Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:31 am BST

PDB ID	:	3ECS
Title	:	Crystal structure of human eIF2B alpha
Authors	:	Hiyama, T.B.; Ito, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2008-09-01
Resolution	:	2.65 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 following versions of software and data (see references ①) were used in the production of this report:

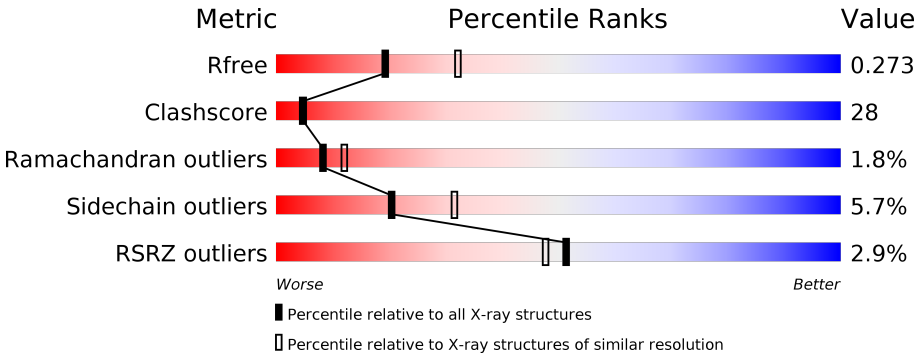
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	315	4% 55% 31% • 11%
1	B	315	5% 50% 36% • 11%
1	C	315	3% 54% 36% • 7%
1	D	315	2% 57% 31% 5% 8%
1	E	315	2% 51% 35% 5% 10%
1	F	315	% 54% 32% • • 9%

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Mol	Chain	Length	Quality of chain
1	G	315	46% 40% • 10%
1	H	315	4% 53% 33% • 10%

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
2	SO4	A	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17958 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	279	Total	C	N	O	S	Se	0	0	0
			2165	1392	362	399	5	7			
1	B	281	Total	C	N	O	S	Se	0	0	0
			2180	1401	365	402	5	7			
1	C	294	Total	C	N	O	S	Se	0	0	0
			2282	1465	380	425	5	7			
1	D	291	Total	C	N	O	S	Se	0	0	0
			2255	1448	377	418	5	7			
1	E	285	Total	C	N	O	S	Se	0	0	0
			2211	1420	368	411	5	7			
1	F	287	Total	C	N	O	S	Se	0	0	0
			2221	1427	372	410	5	7			
1	G	284	Total	C	N	O	S	Se	0	0	0
			2200	1414	368	406	5	7			
1	H	285	Total	C	N	O	S	Se	0	0	0
			2208	1418	369	409	5	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ALA	-	EXPRESSION TAG	UNP Q14232
A	307	ALA	-	EXPRESSION TAG	UNP Q14232
A	308	ALA	-	EXPRESSION TAG	UNP Q14232
A	309	GLU	-	EXPRESSION TAG	UNP Q14232
A	310	HIS	-	EXPRESSION TAG	UNP Q14232
A	311	HIS	-	EXPRESSION TAG	UNP Q14232
A	312	HIS	-	EXPRESSION TAG	UNP Q14232
A	313	HIS	-	EXPRESSION TAG	UNP Q14232
A	314	HIS	-	EXPRESSION TAG	UNP Q14232
A	315	HIS	-	EXPRESSION TAG	UNP Q14232
B	306	ALA	-	EXPRESSION TAG	UNP Q14232
B	307	ALA	-	EXPRESSION TAG	UNP Q14232
B	308	ALA	-	EXPRESSION TAG	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
B	309	GLU	-	EXPRESSION TAG	UNP Q14232
B	310	HIS	-	EXPRESSION TAG	UNP Q14232
B	311	HIS	-	EXPRESSION TAG	UNP Q14232
B	312	HIS	-	EXPRESSION TAG	UNP Q14232
B	313	HIS	-	EXPRESSION TAG	UNP Q14232
B	314	HIS	-	EXPRESSION TAG	UNP Q14232
B	315	HIS	-	EXPRESSION TAG	UNP Q14232
C	306	ALA	-	EXPRESSION TAG	UNP Q14232
C	307	ALA	-	EXPRESSION TAG	UNP Q14232
C	308	ALA	-	EXPRESSION TAG	UNP Q14232
C	309	GLU	-	EXPRESSION TAG	UNP Q14232
C	310	HIS	-	EXPRESSION TAG	UNP Q14232
C	311	HIS	-	EXPRESSION TAG	UNP Q14232
C	312	HIS	-	EXPRESSION TAG	UNP Q14232
C	313	HIS	-	EXPRESSION TAG	UNP Q14232
C	314	HIS	-	EXPRESSION TAG	UNP Q14232
C	315	HIS	-	EXPRESSION TAG	UNP Q14232
D	306	ALA	-	EXPRESSION TAG	UNP Q14232
D	307	ALA	-	EXPRESSION TAG	UNP Q14232
D	308	ALA	-	EXPRESSION TAG	UNP Q14232
D	309	GLU	-	EXPRESSION TAG	UNP Q14232
D	310	HIS	-	EXPRESSION TAG	UNP Q14232
D	311	HIS	-	EXPRESSION TAG	UNP Q14232
D	312	HIS	-	EXPRESSION TAG	UNP Q14232
D	313	HIS	-	EXPRESSION TAG	UNP Q14232
D	314	HIS	-	EXPRESSION TAG	UNP Q14232
D	315	HIS	-	EXPRESSION TAG	UNP Q14232
E	306	ALA	-	EXPRESSION TAG	UNP Q14232
E	307	ALA	-	EXPRESSION TAG	UNP Q14232
E	308	ALA	-	EXPRESSION TAG	UNP Q14232
E	309	GLU	-	EXPRESSION TAG	UNP Q14232
E	310	HIS	-	EXPRESSION TAG	UNP Q14232
E	311	HIS	-	EXPRESSION TAG	UNP Q14232
E	312	HIS	-	EXPRESSION TAG	UNP Q14232
E	313	HIS	-	EXPRESSION TAG	UNP Q14232
E	314	HIS	-	EXPRESSION TAG	UNP Q14232
E	315	HIS	-	EXPRESSION TAG	UNP Q14232
F	306	ALA	-	EXPRESSION TAG	UNP Q14232
F	307	ALA	-	EXPRESSION TAG	UNP Q14232
F	308	ALA	-	EXPRESSION TAG	UNP Q14232
F	309	GLU	-	EXPRESSION TAG	UNP Q14232
F	310	HIS	-	EXPRESSION TAG	UNP Q14232

