:A:185:GLU:HA	1:A:188:ARG:HE	1.65	0.62
2:B:147:LYS:HB3	2:B:180:THR:HG23	1.80	0.62
2:E:51:ILE:O	2:E:53:PRO:HD3	1.98	0.62
2:E:142:LEU:HB3	2:E:214:ILE:HD12	1.82	0.62
2:B:59:ILE:O	2:B:60:TYR:HD1	1.83	0.62
1:A:33:LEU:HD22	1:A:71:TYR:CB	2.30	0.62
2:E:9:ALA:O	2:E:10:GLU:HB2	2.00	0.62
1:D:145:ASN:HB3	1:D:197:THR:OG1	1.99	0.62
3:C:11:ASN:HB2	3:C:26:GLU:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ILE:HD13	1:D:27:GLN:HG2	1.81	0.62
2:B:20:LEU:HD12	2:B:81:LEU:HD12	1.83	0.61
3:C:147:PHE:CD2	3:C:193:ILE:HD12	2.35	0.61
1:D:66:GLY:HA3	1:D:71:TYR:CD1	2.35	0.61
1:D:135:PHE:CE2	2:E:184:SER:HB3	2.34	0.61
3:F:141:LEU:HB3	3:F:145:ASP:CB	2.30	0.61
1:A:147:LYS:HG2	1:A:155:ARG:HH22	1.65	0.61
1:A:6:GLN:HE21	1:A:102:THR:HG23	1.65	0.61
2:B:39:GLN:O	2:B:92:ALA:HB1	2.01	0.61
1:D:108:ARG:HH21	1:D:111:ALA:HB2	1.64	0.61
1:A:170:ASP:O	1:A:172:THR:HG23	2.01	0.61
1:D:152:GLY:O	1:D:154:GLU:N	2.33	0.61
1:A:108:ARG:HH21	1:A:111:ALA:HB2	1.66	0.61
1:D:120:PRO:CG	1:D:130:ALA:HB1	2.31	0.61
2:E:6:GLN:NE2	2:E:96:CYS:SG	2.74	0.61
2:B:20:LEU:HD22	2:B:111:THR:HG21	1.83	0.60
2:E:196:THR:HG23	2:E:213:LYS:HE3	1.83	0.60
1:A:34:ASN:ND2	1:A:49:TYR:HA	2.15	0.60
1:A:196:ALA:HB3	1:A:205:ILE:HB	1.83	0.60
1:D:83:THR:HG21	1:D:166:GLN:CB	2.31	0.60
3:C:74:ARG:HB3	3:C:96:ASN:OD1	2.00	0.60
1:D:129:GLY:HA2	1:D:182:THR:HA	1.82	0.60
2:B:173:VAL:O	2:B:179:TYR:HA	2.02	0.60
3:C:35:THR:HG22	3:C:76:PHE:HB2	1.84	0.60
1:A:6:GLN:NE2	1:A:102:THR:HG23	2.16	0.59
3:C:67:VAL:O	3:C:102:PRO:HB2	2.02	0.59
1:D:44:PRO:HD2	2:E:107:TRP:CE3	2.37	0.59
3:F:32:GLN:HA	3:F:80:ALA:H	1.67	0.59
2:B:12:VAL:CG2	2:B:113:LEU:HD11	2.31	0.59
2:E:130:PRO:HD2	2:E:192:TRP:HH2	1.67	0.59
3:F:38:ILE:HD12	3:F:59:LEU:HD13	1.84	0.59
2:B:50:LEU:HD12	2:B:51:ILE:N	2.18	0.59
1:D:193:THR:HB	1:D:208:SER:OG	2.01	0.59
3:F:135:ARG:HG3	3:F:139:THR:O	2.02	0.59
1:A:199:LYS:HE3	3:F:133:LEU:O	2.01	0.59
3:C:48:LYS:NZ	3:C:48:LYS:HB3	2.18	0.59
2:B:91:THR:HG23	2:B:114:THR:HA	1.84	0.59
1:A:175:MET:O	2:B:170:PHE:CE1	2.56	0.59
2:E:145:LEU:HG	2:E:147:LYS:HD2	1.84	0.59
3:C:42:SER:H	3:C:72:LEU:HD12	1.67	0.58
2:E:18:VAL:O	2:E:82:GLN:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:28:LYS:HG2	3:F:29:PRO:HD2	1.85	0.58
2:B:12:VAL:HG23	2:B:113:LEU:HD11	1.85	0.58
1:A:2:ILE:C	1:A:2:ILE:HD12	2.24	0.58
3:C:69:GLN:HG3	3:C:70:THR:N	2.18	0.58
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.85	0.58
2:B:100:ASN:O	2:B:101:SER:HB2	2.04	0.58
2:B:156:VAL:HG11	2:B:183:SER:HB2	1.84	0.58
1:D:120:PRO:HG2	1:D:130:ALA:HB1	1.85	0.58
3:F:167:THR:HG22	3:F:168:ALA:N	2.18	0.58
3:F:189:VAL:HG12	3:F:205:SER:OG	2.04	0.58
1:D:6:GLN:HA	1:D:22:THR:O	2.04	0.58
1:D:160:LEU:HD13	2:E:175:GLN:HE21	1.68	0.58
3:F:183:GLU:CB	3:F:185:TYR:HE1	2.17	0.57
1:A:187:GLU:HA	1:A:211:ARG:CZ	2.33	0.57
3:C:135:ARG:HH21	3:C:138:ASN:HA	1.69	0.57
1:D:108:ARG:HH11	1:D:108:ARG:CG	2.16	0.57
3:F:76:PHE:CD2	3:F:94:TYR:HB3	2.40	0.57
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.87	0.57
2:B:71:THR:O	2:B:80:TYR:N	2.38	0.57
2:E:142:LEU:HB3	2:E:214:ILE:CD1	2.34	0.57
3:F:114:GLN:HB2	3:F:128:GLU:HB2	1.87	0.57
1:A:18:ARG:HG3	1:A:75:ILE:O	2.05	0.57
2:B:59:ILE:C	2:B:60:TYR:HD1	2.08	0.57
2:B:38:LYS:HG3	2:B:39:GLN:N	2.20	0.57
1:A:147:LYS:CG	1:A:155:ARG:HH22	2.17	0.57
1:A:152:GLY:O	1:A:154:GLU:N	2.38	0.57
3:C:35:THR:CG2	3:C:78:TYR:HE2	2.17	0.57
1:D:6:GLN:HE21	1:D:102:THR:CG2	2.11	0.57
3:C:160:SER:OG	3:C:184:ASN:HB3	2.05	0.56
1:D:153:SER:O	1:D:155:ARG:N	2.38	0.56
1:D:187:GLU:HA	1:D:211:ARG:NE	2.20	0.56
3:F:192:VAL:O	3:F:194:PRO:HD3	2.04	0.56
