Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:04 AM EDT

PDB ID	:	6JLY
Title	:	eIF2a - eIF2B complex
Authors	:	Kashiwagi, K.; Ito, T.
Deposited on	:	2019-03-07
Resolution	:	3.50 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:

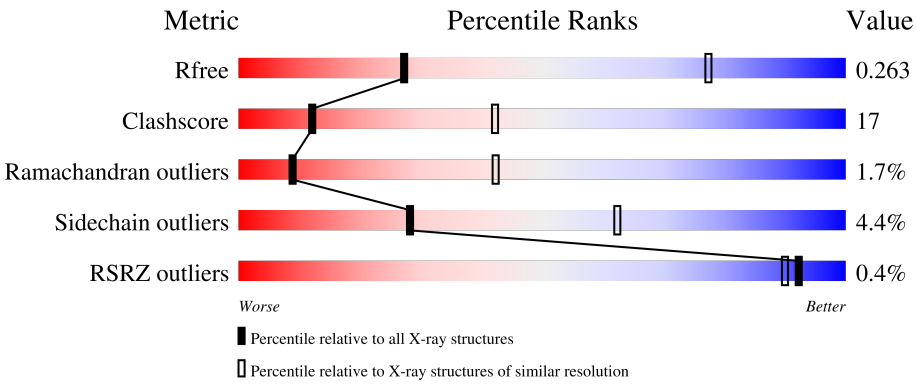
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 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	341	52% 40% • 7%
1	B	341	% 51% 40% • 7%
2	C	399	50% 33% • 15%
2	D	399	54% 29% • 16%
3	E	458	% 50% 37% • 10%

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Mol	Chain	Length	Quality of chain
3	F	458	51% 36% • 10%
4	G	467	49% 26% • 22%
4	H	467	% 48% 28% • 22%
5	I	678	38% 24% • 37%
5	J	678	39% 23% • 37%
6	L	304	% 30% 24% 46%
6	M	304	31% 23% • 45%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31811 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2467	1568	431	455	13	0	0	0
1	B	316	2465	1566	429	457	13	0	0	0

- Molecule 2 is a protein called Probable translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	338	2617	1660	443	502	12	0	0	0
2	D	337	2609	1654	442	501	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q9UT76
C	-4	PRO	-	expression tag	UNP Q9UT76
C	-3	ILE	-	expression tag	UNP Q9UT76
C	-2	SER	-	expression tag	UNP Q9UT76
C	-1	GLU	-	expression tag	UNP Q9UT76
C	0	PHE	-	expression tag	UNP Q9UT76
D	-5	GLY	-	expression tag	UNP Q9UT76
D	-4	PRO	-	expression tag	UNP Q9UT76
D	-3	ILE	-	expression tag	UNP Q9UT76
D	-2	SER	-	expression tag	UNP Q9UT76
D	-1	GLU	-	expression tag	UNP Q9UT76
D	0	PHE	-	expression tag	UNP Q9UT76

- Molecule 3 is a protein called Probable translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	414	3216	2040	555	604	17	0	0	0
3	F	412	3204	2034	553	600	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	157	TYR	ILE	conflict	UNP P56288
E	158	THR	TYR	conflict	UNP P56288
E	159	VAL	GLY	conflict	UNP P56288
F	157	TYR	ILE	conflict	UNP P56288
F	158	THR	TYR	conflict	UNP P56288
F	159	VAL	GLY	conflict	UNP P56288

- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	363	2869	1834	486	536	13	0	0	0
4	H	363	2869	1834	486	536	13	0	0	0

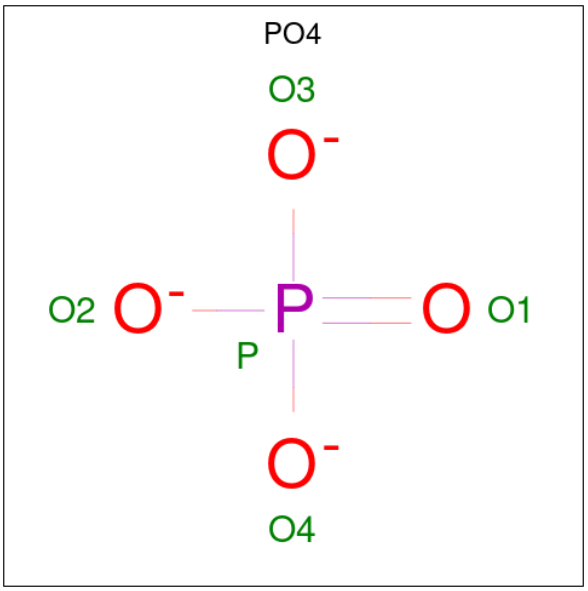
- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	I	428	3377	2123	592	647	15	0	0	0
5	J	426	3362	2115	587	645	15	0	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	165	1353	863	226	258	6	0	0	0
6	M	166	1363	872	227	258	6	0	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



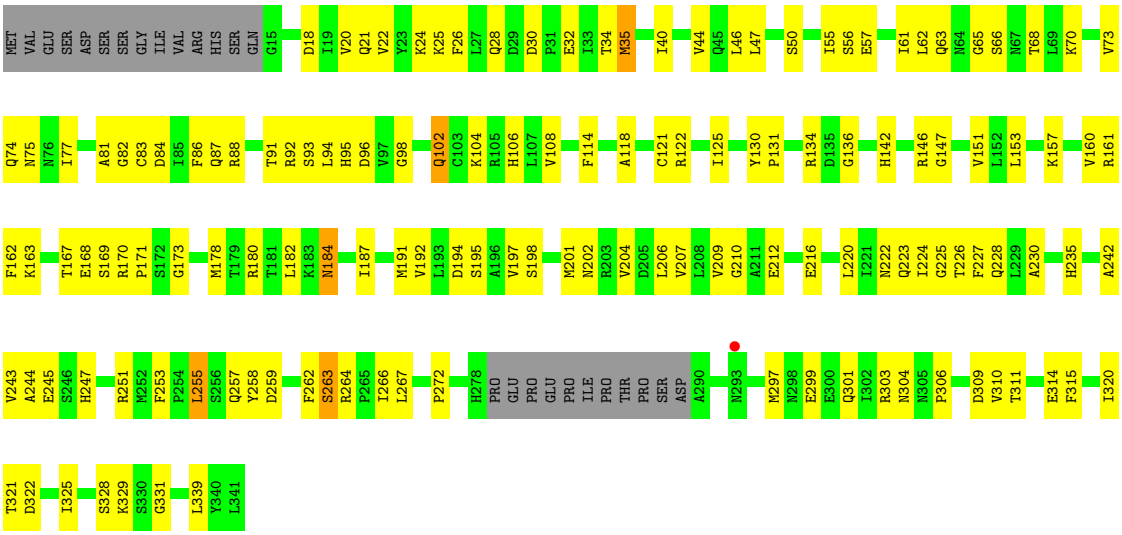
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	C	1	5	4	1	0	0
7	D	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	F	1	5	4	1	0	0
7	F	1	5	4	1	0	0
7	G	1	5	4	1	0	0
7	H	1	5	4	1	0	0

3 Residue-property plots (i)

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

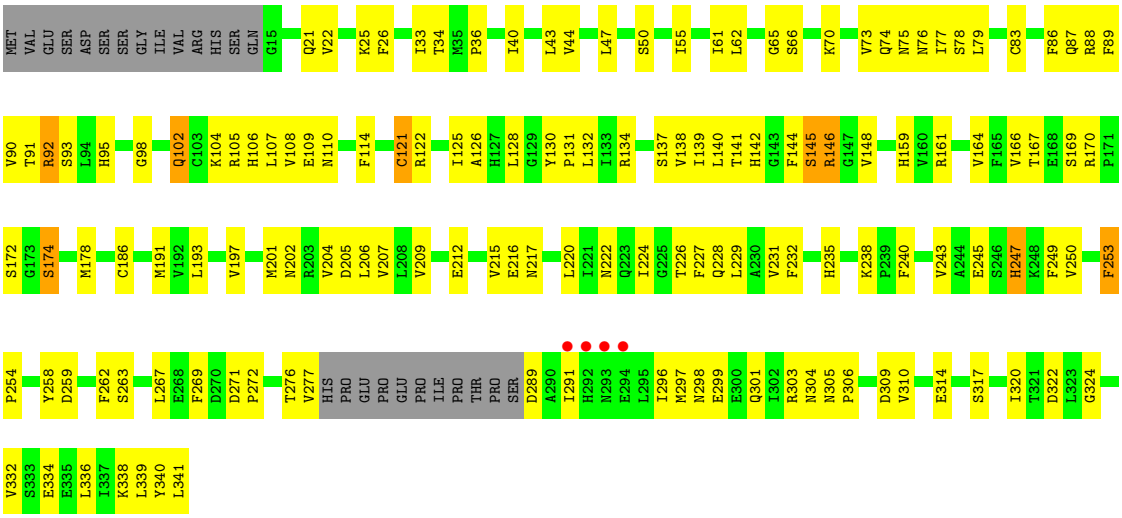
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A: 52% 40% • 7%



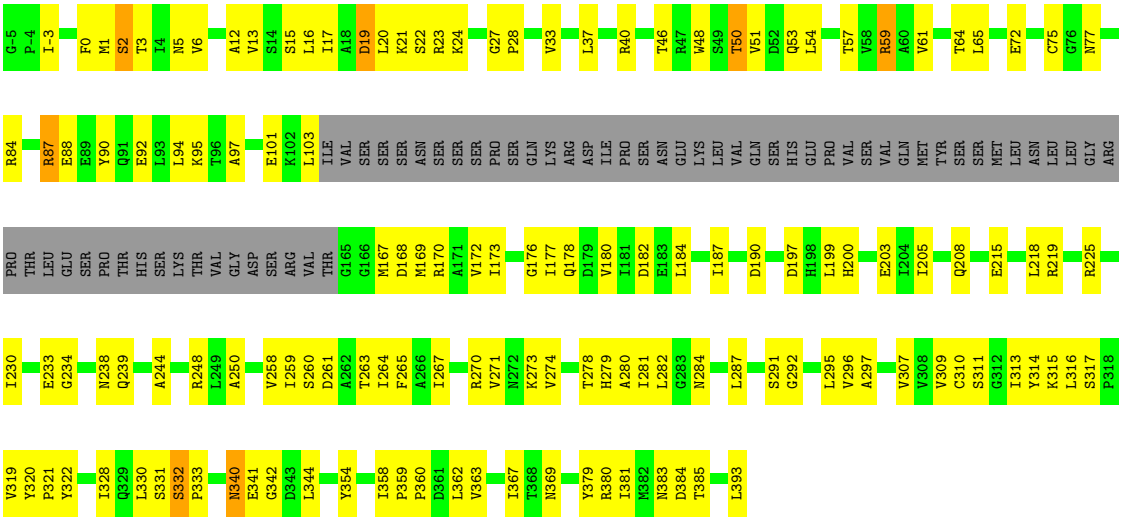
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B: % 51% 40% • 7%



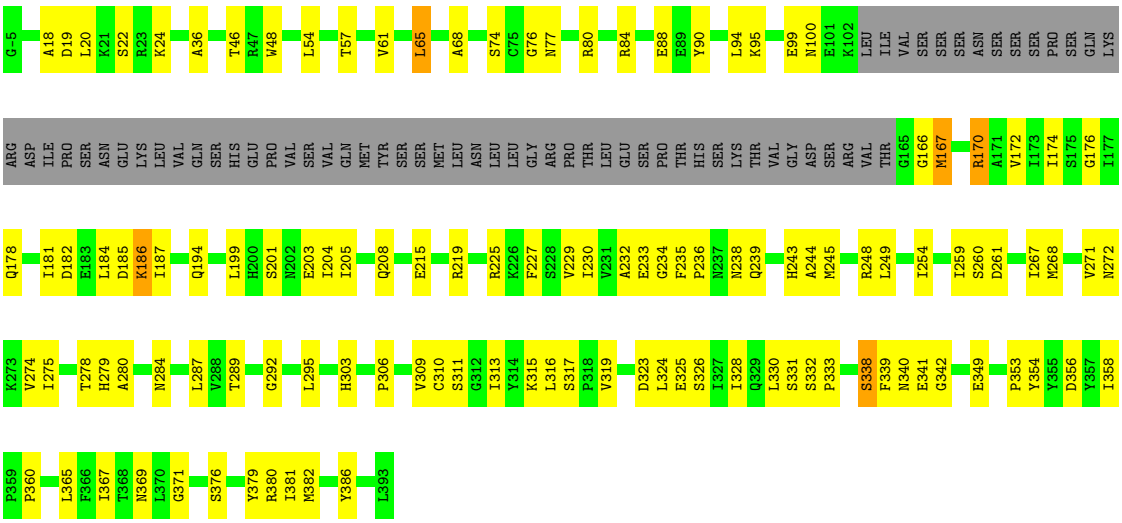
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta

Chain C: 50% 33% • 15%



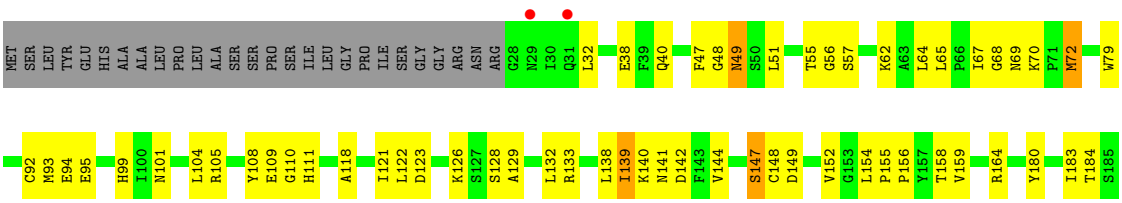
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta

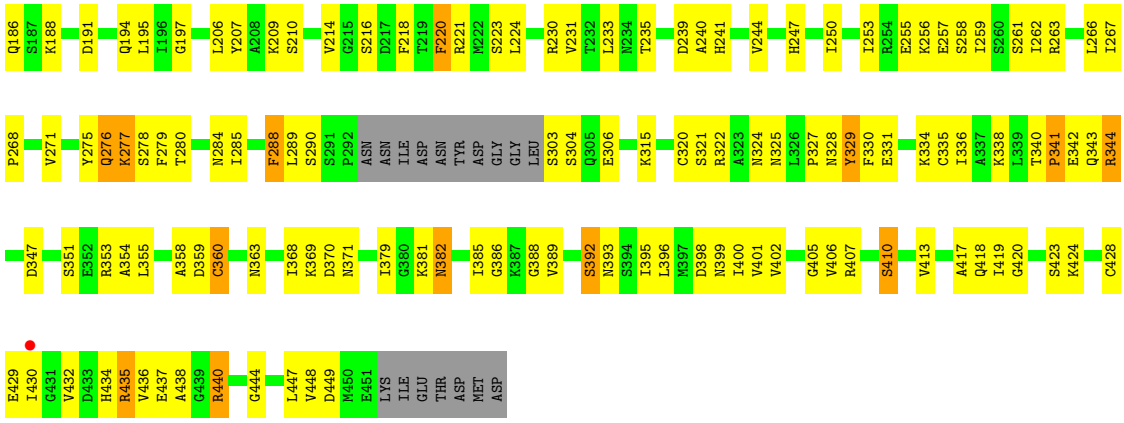
Chain D: 54% 29% • 16%



• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

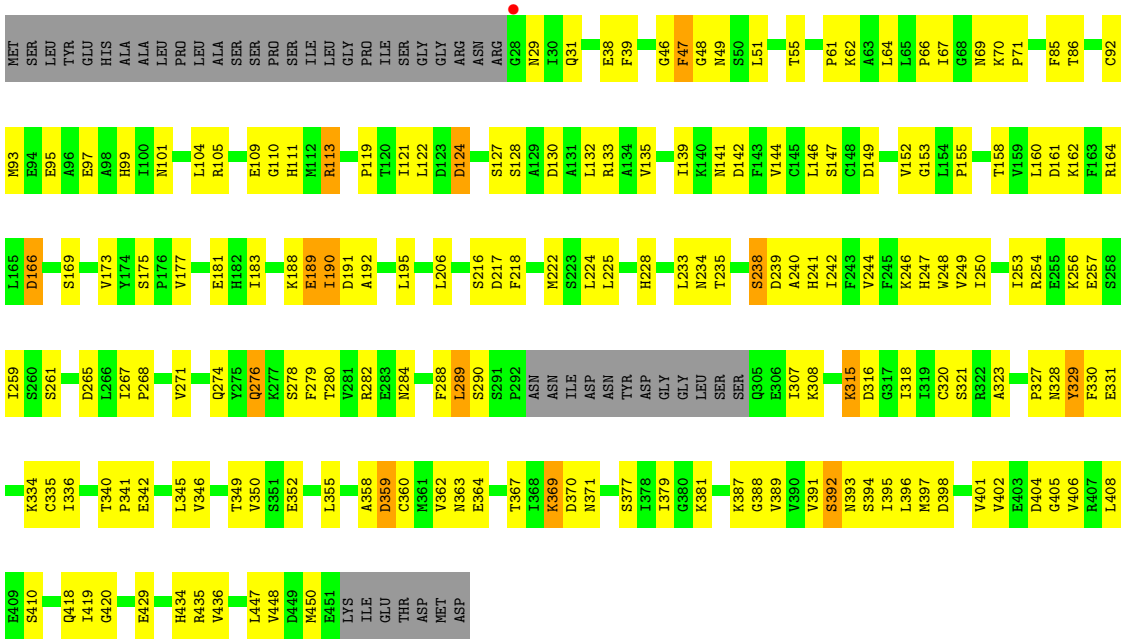
Chain E: % 50% 37% • 10%





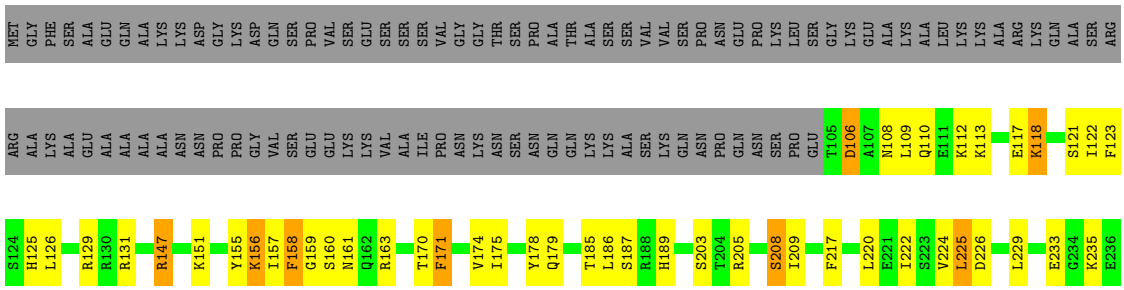
• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

