Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 09:49 AM EDT

PDB ID	:	6JLZ
Title	:	P-eIF2a - eIF2B complex
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Deposited on	:	2019-03-07
Resolution	:	3.35 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:

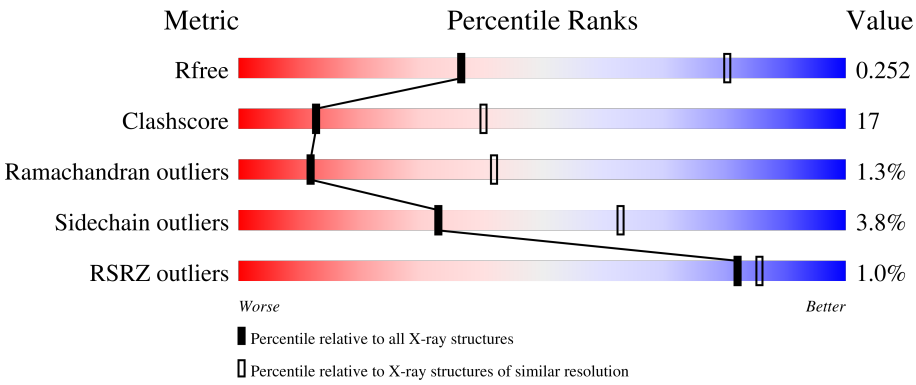
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	% 53% 38% • 7%
1	B	341	% 56% 34% • 8%
2	C	399	51% 32% • 16%
2	D	399	55% 30% 16%
3	E	458	% 55% 31% • 11%

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Mol	Chain	Length	Quality of chain
3	F	458	%, 55%, 31%, 11%
4	G	467	52%, 24%, 23%
4	H	467	48%, 27%, 23%
5	I	678	%, 37%, 25%, 37%
5	J	678	%, 35%, 27%, 37%
6	L	304	3%, 31%, 23%, 45%
6	M	304	2%, 29%, 24%, 44%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	A	401	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31826 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	317	2476	1573	433	457	13	0	0	0
1	B	315	2457	1562	428	454	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	337	2609	1654	442	501	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	409	3178	2018	548	595	17	0	0	0
3	F	409	3178	2018	548	595	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	360	2845	1818	483	531	13	0	0	0
4	H	361	2857	1827	484	533	13	0	0	0

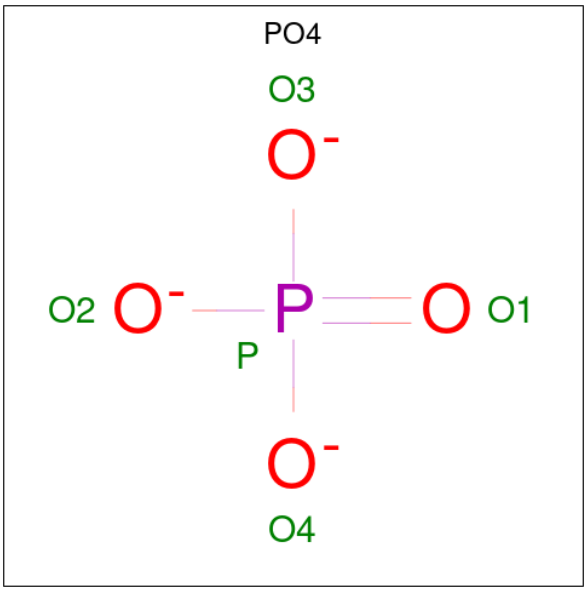
- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	I	430	3393	2134	595	649	15	0	0	0
5	J	428	3377	2123	592	647	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	P	S			
6	L	167	1387	883	237	260	1	6	0	0	0
6	M	169	1400	890	239	264	1	6	0	0	0

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



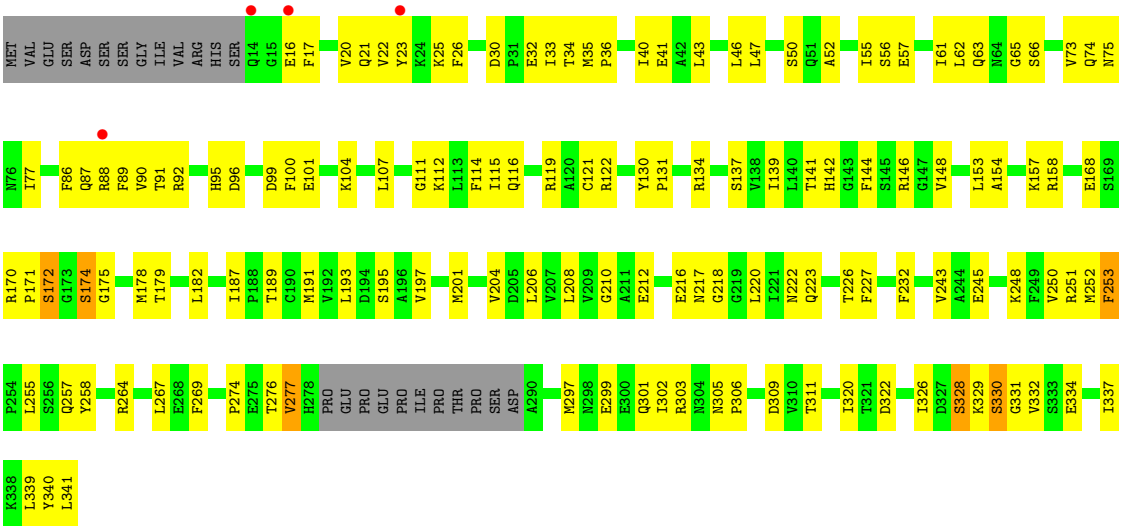
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	A	1	5	4	1	0	0
7	B	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	D	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	F	1	5	4	1	0	0
7	F	1	5	4	1	0	0
7	G	1	5	4	1	0	0
7	H	1	5	4	1	0	0
7	I	1	5	4	1	0	0
7	J	1	5	4	1	0	0

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.

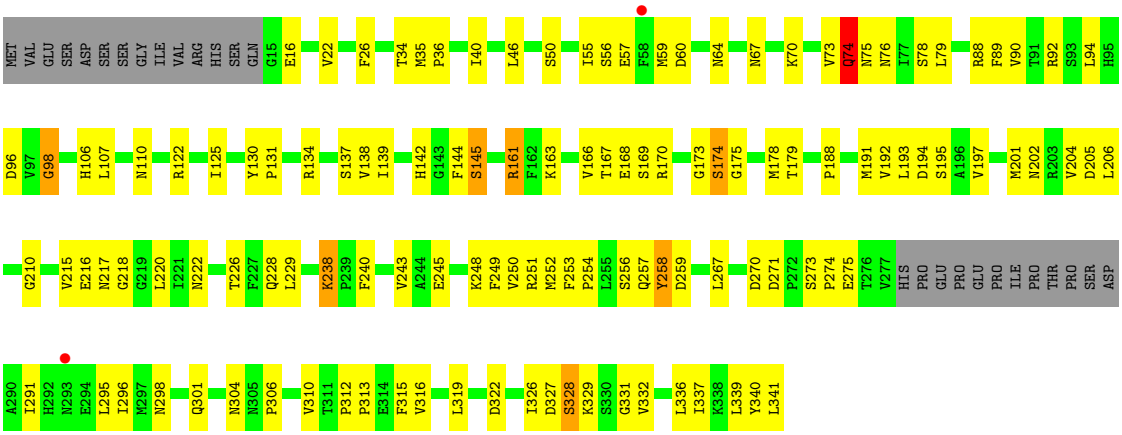
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



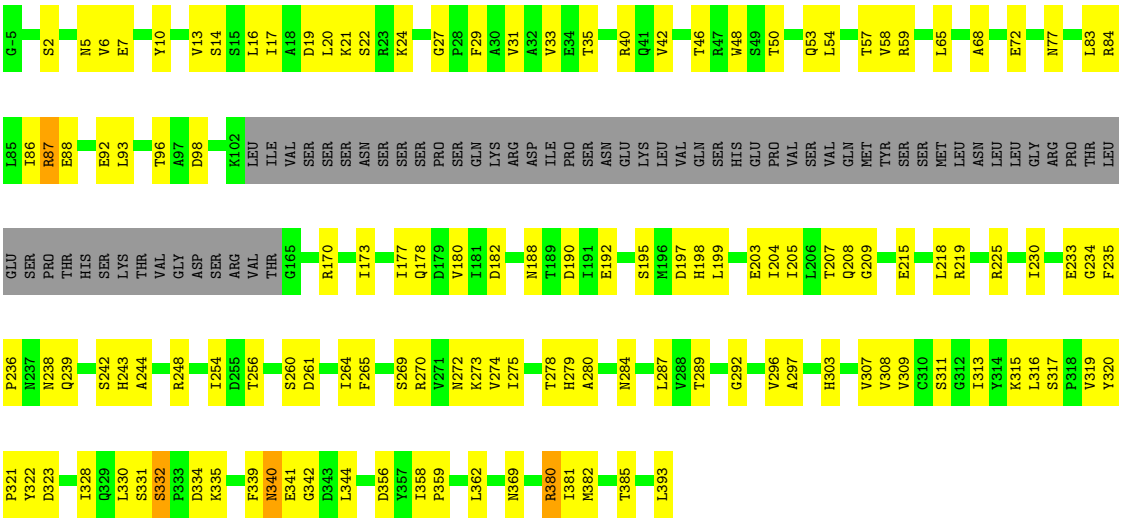
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B:



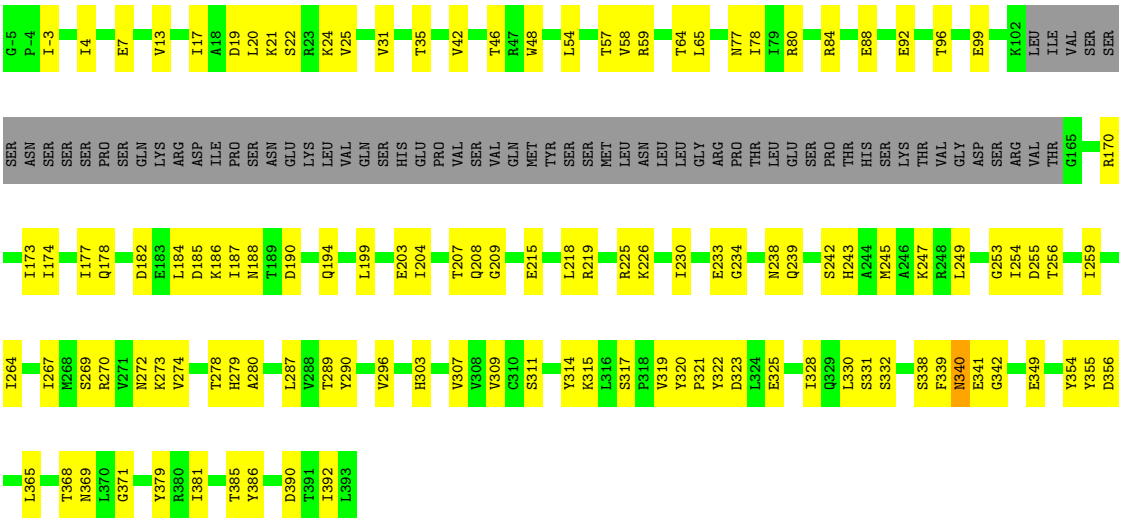
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta

Chain C:



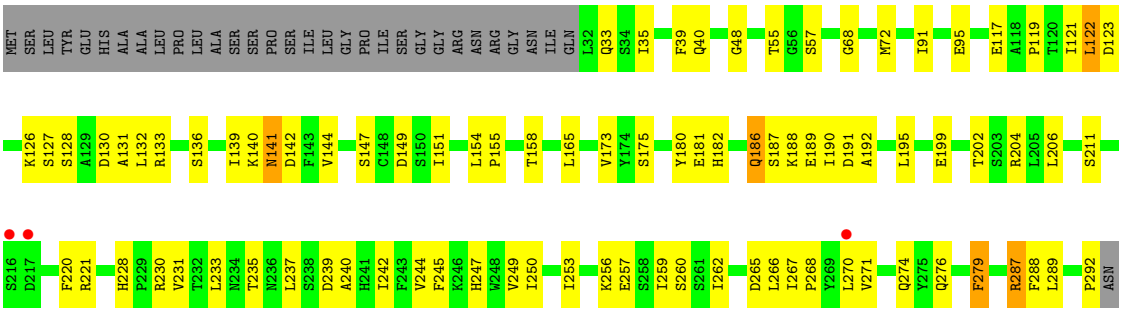
- Molecule 2: Probable translation initiation factor eIF-2B subunit beta

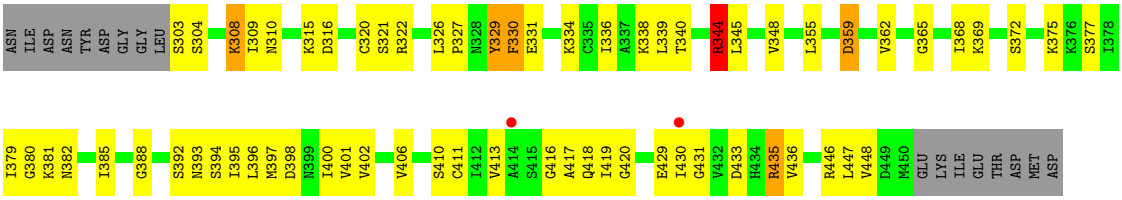
Chain D:



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

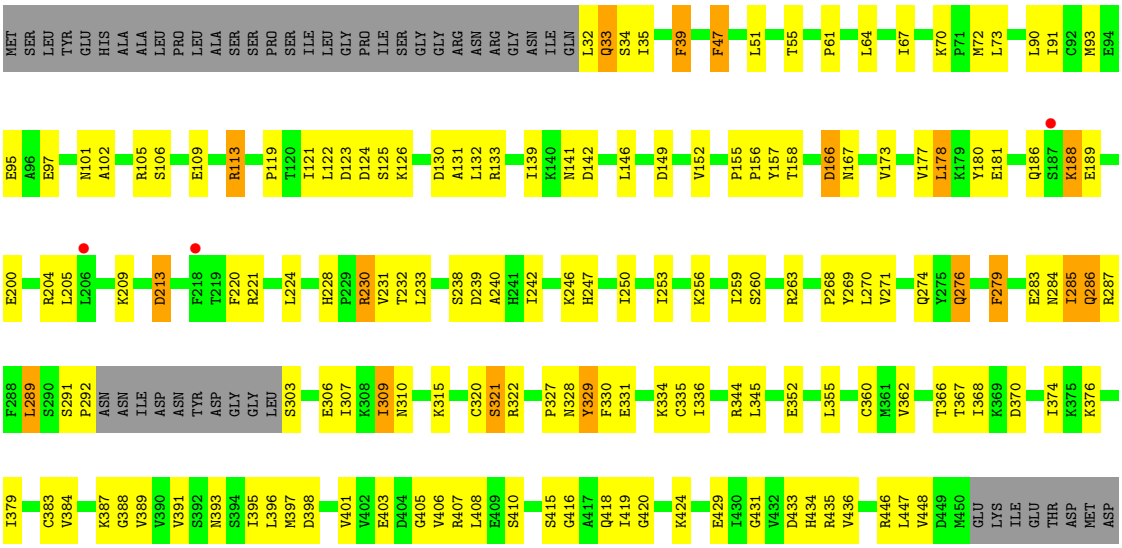
Chain E:





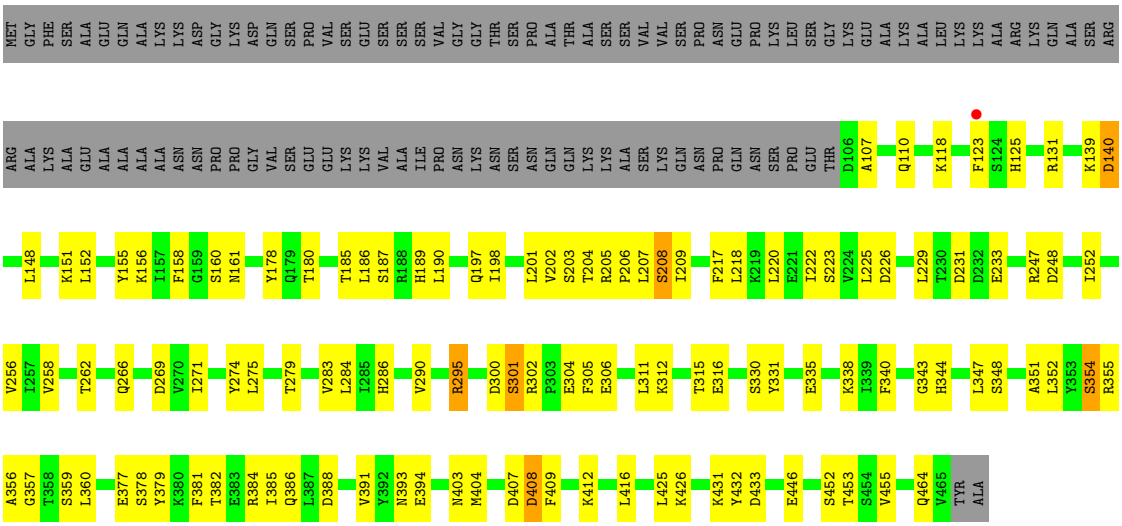
• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

