Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:27 AM GMT

PDB ID	:	2H43
Title	:	Crystal Structure of Human Fragment D Complexed with Ala-His-Arg-Pro-amide
Authors	:	Doolittle, R.F.; Pandi, L.
Deposited on	:	2006-05-23
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

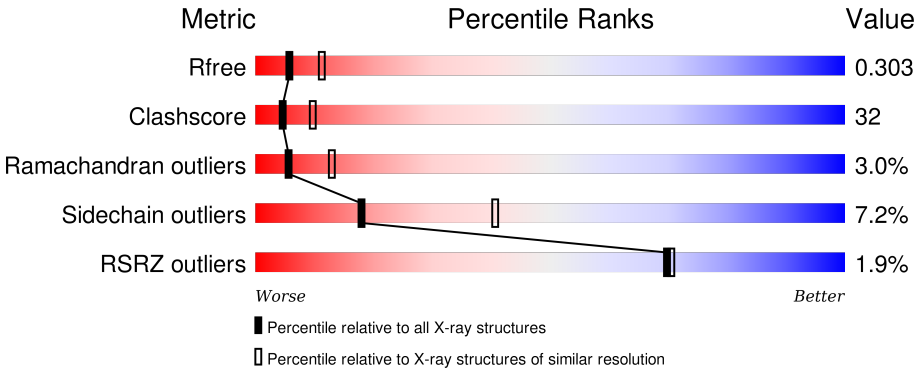
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 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	87	5% 26% 46% 8% 20%
1	D	87	5% 34% 33% 11% 20%
2	B	328	% 50% 36% 6% 8%
2	E	328	2% 47% 40% 5% 8%
3	C	323	% 49% 36% 5% 10%

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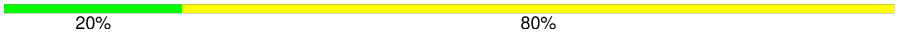
Mol	Chain	Length	Quality of chain
3	F	323	
4	I	5	
4	J	5	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10770 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	70	Total	C	N	O	S	0	0	0
			570	354	106	107	3			
1	D	70	Total	C	N	O	S	0	0	0
			570	354	106	107	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	S	0	0	0
			2421	1510	428	461	22			
2	E	302	Total	C	N	O	S	0	0	0
			2421	1510	428	461	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	290	Total	C	N	O	S	0	0	0
			2329	1477	394	447	11			
3	F	290	Total	C	N	O	S	0	0	0
			2329	1477	394	447	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	408	ALA	-	INSERTION	UNP P02679
C	409	GLY	-	INSERTION	UNP P02679
C	410	ASP	-	INSERTION	UNP P02679
C	411	VAL	-	INSERTION	UNP P02679
F	408	ALA	-	INSERTION	UNP P02679
F	409	GLY	-	INSERTION	UNP P02679
F	410	ASP	-	INSERTION	UNP P02679
F	411	VAL	-	INSERTION	UNP P02679

- Molecule 4 is a protein called GLY-HIS-ARG-PRO-AMIDE peptide ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	5	Total	C	N	O	0	0	1
			34	20	10	4			
4	J	5	Total	C	N	O	0	0	1
			34	20	10	4			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

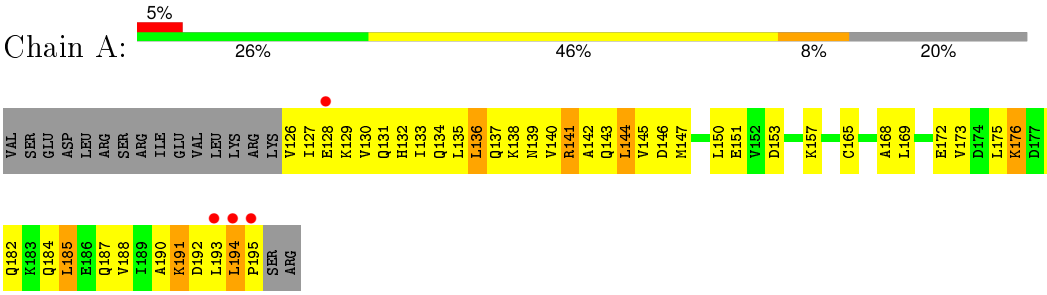
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		
7	F	1	Total	Ca	0	0
			1	1		
7	E	2	Total	Ca	0	0
			2	2		

3 Residue-property plots (i)

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

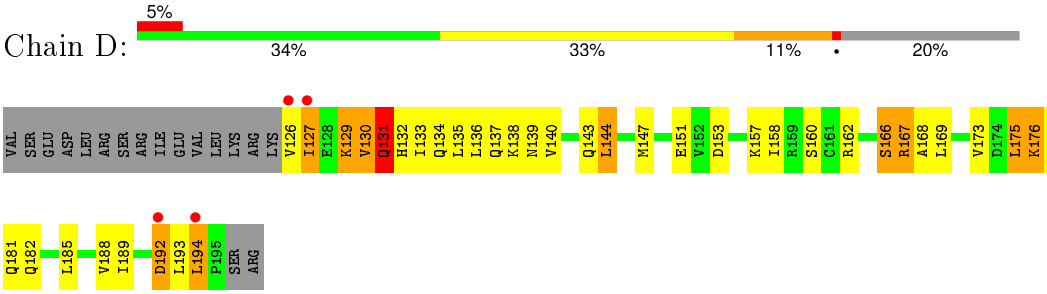
- Molecule 1: Fibrinogen alpha chain

Chain A:



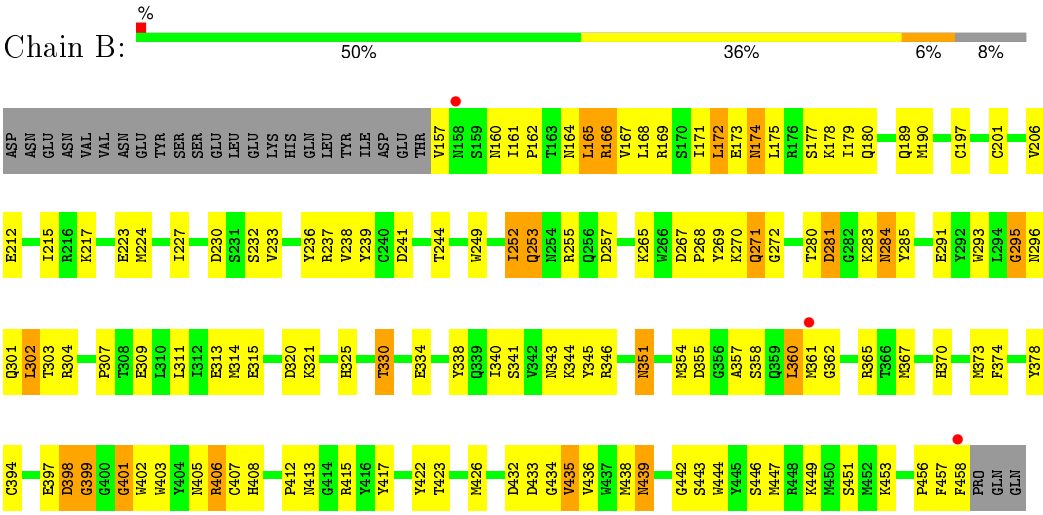
- Molecule 1: Fibrinogen alpha chain

Chain D:



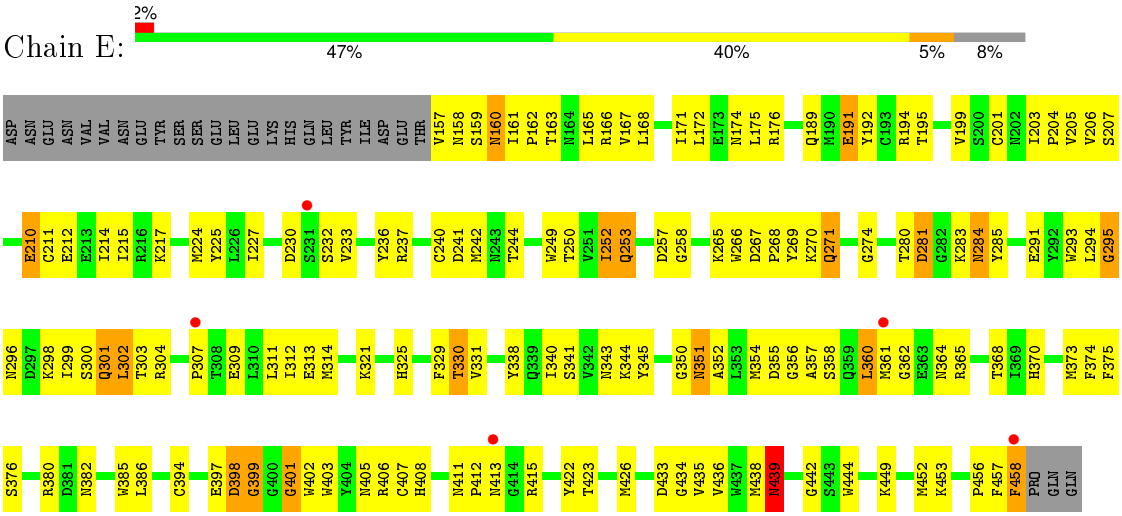
- Molecule 2: Fibrinogen beta chain

Chain B:



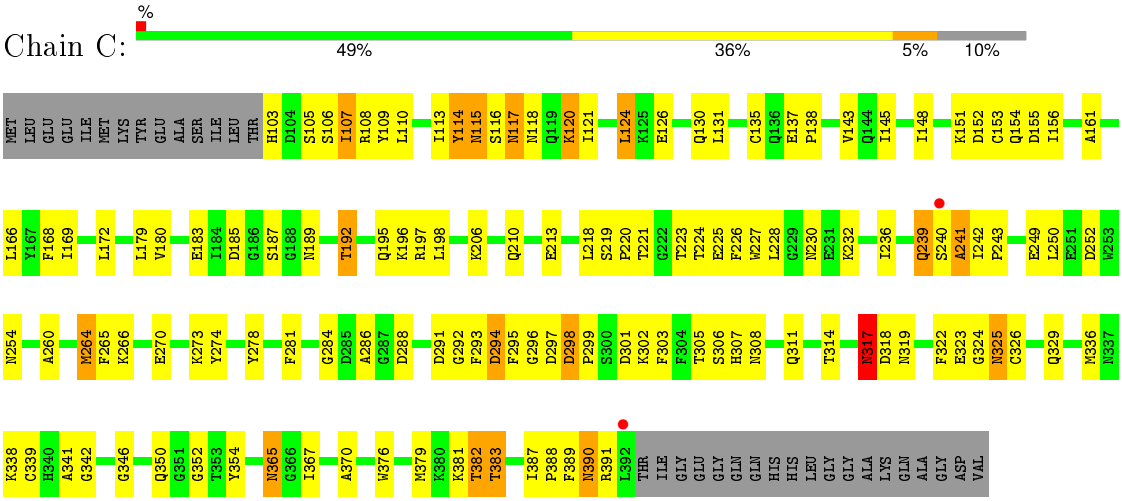
- Molecule 2: Fibrinogen beta chain

Chain E:



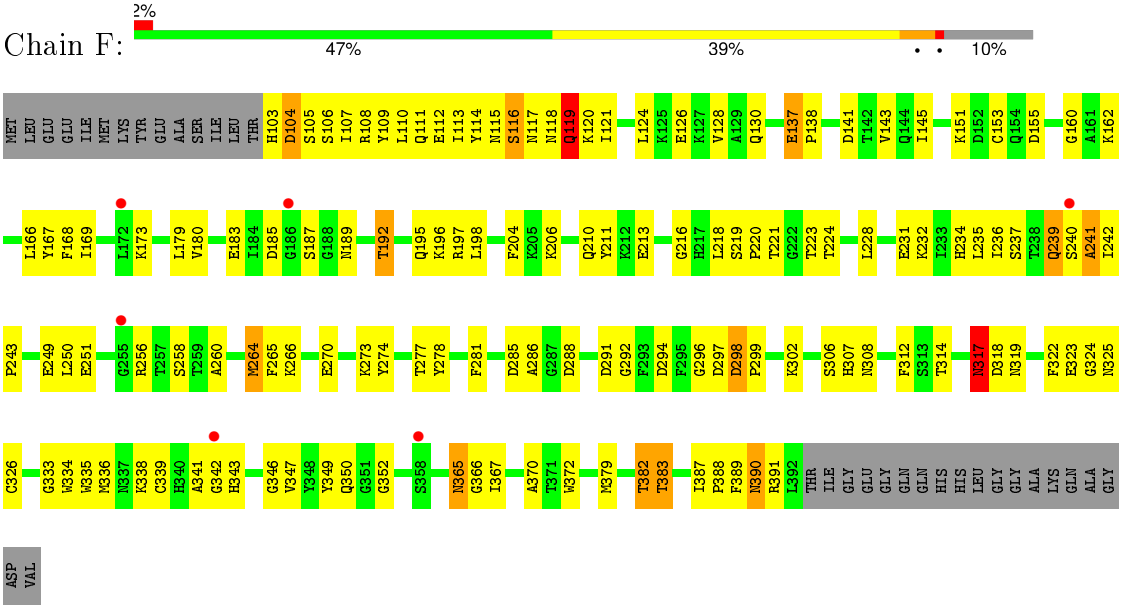
• Molecule 3: Fibrinogen gamma chain

Chain C:



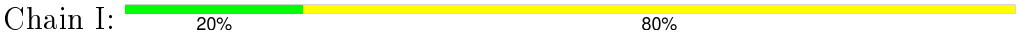
• Molecule 3: Fibrinogen gamma chain

Chain F:



- Molecule 4: GLY-HIS-ARG-PRO-AMIDE peptide ligand

Chain I:



- Molecule 4: GLY-HIS-ARG-PRO-AMIDE peptide ligand

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.00Å 47.90Å 171.40Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 91.8 (29.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.307 0.244 , 0.303	Depositor DCC
R_{free} test set	2053 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 48.8	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 42191 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10770	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, NDG, NH2

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	0.38	0/572	0.66	0/765
1	D	0.39	0/572	0.70	0/765
2	B	0.42	0/2482	0.71	2/3352 (0.1%)
2	E	0.41	0/2482	0.68	2/3352 (0.1%)
3	C	0.41	0/2394	0.62	0/3237
3	F	0.40	0/2394	0.61	0/3237
4	I	0.45	0/34	0.58	0/45
4	J	0.48	0/34	0.59	0/45
All	All	0.41	0/10964	0.66	4/14798 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GLY	N-CA-C	-6.64	96.49	113.10
2	E	399	GLY	N-CA-C	6.50	129.35	113.10
2	B	399	GLY	N-CA-C	6.21	128.64	113.10
2	E	401	GLY	N-CA-C	-5.67	98.93	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	570	0	602	71	0
1	D	570	0	602	61	0
2	B	2421	0	2288	168	0
2	E	2421	0	2288	168	0
3	C	2329	0	2174	139	0
3	F	2329	0	2174	137	0
4	I	34	0	34	3	0
4	J	34	0	34	5	0
5	B	28	0	25	3	0
6	E	28	0	25	1	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
All	All	10770	0	10246	675	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 32.