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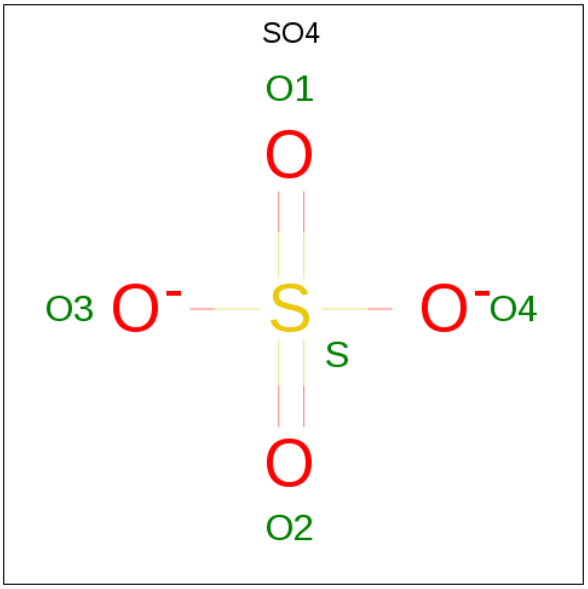
Chain	Residue	Modelled	Actual	Comment	Reference
F	311	HIS	-	EXPRESSION TAG	UNP Q14232
F	312	HIS	-	EXPRESSION TAG	UNP Q14232
F	313	HIS	-	EXPRESSION TAG	UNP Q14232
F	314	HIS	-	EXPRESSION TAG	UNP Q14232
F	315	HIS	-	EXPRESSION TAG	UNP Q14232
G	306	ALA	-	EXPRESSION TAG	UNP Q14232
G	307	ALA	-	EXPRESSION TAG	UNP Q14232
G	308	ALA	-	EXPRESSION TAG	UNP Q14232
G	309	GLU	-	EXPRESSION TAG	UNP Q14232
G	310	HIS	-	EXPRESSION TAG	UNP Q14232
G	311	HIS	-	EXPRESSION TAG	UNP Q14232
G	312	HIS	-	EXPRESSION TAG	UNP Q14232
G	313	HIS	-	EXPRESSION TAG	UNP Q14232
G	314	HIS	-	EXPRESSION TAG	UNP Q14232
G	315	HIS	-	EXPRESSION TAG	UNP Q14232
H	306	ALA	-	EXPRESSION TAG	UNP Q14232
H	307	ALA	-	EXPRESSION TAG	UNP Q14232
H	308	ALA	-	EXPRESSION TAG	UNP Q14232
H	309	GLU	-	EXPRESSION TAG	UNP Q14232
H	310	HIS	-	EXPRESSION TAG	UNP Q14232
H	311	HIS	-	EXPRESSION TAG	UNP Q14232
H	312	HIS	-	EXPRESSION TAG	UNP Q14232
H	313	HIS	-	EXPRESSION TAG	UNP Q14232
H	314	HIS	-	EXPRESSION TAG	UNP Q14232
H	315	HIS	-	EXPRESSION TAG	UNP Q14232

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	27	Total O 27 27	0	0
4	C	20	Total O 20 20	0	0
4	D	24	Total O 24 24	0	0
4	E	15	Total O 15 15	0	0
4	F	26	Total O 26 26	0	0
4	G	28	Total O 28 28	0	0

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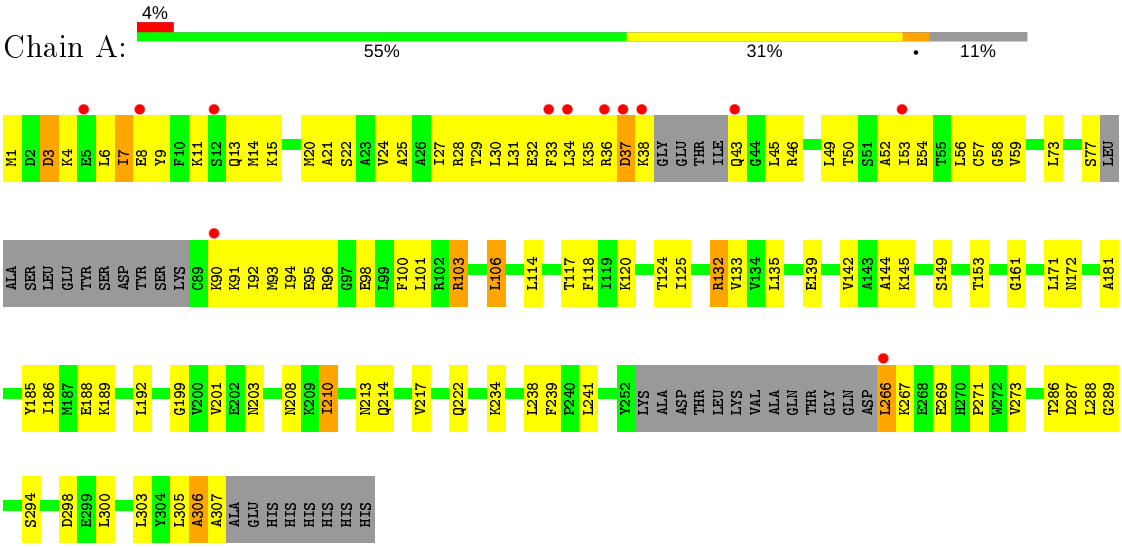
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	15	Total O 15 15	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

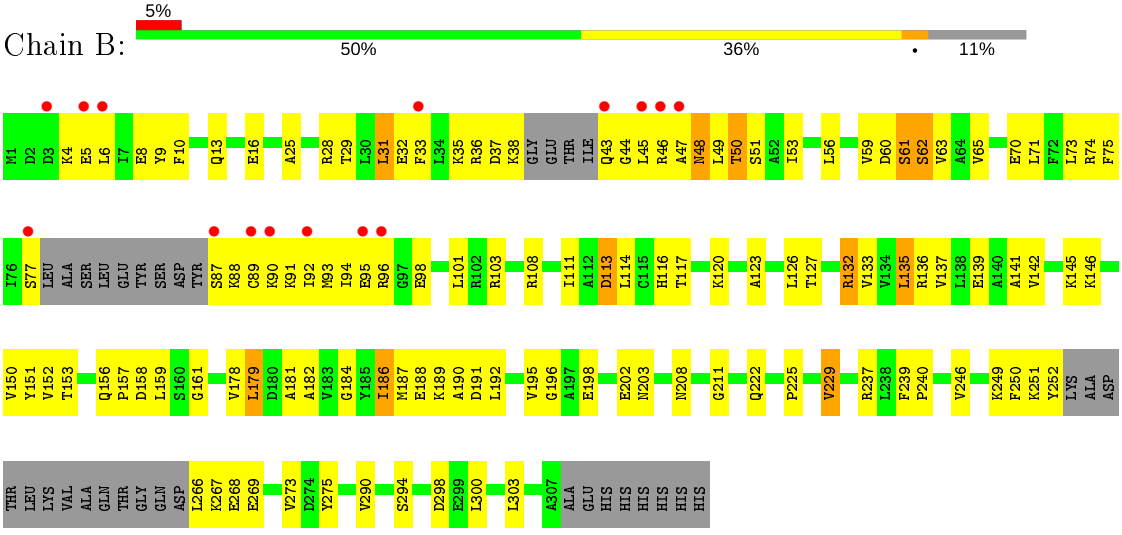
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



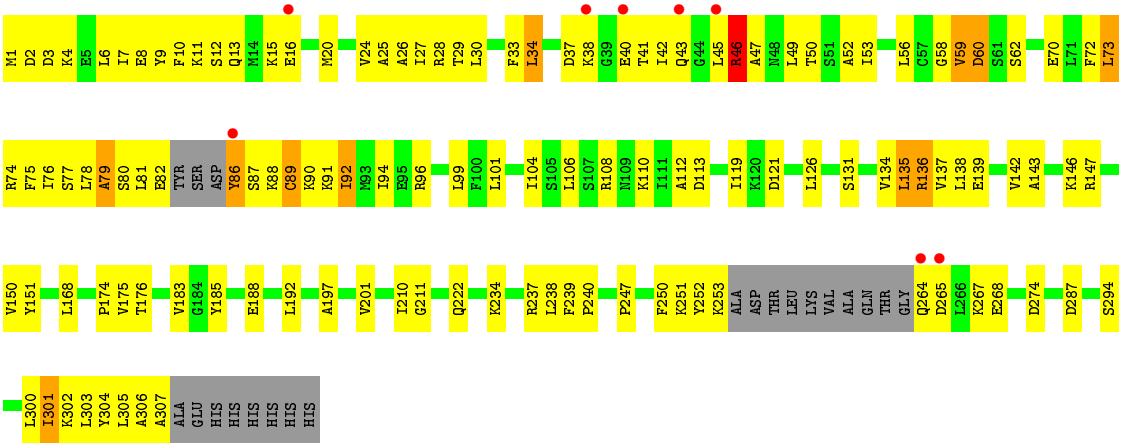
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B:



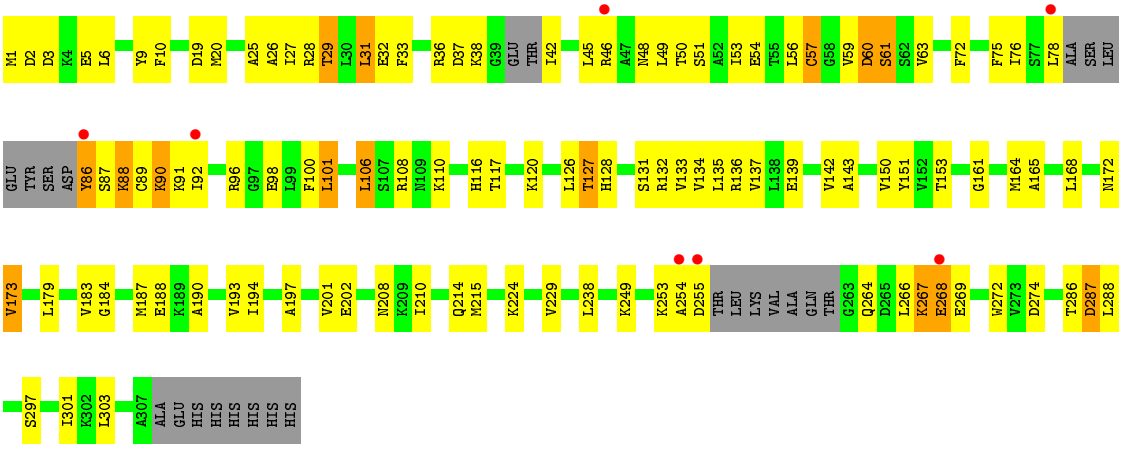
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain C:



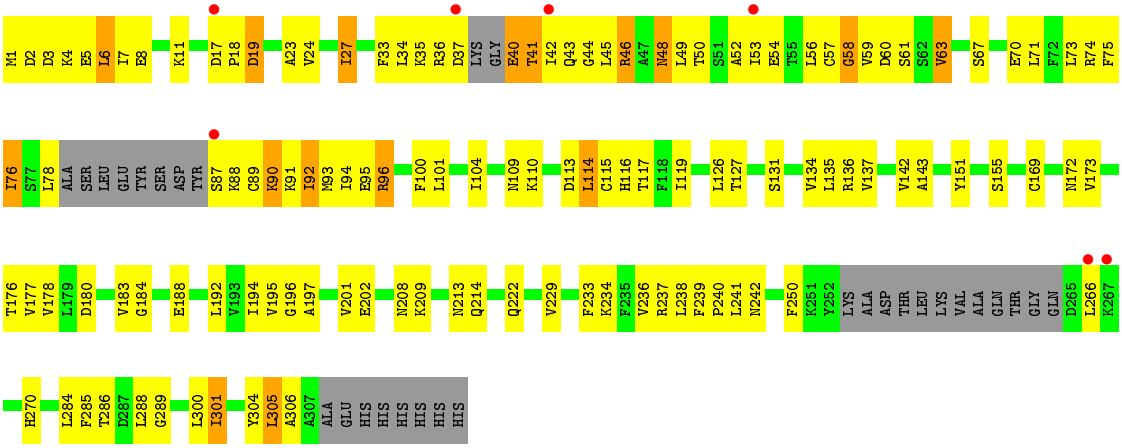
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain D:



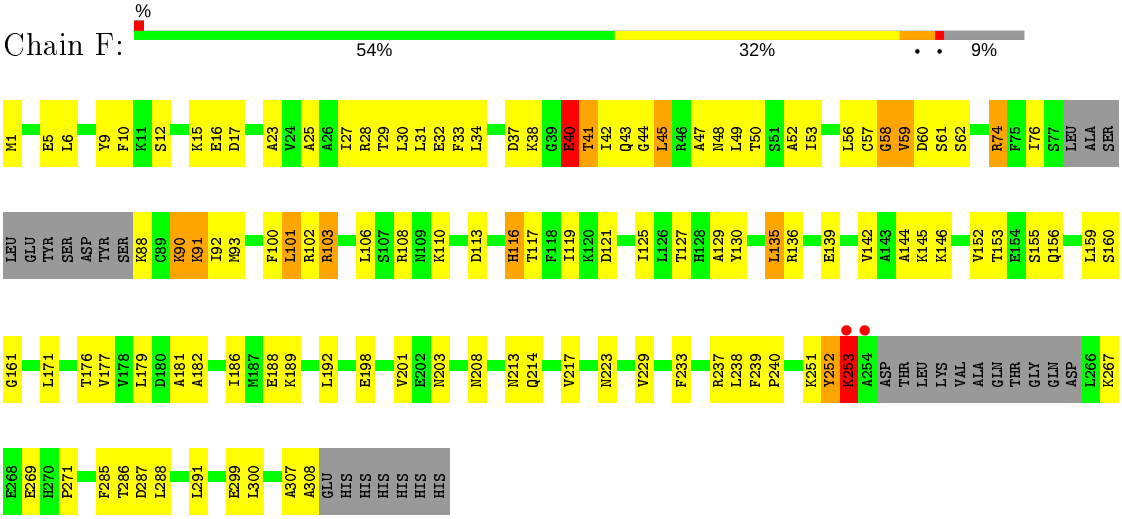
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain E:



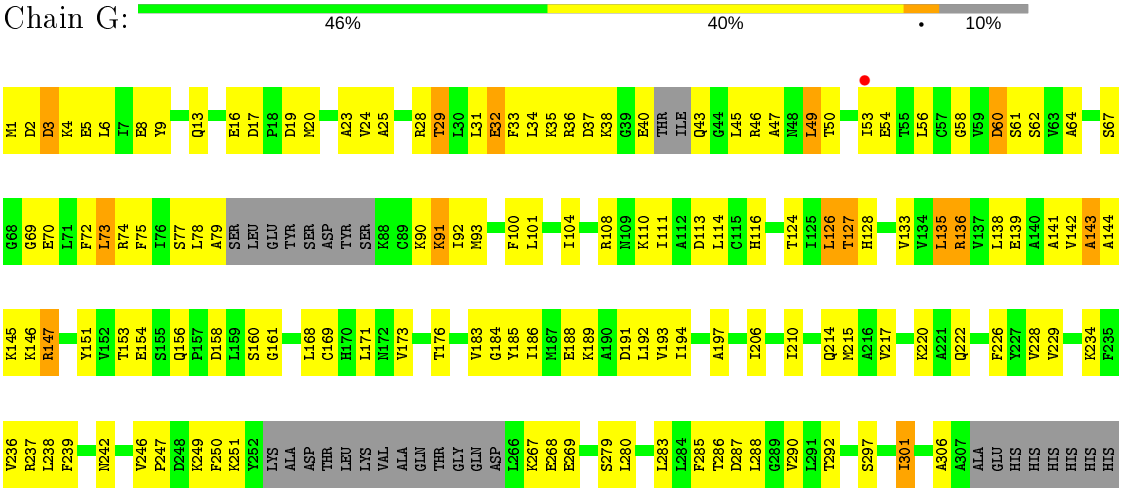
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain F:



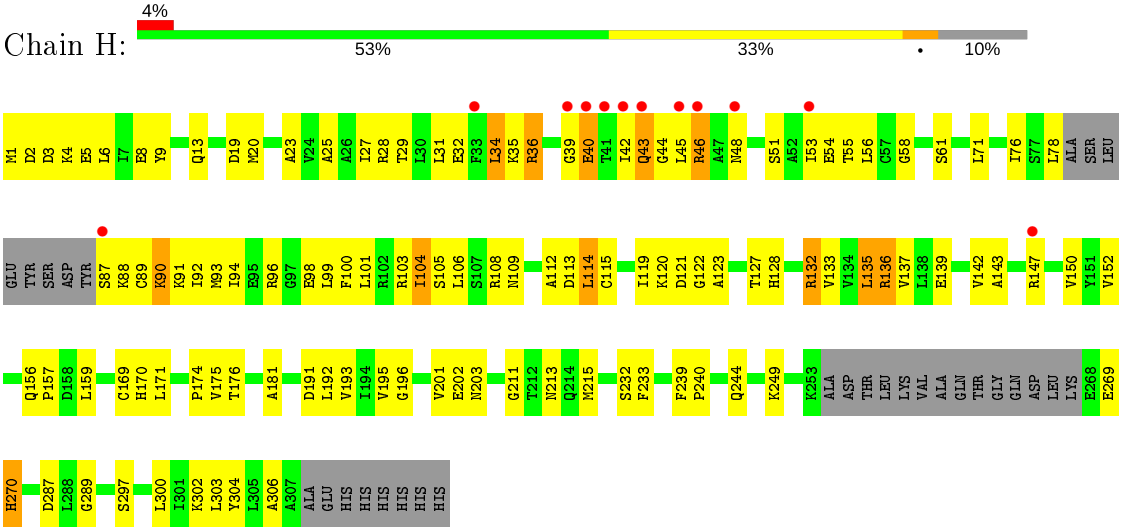
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.89Å 156.39Å 138.44Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 48.59 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.65) 99.2 (48.59-2.65)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.273 0.214 , 0.273	Depositor DCC
R_{free} test set	4200 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17958	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	0.44	0/2191	0.67	0/2945
1	B	0.43	0/2206	0.67	0/2964
1	C	0.43	0/2310	0.70	1/3106 (0.0%)
1	D	0.43	0/2282	0.68	2/3066 (0.1%)
1	E	0.42	0/2237	0.68	1/3008 (0.0%)
1	F	0.44	0/2248	0.67	0/3022
1	G	0.42	0/2226	0.66	0/2991
1	H	0.40	0/2235	0.67	0/3005
All	All	0.43	0/17935	0.68	4/24107 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	92	ILE	N-CA-C	-6.03	94.73	111.00
1	D	60	ASP	N-CA-C	-5.91	95.05	111.00
1	E	58	GLY	N-CA-C	-5.67	98.93	113.10
1	D	267	LYS	N-CA-C	-5.46	96.26	111.00

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	2165	0	2247	122	0
1	B	2180	0	2265	112	0
1	C	2282	0	2365	142	0
1	D	2255	0	2336	143	0
1	E	2211	0	2291	149	0
1	F	2221	0	2311	123	0
1	G	2200	0	2285	141	0
1	H	2208	0	2293	155	0
2	A	10	0	0	4	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	1	0
3	A	1	0	0	0	0
4	A	30	0	0	1	0
4	B	27	0	0	0	0
4	C	20	0	0	3	0
4	D	24	0	0	0	0
4	E	15	0	0	2	0
4	F	26	0	0	1	0
4	G	28	0	0	3	0
4	H	15	0	0	1	0
All	All	17958	0	18393	1011	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 28.