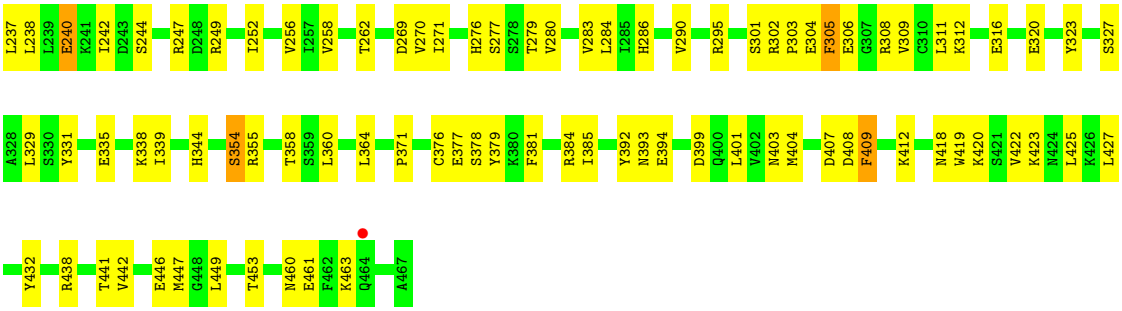
Chain F: 51% 36% • 10%



• Molecule 4: Probable translation initiation factor eIF-2B subunit delta

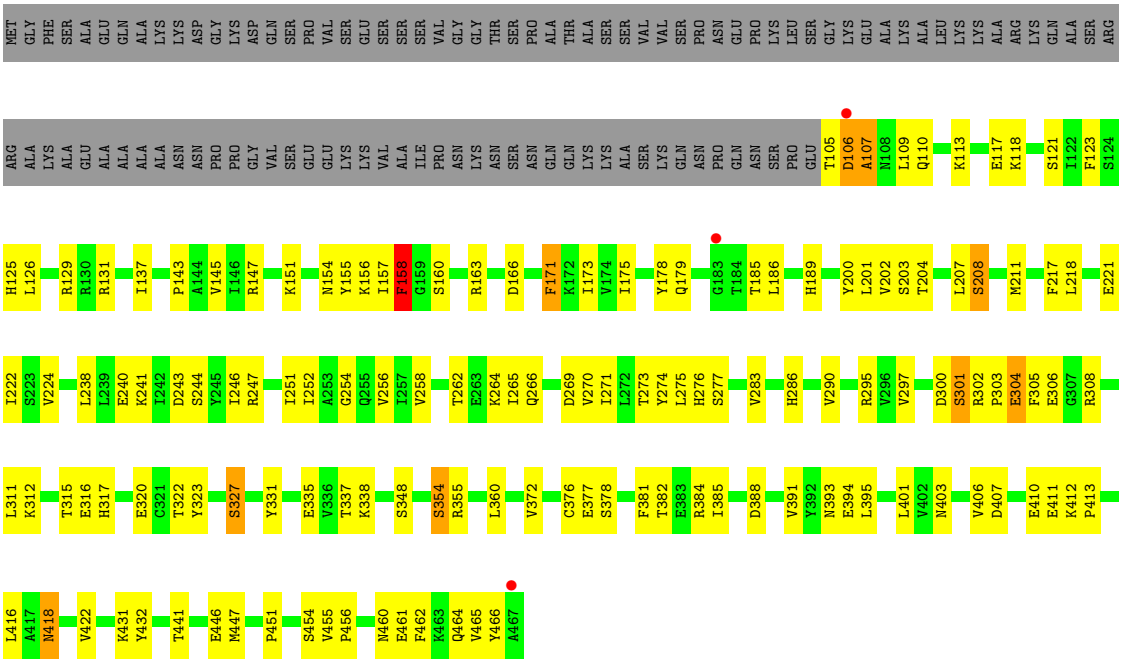
Chain G: 49% 26% • 22%





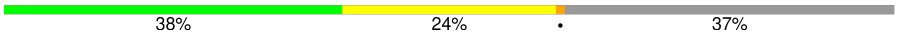
- Molecule 4: Probable translation initiation factor eIF-2B subunit delta

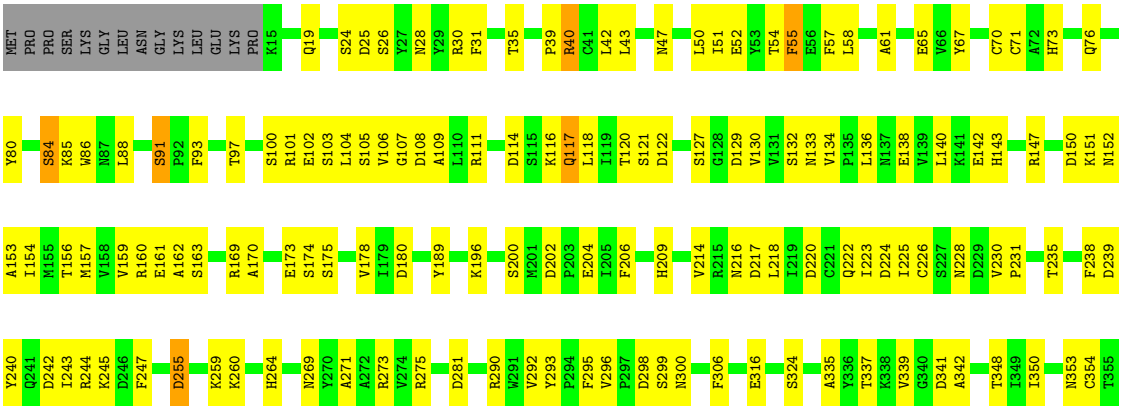
Chain H:

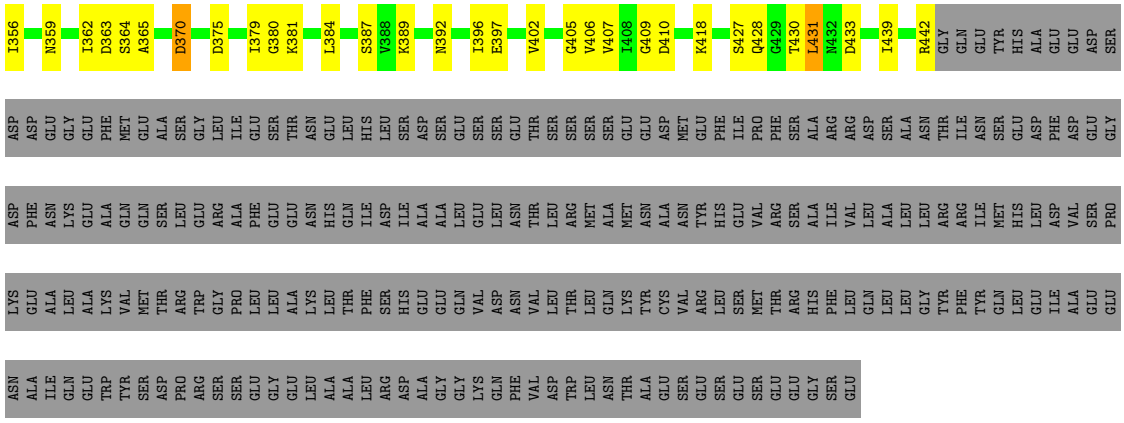


- Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon

Chain I:

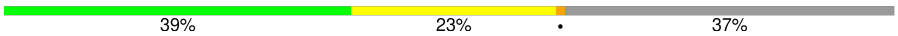


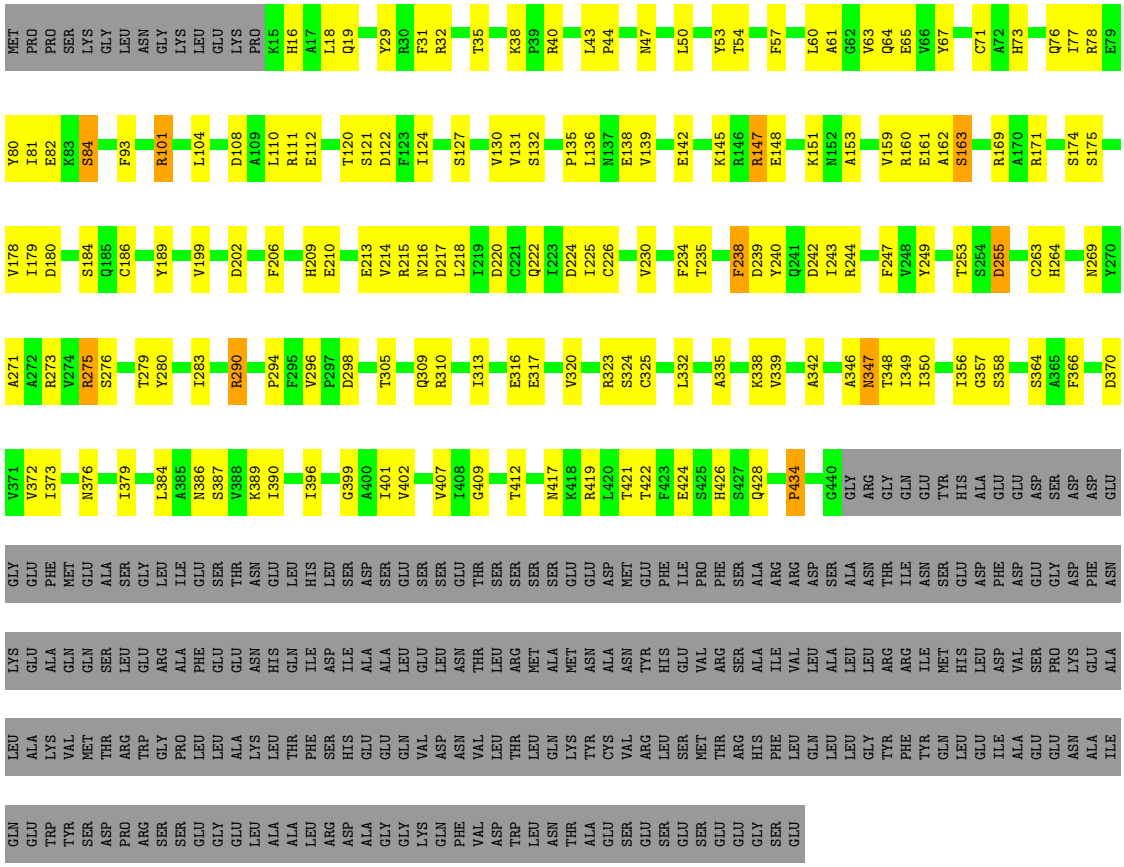




• Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon

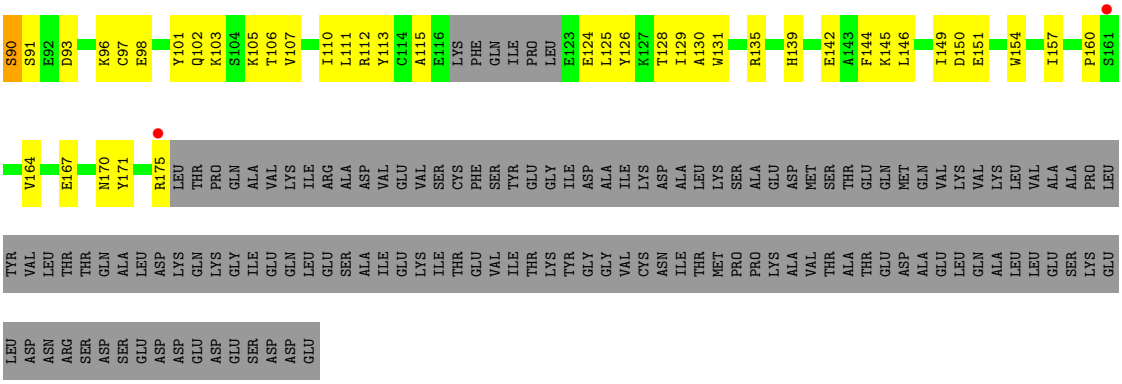
Chain J:





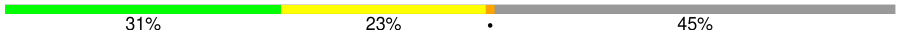
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

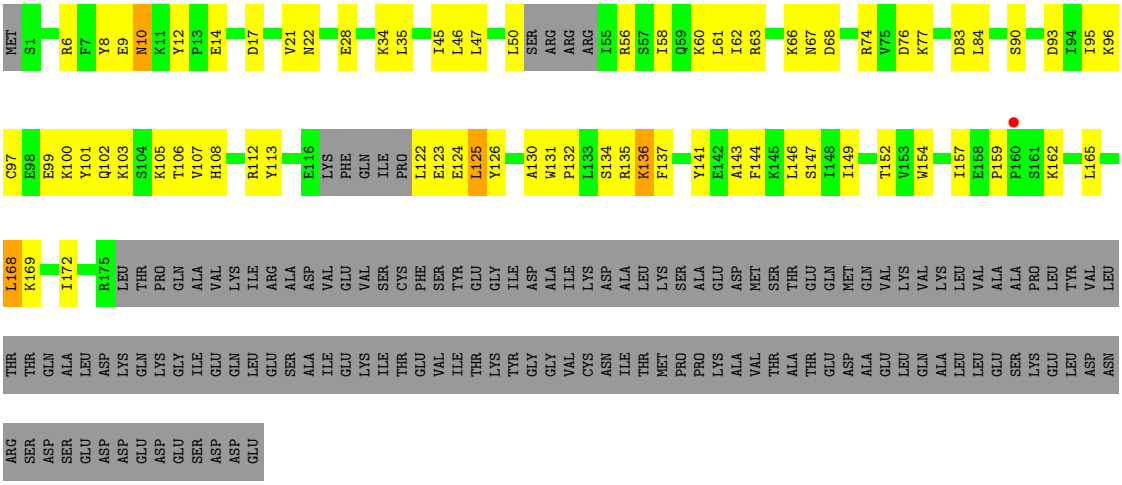
Chain L:



- Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	155.56Å 207.99Å 155.59Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	49.31 – 3.50 49.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.31-3.50) 88.8 (49.31-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.53 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.224 , 0.260 0.227 , 0.263	Depositor DCC
R_{free} test set	1979 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å^2)	122.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.380 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31811	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.28	0/2513	0.44	0/3399
1	B	0.28	0/2510	0.43	0/3395
2	C	0.30	0/2661	0.43	0/3611
2	D	0.30	0/2653	0.44	0/3600
3	E	0.30	0/3272	0.48	0/4427
3	F	0.29	0/3260	0.49	0/4411
4	G	0.31	0/2917	0.45	0/3951
4	H	0.31	0/2917	0.44	0/3951
5	I	0.29	0/3437	0.45	0/4658
5	J	0.29	0/3422	0.47	0/4639
6	L	0.27	0/1374	0.42	0/1845
6	M	0.26	0/1384	0.44	0/1859
All	All	0.29	0/32320	0.45	0/43746

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2467	0	2490	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2465	0	2487	111	0
2	C	2617	0	2653	102	0
2	D	2609	0	2642	83	0
3	E	3216	0	3273	131	0
3	F	3204	0	3263	116	0
4	G	2869	0	2958	90	0
4	H	2869	0	2958	85	0
5	I	3377	0	3361	134	0
5	J	3362	0	3345	121	0
6	L	1353	0	1374	51	0
6	M	1363	0	1391	48	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	1	0
7	F	10	0	0	0	0
7	G	5	0	0	1	0
7	H	5	0	0	1	0
All	All	31811	0	32195	1094	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 17.