1:A:115:VAL:HG12	1:A:116:SER:N	2.20	0.56
1:A:190:ASN:O	1:A:210:ASN:HA	2.06	0.56
3:C:150:ASP:OD1	3:C:195:SER:HB3	2.05	0.56
2:E:13:ARG:HD2	2:E:117:SER:HA	1.86	0.56
3:F:16:SER:HB3	3:F:21:THR:HA	1.87	0.56
3:F:13:THR:O	3:F:24:GLU:HG2	2.05	0.56
1:A:91:HIS:CD2	3:C:169:LYS:NZ	2.73	0.56
2:B:51:ILE:O	2:B:53:PRO:HD3	2.06	0.56
3:C:20:LYS:HD2	3:C:133:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:VAL:HG12	3:C:52:THR:O	2.05	0.56
2:E:100:ASN:O	2:E:101:SER:HB2	2.05	0.56
2:E:102:TYR:OH	3:F:149:LYS:HG2	2.06	0.56
3:F:41:LYS:HA	3:F:72:LEU:HD12	1.88	0.56
1:A:150:ILE:HD13	1:A:192:TYR:HE1	1.71	0.56
2:B:198:THR:HG23	2:B:212:LYS:O	2.06	0.56
3:F:35:THR:HG22	3:F:76:PHE:HB2	1.88	0.56
2:B:1:GLU:OE1	2:B:2:ILE:HG13	2.06	0.56
1:D:34:ASN:ND2	1:D:50:TYR:H	2.04	0.56
1:A:162:SER:OG	2:B:171:PRO:HG2	2.06	0.56
1:A:191:SER:HA	1:A:210:ASN:OD1	2.06	0.56
2:E:34:MET:HB2	2:E:51:ILE:CG2	2.36	0.56
3:F:12:LEU:HD21	3:F:75:VAL:HG23	1.88	0.55
1:D:33:LEU:HD22	1:D:71:TYR:CB	2.36	0.55
1:D:139:PHE:HE2	1:D:175:MET:HB2	1.72	0.55
2:E:86:LEU:HD13	2:E:115:VAL:CG2	2.35	0.55
3:C:60:THR:O	3:C:64:VAL:HG22	2.07	0.55
2:E:28:ASN:ND2	2:E:30:LYS:HG2	2.22	0.55
3:C:70:THR:HA	3:C:100:PHE:O	2.06	0.55
3:F:10:TYR:CZ	3:F:26:GLU:HB3	2.41	0.55
1:A:137:ASN:HA	1:A:174:SER:HA	1.88	0.55
3:C:28:LYS:HD3	3:C:29:PRO:N	2.21	0.55
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.07	0.55
2:E:154:VAL:HG23	2:E:181:LEU:HD13	1.89	0.55
2:E:29:ILE:H	2:E:77:ASN:ND2	2.04	0.55
3:F:74:ARG:HH21	3:F:96:ASN:HD21	1.55	0.54
2:B:145:LEU:HG	2:B:145:LEU:O	2.06	0.54
3:C:115:SER:O	3:C:116:PHE:HB3	2.07	0.54
2:E:55:ASN:O	2:E:57:ASN:N	2.40	0.54
2:B:31:ASP:O	3:C:200:ARG:HD3	2.06	0.54
1:D:179:LEU:HG	1:D:181:LEU:HD13	1.89	0.54
2:E:33:TYR:HB2	2:E:99:ASP:HB3	1.87	0.54
1:A:164:THR:HG23	2:B:170:PHE:CD1	2.42	0.54
3:F:25:TRP:HH2	3:F:57:CYS:HB2	1.72	0.54
1:D:196:ALA:HB3	1:D:205:ILE:CB	2.32	0.54
3:C:110:GLN:NE2	3:C:206:PRO:HD3	2.23	0.54
1:D:136:LEU:HB2	1:D:175:MET:HB3	1.89	0.54
3:F:108:LEU:HD11	3:F:193:ILE:HG12	1.90	0.54
3:F:179:VAL:HB	3:F:185:TYR:CZ	2.42	0.54
2:E:31:ASP:HB3	3:F:200:ARG:CD	2.38	0.54
3:F:155:LEU:HD12	3:F:156:TYR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ARG:HB2	3:C:141:LEU:HD11	1.89	0.53
3:C:149:LYS:HB2	3:C:149:LYS:HZ3	1.73	0.53
1:D:164:THR:HG23	2:E:170:PHE:CD1	2.43	0.53
1:A:193:THR:CB	1:A:208:SER:HB2	2.37	0.53
2:E:5:GLN:HG2	2:E:23:LYS:HB3	1.90	0.53
3:C:39:SER:HB3	3:C:45:TRP:HA	1.90	0.53
3:F:29:PRO:HG3	3:F:53:THR:O	2.08	0.53
3:F:191:ALA:HB3	3:F:202:SER:HB3	1.91	0.53
1:A:39:LYS:HD3	1:A:84:ALA:HB2	1.91	0.53
1:D:15:LEU:O	1:D:17:GLU:N	2.38	0.53
1:D:166:GLN:HE21	1:D:171:SER:HA	1.73	0.53
2:E:13:ARG:HA	2:E:116:SER:O	2.08	0.53
1:A:146:VAL:HA	1:A:195:GLU:O	2.09	0.53
1:D:34:ASN:HD21	1:D:50:TYR:H	1.56	0.53
1:D:148:TRP:HD1	1:D:159:VAL:HG21	1.73	0.53
2:E:164:SER:O	2:E:167:VAL:HG23	2.08	0.53
2:B:174:LEU:HD12	2:B:178:LEU:O	2.09	0.53
1:D:108:ARG:HG2	1:D:109:ALA:N	2.23	0.53
3:F:187:PHE:O	3:F:207:VAL:HA	2.08	0.53
1:A:159:VAL:HA	1:A:178:THR:O	2.09	0.53
2:B:11:LEU:HB2	2:B:151:PRO:HG3	1.91	0.53
1:A:61:ARG:HD2	1:A:77:SER:O	2.09	0.52
1:D:106:ILE:HB	1:D:166:GLN:HE22	1.73	0.52
2:B:2:ILE:HA	2:B:25:SER:O	2.08	0.52
3:C:18:ASN:HB3	3:C:132:THR:HG22	1.91	0.52
2:E:146:VAL:HG12	2:E:146:VAL:O	2.09	0.52
1:A:135:PHE:CE2	2:B:184:SER:HB3	2.44	0.52
2:B:142:LEU:HB3	2:B:214:ILE:CD1	2.40	0.52
2:E:13:ARG:HH11	2:E:116:SER:C	2.13	0.52
1:A:111:ALA:C	1:A:200:THR:HG21	2.29	0.52
1:A:124:GLN:HG3	2:B:126:TYR:CE2	2.44	0.52
2:B:52:ASP:O	2:B:54:GLU:N	2.42	0.52