All (1011) 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)
1:F:53:ILE:HA	1:F:56:LEU:HD12	1.30	1.12
1:H:42:ILE:HA	1:H:45:LEU:HB3	1.32	1.09
1:A:92:ILE:H	1:A:92:ILE:HD12	1.20	1.06
1:E:6:LEU:HD11	1:E:53:ILE:HB	1.41	1.03
1:E:286:THR:HG23	1:E:288:LEU:H	1.21	1.02
1:A:20:MSE:HE3	1:A:25:ALA:HB2	1.40	1.01
1:D:286:THR:HG22	1:D:288:LEU:H	1.23	1.00
1:D:187:MSE:HE2	1:D:224:LYS:HG3	1.46	0.97
1:F:42:ILE:HG13	1:F:44:GLY:H	1.26	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HG12	1:C:43:GLN:H	1.28	0.95
1:C:6:LEU:HD13	1:C:53:ILE:HG13	1.45	0.94
1:H:20:MSE:HE3	1:H:25:ALA:HB2	1.50	0.93
1:D:183:VAL:H	1:E:214:GLN:NE2	1.68	0.91
1:H:4:LYS:O	1:H:8:GLU:HG3	1.71	0.90
1:H:1:MSE:HE2	1:H:36:ARG:HD3	1.53	0.90
1:A:13:GLN:HG3	1:A:20:MSE:HE1	1.55	0.89
1:C:41:THR:HG23	1:C:42:ILE:H	1.38	0.89
1:D:193:VAL:CG1	1:D:215:MSE:HE3	2.04	0.88
1:H:5:GLU:HA	1:H:8:GLU:OE1	1.74	0.87
1:C:43:GLN:NE2	1:C:90:LYS:HG2	1.90	0.86
1:A:50:THR:O	1:A:53:ILE:HG12	1.75	0.86
1:H:78:LEU:H	1:H:78:LEU:HD23	1.41	0.86
1:B:77:SER:H	1:B:96:ARG:HH22	1.17	0.85
1:C:40:GLU:OE2	1:C:41:THR:HG22	1.79	0.83
1:G:77:SER:HA	1:G:93:MSE:HE2	1.60	0.83
1:F:50:THR:O	1:F:53:ILE:HG12	1.79	0.83
1:E:53:ILE:HA	1:E:56:LEU:HG	1.61	0.83
1:H:40:GLU:HA	1:H:42:ILE:HG12	1.61	0.83
1:H:31:LEU:HD22	1:H:35:LYS:HE3	1.61	0.82
1:C:56:LEU:O	1:C:59:VAL:HG22	1.80	0.82
1:G:286:THR:HG22	1:G:288:LEU:H	1.43	0.82
1:H:42:ILE:HG22	1:H:45:LEU:HD12	1.58	0.82
1:H:1:MSE:HE1	1:H:32:GLU:HG3	1.59	0.82
1:A:46:ARG:HA	1:A:49:LEU:HD12	1.60	0.81
1:D:214:GLN:HE21	1:E:184:GLY:H	1.26	0.81
1:A:286:THR:HG23	1:A:288:LEU:H	1.43	0.81
1:C:6:LEU:HD22	1:C:53:ILE:HD11	1.61	0.81
1:B:77:SER:H	1:B:96:ARG:NH2	1.77	0.81
1:G:142:VAL:HG13	1:G:143:ALA:H	1.45	0.81
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.47	0.80
1:F:9:TYR:HD2	1:F:29:THR:HG22	1.47	0.79
1:E:115:CYS:HB3	1:E:285:PHE:CD2	2.16	0.79
1:B:45:LEU:HB3	1:B:48:ASN:OD1	1.83	0.79
1:B:25:ALA:O	1:B:29:THR:HG23	1.83	0.79
1:D:10:PHE:HA	1:D:29:THR:HG21	1.64	0.79
1:B:62:SER:HB2	1:B:65:VAL:HG23	1.63	0.79
1:E:6:LEU:CD1	1:E:53:ILE:HB	2.13	0.79
1:E:23:ALA:O	1:E:27:ILE:HG23	1.83	0.79
1:E:57:CYS:C	1:E:59:VAL:H	1.87	0.78
1:H:42:ILE:HD12	1:H:46:ARG:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HA	1:A:95:GLU:OE1	1.84	0.78
1:D:127:THR:HG23	1:D:194:ILE:O	1.84	0.77
1:D:183:VAL:N	1:E:214:GLN:NE2	2.33	0.77
1:F:25:ALA:O	1:F:29:THR:HG23	1.84	0.77
1:C:70:GLU:O	1:C:74:ARG:HG3	1.85	0.77
1:D:267:LYS:O	1:D:269:GLU:N	2.17	0.77
1:F:47:ALA:O	1:F:50:THR:HG22	1.85	0.77
1:H:99:LEU:HD11	1:H:103:ARG:NH1	2.00	0.77
1:F:286:THR:HG22	1:F:288:LEU:H	1.49	0.76
1:C:6:LEU:CD1	1:C:53:ILE:HG13	2.16	0.76
1:B:266:LEU:HD23	1:H:175:VAL:H	1.50	0.76
1:H:78:LEU:HD11	1:H:90:LYS:HE2	1.66	0.76
1:B:56:LEU:O	1:B:59:VAL:HG12	1.85	0.76
1:G:127:THR:HG23	1:G:194:ILE:O	1.84	0.76
1:H:40:GLU:HG3	1:H:88:LYS:HG3	1.67	0.75
1:D:183:VAL:H	1:E:214:GLN:HE22	1.34	0.75
1:F:108:ARG:HD3	1:F:136:ARG:HG3	1.69	0.75
1:F:286:THR:HG22	1:F:287:ASP:N	2.01	0.75
1:C:79:ALA:HA	1:C:90:LYS:HD2	1.69	0.74
1:H:201:VAL:HG11	1:H:240:PRO:HD2	1.68	0.74
1:E:131:SER:HB3	1:E:134:VAL:HG22	1.68	0.74
1:C:50:THR:O	1:C:53:ILE:HG22	1.87	0.74
1:E:286:THR:HG23	1:E:288:LEU:N	2.01	0.74
1:H:42:ILE:HA	1:H:45:LEU:CB	2.16	0.74
1:C:38:LYS:HA	1:C:91:LYS:HZ1	1.54	0.73
1:C:53:ILE:HA	1:C:56:LEU:HD12	1.69	0.73
1:F:53:ILE:HA	1:F:56:LEU:CD1	2.16	0.73
1:B:43:GLN:HG2	1:B:45:LEU:H	1.54	0.73
1:F:28:ARG:HG2	1:F:101:LEU:HD11	1.71	0.73
1:A:20:MSE:HE3	1:A:25:ALA:CB	2.16	0.73
1:G:20:MSE:HE1	1:G:28:ARG:HE	1.54	0.72
1:B:133:VAL:CG1	1:B:229:VAL:HG13	2.19	0.72
1:B:267:LYS:HG2	1:B:268:GLU:N	2.03	0.72
1:G:70:GLU:O	1:G:74:ARG:HG3	1.89	0.72
1:E:92:ILE:HB	1:E:96:ARG:HH12	1.53	0.72
1:E:53:ILE:HG22	1:E:56:LEU:HD12	1.70	0.72
1:G:108:ARG:HG3	1:G:108:ARG:HH11	1.55	0.72
1:H:121:ASP:OD1	1:H:147:ARG:HG2	1.89	0.72
1:A:1:MSE:HG3	1:A:36:ARG:HG3	1.70	0.72
1:E:286:THR:HG22	1:E:289:GLY:O	1.89	0.71
1:F:253:LYS:HE3	1:F:253:LYS:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MSE:HA	1:H:5:GLU:OE1	1.90	0.71
1:A:45:LEU:HD12	1:A:46:ARG:NH1	2.05	0.71
1:H:46:ARG:HH12	1:H:91:LYS:HE2	1.54	0.71
1:F:9:TYR:CD2	1:F:29:THR:HG22	2.26	0.71
1:F:42:ILE:HG23	1:F:45:LEU:HB2	1.71	0.71
1:G:138:LEU:O	1:G:142:VAL:HG12	1.91	0.71
1:A:92:ILE:H	1:A:92:ILE:CD1	1.96	0.71
1:C:78:LEU:C	1:C:80:SER:H	1.93	0.71