All (1094) 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)
4:H:126:LEU:HB3	4:H:395:LEU:HD11	1.55	0.89
3:E:139:ILE:HG12	3:E:250:ILE:HG12	1.56	0.87
5:I:143:HIS:HD1	5:I:156:THR:HG1	1.21	0.83
5:J:101:ARG:H	5:J:101:ARG:HD3	1.44	0.83
3:E:402:VAL:HG23	3:E:419:ILE:HD11	1.62	0.81
1:B:222:ASN:HB3	1:B:226:THR:HG21	1.63	0.81
3:F:355:LEU:HD11	3:F:370:ASP:HA	1.63	0.80
5:J:290:ARG:NH2	5:J:298:ASP:OD2	2.14	0.80
4:G:161:ASN:OD1	4:G:379:TYR:OH	2.01	0.79
3:F:173:VAL:HG23	3:F:318:ILE:HG23	1.64	0.79
5:J:130:VAL:HG12	5:J:273:ARG:HB3	1.64	0.79
5:I:101:ARG:NH2	5:I:108:ASP:OD2	2.17	0.77
5:I:169:ARG:NH1	5:I:218:LEU:O	2.18	0.77
1:B:140:LEU:HB3	1:B:207:VAL:HG23	1.68	0.76
3:E:368:ILE:HG22	3:E:385:ILE:HB	1.68	0.76
3:F:133:ARG:NH1	3:F:253:ILE:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:152:VAL:HG11	3:F:242:ILE:HD11	1.68	0.76
3:F:97:GLU:O	3:F:101:ASN:ND2	2.19	0.75
1:B:95:HIS:O	1:B:102:GLN:NE2	2.19	0.75
3:F:195:LEU:HD11	3:F:233:LEU:HD12	1.68	0.74
4:G:399:ASP:OD2	4:G:420:LYS:NZ	2.20	0.74
5:I:348:THR:HG21	5:I:362:ILE:HG22	1.69	0.74
3:E:336:ILE:HD12	3:E:395:ILE:HD13	1.68	0.73
5:J:372:VAL:HG22	5:J:389:LYS:HA	1.71	0.73
5:J:169:ARG:NH2	5:J:216:ASN:OD1	2.22	0.73
6:L:6:ARG:NH1	6:L:8:TYR:O	2.22	0.73
3:E:209:LYS:NZ	3:E:210:SER:O	2.21	0.73
4:G:295:ARG:NH2	4:G:335:GLU:OE1	2.22	0.73
2:C:2:SER:H	2:C:5:ASN:HD21	1.37	0.73
2:C:59:ARG:NH2	2:C:393:LEU:O	2.21	0.73
3:F:181:GLU:H	3:F:334:LYS:HE2	1.54	0.73
2:D:338:SER:OG	2:D:340:ASN:ND2	2.22	0.72
4:H:393:ASN:ND2	4:H:432:TYR:O	2.22	0.72
6:L:49:GLU:HG2	6:L:86:LYS:H	1.55	0.72
4:G:302:ARG:NH2	4:G:403:ASN:O	2.22	0.72
1:A:267:LEU:HD21	1:A:306:PRO:HD3	1.72	0.72
5:J:127:SER:HB2	5:J:273:ARG:HH12	1.56	0.71
5:J:19:GLN:OE1	5:J:120:THR:N	2.23	0.71
1:A:46:LEU:O	1:A:50:SER:OG	2.07	0.71
2:C:330:LEU:HB2	5:I:290:ARG:HH11	1.55	0.71
1:B:215:VAL:HG11	1:B:254:PRO:HD3	1.73	0.70
4:H:107:ALA:HB3	4:H:109:LEU:HG	1.72	0.70
6:L:63:ARG:HD3	6:L:66:LYS:HD3	1.73	0.70
3:E:133:ARG:NH1	3:E:256:LYS:O	2.22	0.69
3:F:329:TYR:OH	3:F:429:GLU:OE2	2.10	0.69
1:A:297:MET:HB3	1:A:301:GLN:HG3	1.73	0.69
5:I:28:ASN:HD21	5:I:35:THR:HG21	1.57	0.69
1:B:204:VAL:O	1:B:238:LYS:NZ	2.24	0.69
1:B:142:HIS:HB2	1:B:229:LEU:HD21	1.73	0.69
3:E:186:GLN:HB3	3:E:188:LYS:HE2	1.75	0.69
3:E:392:SER:OG	3:E:393:ASN:OD1	2.11	0.69
4:G:178:TYR:O	4:G:235:LYS:NZ	2.22	0.69
5:J:222:GLN:OE1	5:J:273:ARG:NH1	2.25	0.69
2:D:380:ARG:NH2	4:G:461:GLU:OE1	2.25	0.69
5:I:169:ARG:NH2	5:I:216:ASN:OD1	2.26	0.69
2:C:234:GLY:HA3	2:C:238:ASN:HB2	1.75	0.69
2:C:341:GLU:HB3	2:C:344:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:154:LEU:HD12	3:E:155:PRO:HD2	1.75	0.69
3:E:438:ALA:O	3:E:440:ARG:NH2	2.26	0.69
4:H:403:ASN:ND2	4:H:407:ASP:O	2.26	0.69
3:E:191:ASP:OD1	3:E:328:ASN:ND2	2.26	0.69
4:G:393:ASN:ND2	4:G:432:TYR:O	2.26	0.69
5:I:157:MET:SD	5:I:244:ARG:NH1	2.66	0.69
6:L:7:PHE:O	6:L:131:TRP:NE1	2.20	0.69
3:E:340:THR:O	3:E:342:GLU:N	2.26	0.68
4:G:178:TYR:HH	4:G:189:HIS:HD1	1.40	0.68
5:J:159:VAL:HB	5:J:218:LEU:HD12	1.75	0.68
4:H:295:ARG:NH2	4:H:335:GLU:OE1	2.26	0.68
5:I:114:ASP:HB3	5:I:231:PRO:HB2	1.74	0.68
5:I:19:GLN:NE2	5:I:118:LEU:O	2.25	0.68
2:C:380:ARG:NH2	4:H:461:GLU:OE1	2.20	0.68
1:B:88:ARG:NH2	6:L:28:GLU:OE1	2.26	0.68
5:I:127:SER:O	5:I:273:ARG:NH1	2.26	0.68
1:A:92:ARG:NH2	1:A:339:LEU:O	2.26	0.67
1:A:95:HIS:O	1:A:102:GLN:NE2	2.27	0.67
3:E:382:ASN:ND2	3:E:399:ASN:OD1	2.25	0.67
4:H:355:ARG:NH1	4:H:431:LYS:O	2.28	0.67
3:E:129:ALA:H	3:E:261:SER:HA	1.59	0.67
6:M:157:ILE:HG22	6:M:159:PRO:HD3	1.75	0.67
2:C:203:GLU:OE2	2:C:273:LYS:NZ	2.28	0.67
5:I:156:THR:HB	5:I:225:ILE:HB	1.77	0.67
3:F:284:ASN:HB2	3:F:288:PHE:HE2	1.58	0.67
3:E:147:SER:OG	3:E:149:ASP:OD1	2.10	0.67
2:C:184:LEU:HA	2:C:187:ILE:HG13	1.76	0.67
3:F:70:LYS:NZ	3:F:109:GLU:OE2	2.28	0.67
6:M:22:ASN:ND2	6:M:67:ASN:OD1	2.25	0.67
4:G:441:THR:HG23	4:G:442:VAL:HG12	1.75	0.66
4:G:302:ARG:NH2	4:G:401:LEU:O	2.28	0.66
3:F:336:ILE:HD12	3:F:395:ILE:HD13	1.76	0.66
6:M:136:LYS:NZ	6:M:152:THR:O	2.29	0.66
2:C:330:LEU:O	5:I:290:ARG:NH1	2.29	0.66
4:G:270:VAL:HG12	4:G:295:ARG:HG2	1.77	0.66
6:M:93:ASP:HA	6:M:96:LYS:HB2	1.78	0.66
5:J:309:GLN:HB2	5:J:313:ILE:HG13	1.78	0.66
1:B:55:ILE:N	6:L:83:ASP:OD2	2.29	0.66
1:B:90:VAL:HG11	1:B:107:LEU:HG	1.77	0.66
5:J:339:VAL:HA	5:J:356:ILE:HB	1.78	0.66
1:B:267:LEU:HD21	1:B:306:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:178:TYR:OH	4:G:189:HIS:ND1	2.23	0.66
5:J:169:ARG:NH1	5:J:218:LEU:O	2.29	0.65
5:J:161:GLU:OE2	5:J:215:ARG:NH2	2.29	0.65
3:E:324:ASN:O	3:E:325:ASN:ND2	2.29	0.65
5:J:147:ARG:NH1	5:J:153:ALA:O	2.30	0.65
1:B:276:THR:OG1	1:B:277:VAL:N	2.30	0.65
6:M:102:GLN:HA	6:M:105:LYS:HB3	1.78	0.65
3:E:355:LEU:HD23	3:E:370:ASP:HA	1.77	0.65
5:I:348:THR:HG22	5:I:365:ALA:H	1.62	0.65
5:I:296:VAL:O	5:I:299:SER:OG	2.15	0.65
5:J:61:ALA:HB2	5:J:136:LEU:HD23	1.78	0.65
6:L:126:TYR:HA	6:L:130:ALA:HB3	1.79	0.65
5:J:175:SER:HB3	5:J:189:TYR:HE1	1.62	0.64
2:D:330:LEU:O	5:J:290:ARG:NH1	2.30	0.64
5:I:427:SER:OG	5:I:428:GLN:N	2.30	0.64
6:M:125:LEU:H	6:M:125:LEU:HD23	1.61	0.64
3:E:155:PRO:O	3:E:158:THR:OG1	2.15	0.64
4:H:354:SER:OG	4:H:355:ARG:N	2.31	0.64
2:D:205:ILE:HB	2:D:229:VAL:HG22	1.79	0.64
3:F:420:GLY:N	3:F:436:VAL:O	2.30	0.64
3:E:389:VAL:HG23	3:E:406:VAL:HG12	1.80	0.64
5:I:114:ASP:O	5:I:117:GLN:NE2	2.31	0.64
6:M:102:GLN:O	6:M:106:THR:OG1	2.14	0.64
1:A:66:SER:O	1:A:70:LYS:N	2.26	0.63
3:F:191:ASP:OD1	3:F:328:ASN:ND2	2.31	0.63
6:M:45:ILE:HG22	6:M:84:LEU:HB2	1.80	0.63
2:C:17:ILE:HG22	2:C:21:LYS:HD2	1.79	0.63
4:G:209:ILE:HD11	4:G:384:ARG:HH21	1.63	0.63
6:M:165:LEU:HD21	6:M:168:LEU:HD22	1.80	0.63
3:E:340:THR:H	3:E:341:PRO:HD2	1.63	0.63
4:G:131:ARG:NH1	4:G:203:SER:OG	2.31	0.63
2:C:77:ASN:ND2	2:C:316:LEU:O	2.31	0.63
2:D:340:ASN:O	2:D:342:GLY:N	2.31	0.63
3:E:231:VAL:HG23	5:J:214:VAL:HB	1.80	0.63
3:F:217:ASP:HB3	5:I:200:SER:HB2	1.79	0.63
3:F:389:VAL:HG13	3:F:406:VAL:HG22	1.79	0.63
5:J:18:LEU:HD12	5:J:63:VAL:HA	1.81	0.62
1:B:40:ILE:HD13	1:B:114:PHE:HE2	1.63	0.62
4:H:302:ARG:NH2	4:H:401:LEU:O	2.31	0.62
6:L:90:SER:OG	6:L:91:SER:N	2.32	0.62
3:F:239:ASP:OD1	3:F:240:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:393:ASN:OD1	4:H:394:GLU:N	2.31	0.62
5:J:160:ARG:NH2	5:J:269:ASN:O	2.28	0.62
1:B:121:CYS:SG	1:B:122:ARG:N	2.73	0.62
5:I:409:GLY:H	5:I:433:ASP:HA	1.65	0.62
2:D:77:ASN:ND2	2:D:316:LEU:O	2.33	0.62
4:H:240:GLU:OE2	4:H:244:SER:OG	2.18	0.62
5:I:439:ILE:HG21	5:I:442:ARG:HB2	1.79	0.62
5:I:28:ASN:O	5:I:28:ASN:ND2	2.33	0.62
5:I:132:SER:HB2	5:I:271:ALA:HA	1.80	0.62
6:M:96:LYS:O	6:M:100:LYS:N	2.30	0.62
2:C:16:LEU:HD23	2:C:65:LEU:HD11	1.82	0.62
2:D:313:ILE:HG22	2:D:369:ASN:HD21	1.64	0.61
5:I:52:GLU:OE2	5:I:80:TYR:OH	2.16	0.61
1:A:47:LEU:O	1:A:104:LYS:NZ	2.32	0.61
3:F:267:ILE:O	3:F:315:LYS:NZ	2.34	0.61
3:F:387:LYS:O	3:F:405:GLY:N	2.31	0.61
5:I:298:ASP:OD1	5:I:298:ASP:N	2.32	0.61
6:L:6:ARG:HH12	6:L:9:GLU:C	2.04	0.61
1:B:106:HIS:O	1:B:110:ASN:ND2	2.33	0.61
3:F:149:ASP:O	3:F:327:PRO:HD2	2.00	0.61
4:G:354:SER:OG	4:G:355:ARG:N	2.30	0.61
1:A:198:SER:H	1:B:228:GLN:HE22	1.47	0.61
6:M:60:LYS:O	6:M:62:ILE:N	2.33	0.61
3:F:92:CYS:SG	3:F:93:MET:N	2.73	0.61
4:H:451:PRO:O	4:H:454:SER:OG	2.17	0.61
4:H:372:VAL:O	4:H:441:THR:OG1	2.17	0.61
2:C:178:GLN:NE2	2:C:182:ASP:OD1	2.33	0.61
5:I:170:ALA:O	5:I:174:SER:N	2.31	0.61
5:I:175:SER:HB3	5:I:189:TYR:HE1	1.66	0.61
2:C:313:ILE:HG22	2:C:369:ASN:HD21	1.66	0.61
6:L:102:GLN:O	6:L:106:THR:OG1	2.19	0.61
2:C:40:ARG:NH2	2:C:178:GLN:OE1	2.34	0.61
1:B:215:VAL:HG12	1:B:216:GLU:H	1.66	0.60
2:D:330:LEU:HB2	5:J:290:ARG:HH11	1.64	0.60
3:E:70:LYS:NZ	3:E:109:GLU:OE2	2.34	0.60
5:J:159:VAL:HG12	5:J:220:ASP:HA	1.82	0.60
3:F:47:PHE:O	3:F:55:THR:OG1	2.16	0.60
5:I:142:GLU:OE1	5:I:264:HIS:ND1	2.26	0.60
5:I:204:GLU:OE1	5:I:204:GLU:N	2.34	0.60
1:B:224:ILE:HD11	1:B:306:PRO:HG2	1.83	0.60
1:B:299:GLU:OE1	1:B:303:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:THR:OG1	2:C:279:HIS:N	2.33	0.60
4:G:156:LYS:HG2	4:G:304:GLU:HG2	1.84	0.60
5:I:61:ALA:HB2	5:I:136:LEU:HD13	1.82	0.60
1:A:227:PHE:N	1:A:309:ASP:OD2	2.32	0.60
3:E:327:PRO:HA	3:E:331:GLU:HB2	1.82	0.60
1:B:92:ARG:NH2	1:B:340:TYR:O	2.32	0.60
4:H:382:THR:HG22	4:H:384:ARG:H	1.67	0.60
5:J:65:GLU:OE2	5:J:67:TYR:OH	2.12	0.60
1:A:20:VAL:O	1:A:24:LYS:N	2.31	0.60
1:A:26:PHE:O	1:A:30:ASP:N	2.35	0.60
1:B:272:PRO:HD2	5:J:323:ARG:HH22	1.66	0.60
3:F:288:PHE:O	3:F:290:SER:N	2.34	0.60
6:L:14:GLU:N	6:L:17:ASP:OD2	2.35	0.60
6:M:97:CYS:O	6:M:101:TYR:N	2.34	0.60
2:C:23:ARG:NH1	2:C:354:TYR:OH	2.34	0.60
3:E:288:PHE:O	3:E:290:SER:N	2.35	0.60
5:I:108:ASP:OD1	5:I:111:ARG:NH1	2.27	0.60
1:B:298:ASN:OD1	1:B:301:GLN:N	2.30	0.60
5:I:71:CYS:HB3	5:I:102:GLU:HA	1.84	0.60
3:E:133:ARG:NH1	3:E:253:ILE:O	2.35	0.59
3:E:149:ASP:O	3:E:327:PRO:HD2	2.02	0.59
4:G:408:ASP:OD1	4:G:409:PHE:N	2.35	0.59
4:H:271:ILE:O	4:H:297:VAL:N	2.29	0.59
4:H:312:LYS:NZ	4:H:316:GLU:OE2	2.34	0.59
2:C:380:ARG:NH2	4:H:460:ASN:OD1	2.33	0.59
4:G:378:SER:OG	4:G:446:GLU:OE2	2.18	0.59
4:H:275:LEU:HD22	4:H:306:GLU:HB2	1.84	0.59
6:M:131:TRP:HA	6:M:134:SER:HB3	1.83	0.59
1:B:92:ARG:NH2	1:B:338:LYS:O	2.35	0.59
1:B:245:GLU:OE2	1:B:245:GLU:N	2.29	0.59
6:L:150:ASP:OD1	6:L:151:GLU:N	2.35	0.59
1:A:245:GLU:OE1	1:A:245:GLU:N	2.31	0.59
1:B:169:SER:HG	1:B:172:SER:HG	1.49	0.59
1:B:240:PHE:O	1:B:317:SER:OG	2.20	0.59
4:G:249:ARG:NH2	4:G:378:SER:OG	2.36	0.59
1:A:56:SER:OG	6:M:83:ASP:OD1	2.20	0.59
4:H:258:VAL:HG23	4:H:283:VAL:HA	1.84	0.59
2:D:331:SER:OG	2:D:332:SER:N	2.33	0.59
5:J:138:GLU:OE1	5:J:138:GLU:N	2.36	0.59
1:A:94:LEU:O	1:A:95:HIS:ND1	2.35	0.59
2:C:54:LEU:O	2:C:57:THR:OG1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:381:ILE:O	2:C:385:THR:OG1	2.17	0.59
3:E:149:ASP:OD1	3:E:149:ASP:N	2.36	0.59
5:I:121:SER:OG	5:I:122:ASP:N	2.35	0.59
5:J:240:TYR:OH	5:J:255:ASP:OD1	2.21	0.59
1:B:249:PHE:HB3	1:B:336:LEU:HD13	1.85	0.59
2:C:84:ARG:NH1	2:C:383:ASN:O	2.34	0.59
5:J:224:ASP:OD2	5:J:244:ARG:NH1	2.36	0.59
5:I:178:VAL:HG22	5:I:214:VAL:HG22	1.83	0.58
5:I:281:ASP:OD2	5:I:381:LYS:NZ	2.35	0.58
1:B:146:ARG:H	1:B:146:ARG:HD2	1.68	0.58
3:F:69:ASN:ND2	3:F:379:ILE:O	2.34	0.58
3:F:127:SER:N	3:F:130:ASP:OD2	2.36	0.58
5:J:80:TYR:O	5:J:84:SER:N	2.36	0.58
1:A:88:ARG:NH2	6:M:28:GLU:OE2	2.37	0.58
1:A:216:GLU:OE2	1:A:251:ARG:NH2	2.37	0.58
2:D:380:ARG:NH1	4:G:460:ASN:OD1	2.36	0.58
3:E:329:TYR:OH	3:E:429:GLU:OE2	2.19	0.58
5:I:240:TYR:OH	5:I:255:ASP:OD1	2.20	0.58
6:L:167:GLU:OE2	6:L:171:TYR:HB2	2.04	0.58
2:D:204:ILE:N	2:D:272:ASN:OD1	2.37	0.58
4:H:131:ARG:N	4:H:203:SER:O	2.36	0.58
3:F:38:GLU:OE1	3:F:164:ARG:NH2	2.25	0.58
5:I:101:ARG:NH2	5:I:105:SER:OG	2.37	0.58
5:I:242:ASP:OD1	5:I:245:LYS:N	2.37	0.58
3:E:133:ARG:NH2	3:E:259:ILE:O	2.36	0.58
3:E:239:ASP:OD1	3:E:240:ALA:N	2.37	0.58
1:A:28:GLN:N	1:A:28:GLN:OE1	2.37	0.58
4:H:258:VAL:O	4:H:262:THR:HG22	2.04	0.58
2:D:166:GLY:H	2:D:167:MET:HE3	1.69	0.58
4:H:238:LEU:HA	4:H:241:LYS:HB2	1.86	0.58
5:J:169:ARG:NH1	5:J:216:ASN:O	2.37	0.58
3:F:162:LYS:NZ	3:F:316:ASP:OD2	2.37	0.57
3:F:327:PRO:HA	3:F:331:GLU:HB2	1.86	0.57
4:G:185:THR:OG1	4:G:186:LEU:N	2.33	0.57
4:H:131:ARG:NH1	4:H:203:SER:OG	2.37	0.57
2:C:281:ILE:HG12	2:C:287:LEU:HD22	1.86	0.57
3:F:101:ASN:HA	3:F:104:LEU:HB2	1.85	0.57
2:D:349:GLU:HB3	4:H:322:THR:HG23	1.84	0.57
3:F:95:GLU:OE2	3:F:95:GLU:N	2.28	0.57
1:A:142:HIS:NE2	1:A:224:ILE:O	2.28	0.57
1:A:161:ARG:HD3	5:J:323:ARG:HA	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:403:ASN:ND2	4:G:407:ASP:O	2.38	0.57
2:C:287:LEU:HD11	2:C:309:VAL:HG21	1.87	0.57
2:D:310:CYS:HA	2:D:367:ILE:HB	1.86	0.57
1:A:21:GLN:HA	1:A:24:LYS:HB2	1.87	0.57
2:D:18:ALA:O	2:D:22:SER:OG	2.18	0.57
6:L:49:GLU:HA	6:L:87:ARG:HD2	1.85	0.57
2:D:287:LEU:HB2	2:D:358:ILE:HG13	1.87	0.57
3:E:418:GLN:O	3:E:435:ARG:HA	2.04	0.57
3:F:222:MET:HG3	3:F:225:LEU:HD12	1.87	0.57
3:F:331:GLU:N	3:F:331:GLU:OE1	2.37	0.57
5:I:19:GLN:OE1	5:I:120:THR:N	2.36	0.57
5:I:130:VAL:HG11	5:I:223:ILE:HD11	1.86	0.57
5:J:16:HIS:ND1	5:J:64:GLN:OE1	2.38	0.57
1:B:227:PHE:N	1:B:309:ASP:OD2	2.36	0.57
3:E:69:ASN:ND2	3:E:379:ILE:O	2.23	0.57
3:E:334:LYS:O	3:E:338:LYS:N	2.35	0.57
2:C:50:THR:OG1	2:C:51:VAL:N	2.37	0.56
2:C:331:SER:OG	2:C:332:SER:N	2.36	0.56
5:I:150:ASP:OD2	5:I:260:LYS:NZ	2.37	0.56
5:J:178:VAL:HG22	5:J:214:VAL:HG22	1.86	0.56
4:G:393:ASN:OD1	4:G:394:GLU:N	2.29	0.56
4:H:270:VAL:H	4:H:337:THR:HG22	1.70	0.56
4:H:378:SER:OG	4:H:446:GLU:OE2	2.19	0.56
5:J:132:SER:HB2	5:J:271:ALA:HA	1.86	0.56
2:C:199:LEU:HD21	2:C:218:LEU:HD23	1.87	0.56
2:C:359:PRO:HG2	2:C:362:LEU:HD13	1.86	0.56
3:F:160:LEU:O	3:F:164:ARG:N	2.32	0.56
4:G:329:LEU:HG	4:G:364:LEU:HD12	1.87	0.56
5:J:180:ASP:OD2	5:J:209:HIS:ND1	2.25	0.56
3:E:320:CYS:SG	3:E:321:SER:N	2.77	0.56
1:B:125:ILE:HD13	1:B:243:VAL:HG21	1.88	0.56
2:C:215:GLU:OE2	2:C:248:ARG:NE	2.34	0.56
2:D:61:VAL:O	2:D:65:LEU:N	2.31	0.56
3:E:51:LEU:HD11	3:E:328:ASN:HA	1.88	0.56
3:E:351:SER:HB2	3:E:355:LEU:HD11	1.86	0.56
4:G:269:ASP:OD1	4:G:338:LYS:NZ	2.38	0.56
6:L:93:ASP:HA	6:L:96:LYS:HB3	1.87	0.56
6:M:147:SER:HB2	6:M:169:LYS:HG3	1.87	0.56
2:C:200:HIS:HE2	4:H:391:VAL:HG23	1.71	0.56
2:D:369:ASN:OD1	2:D:369:ASN:N	2.39	0.56
4:H:300:ASP:OD1	4:H:301:SER:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:121:ILE:HD12	3:F:121:ILE:H	1.70	0.56
5:I:363:ASP:OD1	5:I:364:SER:OG	2.22	0.56
3:E:110:GLY:O	3:E:111:HIS:ND1	2.38	0.56
6:L:50:LEU:HD13	6:L:52:ARG:HG3	1.88	0.56
2:D:278:THR:OG1	2:D:279:HIS:N	2.39	0.56
6:M:131:TRP:O	6:M:135:ARG:N	2.37	0.56
3:E:194:GLN:OE1	3:E:239:ASP:N	2.39	0.55
3:F:149:ASP:HB2	3:F:327:PRO:HG2	1.87	0.55
5:J:186:CYS:HB2	5:J:263:CYS:SG	2.47	0.55
6:M:6:ARG:NH2	6:M:9:GLU:O	2.38	0.55
2:D:323:ASP:OD1	2:D:326:SER:N	2.39	0.55
5:I:389:LYS:HB2	5:I:407:VAL:HG23	1.89	0.55
3:F:363:ASN:OD1	3:F:364:GLU:N	2.38	0.55
6:L:139:HIS:HB3	6:L:142:GLU:HB2	1.87	0.55
4:H:178:TYR:OH	4:H:189:HIS:ND1	2.35	0.55
1:B:201:MET:HA	1:B:204:VAL:HG12	1.89	0.55
3:F:429:GLU:OE1	3:F:429:GLU:N	2.39	0.55
6:L:61:LEU:HD13	6:L:63:ARG:HH21	1.71	0.55
1:A:62:LEU:O	1:A:66:SER:OG	2.23	0.55
5:J:16:HIS:O	5:J:64:GLN:NE2	2.38	0.55
5:J:142:GLU:OE2	5:J:264:HIS:ND1	2.40	0.55
1:A:77:ILE:O	1:A:81:ALA:N	2.37	0.55
2:C:258:VAL:HB	4:G:427:LEU:HG	1.89	0.55
3:F:31:GLN:HG2	3:F:86:THR:HG21	1.89	0.55
5:I:428:GLN:N	5:I:428:GLN:OE1	2.40	0.55
1:B:271:ASP:OD1	5:J:323:ARG:NH2	2.40	0.55
1:B:21:GLN:O	1:B:25:LYS:N	2.29	0.54
1:B:34:THR:HG22	1:B:36:PRO:HD2	1.88	0.54
5:I:427:SER:HG	5:I:428:GLN:H	1.54	0.54
5:J:29:TYR:HA	5:J:32:ARG:HD3	1.89	0.54
1:A:258:TYR:CZ	1:B:202:ASN:HB2	2.42	0.54
3:E:381:LYS:N	3:E:398:ASP:OD1	2.36	0.54
3:F:391:VAL:HG13	3:F:394:SER:HB2	1.89	0.54
3:F:119:PRO:HG2	3:F:122:LEU:HG	1.90	0.54
3:F:133:ARG:NH1	3:F:256:LYS:O	2.34	0.54
5:I:147:ARG:NH1	5:I:153:ALA:O	2.41	0.54
5:I:101:ARG:NH1	5:I:103:SER:O	2.40	0.54
3:E:331:GLU:N	3:E:331:GLU:OE1	2.41	0.54
3:F:155:PRO:O	3:F:158:THR:OG1	2.26	0.54
2:C:27:GLY:N	2:C:72:GLU:OE1	2.40	0.54
6:L:129:ILE:HD12	6:L:157:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLU:HB2	1:B:222:ASN:HA	1.89	0.54
3:E:284:ASN:OD1	3:E:284:ASN:N	2.40	0.54
1:A:22:VAL:HG12	1:A:26:PHE:CZ	2.43	0.54
1:B:314:GLU:OE1	1:B:314:GLU:N	2.36	0.54
5:I:85:LYS:HA	5:I:88:LEU:HD13	1.88	0.54
5:I:316:GLU:OE1	5:I:335:ALA:N	2.40	0.54
2:C:380:ARG:NH1	2:C:384:ASP:OD2	2.41	0.54
3:E:51:LEU:O	3:E:55:THR:OG1	2.26	0.54
3:E:303:SER:HA	4:H:173:ILE:HD11	1.90	0.54
4:H:151:LYS:O	4:H:155:TYR:HB2	2.08	0.54
1:A:146:ARG:H	1:A:146:ARG:HD2	1.72	0.54
2:D:178:GLN:NE2	2:D:182:ASP:OD1	2.41	0.54
2:D:313:ILE:HD11	2:D:381:ILE:HG21	1.89	0.54
5:I:65:GLU:OE2	5:I:67:TYR:OH	2.13	0.54
6:L:97:CYS:O	6:L:101:TYR:N	2.41	0.54
1:B:134:ARG:O	1:B:137:SER:OG	2.17	0.53
3:E:40:GLN:NE2	3:E:138:LEU:O	2.35	0.53
3:F:362:VAL:HG22	3:F:379:ILE:HB	1.89	0.53
5:J:47:ASN:ND2	5:J:350:ILE:O	2.32	0.53
5:J:127:SER:O	5:J:273:ARG:NH2	2.36	0.53
5:J:324:SER:OG	5:J:342:ALA:N	2.40	0.53
1:A:182:LEU:HD22	1:A:187:ILE:HD11	1.89	0.53
2:C:340:ASN:O	2:C:342:GLY:N	2.42	0.53
5:J:364:SER:OG	5:J:364:SER:O	2.24	0.53
1:B:145:SER:OG	1:B:148:VAL:HG12	2.08	0.53