Chain F:



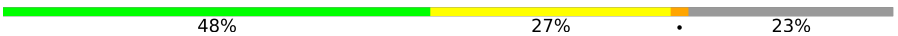
• Molecule 4: Probable translation initiation factor eIF-2B subunit delta

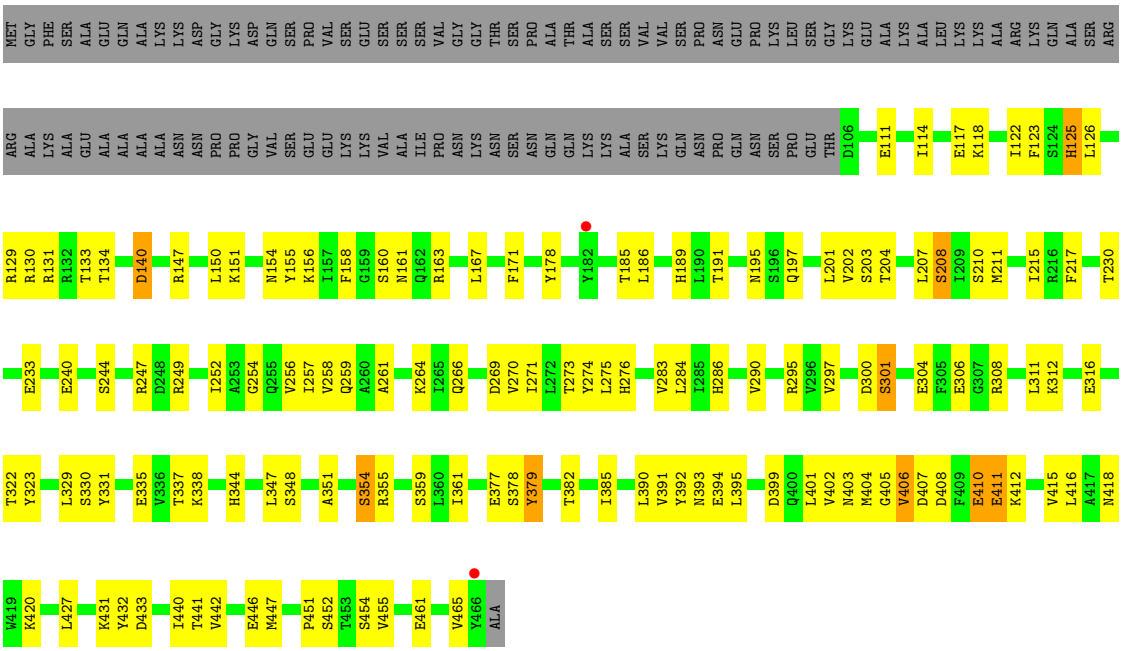
Chain G:



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

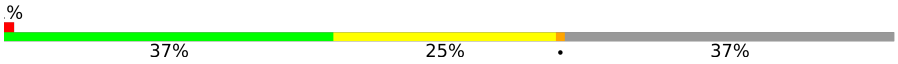
Chain H:

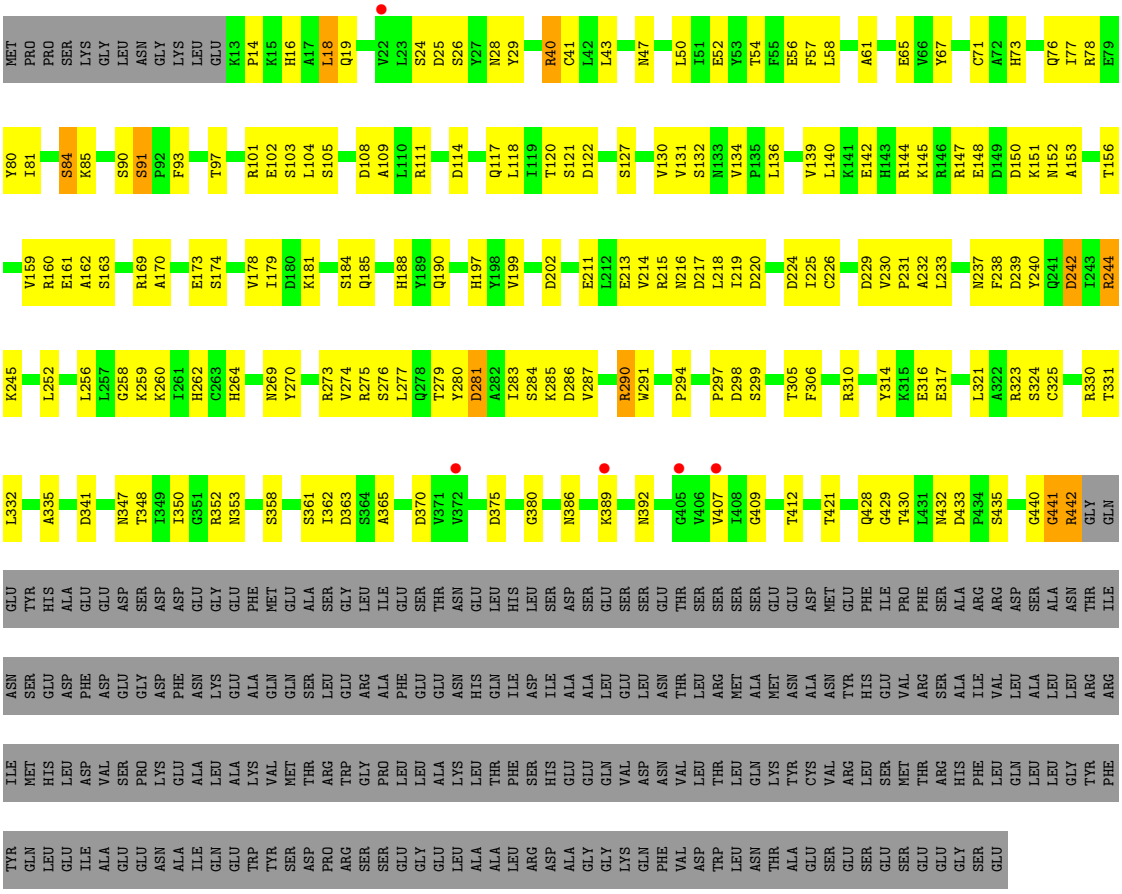




• Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon

Chain I:





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

Chain J: %
35% 27% • 37%

MET PRO PRO SER LYS GLY LEU ASN GLY LYS LEU GLU LYS PRO K15 H16 A17 L18 Q19 A20 I21 S24 D25 S26 Y29 R30 F31 R32 T35 R40 C41 I42 L43 L50 I51 E52 Y53 T54 F55 E56 F57 L58 A61 G62 V63 Q64 E65 V66 Y67 C70 H73

Q76 I77 Y80 I81 S84 L88 P89 S90 T97 R101 E102 S103 L104 S105 D108 R111 E112 L113 D114 L118 I119 T120 S121 D122 F123 I124 S127 G128 D129 V130 V131 S132 N133 V134 P135 L136 N137 E138 V139 L140 H143 R144 K145 R146 R147 E148 D149 D150 K151

T156 V159 R160 E161 A162 S163 R169 A170 R171 T172 E173 S174 V178 I179 D180 S184 Q185 C186 Q190 V199 D202 F206 H209 E210 E211 L212 E213 V214 R215 N216 D217 L218 I219 D220 C221 Q222 I223 D224 I225 N228 A232 L233 F234 F238 D239 Y240 Q241 D242

I243 R244 K245 D246 F247 V248 Y249 T253 S254 D255 L256 L257 G258 K259 K260 I261 H262 C263 K267 E268 N269 Y270 A271 A272 R273 V274 R275 D281 K285 L288 S289 R290 W291 V292 Y293 P294 F295 V296 P297 D298 S299 N300 L301 T305 Y308 Q309 R310 I313 Y314 K315 E316

V320 R323 S324 C325 K328 T331 A335 Y336 T337 K338 A346 N347 T348 G351 R352 N353 C354 T355 I356 G357 S358 L367 D370 V371 V372 I373 G374 D375 N376 I379 G380 K381 L384 S387 V388 K389 I390 S395 I396 E397 D398 V402 G409 D410 N411 T412

I413 I414 E415 K418 T421 E424 S425 Q428 G429 N432 D433 P434 S435 L436 V437 G438 I439 G440 G441 R442 GLY GLN GLU TYR HIS ALA GLU GLU ASP SER ASP ASP GLU GLY GLU PHE MET GLU ALA SER GLY LEU ILE GLU SER THR ASN GLU LEU HIS LEU SER ASP SER GLU

SER SER GLU THR SER SER SER SER GLU GLU ASP MET GLU PHE ILE PRO PHE SER ALA ARG ARG ASP SER ALA ASN THR ILE ASN SER GLU ASP PHE ASP GLU GLY ASP PHE ASN LYS GLU ALA GLN GLN SER LEU GLU GLU ASN HIS GLN ILE ASP ILE ALA ALA LEU

GLU LEU ASN THR LEU ARG MET ALA MET ASN ALA ASN TYR HIS GLU VAL ARG SER ALA ILE VAL LEU ALA LEU LEU ARG ARG ILE MET HIS LEU ASP VAL SER PRO LYS GLU ALA LEU ALA LYS VAL MET THR ARG TRP GLY PRO LEU LEU LEU ALA LYS LEU THR PHE SER HIS GLU GLU GLN

VAL ASP ASN VAL LEU THR LEU GLN LYS TYR VAL ARG LEU SER MET THR ARG HIS PHE LEU GLN LEU LEU GLY TYR PHE TYR GLN LEU GLU ILE ALA GLU GLU ASN ALA ILE GLN GLU TRP TYR SER ASP PRO ARG SER SER GLU GLY GLU LEU ALA ALA LEU ARG ASP ALA GLY GLY

LYS GLN PHE VAL ASP TRP LEU ASN THR ALA GLU SER GLU SER GLU GLU GLY SER GLU

• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain L: 3%
31% 23% • 45%

MET SER THR SER H4 C5 R6 F7 Y8 E9 N10 K11 E14 D17 I18 V19 M20 V21 N22 A27 E28 M29 L35 L36 E37 E42 L46 S51 R52 R53 R54 I55 R56 S57 I58 Q59 K60 K66 N67 D68 R74 V75 D76 K77 E78 Y81 I82 D83 L84 S85

K86 S90 S91 E92 D93 I94 C97 E98 E99 K100 Y101 Q102 K103 S104 K105 T106 L111 R112 Y113 C114 A115 E116 LYS PHE GLN ILE PRO L122 E123 E124 L125 Y126 K127 T128 I129 A130 W131 P132 R135 Y141 K145 L146 S147 I148 I149 D150 E151 T152 Y153 P159 P160 S161 K162

L165 D166 E167 L168 Y171 I172 R175 LEU THR PRO GLN ALA VAL LYS ILE ARG ALA ASP VAL GLU VAL SER CYS PHE SER TYR GLU GLY ILE ASP ALA VAL LYS ASP ALA LEU LYS SER ALA GLU ASP MET SER THR GLU GLN MET GLN VAL LYS VAL LYS LEU VAL ALA PRO

LEU TYR VAL LEU THR THR GLN ALA LEU ASP LYS GLN LYS GLY ILE GLU GLN LEU GLU SER ALA ILE GLU LYS ILE THR GLU VAL ILE THR LYS TYR GLY GLY VAL CYS ASN ILE THR MET PRO PRO LYS ASP VAL THR ALA THR GLU ASP ALA GLU LEU GLN ALA LEU LEU GLU SER LYS

GLU LEU ASP ASN ARG SER ASP SER GLU ASP ASP ASP GLU ASP GLU SER ASP GLU

• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain M:

MET SER T2 C5 R6 F7 Y8 E9 N10 E14 D17 V21 N22 E28 M29 K34 N40 L47 S48 E49 L50 S51 R52 R53 R54 I55 R56 S57 I58 Q59 K60 G65 K66 N67 D68 V69 R74 W75 D76 Y81 I82 D83 R88 I94 I95 K96 C97

E98 E99 K100 Y101 Q102 K103 S104 K105 T106 I110 L111 A115 E116 LYS PHE GLN ILE PRO L122 E123 E124 L125 Y126 K127 T128 I129 A130 W131 P132 L133 S134 R135 K136 H139 A140 Y141 E142 A143 F144 K145 L146 S147 I148 I149 D150 E151 W154 E155 G156 I157 E158 P159 K162 L165

D166 K169 I172 S173 K174 R175 LEU THR PRO GLN ALA VAL LYS ILE ARG ALA ASP VAL GLU VAL SER CYS PHE SER TYR GLU GLY ILE ASP ALA ILE LYS ASP ALA LEU LYS SER ALA GLU ASP MET SER THR GLU GLN MET GLN VAL LYS VAL LYS LEU VAL ALA ALA PRO LEU TYR

VAL LEU THR THR GLN ALA LEU ASP LYS GLN LYS GLY ILE GLU GLN LEU GLU SER ALA ILE GLU LYS ILE THR GLU VAL ILE THR LYS TYR GLY GLY VAL CYS ASN ILE THR MET PRO PRO LYS ALA VAL THR ALA THR GLU ASP ALA GLU LEU GLN ALA LEU LEU GLU SER LYS GLU LEU

ASP ASN ARG SER ASP SER GLU ASP ASP GLU ASP GLU SER ASP ASP GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	155.58Å 207.71Å 155.74Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	49.31 – 3.35 49.31 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.31-3.35) 89.6 (49.31-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.61 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.221 , 0.253 0.221 , 0.252	Depositor DCC
R_{free} test set	1982 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.408 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31826	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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, SEP

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	0.34	0/2522	0.45	0/3411
1	B	0.34	0/2502	0.45	0/3384
2	C	0.37	0/2653	0.45	0/3600
2	D	0.38	0/2653	0.45	0/3600
3	E	0.36	0/3234	0.51	0/4376
3	F	0.36	0/3234	0.51	1/4376 (0.0%)
4	G	0.38	0/2892	0.46	0/3916
4	H	0.37	0/2905	0.45	0/3934
5	I	0.35	0/3454	0.48	0/4681
5	J	0.35	0/3437	0.48	0/4658
6	L	0.29	0/1398	0.44	0/1875
6	M	0.29	0/1411	0.44	0/1893
All	All	0.35	0/32295	0.47	1/43704 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	2
3	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	289	LEU	CA-CB-CG	5.79	128.62	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	340	THR	Peptide
3	E	344	ARG	Peptide
3	F	344	ARG	Peptide