3:C:41:LYS:HA	3:C:72:LEU:HD12	1.91	0.52
1:D:120:PRO:HD3	1:D:132:VAL:CG1	2.40	0.52
2:E:13:ARG:NH1	2:E:118:ALA:O	2.42	0.52
2:B:5:GLN:O	2:B:22:CYS:HA	2.10	0.52
2:B:50:LEU:HG	2:B:59:ILE:HB	1.91	0.52
2:B:94:TYR:N	2:B:94:TYR:CD1	2.77	0.52
1:D:150:ILE:HD12	1:D:156:GLN:CD	2.30	0.52
3:F:153:TYR:HB2	3:F:170:THR:CG2	2.40	0.52
1:D:150:ILE:HD11	1:D:179:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:CG2	2:B:19:LYS:N	2.72	0.52
1:D:139:PHE:HE1	1:D:142:LYS:HA	1.75	0.52
3:F:115:SER:O	3:F:116:PHE:HB3	2.10	0.52
1:A:39:LYS:HB2	1:A:42:LYS:HG3	1.92	0.52
1:A:183:LYS:HG2	1:A:187:GLU:OE1	2.10	0.52
2:B:54:GLU:HG3	2:B:55:ASN:N	2.25	0.52
3:C:35:THR:HG22	3:C:78:TYR:HE2	1.75	0.52
1:D:115:VAL:N	2:E:136:THR:HG21	2.25	0.52
3:F:25:TRP:CH2	3:F:57:CYS:HB2	2.45	0.52
1:D:193:THR:CB	1:D:208:SER:HB2	2.38	0.51
2:E:42:GLU:O	2:E:43:GLN:HG3	2.10	0.51
1:A:145:ASN:HB3	1:A:197:THR:OG1	2.10	0.51
2:B:30:LYS:HA	2:B:53:PRO:HB2	1.93	0.51
1:D:19:VAL:CG2	1:D:75:ILE:HB	2.40	0.51
3:F:28:LYS:HD3	3:F:29:PRO:N	2.25	0.51
1:D:150:ILE:O	1:D:151:ASP:HB2	2.10	0.51
2:B:174:LEU:HD13	2:B:179:TYR:CE2	2.46	0.51
2:E:51:ILE:HB	2:E:70:ILE:HG21	1.91	0.51
1:D:2:ILE:HD13	1:D:27:GLN:CG	2.41	0.51
1:D:150:ILE:CD1	1:D:181:LEU:HD21	2.39	0.51
3:C:74:ARG:HD2	3:C:76:PHE:CZ	2.46	0.51
1:D:21:ILE:HG23	1:D:102:THR:HG21	1.93	0.51
3:F:154:THR:HG22	3:F:156:TYR:CE1	2.45	0.51
1:A:120:PRO:HD2	1:A:186:TYR:OH	2.11	0.51
2:B:200:ASN:HB3	2:B:211:ASP:OD2	2.10	0.51
1:D:13:ALA:O	1:D:107:ASN:HB2	2.11	0.51
3:C:36:VAL:HG22	3:C:75:VAL:HG22	1.93	0.51
3:C:108:LEU:HD11	3:C:193:ILE:HG12	1.91	0.51
2:B:137:ASN:ND2	2:B:139:MET:SD	2.84	0.50
3:C:13:THR:HG21	3:C:15:LYS:CE	2.37	0.50
3:F:35:THR:OG1	3:F:50:PHE:HA	2.11	0.50
1:D:108:ARG:CG	1:D:108:ARG:NH1	2.73	0.50
2:B:57:ASN:HD21	3:C:165:LYS:NZ	2.10	0.50
3:C:119:VAL:HG12	3:C:119:VAL:O	2.09	0.50
1:D:29:ILE:HD11	1:D:71:TYR:CE2	2.47	0.50
1:D:137:ASN:HA	1:D:174:SER:HA	1.93	0.50
2:E:62:PRO:HA	2:E:65:GLN:HG3	1.93	0.50
3:F:42:SER:H	3:F:72:LEU:CD1	2.24	0.50
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.15	0.50
2:B:156:VAL:HG22	2:B:201:VAL:HG22	1.93	0.50
2:E:10:GLU:O	2:E:113:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ASN:HA	1:D:48:ILE:O	2.11	0.50
3:F:135:ARG:HG3	3:F:139:THR:H	1.76	0.50
3:F:158:TRP:CE3	3:F:165:LYS:HG2	2.47	0.50
1:A:12:TYR:HA	1:A:105:GLU:O	2.11	0.49
1:A:33:LEU:HD22	1:A:71:TYR:HB3	1.94	0.49
3:C:144:ARG:NH2	3:C:172:THR:O	2.43	0.49
1:D:185:GLU:HA	1:D:188:ARG:HE	1.76	0.49
3:F:13:THR:CG2	3:F:15:LYS:HE2	2.41	0.49
3:F:78:TYR:CE1	3:F:92:PRO:HG3	2.43	0.49
1:D:55:ALA:O	1:D:57:GLY:N	2.44	0.49
2:E:51:ILE:HB	2:E:70:ILE:CG2	2.42	0.49
1:A:91:HIS:HD2	3:C:169:LYS:HZ3	1.59	0.49
2:B:38:LYS:CG	2:B:39:GLN:N	2.74	0.49
1:D:160:LEU:HD21	2:E:175:GLN:HG3	1.95	0.49
2:E:127:PRO:HB3	2:E:214:ILE:HG22	1.94	0.49
3:C:40:THR:OG1	3:C:41:LYS:N	2.45	0.49
2:E:20:LEU:HD22	2:E:111:THR:HG21	1.94	0.49
2:B:60:TYR:OH	2:B:69:SER:HA	2.13	0.49
2:E:30:LYS:HA	2:E:53:PRO:HB2	1.95	0.49
1:A:199:LYS:NZ	3:F:135:ARG:HB3	2.28	0.49
3:C:42:SER:H	3:C:72:LEU:CD1	2.26	0.49
3:C:70:THR:CG2	3:C:99:GLU:HB3	2.43	0.49
2:B:35:HIS:CD2	2:B:99:ASP:HB2	2.48	0.48
3:C:121:THR:O	3:C:121:THR:HG22	2.12	0.48
3:C:141:LEU:HB3	3:C:145:ASP:CB	2.43	0.48
1:D:134:CYS:HB2	1:D:148:TRP:CH2	2.48	0.48
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.43	0.48
3:C:4:THR:O	3:C:5:ASN:HB2	2.14	0.48
3:C:32:GLN:HE21	3:C:34:TYR:HE1	1.62	0.48
1:D:12:TYR:HD1	1:D:12:TYR:H	1.59	0.48
1:A:190:ASN:OD1	1:A:211:ARG:N	2.46	0.48
2:B:176:SER:O	2:B:178:LEU:N	2.46	0.48
3:F:74:ARG:HD3	3:F:76:PHE:CZ	2.49	0.48
