



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:46 AM UTC

PDB ID : 6JLY / pdb_00006jly
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

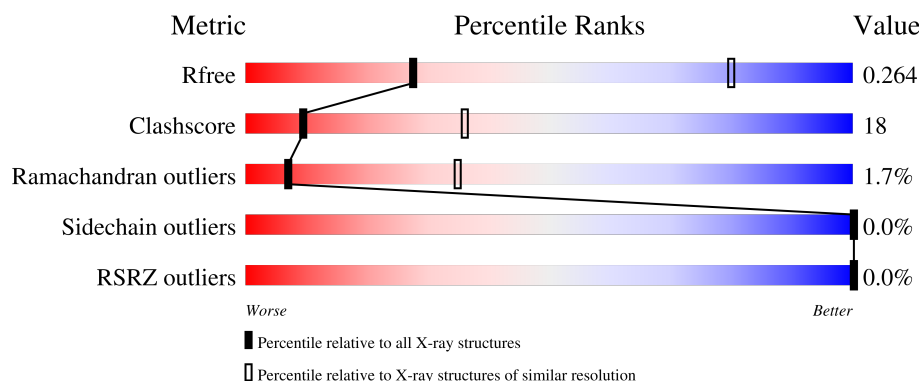
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

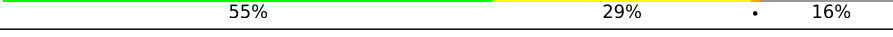
The reported resolution of this entry is 3.50 Å.

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	
2	C	399	
2	D	399	
3	E	458	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	458	
4	G	467	
4	H	467	
5	I	678	
5	J	678	
6	L	304	
6	M	304	

2 Entry composition

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
1	A	316	Total	C	N	O	S	0	0	0
			2467	1568	431	455	13			
1	B	316	Total	C	N	O	S	0	0	0
			2465	1566	429	457	13			

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

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

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
3	E	414	Total	C	N	O	S	0	0	0
			3216	2040	555	604	17			
3	F	412	Total	C	N	O	S	0	0	0
			3204	2034	553	600	17			

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
4	G	363	Total	C	N	O	S	0	0	0
			2869	1834	486	536	13			
4	H	363	Total	C	N	O	S	0	0	0
			2869	1834	486	536	13			

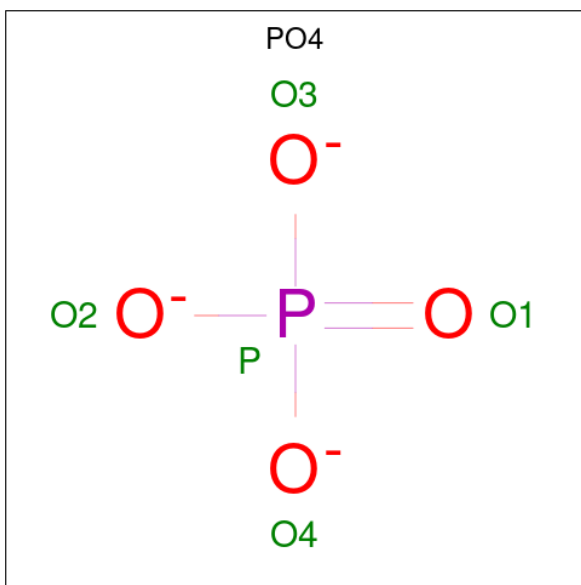
- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

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

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

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

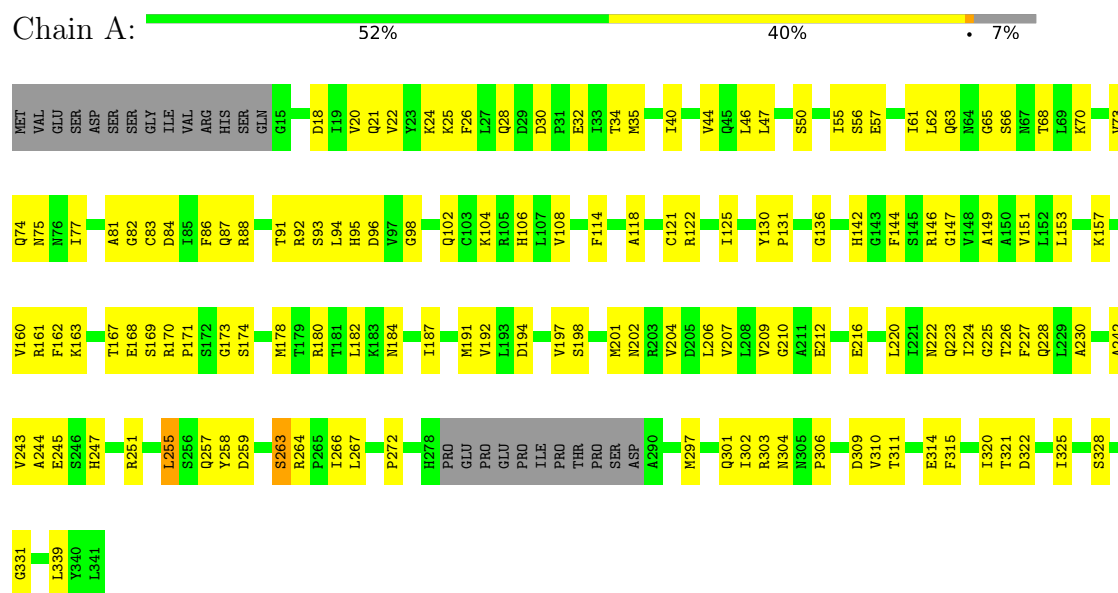


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		
7	G	1	Total	O	P	0	0
			5	4	1		
7	H	1	Total	O	P	0	0
			5	4	1		