2:D:99:GLU:OE2	2:D:100:ASN:ND2	2.41	0.53
2:D:365:LEU:HD13	4:G:385:ILE:HG12	1.90	0.53
5:J:101:ARG:NH1	5:J:112:GLU:OE1	2.42	0.53
5:J:316:GLU:OE1	5:J:335:ALA:N	2.42	0.53
2:D:233:GLU:O	2:D:235:PHE:N	2.41	0.53
1:A:303:ARG:NH2	1:B:289:ASP:OD2	2.41	0.53
2:D:19:ASP:HA	2:D:24:LYS:HD2	1.91	0.53
3:F:61:PRO:HD2	3:F:64:LEU:HB2	1.89	0.53
4:G:163:ARG:HH12	4:G:205:ARG:NH2	2.06	0.53
1:A:44:VAL:HG23	1:A:108:VAL:HG13	1.90	0.53
5:I:73:HIS:HB3	5:I:76:GLN:HB3	1.90	0.53
5:I:104:LEU:HD11	5:I:109:ALA:HB2	1.91	0.53
5:J:226:CYS:HB3	5:J:230:VAL:HG21	1.90	0.53
2:D:199:LEU:O	2:D:225:ARG:NH1	2.40	0.53
5:I:111:ARG:NH2	5:I:240:TYR:O	2.38	0.53
5:I:290:ARG:NH2	5:I:298:ASP:OD2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:GLN:NE2	4:G:404:MET:O	2.41	0.53
2:C:297:ALA:HB1	2:C:362:LEU:HD23	1.91	0.53
3:F:124:ASP:OD1	3:F:124:ASP:N	2.40	0.53
3:F:418:GLN:N	3:F:434:HIS:O	2.40	0.53
5:I:147:ARG:NH1	5:I:151:LYS:O	2.39	0.53
3:E:347:ASP:OD1	3:E:347:ASP:N	2.41	0.52
3:E:354:ALA:O	3:E:371:ASN:N	2.35	0.52
1:A:223:GLN:O	1:A:226:THR:OG1	2.27	0.52
5:J:57:PHE:CZ	5:J:136:LEU:HD21	2.44	0.52
4:G:244:SER:HA	4:G:247:ARG:HG2	1.91	0.52
5:I:173:GLU:OE1	5:I:275:ARG:NH2	2.42	0.52
4:H:201:LEU:O	4:H:204:THR:OG1	2.27	0.52
2:D:184:LEU:O	2:D:186:LYS:N	2.39	0.52
6:M:10:ASN:ND2	6:M:14:GLU:OE2	2.39	0.52
2:C:280:ALA:HA	2:C:315:LYS:HB3	1.92	0.52
2:D:90:TYR:O	2:D:94:LEU:N	2.41	0.52
5:I:339:VAL:HA	5:I:356:ILE:HB	1.92	0.52
2:D:292:GLY:HA3	4:H:327:SER:HB2	1.91	0.52
3:E:268:PRO:HA	3:E:271:VAL:HG12	1.90	0.52
1:A:30:ASP:OD1	1:A:32:GLU:HG2	2.08	0.52
1:A:220:LEU:O	1:A:310:VAL:HA	2.10	0.52
2:D:239:GLN:OE1	4:H:302:ARG:NH1	2.42	0.52
4:G:229:LEU:HD23	4:G:233:GLU:HB3	1.92	0.52
4:H:410:GLU:HG3	4:H:412:LYS:HG3	1.91	0.52
6:L:42:GLU:OE1	6:L:42:GLU:N	2.34	0.52
1:A:61:ILE:O	1:A:65:GLY:N	2.43	0.52
2:D:36:ALA:HB3	2:D:181:ILE:HD11	1.90	0.52
1:A:169:SER:O	1:A:173:GLY:N	2.42	0.52
1:B:66:SER:O	1:B:70:LYS:N	2.42	0.52
5:J:124:ILE:HG22	5:J:225:ILE:HG12	1.91	0.52
6:M:6:ARG:NE	6:M:8:TYR:O	2.40	0.52
1:A:40:ILE:O	1:A:44:VAL:HG12	2.10	0.51
3:E:303:SER:OG	3:E:304:SER:N	2.42	0.51
5:I:224:ASP:OD2	5:I:244:ARG:NH1	2.43	0.51
2:C:40:ARG:HH21	2:C:178:GLN:HB2	1.74	0.51
2:C:215:GLU:O	2:C:219:ARG:HG3	2.10	0.51
2:C:287:LEU:HB2	2:C:358:ILE:HG13	1.93	0.51
5:I:132:SER:OG	5:I:133:ASN:N	2.43	0.51
1:B:259:ASP:OD1	4:H:266:GLN:NE2	2.44	0.51
3:E:241:HIS:O	3:E:241:HIS:ND1	2.43	0.51
5:I:127:SER:O	5:I:127:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:396:ILE:HG22	5:I:397:GLU:H	1.75	0.51
1:A:34:THR:OG1	1:A:35:MET:N	2.44	0.51
2:C:84:ARG:HA	2:C:87:ARG:HD2	1.91	0.51
3:E:94:GLU:HA	3:E:118:ALA:HB1	1.92	0.51
4:H:105:THR:O	4:H:105:THR:OG1	2.27	0.51
4:H:376:CYS:SG	4:H:377:GLU:N	2.83	0.51
6:L:19:VAL:HG11	6:L:35:LEU:HD23	1.91	0.51
1:A:55:ILE:N	6:M:83:ASP:OD2	2.39	0.51
2:C:169:MET:O	2:C:173:ILE:HG12	2.11	0.51
5:I:25:ASP:H	5:I:40:ARG:HH22	1.58	0.51
1:A:257:GLN:HG3	1:A:258:TYR:CZ	2.46	0.51
1:B:93:SER:O	1:B:106:HIS:NE2	2.44	0.51
5:J:384:LEU:HA	5:J:402:VAL:HG22	1.92	0.51
2:D:48:TRP:HZ3	2:D:170:ARG:HH21	1.57	0.51
5:I:239:ASP:OD1	5:I:239:ASP:N	2.43	0.51
6:M:63:ARG:HD3	6:M:66:LYS:HD3	1.92	0.51
6:M:108:HIS:O	6:M:112:ARG:N	2.31	0.51
1:A:125:ILE:HD13	1:A:243:VAL:HG23	1.93	0.51
1:A:243:VAL:HA	1:A:320:ILE:HG23	1.93	0.51
1:B:204:VAL:HG22	1:B:206:LEU:H	1.76	0.51
3:F:342:GLU:OE1	3:F:342:GLU:N	2.43	0.51
2:D:382:MET:O	2:D:386:TYR:N	2.30	0.51
3:E:142:ASP:OD1	3:E:247:HIS:N	2.42	0.51
3:E:420:GLY:N	3:E:436:VAL:O	2.42	0.51
3:E:428:CYS:SG	3:E:444:GLY:N	2.84	0.51
5:I:324:SER:OG	5:I:342:ALA:N	2.43	0.51
3:F:144:VAL:HG22	3:F:244:VAL:HG22	1.93	0.51
5:J:78:ARG:HG2	5:J:82:GLU:HG3	1.93	0.51
6:M:95:ILE:O	6:M:99:GLU:N	2.38	0.51
2:C:172:VAL:O	2:C:176:GLY:N	2.33	0.50
3:F:358:ALA:C	3:F:360:CYS:H	2.13	0.50
4:H:262:THR:HA	4:H:265:ILE:HG13	1.93	0.50
4:H:311:LEU:HD22	4:H:323:TYR:HB2	1.92	0.50
1:B:220:LEU:O	1:B:310:VAL:HA	2.11	0.50
2:C:315:LYS:NZ	7:C:401:PO4:O2	2.44	0.50
3:E:95:GLU:OE2	3:E:95:GLU:N	2.30	0.50
3:E:371:ASN:O	3:E:388:GLY:N	2.44	0.50
5:I:57:PHE:CZ	5:I:136:LEU:HD11	2.47	0.50
5:I:159:VAL:HB	5:I:218:LEU:HD12	1.93	0.50
6:M:103:LYS:HD2	6:M:141:TYR:CD1	2.46	0.50
1:B:43:LEU:HD12	1:B:86:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:208:SER:HB2	4:G:344:HIS:CE1	2.46	0.50
6:M:97:CYS:HA	6:M:100:LYS:HB2	1.93	0.50
4:G:271:ILE:HG22	4:G:338:LYS:HB2	1.94	0.50
5:I:180:ASP:OD2	5:I:209:HIS:ND1	2.37	0.50
3:E:271:VAL:N	3:E:315:LYS:HZ1	2.09	0.50
3:F:110:GLY:O	3:F:111:HIS:ND1	2.44	0.50
3:F:241:HIS:ND1	3:F:241:HIS:O	2.44	0.50
5:I:80:TYR:O	5:I:84:SER:N	2.44	0.50
3:E:370:ASP:OD1	3:E:370:ASP:N	2.44	0.50
3:F:271:VAL:N	3:F:315:LYS:HZ1	2.09	0.50
3:F:370:ASP:N	3:F:370:ASP:OD1	2.45	0.50
3:F:394:SER:OG	3:F:408:LEU:O	2.24	0.50
4:H:308:ARG:NH2	4:H:406:VAL:HG22	2.27	0.50
6:L:126:TYR:HB3	6:L:131:TRP:CE2	2.47	0.50
5:I:300:ASN:OD1	5:I:306:PHE:N	2.31	0.50
3:E:101:ASN:O	3:E:105:ARG:N	2.39	0.50
3:E:230:ARG:NH2	5:J:213:GLU:OE2	2.30	0.50
5:J:428:GLN:N	5:J:428:GLN:OE1	2.45	0.50
1:B:139:ILE:HB	1:B:164:VAL:HG22	1.93	0.50
3:F:146:LEU:HD22	3:F:242:ILE:HG12	1.94	0.50
5:I:392:ASN:N	5:I:410:ASP:OD2	2.43	0.50
1:A:328:SER:OG	1:A:331:GLY:N	2.34	0.49
1:B:36:PRO:HB3	1:B:79:LEU:HA	1.93	0.49
3:E:121:ILE:HD12	3:E:121:ILE:H	1.75	0.49
3:E:220:PHE:HB3	5:J:199:VAL:HB	1.94	0.49
4:G:252:ILE:O	4:G:256:VAL:HG23	2.11	0.49
4:G:304:GLU:O	4:G:306:GLU:N	2.45	0.49
1:B:76:ASN:OD1	1:B:78:SER:OG	2.20	0.49
2:D:330:LEU:HD23	2:D:353:PRO:HA	1.94	0.49
3:E:259:ILE:HG21	3:E:266:LEU:HD23	1.94	0.49
3:E:284:ASN:HB2	3:E:288:PHE:CE2	2.47	0.49
3:F:139:ILE:HG22	3:F:247:HIS:CD2	2.47	0.49
5:J:358:SER:O	5:J:376:ASN:N	2.44	0.49
1:A:18:ASP:O	1:A:21:GLN:HG2	2.13	0.49
1:B:61:ILE:O	1:B:65:GLY:N	2.46	0.49
2:C:344:LEU:HD23	4:G:311:LEU:HD23	1.95	0.49
4:G:131:ARG:N	4:G:203:SER:O	2.44	0.49
4:G:311:LEU:HD22	4:G:323:TYR:HB2	1.93	0.49
1:A:202:ASN:HB3	1:B:258:TYR:CZ	2.48	0.49
1:A:314:GLU:OE1	1:A:314:GLU:N	2.37	0.49
4:H:269:ASP:OD2	4:H:338:LYS:NZ	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:210:GLU:N	5:J:210:GLU:OE1	2.45	0.49
6:L:106:THR:O	6:L:110:ILE:HG13	2.13	0.49
1:A:220:LEU:HB2	1:A:311:THR:HB	1.94	0.49
4:G:403:ASN:HA	4:G:412:LYS:HB3	1.93	0.49
3:E:38:GLU:OE1	3:E:164:ARG:NH2	2.29	0.49
4:H:252:ILE:O	4:H:256:VAL:HG23	2.13	0.49
5:I:384:LEU:HA	5:I:402:VAL:HG22	1.94	0.49
5:J:71:CYS:SG	5:J:104:LEU:HB2	2.53	0.49
6:L:126:TYR:HB3	6:L:131:TRP:CD2	2.47	0.49
3:F:447:LEU:HD12	3:F:448:VAL:H	1.77	0.49
5:I:222:GLN:HA	5:I:244:ARG:NH2	2.27	0.49
5:J:242:ASP:OD1	5:J:244:ARG:N	2.45	0.49
6:M:162:LYS:HG3	6:M:165:LEU:HD22	1.95	0.49
3:F:381:LYS:N	3:F:398:ASP:OD1	2.39	0.49
4:H:447:MET:SD	4:H:447:MET:N	2.86	0.49
5:I:162:ALA:O	5:I:217:ASP:HB2	2.11	0.49
6:L:76:ASP:OD1	6:L:78:GLU:HG2	2.12	0.49
1:A:65:GLY:O	1:A:68:THR:OG1	2.26	0.49
1:A:73:VAL:O	1:A:75:ASN:N	2.45	0.49
1:A:93:SER:O	1:A:106:HIS:NE2	2.46	0.49
2:D:230:ILE:HG21	2:D:267:ILE:HD12	1.95	0.49
4:H:348:SER:HB3	4:H:456:PRO:HB3	1.95	0.49
6:M:21:VAL:N	6:M:68:ASP:O	2.31	0.49
1:A:83:CYS:O	1:A:87:GLN:HG3	2.13	0.49
6:L:131:TRP:O	6:L:135:ARG:N	2.43	0.49
1:A:272:PRO:HB2	1:B:186:CYS:HA	1.95	0.48
1:B:105:ARG:O	1:B:109:GLU:HB2	2.13	0.48
3:E:400:ILE:HG22	3:E:417:ALA:N	2.28	0.48
3:F:48:GLY:HA2	3:F:62:LYS:HD2	1.94	0.48
5:I:160:ARG:NH2	5:I:269:ASN:O	2.42	0.48
1:A:160:VAL:HG23	1:A:162:PHE:HE1	1.78	0.48
1:A:170:ARG:HB3	1:B:193:LEU:HD13	1.96	0.48
1:A:212:GLU:HB2	1:A:222:ASN:HA	1.95	0.48
1:B:243:VAL:HA	1:B:320:ILE:HB	1.96	0.48
3:E:67:ILE:HA	3:E:336:ILE:HG12	1.94	0.48
4:H:178:TYR:HH	4:H:189:HIS:HD1	1.53	0.48
1:A:266:ILE:HG23	1:A:267:LEU:HG	1.95	0.48
1:B:36:PRO:O	1:B:40:ILE:HG13	2.13	0.48
3:F:235:THR:HG21	5:I:206:PHE:HB3	1.95	0.48
4:G:354:SER:HB3	4:G:358:THR:HG21	1.95	0.48
1:A:87:GLN:O	1:A:91:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:413:VAL:HG12	3:E:430:ILE:HB	1.94	0.48
4:G:171:PHE:O	4:G:175:ILE:HG13	2.13	0.48
1:A:258:TYR:CE2	1:B:202:ASN:HB2	2.49	0.48
3:E:379:ILE:HG12	3:E:396:LEU:HD22	1.95	0.48
5:I:341:ASP:O	5:I:359:ASN:N	2.42	0.48
6:L:146:LEU:HA	6:L:149:ILE:HG12	1.94	0.48
6:M:99:GLU:O	6:M:103:LYS:HG3	2.13	0.48
1:A:201:MET:O	1:A:204:VAL:HG22	2.14	0.48
4:H:304:GLU:O	4:H:306:GLU:N	2.46	0.48
5:I:222:GLN:HA	5:I:244:ARG:HH21	1.77	0.48
2:C:307:VAL:HB	2:C:363:VAL:HA	1.95	0.48
5:J:305:THR:OG1	5:J:316:GLU:HG2	2.13	0.48
6:L:29:MET:HA	6:L:47:LEU:HD12	1.94	0.48
4:H:311:LEU:O	4:H:315:THR:OG1	2.27	0.48
5:J:239:ASP:N	5:J:239:ASP:OD1	2.46	0.48
2:D:243:HIS:HB3	4:H:416:LEU:HD21	1.95	0.48
3:F:189:GLU:O	3:F:192:ALA:N	2.45	0.48
5:J:130:VAL:HA	5:J:273:ARG:HA	1.95	0.48
1:B:40:ILE:O	1:B:44:VAL:HG23	2.14	0.48
2:D:215:GLU:OE2	2:D:248:ARG:NE	2.31	0.48
3:E:132:LEU:H	3:E:132:LEU:HD23	1.78	0.48
3:F:379:ILE:HG12	3:F:396:LEU:HB2	1.95	0.48
4:G:449:LEU:HD12	4:G:449:LEU:H	1.78	0.48
5:I:306:PHE:CD1	5:I:316:GLU:HG3	2.48	0.48
2:C:264:ILE:HD13	2:C:296:VAL:HG22	1.95	0.47
3:E:144:VAL:HG22	3:E:244:VAL:HG22	1.96	0.47
5:I:31:PHE:HD2	5:I:40:ARG:HG3	1.79	0.47
5:J:18:LEU:HD13	5:J:19:GLN:N	2.29	0.47
6:M:14:GLU:N	6:M:17:ASP:OD2	2.46	0.47
6:M:122:LEU:O	6:M:124:GLU:N	2.42	0.47
1:A:197:VAL:N	1:B:228:GLN:HE22	2.12	0.47
2:C:244:ALA:O	2:C:248:ARG:HG3	2.13	0.47
4:G:157:ILE:HG21	4:G:309:VAL:HG21	1.96	0.47
5:I:292:VAL:O	5:I:295:PHE:N	2.46	0.47
5:J:332:LEU:HD22	5:J:349:ILE:HG23	1.95	0.47
1:A:96:ASP:OD2	6:M:74:ARG:NE	2.47	0.47
2:D:225:ARG:HD3	4:G:118:LYS:HZ2	1.79	0.47
2:D:274:VAL:HG12	2:D:306:PRO:O	2.14	0.47
3:E:340:THR:N	3:E:341:PRO:HD2	2.28	0.47
3:E:32:LEU:HD22	4:H:179:GLN:NE2	2.28	0.47
3:E:123:ASP:HB2	3:E:126:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:371:ASN:O	3:F:388:GLY:N	2.45	0.47
4:G:110:GLN:OE1	4:G:129:ARG:NH2	2.34	0.47
5:J:401:ILE:HD13	5:J:419:ARG:HG2	1.95	0.47
1:B:134:ARG:HD3	1:B:134:ARG:HA	1.71	0.47
4:G:108:ASN:O	4:G:112:LYS:N	2.48	0.47
4:H:348:SER:OG	4:H:382:THR:O	2.31	0.47
5:J:409:GLY:H	5:J:434:PRO:HD3	1.80	0.47
3:F:340:THR:N	3:F:341:PRO:HD2	2.29	0.47
5:I:189:TYR:CE2	5:I:244:ARG:HG3	2.50	0.47
5:J:38:LYS:HG2	5:J:76:GLN:HE22	1.79	0.47
1:A:121:CYS:HB2	1:A:322:ASP:HB3	1.96	0.47
1:A:267:LEU:N	1:A:304:ASN:OD1	2.47	0.47
2:C:313:ILE:HD11	2:C:381:ILE:HG21	1.97	0.47
2:D:194:GLN:HE22	2:D:371:GLY:HA2	1.80	0.47
3:E:420:GLY:HA3	3:E:437:GLU:HA	1.96	0.47
4:G:376:CYS:SG	4:G:377:GLU:N	2.88	0.47
4:G:447:MET:N	4:G:447:MET:SD	2.88	0.47
5:I:47:ASN:ND2	5:I:350:ILE:O	2.31	0.47
5:I:55:PHE:HB3	5:I:86:TRP:CZ2	2.50	0.47
5:I:71:CYS:SG	5:I:104:LEU:HB2	2.55	0.47
5:I:337:THR:OG1	5:I:354:CYS:N	2.44	0.47
5:J:108:ASP:OD1	5:J:111:ARG:NH2	2.43	0.47
6:M:21:VAL:HG23	6:M:34:LYS:O	2.14	0.47
2:C:5:ASN:OD1	2:C:6:VAL:N	2.48	0.47
5:I:91:SER:OG	5:I:93:PHE:O	2.32	0.47
6:L:90:SER:HG	6:L:91:SER:N	2.12	0.47
1:A:222:ASN:HB3	1:A:226:THR:OG1	2.15	0.47
1:B:138:VAL:HG13	1:B:205:ASP:H	1.79	0.47
2:D:184:LEU:O	2:D:187:ILE:HG12	2.15	0.47
2:D:309:VAL:O	2:D:367:ILE:N	2.43	0.47
4:H:273:THR:OG1	4:H:274:TYR:N	2.47	0.47
5:I:100:SER:OG	5:I:101:ARG:N	2.47	0.47
5:I:405:GLY:O	5:I:407:VAL:N	2.47	0.47
6:L:93:ASP:N	6:L:93:ASP:OD1	2.48	0.47
6:M:46:LEU:HG	6:M:47:LEU:O	2.14	0.47
2:C:282:LEU:HD12	2:C:321:PRO:HB3	1.97	0.47
2:D:201:SER:H	4:G:118:LYS:NZ	2.13	0.47
4:G:446:GLU:HG2	4:G:447:MET:SD	2.55	0.47
1:A:210:GLY:O	1:A:222:ASN:ND2	2.48	0.46
1:B:197:VAL:HG11	1:B:229:LEU:HB3	1.96	0.46
3:F:206:LEU:HD23	3:F:224:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:286:HIS:O	4:G:290:VAL:HG23	2.15	0.46
1:A:136:GLY:N	1:A:161:ARG:O	2.36	0.46
1:B:43:LEU:HD12	1:B:86:PHE:CD2	2.50	0.46
1:B:142:HIS:H	1:B:209:VAL:HG12	1.78	0.46
3:F:177:VAL:HG12	3:F:238:SER:HB3	1.97	0.46
4:G:160:SER:OG	7:G:501:PO4:O1	2.27	0.46
5:I:152:ASN:HB3	5:I:259:LYS:HA	1.97	0.46
5:I:363:ASP:O	5:I:380:GLY:HA2	2.15	0.46
5:J:54:THR:OG1	5:J:130:VAL:N	2.39	0.46
6:M:22:ASN:HA	6:M:67:ASN:HA	1.97	0.46
1:B:92:ARG:HD3	1:B:341:LEU:HG	1.96	0.46
1:B:166:VAL:HG23	1:B:191:MET:HG2	1.96	0.46
2:C:167:MET:HG2	2:C:168:ASP:H	1.79	0.46
2:C:328:ILE:O	2:C:328:ILE:HD12	2.16	0.46
2:D:172:VAL:O	2:D:176:GLY:N	2.46	0.46
4:H:411:GLU:H	4:H:411:GLU:CD	2.17	0.46
5:J:38:LYS:HD2	5:J:386:ASN:HD21	1.80	0.46
1:A:62:LEU:HD12	1:A:63:GLN:N	2.31	0.46
1:A:264:ARG:NH2	1:A:303:ARG:O	2.40	0.46
2:C:84:ARG:NE	2:C:88:GLU:OE2	2.49	0.46
3:E:195:LEU:HD11	3:E:233:LEU:HD23	1.98	0.46
3:F:246:LYS:O	3:F:249:VAL:HG12	2.15	0.46
5:J:249:TYR:CZ	5:J:253:THR:HG21	2.51	0.46
1:A:225:GLY:HA2	1:A:228:GLN:HB2	1.98	0.46
1:B:83:CYS:O	1:B:87:GLN:HG3	2.15	0.46
1:B:132:LEU:HD23	1:B:132:LEU:HA	1.75	0.46
3:E:343:GLN:OE1	3:E:344:ARG:N	2.34	0.46
3:E:429:GLU:N	3:E:429:GLU:OE1	2.49	0.46
4:G:226:ASP:OD1	4:G:226:ASP:N	2.36	0.46
4:H:243:ASP:O	4:H:247:ARG:HG3	2.15	0.46
5:I:105:SER:OG	5:I:108:ASP:OD2	2.33	0.46
5:I:154:ILE:HD11	5:I:259:LYS:HD3	1.98	0.46
6:L:23:VAL:HA	6:L:33:VAL:HG12	1.96	0.46
6:L:93:ASP:HA	6:L:96:LYS:HE2	1.97	0.46
1:A:171:PRO:HB2	1:B:291:ILE:HG23	1.98	0.46
1:B:139:ILE:HA	1:B:206:LEU:O	2.16	0.46
1:B:216:GLU:HG3	1:B:336:LEU:HD23	1.97	0.46
2:C:101:GLU:HG2	2:C:103:LEU:HG	1.98	0.46
2:C:274:VAL:HG13	2:C:307:VAL:HA	1.97	0.46
3:F:66:PRO:HA	3:F:71:PRO:HA	1.98	0.46
3:F:268:PRO:HA	3:F:271:VAL:HG12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:254:GLY:O	4:H:258:VAL:HG12	2.16	0.46
5:I:106:VAL:HG12	5:I:107:GLY:H	1.81	0.46
1:B:267:LEU:N	1:B:304:ASN:OD1	2.49	0.46
2:D:54:LEU:O	2:D:57:THR:OG1	2.30	0.46
3:E:277:LYS:HD2	3:E:278:SER:N	2.31	0.46
3:E:385:ILE:HA	3:E:402:VAL:HG13	1.98	0.46
5:I:40:ARG:O	5:I:43:LEU:HG	2.15	0.46
5:I:418:LYS:HD2	5:I:418:LYS:HA	1.59	0.46
5:J:276:SER:HB2	5:J:279:THR:HG23	1.98	0.46
5:J:320:VAL:HG11	5:J:338:LYS:HD2	1.98	0.46
5:J:379:ILE:HA	5:J:396:ILE:HG23	1.97	0.46
1:B:92:ARG:NH2	1:B:339:LEU:O	2.48	0.46
1:B:104:LYS:O	1:B:108:VAL:HG12	2.16	0.46
3:E:209:LYS:HE2	3:E:214:VAL:HB	1.96	0.46
5:J:357:GLY:H	5:J:373:ILE:HG22	1.81	0.46
6:M:35:LEU:H	6:M:35:LEU:HD12	1.81	0.46
2:C:270:ARG:HH11	4:G:122:ILE:HG22	1.80	0.46
3:F:369:LYS:HG3	3:F:370:ASP:H	1.81	0.46
4:G:108:ASN:N	4:G:108:ASN:OD1	2.49	0.46
5:J:305:THR:OG1	5:J:317:GLU:N	2.48	0.46
6:L:49:GLU:HG3	6:L:87:ARG:HG2	1.97	0.46
1:B:22:VAL:HG12	1:B:26:PHE:CZ	2.51	0.46
3:E:101:ASN:HA	3:E:104:LEU:HD12	1.98	0.46
3:F:247:HIS:O	3:F:250:ILE:HG22	2.16	0.46
5:I:242:ASP:OD1	5:I:244:ARG:N	2.49	0.46
1:A:142:HIS:HE1	1:A:169:SER:HA	1.81	0.45
2:D:245:MET:O	2:D:249:LEU:HG	2.16	0.45
3:E:156:PRO:O	3:E:159:VAL:HG22	2.16	0.45
3:E:447:LEU:HD23	3:E:448:VAL:N	2.31	0.45
3:F:345:LEU:HG	3:F:346:VAL:H	1.81	0.45
1:B:106:HIS:CD2	1:B:110:ASN:HD21	2.35	0.45
2:C:284:ASN:HB3	2:C:320:TYR:CE1	2.51	0.45
2:D:325:GLU:OE1	5:J:310:ARG:NE	2.41	0.45
3:F:271:VAL:HB	3:F:315:LYS:HZ2	1.81	0.45
5:I:42:LEU:HD21	5:I:80:TYR:CD2	2.51	0.45
1:B:62:LEU:HD22	1:B:87:GLN:HG2	1.97	0.45
2:C:284:ASN:O	2:C:360:PRO:HG3	2.17	0.45
2:D:328:ILE:HD12	4:H:331:TYR:CD2	2.52	0.45
3:E:402:VAL:HG23	3:E:419:ILE:CD1	2.41	0.45
3:E:423:SER:O	3:E:424:LYS:HG3	2.17	0.45
5:J:273:ARG:HD3	5:J:275:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:LEU:HD11	4:G:327:SER:HA	1.98	0.45
2:D:284:ASN:O	2:D:360:PRO:HG3	2.16	0.45
4:H:160:SER:N	7:H:501:PO4:O1	2.43	0.45
4:H:286:HIS:O	4:H:290:VAL:HG23	2.17	0.45
5:J:53:TYR:HB3	5:J:131:VAL:HG12	1.99	0.45
5:J:121:SER:OG	5:J:122:ASP:N	2.48	0.45
5:J:162:ALA:O	5:J:217:ASP:HB2	2.16	0.45
2:C:233:GLU:OE2	4:G:302:ARG:HD3	2.17	0.45
2:C:333:PRO:HD3	5:I:290:ARG:HB2	1.98	0.45
3:E:188:LYS:HA	3:E:188:LYS:HD3	1.67	0.45
3:E:206:LEU:HD13	3:E:231:VAL:HG12	1.99	0.45
4:G:187:SER:HB3	4:G:225:LEU:HD11	1.97	0.45
5:I:226:CYS:HB3	5:I:230:VAL:HG21	1.97	0.45
1:B:144:PHE:N	1:B:174:SER:OG	2.38	0.45
3:E:180:TYR:HA	3:E:334:LYS:HG3	1.99	0.45
6:L:167:GLU:O	6:L:171:TYR:N	2.50	0.45
6:M:103:LYS:O	6:M:107:VAL:HG23	2.17	0.45
1:A:212:GLU:N	1:A:222:ASN:OD1	2.50	0.45
1:A:224:ILE:HD12	1:A:309:ASP:HB3	1.97	0.45
2:C:259:ILE:HD12	2:C:263:THR:HB	1.98	0.45
3:F:51:LEU:HD11	3:F:328:ASN:HA	1.98	0.45
4:G:220:LEU:O	4:G:224:VAL:HG13	2.17	0.45
5:J:243:ILE:O	5:J:247:PHE:HB3	2.17	0.45
6:L:49:GLU:HB3	6:L:86:LYS:HB3	1.97	0.45
1:A:167:THR:HG22	1:A:194:ASP:OD1	2.16	0.45
3:F:410:SER:O	3:F:410:SER:OG	2.30	0.45
4:H:171:PHE:O	4:H:175:ILE:HG13	2.16	0.45