1:A:147:LYS:CB	1:A:155:ARG:HH22	2.27	0.48
2:E:127:PRO:CB	2:E:214:ILE:HG22	2.42	0.48
3:F:43:GLY:O	3:F:45:TRP:N	2.47	0.48
3:F:155:LEU:HD12	3:F:156:TYR:H	1.77	0.48
2:B:6:GLN:HB3	2:B:111:THR:OG1	2.14	0.48
2:B:181:LEU:HG	2:B:182:SER:H	1.79	0.48
3:F:16:SER:HG	3:F:100:PHE:HZ	1.61	0.48
1:A:83:THR:HG21	1:A:166:GLN:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:N	1:A:181:LEU:O	2.45	0.48
2:E:17:LEU:HD12	2:E:18:VAL:N	2.28	0.48
3:F:10:TYR:CE1	3:F:27:PRO:HD3	2.48	0.48
3:F:33:VAL:HG21	3:F:51:TYR:HB3	1.95	0.48
3:F:38:ILE:HA	3:F:73:ALA:HA	1.95	0.48
3:F:78:TYR:HE1	3:F:92:PRO:CG	2.25	0.48
3:F:124:ASN:HD21	3:F:174:GLU:HB2	1.79	0.48
3:F:136:ARG:HG3	3:F:137:ASN:ND2	2.29	0.48
1:A:83:THR:HG21	1:A:166:GLN:HB2	1.95	0.48
3:F:136:ARG:NH1	3:F:141:LEU:HD13	2.29	0.48
2:B:2:ILE:O	2:B:3:GLN:HB3	2.14	0.48
1:D:125:LEU:HD22	1:D:183:LYS:HG3	1.96	0.48
2:E:137:ASN:HB3	2:E:139:MET:HG2	1.96	0.48
1:A:34:ASN:O	1:A:88:CYS:HA	2.14	0.48
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.49	0.48
3:C:149:LYS:HB2	3:C:149:LYS:HZ2	1.78	0.48
3:F:42:SER:H	3:F:72:LEU:HD12	1.79	0.48
3:F:196:ARG:HH11	3:F:199:ASN:HB3	1.79	0.48
2:B:167:VAL:HG12	2:B:168:HIS:N	2.29	0.48
3:C:6:THR:OG1	3:C:79:PRO:HB3	2.14	0.48
3:C:28:LYS:HD3	3:C:28:LYS:C	2.33	0.48
2:E:31:ASP:HB3	3:F:200:ARG:HD3	1.96	0.48
3:F:29:PRO:HB2	3:F:32:GLN:O	2.13	0.48
3:C:45:TRP:HZ3	3:C:73:ALA:HA	1.79	0.47
1:D:42:LYS:HB3	1:D:42:LYS:NZ	2.27	0.47
1:D:120:PRO:HD2	1:D:186:TYR:CZ	2.49	0.47
3:F:159:LYS:NZ	3:F:180:ASP:OD2	2.47	0.47
2:B:172:ALA:HB1	2:B:179:TYR:HB3	1.96	0.47
3:C:52:THR:OG1	3:C:53:THR:N	2.47	0.47
3:C:175:PHE:CD1	3:C:175:PHE:N	2.82	0.47
3:F:18:ASN:ND2	3:F:130:GLU:HG2	2.29	0.47
3:F:74:ARG:HH21	3:F:96:ASN:ND2	2.11	0.47
3:F:74:ARG:NE	3:F:94:TYR:CE2	2.82	0.47
2:B:6:GLN:HE21	2:B:108:GLY:HA3	1.79	0.47
3:C:10:TYR:CE1	3:C:27:PRO:HB3	2.50	0.47
1:D:15:LEU:C	1:D:17:GLU:H	2.17	0.47
1:A:14:SER:O	1:A:17:GLU:HB2	2.14	0.47
2:B:5:GLN:HG2	2:B:23:LYS:O	2.13	0.47
3:C:10:TYR:HE1	3:C:27:PRO:HB3	1.79	0.47
3:C:74:ARG:HD3	3:C:94:TYR:CD2	2.49	0.47
1:D:89:LEU:HD23	1:D:98:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:ILE:N	2:E:77:ASN:HD21	2.10	0.47
2:E:48:ILE:HG21	2:E:81:LEU:HD21	1.96	0.47
2:E:156:VAL:HG21	2:E:181:LEU:CD2	2.45	0.47
1:A:116:SER:HB2	1:A:135:PHE:HB2	1.97	0.47
1:D:160:LEU:HD13	2:E:175:GLN:NE2	2.29	0.47
2:E:17:LEU:HD13	2:E:82:GLN:CG	2.45	0.47
1:A:4:MET:HE3	1:A:4:MET:HA	1.97	0.47
2:B:176:SER:C	2:B:178:LEU:H	2.18	0.47
3:C:136:ARG:CB	3:C:141:LEU:HD11	2.44	0.47
1:D:12:TYR:HA	1:D:105:GLU:O	2.14	0.47
1:D:86:TYR:O	1:D:101:GLY:HA2	2.15	0.47
2:E:35:HIS:O	2:E:96:CYS:HA	2.15	0.47
1:A:143:ASP:O	1:A:198:HIS:HD2	1.98	0.47
2:B:17:LEU:O	2:B:17:LEU:HD12	2.14	0.47
3:F:153:TYR:HB2	3:F:170:THR:HG23	1.95	0.47
2:E:100:ASN:O	2:E:101:SER:CB	2.62	0.47
2:E:181:LEU:HG	2:E:182:SER:H	1.80	0.47
3:F:186:CYS:HA	3:F:209:CYS:HA	1.97	0.47
2:E:13:ARG:HD3	2:E:116:SER:O	2.15	0.47
1:D:151:ASP:OD2	1:D:189:HIS:HB3	2.14	0.46
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.97	0.46
2:B:185:VAL:HG13	2:B:185:VAL:O	2.15	0.46
1:D:189:HIS:CD2	1:D:189:HIS:N	2.83	0.46
2:E:13:ARG:CD	2:E:116:SER:O	2.63	0.46
3:C:41:LYS:HE2	3:C:99:GLU:OE2	2.16	0.46
3:F:11:ASN:CB	3:F:26:GLU:HG3	2.37	0.46
2:B:7:SER:O	2:B:9:ALA:N	2.45	0.46
1:D:190:ASN:OD1	1:D:211:ARG:N	2.49	0.46
2:E:5:GLN:O	2:E:22:CYS:HA	2.15	0.46
2:B:156:VAL:HG11	2:B:183:SER:CB	2.45	0.46
2:E:14:PRO:HD2	2:E:116:SER:O	2.15	0.46
1:A:116:SER:HB3	1:A:118:PHE:CE1	2.51	0.46
1:A:142:LYS:HB2	1:A:173:TYR:CZ	2.50	0.46
2:B:30:LYS:HZ2	2:B:30:LYS:HB2	1.81	0.46