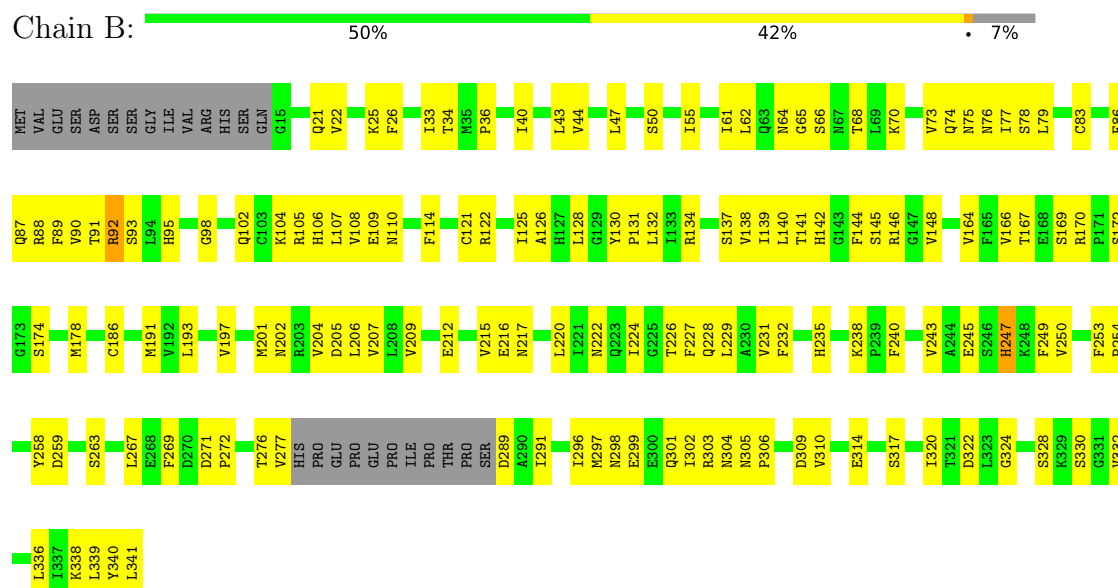
3 Residue-property plots

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.

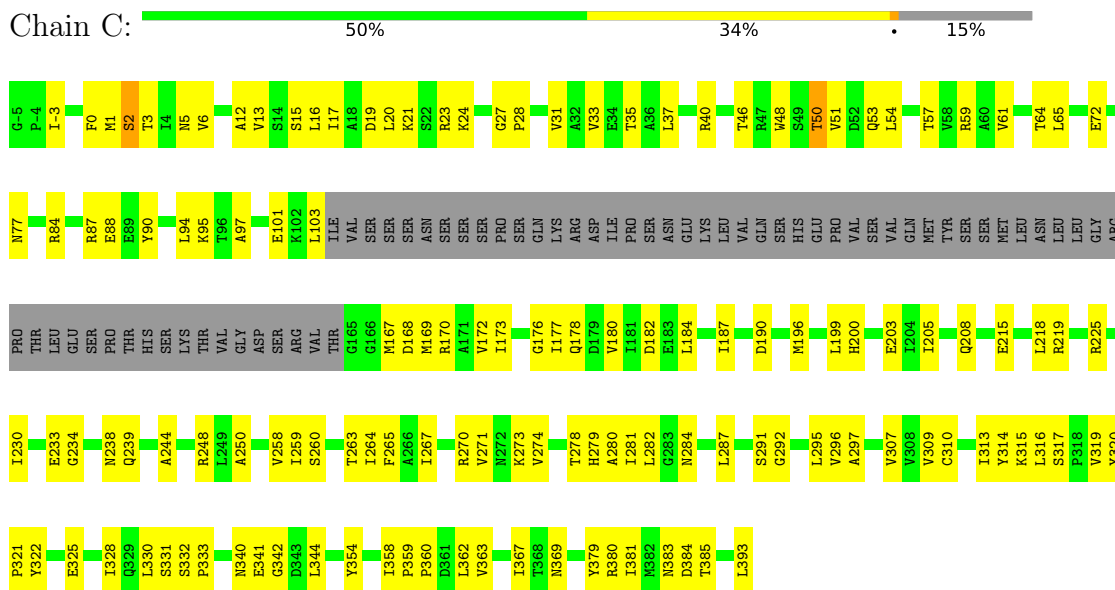
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