4:H:185:THR:OG1	4:H:186:LEU:N	2.49	0.45
5:I:39:PRO:HD3	5:I:73:HIS:CG	2.52	0.45
5:J:421:THR:OG1	5:J:422:THR:N	2.50	0.45
1:B:47:LEU:HD13	1:B:107:LEU:HD21	1.99	0.45
2:C:-3:ILE:HD11	2:C:1:MET:HG3	1.99	0.45
5:I:24:SER:C	5:I:26:SER:H	2.20	0.45
5:J:356:ILE:HA	5:J:373:ILE:HB	1.99	0.45
5:I:159:VAL:HG12	5:I:220:ASP:HA	1.99	0.44
5:J:346:ALA:O	5:J:348:THR:OG1	2.33	0.44
6:M:137:PHE:HB2	6:M:143:ALA:HB2	1.99	0.44
1:A:70:LYS:NZ	1:A:84:ASP:OD1	2.42	0.44
2:C:20:LEU:HA	2:C:20:LEU:HD23	1.71	0.44
2:D:287:LEU:HD21	2:D:309:VAL:HG21	1.98	0.44
3:E:284:ASN:HB2	3:E:288:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:240:GLU:O	4:H:244:SER:OG	2.35	0.44
5:I:51:ILE:O	5:I:55:PHE:N	2.45	0.44
5:J:373:ILE:HD13	5:J:390:ILE:HB	1.98	0.44
1:B:322:ASP:OD1	1:B:322:ASP:N	2.48	0.44
3:E:147:SER:HB3	3:E:241:HIS:ND1	2.31	0.44
3:E:267:ILE:O	3:E:315:LYS:NZ	2.51	0.44
3:F:188:LYS:O	3:F:190:ILE:N	2.50	0.44
4:H:106:ASP:OD1	4:H:106:ASP:N	2.50	0.44
4:H:137:ILE:H	4:H:137:ILE:HG13	1.65	0.44
5:J:60:LEU:HD22	5:J:135:PRO:HA	2.00	0.44
1:B:259:ASP:OD2	4:H:264:LYS:NZ	2.29	0.44
2:D:90:TYR:CZ	2:D:94:LEU:HD13	2.53	0.44
2:D:268:MET:HB3	2:D:303:HIS:CE1	2.53	0.44
3:F:127:SER:OG	3:F:128:SER:N	2.48	0.44
3:F:320:CYS:SG	3:F:321:SER:N	2.88	0.44
4:G:109:LEU:O	4:G:113:LYS:HG3	2.16	0.44
5:I:132:SER:OG	5:I:134:VAL:HG12	2.17	0.44
2:C:177:ILE:O	2:C:180:VAL:HG22	2.17	0.44
2:D:84:ARG:NE	2:D:88:GLU:OE2	2.51	0.44
2:D:317:SER:OG	2:D:319:VAL:HG23	2.18	0.44
4:H:418:ASN:O	4:H:422:VAL:HG23	2.18	0.44
6:M:58:ILE:HB	6:M:60:LYS:HG2	2.00	0.44
1:A:21:GLN:O	1:A:25:LYS:N	2.28	0.44
1:A:191:MET:SD	1:B:297:MET:HG2	2.57	0.44
2:C:200:HIS:N	2:C:203:GLU:OE1	2.46	0.44
2:C:225:ARG:HG2	4:H:118:LYS:HD3	1.99	0.44
2:D:46:THR:HG23	2:D:48:TRP:CZ3	2.52	0.44
2:D:376:SER:OG	4:G:453:THR:OG1	2.24	0.44
3:E:128:SER:HB2	3:E:262:ILE:HG13	2.00	0.44
3:E:276:GLN:OE1	3:E:279:PHE:N	2.36	0.44
3:F:169:SER:HB3	3:F:248:TRP:HZ2	1.82	0.44
5:I:30:ARG:H	5:I:30:ARG:HG2	1.62	0.44
5:J:147:ARG:NH1	5:J:151:LYS:O	2.37	0.44
1:B:126:ALA:C	1:B:128:LEU:H	2.20	0.44
3:E:93:MET:SD	3:E:122:LEU:HB3	2.58	0.44
3:E:379:ILE:HA	3:E:396:LEU:HB2	2.00	0.44
3:E:410:SER:O	3:E:410:SER:OG	2.25	0.44
3:F:276:GLN:HE21	3:F:279:PHE:HB2	1.83	0.44
4:G:240:GLU:O	4:G:244:SER:OG	2.29	0.44
2:C:23:ARG:HH11	5:I:293:TYR:HH	1.64	0.44
3:F:259:ILE:HG23	3:F:265:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:202:ASP:OD1	5:I:202:ASP:N	2.49	0.44
5:J:180:ASP:O	5:J:184:SER:N	2.42	0.44
6:L:124:GLU:O	6:L:128:THR:HG23	2.18	0.44
6:M:126:TYR:HB3	6:M:131:TRP:CD2	2.53	0.44
1:A:121:CYS:SG	1:A:122:ARG:N	2.91	0.44
3:F:239:ASP:OD1	3:F:241:HIS:N	2.36	0.44
4:G:175:ILE:HG13	4:G:175:ILE:H	1.64	0.44
4:G:312:LYS:O	4:G:316:GLU:HG3	2.17	0.44
4:H:208:SER:HB3	4:H:211:MET:SD	2.58	0.44
5:I:243:ILE:O	5:I:247:PHE:HB3	2.17	0.44
5:J:43:LEU:HD12	5:J:50:LEU:HD13	1.99	0.44
5:J:370:ASP:O	5:J:387:SER:HA	2.18	0.44
1:B:131:PRO:HB2	2:C:322:TYR:CD2	2.52	0.43
2:D:324:LEU:HD12	2:D:324:LEU:H	1.83	0.43
3:E:183:ILE:HG23	3:E:184:THR:H	1.83	0.43
3:F:101:ASN:O	3:F:105:ARG:N	2.35	0.43
5:I:101:ARG:HH22	5:I:105:SER:H	1.66	0.43
5:J:139:VAL:HA	5:J:142:GLU:HB2	2.00	0.43
5:J:294:PRO:O	5:J:296:VAL:N	2.50	0.43
6:L:10:ASN:OD1	6:L:10:ASN:N	2.50	0.43
1:A:57:GLU:O	1:A:61:ILE:HG13	2.18	0.43
1:A:114:PHE:O	1:A:118:ALA:N	2.50	0.43
1:B:215:VAL:HG12	1:B:216:GLU:N	2.33	0.43
2:D:295:LEU:HB3	4:H:360:LEU:HD13	1.99	0.43
3:F:358:ALA:O	3:F:360:CYS:N	2.51	0.43
4:G:463:LYS:HA	4:G:463:LYS:HD3	1.81	0.43
4:H:218:LEU:O	4:H:222:ILE:HG12	2.17	0.43
5:I:24:SER:O	5:I:26:SER:N	2.47	0.43
5:J:279:THR:O	5:J:283:ILE:HG12	2.18	0.43
6:L:112:ARG:HA	6:L:115:ALA:HB3	2.00	0.43
3:E:396:LEU:HA	3:E:413:VAL:HG23	1.99	0.43
4:G:305:PHE:O	4:G:308:ARG:HG2	2.17	0.43
4:H:274:TYR:CE1	4:H:275:LEU:HG	2.52	0.43
5:J:73:HIS:HB3	5:J:76:GLN:HB3	2.00	0.43
5:J:305:THR:HG1	5:J:317:GLU:N	2.16	0.43
6:L:51:SER:HB3	6:L:63:ARG:HH22	1.83	0.43
6:M:125:LEU:HG	6:M:126:TYR:CD1	2.54	0.43
1:B:217:ASN:HB3	1:B:253:PHE:CE1	2.54	0.43
2:C:340:ASN:ND2	5:I:161:GLU:HG2	2.33	0.43
3:E:221:ARG:H	3:E:221:ARG:HG2	1.51	0.43
3:E:369:LYS:HD2	3:E:386:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:147:ARG:O	4:G:151:LYS:HG3	2.18	0.43
5:J:110:LEU:HD12	5:J:234:PHE:CD2	2.54	0.43
1:A:206:LEU:HD22	1:A:207:VAL:H	1.84	0.43
2:C:354:TYR:OH	5:I:293:TYR:OH	2.33	0.43
2:D:235:PHE:CD1	2:D:236:PRO:HA	2.53	0.43
3:E:65:LEU:O	3:E:72:MET:N	2.51	0.43
3:E:197:GLY:HA3	3:E:207:TYR:HB3	2.01	0.43
4:G:339:ILE:HB	4:G:371:PRO:O	2.18	0.43
5:I:170:ALA:HB3	5:I:275:ARG:HH22	1.83	0.43
5:J:347:ASN:O	5:J:347:ASN:ND2	2.49	0.43
5:J:412:THR:HG21	5:J:434:PRO:HB3	2.01	0.43
1:A:163:LYS:HB2	1:B:269:PHE:CD2	2.53	0.43
2:C:250:ALA:HB2	4:G:425:LEU:HB2	2.01	0.43
4:H:381:PHE:CD2	4:H:455:VAL:HG13	2.54	0.43
4:H:385:ILE:HD12	4:H:385:ILE:O	2.19	0.43
5:J:31:PHE:O	5:J:35:THR:HG23	2.18	0.43
5:J:54:THR:O	5:J:57:PHE:HB3	2.18	0.43
5:J:338:LYS:HB3	5:J:338:LYS:HE3	1.77	0.43
5:J:399:GLY:O	5:J:417:ASN:HA	2.19	0.43
2:C:190:ASP:OD1	2:C:190:ASP:N	2.51	0.43
3:E:133:ARG:NH1	3:E:257:GLU:HA	2.33	0.43
3:F:113:ARG:NE	3:F:113:ARG:HA	2.34	0.43
3:F:288:PHE:C	3:F:289:LEU:HD23	2.39	0.43
4:H:202:VAL:HG12	4:H:207:LEU:HG	2.01	0.43
5:J:111:ARG:HG2	5:J:235:THR:HA	2.00	0.43
1:A:230:ALA:HB1	1:A:315:PHE:HB3	2.00	0.43
1:B:128:LEU:HD21	1:B:324:GLY:HA2	2.01	0.43
4:G:106:ASP:OD1	4:G:106:ASP:N	2.52	0.43
4:G:277:SER:HB3	4:G:280:VAL:HG22	2.01	0.43
5:I:111:ARG:HD3	5:I:238:PHE:HA	2.01	0.43
5:I:202:ASP:HB2	5:I:204:GLU:OE1	2.19	0.43
1:B:170:ARG:HH22	1:B:296:ILE:HB	1.84	0.43
2:C:95:LYS:HA	2:C:95:LYS:HD3	1.81	0.43
2:C:234:GLY:O	2:C:238:ASN:N	2.52	0.43
2:C:379:TYR:CG	2:C:380:ARG:N	2.87	0.43
3:E:48:GLY:HA2	3:E:62:LYS:HD2	2.01	0.43
6:M:12:TYR:HB2	6:M:77:LYS:HE2	2.01	0.43
1:A:210:GLY:HA2	1:A:243:VAL:HG13	2.00	0.43
1:A:320:ILE:HA	1:A:325:ILE:HA	2.01	0.43
2:C:48:TRP:HZ3	2:C:170:ARG:HH21	1.67	0.43
3:E:38:GLU:HG3	4:H:143:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:149:ASP:HB2	3:E:327:PRO:HG2	2.00	0.43
4:H:110:GLN:O	4:H:113:LYS:HB3	2.19	0.43
5:I:140:LEU:O	5:I:143:HIS:N	2.48	0.43
2:D:77:ASN:OD1	2:D:317:SER:HB2	2.19	0.42
2:D:340:ASN:O	5:J:163:SER:HB3	2.18	0.42
4:H:145:VAL:HG13	4:H:201:LEU:HD21	2.00	0.42
5:I:70:CYS:HG	5:I:97:THR:HG1	1.65	0.42
5:J:202:ASP:OD1	5:J:202:ASP:N	2.39	0.42
6:M:169:LYS:HG3	6:M:172:ILE:HD11	2.01	0.42
2:C:61:VAL:O	2:C:64:THR:OG1	2.35	0.42
3:E:250:ILE:HD12	3:E:253:ILE:HD12	2.01	0.42
3:E:262:ILE:HG13	3:E:262:ILE:H	1.60	0.42
3:F:331:GLU:O	3:F:335:CYS:N	2.36	0.42
3:F:349:THR:OG1	3:F:350:VAL:N	2.51	0.42
3:F:350:VAL:HG23	3:F:367:THR:HG23	2.00	0.42
5:I:111:ARG:HG2	5:I:235:THR:HA	2.00	0.42
1:A:168:GLU:CD	1:B:170:ARG:HH21	2.23	0.42
1:B:130:TYR:CD2	1:B:131:PRO:HD3	2.54	0.42
2:C:46:THR:HG23	2:C:48:TRP:CZ3	2.55	0.42
2:C:265:PHE:HB2	4:G:360:LEU:HD21	2.01	0.42
4:G:170:THR:O	4:G:174:VAL:HG23	2.19	0.42
4:H:221:GLU:HA	4:H:224:VAL:HG12	2.00	0.42
4:H:388:ASP:OD1	4:H:391:VAL:N	2.52	0.42
6:L:35:LEU:HD12	6:L:35:LEU:H	1.84	0.42
2:C:-3:ILE:HD12	2:C:0:PHE:HB2	2.01	0.42
2:D:215:GLU:O	2:D:219:ARG:HG3	2.20	0.42
3:E:69:ASN:ND2	3:E:363:ASN:HB2	2.34	0.42
3:E:247:HIS:O	3:E:250:ILE:HG22	2.20	0.42
3:E:315:LYS:HE2	3:E:315:LYS:HB3	1.86	0.42
3:E:432:VAL:C	3:E:434:HIS:H	2.23	0.42
3:F:278:SER:O	3:F:280:THR:HG22	2.18	0.42
4:G:151:LYS:O	4:G:155:TYR:HB2	2.19	0.42
4:G:158:PHE:CZ	4:G:163:ARG:HG3	2.54	0.42
4:H:200:TYR:O	4:H:203:SER:OG	2.32	0.42
5:I:54:THR:OG1	5:I:130:VAL:N	2.34	0.42
5:I:136:LEU:HD12	5:I:136:LEU:H	1.84	0.42
6:L:58:ILE:HG22	6:L:60:LYS:HG2	2.00	0.42
1:B:87:GLN:O	1:B:91:THR:OG1	2.31	0.42
1:B:217:ASN:HB3	1:B:253:PHE:CZ	2.54	0.42
1:B:334:GLU:OE2	2:C:379:TYR:OH	2.28	0.42
3:E:263:ARG:HH21	7:E:502:PO4:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67:ILE:HA	3:F:336:ILE:HG12	2.02	0.42
5:I:375:ASP:N	5:I:392:ASN:OD1	2.41	0.42
6:M:146:LEU:HA	6:M:149:ILE:HG13	2.01	0.42
1:A:153:LEU:O	1:A:157:LYS:HG2	2.20	0.42
1:B:77:ILE:HD11	1:B:250:VAL:HG11	2.02	0.42
2:C:28:PRO:HB2	2:C:314:TYR:HE2	1.84	0.42
2:D:95:LYS:HD3	2:D:95:LYS:HA	1.78	0.42
2:D:289:THR:O	2:D:356:ASP:N	2.35	0.42
3:F:392:SER:OG	3:F:393:ASN:ND2	2.52	0.42
4:G:258:VAL:O	4:G:262:THR:OG1	2.25	0.42
5:I:409:GLY:N	5:I:433:ASP:HA	2.31	0.42
5:I:430:THR:HB	5:I:431:LEU:H	1.69	0.42
5:J:349:ILE:HD13	5:J:366:PHE:CE2	2.54	0.42
1:A:147:GLY:O	1:A:151:VAL:HG12	2.20	0.42
1:B:50:SER:O	1:B:104:LYS:NZ	2.51	0.42
1:B:92:ARG:HH21	1:B:340:TYR:C	2.22	0.42
2:C:208:GLN:NE2	2:C:292:GLY:O	2.49	0.42
3:F:190:ILE:HG23	3:F:328:ASN:HB2	2.02	0.42
5:I:50:LEU:HB3	5:I:129:ASP:OD2	2.20	0.42
1:A:197:VAL:H	1:B:228:GLN:HE22	1.67	0.42
2:C:12:ALA:HA	2:C:15:SER:HB3	2.01	0.42
2:C:33:VAL:O	2:C:37:LEU:HG	2.20	0.42
2:D:208:GLN:NE2	2:D:292:GLY:O	2.42	0.42
2:D:244:ALA:O	2:D:248:ARG:HG3	2.19	0.42
3:E:152:VAL:HG23	3:E:324:ASN:HD22	1.85	0.42
3:F:331:GLU:HB3	3:F:335:CYS:SG	2.60	0.42
3:F:387:LYS:HG3	3:F:404:ASP:OD1	2.20	0.42
5:J:111:ARG:NH1	5:J:238:PHE:O	2.53	0.42
5:J:218:LEU:HD13	5:J:218:LEU:HA	1.89	0.42
6:L:167:GLU:HA	6:L:170:ASN:HB3	2.02	0.42
1:A:244:ALA:O	1:A:321:THR:HA	2.20	0.42
2:C:270:ARG:NH2	2:D:203:GLU:OE2	2.52	0.42
2:C:317:SER:OG	2:C:319:VAL:HG12	2.20	0.42
3:E:67:ILE:HG22	3:E:68:GLY:N	2.35	0.42
3:E:101:ASN:HA	3:E:104:LEU:HB2	2.01	0.42
3:E:388:GLY:O	3:E:405:GLY:HA2	2.19	0.42
4:H:156:LYS:O	4:H:158:PHE:N	2.52	0.42
6:M:22:ASN:HB3	6:M:34:LYS:HE2	2.02	0.42
1:B:332:VAL:O	1:B:336:LEU:N	2.45	0.42
3:E:407:ARG:HB2	3:E:424:LYS:HG2	2.02	0.42
3:F:166:ASP:OD1	3:F:166:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:391:VAL:HG22	3:F:408:LEU:HB2	2.02	0.42
3:F:402:VAL:HA	3:F:419:ILE:HG23	2.02	0.42
4:G:126:LEU:HA	4:G:126:LEU:HD23	1.78	0.42
4:G:295:ARG:HB2	4:G:320:GLU:HB2	2.01	0.42
5:J:217:ASP:OD1	5:J:217:ASP:N	2.49	0.42
2:C:19:ASP:N	2:C:19:ASP:OD1	2.52	0.41
2:D:170:ARG:O	2:D:174:ILE:HG12	2.20	0.41
2:D:235:PHE:N	2:D:261:ASP:OD2	2.52	0.41
5:I:353:ASN:HB3	5:I:370:ASP:HB3	2.02	0.41
5:J:44:PRO:O	5:J:280:TYR:OH	2.23	0.41
6:L:6:ARG:HD2	6:L:11:LYS:HA	2.02	0.41
6:L:102:GLN:HA	6:L:105:LYS:HB3	2.01	0.41
6:L:103:LYS:O	6:L:107:VAL:HG23	2.20	0.41
2:C:97:ALA:O	2:C:101:GLU:HB2	2.21	0.41
2:C:205:ILE:O	2:C:230:ILE:N	2.53	0.41
4:G:446:GLU:OE1	4:G:446:GLU:N	2.47	0.41
5:I:19:GLN:CD	5:I:120:THR:H	2.23	0.41
5:I:116:LYS:HB2	5:I:118:LEU:HD22	2.01	0.41
5:I:379:ILE:HG12	5:I:396:ILE:HG13	2.01	0.41
1:A:163:LYS:HB2	1:B:269:PHE:CE2	2.55	0.41
1:B:142:HIS:HD1	1:B:167:THR:HB	1.85	0.41
1:B:144:PHE:HB2	1:B:178:MET:HB2	2.02	0.41
2:C:19:ASP:HB3	2:C:24:LYS:HB2	2.01	0.41
2:D:280:ALA:HA	2:D:315:LYS:HB3	2.02	0.41
3:F:142:ASP:OD1	3:F:247:HIS:N	2.49	0.41
3:F:360:CYS:HB3	3:F:377:SER:O	2.19	0.41
5:I:196:LYS:HE2	5:I:196:LYS:HB2	1.93	0.41
6:L:111:LEU:HD21	6:L:125:LEU:HB3	2.02	0.41
1:A:322:ASP:N	1:A:322:ASP:OD1	2.54	0.41
1:B:305:ASN:H	1:B:305:ASN:HD22	1.68	0.41
2:C:310:CYS:HA	2:C:367:ILE:HB	2.01	0.41
3:E:358:ALA:O	3:E:360:CYS:N	2.52	0.41
3:F:133:ARG:NH1	3:F:257:GLU:HA	2.36	0.41
3:F:352:GLU:N	3:F:355:LEU:HD22	2.35	0.41
4:G:113:LYS:O	4:G:117:GLU:HG3	2.20	0.41
4:G:179:GLN:NE2	4:G:179:GLN:O	2.53	0.41
5:J:347:ASN:O	5:J:364:SER:HA	2.20	0.41
6:L:171:TYR:OH	6:L:175:ARG:NE	2.53	0.41
1:B:73:VAL:O	1:B:75:ASN:N	2.53	0.41
2:C:2:SER:HB3	2:C:3:THR:H	1.72	0.41
2:C:59:ARG:HH12	2:C:393:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:ILE:HG13	2:C:260:SER:O	2.21	0.41
2:D:230:ILE:HG21	2:D:267:ILE:CD1	2.50	0.41
3:E:235:THR:HG21	5:J:206:PHE:HB3	2.01	0.41
3:E:331:GLU:HB3	3:E:335:CYS:SG	2.61	0.41
3:E:344:ARG:HB2	3:E:344:ARG:NH1	2.36	0.41
3:E:353:ARG:O	3:E:355:LEU:N	2.49	0.41
3:F:250:ILE:O	3:F:254:ARG:HG3	2.21	0.41
2:C:291:SER:HB3	2:C:354:TYR:HA	2.03	0.41
2:D:199:LEU:HD21	2:D:275:ILE:HD11	2.02	0.41
3:E:401:VAL:O	3:E:418:GLN:HA	2.20	0.41
3:F:190:ILE:HG21	3:F:331:GLU:OE2	2.21	0.41
4:H:160:SER:HA	4:H:163:ARG:HD3	2.02	0.41
5:I:31:PHE:CD2	5:I:40:ARG:HG3	2.56	0.41
5:J:145:LYS:O	5:J:148:GLU:HG2	2.21	0.41
5:J:389:LYS:O	5:J:407:VAL:HA	2.20	0.41
6:M:50:LEU:HD21	6:M:56:ARG:HG3	2.02	0.41
6:M:131:TRP:N	6:M:132:PRO:HD2	2.36	0.41
2:D:232:ALA:HB2	2:D:259:ILE:HD11	2.02	0.41
2:D:379:TYR:CG	2:D:380:ARG:N	2.88	0.41
3:F:379:ILE:HG12	3:F:396:LEU:HD22	2.03	0.41
4:G:279:THR:O	4:G:283:VAL:HG23	2.20	0.41
4:H:154:ASN:OD1	4:H:154:ASN:N	2.53	0.41
5:I:54:THR:O	5:I:58:LEU:HD23	2.20	0.41
1:A:82:GLY:O	1:A:86:PHE:N	2.44	0.41
2:D:20:LEU:HA	2:D:20:LEU:HD23	1.79	0.41
3:F:261:SER:N	3:F:265:ASP:OD2	2.46	0.41
3:F:276:GLN:NE2	3:F:276:GLN:O	2.54	0.41
4:H:117:GLU:OE1	4:H:129:ARG:NH1	2.47	0.41
5:J:179:ILE:HG22	5:J:184:SER:HA	2.03	0.41
1:A:87:GLN:HG3	1:A:87:GLN:H	1.72	0.41
1:A:180:ARG:O	1:A:184:ASN:N	2.29	0.41
1:A:255:LEU:N	1:A:259:ASP:OD2	2.47	0.41
1:B:87:GLN:HB3	6:L:29:MET:CE	2.51	0.41
1:B:140:LEU:HD23	1:B:141:THR:N	2.36	0.41
2:C:40:ARG:NH2	2:C:178:GLN:HB2	2.36	0.41
2:C:90:TYR:CZ	2:C:94:LEU:HD13	2.56	0.41
3:E:104:LEU:HD23	3:E:108:TYR:HB2	2.01	0.41
3:E:255:GLU:OE1	3:E:285:ILE:HG12	2.20	0.41
3:F:46:GLY:O	3:F:48:GLY:N	2.54	0.41
3:F:153:GLY:N	3:F:323:ALA:O	2.51	0.41
3:F:401:VAL:HG13	3:F:418:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:222:ILE:HD13	4:G:222:ILE:HA	1.87	0.41
4:G:238:LEU:O	4:G:242:ILE:N	2.46	0.41
4:G:381:PHE:N	4:G:381:PHE:CD1	2.88	0.41
4:G:384:ARG:HD2	4:G:392:TYR:CD2	2.56	0.41
4:H:462:PHE:O	4:H:466:TYR:HB2	2.21	0.41
5:I:356:ILE:HD13	5:I:356:ILE:HA	1.89	0.41
5:J:77:ILE:O	5:J:81:ILE:HG13	2.21	0.41
6:L:20:MET:HE1	6:L:98:GLU:HG2	2.03	0.41
6:M:126:TYR:HA	6:M:130:ALA:HB3	2.03	0.41
1:A:263:SER:OG	1:A:264:ARG:N	2.53	0.41
2:D:333:PRO:HD3	5:J:290:ARG:HB2	2.03	0.41
3:E:64:LEU:HD23	3:E:64:LEU:HA	1.87	0.41
3:F:352:GLU:CD	3:F:370:ASP:HB3	2.41	0.41
3:F:418:GLN:O	3:F:435:ARG:HA	2.21	0.41
5:I:370:ASP:O	5:I:387:SER:HA	2.21	0.41
2:C:13:VAL:O	2:C:17:ILE:HG13	2.20	0.40
3:F:274:GLN:OE1	3:F:315:LYS:N	2.54	0.40
4:G:418:ASN:O	4:G:422:VAL:HG23	2.21	0.40
4:G:419:TRP:CG	4:G:427:LEU:HD13	2.56	0.40
4:H:246:ILE:O	4:H:251:ILE:HG13	2.21	0.40
5:J:63:VAL:O	5:J:93:PHE:HB3	2.21	0.40
1:A:130:TYR:CD2	1:A:131:PRO:HD3	2.56	0.40
1:A:192:VAL:HA	1:B:305:ASN:OD1	2.22	0.40
1:A:197:VAL:H	1:B:228:GLN:NE2	2.19	0.40
1:B:33:ILE:HD12	1:B:33:ILE:O	2.21	0.40
1:B:247:HIS:CD2	1:B:247:HIS:H	2.38	0.40
2:C:50:THR:OG1	2:C:53:GLN:HG2	2.21	0.40
3:E:224:LEU:HD12	3:E:275:TYR:CE1	2.56	0.40
3:F:132:LEU:HD11	3:F:139:ILE:HD11	2.03	0.40
3:F:161:ASP:HA	3:F:164:ARG:HB2	2.03	0.40
5:I:40:ARG:O	5:I:40:ARG:HG2	2.21	0.40
1:A:182:LEU:HB3	1:A:187:ILE:HD11	2.03	0.40
1:B:231:VAL:O	1:B:235:HIS:N	2.52	0.40
2:D:80:ARG:H	2:D:80:ARG:HG3	1.64	0.40
2:D:340:ASN:OD1	5:J:161:GLU:HG2	2.21	0.40
3:E:220:PHE:O	5:J:199:VAL:N	2.50	0.40
3:F:173:VAL:CG1	3:F:242:ILE:HB	2.52	0.40
5:I:51:ILE:HG12	5:I:55:PHE:CD2	2.56	0.40
1:B:229:LEU:HA	1:B:232:PHE:CD2	2.56	0.40
2:C:267:ILE:O	2:C:271:VAL:HG23	2.21	0.40
3:E:440:ARG:HB3	3:E:440:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:133:ARG:HH22	3:F:259:ILE:HB	1.87	0.40
4:G:159:GLY:HA3	4:G:163:ARG:HD2	2.03	0.40
4:G:280:VAL:O	4:G:284:LEU:HG	2.22	0.40
5:J:171:ARG:HA	5:J:171:ARG:HD3	1.85	0.40
6:L:128:THR:OG1	6:L:129:ILE:HG12	2.21	0.40
1:A:209:VAL:O	1:A:242:ALA:HA	2.21	0.40
2:D:19:ASP:HB3	2:D:24:LYS:HB2	2.04	0.40
2:D:76:GLY:O	2:D:80:ARG:HG3	2.21	0.40
2:D:227:PHE:O	2:D:254:ILE:HG13	2.22	0.40
2:D:267:ILE:O	2:D:271:VAL:HG23	2.21	0.40
3:E:216:SER:O	3:E:218:PHE:N	2.54	0.40
5:J:35:THR:HA	5:J:38:LYS:O	2.20	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	312/341 (92%)	271 (87%)	36 (12%)	5 (2%)	9 43
1	B	312/341 (92%)	268 (86%)	39 (12%)	5 (2%)	9 43
2	C	334/399 (84%)	299 (90%)	33 (10%)	2 (1%)	25 64
2	D	333/399 (84%)	300 (90%)	27 (8%)	6 (2%)	8 41
3	E	410/458 (90%)	327 (80%)	72 (18%)	11 (3%)	5 33
3	F	408/458 (89%)	344 (84%)	51 (12%)	13 (3%)	4 29
4	G	361/467 (77%)	321 (89%)	36 (10%)	4 (1%)	14 52
4	H	361/467 (77%)	330 (91%)	20 (6%)	11 (3%)	4 30
5	I	426/678 (63%)	369 (87%)	54 (13%)	3 (1%)	22 61
5	J	424/678 (62%)	378 (89%)	43 (10%)	3 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	L	159/304 (52%)	134 (84%)	23 (14%)	2 (1%)	12 48
6	M	160/304 (53%)	133 (83%)	23 (14%)	4 (2%)	5 34
All	All	4000/5294 (76%)	3474 (87%)	457 (11%)	69 (2%)	9 42