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	2476	0	2498	109	0
1	B	2457	0	2483	102	0
2	C	2609	0	2642	92	0
2	D	2609	0	2642	81	0
3	E	3178	0	3239	99	0
3	F	3178	0	3239	106	1
4	G	2845	0	2937	80	0
4	H	2857	0	2946	91	0
5	I	3393	0	3381	126	0
5	J	3377	0	3361	143	0
6	L	1387	0	1415	61	1
6	M	1400	0	1425	64	0
7	A	5	0	0	2	0
7	B	5	0	0	0	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	0	0
7	F	10	0	0	1	0
7	G	5	0	0	1	0
7	H	5	0	0	0	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
All	All	31826	0	32208	1063	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1063) 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)
6:L:68:ASP:OD2	6:L:86:LYS:HE2	1.39	1.19
5:I:290:ARG:NH1	5:I:298:ASP:OD2	1.90	1.05
1:A:216:GLU:OE2	1:A:251:ARG:NH1	1.93	1.01
5:J:242:ASP:OD1	5:J:245:LYS:N	1.99	0.95
3:E:230:ARG:NH2	5:J:213:GLU:OE2	2.01	0.94
6:L:68:ASP:OD2	6:L:86:LYS:CE	2.16	0.93
5:I:56:GLU:OE2	5:I:85:LYS:NZ	2.01	0.93
5:I:242:ASP:OD1	5:I:245:LYS:N	2.05	0.90
1:B:216:GLU:OE2	1:B:251:ARG:NE	2.05	0.90
4:H:359:SER:OG	4:H:433:ASP:OD2	1.90	0.89
4:H:312:LYS:NZ	4:H:316:GLU:OE2	2.04	0.89
3:F:329:TYR:OH	3:F:429:GLU:OE2	1.92	0.87
5:I:65:GLU:OE2	5:I:67:TYR:OH	1.94	0.86
5:I:150:ASP:OD2	5:I:260:LYS:NZ	2.09	0.85
5:J:65:GLU:OE2	5:J:67:TYR:OH	1.92	0.85
3:F:123:ASP:OD1	3:F:125:SER:N	2.09	0.85
3:E:329:TYR:OH	3:E:429:GLU:OE2	1.95	0.84
5:I:25:ASP:H	5:I:40:ARG:HH22	1.23	0.84
1:B:56:SER:OG	6:L:83:ASP:OD1	1.95	0.84
3:F:95:GLU:OE2	3:F:95:GLU:N	2.10	0.83
2:C:17:ILE:HG22	2:C:21:LYS:HD2	1.61	0.83
3:E:199:GLU:OE2	3:E:202:THR:OG1	1.96	0.83
1:B:259:ASP:OD2	4:H:264:LYS:NZ	2.12	0.82
4:H:240:GLU:OE2	4:H:244:SER:OG	1.97	0.82
1:A:56:SER:OG	6:M:83:ASP:OD1	1.98	0.81
5:J:421:THR:H	5:J:429:GLY:HA3	1.45	0.81
4:G:384:ARG:NH1	4:G:386:GLN:OE1	2.14	0.81
3:E:95:GLU:N	3:E:95:GLU:OE2	2.14	0.80
3:F:152:VAL:HG11	3:F:242:ILE:HD11	1.63	0.80
4:H:399:ASP:OD2	4:H:420:LYS:NZ	2.12	0.80
4:G:378:SER:OG	4:G:446:GLU:OE2	1.99	0.80
5:J:111:ARG:NH1	5:J:234:PHE:O	2.14	0.79
2:D:338:SER:OG	2:D:340:ASN:OD1	2.00	0.79
5:J:290:ARG:NH2	5:J:298:ASP:OD2	2.17	0.78
5:J:105:SER:OG	5:J:108:ASP:OD2	2.02	0.78
1:A:303:ARG:HE	1:B:291:ILE:HG13	1.47	0.78
2:D:178:GLN:NE2	2:D:182:ASP:OD1	2.16	0.77
2:C:86:ILE:HG22	2:C:173:ILE:HD12	1.66	0.77
5:J:111:ARG:NH2	5:J:240:TYR:O	2.17	0.77
6:M:69:VAL:HG11	6:M:94:ILE:HG23	1.66	0.77
3:F:181:GLU:H	3:F:334:LYS:HE2	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:410:GLU:OE2	4:H:412:LYS:NZ	2.17	0.76
5:J:19:GLN:NE2	5:J:118:LEU:O	2.18	0.76
6:L:159:PRO:HG3	6:L:165:LEU:HG	1.67	0.76
4:G:271:ILE:HD11	4:G:284:LEU:HD21	1.68	0.76
5:I:111:ARG:NH2	5:I:240:TYR:O	2.17	0.75
5:I:220:ASP:OD1	5:I:244:ARG:NH2	2.20	0.75
3:E:320:CYS:SG	3:E:321:SER:N	2.59	0.75
3:F:97:GLU:O	3:F:101:ASN:ND2	2.19	0.75
4:H:378:SER:OG	4:H:446:GLU:OE2	2.00	0.75
2:D:233:GLU:OE2	2:D:243:HIS:NE2	2.20	0.75
2:C:270:ARG:NH2	2:D:203:GLU:OE2	2.19	0.74
3:F:133:ARG:NH1	3:F:253:ILE:O	2.19	0.74
5:I:127:SER:O	5:I:273:ARG:NH1	2.20	0.74
1:B:222:ASN:HB3	1:B:226:THR:HG21	1.68	0.74
6:L:53:ARG:HB3	6:L:58:ILE:HG13	1.70	0.74
6:L:14:GLU:N	6:L:17:ASP:OD2	2.20	0.73
4:H:331:TYR:O	5:J:310:ARG:NH2	2.20	0.73
4:G:331:TYR:O	5:I:310:ARG:NH2	2.19	0.73
5:J:160:ARG:NH2	5:J:269:ASN:O	2.21	0.73
5:I:421:THR:H	5:I:429:GLY:HA3	1.53	0.72
3:F:418:GLN:OE1	3:F:435:ARG:NH1	2.22	0.72
4:G:354:SER:OG	4:G:355:ARG:N	2.20	0.72
5:I:316:GLU:OE2	5:I:352:ARG:NH2	2.20	0.72
2:C:40:ARG:NH2	2:C:178:GLN:OE1	2.20	0.72
4:G:295:ARG:NH2	4:G:335:GLU:OE1	2.23	0.72
4:G:393:ASN:OD1	4:G:394:GLU:N	2.21	0.72
5:I:173:GLU:OE2	5:I:275:ARG:NE	2.22	0.71
5:J:424:GLU:OE2	5:J:424:GLU:N	2.23	0.71
5:I:40:ARG:HH21	5:I:41:CYS:HB3	1.55	0.71
2:C:178:GLN:NE2	2:C:182:ASP:OD1	2.23	0.71
5:J:290:ARG:HH21	5:J:296:VAL:HG11	1.56	0.71
4:G:140:ASP:O	4:G:197:GLN:NE2	2.22	0.71
3:E:276:GLN:OE1	3:E:279:PHE:N	2.24	0.70
3:E:362:VAL:HG12	3:E:379:ILE:HB	1.74	0.70
4:G:393:ASN:ND2	4:G:432:TYR:O	2.24	0.70
5:I:181:LYS:NZ	5:I:211:GLU:OE2	2.17	0.70
4:H:264:LYS:O	4:H:338:LYS:NZ	2.25	0.70
4:G:355:ARG:HH12	4:G:431:LYS:HB2	1.56	0.69
4:H:393:ASN:OD1	4:H:394:GLU:N	2.20	0.69
5:J:180:ASP:OD2	5:J:209:HIS:ND1	2.18	0.69
2:C:233:GLU:OE1	2:C:243:HIS:NE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:340:ASN:ND2	5:I:161:GLU:OE1	2.23	0.69
3:E:130:ASP:OD1	3:E:260:SER:HA	1.93	0.69
6:M:100:LYS:HA	6:M:103:LYS:HZ2	1.58	0.68
1:A:146:ARG:NH1	7:A:401:PO4:O1	2.26	0.68
2:D:7:GLU:OE2	5:J:90:SER:OG	2.06	0.68
3:F:327:PRO:HA	3:F:331:GLU:HB2	1.76	0.68
1:B:298:ASN:OD1	1:B:301:GLN:N	2.25	0.68
2:D:330:LEU:O	5:J:290:ARG:NH1	2.26	0.68
5:J:354:CYS:SG	5:J:355:THR:N	2.66	0.68
1:B:60:ASP:O	1:B:64:ASN:ND2	2.24	0.68
5:J:210:GLU:OE1	5:J:210:GLU:N	2.25	0.68
6:L:6:ARG:NH1	6:L:8:TYR:O	2.27	0.68
5:I:156:THR:HB	5:I:225:ILE:HB	1.76	0.68
1:A:92:ARG:NH2	1:A:339:LEU:O	2.26	0.68
4:H:300:ASP:OD1	4:H:301:SER:N	2.26	0.68
1:B:271:ASP:OD1	5:J:323:ARG:NH2	2.27	0.68
5:I:52:GLU:OE2	5:I:80:TYR:OH	2.07	0.68
3:F:180:TYR:OH	3:F:331:GLU:OE2	2.10	0.67
4:H:354:SER:OG	4:H:355:ARG:N	2.27	0.67
4:H:355:ARG:NH1	4:H:431:LYS:O	2.28	0.67
1:A:264:ARG:NH1	1:A:303:ARG:O	2.28	0.67
3:E:336:ILE:HD12	3:E:395:ILE:HD13	1.77	0.67
4:H:451:PRO:O	4:H:454:SER:OG	2.13	0.67
5:I:101:ARG:NH1	5:I:103:SER:O	2.28	0.67
3:F:320:CYS:SG	3:F:321:SER:N	2.68	0.67
6:M:148:ILE:HD13	6:M:172:ILE:HB	1.76	0.67
2:C:199:LEU:HD21	2:C:218:LEU:HD23	1.77	0.67
2:D:17:ILE:HG22	2:D:21:LYS:HD2	1.77	0.67
4:H:140:ASP:O	4:H:197:GLN:NE2	2.28	0.67
5:I:111:ARG:HE	5:I:238:PHE:HA	1.58	0.67
5:I:280:TYR:O	5:I:284:SER:OG	2.11	0.67
2:D:230:ILE:HD13	2:D:267:ILE:HD12	1.76	0.67
6:M:96:LYS:NZ	6:M:99:GLU:OE2	2.17	0.67
2:C:280:ALA:HA	2:C:315:LYS:HB3	1.77	0.66
2:C:341:GLU:HB3	2:C:344:LEU:HD13	1.77	0.66
2:D:270:ARG:HH11	4:H:122:ILE:HG23	1.60	0.66
2:C:381:ILE:O	2:C:385:THR:OG1	2.08	0.66
5:I:19:GLN:NE2	5:I:118:LEU:O	2.28	0.66
5:I:173:GLU:OE1	5:I:275:ARG:NH2	2.29	0.66
6:M:159:PRO:HG3	6:M:165:LEU:HD12	1.78	0.66
2:D:330:LEU:HB2	5:J:290:ARG:HH11	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:148:LEU:HD23	4:G:201:LEU:HD21	1.76	0.66
2:C:203:GLU:OE2	2:D:270:ARG:NH2	2.29	0.66
4:G:269:ASP:OD1	4:G:338:LYS:NZ	2.27	0.66
5:I:409:GLY:O	5:I:412:THR:OG1	2.10	0.66
2:D:239:GLN:NE2	4:H:404:MET:O	2.28	0.65
4:H:244:SER:OG	4:H:247:ARG:NH2	2.30	0.65
5:J:169:ARG:NH2	5:J:216:ASN:OD1	2.29	0.65
1:A:100:PHE:HD2	6:M:74:ARG:HE	1.43	0.65
4:G:189:HIS:O	4:G:189:HIS:ND1	2.29	0.65
5:J:173:GLU:OE2	5:J:275:ARG:NE	2.29	0.65
2:D:199:LEU:O	2:D:225:ARG:NH1	2.29	0.65
6:L:92:GLU:OE2	6:L:92:GLU:N	2.29	0.65
4:G:403:ASN:ND2	4:G:407:ASP:O	2.29	0.65
3:E:133:ARG:NH2	3:E:259:ILE:O	2.30	0.65
4:H:335:GLU:OE2	5:J:310:ARG:NH1	2.29	0.65
4:H:393:ASN:ND2	4:H:432:TYR:O	2.29	0.65
5:J:130:VAL:HG12	5:J:273:ARG:HB3	1.78	0.65
1:B:92:ARG:NH2	1:B:339:LEU:O	2.27	0.65
2:D:187:ILE:HG22	2:D:369:ASN:HD22	1.62	0.65
4:H:447:MET:SD	4:H:447:MET:N	2.69	0.65
6:L:111:LEU:HB3	6:L:122:LEU:HD22	1.78	0.65
3:E:308:LYS:HD2	3:E:309:ILE:HG23	1.77	0.65
4:H:156:LYS:HD3	4:H:304:GLU:HG2	1.77	0.65
4:G:156:LYS:HD3	4:G:304:GLU:HG2	1.79	0.65
5:J:222:GLN:OE1	5:J:273:ARG:NH1	2.29	0.65
6:L:141:TYR:O	6:L:145:LYS:NZ	2.28	0.65
6:M:14:GLU:N	6:M:17:ASP:OD2	2.29	0.64
6:M:150:ASP:OD1	6:M:151:GLU:N	2.30	0.64
6:L:66:LYS:NZ	6:L:67:ASN:O	2.27	0.64
4:G:300:ASP:OD1	4:G:301:SER:N	2.29	0.64
1:A:193:LEU:HD12	1:B:170:ARG:HB3	1.80	0.64
2:C:316:LEU:HD11	2:C:382:MET:HG2	1.79	0.64
5:I:169:ARG:NH2	5:I:216:ASN:OD1	2.30	0.64
2:C:315:LYS:NZ	7:C:401:PO4:O1	2.26	0.64
6:M:136:LYS:NZ	6:M:155:GLU:O	2.31	0.64
5:J:150:ASP:OD2	5:J:260:LYS:NZ	2.18	0.64
1:A:328:SER:OG	1:A:331:GLY:N	2.28	0.63
3:F:431:GLY:HA3	3:F:447:LEU:HD23	1.79	0.63
5:J:61:ALA:HB2	5:J:136:LEU:HD23	1.80	0.63
6:L:42:GLU:OE2	6:L:42:GLU:N	2.26	0.63
3:F:263:ARG:NH2	7:F:502:PO4:O3	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:GLU:HB3	4:H:322:THR:HG23	1.81	0.63
3:E:154:LEU:HD12	3:E:155:PRO:HD2	1.80	0.63
5:J:409:GLY:O	5:J:412:THR:OG1	2.14	0.63
4:G:275:LEU:HD22	4:G:306:GLU:HB2	1.80	0.63
4:H:410:GLU:HG3	4:H:412:LYS:HD3	1.78	0.63
5:I:54:THR:HG1	5:I:130:VAL:H	1.45	0.63
6:L:22:ASN:ND2	6:L:67:ASN:OD1	2.26	0.63
1:A:299:GLU:OE2	1:A:303:ARG:NH2	2.32	0.63
5:I:47:ASN:ND2	5:I:350:ILE:O	2.25	0.63
1:B:249:PHE:HB3	1:B:336:LEU:HD13	1.81	0.63
5:I:348:THR:HG22	5:I:365:ALA:H	1.64	0.62
6:L:115:ALA:HB2	6:L:122:LEU:HD21	1.79	0.62
2:C:77:ASN:ND2	2:C:316:LEU:O	2.32	0.62
4:G:180:THR:HG21	4:G:231:ASP:OD1	2.00	0.62
5:I:178:VAL:HG22	5:I:214:VAL:HG22	1.79	0.62
6:M:5:CYS:SG	6:M:6:ARG:N	2.72	0.62
1:B:204:VAL:O	1:B:238:LYS:NZ	2.30	0.62
1:A:227:PHE:N	1:A:309:ASP:OD2	2.31	0.62
1:B:134:ARG:O	1:B:137:SER:OG	2.12	0.62
2:C:287:LEU:HB2	2:C:358:ILE:HG12	1.81	0.61
4:H:178:TYR:OH	4:H:189:HIS:O	2.15	0.61
4:H:189:HIS:O	4:H:189:HIS:ND1	2.32	0.61
4:H:348:SER:OG	4:H:382:THR:O	2.16	0.61
2:D:365:LEU:HD13	4:G:385:ILE:HD13	1.82	0.61
1:A:73:VAL:O	1:A:75:ASN:N	2.32	0.61
4:H:258:VAL:HG23	4:H:283:VAL:HA	1.82	0.61
2:C:234:GLY:HA3	2:C:238:ASN:HB2	1.83	0.61
5:J:372:VAL:HG22	5:J:389:LYS:HA	1.81	0.61
5:I:428:GLN:OE1	5:I:428:GLN:N	2.33	0.61
1:B:55:ILE:N	6:L:83:ASP:OD2	2.32	0.61
2:C:334:ASP:OD2	2:C:335:LYS:NZ	2.34	0.61
5:J:53:TYR:HB3	5:J:131:VAL:HG12	1.83	0.61
5:J:239:ASP:N	5:J:239:ASP:OD1	2.31	0.61
1:A:95:HIS:NE2	6:M:48:SER:OG	2.33	0.61
3:E:149:ASP:O	3:E:327:PRO:HD2	2.00	0.61
3:E:231:VAL:HG23	5:J:214:VAL:HB	1.82	0.61
4:H:275:LEU:HD22	4:H:306:GLU:HB2	1.81	0.61
3:E:239:ASP:OD1	3:E:240:ALA:N	2.34	0.61
3:F:268:PRO:HA	3:F:271:VAL:HG12	1.83	0.61
5:I:432:ASN:OD1	5:I:433:ASP:N	2.31	0.61
5:J:316:GLU:OE1	5:J:335:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:6:ARG:NH2	6:M:9:GLU:O	2.34	0.61
2:C:208:GLN:NE2	2:C:292:GLY:O	2.27	0.60
2:D:59:ARG:NH2	2:D:392:ILE:O	2.34	0.60
3:F:220:PHE:HB2	5:I:199:VAL:HB	1.83	0.60
4:G:209:ILE:HD11	4:G:384:ARG:HH21	1.64	0.60
6:L:102:GLN:O	6:L:106:THR:OG1	2.19	0.60
1:A:146:ARG:N	7:A:401:PO4:O2	2.34	0.60
4:G:161:ASN:OD1	4:G:379:TYR:OH	2.16	0.60
5:J:432:ASN:O	5:J:435:SER:OG	2.15	0.60
3:F:149:ASP:O	3:F:327:PRO:HD2	2.01	0.60
4:G:202:VAL:HG22	4:G:207:LEU:HG	1.83	0.60
6:M:139:HIS:HB3	6:M:142:GLU:OE2	2.02	0.60
2:D:331:SER:OG	2:D:332:SER:N	2.35	0.60
4:G:377:GLU:OE2	4:G:377:GLU:N	2.34	0.60
2:C:356:ASP:OD1	4:G:330:SER:OG	2.20	0.59
3:F:124:ASP:OD1	3:F:124:ASP:N	2.35	0.59
5:J:202:ASP:OD1	5:J:202:ASP:N	2.35	0.59
6:M:111:LEU:O	6:M:115:ALA:N	2.34	0.59
6:M:146:LEU:HA	6:M:149:ILE:HG12	1.84	0.59
2:C:233:GLU:OE2	4:G:302:ARG:HD3	2.02	0.59
3:E:413:VAL:HG12	3:E:430:ILE:HB	1.83	0.59
3:F:230:ARG:NH1	5:I:213:GLU:OE1	2.32	0.59
4:H:295:ARG:NH2	4:H:335:GLU:OE1	2.36	0.59
5:I:202:ASP:N	5:I:202:ASP:OD1	2.35	0.59
6:M:144:PHE:O	6:M:147:SER:OG	2.19	0.59
2:C:16:LEU:HD23	2:C:65:LEU:HD11	1.84	0.59
3:F:307:ILE:HG21	3:F:310:ASN:HB3	1.83	0.59
2:D:80:ARG:NH1	2:D:390:ASP:O	2.33	0.59
2:D:225:ARG:HD3	4:G:118:LYS:HZ1	1.68	0.58
3:E:133:ARG:NH1	3:E:253:ILE:O	2.35	0.58
5:I:114:ASP:HB3	5:I:231:PRO:HB2	1.84	0.58
1:A:33:ILE:HG21	1:A:119:ARG:HH21	1.66	0.58
2:C:225:ARG:HG2	4:H:118:LYS:HE2	1.85	0.58
2:C:330:LEU:O	5:I:290:ARG:NH2	2.36	0.58
4:G:198:ILE:O	4:G:202:VAL:N	2.30	0.58
5:I:217:ASP:OD1	5:I:218:LEU:HD22	2.02	0.58
5:J:54:THR:OG1	5:J:130:VAL:N	2.34	0.58
1:B:88:ARG:NH2	6:L:28:GLU:OE2	2.37	0.58
3:E:155:PRO:O	3:E:158:THR:OG1	2.21	0.58
3:E:355:LEU:HD13	3:E:368:ILE:HG22	1.85	0.58
3:E:230:ARG:HD2	5:J:217:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:270:LEU:C	3:F:315:LYS:HZ1	2.06	0.58
1:B:106:HIS:O	1:B:110:ASN:ND2	2.26	0.58
4:G:347:LEU:HD12	4:G:351:ALA:HB3	1.85	0.58
1:A:130:TYR:CD1	1:A:131:PRO:HD3	2.38	0.58
2:C:50:THR:N	2:C:53:GLN:OE1	2.37	0.58
3:E:147:SER:OG	3:E:149:ASP:OD1	2.10	0.58
5:I:147:ARG:NH1	5:I:153:ALA:O	2.37	0.58
5:I:305:THR:HG1	5:I:317:GLU:H	1.49	0.58
3:E:211:SER:OG	3:E:211:SER:O	2.20	0.58
2:C:7:GLU:OE2	5:I:90:SER:OG	2.19	0.58
3:F:155:PRO:O	3:F:158:THR:OG1	2.22	0.58
5:I:432:ASN:O	5:I:435:SER:OG	2.19	0.58
5:J:19:GLN:OE1	5:J:120:THR:N	2.37	0.58
6:M:6:ARG:NE	6:M:8:TYR:O	2.33	0.58
1:A:297:MET:HB3	1:A:301:GLN:HG3	1.86	0.58
3:E:418:GLN:O	3:E:435:ARG:HA	2.04	0.58
4:H:408:ASP:OD1	4:H:408:ASP:N	2.36	0.58
5:I:159:VAL:HG12	5:I:220:ASP:HA	1.85	0.58
1:A:334:GLU:OE1	2:D:379:TYR:OH	2.20	0.58
2:D:340:ASN:O	2:D:342:GLY:N	2.36	0.58
3:E:144:VAL:HG13	3:E:244:VAL:HG22	1.86	0.57
1:B:197:VAL:HG11	1:B:229:LEU:HB3	1.85	0.57
1:B:337:ILE:HD12	6:L:56:ARG:HE	1.69	0.57
2:D:328:ILE:HG22	2:D:355:TYR:HB2	1.86	0.57
5:I:239:ASP:OD1	5:I:239:ASP:N	2.37	0.57
1:A:61:ILE:O	1:A:65:GLY:N	2.33	0.57
2:C:93:LEU:HA	2:C:96:THR:HG22	1.85	0.57
3:E:40:GLN:OE1	3:E:140:LYS:N	2.35	0.57
3:E:401:VAL:HG13	3:E:418:GLN:HG3	1.85	0.57
5:J:58:LEU:HB3	5:J:63:VAL:HG11	1.85	0.57
5:J:173:GLU:CD	5:J:275:ARG:HE	2.08	0.57
5:J:57:PHE:CZ	5:J:136:LEU:HD21	2.39	0.57
3:F:123:ASP:OD1	3:F:124:ASP:N	2.37	0.57
4:G:160:SER:OG	7:G:501:PO4:O3	2.21	0.57
5:J:70:CYS:HG	5:J:97:THR:HG1	1.52	0.57
1:A:47:LEU:O	1:A:104:LYS:NZ	2.38	0.57
1:A:131:PRO:HB2	2:D:322:TYR:CD1	2.39	0.57
3:E:406:VAL:HG21	3:E:419:ILE:HD11	1.86	0.57
3:F:119:PRO:HG2	3:F:122:LEU:HG	1.86	0.57
5:J:381:LYS:HD3	5:J:398:ASP:OD1	2.04	0.57
6:M:49:GLU:OE2	6:M:88:ARG:NH2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:HB2	1:B:229:LEU:HD21	1.87	0.57
4:H:126:LEU:HB3	4:H:395:LEU:HD11	1.87	0.57
5:J:138:GLU:OE1	5:J:138:GLU:N	2.37	0.57
6:L:132:PRO:HA	6:L:135:ARG:HB2	1.86	0.57
6:M:154:TRP:HD1	6:M:157:ILE:HG21	1.69	0.57
1:B:169:SER:O	1:B:169:SER:OG	2.20	0.57
1:B:245:GLU:OE2	1:B:248:LYS:NZ	2.33	0.57
2:C:173:ILE:O	2:C:177:ILE:N	2.34	0.57
3:E:180:TYR:HD1	3:E:334:LYS:HG3	1.70	0.57
1:A:52:ALA:HB1	1:A:57:GLU:HB3	1.87	0.56
1:A:134:ARG:O	1:A:137:SER:OG	2.13	0.56
3:F:188:LYS:H	3:F:188:LYS:HD3	1.69	0.56
3:F:327:PRO:O	3:F:328:ASN:ND2	2.38	0.56
4:G:304:GLU:O	4:G:306:GLU:N	2.38	0.56
5:I:101:ARG:NH2	5:I:105:SER:OG	2.37	0.56
5:J:80:TYR:O	5:J:84:SER:N	2.36	0.56
5:J:213:GLU:HG2	5:J:215:ARG:HG2	1.86	0.56
1:A:46:LEU:O	1:A:50:SER:OG	2.15	0.56
1:A:220:LEU:HB3	1:A:311:THR:HB	1.88	0.56
5:J:273:ARG:NH1	5:J:275:ARG:HH12	2.03	0.56
1:A:144:PHE:N	1:A:174:SER:OG	2.37	0.56
3:F:276:GLN:OE1	3:F:279:PHE:N	2.32	0.56
6:M:102:GLN:O	6:M:106:THR:N	2.31	0.56
2:C:54:LEU:O	2:C:57:THR:N	2.38	0.56
1:B:166:VAL:HG21	1:B:179:THR:HB	1.88	0.56
2:C:340:ASN:O	2:C:342:GLY:N	2.39	0.56
2:D:280:ALA:HA	2:D:315:LYS:HB3	1.86	0.56
4:G:258:VAL:O	4:G:262:THR:OG1	2.21	0.56
4:G:348:SER:OG	4:G:382:THR:O	2.21	0.56
4:G:359:SER:OG	4:G:433:ASP:OD2	2.13	0.56
5:J:52:GLU:OE2	5:J:80:TYR:OH	2.15	0.56
3:F:167:ASN:OD1	3:F:246:LYS:NZ	2.37	0.56
1:A:245:GLU:OE1	1:A:248:LYS:NZ	2.29	0.56
5:J:40:ARG:HH22	5:J:41:CYS:HB3	1.71	0.56
4:G:311:LEU:O	4:G:315:THR:OG1	2.22	0.55
6:L:97:CYS:O	6:L:101:TYR:N	2.35	0.55
6:L:150:ASP:OD1	6:L:152:THR:N	2.39	0.55
3:E:303:SER:OG	3:E:304:SER:N	2.38	0.55
4:G:266:GLN:N	4:G:269:ASP:OD2	2.33	0.55
5:I:73:HIS:HB3	5:I:76:GLN:HG2	1.88	0.55
6:L:150:ASP:OD1	6:L:151:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:O	1:B:75:ASN:N	2.35	0.55
2:D:234:GLY:HA3	2:D:238:ASN:HB2	1.88	0.55
3:F:355:LEU:HD21	3:F:368:ILE:HB	1.88	0.55
1:A:168:GLU:OE2	1:B:170:ARG:NH2	2.40	0.55
5:J:249:TYR:O	5:J:253:THR:OG1	2.17	0.55
5:J:29:TYR:HA	5:J:32:ARG:HD3	1.89	0.55
2:C:215:GLU:OE2	2:C:248:ARG:NE	2.36	0.55
1:B:22:VAL:HG12	1:B:26:PHE:HE2	1.70	0.55
5:I:316:GLU:OE1	5:I:335:ALA:N	2.38	0.55
1:A:195:SER:O	1:A:195:SER:OG	2.20	0.55
3:F:239:ASP:OD1	3:F:240:ALA:N	2.39	0.55
5:I:224:ASP:OD2	5:I:244:ARG:NH1	2.40	0.55
5:J:294:PRO:O	5:J:296:VAL:N	2.39	0.55
6:L:99:GLU:O	6:L:103:LYS:NZ	2.39	0.55
1:A:55:ILE:N	6:M:83:ASP:OD2	2.38	0.55
3:F:403:GLU:OE2	3:F:420:GLY:HA2	2.07	0.55
4:H:202:VAL:HG12	4:H:207:LEU:HG	1.89	0.55