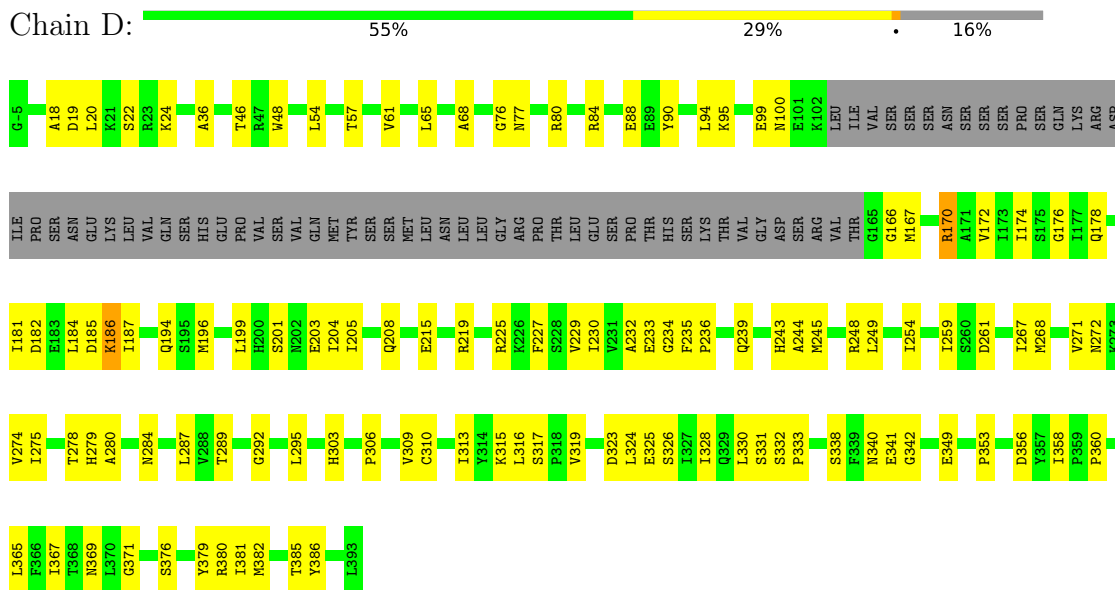
- Molecule 1: Translation initiation factor eIF-2B subunit alpha



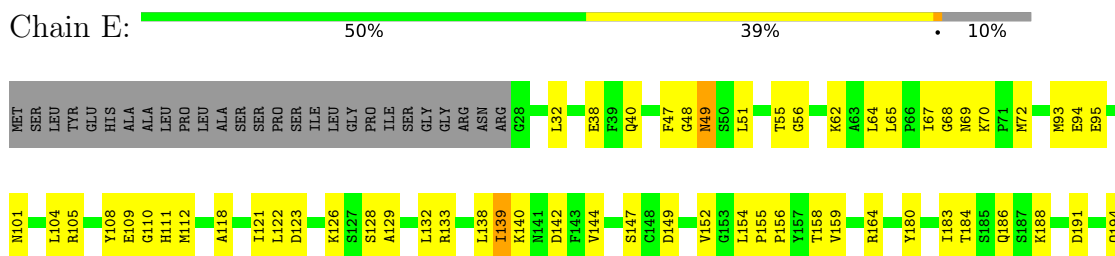
- Molecule 2: Probable translation initiation factor eIF-2B subunit beta

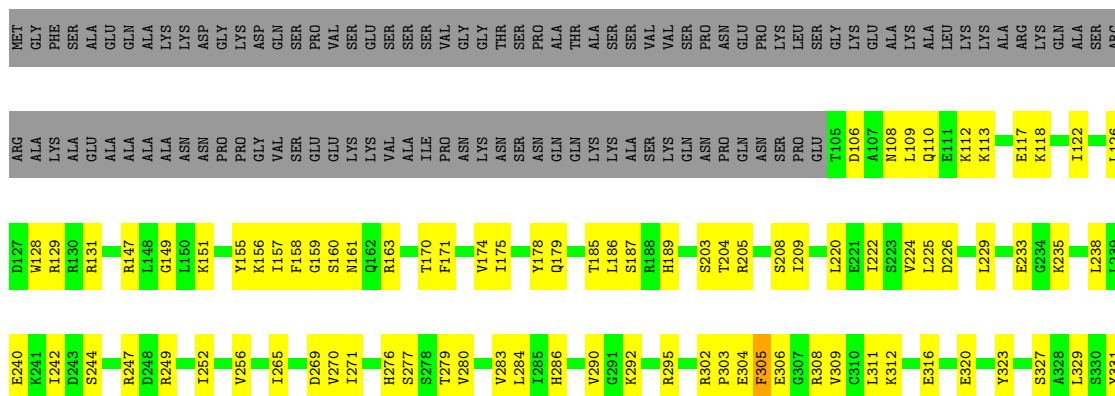


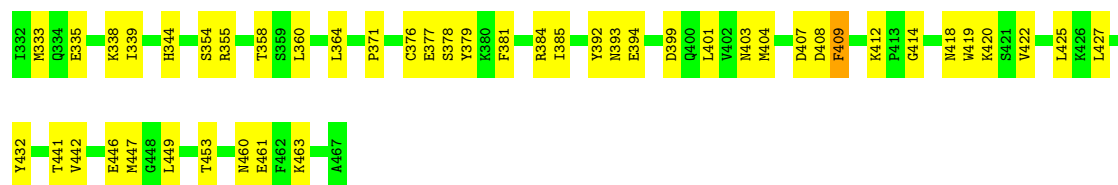
- Molecule 2: Probable translation initiation factor eIF-2B subunit beta



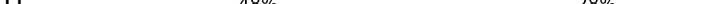
- Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