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	289	LEU
3	E	359	ASP
4	G	303	PRO
4	H	303	PRO
6	M	61	LEU
1	A	263	SER
1	B	92	ARG
2	D	186	LYS
2	D	234	GLY
2	D	341	GLU
3	E	258	SER
3	E	341	PRO
3	F	49	ASN
3	F	190	ILE
3	F	216	SER
3	F	289	LEU
3	F	359	ASP
3	F	450	MET
1	A	98	GLY
1	B	74	GLN
1	B	98	GLY
2	D	68	ALA
3	E	139	ILE
3	F	189	GLU
4	G	276	HIS
4	G	305	PHE
4	G	409	PHE
4	H	276	HIS
6	L	160	PRO
6	M	168	LEU
1	A	255	LEU
1	B	263	SER
2	C	50	THR
2	D	185	ASP

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Mol	Chain	Res	Type
3	E	56	GLY
3	E	288	PHE
3	F	47	PHE
3	F	329	TYR
4	H	158	PHE
4	H	304	GLU
4	H	305	PHE
5	I	431	LEU
6	M	123	GLU
6	M	136	LYS
1	A	74	GLN
1	B	247	HIS
2	C	2	SER
3	E	49	ASN
3	E	140	LYS
3	E	280	THR
3	E	329	TYR
3	F	307	ILE
3	F	397	MET
4	H	107	ALA
4	H	157	ILE
4	H	320	GLU
4	H	327	SER
5	I	117	GLN
5	I	406	VAL
5	J	174	SER
6	L	164	VAL
1	A	247	HIS
2	D	170	ARG
5	J	426	HIS
5	J	434	PRO
4	H	465	VAL
4	H	413	PRO
3	F	135	VAL
3	F	183	ILE