All (675) 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:357:ALA:HB3	2:E:360:LEU:HD21	1.37	1.05
1:D:134:GLN:HE21	1:D:193:LEU:HD13	1.16	1.01
1:D:181:GLN:HE22	2:E:174:ASN:ND2	1.60	1.00
3:C:110:LEU:H	3:C:110:LEU:HD12	1.19	1.00
3:C:153:CYS:HB2	3:C:192:THR:HG22	1.43	0.98
3:C:117:ASN:C	3:C:117:ASN:HD22	1.63	0.98
3:F:281:PHE:HB2	3:F:288:ASP:OD2	1.64	0.98
1:D:185:LEU:HD23	2:E:171:ILE:HD12	1.46	0.97
3:C:281:PHE:HB2	3:C:288:ASP:OD2	1.66	0.96
3:F:307:HIS:HE1	3:F:341:ALA:H	1.09	0.94
1:D:134:GLN:NE2	1:D:193:LEU:HD13	1.81	0.94
2:B:357:ALA:HB3	2:B:360:LEU:HD21	1.51	0.93
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.37	0.90
1:A:153:ASP:O	1:A:157:LYS:HG2	1.72	0.90
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.54	0.89
3:C:307:HIS:HE1	3:C:341:ALA:H	1.14	0.89
2:E:358:SER:HA	2:E:365:ARG:HH12	1.34	0.89
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.55	0.87
2:E:176:ARG:HH21	3:F:113:ILE:HD11	1.37	0.86
1:A:143:GLN:HE22	3:C:118:ASN:HB2	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.57	0.86
2:E:360:LEU:O	2:E:365:ARG:HB2	1.77	0.85
2:E:172:LEU:HB3	3:F:113:ILE:HG21	1.59	0.84
2:B:172:LEU:HD12	3:C:113:ILE:HG22	1.58	0.84
1:A:169:LEU:H	2:B:189:GLN:NE2	1.76	0.83
2:E:412:PRO:O	2:E:413:ASN:HB2	1.75	0.83
2:E:357:ALA:HA	2:E:439:ASN:HD21	1.42	0.83
2:B:412:PRO:O	2:B:413:ASN:HB2	1.77	0.82
3:C:110:LEU:H	3:C:110:LEU:CD1	1.92	0.82
2:B:172:LEU:HD21	3:C:114:TYR:HB2	1.58	0.82
1:D:177:ASP:O	1:D:181:GLN:HG3	1.79	0.82
1:A:126:VAL:HG23	1:A:127:ILE:H	1.44	0.82
1:A:129:LYS:CA	1:A:131:GLN:HE22	1.93	0.81
2:E:406:ARG:N	2:E:407:CYS:HA	1.95	0.81
1:A:131:GLN:HA	1:A:134:GLN:HG2	1.62	0.81
2:E:176:ARG:NH2	3:F:113:ILE:HD11	1.96	0.80
3:F:153:CYS:SG	3:F:192:THR:HB	2.22	0.80
2:B:406:ARG:N	2:B:407:CYS:HA	1.98	0.78
1:A:129:LYS:HA	1:A:131:GLN:HE22	1.46	0.78
3:F:103:HIS:C	3:F:105:SER:H	1.85	0.78
3:C:153:CYS:SG	3:C:192:THR:HB	2.23	0.78
3:C:117:ASN:HA	3:C:120:LYS:HG3	1.65	0.78
3:C:307:HIS:CE1	3:C:341:ALA:H	2.00	0.78
3:C:221:THR:O	3:C:223:THR:HG23	1.84	0.78
2:B:360:LEU:O	2:B:365:ARG:HB2	1.83	0.77
2:E:439:ASN:N	2:E:439:ASN:HD22	1.80	0.77
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.48	0.77
1:A:169:LEU:H	2:B:189:GLN:HE22	1.30	0.77
3:F:219:SER:OG	3:F:224:THR:HG22	1.84	0.77
3:F:307:HIS:CE1	3:F:341:ALA:H	1.99	0.77
2:E:357:ALA:CB	2:E:360:LEU:HD21	2.13	0.76
3:C:110:LEU:N	3:C:110:LEU:HD12	1.98	0.76
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.66	0.76
2:B:439:ASN:HD22	2:B:439:ASN:N	1.81	0.76
1:A:131:GLN:HE21	1:A:132:HIS:H	1.34	0.75
3:C:197:ARG:HB2	3:C:382:THR:HG22	1.66	0.75
1:A:131:GLN:NE2	1:A:132:HIS:H	1.85	0.75
3:F:153:CYS:HB2	3:F:192:THR:HG22	1.68	0.75
3:C:117:ASN:HD22	3:C:118:ASN:N	1.84	0.74
2:E:165:LEU:HD11	3:F:106:SER:HB2	1.69	0.74
1:D:129:LYS:HA	1:D:129:LYS:NZ	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:VAL:HG23	1:D:131:GLN:H	1.52	0.74
2:E:201:CYS:O	3:F:143:VAL:HG21	1.87	0.74
3:C:265:PHE:O	3:C:266:LYS:HG3	1.86	0.74
1:A:143:GLN:NE2	3:C:118:ASN:HB2	2.03	0.74
2:B:271:GLN:HE21	2:B:271:GLN:HA	1.52	0.74
3:F:326:CYS:HB3	3:F:336:MET:HE2	1.70	0.74
2:B:358:SER:HA	2:B:365:ARG:HH12	1.53	0.73
2:B:173:GLU:OE2	2:B:173:GLU:HA	1.88	0.73
3:F:228:LEU:O	3:F:232:LYS:HD2	1.88	0.73
1:A:144:LEU:HD23	2:B:175:LEU:HD11	1.71	0.73
1:A:147:MET:HE1	3:C:121:ILE:HD11	1.70	0.73
3:C:109:TYR:HB2	3:C:110:LEU:HD12	1.71	0.72
2:E:159:SER:C	2:E:162:PRO:HD2	2.09	0.72
1:D:162:ARG:HH11	1:D:168:ALA:HB3	1.55	0.72
2:B:174:ASN:HD21	2:B:178:LYS:NZ	1.87	0.72
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.24	0.72
1:D:127:ILE:HG23	1:D:194:LEU:HD13	1.71	0.72
2:E:237:ARG:HH11	2:E:237:ARG:HG3	1.54	0.71
3:C:117:ASN:C	3:C:117:ASN:ND2	2.37	0.71
2:E:438:MET:HA	2:E:442:GLY:O	1.89	0.71
1:D:129:LYS:HA	1:D:129:LYS:HZ3	1.55	0.71
2:B:177:SER:O	2:B:180:GLN:HB2	1.90	0.70
2:E:157:VAL:HA	2:E:161:ILE:HD13	1.71	0.70
3:C:365:ASN:C	3:C:365:ASN:HD22	1.93	0.70
2:E:358:SER:HA	2:E:365:ARG:NH1	2.06	0.69
2:B:252:ILE:HG13	2:B:299:ILE:CD1	2.21	0.69
3:F:195:GLN:HE22	3:F:382:THR:CG2	2.05	0.69
2:B:343:ASN:HD22	2:B:344:LYS:HG3	1.55	0.69
1:A:132:HIS:HB3	3:C:107:ILE:HD13	1.75	0.69
1:A:128:GLU:C	1:A:129:LYS:HD2	2.13	0.68
3:C:117:ASN:HA	3:C:120:LYS:CG	2.24	0.68
1:A:188:VAL:CG1	2:B:165:LEU:HG	2.24	0.68
3:F:250:LEU:HB3	3:F:379:MET:HE2	1.75	0.68
1:A:141:ARG:HG3	1:A:142:ALA:N	2.09	0.68
2:E:161:ILE:HD12	2:E:161:ILE:H	1.58	0.68
2:B:340:ILE:HG12	2:B:341:SER:N	2.09	0.68
5:B:470:NAG:O6	5:B:471:NAG:H82	1.94	0.68
2:E:364:ASN:ND2	6:E:470:NAG:H62	2.09	0.68
3:F:241:ALA:O	3:F:242:ILE:HG23	1.93	0.67
2:B:373:MET:CG	2:B:405:ASN:HB2	2.23	0.67
2:E:423:THR:N	2:E:426:MET:HE3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:SER:OG	2:E:195:THR:HG22	1.93	0.67
2:B:172:LEU:HD11	3:C:114:TYR:HA	1.75	0.67
2:B:386:LEU:H	2:B:386:LEU:HD23	1.57	0.67
1:A:194:LEU:N	1:A:195:PRO:HD3	2.09	0.67
1:D:127:ILE:HG21	1:D:194:LEU:HB2	1.77	0.66
3:F:104:ASP:O	3:F:108:ARG:NH1	2.28	0.66
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.76	0.66
2:B:357:ALA:HA	2:B:439:ASN:ND2	2.07	0.66
1:D:127:ILE:CG2	1:D:194:LEU:HB2	2.26	0.66
3:C:145:ILE:HG21	3:C:168:PHE:CE1	2.31	0.66
3:F:221:THR:O	3:F:223:THR:HG23	1.95	0.66
2:E:394:CYS:O	2:E:398:ASP:HB2	1.96	0.65
1:A:140:VAL:HG21	2:B:168:LEU:HD11	1.78	0.65
2:E:373:MET:CG	2:E:405:ASN:HB2	2.27	0.65
2:E:230:ASP:OD2	2:E:232:SER:HB3	1.96	0.65
1:A:194:LEU:H	1:A:195:PRO:HD3	1.61	0.65
2:E:210:GLU:O	2:E:214:ILE:HG13	1.96	0.65
2:E:159:SER:O	2:E:163:THR:HG23	1.97	0.65
3:F:250:LEU:HB3	3:F:379:MET:CE	2.26	0.65
2:E:343:ASN:HD22	2:E:344:LYS:HG3	1.62	0.65
3:C:197:ARG:NH2	3:C:346:GLY:O	2.30	0.65
2:B:415:ARG:O	2:B:434:GLY:HA2	1.96	0.65
3:C:389:PHE:C	3:C:391:ARG:H	2.01	0.65
3:F:243:PRO:HB2	3:F:389:PHE:HB3	1.79	0.64
2:E:386:LEU:HD23	2:E:386:LEU:H	1.62	0.64
1:A:128:GLU:O	1:A:129:LYS:HD2	1.97	0.64
1:A:188:VAL:HG11	2:B:165:LEU:HG	1.77	0.64
3:C:241:ALA:O	3:C:242:ILE:HG23	1.98	0.64
3:C:322:PHE:HD2	3:C:338:LYS:HG3	1.63	0.64
2:B:237:ARG:HH11	2:B:237:ARG:HG3	1.62	0.64
3:C:219:SER:OG	3:C:224:THR:HG22	1.97	0.64
3:C:281:PHE:CG	3:C:288:ASP:HB2	2.33	0.64
1:D:134:GLN:O	1:D:138:LYS:HG2	1.98	0.64
2:B:169:ARG:HH21	3:C:109:TYR:CB	2.11	0.63
2:E:165:LEU:HD11	3:F:106:SER:CB	2.29	0.63
3:C:250:LEU:HB3	3:C:379:MET:HE2	1.80	0.63
3:F:265:PHE:O	3:F:266:LYS:HG3	1.98	0.63
1:D:126:VAL:O	1:D:194:LEU:HD22	1.99	0.63
1:D:126:VAL:O	1:D:127:ILE:HG23	1.98	0.63
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.33	0.63
2:E:172:LEU:HB3	3:F:113:ILE:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:CYS:O	2:B:398:ASP:HB2	1.98	0.63
3:F:273:LYS:HG3	3:F:319:ASN:OD1	1.99	0.63
3:C:189:ASN:ND2	3:C:391:ARG:HE	1.97	0.63
2:B:439:ASN:ND2	2:B:439:ASN:N	2.47	0.62
1:A:131:GLN:HA	1:A:134:GLN:CG	2.29	0.62
3:F:103:HIS:O	3:F:105:SER:N	2.31	0.62
2:B:405:ASN:O	2:B:406:ARG:HB3	1.99	0.62
1:D:167:ARG:NH1	1:D:167:ARG:HB3	2.14	0.62
3:C:107:ILE:HG22	3:C:107:ILE:O	1.97	0.62
3:C:197:ARG:CB	3:C:382:THR:HG22	2.30	0.62
1:A:184:GLN:O	1:A:187:GLN:HB3	1.99	0.62
2:E:293:TRP:HE1	2:E:296:ASN:ND2	1.97	0.62
1:A:141:ARG:HG3	1:A:142:ALA:H	1.65	0.62
1:D:185:LEU:HD23	2:E:171:ILE:CD1	2.26	0.62
2:B:357:ALA:CB	2:B:360:LEU:HD21	2.27	0.62
3:F:115:ASN:HD22	3:F:115:ASN:N	1.98	0.62
2:E:360:LEU:HD23	2:E:360:LEU:N	2.15	0.62
3:C:291:ASP:O	3:C:302:LYS:HD2	1.99	0.61
2:E:252:ILE:HG13	2:E:299:ILE:CD1	2.30	0.61
2:B:201:CYS:O	3:C:143:VAL:HG21	2.01	0.61
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.00	0.61
2:B:230:ASP:HB3	2:B:233:VAL:HG12	1.83	0.61
3:C:120:LYS:HZ2	3:C:120:LYS:HB3	1.65	0.61
1:A:191:LYS:HZ1	1:A:193:LEU:HD21	1.66	0.61
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.81	0.61
2:B:405:ASN:CG	2:B:405:ASN:O	2.39	0.61