5:I:61:ALA:HB2	5:I:136:LEU:HD13	1.88	0.55
6:L:91:SER:N	6:L:92:GLU:OE2	2.40	0.55
6:L:148:ILE:HD11	6:L:172:ILE:HB	1.88	0.55
3:E:48:GLY:HA3	3:E:55:THR:HG21	1.88	0.54
3:E:133:ARG:NH1	3:E:256:LYS:O	2.36	0.54
3:F:91:ILE:HG21	3:F:131:ALA:HB1	1.89	0.54
2:C:239:GLN:NE2	4:G:404:MET:O	2.39	0.54
3:E:327:PRO:HA	3:E:331:GLU:HB2	1.88	0.54
4:G:408:ASP:OD1	4:G:409:PHE:N	2.39	0.54
5:I:71:CYS:HB3	5:I:102:GLU:HA	1.89	0.54
3:E:139:ILE:HG12	3:E:250:ILE:HG13	1.89	0.54
3:F:366:THR:HG22	3:F:383:CYS:H	1.72	0.54
6:M:142:GLU:OE2	6:M:142:GLU:N	2.41	0.54
3:E:181:GLU:HB3	3:E:334:LYS:NZ	2.22	0.54
4:G:312:LYS:NZ	4:G:316:GLU:OE2	2.22	0.54
6:M:58:ILE:HD11	6:M:60:LYS:HE2	1.89	0.54
3:F:331:GLU:O	3:F:335:CYS:N	2.35	0.54
4:H:161:ASN:OD1	4:H:379:TYR:OH	2.18	0.54
3:E:292:PRO:HG3	3:E:309:ILE:HG12	1.88	0.54
3:E:375:LYS:O	3:E:377:SER:OG	2.20	0.54
3:F:173:VAL:HB	3:F:242:ILE:HB	1.90	0.54
1:B:163:LYS:HA	1:B:188:PRO:HG2	1.89	0.54
1:B:328:SER:OG	1:B:331:GLY:N	2.26	0.54
5:I:375:ASP:N	5:I:392:ASN:OD1	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:156:THR:HG23	5:J:225:ILE:HB	1.89	0.54
1:B:195:SER:O	1:B:195:SER:OG	2.24	0.54
4:G:302:ARG:NH2	4:G:403:ASN:O	2.41	0.54
6:M:132:PRO:O	6:M:136:LYS:N	2.41	0.54
1:B:130:TYR:CD1	1:B:131:PRO:HD3	2.43	0.54
1:B:273:SER:O	1:B:275:GLU:N	2.41	0.54
3:E:260:SER:OG	3:E:265:ASP:OD2	2.22	0.54
3:F:73:LEU:HD21	3:F:90:LEU:HD11	1.90	0.53
3:F:189:GLU:OE1	3:F:189:GLU:N	2.39	0.53
5:I:57:PHE:CZ	5:I:136:LEU:HD11	2.43	0.53
1:A:30:ASP:OD1	1:A:32:GLU:HG2	2.08	0.53
1:B:210:GLY:O	1:B:222:ASN:ND2	2.41	0.53
3:F:307:ILE:HG22	3:F:309:ILE:H	1.73	0.53
2:C:84:ARG:NE	2:C:88:GLU:OE2	2.29	0.53
5:J:335:ALA:H	5:J:352:ARG:HG2	1.73	0.53
5:J:397:GLU:OE2	5:J:415:GLU:HA	2.09	0.53
3:F:200:GLU:OE2	3:F:232:THR:HG21	2.08	0.53
5:J:240:TYR:OH	5:J:255:ASP:OD1	2.25	0.53
6:M:22:ASN:ND2	6:M:65:GLY:O	2.33	0.53
3:E:287:ARG:O	3:E:289:LEU:N	2.40	0.53
5:J:242:ASP:OD1	5:J:244:ARG:N	2.41	0.53
1:A:87:GLN:NE2	6:M:29:MET:SD	2.81	0.53
1:A:148:VAL:HG22	1:A:208:LEU:HG	1.90	0.53
3:E:187:SER:HG	3:E:330:PHE:HE2	1.54	0.53
5:I:440:GLY:O	5:I:442:ARG:N	2.42	0.53
1:B:201:MET:O	1:B:204:VAL:HG12	2.09	0.53
1:A:243:VAL:HA	1:A:320:ILE:HG23	1.91	0.53
2:C:27:GLY:N	2:C:72:GLU:OE1	2.41	0.53
3:E:400:ILE:HG22	3:E:417:ALA:H	1.74	0.53
3:F:389:VAL:HG13	3:F:406:VAL:HG22	1.91	0.53
5:J:114:ASP:OD2	5:J:232:ALA:HA	2.08	0.53
5:J:305:THR:OG1	5:J:316:GLU:HG2	2.09	0.53
1:A:223:GLN:N	1:A:223:GLN:OE1	2.42	0.52
2:C:19:ASP:HA	2:C:24:LYS:HD2	1.91	0.52
2:C:287:LEU:HD11	2:C:309:VAL:HG21	1.91	0.52
3:F:142:ASP:OD1	3:F:247:HIS:N	2.41	0.52
3:F:362:VAL:HG22	3:F:379:ILE:HB	1.90	0.52
6:M:97:CYS:O	6:M:101:TYR:N	2.41	0.52
2:C:287:LEU:HD12	2:C:358:ILE:HD11	1.92	0.52
5:J:228:ASN:OD1	5:J:228:ASN:N	2.42	0.52
5:J:309:GLN:HB2	5:J:313:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:54:THR:O	5:J:58:LEU:HD12	2.10	0.52
6:M:103:LYS:HE2	6:M:141:TYR:HB3	1.90	0.52
1:B:76:ASN:OD1	1:B:78:SER:N	2.43	0.52
2:D:54:LEU:O	2:D:57:THR:OG1	2.20	0.52
3:E:91:ILE:HG22	3:E:117:GLU:HB3	1.92	0.52
4:H:377:GLU:N	4:H:377:GLU:OE1	2.42	0.52
6:L:145:LYS:H	6:L:145:LYS:HD2	1.75	0.52
4:H:208:SER:HB2	4:H:344:HIS:NE2	2.25	0.52
5:I:152:ASN:OD1	5:I:259:LYS:NZ	2.43	0.52
5:J:353:ASN:HB3	5:J:370:ASP:OD1	2.10	0.52
5:J:244:ARG:HA	5:J:248:VAL:HG23	1.92	0.52
5:J:288:LEU:O	5:J:314:TYR:OH	2.21	0.52
2:D:204:ILE:N	2:D:272:ASN:OD1	2.37	0.52
3:E:121:ILE:O	3:E:123:ASP:N	2.43	0.52
5:I:142:GLU:OE1	5:I:264:HIS:ND1	2.36	0.52
5:J:346:ALA:O	5:J:348:THR:OG1	2.26	0.52
6:L:35:LEU:HD21	6:L:84:LEU:HD21	1.91	0.52
1:A:326:ILE:O	1:A:329:LYS:NZ	2.42	0.52
2:C:204:ILE:N	2:C:272:ASN:OD1	2.36	0.52
3:E:165:LEU:HD23	4:H:150:LEU:HB3	1.92	0.52
4:H:347:LEU:HD23	4:H:351:ALA:HB3	1.92	0.52
5:J:121:SER:OG	5:J:122:ASP:N	2.41	0.52
5:J:409:GLY:H	5:J:434:PRO:HA	1.75	0.52
1:A:170:ARG:HB3	1:B:193:LEU:HD13	1.92	0.51
5:J:140:LEU:HD13	5:J:144:ARG:HE	1.75	0.51
6:L:162:LYS:HG2	6:L:166:ASP:OD2	2.09	0.51
2:C:197:ASP:OD1	4:H:392:TYR:OH	2.28	0.51
4:H:252:ILE:HG21	6:L:60:LYS:HG3	1.91	0.51
1:B:131:PRO:HB2	2:C:322:TYR:CD1	2.45	0.51
3:F:102:ALA:O	3:F:106:SER:N	2.39	0.51
5:I:348:THR:HG21	5:I:362:ILE:HG22	1.92	0.51
5:J:24:SER:O	5:J:26:SER:N	2.42	0.51
1:A:141:THR:HA	1:A:208:LEU:O	2.11	0.51
5:I:152:ASN:ND2	5:I:258:GLY:O	2.43	0.51
6:M:131:TRP:O	6:M:135:ARG:N	2.41	0.51
1:A:88:ARG:NH2	6:M:28:GLU:OE1	2.33	0.51
4:H:208:SER:OG	4:H:210:SER:OG	2.24	0.51
1:A:88:ARG:NH1	1:A:340:TYR:HB3	2.25	0.51
1:A:96:ASP:O	6:M:88:ARG:NH2	2.39	0.51
2:D:287:LEU:HD21	2:D:309:VAL:HG21	1.92	0.51
2:D:381:ILE:O	2:D:385:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:256:LYS:HE3	3:F:269:TYR:HE2	1.75	0.51
3:F:310:ASN:OD1	3:F:310:ASN:N	2.43	0.51
4:H:401:LEU:HD11	4:H:427:LEU:HB3	1.93	0.51
5:J:379:ILE:HA	5:J:396:ILE:HG23	1.91	0.51
1:A:170:ARG:HE	1:B:170:ARG:HH21	1.58	0.51
1:B:313:PRO:HB2	1:B:329:LYS:HG3	1.92	0.51
3:E:195:LEU:HD11	3:E:233:LEU:HG	1.93	0.51
5:J:111:ARG:NH1	5:J:238:PHE:HA	2.25	0.51
5:J:173:GLU:HG3	5:J:275:ARG:HH21	1.76	0.51
1:A:16:GLU:OE1	1:A:16:GLU:N	2.44	0.50
4:G:343:GLY:HA2	4:G:354:SER:HB2	1.93	0.50
4:H:286:HIS:O	4:H:290:VAL:HG23	2.11	0.50
3:E:128:SER:OG	3:E:262:ILE:N	2.39	0.50
3:F:247:HIS:O	3:F:250:ILE:HG22	2.12	0.50
3:F:307:ILE:HD12	3:F:307:ILE:H	1.76	0.50
3:F:336:ILE:HD12	3:F:395:ILE:HD13	1.93	0.50
4:G:131:ARG:NH1	4:G:203:SER:OG	2.45	0.50
4:H:140:ASP:N	4:H:140:ASP:OD1	2.42	0.50
4:H:230:THR:N	4:H:233:GLU:OE1	2.43	0.50
5:I:276:SER:O	5:I:279:THR:OG1	2.27	0.50
1:A:87:GLN:O	1:A:91:THR:HG22	2.10	0.50
3:E:375:LYS:HD2	3:E:392:SER:HB2	1.92	0.50
4:G:218:LEU:O	4:G:222:ILE:HG12	2.12	0.50
5:I:160:ARG:NH2	5:I:269:ASN:O	2.31	0.50
5:J:127:SER:HB2	5:J:273:ARG:NH2	2.26	0.50
1:B:166:VAL:HG23	1:B:191:MET:HG2	1.94	0.50
3:F:434:HIS:ND1	3:F:448:VAL:HG22	2.26	0.50
4:G:186:LEU:HB2	4:G:231:ASP:OD1	2.12	0.50
4:G:335:GLU:OE2	5:I:310:ARG:NH1	2.44	0.50
6:L:53:ARG:HE	6:L:58:ILE:HB	1.76	0.50
4:H:131:ARG:NH1	4:H:203:SER:OG	2.44	0.50
5:J:54:THR:O	5:J:57:PHE:HB3	2.11	0.50
1:A:258:TYR:CZ	1:B:202:ASN:HB3	2.46	0.50
1:B:267:LEU:N	1:B:304:ASN:OD1	2.44	0.50
2:D:320:TYR:O	2:D:322:TYR:N	2.44	0.50
2:D:356:ASP:OD1	4:H:330:SER:OG	2.27	0.50
5:I:242:ASP:OD1	5:I:244:ARG:N	2.42	0.50
4:H:304:GLU:O	4:H:306:GLU:N	2.45	0.50
2:C:54:LEU:O	2:C:58:VAL:HG12	2.12	0.50
2:D:187:ILE:HG13	2:D:188:ASN:H	1.77	0.50
2:D:289:THR:O	2:D:356:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:ASP:OD1	3:E:247:HIS:N	2.41	0.50
3:F:284:ASN:C	3:F:286:GLN:H	2.13	0.50
2:C:264:ILE:HD13	2:C:296:VAL:HG22	1.94	0.50
3:F:387:LYS:O	3:F:405:GLY:N	2.43	0.50
4:G:185:THR:OG1	4:G:186:LEU:N	2.45	0.50
6:L:6:ARG:HH12	6:L:9:GLU:HA	1.77	0.50
6:L:7:PHE:O	6:L:131:TRP:NE1	2.32	0.50
6:L:19:VAL:HA	6:L:37:GLU:OE2	2.12	0.50
6:M:2:THR:HB	6:M:122:LEU:HB3	1.94	0.50
1:A:30:ASP:OD1	1:A:32:GLU:N	2.45	0.49
2:D:77:ASN:HB3	2:D:386:TYR:OH	2.12	0.49
6:L:55:ILE:HG22	6:L:57:SER:H	1.77	0.49
1:B:94:LEU:HB3	6:L:46:LEU:HD21	1.94	0.49
5:J:289:SER:O	5:J:291:TRP:N	2.40	0.49
5:J:440:GLY:O	5:J:442:ARG:N	2.39	0.49
3:E:119:PRO:HD2	3:E:122:LEU:HD11	1.94	0.49
3:E:190:ILE:O	3:E:192:ALA:N	2.45	0.49
4:H:461:GLU:HG2	6:L:56:ARG:HB2	1.93	0.49
5:I:224:ASP:CG	5:I:244:ARG:HH12	2.15	0.49
3:E:309:ILE:HD13	3:E:310:ASN:OD1	2.12	0.49
3:F:205:LEU:O	3:F:274:GLN:NE2	2.45	0.49
3:F:401:VAL:HG13	3:F:418:GLN:HG3	1.93	0.49
4:G:178:TYR:OH	4:G:189:HIS:O	2.24	0.49
4:H:122:ILE:HG21	4:H:390:LEU:HD13	1.93	0.49
6:M:140:ALA:O	6:M:144:PHE:HB2	2.13	0.49
2:C:31:VAL:O	2:C:35:THR:OG1	2.22	0.49
2:D:247:LYS:HD2	4:H:415:VAL:HG12	1.93	0.49
2:D:254:ILE:O	2:D:256:THR:N	2.46	0.49
3:F:121:ILE:O	3:F:123:ASP:N	2.45	0.49
4:G:229:LEU:HD22	4:G:233:GLU:HB3	1.95	0.49
5:I:50:LEU:HD21	5:I:274:VAL:HG11	1.95	0.49
5:I:145:LYS:O	5:I:148:GLU:HG2	2.12	0.49
6:M:126:TYR:HA	6:M:130:ALA:HB3	1.94	0.49
2:C:269:SER:HA	2:C:303:HIS:HD2	1.77	0.49
3:E:267:ILE:HG13	3:E:315:LYS:HZ1	1.77	0.49
3:E:381:LYS:N	3:E:398:ASP:OD1	2.34	0.49
4:H:201:LEU:O	4:H:204:THR:OG1	2.31	0.49
2:C:313:ILE:HD11	2:C:381:ILE:HG21	1.94	0.49
2:C:317:SER:OG	2:C:319:VAL:HG12	2.13	0.49
3:F:429:GLU:OE1	3:F:429:GLU:N	2.46	0.49
5:J:19:GLN:CD	5:J:120:THR:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:161:GLU:OE2	5:J:267:LYS:HE2	2.12	0.49
1:B:218:GLY:HA2	1:B:332:VAL:HG21	1.94	0.49
2:C:369:ASN:N	2:C:369:ASN:OD1	2.44	0.49
2:D:84:ARG:NE	2:D:88:GLU:OE2	2.37	0.49
4:G:151:LYS:O	4:G:155:TYR:HB2	2.13	0.49
5:I:54:THR:O	5:I:58:LEU:HD23	2.13	0.49
6:M:165:LEU:HD22	6:M:169:LYS:HE3	1.95	0.49
2:C:278:THR:OG1	2:C:279:HIS:N	2.46	0.48
3:F:149:ASP:OD1	3:F:149:ASP:N	2.40	0.48
3:F:204:ARG:HH21	3:F:274:GLN:HG2	1.78	0.48
5:J:101:ARG:NH1	5:J:112:GLU:OE1	2.46	0.48
5:J:159:VAL:HG12	5:J:220:ASP:HA	1.93	0.48
6:L:168:LEU:O	6:L:172:ILE:HG13	2.12	0.48
1:A:43:LEU:O	1:A:47:LEU:N	2.42	0.48
2:C:209:GLY:HA2	2:C:242:SER:HB2	1.94	0.48
3:F:186:GLN:HG3	3:F:188:LYS:HZ3	1.78	0.48
3:F:285:ILE:HD12	3:F:285:ILE:H	1.78	0.48
4:H:308:ARG:NH2	4:H:406:VAL:HG22	2.28	0.48
1:A:220:LEU:HD12	1:A:226:THR:HG21	1.94	0.48
2:D:187:ILE:HD13	2:D:314:TYR:HE1	1.78	0.48
5:I:121:SER:OG	5:I:122:ASP:N	2.44	0.48
5:J:296:VAL:HG12	5:J:298:ASP:H	1.78	0.48
6:M:102:GLN:HA	6:M:105:LYS:HB3	1.95	0.48
1:A:226:THR:HB	1:A:309:ASP:OD1	2.12	0.48
2:C:40:ARG:HH21	2:C:178:GLN:HB2	1.79	0.48
2:C:13:VAL:O	2:C:17:ILE:HG13	2.13	0.48
5:I:188:HIS:HA	5:I:252:LEU:HD13	1.96	0.48
6:M:53:ARG:HD2	6:M:58:ILE:HB	1.96	0.48
2:C:274:VAL:HG13	2:C:307:VAL:HA	1.95	0.48
3:E:447:LEU:HD22	3:E:448:VAL:H	1.79	0.48
4:H:271:ILE:O	4:H:297:VAL:N	2.34	0.48
5:J:127:SER:O	5:J:273:ARG:NH2	2.47	0.48
1:A:175:GLY:O	1:A:179:THR:OG1	2.24	0.48
1:B:175:GLY:O	1:B:179:THR:HG22	2.14	0.48
2:C:42:VAL:O	2:C:46:THR:HG22	2.14	0.48
2:D:226:LYS:NZ	2:D:253:GLY:O	2.41	0.48
3:F:61:PRO:HD2	3:F:64:LEU:HB2	1.94	0.48
1:A:189:THR:N	1:B:270:ASP:OD1	2.34	0.48
3:F:447:LEU:HD22	3:F:448:VAL:H	1.78	0.48
5:I:226:CYS:HB3	5:I:230:VAL:HG21	1.95	0.48
1:B:166:VAL:HG23	1:B:191:MET:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:ILE:O	2:C:230:ILE:N	2.47	0.47
2:D:170:ARG:O	2:D:174:ILE:HG12	2.14	0.47
3:E:394:SER:OG	3:E:411:CYS:N	2.34	0.47
5:I:101:ARG:NH2	5:I:108:ASP:OD2	2.46	0.47
6:M:22:ASN:ND2	6:M:67:ASN:OD1	2.43	0.47
2:D:31:VAL:O	2:D:35:THR:OG1	2.24	0.47
1:A:154:ALA:O	1:A:158:ARG:HD3	2.14	0.47
2:D:184:LEU:O	2:D:187:ILE:HG12	2.14	0.47
5:I:132:SER:OG	5:I:134:VAL:HG12	2.14	0.47
1:B:161:ARG:H	1:B:161:ARG:HG2	1.54	0.47
1:B:327:ASP:OD2	2:C:284:ASN:HA	2.14	0.47
2:C:254:ILE:O	2:C:256:THR:N	2.48	0.47
2:D:328:ILE:HD12	4:H:331:TYR:HD1	1.79	0.47
3:E:380:GLY:N	3:E:396:LEU:O	2.47	0.47
1:B:322:ASP:OD1	1:B:322:ASP:N	2.47	0.47
4:H:211:MET:O	4:H:215:ILE:HG12	2.14	0.47
2:D:317:SER:OG	2:D:319:VAL:HG23	2.15	0.47
6:M:34:LYS:HD2	6:M:40:ASN:HB3	1.95	0.47
1:A:121:CYS:SG	1:A:122:ARG:N	2.87	0.47
1:B:250:VAL:HG23	1:B:252:MET:HG2	1.96	0.47
2:C:188:ASN:O	2:C:192:GLU:HG2	2.15	0.47
2:C:244:ALA:O	2:C:248:ARG:HG3	2.15	0.47
2:C:359:PRO:HG2	2:C:362:LEU:HD13	1.97	0.47
3:E:268:PRO:HA	3:E:271:VAL:HG12	1.96	0.47
3:F:188:LYS:H	3:F:188:LYS:CD	2.27	0.47
3:F:256:LYS:HE3	3:F:269:TYR:CE2	2.50	0.47
3:F:352:GLU:OE1	3:F:370:ASP:HA	2.15	0.47
4:H:160:SER:HA	4:H:163:ARG:HD3	1.96	0.47
5:I:25:ASP:HA	5:I:28:ASN:HB2	1.96	0.47
5:I:286:ASP:O	5:I:291:TRP:HB2	2.15	0.47
5:I:363:ASP:O	5:I:380:GLY:HA2	2.14	0.47
5:J:145:LYS:O	5:J:148:GLU:HG2	2.15	0.47
5:J:281:ASP:O	5:J:285:LYS:HG3	2.15	0.47
5:J:335:ALA:N	5:J:352:ARG:HG2	2.29	0.47
6:M:115:ALA:HB1	6:M:122:LEU:HD12	1.97	0.47
4:G:226:ASP:OD1	4:G:226:ASP:N	2.46	0.47
4:H:254:GLY:O	4:H:258:VAL:HG12	2.15	0.47
5:J:173:GLU:HB3	5:J:219:ILE:O	2.15	0.47
3:E:91:ILE:HD12	3:E:131:ALA:HB1	1.97	0.47
5:J:305:THR:OG1	5:J:305:THR:O	2.32	0.47
5:J:337:THR:HA	5:J:354:CYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PHE:N	1:B:174:SER:OG	2.45	0.47
1:B:169:SER:O	1:B:173:GLY:N	2.46	0.47
3:E:394:SER:HG	3:E:411:CYS:H	1.61	0.47
4:H:402:VAL:O	4:H:404:MET:N	2.48	0.47
5:I:323:ARG:O	5:I:324:SER:OG	2.28	0.47
5:J:328:LYS:O	5:J:331:THR:OG1	2.26	0.47
1:A:41:GLU:OE1	1:A:115:ILE:HG21	2.15	0.46
2:C:22:SER:O	2:C:22:SER:OG	2.30	0.46
2:C:177:ILE:O	2:C:180:VAL:HG22	2.15	0.46
4:G:107:ALA:HA	4:G:110:GLN:HB3	1.96	0.46
6:M:76:ASP:OD1	6:M:76:ASP:C	2.53	0.46
1:B:319:LEU:N	1:B:326:ILE:O	2.45	0.46
3:E:266:LEU:HD13	3:E:270:LEU:HD13	1.96	0.46
5:I:78:ARG:HG3	5:I:97:THR:HG21	1.97	0.46
5:I:140:LEU:O	5:I:144:ARG:N	2.34	0.46
1:A:191:MET:SD	1:B:301:GLN:NE2	2.89	0.46
3:E:368:ILE:HA	3:E:385:ILE:HB	1.98	0.46
3:F:132:LEU:HD11	3:F:139:ILE:HD11	1.96	0.46
4:H:385:ILE:HD12	4:H:385:ILE:O	2.14	0.46
6:L:6:ARG:HD2	6:L:11:LYS:HA	1.96	0.46
1:A:222:ASN:HB3	1:A:226:THR:OG1	2.15	0.46
2:C:331:SER:OG	2:C:332:SER:N	2.49	0.46
3:F:384:VAL:HB	3:F:401:VAL:HA	1.97	0.46
4:G:208:SER:HB2	4:G:344:HIS:NE2	2.31	0.46
4:G:355:ARG:NH1	4:G:431:LYS:O	2.48	0.46
5:J:434:PRO:HG2	5:J:438:GLY:HA3	1.97	0.46
6:M:21:VAL:HG23	6:M:34:LYS:O	2.15	0.46
3:F:113:ARG:NE	3:F:113:ARG:HA	2.30	0.46
5:I:114:ASP:OD2	5:I:232:ALA:HA	2.15	0.46
5:J:43:LEU:HD12	5:J:50:LEU:HD13	1.96	0.46
5:J:170:ALA:O	5:J:174:SER:N	2.49	0.46
5:J:428:GLN:N	5:J:428:GLN:OE1	2.49	0.46
1:B:312:PRO:HG2	1:B:315:PHE:CD1	2.50	0.46
3:E:393:ASN:O	3:E:410:SER:HA	2.16	0.46
1:A:212:GLU:N	1:A:222:ASN:OD1	2.48	0.46
2:C:2:SER:O	2:C:6:VAL:HG23	2.15	0.46
1:A:20:VAL:HA	1:A:23:TYR:HB3	1.97	0.46
1:A:46:LEU:HD21	1:A:61:ILE:HG22	1.96	0.46
1:B:88:ARG:NE	6:L:28:GLU:OE1	2.49	0.46
1:B:240:PHE:CD2	1:B:316:VAL:HG12	2.51	0.46
2:D:13:VAL:O	2:D:17:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:271:ILE:HG21	4:H:284:LEU:HD21	1.98	0.46
1:B:22:VAL:HG12	1:B:26:PHE:CE2	2.51	0.46
3:E:431:GLY:HA3	3:E:447:LEU:HD23	1.97	0.46
5:I:19:GLN:CD	5:I:120:THR:H	2.17	0.46
1:A:322:ASP:N	1:A:322:ASP:OD1	2.45	0.46
2:D:65:LEU:HD23	2:D:65:LEU:HA	1.74	0.46
3:E:33:GLN:C	3:E:35:ILE:H	2.20	0.46
3:E:235:THR:HG21	5:J:206:PHE:HB3	1.98	0.46
3:E:400:ILE:HG22	3:E:417:ALA:N	2.31	0.46
5:J:73:HIS:HB3	5:J:76:GLN:HB3	1.98	0.46
5:J:370:ASP:O	5:J:387:SER:HA	2.15	0.46
6:M:96:LYS:HD3	6:M:96:LYS:HA	1.59	0.46
1:B:337:ILE:HD12	6:L:56:ARG:NE	2.31	0.45
1:B:337:ILE:O	1:B:341:LEU:HD23	2.15	0.45
2:D:96:THR:HA	2:D:99:GLU:HG2	1.98	0.45
2:D:323:ASP:OD1	2:D:325:GLU:N	2.48	0.45
4:H:185:THR:OG1	4:H:186:LEU:N	2.49	0.45
4:H:257:ILE:O	4:H:261:ALA:N	2.42	0.45
5:J:297:PRO:O	5:J:300:ASN:ND2	2.49	0.45
1:A:153:LEU:O	1:A:157:LYS:HG2	2.16	0.45
2:C:7:GLU:OE2	2:C:14:SER:OG	2.28	0.45
2:C:59:ARG:NH1	2:C:393:LEU:O	2.47	0.45
2:C:380:ARG:NH2	4:H:461:GLU:OE2	2.49	0.45
3:F:166:ASP:OD1	3:F:166:ASP:N	2.49	0.45
5:I:190:GLN:NE2	5:I:199:VAL:HG22	2.31	0.45
6:L:101:TYR:O	6:L:104:SER:N	2.50	0.45
1:A:115:ILE:O	1:A:119:ARG:HG3	2.16	0.45
2:C:215:GLU:O	2:C:219:ARG:HG3	2.16	0.45
4:G:431:LYS:HB2	4:G:431:LYS:HE3	1.66	0.45
4:H:270:VAL:H	4:H:337:THR:CG2	2.29	0.45
4:H:412:LYS:N	4:H:412:LYS:HD2	2.31	0.45
5:J:147:ARG:NH1	5:J:151:LYS:O	2.45	0.45
2:C:203:GLU:OE1	2:C:273:LYS:NZ	2.50	0.45
3:F:70:LYS:NZ	3:F:109:GLU:OE1	2.43	0.45
1:A:62:LEU:O	1:A:66:SER:N	2.34	0.45
1:B:36:PRO:HB3	1:B:79:LEU:HA	1.98	0.45
1:B:312:PRO:HG2	1:B:315:PHE:HD1	1.81	0.45
2:D:186:LYS:HE2	2:D:190:ASP:OD2	2.15	0.45
3:E:133:ARG:O	3:E:136:SER:OG	2.34	0.45
3:E:186:GLN:OE1	3:E:188:LYS:HB2	2.17	0.45
5:I:104:LEU:HD11	5:I:109:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:GLU:OE1	2:D:273:LYS:NZ	2.45	0.45
2:D:259:ILE:HD13	2:D:267:ILE:HD11	1.98	0.45
3:E:165:LEU:HD21	4:H:154:ASN:HB2	1.98	0.45
3:E:303:SER:O	3:E:304:SER:OG	2.31	0.45
3:E:420:GLY:N	3:E:436:VAL:O	2.48	0.45
4:H:151:LYS:O	4:H:155:TYR:HB2	2.17	0.45
4:H:405:GLY:C	4:H:407:ASP:H	2.20	0.45
5:I:24:SER:OG	5:I:40:ARG:NH2	2.49	0.45