1:D:35:TRP:CZ3	1:D:88:CYS:HB3	2.50	0.46
3:F:37:GLN:CG	3:F:45:TRP:HB3	2.44	0.46
2:E:153:PRO:O	2:E:204:PRO:HD2	2.16	0.46
3:F:23:LEU:HG	3:F:25:TRP:CE3	2.51	0.46
3:F:93:LEU:HD23	3:F:93:LEU:N	2.29	0.46
1:A:1:ASP:OD2	1:A:2:ILE:HG22	2.16	0.46
3:C:10:TYR:O	3:C:11:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:SER:O	1:D:102:THR:HA	2.15	0.46
2:B:11:LEU:HD21	2:B:13:ARG:HH12	1.81	0.46
3:C:46:LYS:HG2	3:C:48:LYS:HD3	1.97	0.46
2:E:123:PRO:HB3	2:E:149:TYR:HB3	1.98	0.46
3:F:75:VAL:O	3:F:94:TYR:HB2	2.15	0.46
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.98	0.46
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.81	0.46
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.31	0.46
1:A:116:SER:HB3	1:A:118:PHE:HE1	1.80	0.46
3:C:41:LYS:HD2	3:C:72:LEU:HD11	1.97	0.46
2:E:2:ILE:HD13	2:E:98:ARG:NH1	2.30	0.46
3:F:10:TYR:HE1	3:F:27:PRO:HD3	1.79	0.46
3:C:141:LEU:HB3	3:C:145:ASP:HB2	1.97	0.45
1:D:115:VAL:O	2:E:136:THR:HG21	2.17	0.45
3:F:74:ARG:CZ	3:F:94:TYR:CE2	3.00	0.45
2:B:70:ILE:N	2:B:70:ILE:HD12	2.31	0.45
3:C:167:THR:HG22	3:C:168:ALA:N	2.32	0.45
3:C:210:MET:HB3	3:C:211:GLY:H	1.52	0.45
2:E:35:HIS:NE2	2:E:99:ASP:HB2	2.32	0.45
3:F:193:ILE:CG2	3:F:196:ARG:HG3	2.47	0.45
1:A:36:TYR:O	1:A:86:TYR:HA	2.16	0.45
1:D:118:PHE:HA	1:D:119:PRO:HD3	1.79	0.45
3:F:94:TYR:HE2	3:F:96:ASN:OD1	1.99	0.45
2:B:55:ASN:O	2:B:57:ASN:N	2.50	0.45
3:C:124:ASN:C	3:C:124:ASN:ND2	2.69	0.45
1:D:166:GLN:HG3	1:D:173:TYR:OH	2.16	0.45
2:B:214:ILE:OXT	2:B:214:ILE:HG13	2.16	0.45
3:F:38:ILE:HD12	3:F:59:LEU:CD1	2.45	0.45
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.52	0.45
2:B:58:THR:C	2:B:59:ILE:HD12	2.38	0.45
1:D:191:SER:HA	1:D:210:ASN:OD1	2.16	0.45
3:F:136:ARG:CG	3:F:141:LEU:HD21	2.46	0.45
1:A:29:ILE:HD11	1:A:71:TYR:CD2	2.52	0.45
2:B:18:VAL:O	2:B:82:GLN:HA	2.17	0.45
2:E:5:GLN:C	2:E:6:GLN:HG2	2.37	0.45
2:E:71:THR:O	2:E:80:TYR:N	2.48	0.45
1:A:9:SER:O	1:A:102:THR:HA	2.17	0.45
1:A:135:PHE:CZ	2:B:184:SER:HB3	2.52	0.44
1:D:34:ASN:ND2	1:D:49:TYR:CA	2.73	0.44
3:F:187:PHE:N	3:F:208:GLU:O	2.50	0.44
1:A:115:VAL:CG1	1:A:116:SER:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:GLN:HG3	2:B:23:LYS:HB3	1.99	0.44
1:D:14:SER:O	1:D:17:GLU:CB	2.63	0.44
1:D:61:ARG:NH2	1:D:82:ASP:OD1	2.49	0.44
1:D:108:ARG:NH2	1:D:111:ALA:HB2	2.30	0.44
2:E:2:ILE:HG22	2:E:3:GLN:N	2.31	0.44
2:E:17:LEU:HD12	2:E:17:LEU:C	2.38	0.44
2:E:108:GLY:C	2:E:109:GLN:O	2.54	0.44
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.79	0.44
1:A:189:HIS:CD2	1:A:189:HIS:N	2.85	0.44
2:B:123:PRO:HB2	2:B:146:VAL:HG13	1.99	0.44
2:B:149:TYR:CZ	2:B:154:VAL:HG22	2.52	0.44
3:C:15:LYS:HG3	3:C:24:GLU:OE1	2.17	0.44
3:F:63:ILE:C	3:F:63:ILE:HD12	2.37	0.44
3:F:155:LEU:HG	3:F:157:TYR:HD2	1.82	0.44
2:B:17:LEU:HD12	2:B:17:LEU:C	2.38	0.44
3:C:10:TYR:HE1	3:C:27:PRO:CD	2.30	0.44
1:D:147:LYS:O	1:D:194:CYS:HA	2.17	0.44
1:A:26:SER:O	1:A:27:GLN:CB	2.65	0.44
1:A:149:LYS:HD2	1:A:153:SER:HA	1.99	0.44
3:C:143:LEU:HA	3:C:143:LEU:HD12	1.74	0.44
1:D:36:TYR:CE1	1:D:46:THR:HB	2.52	0.44
1:D:132:VAL:HG23	1:D:179:LEU:HB3	2.00	0.44
1:A:24:LYS:HA	1:A:69:GLN:O	2.18	0.44
1:D:166:GLN:NE2	1:D:171:SER:HB3	2.32	0.44
1:A:39:LYS:NZ	1:A:81:ASP:C	2.71	0.44
3:C:10:TYR:HE1	3:C:27:PRO:CB	2.30	0.44
3:C:135:ARG:NE	3:C:138:ASN:HA	2.32	0.44
2:E:145:LEU:CG	2:E:147:LYS:HD2	2.48	0.44
3:F:72:LEU:HD21	3:F:99:GLU:HG3	1.99	0.44
3:C:169:LYS:HB2	3:C:169:LYS:HE3	1.80	0.44
1:D:133:VAL:HG22	1:D:178:THR:OG1	2.18	0.44
1:D:148:TRP:CD1	1:D:159:VAL:HG21	2.52	0.44
2:E:17:LEU:HD13	2:E:82:GLN:HG3	1.99	0.44