2:E:210:GLU:OE2	2:E:212:GLU:HB3	2.01	0.61
2:E:271:GLN:HA	2:E:271:GLN:HE21	1.65	0.61
3:C:105:SER:HA	3:C:108:ARG:CD	2.31	0.61
2:E:406:ARG:O	2:E:406:ARG:HG2	2.00	0.61
2:E:434:GLY:O	2:E:436:VAL:HG23	2.00	0.61
2:E:157:VAL:HG12	2:E:157:VAL:O	2.01	0.60
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.81	0.60
2:B:166:ARG:NH2	2:B:169:ARG:HD2	2.16	0.60
2:B:373:MET:SD	2:B:405:ASN:HB2	2.41	0.60
2:B:309:GLU:HB2	2:B:325:HIS:HE1	1.67	0.60
3:F:281:PHE:CG	3:F:288:ASP:HB2	2.37	0.60
3:F:197:ARG:HB2	3:F:382:THR:HG22	1.82	0.60
2:E:439:ASN:N	2:E:439:ASN:ND2	2.50	0.60
2:B:351:ASN:CG	2:B:354:MET:HB2	2.22	0.60
2:B:157:VAL:O	2:B:157:VAL:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:PRO:HB2	3:C:389:PHE:HB3	1.84	0.60
1:A:140:VAL:CG2	1:A:185:LEU:HD11	2.30	0.60
3:C:250:LEU:HB3	3:C:379:MET:CE	2.31	0.60
1:D:167:ARG:HG3	2:E:192:TYR:CG	2.36	0.60
2:B:406:ARG:H	2:B:407:CYS:HA	1.67	0.59
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.66	0.59
2:B:438:MET:HA	2:B:442:GLY:O	2.02	0.59
1:A:153:ASP:OD1	1:A:157:LYS:HE3	2.02	0.59
2:B:412:PRO:O	2:B:413:ASN:CB	2.50	0.59
1:A:181:GLN:NE2	2:B:174:ASN:OD1	2.35	0.59
3:F:389:PHE:C	3:F:391:ARG:H	2.05	0.59
3:C:387:ILE:HG13	3:C:388:PRO:HD2	1.83	0.59
2:E:227:ILE:HD11	2:E:236:TYR:CE2	2.38	0.59
1:A:131:GLN:CA	1:A:134:GLN:HG2	2.33	0.59
2:B:340:ILE:HG12	2:B:341:SER:H	1.65	0.59
3:C:228:LEU:O	3:C:232:LYS:HD2	2.02	0.59
1:A:133:ILE:CG2	2:B:165:LEU:HD22	2.33	0.59
3:F:103:HIS:C	3:F:105:SER:N	2.55	0.59
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.85	0.59
1:A:147:MET:CE	3:C:121:ILE:HD11	2.33	0.58
2:E:295:GLY:O	2:E:299:ILE:HG13	2.03	0.58
1:A:131:GLN:H	1:A:131:GLN:CD	2.07	0.58
1:A:181:GLN:OE1	2:B:171:ILE:HG23	2.03	0.58
2:B:406:ARG:O	2:B:406:ARG:HG2	2.04	0.58
3:C:106:SER:O	3:C:110:LEU:HD13	2.04	0.58
2:E:406:ARG:H	2:E:407:CYS:HA	1.67	0.58
3:C:307:HIS:CE1	3:C:342:GLY:H	2.22	0.58
3:F:114:TYR:HD1	3:F:115:ASN:ND2	2.01	0.58
2:E:157:VAL:HA	2:E:161:ILE:CD1	2.33	0.58
3:C:281:PHE:CD2	3:C:288:ASP:HB2	2.39	0.58
3:C:260:ALA:HB2	3:C:286:ALA:HB3	1.86	0.57
1:A:127:ILE:O	1:A:130:VAL:HG22	2.04	0.57
3:C:120:LYS:NZ	3:C:120:LYS:HB3	2.19	0.57
1:D:181:GLN:HE22	2:E:174:ASN:HD21	1.49	0.57
2:E:212:GLU:O	2:E:215:ILE:HG22	2.04	0.57
2:E:309:GLU:HB2	2:E:325:HIS:HE1	1.68	0.57
2:E:405:ASN:O	2:E:406:ARG:HB3	2.05	0.57
2:E:210:GLU:OE1	2:E:456:PRO:HG2	2.04	0.57
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.39	0.57
1:A:133:ILE:HG23	2:B:165:LEU:HD22	1.86	0.56
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:GLU:HG2	2:B:458:PHE:CE2	2.39	0.56
3:C:326:CYS:HB3	3:C:336:MET:HE2	1.86	0.56
3:F:197:ARG:HD3	3:F:204:PHE:CE2	2.41	0.56
3:F:322:PHE:CD1	3:F:324:GLY:N	2.73	0.56
3:F:116:SER:O	3:F:120:LYS:HG2	2.06	0.56
2:E:300:SER:OG	2:E:331:VAL:O	2.20	0.56
1:A:136:LEU:O	1:A:140:VAL:HG22	2.06	0.56
3:F:189:ASN:ND2	3:F:391:ARG:HE	2.03	0.55
2:E:340:ILE:HG12	2:E:341:SER:N	2.21	0.55
2:B:351:ASN:ND2	2:B:354:MET:H	2.04	0.55
3:F:288:ASP:OD1	3:F:291:ASP:HB2	2.07	0.55
3:C:365:ASN:C	3:C:365:ASN:ND2	2.60	0.55
2:B:252:ILE:HG13	2:B:299:ILE:HD13	1.87	0.55
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.87	0.55
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.71	0.55
3:C:270:GLU:HG3	3:C:274:TYR:CE1	2.42	0.55
3:F:117:ASN:O	3:F:119:GLN:N	2.33	0.55
2:B:360:LEU:HD23	2:B:360:LEU:N	2.22	0.55
3:C:326:CYS:HB3	3:C:336:MET:CE	2.36	0.55
2:B:280:THR:O	2:B:281:ASP:OD2	2.24	0.55
3:C:288:ASP:OD1	3:C:291:ASP:HB2	2.06	0.55
3:C:322:PHE:CD1	3:C:324:GLY:N	2.75	0.55
2:E:370:HIS:HE1	2:E:408:HIS:HB2	1.72	0.55
2:B:311:LEU:HD23	2:B:453:LYS:HD2	1.88	0.55
2:E:439:ASN:H	2:E:439:ASN:HD22	1.50	0.55
3:F:291:ASP:O	3:F:302:LYS:HD2	2.06	0.55
2:E:415:ARG:O	2:E:434:GLY:HA2	2.06	0.55
2:B:257:ASP:O	2:B:291:GLU:OE2	2.24	0.55
3:F:347:VAL:HB	3:F:349:TYR:CE1	2.41	0.55
2:E:206:VAL:HG22	2:E:207:SER:N	2.22	0.55
2:E:162:PRO:O	2:E:166:ARG:HG3	2.07	0.54
2:B:295:GLY:O	2:B:299:ILE:HG13	2.07	0.54
1:A:192:ASP:O	1:A:193:LEU:HD23	2.07	0.54
3:C:195:GLN:HE22	3:C:382:THR:HG21	1.72	0.54
1:D:167:ARG:HD2	2:E:192:TYR:CD1	2.42	0.54
2:B:230:ASP:OD2	2:B:232:SER:HB3	2.08	0.54
2:B:169:ARG:NH2	3:C:109:TYR:HB3	2.23	0.54
3:F:197:ARG:NH2	3:F:346:GLY:O	2.40	0.54
2:E:434:GLY:O	2:E:436:VAL:N	2.40	0.54
2:E:265:LYS:O	2:E:268:PRO:HD2	2.08	0.54
2:E:405:ASN:CG	2:E:405:ASN:O	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ASN:C	2:B:166:ARG:H	2.11	0.54
3:C:307:HIS:HE1	3:C:342:GLY:H	1.55	0.54
2:B:210:GLU:OE2	2:B:212:GLU:N	2.41	0.54
2:B:212:GLU:O	2:B:215:ILE:HG22	2.07	0.54
3:C:350:GLN:C	3:C:352:GLY:H	2.11	0.54
1:D:130:VAL:O	1:D:133:ILE:HG12	2.09	0.54
1:D:193:LEU:C	1:D:194:LEU:HD12	2.28	0.54
2:B:456:PRO:O	2:B:457:PHE:HB3	2.08	0.54
3:C:169:ILE:HD11	3:C:180:VAL:HG11	1.90	0.54
2:B:367:MET:SD	4:I:2:HIS:HB2	2.49	0.53
1:D:158:ILE:HG23	2:E:189:GLN:NE2	2.23	0.53
2:E:345:TYR:HB2	2:E:354:MET:CE	2.38	0.53
2:E:397:GLU:O	2:E:399:GLY:N	2.42	0.53
3:C:148:ILE:HG22	3:C:156:ILE:HG23	1.91	0.53
1:A:165:CYS:O	2:B:197:CYS:HB3	2.08	0.53
3:C:105:SER:HA	3:C:108:ARG:HD3	1.91	0.53
2:E:397:GLU:C	2:E:399:GLY:H	2.12	0.53
2:B:423:THR:N	2:B:426:MET:HE3	2.24	0.53
2:B:432:ASP:OD1	2:B:443:SER:OG	2.27	0.53
3:C:232:LYS:O	3:C:236:ILE:HG13	2.09	0.53
1:D:144:LEU:HD22	1:D:182:GLN:HG3	1.91	0.53
2:E:357:ALA:HA	2:E:439:ASN:ND2	2.17	0.53
2:E:439:ASN:H	2:E:439:ASN:ND2	2.07	0.53
2:B:345:TYR:HB2	2:B:354:MET:CE	2.39	0.53
1:A:151:GLU:CG	1:A:173:VAL:HG13	2.38	0.53
1:D:151:GLU:HG2	1:D:173:VAL:CG1	2.39	0.53
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.44	0.53
2:B:358:SER:HA	2:B:365:ARG:NH1	2.21	0.53
2:B:345:TYR:CZ	2:B:346:ARG:O	2.62	0.53
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.44	0.53
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.73	0.53
5:B:470:NAG:H62	5:B:471:NAG:O5	2.09	0.53
1:D:153:ASP:O	1:D:157:LYS:HG2	2.09	0.53
1:D:151:GLU:HG2	1:D:173:VAL:HG13	1.91	0.53
3:F:307:HIS:CE1	3:F:342:GLY:H	2.27	0.52
1:A:131:GLN:N	1:A:131:GLN:CD	2.62	0.52
2:E:412:PRO:O	2:E:413:ASN:CB	2.49	0.52
2:B:271:GLN:NE2	2:B:271:GLN:HA	2.22	0.52
2:B:174:ASN:HD21	2:B:178:LYS:HZ1	1.54	0.52
2:E:210:GLU:OE2	2:E:212:GLU:N	2.40	0.52
2:B:439:ASN:H	2:B:439:ASN:ND2	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:O	1:A:127:ILE:HG22	2.09	0.52
3:F:219:SER:N	3:F:224:THR:HG21	2.25	0.52
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.24	0.52
2:E:356:GLY:HA2	2:E:368:THR:O	2.09	0.52
1:A:144:LEU:HD23	2:B:175:LEU:HD21	1.92	0.52
2:B:227:ILE:HD13	2:B:238:VAL:HG11	1.90	0.52
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.91	0.52
2:B:370:HIS:CE1	2:B:408:HIS:HB2	2.44	0.52
2:B:180:GLN:OE1	2:B:180:GLN:HA	2.10	0.52
2:B:434:GLY:O	2:B:436:VAL:HG23	2.10	0.52
1:D:136:LEU:O	1:D:140:VAL:HG23	2.10	0.52
3:C:151:LYS:HE2	3:C:172:LEU:HB2	1.91	0.52
1:D:137:GLN:NE2	1:D:188:VAL:HG12	2.25	0.52
2:B:174:ASN:HD21	2:B:178:LYS:HZ3	1.56	0.52
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.10	0.52
3:F:166:LEU:HD12	3:F:220:PRO:HG3	1.92	0.52
1:D:134:GLN:HE21	1:D:193:LEU:CD1	2.06	0.52
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.92	0.52
2:E:283:LYS:HB3	2:E:285:TYR:CE1	2.44	0.52
3:F:365:ASN:HD22	3:F:365:ASN:C	2.13	0.51
3:F:117:ASN:C	3:F:119:GLN:H	2.14	0.51
2:E:311:LEU:HD23	2:E:453:LYS:HD2	1.91	0.51
3:C:114:TYR:O	3:C:118:ASN:HB2	2.11	0.51
3:F:278:TYR:CE2	3:F:308:ASN:HB2	2.45	0.51
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.08	0.51
1:D:130:VAL:HG23	1:D:131:GLN:N	2.22	0.51
3:C:252:ASP:OD2	3:C:254:ASN:HB2	2.10	0.51
2:B:374:PHE:O	2:B:403:TRP:HA	2.10	0.51
1:D:167:ARG:HH11	1:D:167:ARG:HB3	1.76	0.51
3:C:297:ASP:O	3:C:298:ASP:HB2	2.11	0.51
3:F:326:CYS:HB3	3:F:336:MET:CE	2.39	0.50