1:A:90:VAL:HG12	1:A:107:LEU:HD22	1.98	0.45
2:D:215:GLU:O	2:D:219:ARG:HG3	2.16	0.45
3:F:130:ASP:OD1	3:F:260:SER:HA	2.17	0.45
4:G:425:LEU:O	4:G:426:LYS:HD2	2.17	0.45
6:L:128:THR:HG21	6:L:160:PRO:HD3	1.99	0.45
1:B:98:GLY:O	6:L:74:ARG:NH2	2.44	0.45
4:G:412:LYS:HA	4:G:412:LYS:HD3	1.75	0.45
5:I:353:ASN:O	5:I:353:ASN:ND2	2.50	0.45
2:C:65:LEU:HD12	2:C:65:LEU:HA	1.77	0.45
2:C:207:THR:OG1	2:C:208:GLN:N	2.50	0.45
2:D:42:VAL:O	2:D:46:THR:HG22	2.16	0.45
2:D:46:THR:O	2:D:170:ARG:NH2	2.50	0.45
3:F:407:ARG:HB2	3:F:424:LYS:HG2	1.99	0.45
6:L:126:TYR:HA	6:L:130:ALA:HB3	1.99	0.45
1:A:112:LYS:HB2	1:A:112:LYS:HE3	1.85	0.45
1:B:295:LEU:HD23	1:B:295:LEU:HA	1.75	0.45
3:E:127:SER:N	3:E:130:ASP:OD2	2.49	0.45
5:I:179:ILE:HG22	5:I:184:SER:HA	1.98	0.45
3:F:303:SER:N	3:F:306:GLU:O	2.50	0.44
5:I:111:ARG:NH2	5:I:238:PHE:O	2.50	0.44
5:J:18:LEU:HD12	5:J:63:VAL:HA	1.99	0.44
5:J:21:ILE:HG21	5:J:113:LEU:HD21	1.98	0.44
5:J:169:ARG:HD2	5:J:218:LEU:O	2.16	0.44
5:J:384:LEU:HA	5:J:402:VAL:HG22	1.98	0.44
6:M:101:TYR:O	6:M:104:SER:OG	2.24	0.44
1:B:204:VAL:HG22	1:B:206:LEU:H	1.82	0.44
5:I:105:SER:OG	5:I:108:ASP:OD2	2.35	0.44
5:I:341:ASP:H	5:I:358:SER:HB3	1.82	0.44
5:J:256:LEU:O	5:J:258:GLY:N	2.49	0.44
1:A:172:SER:OG	1:A:174:SER:HB3	2.17	0.44
2:C:328:ILE:O	2:C:328:ILE:HD12	2.17	0.44
5:J:133:ASN:ND2	5:J:292:VAL:HA	2.33	0.44
5:J:433:ASP:OD1	5:J:433:ASP:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLN:HG3	1:A:258:TYR:CZ	2.53	0.44
2:D:20:LEU:HD23	2:D:25:VAL:HG23	2.00	0.44
3:F:286:GLN:OE1	3:F:287:ARG:HB3	2.16	0.44
5:J:73:HIS:O	5:J:77:ILE:N	2.43	0.44
6:M:129:ILE:O	6:M:133:LEU:HB2	2.17	0.44
1:B:267:LEU:HD21	1:B:306:PRO:HD3	2.00	0.44
2:D:245:MET:O	2:D:249:LEU:HG	2.17	0.44
3:E:416:GLY:HA3	3:E:433:ASP:OD1	2.17	0.44
3:F:47:PHE:CZ	3:F:93:MET:HE2	2.52	0.44
1:A:89:PHE:CD2	1:A:114:PHE:HD2	2.35	0.44
3:E:372:SER:OG	3:E:388:GLY:N	2.51	0.44
3:F:51:LEU:HB2	3:F:55:THR:HG22	1.99	0.44
5:J:77:ILE:O	5:J:81:ILE:HG13	2.18	0.44
1:A:21:GLN:O	1:A:25:LYS:N	2.42	0.44
1:A:107:LEU:O	1:A:111:GLY:N	2.38	0.44
2:D:7:GLU:HG3	5:J:88:LEU:HD13	2.00	0.44
5:I:440:GLY:C	5:I:442:ARG:H	2.21	0.44
5:J:40:ARG:NH2	5:J:41:CYS:HB3	2.31	0.44
5:J:178:VAL:HG22	5:J:214:VAL:HG22	1.99	0.44
1:A:34:THR:OG1	1:A:35:MET:N	2.50	0.44
1:B:92:ARG:HD3	1:B:341:LEU:HD12	2.00	0.44
2:D:4:ILE:HD12	2:D:4:ILE:H	1.83	0.44
5:I:277:LEU:H	5:I:277:LEU:HD23	1.83	0.44
5:J:418:LYS:HD3	5:J:418:LYS:HA	1.75	0.44
6:M:126:TYR:HB3	6:M:131:TRP:CD2	2.53	0.44
1:B:170:ARG:HH22	1:B:296:ILE:HB	1.83	0.44
2:C:17:ILE:HG23	2:C:68:ALA:HB2	1.98	0.44
3:E:274:GLN:NE2	3:E:315:LYS:HB3	2.32	0.44
4:H:167:LEU:HD21	4:H:215:ILE:HD11	2.00	0.44
5:I:162:ALA:O	5:I:217:ASP:HB2	2.18	0.44
1:A:201:MET:O	1:A:204:VAL:HG22	2.17	0.43
1:A:330:SER:HB2	4:G:453:THR:HG23	2.00	0.43
2:C:243:HIS:CG	4:G:416:LEU:HD11	2.53	0.43
3:E:204:ARG:HA	3:E:316:ASP:HA	2.00	0.43
3:E:396:LEU:HG	3:E:413:VAL:HG21	2.00	0.43
4:G:190:LEU:HD23	4:G:222:ILE:HD12	2.00	0.43
4:H:208:SER:OG	4:H:211:MET:HG3	2.18	0.43
5:J:356:ILE:HA	5:J:373:ILE:HB	1.99	0.43
2:D:264:ILE:HD12	2:D:296:VAL:HG12	1.99	0.43
3:F:35:ILE:HD13	4:G:139:LYS:O	2.18	0.43
3:F:374:ILE:HD13	3:F:391:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:186:CYS:HB2	5:J:263:CYS:SG	2.58	0.43
2:C:20:LEU:HA	2:C:20:LEU:HD23	1.74	0.43
2:D:368:THR:OG1	2:D:371:GLY:O	2.25	0.43
3:E:348:VAL:O	3:E:365:GLY:N	2.48	0.43
3:F:177:VAL:HG12	3:F:238:SER:HB3	2.00	0.43
4:G:152:LEU:HD23	4:G:152:LEU:HA	1.81	0.43
4:G:274:TYR:OH	4:G:357:GLY:N	2.49	0.43
4:H:329:LEU:HD21	4:H:361:ILE:HA	2.00	0.43
5:I:24:SER:C	5:I:26:SER:H	2.22	0.43
6:M:165:LEU:O	6:M:169:LYS:HG3	2.18	0.43
1:A:95:HIS:CE1	6:M:48:SER:HG	2.34	0.43
3:E:245:PHE:HB3	3:E:249:VAL:HG21	2.00	0.43
3:F:398:ASP:H	3:F:415:SER:HB3	1.84	0.43
5:I:173:GLU:HB3	5:I:219:ILE:O	2.18	0.43
1:A:36:PRO:O	1:A:40:ILE:HG13	2.19	0.43
1:B:254:PRO:HB3	1:B:259:ASP:HB3	2.00	0.43
3:E:149:ASP:OD1	3:E:149:ASP:N	2.41	0.43
3:F:388:GLY:O	3:F:405:GLY:HA2	2.18	0.43
3:F:393:ASN:O	3:F:410:SER:HA	2.18	0.43
4:G:343:GLY:HA3	4:G:352:LEU:HD11	2.00	0.43
4:G:452:SER:O	4:G:455:VAL:HG23	2.17	0.43
4:H:266:GLN:N	4:H:269:ASP:OD2	2.39	0.43
5:I:358:SER:OG	5:I:375:ASP:OD1	2.33	0.43
6:L:55:ILE:HB	6:L:58:ILE:HG12	2.00	0.43
1:A:329:LYS:HD2	1:A:329:LYS:N	2.33	0.43
1:B:215:VAL:HG12	1:B:217:ASN:H	1.84	0.43
2:D:19:ASP:HA	2:D:24:LYS:HB2	2.01	0.43
2:D:48:TRP:CD2	2:D:54:LEU:HD13	2.54	0.43
4:G:425:LEU:C	4:G:426:LYS:HD2	2.39	0.43
2:D:78:ILE:HD13	2:D:78:ILE:HA	1.85	0.43
3:E:268:PRO:O	3:E:271:VAL:HG12	2.19	0.43
4:G:252:ILE:O	4:G:256:VAL:HG23	2.18	0.43
5:J:243:ILE:O	5:J:247:PHE:HB3	2.19	0.43
6:M:2:THR:HB	6:M:122:LEU:HD22	2.01	0.43
6:M:106:THR:O	6:M:110:ILE:HG13	2.18	0.43
1:B:36:PRO:O	1:B:40:ILE:HG13	2.18	0.43
1:B:96:ASP:OD2	6:L:74:ARG:NE	2.51	0.43
2:C:77:ASN:HD21	2:C:317:SER:HB2	1.82	0.43
2:D:54:LEU:O	2:D:58:VAL:HG22	2.18	0.43
3:F:157:TYR:CE1	3:F:158:THR:HG23	2.53	0.43
4:G:201:LEU:HD12	4:G:201:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:43:LEU:HD12	5:I:50:LEU:HD13	2.01	0.43
5:I:77:ILE:O	5:I:81:ILE:HG13	2.19	0.43
5:I:283:ILE:O	5:I:287:VAL:HG13	2.18	0.43
5:I:305:THR:OG1	5:I:316:GLU:HG2	2.19	0.43
1:A:197:VAL:H	1:B:228:GLN:HE22	1.66	0.43
2:D:243:HIS:CG	4:H:416:LEU:HD11	2.54	0.43
3:F:420:GLY:N	3:F:436:VAL:O	2.47	0.43
4:G:201:LEU:O	4:G:204:THR:HG22	2.19	0.43
4:G:271:ILE:HD12	4:G:340:PHE:CD1	2.54	0.43
2:C:297:ALA:HB1	2:C:362:LEU:HD23	2.01	0.43
2:D:199:LEU:HD11	2:D:218:LEU:HD23	2.00	0.43
3:F:289:LEU:HD12	3:F:289:LEU:O	2.19	0.43
3:F:416:GLY:HA3	3:F:433:ASP:OD1	2.18	0.43
1:A:139:ILE:HD13	1:A:206:LEU:HB3	2.01	0.42
1:A:144:PHE:HA	1:A:178:MET:HB2	2.00	0.42
1:B:34:THR:HG22	1:B:35:MET:H	1.83	0.42
2:C:16:LEU:O	2:C:20:LEU:N	2.52	0.42
4:G:247:ARG:HG3	4:G:248:ASP:N	2.34	0.42
4:H:191:THR:O	4:H:195:ASN:N	2.25	0.42
5:I:389:LYS:O	5:I:407:VAL:HA	2.19	0.42
1:B:328:SER:HG	1:B:331:GLY:H	1.60	0.42
2:C:83:LEU:O	2:C:87:ARG:HD2	2.20	0.42
2:D:264:ILE:H	2:D:264:ILE:HG12	1.69	0.42
3:F:146:LEU:HD22	3:F:242:ILE:HG12	2.01	0.42
6:L:146:LEU:HA	6:L:149:ILE:HG12	2.01	0.42
1:A:297:MET:HE2	1:A:302:ILE:HG12	2.02	0.42
2:C:40:ARG:NH2	2:C:178:GLN:HB2	2.33	0.42
2:C:265:PHE:HB2	4:G:360:LEU:HD21	2.01	0.42
2:D:209:GLY:HA2	2:D:242:SER:HB2	2.02	0.42
2:D:274:VAL:HG13	2:D:307:VAL:HA	2.01	0.42
3:F:155:PRO:HA	3:F:156:PRO:HD3	1.90	0.42
5:I:25:ASP:H	5:I:40:ARG:NH2	2.03	0.42
3:F:270:LEU:HB3	3:F:315:LYS:NZ	2.33	0.42
4:G:279:THR:O	4:G:283:VAL:HG23	2.19	0.42
4:G:407:ASP:OD1	4:G:408:ASP:N	2.52	0.42
5:I:131:VAL:HG23	5:I:270:TYR:HE2	1.84	0.42
5:I:170:ALA:O	5:I:174:SER:N	2.53	0.42
5:J:50:LEU:HB3	5:J:129:ASP:OD2	2.19	0.42
5:J:111:ARG:NH2	5:J:238:PHE:O	2.52	0.42
5:J:143:HIS:HB2	5:J:156:THR:HG21	2.01	0.42
1:A:22:VAL:HG12	1:A:26:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LYS:HE3	5:J:301:LEU:HA	2.00	0.42
3:E:173:VAL:HB	3:E:242:ILE:HB	2.01	0.42
5:I:409:GLY:HA2	5:I:433:ASP:HB2	2.02	0.42
5:J:132:SER:HB2	5:J:271:ALA:HA	2.01	0.42
6:L:94:ILE:O	6:L:98:GLU:HG3	2.20	0.42
6:L:124:GLU:O	6:L:128:THR:HG23	2.19	0.42
6:M:162:LYS:HB2	6:M:166:ASP:OD1	2.20	0.42
1:B:125:ILE:HD13	1:B:243:VAL:CG2	2.49	0.42
1:B:134:ARG:HD3	1:B:134:ARG:HA	1.91	0.42
2:D:22:SER:O	2:D:22:SER:OG	2.32	0.42
2:D:238:ASN:HD21	2:D:290:TYR:HB3	1.85	0.42
2:D:269:SER:HA	2:D:303:HIS:HD2	1.84	0.42
3:E:322:ARG:HA	3:E:322:ARG:HD3	1.90	0.42
3:F:67:ILE:HA	3:F:336:ILE:HG12	2.02	0.42
5:I:215:ARG:HE	5:I:215:ARG:HB3	1.74	0.42
5:J:320:VAL:HG11	5:J:338:LYS:HG2	2.00	0.42
6:M:10:ASN:OD1	6:M:10:ASN:N	2.52	0.42
1:A:258:TYR:CE2	1:B:202:ASN:HB3	2.55	0.42
1:A:297:MET:SD	1:B:168:GLU:HB2	2.60	0.42
1:B:67:ASN:HA	1:B:70:LYS:HB2	2.02	0.42
2:D:278:THR:OG1	2:D:279:HIS:N	2.52	0.42
3:E:126:LYS:HB3	3:E:130:ASP:HB2	2.01	0.42
3:F:133:ARG:NH2	3:F:259:ILE:O	2.52	0.42
3:F:408:LEU:HD11	3:F:419:ILE:HD13	2.02	0.42
4:H:249:ARG:HD2	4:H:249:ARG:HA	1.82	0.42
5:I:256:LEU:HD12	5:I:256:LEU:HA	1.77	0.42
5:J:132:SER:OG	5:J:134:VAL:HG23	2.20	0.42
5:J:320:VAL:HG13	5:J:338:LYS:HA	2.01	0.42
5:J:355:THR:HG23	5:J:372:VAL:HA	2.01	0.42
1:B:60:ASP:OD1	1:B:64:ASN:ND2	2.52	0.42
2:C:29:PHE:O	2:C:33:VAL:HG12	2.19	0.42
2:C:190:ASP:OD1	2:C:190:ASP:N	2.42	0.42
3:F:178:LEU:HD23	3:F:178:LEU:HA	1.85	0.42
5:I:19:GLN:OE1	5:I:120:THR:N	2.37	0.42
5:I:245:LYS:HE2	5:I:245:LYS:HB3	1.83	0.42
5:I:316:GLU:HB3	5:I:335:ALA:HB2	2.00	0.42
6:L:103:LYS:HD2	6:L:141:TYR:CG	2.55	0.42
6:L:122:LEU:O	6:L:125:LEU:N	2.53	0.42
1:A:30:ASP:OD1	1:A:30:ASP:C	2.58	0.42
2:C:243:HIS:ND1	4:G:416:LEU:HD11	2.35	0.42
3:F:123:ASP:HB3	3:F:126:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:ASP:HB2	3:F:327:PRO:HD2	2.02	0.42
3:F:291:SER:HA	3:F:292:PRO:HD2	1.76	0.42
4:G:220:LEU:O	4:G:223:SER:N	2.51	0.42
4:H:125:HIS:HE2	4:H:391:VAL:HA	1.85	0.42
4:H:273:THR:OG1	4:H:274:TYR:N	2.52	0.42
4:H:452:SER:O	4:H:455:VAL:HG23	2.20	0.42
1:A:35:MET:HB2	1:A:36:PRO:HD3	2.01	0.42
2:D:173:ILE:O	2:D:177:ILE:N	2.44	0.42
2:D:207:THR:HG22	2:D:208:GLN:H	1.85	0.42
3:E:447:LEU:HD13	3:E:448:VAL:O	2.20	0.42
3:F:33:GLN:H	3:F:33:GLN:CD	2.22	0.42
3:F:379:ILE:HG12	3:F:396:LEU:HB2	2.02	0.42
4:H:252:ILE:O	4:H:256:VAL:HG23	2.20	0.42
5:I:281:ASP:O	5:I:285:LYS:HG3	2.20	0.42
5:I:386:ASN:ND2	5:I:386:ASN:H	2.18	0.42
5:J:243:ILE:HG23	5:J:244:ARG:HG2	2.02	0.42
6:L:7:PHE:HB2	6:L:37:GLU:O	2.19	0.42
1:A:62:LEU:HD12	1:A:63:GLN:N	2.34	0.41
1:A:86:PHE:O	1:A:90:VAL:HG23	2.20	0.41
1:A:95:HIS:CD2	6:M:48:SER:HG	2.35	0.41
3:E:186:GLN:OE1	3:E:188:LYS:N	2.53	0.41
5:I:114:ASP:O	5:I:117:GLN:HG2	2.20	0.41
5:I:409:GLY:CA	5:I:433:ASP:HB2	2.50	0.41
5:J:24:SER:C	5:J:26:SER:H	2.21	0.41
6:L:111:LEU:O	6:L:115:ALA:N	2.53	0.41
6:L:167:GLU:OE2	6:L:171:TYR:CD1	2.72	0.41
6:M:2:THR:O	6:M:122:LEU:HD13	2.20	0.41
1:B:59:MET:SD	6:L:29:MET:HB3	2.60	0.41
3:E:68:GLY:HA3	3:E:339:LEU:HD23	2.02	0.41
3:E:233:LEU:N	5:J:212:LEU:O	2.48	0.41
3:E:402:VAL:HG23	3:E:419:ILE:HG12	2.02	0.41
4:G:388:ASP:OD1	4:G:391:VAL:HG23	2.19	0.41
4:H:230:THR:H	4:H:233:GLU:HB2	1.83	0.41
5:I:294:PRO:O	5:I:299:SER:OG	2.25	0.41
5:J:169:ARG:O	5:J:171:ARG:NH2	2.53	0.41
5:J:298:ASP:CG	5:J:308:TYR:HB2	2.41	0.41
1:A:171:PRO:HB3	1:B:193:LEU:HD11	2.02	0.41
1:B:220:LEU:O	1:B:310:VAL:HA	2.21	0.41
1:B:339:LEU:O	1:B:341:LEU:N	2.53	0.41
2:C:195:SER:O	2:C:198:HIS:N	2.48	0.41
3:F:39:PHE:HD1	3:F:142:ASP:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:205:ARG:HG3	4:G:206:PRO:HD2	2.02	0.41
4:G:381:PHE:CD2	4:G:455:VAL:HG13	2.55	0.41
5:I:331:THR:OG1	5:I:332:LEU:N	2.54	0.41
5:J:224:ASP:CG	5:J:244:ARG:HH12	2.23	0.41
6:L:162:LYS:NZ	6:L:166:ASP:OD1	2.35	0.41
1:A:210:GLY:O	1:A:222:ASN:ND2	2.54	0.41
1:B:256:SER:C	1:B:258:TYR:H	2.23	0.41
3:E:149:ASP:O	3:E:151:ILE:N	2.51	0.41
4:G:286:HIS:O	4:G:290:VAL:HG23	2.20	0.41
4:H:117:GLU:OE1	4:H:129:ARG:NH1	2.44	0.41
5:J:376:ASN:O	5:J:376:ASN:ND2	2.54	0.41
6:M:50:LEU:HD12	6:M:51:SEP:H	1.86	0.41
6:M:148:ILE:HD12	6:M:148:ILE:HA	1.89	0.41
1:B:74:GLN:H	1:B:74:GLN:HG3	1.59	0.41
1:B:215:VAL:HG11	1:B:254:PRO:HD3	2.02	0.41
2:C:2:SER:H	2:C:5:ASN:HD21	1.68	0.41
2:D:20:LEU:HD23	2:D:20:LEU:HA	1.71	0.41
3:F:101:ASN:O	3:F:105:ARG:N	2.52	0.41
3:F:123:ASP:OD1	3:F:123:ASP:C	2.58	0.41
1:A:57:GLU:O	1:A:61:ILE:HG13	2.21	0.41
1:A:168:GLU:HB2	1:A:193:LEU:HA	2.02	0.41
1:A:267:LEU:HD21	1:A:306:PRO:HD3	2.03	0.41
1:A:269:PHE:CE2	1:B:163:LYS:HB3	2.55	0.41
1:B:139:ILE:HA	1:B:206:LEU:O	2.21	0.41
1:B:210:GLY:HA2	1:B:243:VAL:HG13	2.02	0.41
2:D:-3:ILE:HG22	2:D:64:THR:OG1	2.21	0.41
3:F:209:LYS:HE2	3:F:213:ASP:HB2	2.01	0.41
4:G:180:THR:HG21	4:G:231:ASP:CG	2.41	0.41
4:H:441:THR:HG22	4:H:442:VAL:HG23	2.03	0.41
5:I:91:SER:OG	5:I:93:PHE:O	2.35	0.41
5:I:314:TYR:HB2	5:I:332:LEU:HD13	2.01	0.41
5:I:321:LEU:HD23	5:I:321:LEU:HA	1.76	0.41
5:I:430:THR:HG21	5:I:441:GLY:HA3	2.02	0.41
5:J:101:ARG:CD	5:J:101:ARG:H	2.34	0.41
5:J:338:LYS:HE2	5:J:338:LYS:HB3	1.67	0.41
1:A:182:LEU:HB3	1:A:187:ILE:HD11	2.02	0.41
1:A:276:THR:O	1:A:277:VAL:HG12	2.21	0.41
1:B:201:MET:O	1:B:204:VAL:N	2.50	0.41
3:E:396:LEU:HA	3:E:413:VAL:HG23	2.02	0.41
3:F:122:LEU:HD23	3:F:122:LEU:HA	1.88	0.41
4:H:440:ILE:HG21	4:H:452:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:16:HIS:C	5:I:18:LEU:H	2.24	0.41
5:J:290:ARG:NH2	5:J:296:VAL:HG11	2.29	0.41
1:A:101:GLU:H	1:A:101:GLU:CD	2.24	0.41
1:A:232:PHE:HZ	1:B:228:GLN:HG3	1.86	0.41
1:B:134:ARG:HG3	2:C:323:ASP:OD2	2.19	0.41
2:C:235:PHE:CD1	2:C:236:PRO:HA	2.56	0.41
2:C:235:PHE:CG	2:C:236:PRO:HA	2.55	0.41
3:E:355:LEU:HD21	3:E:369:LYS:O	2.21	0.41
5:I:80:TYR:O	5:I:84:SER:N	2.53	0.41
5:I:229:ASP:O	5:I:233:LEU:HG	2.21	0.41
5:J:58:LEU:HD23	5:J:124:ILE:HD11	2.03	0.41
5:J:351:GLY:N	5:J:367:LEU:O	2.52	0.41
6:L:76:ASP:OD1	6:L:78:GLU:HG2	2.20	0.41
6:M:47:LEU:H	6:M:47:LEU:HD22	1.86	0.41
6:M:173:SER:O	6:M:175:ARG:N	2.51	0.41
1:A:210:GLY:HA2	1:A:243:VAL:HG13	2.02	0.41
1:A:337:ILE:HD12	6:M:56:ARG:HH11	1.85	0.41
1:B:138:VAL:HG13	1:B:205:ASP:H	1.85	0.41
1:B:145:SER:H	1:B:178:MET:HE1	1.86	0.41
2:C:275:ILE:HD13	2:C:308:VAL:HB	2.02	0.41
3:E:206:LEU:HD13	3:E:231:VAL:HG12	2.03	0.41
3:E:250:ILE:HD13	3:E:253:ILE:HD12	2.02	0.41
3:F:360:CYS:SG	3:F:376:LYS:N	2.94	0.41
5:I:71:CYS:SG	5:I:104:LEU:HB2	2.61	0.41
5:I:147:ARG:NH1	5:I:151:LYS:O	2.51	0.41
6:L:131:TRP:O	6:L:135:ARG:N	2.45	0.41
1:A:50:SER:O	1:A:104:LYS:NZ	2.47	0.41
1:A:57:GLU:HB2	6:M:81:TYR:CD2	2.56	0.41
1:A:218:GLY:HA2	1:A:332:VAL:HG11	2.02	0.41
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.93	0.41
1:B:170:ARG:HB2	1:B:194:ASP:OD2	2.21	0.41
3:E:344:ARG:HD2	3:E:345:LEU:HG	2.03	0.41
3:F:231:VAL:O	5:I:214:VAL:N	2.46	0.41
4:H:270:VAL:H	4:H:337:THR:HG22	1.86	0.41
5:I:297:PRO:HB3	5:I:306:PHE:CD2	2.56	0.41
5:J:190:GLN:OE1	5:J:199:VAL:HG22	2.21	0.41
5:J:305:THR:O	5:J:316:GLU:HA	2.21	0.41
1:A:77:ILE:H	1:A:77:ILE:HG12	1.65	0.40
1:B:46:LEU:O	1:B:50:SER:OG	2.39	0.40
1:B:57:GLU:HB2	6:L:81:TYR:CD2	2.56	0.40
1:B:167:THR:HG22	1:B:194:ASP:OD1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:320:TYR:O	2:C:322:TYR:N	2.54	0.40
4:H:133:THR:OG1	4:H:134:THR:N	2.54	0.40
4:H:311:LEU:HD22	4:H:323:TYR:HB2	2.03	0.40
5:I:185:GLN:HB2	5:I:262:HIS:CE1	2.56	0.40
5:J:374:GLY:N	5:J:390:ILE:O	2.54	0.40
6:L:20:MET:HG2	6:L:101:TYR:CE2	2.56	0.40
6:M:131:TRP:N	6:M:132:PRO:HD2	2.36	0.40
1:A:141:THR:OG1	1:A:142:HIS:N	2.54	0.40
2:C:289:THR:O	2:C:356:ASP:N	2.54	0.40
3:E:33:GLN:O	3:E:35:ILE:N	2.54	0.40
3:E:237:LEU:HD23	3:E:237:LEU:HA	1.87	0.40
3:E:338:LYS:N	3:E:338:LYS:HD2	2.35	0.40
3:F:221:ARG:O	3:F:224:LEU:HB3	2.20	0.40
5:I:136:LEU:O	5:I:139:VAL:N	2.55	0.40
5:J:31:PHE:O	5:J:35:THR:HG23	2.21	0.40
5:J:55:PHE:HD1	5:J:55:PHE:HA	1.78	0.40
5:J:358:SER:O	5:J:376:ASN:N	2.46	0.40
6:M:124:GLU:O	6:M:128:THR:HG23	2.21	0.40
1:A:92:ARG:HE	1:A:341:LEU:HB3	1.87	0.40
1:A:217:ASN:HB3	1:A:253:PHE:CZ	2.56	0.40
1:B:90:VAL:HG12	1:B:107:LEU:HD12	2.03	0.40
2:D:328:ILE:HD12	4:H:331:TYR:CD1	2.57	0.40
3:F:32:LEU:C	3:F:34:SER:H	2.25	0.40
3:F:446:ARG:HD3	3:F:446:ARG:HA	1.63	0.40
4:G:140:ASP:OD1	4:G:140:ASP:N	2.53	0.40
4:H:411:GLU:H	4:H:411:GLU:CD	2.24	0.40
5:I:330:ARG:O	5:I:347:ASN:HA	2.20	0.40
3:E:141:ASN:OD1	3:E:141:ASN:N	2.54	0.40
5:I:40:ARG:NH2	5:I:41:CYS:HB3	2.28	0.40
5:J:184:SER:O	5:J:262:HIS:ND1	2.49	0.40
6:L:128:THR:OG1	6:L:129:ILE:HG12	2.21	0.40
1:A:250:VAL:HG23	1:A:252:MET:HG2	2.03	0.40
1:A:305:ASN:HD21	1:B:192:VAL:HA	1.87	0.40
2:C:48:TRP:HH2	2:C:170:ARG:HB3	1.86	0.40
2:D:194:GLN:HE21	2:D:194:GLN:HB3	1.62	0.40
3:E:326:LEU:HA	3:E:327:PRO:HD2	1.91	0.40
4:H:111:GLU:O	4:H:114:ILE:HG22	2.21	0.40
6:M:103:LYS:HD2	6:M:141:TYR:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:367:THR:OG1	6:L:14:GLU:OE2[1_556]	2.03	0.17