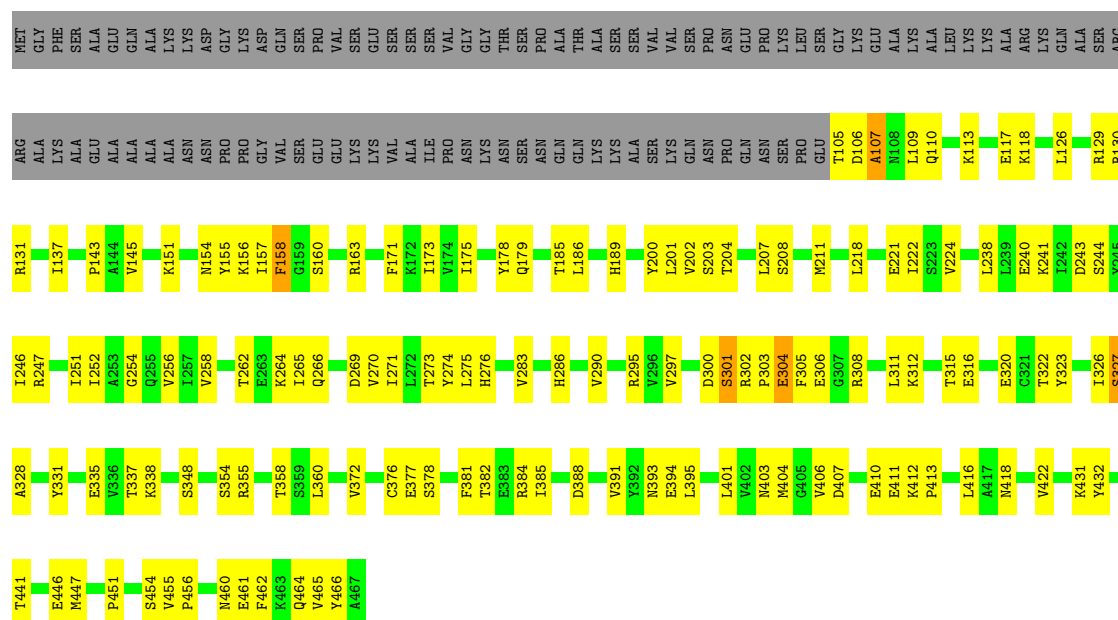






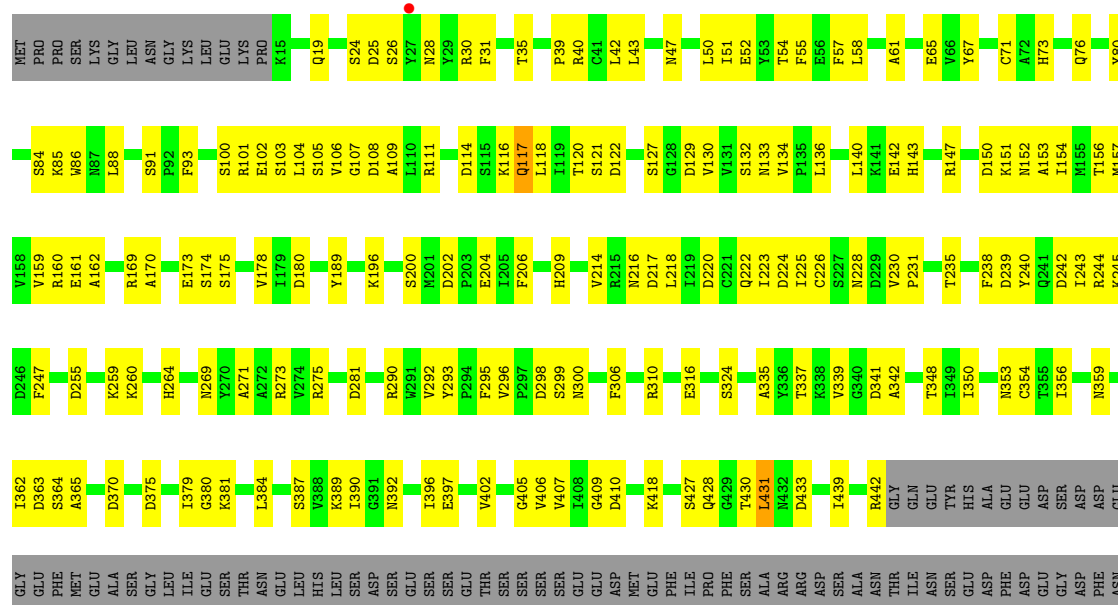
- Molecule 4: Probable translation initiation factor eIF-2B subunit delta

Chain H:  48% 28% 2% 22%



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

Chain I: 38% 25% 37%



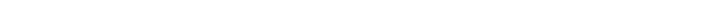
[illegible]