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.93	0.50
3:C:169:ILE:CD1	3:C:180:VAL:HG11	2.41	0.50
4:J:3:ARG:HG2	4:J:3:ARG:HH21	1.76	0.50
2:B:397:GLU:C	2:B:399:GLY:H	2.15	0.50
1:A:132:HIS:CB	3:C:107:ILE:HD13	2.40	0.50
2:B:271:GLN:HE21	2:B:271:GLN:CA	2.15	0.50
1:A:178:TYR:O	1:A:182:GLN:HG3	2.11	0.50
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.93	0.50
2:B:210:GLU:OE1	2:B:456:PRO:HG2	2.11	0.50
3:F:145:ILE:HG21	3:F:168:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:243:PRO:HB3	3:F:264:MET:SD	2.52	0.50
3:C:325:ASN:O	3:C:329:GLN:HG3	2.10	0.50
2:E:166:ARG:HH11	2:E:166:ARG:HG2	1.77	0.50
2:B:283:LYS:HB3	2:B:285:TYR:CE1	2.47	0.50
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.23	0.49
2:E:423:THR:H	2:E:426:MET:HE3	1.76	0.49
2:B:280:THR:O	2:B:281:ASP:O	2.29	0.49
3:F:219:SER:H	3:F:224:THR:HG21	1.77	0.49
1:D:143:GLN:HE22	3:F:117:ASN:HB2	1.77	0.49
2:B:334:GLU:HB2	2:B:338:TYR:CZ	2.46	0.49
3:C:114:TYR:O	3:C:118:ASN:CB	2.61	0.49
3:F:213:GLU:HA	3:F:213:GLU:OE2	2.11	0.49
1:D:132:HIS:HD2	3:F:107:ILE:HG21	1.77	0.49
1:D:181:GLN:HE22	2:E:174:ASN:CG	2.14	0.49
2:E:351:ASN:OD1	2:E:354:MET:HB2	2.12	0.49
2:B:334:GLU:HB2	2:B:338:TYR:OH	2.12	0.49
3:F:298:ASP:OD2	3:F:299:PRO:HD2	2.12	0.49
2:B:169:ARG:HH21	3:C:109:TYR:HB3	1.75	0.49
2:B:432:ASP:OD2	4:I:1:ALA:N	2.46	0.49
3:F:197:ARG:CB	3:F:382:THR:HG22	2.42	0.49
2:E:456:PRO:O	2:E:457:PHE:HB3	2.12	0.49
3:F:338:LYS:N	3:F:339:CYS:HA	2.28	0.49
2:B:190:MET:HE2	3:C:131:LEU:HD13	1.94	0.49
1:A:169:LEU:N	2:B:189:GLN:HE22	2.05	0.49
3:C:301:ASP:O	3:C:305:THR:HG23	2.13	0.49
2:E:159:SER:O	2:E:162:PRO:HD2	2.13	0.49
2:E:253:GLN:HB2	2:E:293:TRP:CE3	2.48	0.49
1:A:191:LYS:N	1:A:191:LYS:HD3	2.28	0.49
2:E:385:TRP:CZ2	4:J:3:ARG:HD2	2.48	0.49
2:B:227:ILE:HD11	2:B:236:TYR:CE2	2.47	0.48
2:E:217:LYS:HB3	3:F:213:GLU:HG3	1.94	0.48
2:B:307:PRO:O	2:B:456:PRO:O	2.31	0.48
2:E:206:VAL:CG2	2:E:207:SER:N	2.77	0.48
3:C:273:LYS:HB2	3:C:311:GLN:HB3	1.95	0.48
2:E:157:VAL:N	2:E:160:ASN:ND2	2.61	0.48
3:C:296:GLY:C	3:C:298:ASP:H	2.16	0.48
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.95	0.48
3:F:179:LEU:HD23	3:F:218:LEU:HD12	1.96	0.48
3:C:322:PHE:HA	3:C:338:LYS:HD2	1.96	0.48
3:C:338:LYS:N	3:C:339:CYS:HA	2.27	0.48
2:B:166:ARG:C	2:B:168:LEU:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:LEU:HD21	3:F:106:SER:CB	2.44	0.48
1:A:144:LEU:CD2	2:B:175:LEU:HD21	2.43	0.48
2:E:386:LEU:HG	2:E:386:LEU:O	2.13	0.48
3:C:156:ILE:HG22	3:C:161:ALA:CB	2.44	0.48
2:B:269:TYR:CE2	2:B:401:GLY:HA3	2.49	0.48
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.48	0.48
3:C:367:ILE:O	3:C:379:MET:HG2	2.14	0.48
2:E:269:TYR:CE2	2:E:401:GLY:HA3	2.49	0.48
2:E:402:TRP:CG	2:E:403:TRP:N	2.82	0.48
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.95	0.47
2:B:166:ARG:C	2:B:168:LEU:N	2.67	0.47
2:B:166:ARG:HG2	2:B:166:ARG:HH11	1.79	0.47
3:C:197:ARG:O	3:C:381:LYS:HA	2.14	0.47
5:B:470:NAG:C6	5:B:471:NAG:C1	2.93	0.47
2:B:166:ARG:CG	2:B:166:ARG:HH11	2.27	0.47
2:E:171:ILE:O	2:E:175:LEU:HG	2.14	0.47
2:B:385:TRP:HA	2:B:406:ARG:HD2	1.96	0.47
1:A:126:VAL:HG23	1:A:127:ILE:N	2.21	0.47
2:E:224:MET:CE	2:E:237:ARG:HD3	2.44	0.47
2:E:340:ILE:HG12	2:E:341:SER:H	1.79	0.47
1:A:193:LEU:O	1:A:194:LEU:HB2	2.14	0.47
2:E:357:ALA:HB3	2:E:360:LEU:CD2	2.28	0.47
1:D:130:VAL:HA	1:D:133:ILE:HG12	1.96	0.47
2:E:345:TYR:HB2	2:E:354:MET:HE3	1.97	0.47
2:E:211:CYS:SG	2:E:250:THR:HA	2.55	0.47
1:D:160:SER:HA	2:E:258:GLY:O	2.14	0.47
1:A:169:LEU:C	1:A:169:LEU:HD13	2.35	0.47
2:B:386:LEU:HG	2:B:386:LEU:O	2.14	0.47
3:C:148:ILE:CG2	3:C:156:ILE:HG23	2.44	0.47
2:B:169:ARG:O	2:B:173:GLU:HG2	2.14	0.47
1:D:185:LEU:CD1	1:D:189:ILE:HD11	2.45	0.47
3:F:307:HIS:HE1	3:F:341:ALA:N	1.93	0.47
2:E:373:MET:SD	2:E:405:ASN:HB2	2.55	0.47
1:A:127:ILE:C	1:A:129:LYS:H	2.17	0.47
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.96	0.47
1:A:151:GLU:HG2	1:A:173:VAL:HG13	1.97	0.47
3:F:278:TYR:CZ	3:F:308:ASN:HB2	2.50	0.47
3:F:196:LYS:C	3:F:197:ARG:HG2	2.35	0.47
2:B:439:ASN:HD22	2:B:439:ASN:H	1.58	0.47
2:B:304:ARG:HH11	2:B:304:ARG:CB	2.27	0.47
2:E:304:ARG:NH1	2:E:304:ARG:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:O	1:D:189:ILE:HG13	2.15	0.46
3:C:166:LEU:HD12	3:C:220:PRO:HG3	1.97	0.46
3:F:169:ILE:CD1	3:F:180:VAL:HG11	2.45	0.46
2:B:164:ASN:O	2:B:166:ARG:N	2.43	0.46
1:A:134:GLN:HA	1:A:137:GLN:HB2	1.96	0.46
3:C:156:ILE:HG22	3:C:161:ALA:HB2	1.98	0.46
2:B:397:GLU:O	2:B:399:GLY:N	2.47	0.46
2:B:271:GLN:NE2	2:B:271:GLN:CA	2.78	0.46
1:A:138:LYS:HA	1:A:141:ARG:HG2	1.97	0.46
2:E:351:ASN:CG	2:E:354:MET:HB2	2.36	0.46
2:B:272:GLY:HA2	2:B:293:TRP:O	2.16	0.46
2:E:304:ARG:HH11	2:E:304:ARG:CB	2.29	0.46
3:F:160:GLY:O	3:F:162:LYS:HG2	2.14	0.46
2:E:274:GLY:O	3:F:138:PRO:HB3	2.15	0.46
2:B:340:ILE:CG1	2:B:341:SER:N	2.78	0.46
2:E:374:PHE:O	2:E:403:TRP:HA	2.15	0.46
3:C:206:LYS:HB3	3:C:210:GLN:HB2	1.97	0.46
3:C:196:LYS:C	3:C:197:ARG:HG2	2.36	0.46
3:C:389:PHE:O	3:C:391:ARG:N	2.44	0.46
3:F:296:GLY:C	3:F:298:ASP:H	2.19	0.46
2:E:280:THR:O	2:E:281:ASP:O	2.33	0.46
3:C:284:GLY:C	3:C:286:ALA:H	2.19	0.46
4:J:3:ARG:HG2	4:J:3:ARG:NH2	2.31	0.46
3:C:225:GLU:O	3:C:226:PHE:HB3	2.16	0.46
3:F:294:ASP:OD2	3:F:302:LYS:HB2	2.16	0.46
3:F:322:PHE:HA	3:F:338:LYS:HD2	1.98	0.46
3:F:117:ASN:C	3:F:119:GLN:N	2.70	0.46
3:F:169:ILE:HD11	3:F:180:VAL:HG11	1.97	0.46
3:F:270:GLU:HG3	3:F:274:TYR:CE1	2.50	0.46
1:A:135:LEU:HD13	1:A:139:ASN:ND2	2.31	0.46
2:B:298:LYS:O	2:B:302:LEU:HB2	2.16	0.46
2:B:315:GLU:HA	2:B:320:ASP:O	2.16	0.46
2:E:252:ILE:HG13	2:E:299:ILE:HD13	1.98	0.45
2:B:351:ASN:C	2:B:351:ASN:HD22	2.19	0.45
2:B:304:ARG:HB3	2:B:304:ARG:HH11	1.81	0.45
2:E:199:VAL:O	3:F:141:ASP:HA	2.16	0.45
2:E:157:VAL:N	2:E:160:ASN:HD22	2.15	0.45
3:F:318:ASP:C	3:F:319:ASN:HD22	2.19	0.45
2:B:265:LYS:O	2:B:268:PRO:HD2	2.15	0.45
3:F:115:ASN:N	3:F:115:ASN:ND2	2.63	0.45
2:E:204:PRO:HG2	2:E:224:MET:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:347:VAL:H	3:F:366:GLY:HA2	1.81	0.45
3:C:106:SER:C	3:C:108:ARG:H	2.20	0.45
2:E:284:ASN:ND2	2:E:284:ASN:H	2.13	0.45
1:D:130:VAL:HB	1:D:134:GLN:OE1	2.17	0.45
2:B:457:PHE:O	2:B:458:PHE:C	2.55	0.45
2:B:422:TYR:O	2:B:444:TRP:HB3	2.16	0.45
1:A:175:LEU:O	1:A:176:LYS:C	2.55	0.45
2:B:172:LEU:HD11	3:C:114:TYR:CA	2.44	0.45
3:F:206:LYS:HD2	3:F:210:GLN:OE1	2.16	0.45
2:E:329:PHE:HE1	2:E:340:ILE:HG13	1.81	0.45
1:A:173:VAL:HG12	1:A:175:LEU:HD22	1.97	0.45
2:E:304:ARG:NH1	2:E:304:ARG:CB	2.80	0.45
3:C:152:ASP:OD1	3:C:154:GLN:N	2.42	0.45
3:F:126:GLU:O	3:F:130:GLN:HG3	2.17	0.45
3:C:303:PHE:CE1	3:F:277:THR:HG21	2.52	0.45
3:C:153:CYS:CB	3:C:192:THR:HG22	2.30	0.45
2:E:406:ARG:O	2:E:406:ARG:CG	2.63	0.45
3:F:318:ASP:OD1	3:F:318:ASP:C	2.55	0.45
2:E:298:LYS:O	2:E:302:LEU:HB2	2.17	0.45
3:F:113:ILE:HA	3:F:113:ILE:HD13	1.74	0.45
1:A:132:HIS:HD2	3:C:107:ILE:HG21	1.81	0.44
3:C:197:ARG:HB2	3:C:382:THR:CG2	2.41	0.44
2:B:252:ILE:HD12	2:B:252:ILE:HA	1.72	0.44
2:E:215:ILE:HD13	2:E:242:MET:HB3	1.99	0.44
3:C:143:VAL:HA	3:C:220:PRO:HG2	1.99	0.44
2:B:370:HIS:HE1	2:B:408:HIS:CB	2.29	0.44
2:E:397:GLU:OE1	4:J:3:ARG:NH1	2.37	0.44
3:F:114:TYR:CD1	3:F:115:ASN:ND2	2.82	0.44
2:E:457:PHE:O	2:E:458:PHE:O	2.36	0.44
3:C:143:VAL:O	3:C:143:VAL:HG23	2.17	0.44
2:E:280:THR:O	2:E:281:ASP:OD2	2.35	0.44
3:F:292:GLY:N	3:F:306:SER:HA	2.32	0.44
2:B:361:MET:HG3	2:B:362:GLY:N	2.32	0.44
3:F:211:TYR:CE1	3:F:333:GLY:HA3	2.52	0.44
2:B:178:LYS:C	2:B:180:GLN:N	2.71	0.44
3:F:237:SER:HB2	3:F:266:LYS:HA	2.00	0.44
3:C:314:THR:O	3:C:317:ASN:N	2.47	0.44
3:C:137:GLU:HA	3:C:138:PRO:HD3	1.84	0.44
3:C:389:PHE:C	3:C:391:ARG:N	2.69	0.44
1:D:176:LYS:HD2	1:D:179:GLU:OE2	2.18	0.44