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	313/341 (92%)	279 (89%)	30 (10%)	4 (1%)	12 42
1	B	311/341 (91%)	281 (90%)	25 (8%)	5 (2%)	9 38
2	C	333/399 (84%)	307 (92%)	25 (8%)	1 (0%)	41 73
2	D	333/399 (84%)	306 (92%)	24 (7%)	3 (1%)	17 51
3	E	405/458 (88%)	332 (82%)	66 (16%)	7 (2%)	9 36
3	F	405/458 (88%)	338 (84%)	61 (15%)	6 (2%)	10 39
4	G	358/467 (77%)	317 (88%)	38 (11%)	3 (1%)	19 53
4	H	359/467 (77%)	325 (90%)	28 (8%)	6 (2%)	9 36
5	I	428/678 (63%)	377 (88%)	46 (11%)	5 (1%)	13 44
5	J	426/678 (63%)	380 (89%)	39 (9%)	7 (2%)	9 38
6	L	162/304 (53%)	148 (91%)	13 (8%)	1 (1%)	25 59
6	M	164/304 (54%)	146 (89%)	16 (10%)	2 (1%)	13 44
All	All	3997/5294 (76%)	3536 (88%)	411 (10%)	50 (1%)	12 42

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	356	ALA
1	A	74	GLN
1	A	255	LEU
1	B	98	GLY
2	D	255	ASP
3	E	122	LEU
3	E	191	ASP