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

Chain J: 38% 24% 37%

ALA	ILE	GLU	PHE	ASP	A365	Y270	I179	E82	MET
ILE	ALA	ALA	ASN	GLU	F366	A271	D180	K83	PRO
GLN	LEU	GLN	LYS	GLY	A272	A272	S94	S84	PRO
ALA	ALA	GLU	GLU	GLU	D370	R273	S184	S185	SER
TRP	GLN	LYS	ALA	PHE	V371	V274	G185	F93	LYS
TYR	VAL	GLN	GLN	MET	V372	R275	C186		GLY
SER	MET	GLN	GLN	GLU	I373	S276		R101	LEU
ASP	THR	SER	SER	ALA		L277	Y189		ASN
PRO	PRO	ARG	LEU	SER	N376	Q278		L104	GLY
ARG	TRP	GLU	GLU	GLY	T279	T279	V199		LYS
SER	GLY	ARG	ARG	LEU	I379	Y280		D108	LEU
SER	SER	ALA	ILE	ILE			D202		GLU
GLU	GLU	LEU	PHE	GLU	L384	T283		D109	LYS
GLY	GLU	LEU	GLU	THR	A385		F206	L110	PRO
GLU	ALA	ALA	GLU	THR	N386	R290		R111	
LEU	LEU	LYS	GLU	ASN	S387		H209	E112	
ALA	ALA	LEU	HTS	GLU	V388	P294	E210	T120	
ALA	ALA	LEU	GLN	LEU	K389	F295		S121	
THR	PHE	ALA	ILE	HIS	I390	V296	E213	D122	
LEU	LEU	ARG	ILE	LEU		P297	V214	F123	
ARG	ARG	SER	ILE	LEU		D298	R215	I124	
ASP	ALA	HIS	ILE	ASP	I396		N216	Y29	
ALA	ALA	GLU	ALA	SER		T305	D217	F31	
GLY	GLY	ALA	LEU	GLU	G399		L218	R32	
GLN	GLN	LEU	LEU	SER	A400				
LYS	VAL	GLU	GLU	SER	I401	Q309	T219	V130	
GLN	ASP	LEU	LEU	SER	V402	R310	D220	S131	
PHE	PHE	ASN	ASN	GLU			C221	S132	
VAL	VAL	VAL	THR	THR	V407	I313	Q222	K38	
LEU	LEU	LEU	LEU	SER	A408		I223	P135	
ASP	ASP	LEU	ARG	SER	G409	E316	D224	L136	
TRP	TRP	LEU	MET	SER		E317	I225	R137	
LEU	LEU	GLN	ALA	SER	T412		C226	E138	
ASN	ASN	GLN	ALA	SER		V320		V139	
THR	THR	LYS	MET	GLU			V230	N47	
ALA	TYR	ASN	ASN	GLU	N417			L50	
GLU	GLU	ALA	ALA	ASP	K418	R323		E142	
SER	SER	VAL	ASN	MET	R419	S324	F334	K145	
GLU	GLU	ARG	TYR	GLU	L420		T235		
LEU	LEU	SER	HTS	PHE	T421	K328		R146	
GLU	GLU	LEU	ILE	ILE	T422		F238	R147	
SER	SER	MET	VAL	PRO		T331	D239	E148	
GLU	GLU	THR	ARG	PHE	H426	L332	Y240	D149	
ARG	ARG	THR	SER	SER	S427		Q241	D150	
GLU	HIS	ALA	ALA	ALA	Q428	A335	D242	K151	
GLY	PHE	LEU	ILE	ARG			I243	N152	
SER	SER	LEU	VAL	ARG	P434	K338	R244	A153	
GLU	GLN	LEU	LEU	ASP		V339		Q64	
LEU	LEU	LEU	ALA	SER	G440		F247	V159	
LEU	LEU	LEU	LEU	GLY	GLY	A342	V248	E65	
GLY	GLY	GLY	LEU	ASN	THR		Y249	R160	
TYR	TYR	ARG	THR	GLN	GLY	A346		E161	
PHE	PHE	ARG	ILE	GLN	N347		T253	S163	
TYR	TYR	ILE	ILE	ASN	GLU	T348	S254	A72	
GLN	GLN	MET	SER	SER	TYR	I349	D255	R169	
LEU	LEU	HTS	GLU	GLU	HIS	I350		A170	
GLU	GLU	LEU	LEU	ASP	ALA		K260	R171	
ASP	PHE	GLU	ASP	GLU	GLU	I356		I77	
ILE	ILE	VAL	VAL	ASP	GLU	S357	C263	S174	
ALA	ALA	GLU	SER	GLU	ASP	S358	H264	S175	
GLU	GLU	GLU	GLY	SER	GLY			Y80	
ASN	ASN	ASN	ASN	ASN	ASN	S264	N269	V172	

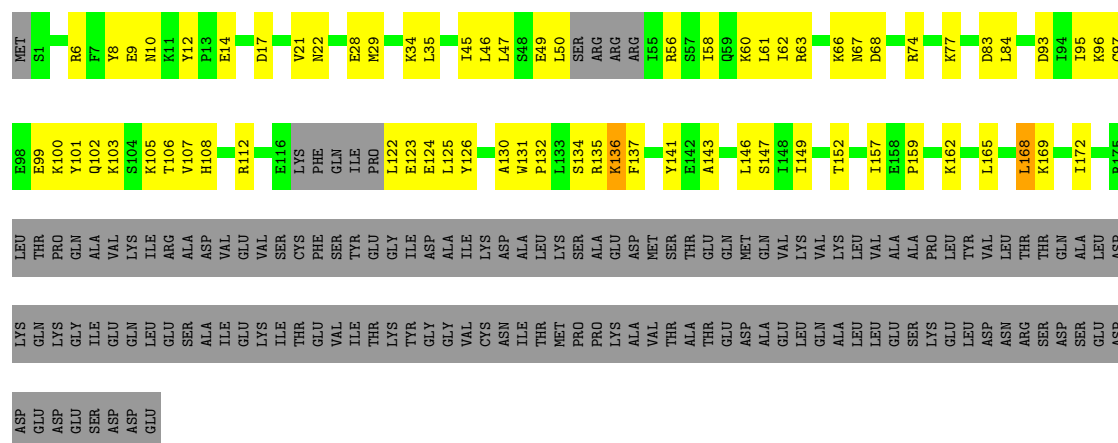
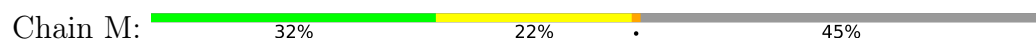
- Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain L:  31% 23% 46%

Y171	S90	MET
R175	S91	S1
THR	E92	
PRO	D93	R6
GLN	K96	F7
ALA	C97	Y8
VAL	Y101	E9
LYS	Y102	N10
ILE	K103	K11
ARG	K104	
ALA	K105	E14
ASP	T106	D17
VAL	V107	I18
GLU	I110	V19
VAL	L111	M20
SER	R112	M22
CYS	Y113	V23
PHE	C114	
SER	A115	E28
TYR	E116	M29
GLY	LYS	
ILE	PHE	V33
ASP	GLN	K34
ALA	ILE	L36
ILE	PRO	
LYS	LEU	E42
ASP	E123	L47
ALA	E124	S48
LEU	L125	E49
LYS	Y126	L50
SER	K127	S51
ALA	T128	B52
GLU	I129	ARG
ASP	A130	ARG
MET	W131	ILE
SER		ARG
THR	R135	S57
GLU		I58
GLN	H139	C59
MET		K60
LYS	E142	L61
VAL	L143	I62
LYS	L146	R63
VAL		
LYS	I149	K66
LEU	D150	M67
VAL	E151	D68
ALA		
ALA	I157	D76
PRO	P160	K77
LEU		E78
TYR	V164	
VAL		D83
THR	E167	K86
THR		R87
THR	N170	