1:D:267:LYS:C	1:D:269:GLU:H	1.94	0.71
1:C:42:ILE:HG12	1:C:43:GLN:N	2.04	0.70
1:D:187:MSE:HE3	1:D:190:ALA:HB3	1.73	0.70
1:D:184:GLY:H	1:E:214:GLN:HE21	1.37	0.70
1:C:34:LEU:HD13	1:C:94:ILE:HG12	1.73	0.70
1:A:52:ALA:O	1:A:56:LEU:HG	1.91	0.70
1:B:188:GLU:HA	1:B:222:GLN:HE22	1.57	0.70
1:F:201:VAL:HG11	1:F:240:PRO:HD2	1.72	0.70
1:C:33:PHE:O	1:C:37:ASP:HB2	1.91	0.70
1:H:27:ILE:HG13	1:H:101:LEU:HD21	1.72	0.70
1:C:47:ALA:HB1	4:C:1024:HOH:O	1.92	0.69
1:A:1:MSE:HG3	1:A:36:ARG:HE	1.57	0.69
1:A:77:SER:HB3	1:A:93:MSE:HE2	1.75	0.69
1:B:38:LYS:NZ	1:B:91:LYS:HE3	2.08	0.69
1:E:40:GLU:O	1:E:88:LYS:HE2	1.92	0.69
1:D:31:LEU:HD12	1:D:101:LEU:HD12	1.74	0.69
1:G:4:LYS:O	1:G:8:GLU:HG3	1.91	0.69
1:A:94:ILE:O	1:A:98:GLU:HG3	1.92	0.69
1:B:184:GLY:HA3	1:H:213:ASN:HD22	1.57	0.69
1:H:89:CYS:O	1:H:92:ILE:HG23	1.92	0.69
1:D:193:VAL:HG11	1:D:215:MSE:HE3	1.73	0.69
1:D:6:LEU:HD11	1:D:53:ILE:HB	1.73	0.69
1:C:12:SER:HA	1:C:15:LYS:HD3	1.74	0.69
1:A:294:SER:HB3	1:B:298:ASP:OD1	1.93	0.69
1:C:38:LYS:HA	1:C:91:LYS:NZ	2.08	0.69
1:H:139:GLU:O	1:H:142:VAL:HG22	1.93	0.68
1:C:28:ARG:HH11	1:C:28:ARG:HG2	1.58	0.68
1:E:35:LYS:HG2	1:E:94:ILE:HD13	1.75	0.68
1:G:28:ARG:NH1	1:G:101:LEU:HD21	2.09	0.68
1:E:60:ASP:O	1:E:61:SER:HB2	1.92	0.68
1:C:81:LEU:HD23	1:C:92:ILE:HD13	1.74	0.68
1:H:46:ARG:HH11	1:H:46:ARG:HG2	1.59	0.68
1:C:301:ILE:O	1:C:305:LEU:HG	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LYS:HG2	1:B:268:GLU:H	1.59	0.68
1:D:197:ALA:HA	1:D:208:ASN:ND2	2.08	0.68
1:D:210:ILE:HD12	1:D:274:ASP:HB3	1.76	0.68
1:A:57:CYS:C	1:A:59:VAL:H	1.97	0.67
1:G:23:ALA:HB2	1:G:64:ALA:HB1	1.75	0.67
1:E:229:VAL:HG12	1:E:285:PHE:HB2	1.74	0.67
1:B:187:MSE:HE3	1:B:190:ALA:HB3	1.75	0.67
1:C:108:ARG:HD3	1:C:136:ARG:HG3	1.76	0.67
1:D:214:GLN:NE2	1:E:183:VAL:N	2.42	0.67
1:B:269:GLU:HG3	1:H:176:THR:HG21	1.77	0.67
1:F:1:MSE:HE1	1:F:9:TYR:HB2	1.77	0.67
1:B:188:GLU:CA	1:B:222:GLN:HE22	2.07	0.67
1:E:49:LEU:O	1:E:53:ILE:HG23	1.94	0.67
1:A:43:GLN:C	1:A:45:LEU:H	1.97	0.66
1:B:188:GLU:HA	1:B:222:GLN:NE2	2.11	0.66
1:B:132:ARG:HG2	2:B:502:SO4:O4	1.95	0.66
1:E:1:MSE:HE3	1:E:36:ARG:NH1	2.10	0.66
1:F:10:PHE:HA	1:F:29:THR:HG21	1.77	0.66
1:D:266:LEU:O	1:E:176:THR:HA	1.94	0.66
1:H:28:ARG:HG3	1:H:28:ARG:HH11	1.59	0.66
1:G:297:SER:O	1:G:301:ILE:HG22	1.95	0.66
1:H:55:THR:HG23	1:H:56:LEU:H	1.61	0.66
1:H:56:LEU:C	1:H:58:GLY:H	1.99	0.66
1:H:25:ALA:O	1:H:29:THR:HG23	1.96	0.65
1:C:33:PHE:HZ	1:C:49:LEU:HG	1.60	0.65
1:B:114:LEU:CD2	1:D:117:THR:HG21	2.26	0.65
1:H:31:LEU:CD2	1:H:35:LYS:HE3	2.25	0.65
1:A:188:GLU:HA	1:A:222:GLN:HE22	1.59	0.65
1:E:92:ILE:HB	1:E:96:ARG:NH1	2.12	0.65
1:F:1:MSE:CE	1:F:5:GLU:HB3	2.27	0.65
1:F:42:ILE:HG13	1:F:44:GLY:N	2.06	0.65
1:E:53:ILE:HA	1:E:56:LEU:CG	2.26	0.65
1:F:108:ARG:HH11	1:F:136:ARG:HH12	1.42	0.65
1:H:201:VAL:CG1	1:H:240:PRO:HD2	2.26	0.65
1:H:90:LYS:O	1:H:93:MSE:HG3	1.97	0.65
1:A:286:THR:HG22	1:A:289:GLY:O	1.98	0.64
1:C:73:LEU:O	1:C:76:ILE:HG22	1.97	0.64
1:D:183:VAL:N	1:E:214:GLN:HE21	1.93	0.64
1:C:43:GLN:HE22	1:C:90:LYS:HG2	1.60	0.64
1:G:1:MSE:HE2	1:G:5:GLU:HB3	1.80	0.64
1:H:90:LYS:C	1:H:92:ILE:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:CYS:C	1:E:91:LYS:H	2.01	0.64
1:H:55:THR:HG23	1:H:56:LEU:N	2.13	0.64
1:B:133:VAL:HG12	1:B:229:VAL:HG13	1.80	0.64
1:G:25:ALA:O	1:G:29:THR:HG23	1.98	0.64
1:D:133:VAL:HG23	1:D:229:VAL:HG23	1.79	0.64
1:G:20:MSE:CE	1:G:28:ARG:HE	2.10	0.64
1:B:4:LYS:O	1:B:8:GLU:HG3	1.98	0.63
1:C:201:VAL:HG11	1:C:240:PRO:HD2	1.79	0.63
1:E:304:TYR:C	1:E:306:ALA:H	2.00	0.63
1:A:286:THR:HG23	1:A:288:LEU:N	2.13	0.63
1:A:269:GLU:HG3	1:C:176:THR:HG21	1.79	0.63
1:C:4:LYS:O	1:C:8:GLU:HG3	1.97	0.63
1:A:92:ILE:N	1:A:92:ILE:HD12	2.03	0.63
1:E:114:LEU:HD11	1:E:289:GLY:HA2	1.80	0.63
1:D:61:SER:HB2	1:D:249:LYS:O	1.98	0.63
1:E:127:THR:HG22	1:E:194:ILE:O	1.98	0.63
1:B:48:ASN:N	1:B:48:ASN:HD22	1.96	0.63
1:C:26:ALA:O	1:C:30:LEU:HD23	1.98	0.63
1:H:28:ARG:NH1	1:H:101:LEU:HD22	2.13	0.63
1:F:42:ILE:HD12	1:F:43:GLN:H	1.64	0.63
1:G:37:ASP:O	1:G:46:ARG:NH1	2.31	0.63
1:A:54:GLU:N	1:A:54:GLU:OE2	2.32	0.63
1:B:114:LEU:HD23	1:D:117:THR:HG21	1.81	0.62
1:C:304:TYR:O	1:C:305:LEU:HD23	1.99	0.62
1:F:229:VAL:HG12	1:F:285:PHE:HB2	1.79	0.62
1:A:6:LEU:HD21	1:A:33:PHE:HD2	1.65	0.62
1:D:46:ARG:NH2	1:D:88:LYS:HE3	2.14	0.62
1:F:102:ARG:O	1:F:106:LEU:HD13	1.99	0.62
1:B:198:GLU:HG3	1:B:208:ASN:HA	1.81	0.62