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	274/298 (92%)	263 (96%)	11 (4%)	31	64
1	B	274/298 (92%)	264 (96%)	10 (4%)	35	66
2	C	291/350 (83%)	280 (96%)	11 (4%)	33	65
2	D	290/350 (83%)	281 (97%)	9 (3%)	40	70
3	E	359/395 (91%)	334 (93%)	25 (7%)	15	46
3	F	357/395 (90%)	335 (94%)	22 (6%)	18	51
4	G	326/408 (80%)	307 (94%)	19 (6%)	20	53
4	H	326/408 (80%)	310 (95%)	16 (5%)	25	59
5	I	379/596 (64%)	370 (98%)	9 (2%)	49	76
5	J	378/596 (63%)	366 (97%)	12 (3%)	39	69
6	L	152/274 (56%)	145 (95%)	7 (5%)	27	61
6	M	153/274 (56%)	146 (95%)	7 (5%)	27	61
All	All	3559/4642 (77%)	3401 (96%)	158 (4%)	28	62

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	102	GLN
1	A	134	ARG
1	A	178	MET
1	A	184	ASN
1	A	195	SER
1	A	235	HIS
1	A	253	PHE
1	A	262	PHE
1	A	299	GLU
1	A	329	LYS
1	B	89	PHE
1	B	102	GLN
1	B	121	CYS
1	B	145	SER
1	B	146	ARG
1	B	159	HIS
1	B	161	ARG
1	B	174	SER
1	B	253	PHE