[illegible]

- Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha



4 Data and refinement statistics

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) 88.9 (49.31-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.224 , 0.260 0.227 , 0.264	Depositor DCC
R_{free} test set	1979 reflections (1.60%)	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 , 117.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.380 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.19	0/2513	0.40	0/3399
1	B	0.19	0/2510	0.38	0/3395
2	C	0.22	0/2661	0.40	0/3611
2	D	0.23	0/2653	0.39	0/3600
3	E	0.21	0/3272	0.45	0/4427
3	F	0.22	0/3260	0.47	0/4411
4	G	0.24	0/2917	0.40	0/3951
4	H	0.25	1/2917 (0.0%)	0.39	0/3951
5	I	0.20	0/3437	0.40	0/4658
5	J	0.20	0/3422	0.40	0/4639
6	L	0.16	0/1374	0.41	0/1845
6	M	0.16	0/1384	0.41	0/1859
All	All	0.21	1/32320 (0.0%)	0.41	0/43746

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	SER	C-N	-5.70	1.25	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2467	0	2490	102	0
1	B	2465	0	2487	114	0
2	C	2617	0	2653	105	0
2	D	2609	0	2642	85	0
3	E	3216	0	3273	140	0
3	F	3204	0	3263	122	0
4	G	2869	0	2958	96	0
4	H	2869	0	2958	90	0
5	I	3377	0	3361	137	0
5	J	3362	0	3345	125	0
6	L	1353	0	1374	54	0
6	M	1363	0	1391	51	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	1144	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 18.

All (1144) 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

Continued on next page...

Continued from previous page...