2:E:97:ALA:HA	2:E:106:TYR:O	2.18	0.44
3:C:124:ASN:HA	3:C:176:LEU:HD12	2.00	0.44
2:E:156:VAL:HG21	2:E:181:LEU:HD21	2.00	0.44
3:C:135:ARG:NH2	3:C:138:ASN:CA	2.75	0.43
3:C:198:VAL:HG23	3:C:199:ASN:H	1.82	0.43
1:D:35:TRP:CD2	1:D:73:LEU:HB2	2.53	0.43
2:E:150:PHE:CD1	2:E:150:PHE:C	2.92	0.43
1:A:13:ALA:HB3	1:A:78:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:HE2	3:C:149:LYS:HE3	1.83	0.43
1:D:36:TYR:O	1:D:86:TYR:HA	2.18	0.43
2:E:140:VAL:O	2:E:186:THR:HA	2.18	0.43
3:F:111:PRO:HB2	3:F:189:VAL:HG13	1.99	0.43
3:F:158:TRP:CE2	3:F:186:CYS:HB2	2.53	0.43
3:C:183:GLU:HB2	3:C:185:TYR:HE1	1.83	0.43
2:E:163:LEU:HG	2:E:185:VAL:HG21	2.00	0.43
1:A:4:MET:HE2	1:A:4:MET:HB3	1.89	0.43
1:A:134:CYS:HB3	1:A:177:SER:HB3	2.01	0.43
1:D:150:ILE:O	1:D:150:ILE:HG22	2.18	0.43
1:A:50:TYR:CE2	3:C:149:LYS:HE3	2.54	0.43
3:C:31:ASN:C	3:C:80:ALA:HB3	2.39	0.43
3:C:43:GLY:O	3:C:45:TRP:CD1	2.71	0.43
3:C:125:VAL:HG12	3:C:126:THR:N	2.33	0.43
2:E:33:TYR:HE1	3:F:156:TYR:OH	2.01	0.43
2:E:48:ILE:HD13	2:E:64:PHE:CE2	2.54	0.43
1:A:15:LEU:C	1:A:17:GLU:H	2.22	0.43
1:D:106:ILE:N	1:D:166:GLN:OE1	2.51	0.43
1:A:39:LYS:HZ3	1:A:81:ASP:C	2.22	0.43
1:A:133:VAL:HG22	1:A:178:THR:OG1	2.19	0.43
2:E:142:LEU:HD13	2:E:214:ILE:HD11	2.01	0.43
1:A:89:LEU:HG	1:A:98:PHE:CE1	2.54	0.43
2:B:118:ALA:HB3	2:B:150:PHE:CE2	2.54	0.43
2:B:174:LEU:HD13	2:B:179:TYR:CD2	2.54	0.43
1:D:113:PRO:HB3	1:D:139:PHE:HB3	2.01	0.43
3:F:152:ILE:HD13	3:F:152:ILE:HA	1.84	0.43
3:F:37:GLN:HA	3:F:46:LYS:O	2.19	0.42
2:B:40:ARG:HG2	2:B:92:ALA:HB2	2.01	0.42
1:D:119:PRO:HG3	1:D:209:PHE:CG	2.55	0.42
3:F:135:ARG:HA	3:F:139:THR:O	2.19	0.42
3:C:32:GLN:HA	3:C:80:ALA:N	2.34	0.42
3:C:134:VAL:HG21	3:C:146:VAL:HG21	2.00	0.42
1:D:1:ASP:OD2	1:D:2:ILE:HG22	2.18	0.42
3:F:74:ARG:HG3	3:F:76:PHE:CE1	2.54	0.42
2:B:4:LEU:HD23	2:B:96:CYS:SG	2.58	0.42
2:B:38:LYS:HG3	2:B:39:GLN:H	1.83	0.42
1:D:165:ASP:O	1:D:166:GLN:C	2.58	0.42
2:E:39:GLN:HB2	2:E:45:LEU:HD23	2.01	0.42
3:F:16:SER:OG	3:F:100:PHE:HZ	2.02	0.42
1:A:38:GLN:HG3	1:A:44:PRO:HG3	2.02	0.42
3:C:12:LEU:HD21	3:C:75:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:LEU:HG	3:C:157:TYR:HD2	1.83	0.42
3:F:159:LYS:HA	3:F:185:TYR:HA	2.01	0.42
3:F:190:GLN:O	3:F:190:GLN:HG3	2.19	0.42
3:C:162:SER:OG	3:C:163:SER:N	2.53	0.42
1:D:121:SER:C	1:D:123:GLU:N	2.73	0.42
3:F:185:TYR:O	3:F:209:CYS:HA	2.20	0.42
1:A:144:ILE:HG13	1:A:198:HIS:HB2	2.01	0.42
2:B:135:GLN:C	2:B:135:GLN:CD	2.77	0.42
1:D:120:PRO:HD3	1:D:132:VAL:HG13	2.01	0.42
1:A:1:ASP:CG	1:A:2:ILE:N	2.73	0.42
1:A:91:HIS:CD2	3:C:169:LYS:HZ2	2.38	0.42
2:B:164:SER:O	2:B:167:VAL:HG23	2.20	0.42
3:C:152:ILE:HG13	3:C:194:PRO:HG2	2.02	0.42
2:E:5:GLN:HG3	2:E:23:LYS:HB3	2.01	0.42
2:E:135:GLN:C	2:E:135:GLN:CD	2.78	0.42
2:E:137:ASN:CG	2:E:139:MET:SD	2.98	0.42
3:F:186:CYS:HA	3:F:208:GLU:O	2.20	0.42
1:A:175:MET:O	2:B:170:PHE:CZ	2.73	0.42
2:B:139:MET:CB	2:B:188:PRO:HA	2.49	0.42
3:C:4:THR:HB	3:C:5:ASN:H	1.54	0.42
1:A:26:SER:O	1:A:27:GLN:HB3	2.20	0.42
1:A:170:ASP:OD1	1:A:170:ASP:C	2.58	0.42
3:C:156:TYR:HB3	3:C:165:LYS:HZ3	1.85	0.42
2:E:11:LEU:HD21	2:E:13:ARG:HH22	1.84	0.42
1:D:151:ASP:HA	1:D:191:SER:OG	2.20	0.41
2:E:142:LEU:O	2:E:184:SER:HA	2.20	0.41
3:C:106:THR:O	3:C:106:THR:CG2	2.67	0.41
1:A:44:PRO:HD2	2:B:107:TRP:CE3	2.55	0.41
1:D:119:PRO:HA	1:D:132:VAL:HG12	2.02	0.41
1:D:161:ASN:HB3	1:D:175:MET:HE2	2.02	0.41
2:E:2:ILE:O	2:E:3:GLN:HB3	2.19	0.41
2:E:51:ILE:O	2:E:51:ILE:HG23	2.20	0.41
3:F:13:THR:HG21	3:F:15:LYS:HE2	2.02	0.41
3:F:38:ILE:HG13	3:F:72:LEU:O	2.20	0.41
3:F:48:LYS:HA	3:F:48:LYS:HD2	1.90	0.41