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Mol	Chain	Res	Type
3	E	288	PHE
3	F	397	MET
4	H	465	VAL
6	L	130	ALA
1	B	74	GLN
1	B	257	GLN
3	E	329	TYR
3	F	213	ASP
4	G	305	PHE
4	H	403	ASN
5	I	18	LEU
5	I	370	ASP
6	M	56	ARG
6	M	130	ALA
1	B	340	TYR
3	E	359	ASP
3	E	397	MET
3	F	33	GLN
3	F	285	ILE
3	F	329	TYR
4	H	140	ASP
4	H	410	GLU
5	I	14	PRO
5	I	441	GLY
5	J	16	HIS
5	J	35	THR
5	J	290	ARG
5	J	425	SER
5	J	441	GLY
1	B	274	PRO
2	D	185	ASP
3	E	382	ASN
4	G	408	ASP
4	H	276	HIS
5	J	295	PHE
3	F	309	ILE
5	I	290	ARG
5	J	257	LEU
2	D	321	PRO
1	A	277	VAL
2	C	321	PRO
1	A	274	PRO

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Mol	Chain	Res	Type
4	H	406	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/298 (92%)	267 (97%)	8 (3%)	42	70
1	B	273/298 (92%)	262 (96%)	11 (4%)	31	62
2	C	290/350 (83%)	279 (96%)	11 (4%)	33	63
2	D	290/350 (83%)	284 (98%)	6 (2%)	53	77
3	E	355/395 (90%)	334 (94%)	21 (6%)	19	51
3	F	355/395 (90%)	336 (95%)	19 (5%)	22	54
4	G	324/408 (79%)	312 (96%)	12 (4%)	34	63
4	H	325/408 (80%)	311 (96%)	14 (4%)	29	60
5	I	381/596 (64%)	368 (97%)	13 (3%)	37	66
5	J	379/596 (64%)	368 (97%)	11 (3%)	42	70
6	L	153/273 (56%)	150 (98%)	3 (2%)	55	78
6	M	155/273 (57%)	148 (96%)	7 (4%)	27	59
All	All	3555/4640 (77%)	3419 (96%)	136 (4%)	33	63