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
3:F:397:MET:HE2	3:F:414:ALA:HA	1.71	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:204:VAL:O	1:B:238:LYS:NZ	2.24	0.70
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:GLU:HB3	2:C:344:LEU:HD13	1.73	0.69
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
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
4:G:178:TYR:HH	4:G:189:HIS:HD1	1.42	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:L:6:ARG:HH12	6:L:9:GLU:C	2.04	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:I:65:GLU:OE2	5:I:67:TYR:OH	2.13	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
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
4:G:333:MET:HE1	4:G:339:ILE:HD11	1.79	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
1:B:169:SER:HG	1:B:172:SER:HG	1.45	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
1:B:87:GLN:HB3	6:L:29:MET:HE3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:239:ASP:OD1	3:F:240:ALA:N	2.32	0.62
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
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
4:H:378:SER:OG	4:H:446:GLU:OE2	2.19	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:H:354:SER:OG	4:H:355:ARG:N	2.31	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:76:ASN:OD1	1:B:78:SER:OG	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:E:65:LEU:HD12	3:E:397:MET:HE1	1.84	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:H:269:ASP:OD2	4:H:338:LYS:NZ	2.38	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
3:F:271:VAL:N	3:F:315:LYS:HZ1	2.03	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:394:SER:OG	3:F:408:LEU:O	2.24	0.56
4:H:300:ASP:OD1	4:H:301:SER:N	2.37	0.56
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
6:L:90:SER:OG	6:L:91:SER:N	2.32	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:358:ALA:C	3:F:360:CYS:H	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
4:G:265:ILE:O	4:G:292:LYS:NZ	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:L:102:GLN:O	6:L:106:THR:OG1	2.19	0.53
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:271:VAL:N	3:E:315:LYS:HZ1	2.07	0.52
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
2:D:184:LEU:O	2:D:186:LYS:N	2.39	0.52
5:J:364:SER:O	5:J:364:SER:OG	2.24	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
5:J:276:SER:O	5:J:279:THR:OG1	2.19	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
2:D:166:GLY:H	2:D:167:MET:HE3	1.75	0.52
1:A:169:SER:O	1:A:173:GLY:N	2.42	0.52
1:B:64:ASN:O	1:B:68:THR:OG1	2.25	0.52
1:B:66:SER:O	1:B:70:LYS:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:H:411:GLU:H	4:H:411:GLU:CD	2.17	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
4:G:128:TRP:H	4:G:128:TRP:CD1	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:370:ASP:N	3:F:370:ASP:OD1	2.45	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
1:B:297:MET:HE3	1:B:302:ILE:HG12	1.94	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:410:SER:O	3:E:410:SER:OG	2.25	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
5:I:24:SER:C	5:I:26:SER:H	2.20	0.49
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
6:L:101:TYR:O	6:L:104:SER:OG	2.29	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
1:B:126:ALA:C	1:B:128:LEU:H	2.20	0.48
3:E:400:ILE:HG22	3:E:417:ALA:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:288:PHE:C	3:F:289:LEU:HD23	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:31:VAL:O	2:C:35:THR:OG1	2.27	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
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:201:LEU:O	4:H:204:THR:OG1	2.27	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
1:A:168:GLU:CD	1:B:170:ARG:HH21	2.23	0.47
2:D:381:ILE:O	2:D:385:THR:OG1	2.28	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
3:E:432:VAL:C	3:E:434:HIS:H	2.23	0.47
4:G:149:GLY:O	4:G:204:THR:OG1	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:G:404:MET:HE2	4:G:414:GLY:HA2	1.97	0.47
5:I:91:SER:OG	5:I:93:PHE:O	2.32	0.47
1:A:222:ASN:HB3	1:A:226:THR:OG1	2.15	0.47
1:B:92:ARG:HH21	1:B:340:TYR:C	2.22	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: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:A:297:MET:HE3	1:A:302:ILE:HG12	1.97	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:352:GLU:CD	3:F:370:ASP:HB3	2.41	0.46
5:I:19:GLN:CD	5:I:120:THR:H	2.23	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:112:MET:HE2	3:E:112:MET:HB3	1.84	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
6:L:93:ASP:OD1	6:L:93:ASP:N	2.48	0.46
1:A:142:HIS:HE1	1:A:169:SER:HA	1.81	0.45
2:D:54:LEU:O	2:D:57:THR:OG1	2.30	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
6:L:90:SER:HG	6:L:91:SER:N	2.14	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:I:39:PRO:HD3	5:I:73:HIS:CG	2.52	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:J:356:ILE:HA	5:J:373:ILE:HB	1.99	0.45
4:H:355:ARG:O	4:H:358:THR:OG1	2.25	0.44
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
4:H:185:THR:OG1	4:H:186:LEU:N	2.49	0.44
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
3:E:47:PHE:CD2	3:E:93:MET:HE3	2.52	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:188:LYS:C	3:F:190:ILE:H	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:322:ASP:OD1	1:B:322:ASP:N	2.48	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:257:GLU:C	3:E:259:ILE:H	2.25	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
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: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
4:H:404:MET:HE2	4:H:404:MET:HB3	1.84	0.44
1:B:328:SER:C	1:B:330:SER:H	2.26	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:J:421:THR:OG1	5:J:422:THR:N	2.50	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:331:TYR:CD1	4:G:331:TYR:C	2.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:L:68:ASP:CG	6:L:86:LYS:HZ2	2.27	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
3:F:48:GLY:O	3:F:49:ASN:C	2.62	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
5:I:152:ASN:OD1	5:I:259:LYS:NZ	2.43	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
2:C:84:ARG:HH12	2:C:383:ASN:C	2.25	0.43
3:E:38:GLU:HG3	4:H:143:PRO:HB3	2.00	0.43
3:E:149:ASP:HB2	3:E:327:PRO:HG2	2.00	0.43
3:E:375:LYS:O	3:E:377:SER:OG	2.33	0.43
4:H:110:GLN:O	4:H:113:LYS:HB3	2.19	0.43
4:H:326:ILE:C	4:H:328:ALA:H	2.26	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:J:202:ASP:OD1	5:J:202:ASP:N	2.39	0.42
6:L:111:LEU:C	6:L:113:TYR:H	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:G:106:ASP:OD1	4:G:106:ASP:N	2.52	0.42
5:I:111:ARG:HG2	5:I:235:THR:HA	2.00	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: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
3:E:263:ARG:HH21	7:E:502:PO4:P	2.42	0.42
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:127:SER:OG	3:F:128:SER:N	2.48	0.42
3:F:392:SER:OG	3:F:393:ASN:ND2	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:SER:O	1:B:104:LYS:NZ	2.51	0.42
2:C:208:GLN:NE2	2:C:292:GLY:O	2.49	0.42
3:E:358:ALA:C	3:E:360:CYS:H	2.27	0.42
3:F:190:ILE:HG23	3:F:328:ASN:HB2	2.02	0.42
3:F:358:ALA:C	3:F:360:CYS:N	2.78	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:I:228:ASN:HD22	5:I:228:ASN:C	2.26	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:L:21:VAL:HG23	6:L:34:LYS:C	2.45	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
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
3:F:202:THR:C	3:F:204:ARG:H	2.28	0.41
4:G:331:TYR:C	4:G:331:TYR:HD1	2.28	0.41
5:I:353:ASN:HB3	5:I:370:ASP:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:149:ALA:HB2	1:A:178:MET:HE1	2.02	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
3:E:202:THR:C	3:E:204:ARG:H	2.27	0.41
4:G:446:GLU:OE1	4:G:446:GLU:N	2.47	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
3:F:363:ASN:CG	3:F:364:GLU:H	2.28	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
6:M:47:LEU:C	6:M:49:GLU:H	2.27	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
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:343:GLN:CD	3:E:344:ARG:H	2.24	0.41
3:E:344:ARG:HB2	3:E:344:ARG:NH1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:ASN:HD22	5:J:347:ASN:C	2.28	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:196:MET:HE3	2:D:196:MET:HB3	1.86	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
4:H:331:TYR:C	4:H:331:TYR:CD1	2.99	0.41
5:I:54:THR:O	5:I:58:LEU:HD23	2.20	0.41
6:M:21:VAL:HG23	6:M:34:LYS:C	2.45	0.41
6:M:29:MET:HE2	6:M:29:MET:HB3	1.98	0.41
1:A:82:GLY:O	1:A:86:PHE:N	2.44	0.41
2:C:196:MET:HE3	2:C:196:MET:HB3	1.81	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:144:PHE:H	1:A:174:SER:HG	1.60	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:288:PHE:C	3:F:290:SER:H	2.28	0.41
3:F:401:VAL:HG13	3:F:418:GLN:HG3	2.03	0.41
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
5:J:150:ASP:OD2	5:J:260:LYS:NZ	2.43	0.41
5:J:278:GLN:H	5:J:278:GLN:CD	2.28	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: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
1:B:89:PHE:C	1:B:89:PHE:CD1	2.98	0.40
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
5:J:328:LYS:O	5:J:331:THR:OG1	2.39	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
4:H:464:GLN:C	4:H:466:TYR:H	2.29	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:389:LYS:C	5:I:390:ILE:HD12	2.46	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:C:325:GLU:CD	5:I:310:ARG:HE	2.29	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
3:E:222:MET:HE3	3:E:222:MET:HB2	1.90	0.40
4:H:129:ARG:C	4:H:130:ARG:HD2	2.47	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	7	36
1	B	312/341 (92%)	268 (86%)	39 (12%)	5 (2%)	7	36
2	C	334/399 (84%)	299 (90%)	33 (10%)	2 (1%)	21	54
2	D	333/399 (84%)	300 (90%)	27 (8%)	6 (2%)	6	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	410/458 (90%)	327 (80%)	72 (18%)	11 (3%)	4	27
3	F	408/458 (89%)	344 (84%)	51 (12%)	13 (3%)	3	24
4	G	361/467 (77%)	321 (89%)	36 (10%)	4 (1%)	11	43
4	H	361/467 (77%)	330 (91%)	20 (6%)	11 (3%)	3	25
5	I	426/678 (63%)	369 (87%)	54 (13%)	3 (1%)	18	51
5	J	424/678 (62%)	378 (89%)	43 (10%)	3 (1%)	18	51
6	L	159/304 (52%)	134 (84%)	23 (14%)	2 (1%)	9	39
6	M	160/304 (53%)	133 (83%)	23 (14%)	4 (2%)	4	28
All	All	4000/5294 (76%)	3474 (87%)	457 (11%)	69 (2%)	7	35