3:F:63:ILE:HD12	3:F:64:VAL:N	2.34	0.41
3:F:111:PRO:HD2	3:F:203:THR:O	2.19	0.41
3:F:157:TYR:CE1	3:F:166:LYS:HB2	2.55	0.41
1:A:89:LEU:HB2	1:A:98:PHE:CD1	2.55	0.41
1:A:131:SER:OG	1:A:180:THR:HG23	2.20	0.41
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:ASN:HB3	2:E:139:MET:O	2.20	0.41
3:F:180:ASP:HB2	3:F:185:TYR:OH	2.20	0.41
1:A:89:LEU:HD23	1:A:98:PHE:CD1	2.56	0.41
2:B:156:VAL:HG21	2:B:181:LEU:CD2	2.50	0.41
2:E:93:VAL:HA	2:E:111:THR:O	2.20	0.41
2:E:149:TYR:CE1	2:E:179:TYR:HB2	2.56	0.41
3:F:19:PHE:O	3:F:63:ILE:HD11	2.21	0.41
3:F:51:TYR:HE1	3:F:78:TYR:CE2	2.38	0.41
1:A:11:MET:O	1:A:11:MET:HG3	2.20	0.41
2:E:139:MET:HG3	2:E:186:THR:CG2	2.50	0.41
2:E:174:LEU:HD12	2:E:178:LEU:O	2.20	0.41
3:F:183:GLU:HB2	3:F:185:TYR:CE1	2.38	0.41
2:B:181:LEU:HG	2:B:182:SER:N	2.35	0.41
3:C:29:PRO:HG3	3:C:53:THR:O	2.21	0.41
3:C:32:GLN:HA	3:C:80:ALA:H	1.85	0.41
3:C:132:THR:O	3:C:140:PHE:HD2	2.04	0.41
2:E:1:GLU:O	2:E:26:GLY:HA3	2.21	0.41
3:F:34:TYR:HD1	3:F:77:SER:HA	1.86	0.41
1:A:165:ASP:O	1:A:166:GLN:C	2.59	0.41
2:B:128:LEU:HD12	2:B:143:GLY:C	2.41	0.41
3:C:25:TRP:O	3:C:55:THR:HB	2.21	0.41
1:D:94:SER:OG	2:E:59:ILE:HG21	2.20	0.41
1:D:170:ASP:OD1	1:D:170:ASP:C	2.59	0.41
1:D:183:LYS:O	1:D:186:TYR:HB3	2.20	0.41
2:E:212:LYS:HA	2:E:212:LYS:HD3	1.85	0.41
3:F:74:ARG:HD3	3:F:94:TYR:CD2	2.56	0.41
3:F:94:TYR:CE2	3:F:96:ASN:OD1	2.74	0.41
2:B:84:SER:O	2:B:85:SER:C	2.59	0.41
2:B:105:ASP:O	2:B:106:TYR:CD2	2.74	0.41
1:D:139:PHE:CE2	1:D:175:MET:HB2	2.52	0.41
1:D:141:PRO:C	1:D:143:ASP:N	2.73	0.41
2:E:11:LEU:HD21	2:E:13:ARG:NH2	2.36	0.41
2:E:117:SER:OG	2:E:118:ALA:N	2.54	0.41
3:F:169:LYS:HE2	3:F:169:LYS:HB2	1.24	0.41
3:F:176:LEU:HD13	3:F:176:LEU:HA	1.84	0.41
2:B:154:VAL:HA	2:B:202:ALA:O	2.21	0.40
3:C:166:LYS:HE2	3:C:166:LYS:HB3	1.93	0.40
1:D:12:TYR:CD2	1:D:105:GLU:HB3	2.57	0.40
2:E:174:LEU:HD12	2:E:174:LEU:HA	1.74	0.40
1:A:155:ARG:H	1:A:155:ARG:HG3	1.65	0.40
1:A:161:ASN:HB3	1:A:175:MET:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:THR:O	2:B:89:GLU:N	2.54	0.40
2:B:145:LEU:HD21	2:B:147:LYS:CD	2.48	0.40
2:B:157:THR:O	2:B:200:ASN:OD1	2.40	0.40
3:C:69:GLN:O	3:C:102:PRO:HD2	2.20	0.40
3:C:154:THR:HB	3:C:190:GLN:HG2	2.04	0.40
3:F:51:TYR:CE1	3:F:78:TYR:CE2	3.09	0.40
3:C:204:ASP:OD1	3:C:204:ASP:N	2.54	0.40
3:F:34:TYR:HB3	3:F:75:VAL:HG12	2.02	0.40
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.56	0.40
2:B:3:GLN:HG2	2:B:25:SER:HB2	2.03	0.40
1:D:131:SER:OG	1:D:180:THR:HG23	2.22	0.40
2:E:181:LEU:CG	2:E:182:SER:N	2.84	0.40
1:A:142:LYS:HB2	1:A:173:TYR:CE1	2.57	0.40
2:B:121:THR:O	2:B:149:TYR:HA	2.22	0.40
2:B:196:THR:CG2	2:B:213:LYS:HE3	2.49	0.40
3:C:192:VAL:HA	3:C:200:ARG:O	2.22	0.40
2:E:27:PHE:HD2	2:E:32:TYR:CD2	2.40	0.40
3:F:29:PRO:HA	3:F:34:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

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	212/214 (99%)	176 (83%)	29 (14%)	7 (3%)	4 21
1	D	212/214 (99%)	177 (84%)	29 (14%)	6 (3%)	5 25
2	B	212/214 (99%)	177 (84%)	26 (12%)	9 (4%)	3 16
2	E	212/214 (99%)	175 (82%)	30 (14%)	7 (3%)	4 21
3	C	196/219 (90%)	158 (81%)	31 (16%)	7 (4%)	3 19
3	F	196/219 (90%)	161 (82%)	29 (15%)	6 (3%)	4 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1240/1294 (96%)	1024 (83%)	174 (14%)	42 (3%)	3 20

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	153	SER
2	B	41	PRO
2	B	56	GLY
3	C	5	ASN
3	C	51	TYR
3	C	130	GLU
1	D	56	ASP
1	D	153	SER
2	E	10	GLU
2	E	56	GLY
2	E	101	SER
3	F	44	ASP
1	A	154	GLU
2	B	7	SER
2	B	101	SER
2	B	132	SER
1	D	154	GLU
2	E	41	PRO