2:B:304:ARG:HB2	2:B:304:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:VAL:CG1	2:B:447:MET:HB2	2.47	0.44
2:B:217:LYS:HB3	3:C:213:GLU:HG3	2.00	0.44
1:D:127:ILE:HG21	1:D:193:LEU:O	2.17	0.44
3:F:196:LYS:O	3:F:197:ARG:HG2	2.18	0.44
2:E:293:TRP:O	2:E:294:LEU:C	2.56	0.44
2:E:271:GLN:HA	2:E:271:GLN:NE2	2.30	0.44
3:F:297:ASP:O	3:F:298:ASP:HB2	2.16	0.44
3:F:185:ASP:OD1	3:F:189:ASN:HB2	2.18	0.44
1:D:129:LYS:NZ	1:D:129:LYS:CA	2.77	0.44
3:F:307:HIS:HD2	3:F:335:TRP:O	1.99	0.44
1:D:153:ASP:OD1	2:E:415:ARG:NH2	2.50	0.44
2:E:205:VAL:HG23	3:F:216:GLY:C	2.38	0.44
3:C:196:LYS:HD2	3:C:383:THR:HB	2.00	0.44
2:B:265:LYS:HE3	2:B:378:TYR:OH	2.17	0.44
3:C:179:LEU:HD23	3:C:218:LEU:HD12	2.00	0.44
2:B:405:ASN:O	2:B:406:ARG:CB	2.66	0.43
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.82	0.43
2:B:267:ASP:O	2:B:270:LYS:HB3	2.18	0.43
3:F:124:LEU:O	3:F:128:VAL:HG23	2.18	0.43
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.99	0.43
2:B:161:ILE:O	2:B:164:ASN:HB3	2.18	0.43
2:B:169:ARG:NH2	3:C:109:TYR:CG	2.86	0.43
2:B:386:LEU:HD23	2:B:386:LEU:N	2.30	0.43
2:E:271:GLN:CA	2:E:271:GLN:HE21	2.27	0.43
3:F:322:PHE:HD2	3:F:338:LYS:HG3	1.82	0.43
3:C:115:ASN:O	3:C:118:ASN:HB3	2.18	0.43
3:F:367:ILE:O	3:F:379:MET:HG2	2.18	0.43
3:C:242:ILE:HA	3:C:243:PRO:HD3	1.85	0.43
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.67	0.43
1:D:143:GLN:NE2	3:F:117:ASN:HB2	2.33	0.43
2:B:304:ARG:NH1	2:B:304:ARG:CB	2.82	0.43
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.66	0.43
2:E:376:SER:OG	2:E:382:ASN:HB2	2.19	0.43
2:B:402:TRP:CG	2:B:403:TRP:N	2.86	0.43
3:F:235:LEU:HD12	3:F:235:LEU:N	2.33	0.43
3:F:196:LYS:HD2	3:F:383:THR:HB	2.00	0.43
3:F:249:GLU:HB3	3:F:383:THR:CG2	2.38	0.43
3:F:219:SER:H	3:F:224:THR:CG2	2.32	0.43
3:C:354:TYR:O	3:C:376:TRP:HB3	2.17	0.43
1:D:130:VAL:O	1:D:132:HIS:N	2.51	0.43
1:A:128:GLU:O	1:A:128:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:SER:N	3:C:224:THR:HG21	2.33	0.43
2:B:164:ASN:C	2:B:166:ARG:N	2.72	0.43
2:E:165:LEU:HD21	3:F:106:SER:OG	2.19	0.43
2:E:375:PHE:CE1	2:E:402:TRP:HA	2.53	0.43
1:A:134:GLN:NE2	1:A:191:LYS:HZ1	2.17	0.43
2:B:340:ILE:CG1	2:B:341:SER:H	2.32	0.43
3:C:151:LYS:HB2	3:C:155:ASP:OD1	2.18	0.43
2:B:321:LYS:HE2	2:B:321:LYS:HB3	1.75	0.43
2:B:284:ASN:H	2:B:284:ASN:ND2	2.16	0.43
2:E:160:ASN:HB2	2:E:161:ILE:HD12	2.00	0.43
1:A:137:GLN:OE1	2:B:165:LEU:HD21	2.19	0.43
2:E:370:HIS:HE1	2:E:408:HIS:CB	2.31	0.43
4:J:2:HIS:O	4:J:3:ARG:NH2	2.48	0.43
1:D:175:LEU:HD13	1:D:179:GLU:OE2	2.18	0.43
3:F:137:GLU:OE1	3:F:137:GLU:CA	2.67	0.43
3:F:372:TRP:HZ3	3:F:379:MET:HE3	1.84	0.43
3:C:185:ASP:OD1	3:C:189:ASN:HB2	2.18	0.43
3:C:278:TYR:CE2	3:C:308:ASN:HB2	2.53	0.42
1:D:181:GLN:NE2	2:E:174:ASN:ND2	2.45	0.42
3:F:312:PHE:CE1	3:F:334:TRP:HA	2.53	0.42
1:D:139:ASN:HB3	3:F:114:TYR:CE2	2.54	0.42
3:F:343:HIS:O	3:F:367:ILE:HA	2.19	0.42
2:B:438:MET:HE2	2:B:443:SER:HB2	2.01	0.42
2:E:304:ARG:HH11	2:E:304:ARG:HB3	1.83	0.42
1:A:150:LEU:HD21	3:C:124:LEU:HD13	2.01	0.42
3:F:231:GLU:O	3:F:234:HIS:HB3	2.19	0.42
1:D:192:ASP:O	1:D:193:LEU:HG	2.19	0.42
2:B:373:MET:HA	2:B:373:MET:HE3	2.01	0.42
3:C:197:ARG:CG	3:C:382:THR:HG22	2.50	0.42
3:C:109:TYR:HB3	3:C:113:ILE:HD11	2.01	0.42
3:C:153:CYS:SG	3:C:192:THR:CB	3.02	0.42
3:C:294:ASP:OD2	3:C:302:LYS:HB2	2.17	0.42
3:C:219:SER:HA	3:C:220:PRO:HD3	1.92	0.42
2:B:303:THR:HB	2:B:330:THR:HA	2.00	0.42
2:E:321:LYS:HE2	2:E:321:LYS:HB3	1.73	0.42
4:I:3:ARG:HA	4:I:4:PRO:HD2	1.90	0.42
3:F:251:GLU:HA	3:F:256:ARG:O	2.19	0.42
3:F:104:ASP:OD2	3:F:104:ASP:O	2.37	0.42
3:C:292:GLY:N	3:C:306:SER:HA	2.33	0.42
2:E:351:ASN:ND2	2:E:354:MET:H	2.17	0.42
2:E:301:GLN:HB3	2:E:301:GLN:HE21	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:288:ASP:O	3:C:288:ASP:OD1	2.37	0.42
3:C:195:GLN:OE1	3:C:382:THR:HG23	2.19	0.42
2:E:252:ILE:HG13	2:E:299:ILE:HG12	2.01	0.42
3:F:338:LYS:HG2	3:F:338:LYS:O	2.20	0.42
2:B:296:ASN:HD22	2:B:296:ASN:HA	1.62	0.42
2:B:253:GLN:HE22	2:B:451:SER:HA	1.84	0.42
3:F:239:GLN:HB3	3:F:240:SER:H	1.54	0.42
1:D:185:LEU:HD13	1:D:185:LEU:O	2.19	0.42
3:C:292:GLY:C	3:C:302:LYS:HD3	2.40	0.42
3:F:258:SER:HA	3:F:285:ASP:OD2	2.19	0.42
2:E:307:PRO:O	2:E:456:PRO:O	2.37	0.42
2:B:314:MET:HA	2:B:449:LYS:O	2.20	0.42
2:B:417:TYR:HB2	2:B:446:SER:CB	2.48	0.42
3:F:232:LYS:O	3:F:236:ILE:HG13	2.19	0.42
2:E:386:LEU:N	2:E:386:LEU:HD23	2.32	0.42
2:B:417:TYR:HB2	2:B:446:SER:HB2	2.02	0.42
1:D:133:ILE:HG13	1:D:134:GLN:N	2.34	0.42
2:E:172:LEU:HD22	3:F:113:ILE:HG22	2.00	0.42
1:A:147:MET:HE1	2:B:179:ILE:HD11	2.01	0.42
2:B:224:MET:CE	2:B:237:ARG:HD3	2.50	0.42
2:B:255:ARG:HA	2:B:255:ARG:HD2	1.96	0.42
1:D:126:VAL:HA	2:E:157:VAL:HG21	2.02	0.41
3:C:116:SER:O	3:C:120:LYS:HG2	2.20	0.41
1:A:133:ILE:CD1	3:C:107:ILE:HD11	2.49	0.41
3:F:389:PHE:C	3:F:391:ARG:N	2.73	0.41
2:E:312:ILE:HG12	2:E:452:MET:HG2	2.01	0.41
2:E:267:ASP:O	2:E:270:LYS:HB3	2.19	0.41
2:B:406:ARG:O	2:B:406:ARG:CG	2.63	0.41
3:C:250:LEU:N	3:C:250:LEU:HD22	2.35	0.41
2:B:398:ASP:CA	2:B:433:ASP:HB3	2.50	0.41
2:E:252:ILE:HA	2:E:252:ILE:HD12	1.65	0.41
2:E:370:HIS:CE1	2:E:408:HIS:HA	2.55	0.41
1:A:151:GLU:HG3	1:A:173:VAL:HG13	2.01	0.41
2:B:241:ASP:HB3	2:B:249:TRP:HB2	2.01	0.41
2:E:314:MET:HA	2:E:449:LYS:O	2.21	0.41
2:E:350:GLY:O	2:E:352:ALA:N	2.53	0.41
2:E:361:MET:HG3	2:E:362:GLY:N	2.36	0.41
3:C:318:ASP:O	3:C:319:ASN:ND2	2.48	0.41
1:D:127:ILE:HG23	1:D:194:LEU:HB2	1.98	0.41
1:D:132:HIS:CD2	3:F:107:ILE:HG21	2.55	0.41
3:F:151:LYS:HB2	3:F:155:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:GLU:HG2	2:B:458:PHE:HE2	1.83	0.41
1:A:129:LYS:HA	1:A:131:GLN:NE2	2.26	0.41
3:F:242:ILE:HA	3:F:243:PRO:HD3	1.90	0.41
1:A:145:VAL:O	1:A:146:ASP:C	2.58	0.41
3:C:239:GLN:HB3	3:C:240:SER:H	1.55	0.41
1:D:147:MET:SD	3:F:121:ILE:HD11	2.59	0.41
2:E:244:THR:HG21	2:E:313:GLU:OE2	2.21	0.41
3:C:243:PRO:HB3	3:C:264:MET:SD	2.61	0.41
3:C:338:LYS:HG2	3:C:338:LYS:O	2.21	0.41
2:E:253:GLN:HE21	2:E:253:GLN:C	2.23	0.41
2:E:199:VAL:HG23	3:F:141:ASP:HA	2.03	0.41
3:C:103:HIS:C	3:C:105:SER:H	2.21	0.41
3:F:107:ILE:O	3:F:108:ARG:C	2.58	0.41
3:F:195:GLN:OE1	3:F:195:GLN:C	2.59	0.41
3:F:365:ASN:ND2	3:F:365:ASN:C	2.74	0.41
2:B:253:GLN:NE2	2:B:451:SER:HA	2.36	0.41
2:B:244:THR:HG21	2:B:313:GLU:OE2	2.21	0.41
2:E:303:THR:HB	2:E:330:THR:HA	2.03	0.41
3:F:334:TRP:CG	3:F:335:TRP:N	2.89	0.41
3:C:298:ASP:OD2	3:C:299:PRO:HD2	2.21	0.41
3:F:350:GLN:C	3:F:352:GLY:H	2.25	0.41
2:E:191:GLU:O	2:E:194:ARG:HG3	2.20	0.41
2:E:331:VAL:HG13	2:E:338:TYR:O	2.21	0.40
1:D:179:GLU:O	1:D:182:GLN:N	2.55	0.40
3:F:109:TYR:O	3:F:112:GLU:HB2	2.21	0.40
3:F:173:LYS:HB2	3:F:173:LYS:HE3	1.85	0.40
2:E:172:LEU:CD1	3:F:110:LEU:HB3	2.51	0.40
3:F:347:VAL:HB	3:F:349:TYR:HE1	1.86	0.40
2:B:206:VAL:HG22	2:B:207:SER:N	2.36	0.40
3:C:293:PHE:HD1	3:C:295:PHE:CD2	2.39	0.40
2:E:167:VAL:O	2:E:171:ILE:HG13	2.21	0.40
1:D:129:LYS:O	1:D:130:VAL:C	2.60	0.40
3:F:145:ILE:HG23	3:F:166:LEU:O	2.22	0.40
3:F:314:THR:O	3:F:317:ASN:N	2.53	0.40
2:E:225:TYR:HD2	2:E:240:CYS:HB2	1.87	0.40
2:B:223:GLU:HA	2:B:239:TYR:CE2	2.57	0.40
3:F:307:HIS:HE1	3:F:342:GLY:H	1.69	0.40
2:E:284:ASN:N	2:E:284:ASN:ND2	2.68	0.40
2:E:257:ASP:O	2:E:291:GLU:OE2	2.39	0.40
2:E:422:TYR:O	2:E:444:TRP:HB3	2.22	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	68/87 (78%)	52 (76%)	13 (19%)	3 (4%)	3 6
1	D	68/87 (78%)	58 (85%)	4 (6%)	6 (9%)	1 1
2	B	300/328 (92%)	248 (83%)	47 (16%)	5 (2%)	11 29
2	E	300/328 (92%)	249 (83%)	45 (15%)	6 (2%)	9 24
3	C	288/323 (89%)	247 (86%)	31 (11%)	10 (4%)	4 10
3	F	288/323 (89%)	243 (84%)	35 (12%)	10 (4%)	4 10
4	I	3/5 (60%)	3 (100%)	0	0	100 100
4	J	3/5 (60%)	1 (33%)	2 (67%)	0	100 100
All	All	1318/1486 (89%)	1101 (84%)	177 (13%)	40 (3%)	5 13