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	183	ILE

5.3.2 Protein sidechains ⓘ

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%)	274 (100%)	0	100	100
1	B	274/298 (92%)	274 (100%)	0	100	100
2	C	291/350 (83%)	291 (100%)	0	100	100
2	D	290/350 (83%)	290 (100%)	0	100	100
3	E	359/395 (91%)	358 (100%)	1 (0%)	86	83
3	F	357/395 (90%)	357 (100%)	0	100	100
4	G	326/408 (80%)	326 (100%)	0	100	100
4	H	326/408 (80%)	326 (100%)	0	100	100
5	I	379/596 (64%)	379 (100%)	0	100	100
5	J	378/596 (63%)	378 (100%)	0	100	100
6	L	152/274 (56%)	152 (100%)	0	100	100
6	M	153/274 (56%)	153 (100%)	0	100	100
All	All	3559/4642 (77%)	3558 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	247	HIS
1	A	257	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	21	GLN
1	B	110	ASN
1	B	228	GLN
2	C	41	GLN
2	C	45	GLN
2	C	202	ASN
2	D	194	GLN
2	D	202	ASN
2	D	302	HIS
2	D	340	ASN
3	E	33	GLN
3	F	310	ASN
3	F	393	ASN
3	F	418	GLN
4	G	179	GLN
4	H	193	HIS
5	I	28	ASN
5	I	117	GLN
5	I	311	HIS
5	I	432	ASN
5	J	137	ASN
5	J	190	GLN
6	L	24	GLN
6	M	59	GLN
6	M	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	D	401	-	4,4,4	1.02	0	6,6,6	0.42	0
7	PO4	G	501	-	4,4,4	1.02	0	6,6,6	0.53	0
7	PO4	E	501	-	4,4,4	1.03	0	6,6,6	0.48	0
7	PO4	F	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	C	401	-	4,4,4	1.01	0	6,6,6	0.46	0
7	PO4	F	501	-	4,4,4	1.05	0	6,6,6	0.42	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	G	501	PO4	1	0
7	H	501	PO4	1	0
7	C	401	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-1.23	0 100 100	109, 145, 196, 237	0
1	B	316/341 (92%)	-1.18	0 100 100	106, 146, 196, 238	0
2	C	338/399 (84%)	-1.20	0 100 100	79, 121, 185, 214	0
2	D	337/399 (84%)	-1.25	0 100 100	76, 120, 189, 232	0
3	E	414/458 (90%)	-1.07	0 100 100	88, 139, 206, 234	0
3	F	412/458 (89%)	-1.08	0 100 100	93, 138, 205, 236	0
4	G	363/467 (77%)	-1.14	0 100 100	87, 122, 187, 235	0
4	H	363/467 (77%)	-1.21	0 100 100	88, 119, 191, 228	0
5	I	428/678 (63%)	-1.13	1 (0%) 91 82	101, 141, 187, 209	0
5	J	426/678 (62%)	-1.22	0 100 100	100, 141, 184, 222	0
6	L	165/304 (54%)	-0.84	0 100 100	121, 203, 232, 244	0
6	M	166/304 (54%)	-0.99	0 100 100	121, 202, 236, 253	0
All	All	4044/5294 (76%)	-1.15	1 (0%) 100 100	76, 137, 209, 253	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	27	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	D	401	5/5	0.97	0.06	80,107,166,167	0
7	PO4	C	401	5/5	0.98	0.05	98,137,158,184	0
7	PO4	E	502	5/5	0.98	0.05	171,171,195,223	0
7	PO4	F	502	5/5	0.98	0.04	172,179,190,228	0
7	PO4	H	501	5/5	0.98	0.06	105,106,166,171	0
7	PO4	E	501	5/5	0.99	0.10	114,122,147,186	0
7	PO4	G	501	5/5	0.99	0.05	115,136,151,154	0
7	PO4	F	501	5/5	0.99	0.13	113,128,142,183	0

6.5 Other polymers [i](#)

There are no such residues in this entry.