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Mol	Chain	Res	Type
1	B	262	PHE
2	C	19	ASP
2	C	22	SER
2	C	59	ARG
2	C	75	CYS
2	C	87	ARG
2	C	92	GLU
2	C	197	ASP
2	C	261	ASP
2	C	311	SER
2	C	332	SER
2	C	340	ASN
2	D	65	LEU
2	D	74	SER
2	D	167	MET
2	D	238	ASN
2	D	260	SER
2	D	311	SER
2	D	338	SER
2	D	339	PHE
2	D	354	TYR
3	E	47	PHE
3	E	49	ASN
3	E	57	SER
3	E	72	MET
3	E	79	TRP
3	E	92	CYS
3	E	99	HIS
3	E	141	ASN
3	E	147	SER
3	E	148	CYS
3	E	220	PHE
3	E	223	SER
3	E	276	GLN
3	E	277	LYS
3	E	306	GLU
3	E	322	ARG
3	E	330	PHE
3	E	344	ARG
3	E	360	CYS
3	E	382	ASN
3	E	392	SER

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Mol	Chain	Res	Type
3	E	410	SER
3	E	435	ARG
3	E	440	ARG
3	E	449	ASP
3	F	29	ASN
3	F	39	PHE
3	F	85	PHE
3	F	99	HIS
3	F	113	ARG
3	F	124	ASP
3	F	141	ASN
3	F	147	SER
3	F	166	ASP
3	F	175	SER
3	F	218	PHE
3	F	228	HIS
3	F	234	ASN
3	F	238	SER
3	F	276	GLN
3	F	282	ARG
3	F	308	LYS
3	F	315	LYS
3	F	330	PHE
3	F	359	ASP
3	F	369	LYS
3	F	392	SER
4	G	106	ASP
4	G	118	LYS
4	G	121	SER
4	G	123	PHE
4	G	125	HIS
4	G	147	ARG
4	G	156	LYS
4	G	158	PHE
4	G	171	PHE
4	G	208	SER
4	G	217	PHE
4	G	225	LEU
4	G	237	LEU
4	G	240	GLU
4	G	301	SER
4	G	331	TYR

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Mol	Chain	Res	Type
4	G	354	SER
4	G	423	LYS
4	G	438	ARG
4	H	106	ASP
4	H	121	SER
4	H	123	PHE
4	H	125	HIS
4	H	147	ARG
4	H	158	PHE
4	H	166	ASP
4	H	171	PHE
4	H	208	SER
4	H	217	PHE
4	H	277	SER
4	H	301	SER
4	H	317	HIS
4	H	354	SER
4	H	418	ASN
4	H	464	GLN
5	I	40	ARG
5	I	55	PHE
5	I	84	SER
5	I	91	SER
5	I	138	GLU
5	I	163	SER
5	I	228	ASN
5	I	255	ASP
5	I	370	ASP
5	J	40	ARG
5	J	84	SER
5	J	101	ARG
5	J	147	ARG
5	J	163	SER
5	J	238	PHE
5	J	255	ASP
5	J	275	ARG
5	J	290	ARG
5	J	325	CYS
5	J	347	ASN
5	J	424	GLU
6	L	4	HIS
6	L	36	LEU

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Mol	Chain	Res	Type
6	L	90	SER
6	L	113	TYR
6	L	144	PHE
6	L	145	LYS
6	L	154	TRP
6	M	10	ASN
6	M	76	ASP
6	M	90	SER
6	M	113	TYR
6	M	125	LEU
6	M	144	PHE
6	M	154	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	ASN
1	B	228	GLN
2	C	45	GLN
2	D	194	GLN
2	D	198	HIS
2	D	302	HIS
3	F	325	ASN
3	F	393	ASN
4	G	179	GLN
5	I	28	ASN
5	I	117	GLN
6	M	59	GLN
6	M	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
7	PO4	E	502	-	4,4,4	0.99	0	6,6,6	0.48	0
7	PO4	H	501	-	4,4,4	1.03	0	6,6,6	0.47	0
7	PO4	F	502	-	4,4,4	0.99	0	6,6,6	0.48	0
7	PO4	E	501	-	4,4,4	1.03	0	6,6,6	0.48	0
7	PO4	G	501	-	4,4,4	1.02	0	6,6,6	0.53	0
7	PO4	F	501	-	4,4,4	1.05	0	6,6,6	0.42	0
7	PO4	D	401	-	4,4,4	1.02	0	6,6,6	0.42	0
7	PO4	C	401	-	4,4,4	1.01	0	6,6,6	0.46	0

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	502	PO4	1	0
7	H	501	PO4	1	0
7	G	501	PO4	1	0
7	C	401	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	316/341 (92%)	-0.40	1 (0%)	94	91	109, 145, 196, 237	0
1	B	316/341 (92%)	-0.31	4 (1%)	77	71	106, 146, 196, 238	0
2	C	338/399 (84%)	-0.31	0	100	100	79, 121, 185, 214	0
2	D	337/399 (84%)	-0.31	0	100	100	76, 120, 189, 232	0
3	E	414/458 (90%)	-0.31	3 (0%)	87	83	88, 139, 206, 234	0
3	F	412/458 (89%)	-0.35	1 (0%)	95	93	93, 138, 205, 236	0
4	G	363/467 (77%)	-0.31	1 (0%)	94	91	87, 122, 187, 235	0
4	H	363/467 (77%)	-0.26	3 (0%)	86	81	88, 119, 191, 228	0
5	I	428/678 (63%)	-0.38	0	100	100	101, 141, 187, 209	0
5	J	426/678 (62%)	-0.40	0	100	100	100, 141, 184, 222	0
6	L	165/304 (54%)	-0.36	2 (1%)	79	73	121, 203, 232, 244	0
6	M	166/304 (54%)	-0.43	1 (0%)	89	86	121, 202, 236, 253	0
All	All	4044/5294 (76%)	-0.34	16 (0%)	92	90	76, 137, 209, 253	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	467	ALA	5.9
3	E	31	GLN	5.5
3	E	29	ASN	4.3
1	B	292	HIS	3.6
3	F	28	GLY	3.1
1	A	293	ASN	3.1
4	H	183	GLY	3.0
4	H	106	ASP	2.5
6	L	161	SER	2.4
1	B	294	GLU	2.4
3	E	430	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	293	ASN	2.3
6	M	160	PRO	2.2
1	B	291	ILE	2.1
6	L	175	ARG	2.0
4	G	464	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PO4	F	502	5/5	0.89	0.19	172,179,190,228	0
7	PO4	G	501	5/5	0.90	0.23	115,136,151,154	0
7	PO4	E	501	5/5	0.91	0.19	114,122,147,186	0
7	PO4	C	401	5/5	0.92	0.19	98,137,158,184	0
7	PO4	H	501	5/5	0.92	0.20	105,106,166,171	0
7	PO4	F	501	5/5	0.93	0.24	113,128,142,183	0
7	PO4	D	401	5/5	0.95	0.26	80,107,166,167	0
7	PO4	E	502	5/5	0.95	0.20	171,171,195,223	0

6.5 Other polymers (i)

There are no such residues in this entry.