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ALA
2	B	281	ASP
2	B	295	GLY
1	D	127	ILE
1	D	130	VAL
1	D	166	SER
2	E	281	ASP
3	F	370	ALA
3	C	370	ALA
2	E	160	ASN
2	E	295	GLY
2	E	398	ASP
2	E	435	VAL
3	F	104	ASP
3	F	317	ASN
1	A	176	LYS
2	B	435	VAL

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Mol	Chain	Res	Type
3	C	135	CYS
3	C	239	GLN
3	C	390	ASN
1	D	131	GLN
3	F	119	GLN
3	F	187	SER
3	F	239	GLN
3	F	241	ALA
2	B	398	ASP
3	C	187	SER
3	C	241	ALA
3	C	294	ASP
1	D	194	LEU
2	E	439	ASN
3	F	390	ASN
3	C	107	ILE
3	C	317	ASN
1	D	192	ASP
3	F	118	ASN
1	A	194	LEU
2	B	406	ARG
3	C	298	ASP
3	F	298	ASP

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	65/82 (79%)	58 (89%)	7 (11%)	8 18
1	D	65/82 (79%)	57 (88%)	8 (12%)	6 14
2	B	260/286 (91%)	243 (94%)	17 (6%)	21 46
2	E	260/286 (91%)	244 (94%)	16 (6%)	23 49
3	C	244/269 (91%)	226 (93%)	18 (7%)	17 39
3	F	244/269 (91%)	228 (93%)	16 (7%)	21 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	I	3/3 (100%)	3 (100%)	0	100 100
4	J	3/3 (100%)	3 (100%)	0	100 100
All	All	1144/1280 (89%)	1062 (93%)	82 (7%)	18 41