3	F	42	SER
3	F	81	GLY
3	F	160	SER
1	A	27	GLN
2	B	177	ASP
3	C	40	THR
3	C	160	SER
1	D	110	ASP
1	D	184	ASP
2	E	54	GLU
3	F	40	THR
3	C	124	ASN
2	E	165	SER
2	E	177	ASP
1	A	184	ASP
1	A	204	PRO
2	B	163	LEU
1	D	152	GLY

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Mol	Chain	Res	Type
3	F	161	SER
1	A	16	GLY
2	B	176	SER
3	C	198	VAL
2	B	53	PRO

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	191/191 (100%)	154 (81%)	37 (19%)	1 7
1	D	191/191 (100%)	154 (81%)	37 (19%)	1 7
2	B	185/185 (100%)	155 (84%)	30 (16%)	2 12
2	E	185/185 (100%)	167 (90%)	18 (10%)	8 31
3	C	186/200 (93%)	158 (85%)	28 (15%)	3 14
3	F	186/200 (93%)	162 (87%)	24 (13%)	4 19
All	All	1124/1152 (98%)	950 (84%)	174 (16%)	2 13

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	2	ILE
1	A	8	PRO
1	A	11	MET
1	A	22	THR
1	A	29	ILE
1	A	56	ASP
1	A	67	SER
1	A	73	LEU
1	A	77	SER
1	A	83	THR
1	A	90	GLN
1	A	102	THR

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Mol	Chain	Res	Type
1	A	104	LEU
1	A	105	GLU
1	A	107	ASN
1	A	108	ARG
1	A	122	SER
1	A	143	ASP
1	A	145	ASN
1	A	146	VAL
1	A	153	SER
1	A	154	GLU
1	A	155	ARG
1	A	159	VAL
1	A	160	LEU
1	A	165	ASP
1	A	166	GLN
1	A	175	MET
1	A	181	LEU
1	A	184	ASP
1	A	185	GLU
1	A	199	LYS
1	A	200	THR
1	A	203	SER
1	A	213	GLU
1	A	214	CYS
2	B	5	GLN
2	B	7	SER
2	B	17	LEU
2	B	18	VAL
2	B	22	CYS
2	B	30	LYS
2	B	41	PRO
2	B	57	ASN
2	B	58	THR
2	B	62	PRO
2	B	74	THR
2	B	77	ASN
2	B	81	LEU
2	B	84	SER
2	B	123	PRO
2	B	135	GLN
2	B	136	THR
2	B	139	MET

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Mol	Chain	Res	Type
2	B	144	CYS
2	B	152	GLU
2	B	154	VAL
2	B	155	THR
2	B	157	THR
2	B	162	SER
2	B	178	LEU
2	B	181	LEU
2	B	189	SER
2	B	195	GLU
2	B	199	CYS
2	B	200	ASN
3	C	4	THR
3	C	16	SER
3	C	23	LEU
3	C	28	LYS
3	C	33	VAL
3	C	35	THR
3	C	44	ASP
3	C	47	SER
3	C	53	THR
3	C	56	GLU
3	C	61	ASP
3	C	102	PRO
3	C	105	GLU
3	C	115	SER
3	C	117	GLU
3	C	124	ASN
3	C	130	GLU
3	C	131	ARG
3	C	132	THR
3	C	152	ILE
3	C	163	SER
3	C	172	THR
3	C	176	LEU
3	C	177	ILE
3	C	195	SER
3	C	203	THR
3	C	204	ASP
3	C	210	MET
1	D	1	ASP
1	D	2	ILE

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Mol	Chain	Res	Type
1	D	7	SER
1	D	11	MET
1	D	12	TYR
1	D	17	GLU
1	D	19	VAL
1	D	22	THR
1	D	56	ASP
1	D	67	SER
1	D	73	LEU
1	D	77	SER
1	D	83	THR
1	D	90	GLN
1	D	102	THR
1	D	105	GLU
1	D	107	ASN
1	D	108	ARG
1	D	122	SER
1	D	143	ASP
1	D	145	ASN
1	D	146	VAL
1	D	154	GLU
1	D	155	ARG
1	D	159	VAL
1	D	160	LEU
1	D	165	ASP
1	D	166	GLN
1	D	175	MET
1	D	184	ASP
1	D	185	GLU
1	D	194	CYS
1	D	199	LYS
1	D	200	THR
1	D	203	SER
1	D	213	GLU
1	D	214	CYS
2	E	2	ILE
2	E	5	GLN
2	E	17	LEU
2	E	30	LYS
2	E	73	ASP
2	E	77	ASN
2	E	135	GLN

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Mol	Chain	Res	Type
2	E	136	THR
2	E	139	MET
2	E	144	CYS
2	E	152	GLU
2	E	154	VAL
2	E	165	SER
2	E	176	SER
2	E	178	LEU
2	E	195	GLU
2	E	199	CYS
2	E	200	ASN
3	F	4	THR
3	F	13	THR
3	F	27	PRO
3	F	28	LYS
3	F	35	THR
3	F	42	SER
3	F	53	THR
3	F	61	ASP
3	F	70	THR
3	F	93	LEU
3	F	101	THR
3	F	115	SER
3	F	117	GLU
3	F	126	THR
3	F	165	LYS
3	F	169	LYS
3	F	172	THR
3	F	176	LEU
3	F	190	GLN
3	F	194	PRO
3	F	197	THR
3	F	198	VAL
3	F	199	ASN
3	F	203	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	91	HIS
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	156	GLN
2	B	6	GLN
2	B	57	ASN
2	B	77	ASN
3	C	118	GLN
3	C	124	ASN
3	C	184	ASN
1	D	34	ASN
1	D	124	GLN
1	D	145	ASN
2	E	6	GLN
2	E	28	ASN
2	E	77	ASN
2	E	175	GLN
3	F	32	GLN
3	F	118	GLN
3	F	124	ASN
3	F	137	ASN
3	F	190	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.