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	99	ASP
1	A	116	GLN
1	A	172	SER
1	A	174	SER
1	A	253	PHE
1	A	328	SER
1	A	330	SER
1	B	16	GLU

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Mol	Chain	Res	Type
1	B	74	GLN
1	B	89	PHE
1	B	122	ARG
1	B	145	SER
1	B	161	ARG
1	B	174	SER
1	B	238	LYS
1	B	253	PHE
1	B	258	TYR
1	B	328	SER
2	C	10	TYR
2	C	87	ARG
2	C	92	GLU
2	C	98	ASP
2	C	260	SER
2	C	261	ASP
2	C	311	SER
2	C	332	SER
2	C	339	PHE
2	C	340	ASN
2	C	380	ARG
2	D	92	GLU
2	D	311	SER
2	D	339	PHE
2	D	340	ASN
2	D	341	GLU
2	D	354	TYR
3	E	39	PHE
3	E	57	SER
3	E	72	MET
3	E	132	LEU
3	E	141	ASN
3	E	175	SER
3	E	182	HIS
3	E	186	GLN
3	E	189	GLU
3	E	220	PHE
3	E	221	ARG
3	E	228	HIS
3	E	257	GLU
3	E	279	PHE
3	E	287	ARG

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Mol	Chain	Res	Type
3	E	308	LYS
3	E	330	PHE
3	E	344	ARG
3	E	359	ASP
3	E	435	ARG
3	E	446	ARG
3	F	39	PHE
3	F	47	PHE
3	F	72	MET
3	F	113	ARG
3	F	141	ASN
3	F	166	ASP
3	F	178	LEU
3	F	188	LYS
3	F	228	HIS
3	F	230	ARG
3	F	233	LEU
3	F	276	GLN
3	F	279	PHE
3	F	283	GLU
3	F	286	GLN
3	F	321	SER
3	F	322	ARG
3	F	330	PHE
3	F	345	LEU
4	G	123	PHE
4	G	125	HIS
4	G	140	ASP
4	G	158	PHE
4	G	187	SER
4	G	208	SER
4	G	217	PHE
4	G	225	LEU
4	G	295	ARG
4	G	301	SER
4	G	354	SER
4	G	464	GLN
4	H	123	PHE
4	H	125	HIS
4	H	130	ARG
4	H	147	ARG
4	H	158	PHE

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Mol	Chain	Res	Type
4	H	171	PHE
4	H	208	SER
4	H	217	PHE
4	H	259	GLN
4	H	301	SER
4	H	354	SER
4	H	379	TYR
4	H	411	GLU
4	H	418	ASN
5	I	29	TYR
5	I	40	ARG
5	I	84	SER
5	I	91	SER
5	I	163	SER
5	I	197	HIS
5	I	237	ASN
5	I	242	ASP
5	I	244	ARG
5	I	281	ASP
5	I	325	CYS
5	I	361	SER
5	I	442	ARG
5	J	40	ARG
5	J	101	ARG
5	J	163	SER
5	J	238	PHE
5	J	242	ASP
5	J	257	LEU
5	J	273	ARG
5	J	325	CYS
5	J	381	LYS
5	J	410	ASP
5	J	442	ARG
6	L	90	SER
6	L	145	LYS
6	L	171	TYR
6	M	5	CYS
6	M	10	ASN
6	M	54	ARG
6	M	66	LYS
6	M	122	LEU
6	M	151	GLU

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Mol	Chain	Res	Type
6	M	175	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	100	ASN
2	C	329	GLN
2	D	329	GLN
3	F	328	ASN
4	H	176	GLN
4	H	400	GLN
5	I	96	ASN
5	I	303	ASN
5	J	117	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
6	SEP	L	51	6	8,9,10	1.48	1 (12%)	8,12,14	1.82	2 (25%)
6	SEP	M	51	6	8,9,10	1.50	1 (12%)	8,12,14	1.74	2 (25%)

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
6	SEP	L	51	6	-	3/5/8/10	-
6	SEP	M	51	6	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	51	SEP	P-O1P	3.31	1.61	1.50
6	L	51	SEP	P-O1P	3.25	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	51	SEP	P-OG-CB	-3.78	107.88	118.30
6	M	51	SEP	P-OG-CB	-3.46	108.76	118.30
6	M	51	SEP	OG-CB-CA	3.02	111.08	108.14
6	L	51	SEP	OG-CB-CA	2.97	111.03	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	51	SEP	CB-OG-P-O1P
6	L	51	SEP	CB-OG-P-O2P
6	L	51	SEP	CB-OG-P-O3P
6	M	51	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	51	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	D	401	-	4,4,4	1.14	0	6,6,6	0.39	0
7	PO4	F	502	-	4,4,4	1.04	0	6,6,6	0.44	0
7	PO4	G	501	-	4,4,4	1.10	0	6,6,6	0.53	0
7	PO4	B	401	-	4,4,4	1.00	0	6,6,6	0.41	0
7	PO4	C	401	-	4,4,4	1.11	0	6,6,6	0.44	0
7	PO4	E	501	-	4,4,4	1.19	0	6,6,6	0.51	0
7	PO4	F	501	-	4,4,4	1.22	0	6,6,6	0.44	0
7	PO4	E	502	-	4,4,4	1.03	0	6,6,6	0.41	0
7	PO4	H	501	-	4,4,4	1.14	0	6,6,6	0.42	0
7	PO4	I	701	-	4,4,4	1.10	0	6,6,6	0.47	0
7	PO4	A	401	-	4,4,4	1.03	0	6,6,6	0.41	0
7	PO4	J	701	-	4,4,4	1.03	0	6,6,6	0.49	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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	502	PO4	1	0
7	G	501	PO4	1	0
7	C	401	PO4	1	0
7	A	401	PO4	2	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	317/341 (92%)	-0.06	4 (1%)	77	80	76, 112, 160, 206	0
1	B	315/341 (92%)	0.00	2 (0%)	89	92	74, 110, 157, 180	0
2	C	337/399 (84%)	0.02	0	100	100	53, 90, 149, 189	0
2	D	337/399 (84%)	0.03	0	100	100	58, 90, 152, 208	0
3	E	409/458 (89%)	0.04	5 (1%)	79	82	66, 105, 169, 201	0
3	F	409/458 (89%)	-0.00	3 (0%)	87	91	69, 107, 170, 196	0
4	G	360/467 (77%)	0.04	1 (0%)	94	95	62, 89, 148, 183	0
4	H	361/467 (77%)	0.03	2 (0%)	89	92	62, 89, 151, 184	0
5	I	430/678 (63%)	0.00	5 (1%)	79	82	71, 108, 159, 199	0
5	J	428/678 (63%)	-0.00	5 (1%)	79	82	72, 108, 156, 194	0
6	L	166/304 (54%)	0.13	9 (5%)	25	28	87, 161, 204, 222	0
6	M	168/304 (55%)	0.04	5 (2%)	50	53	89, 159, 206, 215	0
All	All	4037/5294 (76%)	0.02	41 (1%)	82	86	53, 104, 175, 222	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	L	57	SER	5.1
6	L	56	ARG	4.7
6	M	55	ILE	4.1
5	J	103	SER	3.8
5	I	372	VAL	3.6
6	M	56	ARG	3.6
4	H	182	TYR	3.5
3	E	217	ASP	3.4
6	M	29	MET	3.3
1	A	14	GLN	3.3
6	M	54	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
5	I	407	VAL	3.1
1	A	23	TYR	3.0
5	I	405	GLY	3.0
3	F	187	SER	3.0
3	E	216	SER	3.0
1	B	293	ASN	3.0
6	L	28	GLU	2.9
5	I	389	LYS	2.9
5	J	436	LEU	2.4
4	G	123	PHE	2.4
1	B	58	PHE	2.4
6	L	153	VAL	2.4
1	A	16	GLU	2.3
6	L	113	TYR	2.3
3	E	430	ILE	2.3
6	L	27	ALA	2.3
5	J	413	ILE	2.3
5	J	395	SER	2.2
3	F	206	LEU	2.2
3	E	414	ALA	2.1
5	J	433	ASP	2.1
3	E	270	LEU	2.1
6	M	28	GLU	2.1
6	L	145	LYS	2.1
4	H	466	TYR	2.1
5	I	22	VAL	2.1
6	L	160	PRO	2.1
1	A	88	ARG	2.0
3	F	218	PHE	2.0
6	L	152	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
6	SEP	M	51	10/11	0.92	0.10	137,154,182,184	0
6	SEP	L	51	10/11	0.95	0.11	132,141,152,159	0

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	B	401	5/5	0.81	0.13	137,161,171,193	0
7	PO4	I	701	5/5	0.82	0.40	111,124,146,169	0
7	PO4	J	701	5/5	0.85	0.95	136,141,152,185	0
7	PO4	A	401	5/5	0.86	0.15	149,154,168,180	0
7	PO4	D	401	5/5	0.91	0.23	56,91,105,123	0
7	PO4	H	501	5/5	0.91	0.23	91,93,111,124	0
7	PO4	F	501	5/5	0.92	0.23	84,99,115,117	0
7	PO4	C	401	5/5	0.93	0.18	63,115,116,137	0
7	PO4	E	502	5/5	0.93	0.20	114,130,143,164	0
7	PO4	E	501	5/5	0.94	0.32	61,91,121,127	0
7	PO4	F	502	5/5	0.94	0.17	131,139,155,167	0
7	PO4	G	501	5/5	0.94	0.23	81,92,120,121	0

6.5 Other polymers (i)

There are no such residues in this entry.