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	141	ARG
1	A	144	LEU
1	A	172	GLU
1	A	180	ASP
1	A	185	LEU
1	A	191	LYS
2	B	160	ASN
2	B	165	LEU
2	B	166	ARG
2	B	172	LEU
2	B	174	ASN
2	B	210	GLU
2	B	252	ILE
2	B	253	GLN
2	B	271	GLN
2	B	284	ASN
2	B	301	GLN
2	B	302	LEU
2	B	330	THR
2	B	351	ASN
2	B	355	ASP
2	B	360	LEU
2	B	439	ASN
3	C	114	TYR
3	C	115	ASN
3	C	117	ASN
3	C	120	LYS
3	C	124	LEU
3	C	126	GLU
3	C	130	GLN
3	C	183	GLU
3	C	192	THR
3	C	198	LEU

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Mol	Chain	Res	Type
3	C	264	MET
3	C	317	ASN
3	C	323	GLU
3	C	325	ASN
3	C	365	ASN
3	C	382	THR
3	C	383	THR
3	C	390	ASN
1	D	129	LYS
1	D	131	GLN
1	D	135	LEU
1	D	144	LEU
1	D	167	ARG
1	D	169	LEU
1	D	175	LEU
1	D	176	LYS
2	E	158	ASN
2	E	168	LEU
2	E	191	GLU
2	E	210	GLU
2	E	252	ILE
2	E	253	GLN
2	E	271	GLN
2	E	284	ASN
2	E	301	GLN
2	E	302	LEU
2	E	330	THR
2	E	351	ASN
2	E	355	ASP
2	E	360	LEU
2	E	439	ASN
2	E	458	PHE
3	F	111	GLN
3	F	116	SER
3	F	119	GLN
3	F	137	GLU
3	F	167	TYR
3	F	183	GLU
3	F	192	THR
3	F	198	LEU
3	F	264	MET
3	F	317	ASN

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Mol	Chain	Res	Type
3	F	323	GLU
3	F	325	ASN
3	F	365	ASN
3	F	382	THR
3	F	383	THR
3	F	390	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	132	HIS
1	A	134	GLN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
2	B	158	ASN
2	B	174	ASN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	339	GLN
2	B	343	ASN
2	B	351	ASN
2	B	359	GLN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	117	ASN
3	C	123	ASN
3	C	134	GLN
3	C	177	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	350	GLN

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Mol	Chain	Res	Type
3	C	365	ASN
1	D	131	GLN
1	D	132	HIS
1	D	137	GLN
1	D	187	GLN
2	E	158	ASN
2	E	174	ASN
2	E	189	GLN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	115	ASN
3	F	117	ASN
3	F	123	ASN
3	F	134	GLN
3	F	176	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	340	HIS
3	F	350	GLN
3	F	365	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	470	2,5	14,14,15	0.81	0	15,19,21	0.95	1 (6%)
5	NAG	B	471	5	14,14,15	0.85	1 (7%)	15,19,21	0.78	0
6	NAG	E	470	2,6	14,14,15	0.78	0	15,19,21	1.20	3 (20%)
6	NDG	E	471	6	14,14,15	0.73	1 (7%)	15,19,21	0.77	1 (6%)

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
5	NAG	B	470	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	471	5	-	0/6/23/26	0/1/1/1
6	NAG	E	470	2,6	-	0/6/23/26	0/1/1/1
6	NDG	E	471	6	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	471	NDG	C1-C2	2.05	1.55	1.52
5	B	471	NAG	C1-C2	2.30	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	470	NAG	C2-N2-C7	-2.78	119.46	123.04
6	E	470	NAG	C4-C3-C2	-2.55	107.26	111.23
5	B	470	NAG	C2-N2-C7	-2.18	120.24	123.04
6	E	471	NDG	C2-N2-C7	-2.17	120.25	123.04
6	E	470	NAG	C1-O5-C5	2.11	114.93	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	471	NDG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	3	0
5	B	471	NAG	3	0
6	E	470	NAG	1	0

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	70/87 (80%)	-0.22	4 (5%) 27 26	37, 65, 114, 146	0
1	D	70/87 (80%)	0.10	4 (5%) 27 26	38, 64, 122, 162	0
2	B	302/328 (92%)	-0.16	4 (1%) 79 79	29, 51, 87, 115	0
2	E	302/328 (92%)	-0.08	5 (1%) 73 74	30, 61, 91, 111	0
3	C	290/323 (89%)	-0.11	2 (0%) 89 90	36, 62, 92, 112	0
3	F	290/323 (89%)	0.16	6 (2%) 67 68	38, 66, 97, 131	0
4	I	4/5 (80%)	0.35	0 100 100	56, 61, 65, 76	0
4	J	4/5 (80%)	-0.16	0 100 100	61, 65, 68, 81	0
All	All	1332/1486 (89%)	-0.05	25 (1%) 70 70	29, 61, 95, 162	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	ILE	9.8
3	F	172	LEU	4.6
3	F	358	SER	4.1
1	A	195	PRO	3.8
1	D	194	LEU	3.8
1	A	194	LEU	3.5
2	E	361	MET	3.5
2	B	458	PHE	3.3
3	F	240	SER	3.2
3	C	240	SER	3.2
2	E	307	PRO	3.1
3	F	342	GLY	3.0
2	E	231	SER	3.0
3	F	186	GLY	2.9
3	F	255	GLY	2.8
1	A	128	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	392	LEU	2.5
2	B	361	MET	2.4
1	D	126	VAL	2.4
1	D	192	ASP	2.4
2	E	458	PHE	2.3
1	A	193	LEU	2.2
2	B	158	ASN	2.2
2	B	386	LEU	2.2
2	E	413	ASN	2.1

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

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

6.3 Carbohydrates (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	B	470	14/15	0.87	0.28	1.20	103,108,111,113	0
6	NAG	E	470	14/15	0.90	0.21	-0.81	69,89,98,100	0
6	NDG	E	471	14/15	0.89	0.27	-	73,99,110,113	0
5	NAG	B	471	14/15	0.75	0.34	-	90,107,115,116	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	CA	B	2	1/1	0.94	0.22	0.20	52,52,52,52	0
7	CA	E	2	1/1	0.96	0.16	-0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	CA	C	1	1/1	0.94	0.14	-0.69	60,60,60,60	0
7	CA	F	1	1/1	0.94	0.08	-2.06	62,62,62,62	0
7	CA	E	3	1/1	0.71	0.20	-	111,111,111,111	0
7	CA	B	3	1/1	0.76	0.29	-	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.