1:E:49:LEU:HA	1:E:52:ALA:HB3	1.82	0.62
1:F:119:ILE:O	1:F:146:LYS:HD3	2.00	0.62
1:A:4:LYS:O	1:A:8:GLU:HG3	2.00	0.62
1:G:136:ARG:CZ	1:G:136:ARG:HB3	2.30	0.62
1:C:12:SER:O	1:C:16:GLU:HG2	1.99	0.62
1:C:42:ILE:CG1	1:C:43:GLN:H	2.10	0.62
1:H:53:ILE:HG22	1:H:56:LEU:HD12	1.80	0.62
1:A:213:ASN:O	1:A:217:VAL:HG23	2.00	0.62
1:B:94:ILE:O	1:B:98:GLU:HG3	1.99	0.62
1:D:214:GLN:HE21	1:E:184:GLY:N	1.96	0.62
1:E:6:LEU:HD11	1:E:53:ILE:CB	2.26	0.62
1:H:42:ILE:CA	1:H:45:LEU:HB3	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:THR:O	1:E:54:GLU:HG3	1.99	0.61
1:B:33:PHE:CE1	1:B:53:ILE:HG12	2.35	0.61
1:D:139:GLU:O	1:D:142:VAL:HG22	2.00	0.61
1:G:6:LEU:HD11	1:G:53:ILE:HB	1.83	0.61
1:A:46:ARG:HB3	1:A:90:LYS:HZ3	1.66	0.61
1:C:86:TYR:CD1	1:C:87:SER:N	2.69	0.61
1:D:187:MSE:CE	1:D:190:ALA:HB3	2.30	0.61
1:D:45:LEU:O	1:D:49:LEU:HG	2.00	0.61
1:H:113:ASP:C	1:H:115:CYS:H	2.02	0.61
1:H:42:ILE:HB	1:H:46:ARG:HB3	1.82	0.61
1:F:286:THR:CG2	1:F:287:ASP:N	2.64	0.61
1:H:40:GLU:HG3	1:H:88:LYS:CG	2.30	0.61
1:E:104:ILE:HD12	1:E:104:ILE:C	2.21	0.61
1:G:147:ARG:HG3	1:G:147:ARG:HH11	1.65	0.61
1:H:269:GLU:O	1:H:270:HIS:HB2	2.00	0.61
1:C:46:ARG:HG3	1:C:46:ARG:HH21	1.65	0.61
1:D:127:THR:HG22	1:D:128:HIS:H	1.66	0.60
1:D:214:GLN:NE2	1:E:183:VAL:H	1.99	0.60
1:G:60:ASP:C	1:G:62:SER:H	2.04	0.60
1:H:42:ILE:HB	1:H:46:ARG:H	1.66	0.60
1:F:192:LEU:HD23	1:F:192:LEU:N	2.16	0.60
1:F:251:LYS:O	1:F:252:TYR:HB2	2.00	0.60
1:B:62:SER:HB2	1:B:65:VAL:CG2	2.31	0.60
1:F:6:LEU:HD21	1:F:33:PHE:CD2	2.36	0.60
1:G:33:PHE:HZ	1:G:49:LEU:HD22	1.66	0.60
1:F:198:GLU:HG2	1:F:208:ASN:HD22	1.66	0.60
1:G:133:VAL:CG1	1:G:229:VAL:HG12	2.32	0.60
1:G:136:ARG:HB3	1:G:136:ARG:NH1	2.16	0.60
1:F:176:THR:OG1	1:G:267:LYS:HE3	2.00	0.60
1:C:3:ASP:HA	1:C:6:LEU:HD12	1.84	0.60
1:D:46:ARG:NH2	1:D:91:LYS:NZ	2.49	0.60
1:E:201:VAL:CG1	1:E:240:PRO:HD2	2.32	0.60
1:G:111:ILE:HG21	1:G:229:VAL:HG13	1.82	0.60
1:A:3:ASP:OD2	1:A:56:LEU:HD22	2.02	0.59
1:F:1:MSE:HE2	1:F:5:GLU:HB3	1.84	0.59
1:A:9:TYR:O	1:A:13:GLN:HB2	2.01	0.59
1:B:237:ARG:HG3	1:B:237:ARG:HH11	1.67	0.59
1:F:108:ARG:HH11	1:F:136:ARG:NH1	1.99	0.59
1:F:53:ILE:CA	1:F:56:LEU:HD12	2.21	0.59
1:A:45:LEU:O	1:A:49:LEU:HG	2.03	0.59
1:B:44:GLY:C	1:B:45:LEU:HD12	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:VAL:HG13	1:F:238:LEU:O	2.03	0.59
1:F:291:LEU:HD21	1:F:299:GLU:HG3	1.83	0.59
1:H:46:ARG:HH21	1:H:93:MSE:SE	2.36	0.59
1:A:21:ALA:HB3	1:A:24:VAL:HG23	1.84	0.59
1:C:52:ALA:O	1:C:56:LEU:HG	2.02	0.59
1:E:45:LEU:O	1:E:49:LEU:HG	2.02	0.59
1:E:78:LEU:HA	1:E:90:LYS:HZ1	1.67	0.59
1:H:78:LEU:HD23	1:H:78:LEU:N	2.17	0.59
1:F:103:ARG:HG2	1:F:103:ARG:NH1	2.13	0.59
1:B:46:ARG:HH11	1:B:49:LEU:CD1	2.16	0.59
1:D:86:TYR:HD1	1:D:87:SER:H	1.50	0.59
1:A:22:SER:HB2	4:A:1025:HOH:O	2.01	0.59
1:A:34:LEU:HD22	1:A:90:LYS:HE2	1.85	0.59
1:B:16:GLU:O	1:B:16:GLU:HG2	2.03	0.59
1:A:13:GLN:CG	1:A:20:MSE:HE1	2.30	0.59
1:B:137:VAL:HG21	1:B:229:VAL:HG21	1.85	0.59
1:D:1:MSE:HA	1:D:5:GLU:OE1	2.02	0.59
1:A:124:THR:HG21	1:A:189:LYS:O	2.03	0.59
1:A:90:LYS:HG3	1:A:93:MSE:SE	2.53	0.59
1:D:134:VAL:HG13	1:D:164:MSE:HE1	1.84	0.59
1:G:188:GLU:HA	1:G:222:GLN:HE22	1.68	0.59
1:C:41:THR:HG23	1:C:45:LEU:HB2	1.85	0.58
1:D:214:GLN:HE22	1:E:183:VAL:H	1.51	0.58
1:D:56:LEU:O	1:D:59:VAL:HG23	2.03	0.58
1:E:87:SER:C	1:E:89:CYS:H	2.06	0.58
1:H:169:CYS:C	1:H:171:LEU:H	2.07	0.58
1:C:188:GLU:HA	1:C:222:GLN:HE22	1.68	0.58
1:C:59:VAL:O	1:C:59:VAL:HG23	2.02	0.58
1:A:30:LEU:O	1:A:33:PHE:N	2.37	0.58
1:B:111:ILE:CG2	1:B:229:VAL:HG22	2.34	0.58
1:B:133:VAL:O	1:B:137:VAL:HG23	2.02	0.58
1:C:25:ALA:O	1:C:29:THR:HG23	2.03	0.58
1:D:28:ARG:HG2	1:D:28:ARG:HH11	1.68	0.58
1:D:133:VAL:O	1:D:137:VAL:HG23	2.04	0.58
1:F:42:ILE:HD12	1:F:43:GLN:N	2.18	0.58
1:H:27:ILE:CD1	1:H:104:ILE:HD11	2.33	0.58
1:A:46:ARG:N	1:A:46:ARG:HD2	2.19	0.58
1:B:43:GLN:HG2	1:B:44:GLY:N	2.19	0.58
1:G:56:LEU:C	1:G:58:GLY:H	2.05	0.58
1:A:43:GLN:C	1:A:45:LEU:N	2.56	0.58
1:B:187:MSE:CE	1:B:190:ALA:HB3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:VAL:HG13	1:B:59:VAL:O	2.02	0.58
1:C:237:ARG:CZ	1:E:301:ILE:HD11	2.33	0.58
1:H:40:GLU:HG3	1:H:88:LYS:HD2	1.86	0.58
1:A:6:LEU:C	1:A:8:GLU:H	2.06	0.58
1:A:91:LYS:O	1:A:95:GLU:HG3	2.03	0.58
1:C:46:ARG:HB2	1:C:46:ARG:CZ	2.33	0.58
1:G:108:ARG:NH1	1:G:108:ARG:HG3	2.18	0.58
1:C:28:ARG:HG2	1:C:101:LEU:HD11	1.86	0.58
1:D:106:LEU:HB3	1:D:110:LYS:NZ	2.18	0.58
1:G:133:VAL:HG12	1:G:229:VAL:CG1	2.34	0.58
1:H:31:LEU:HD12	1:H:101:LEU:HD12	1.85	0.58
1:H:40:GLU:CA	1:H:42:ILE:HG12	2.34	0.57
1:E:195:VAL:HG12	1:E:196:GLY:O	2.03	0.57
1:C:201:VAL:CG1	1:C:240:PRO:HD2	2.34	0.57
1:C:20:MSE:CE	1:C:28:ARG:HE	2.17	0.57
1:B:192:LEU:N	1:B:192:LEU:HD23	2.20	0.57
1:H:54:GLU:OE1	1:H:54:GLU:HA	2.04	0.57
1:C:237:ARG:NH2	1:E:301:ILE:HD11	2.20	0.57
1:D:197:ALA:HA	1:D:208:ASN:HD22	1.69	0.57
1:D:131:SER:O	1:D:134:VAL:HG12	2.02	0.57
1:E:37:ASP:O	1:E:40:GLU:HG3	2.05	0.57
1:F:6:LEU:HD11	1:F:53:ILE:HG22	1.85	0.57
1:C:41:THR:HG23	1:C:42:ILE:N	2.14	0.57
1:C:43:GLN:O	1:C:46:ARG:HG2	2.04	0.57
1:C:60:ASP:C	1:C:62:SER:H	2.07	0.57
1:D:50:THR:HA	1:D:53:ILE:HD11	1.85	0.57
1:H:31:LEU:HD11	1:H:98:GLU:HG2	1.86	0.57
1:F:58:GLY:C	1:F:60:ASP:H	2.08	0.57
1:G:246:VAL:HB	1:G:251:LYS:HZ2	1.70	0.57
1:H:156:GLN:NE2	1:H:159:LEU:HD21	2.19	0.57
1:C:139:GLU:O	1:C:142:VAL:HG22	2.03	0.57
1:C:86:TYR:HD1	1:C:87:SER:N	2.02	0.57
1:G:267:LYS:HG2	1:G:268:GLU:N	2.20	0.57
1:H:109:ASN:ND2	1:H:136:ARG:HE	2.03	0.57
1:H:202:GLU:O	1:H:297:SER:HB3	2.04	0.57
1:F:1:MSE:HE2	1:F:5:GLU:C	2.25	0.57
1:A:53:ILE:HA	1:A:56:LEU:HD12	1.86	0.56
1:G:45:LEU:CD2	1:G:49:LEU:HD12	2.35	0.56
1:H:232:SER:N	1:H:287:ASP:OD1	2.38	0.56
1:H:88:LYS:N	1:H:88:LYS:HZ3	2.03	0.56
1:A:7:ILE:O	1:A:7:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:ARG:HG2	2:H:508:SO4:O3	2.04	0.56
1:A:1:MSE:HG3	1:A:36:ARG:CG	2.35	0.56
1:B:135:LEU:O	1:B:139:GLU:HG3	2.04	0.56
1:E:201:VAL:HG11	1:E:240:PRO:HD2	1.86	0.56
1:E:56:LEU:C	1:E:58:GLY:H	2.07	0.56
1:E:4:LYS:O	1:E:8:GLU:HG3	2.04	0.56
1:G:92:ILE:HD12	1:G:92:ILE:C	2.26	0.56
1:B:92:ILE:O	1:B:95:GLU:HB3	2.05	0.56
1:C:6:LEU:HD21	1:C:33:PHE:HD1	1.71	0.56
1:E:304:TYR:O	1:E:306:ALA:N	2.35	0.56
1:F:144:ALA:O	1:F:145:LYS:HB2	2.04	0.56
1:F:1:MSE:HG3	1:F:5:GLU:HB3	1.87	0.56
1:E:27:ILE:HD11	1:E:101:LEU:HD13	1.87	0.56
1:F:90:LYS:C	1:F:90:LYS:HD2	2.26	0.56
1:B:300:LEU:O	1:B:300:LEU:HD23	2.06	0.56
1:E:188:GLU:HA	1:E:222:GLN:HE22	1.70	0.56
1:H:215:MSE:HE3	4:H:1170:HOH:O	2.06	0.56
1:D:267:LYS:C	1:D:269:GLU:N	2.59	0.56
1:H:150:VAL:O	1:H:175:VAL:HA	2.06	0.56
1:H:42:ILE:O	1:H:44:GLY:N	2.40	0.55
1:H:46:ARG:HD2	1:H:46:ARG:O	2.06	0.55
1:E:92:ILE:O	1:E:95:GLU:HG2	2.06	0.55
1:H:94:ILE:O	1:H:98:GLU:HG3	2.06	0.55
1:A:11:LYS:O	1:A:15:LYS:HG2	2.07	0.55
1:D:3:ASP:OD1	1:D:56:LEU:HG	2.06	0.55
1:E:76:ILE:O	1:E:76:ILE:HG13	2.05	0.55
1:H:34:LEU:HD13	1:H:94:ILE:HG12	1.89	0.55
1:C:72:PHE:O	1:C:76:ILE:HB	2.06	0.55
1:D:266:LEU:HB3	1:D:268:GLU:HB2	1.89	0.55
1:C:294:SER:HB2	1:E:239:PHE:CD2	2.41	0.55
1:G:286:THR:HG22	1:G:287:ASP:N	2.21	0.55
1:D:214:GLN:HG3	1:E:184:GLY:H	1.71	0.55
1:C:1:MSE:SE	1:C:6:LEU:HD23	2.57	0.55
1:D:46:ARG:HH21	1:D:91:LYS:HD3	1.72	0.55
1:F:10:PHE:CA	1:F:29:THR:HG21	2.36	0.55
1:B:28:ARG:HG2	1:B:101:LEU:HD11	1.87	0.55
1:D:165:ALA:HB1	1:E:266:LEU:CD1	2.37	0.55
1:D:27:ILE:HD11	1:D:101:LEU:HG	1.88	0.55
1:F:125:ILE:HG12	1:F:192:LEU:HD21	1.87	0.55
1:G:246:VAL:HB	1:G:251:LYS:NZ	2.22	0.55
1:G:54:GLU:OE1	1:G:73:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:ARG:C	1:H:48:ASN:N	2.57	0.55
1:G:246:VAL:O	1:G:251:LYS:NZ	2.39	0.55
1:A:1:MSE:CG	1:A:36:ARG:HE	2.18	0.55
1:B:141:ALA:O	1:B:146:LYS:HB2	2.07	0.54
1:C:252:TYR:O	1:C:253:LYS:HB2	2.07	0.54
1:C:82:GLU:HB2	1:C:90:LYS:NZ	2.22	0.54
1:E:78:LEU:HA	1:E:90:LYS:NZ	2.22	0.54
1:G:215:MSE:HE3	4:G:1023:HOH:O	2.06	0.54
1:H:40:GLU:O	1:H:42:ILE:HG23	2.08	0.54
1:F:10:PHE:HA	1:F:29:THR:CG2	2.36	0.54
1:F:92:ILE:C	1:F:92:ILE:HD12	2.27	0.54
1:A:46:ARG:HA	1:A:49:LEU:CD1	2.34	0.54
1:G:286:THR:CG2	1:G:287:ASP:N	2.70	0.54
1:H:42:ILE:O	1:H:43:GLN:C	2.45	0.54
1:C:50:THR:C	1:C:53:ILE:HG22	2.27	0.54
1:D:133:VAL:CG2	1:D:229:VAL:HG23	2.38	0.54
1:D:78:LEU:HB3	1:D:96:ARG:HH12	1.73	0.54
1:B:87:SER:C	1:B:89:CYS:H	2.10	0.54
1:D:92:ILE:HD12	1:D:92:ILE:C	2.28	0.54
1:E:119:ILE:HD11	1:E:137:VAL:HG12	1.88	0.54
1:F:12:SER:HA	1:F:15:LYS:CB	2.38	0.54
1:H:192:LEU:HD23	1:H:192:LEU:N	2.23	0.54
1:G:79:ALA:HB1	1:G:90:LYS:HG3	1.89	0.54
1:C:76:ILE:CG2	1:C:77:SER:N	2.71	0.54
1:D:56:LEU:O	1:D:56:LEU:HD13	2.07	0.54
1:B:153:THR:O	1:B:161:GLY:HA3	2.08	0.54
1:A:266:LEU:HD13	1:C:174:PRO:HB3	1.89	0.54
1:C:201:VAL:HG13	1:C:238:LEU:O	2.08	0.54
1:E:61:SER:O	1:E:250:PHE:HA	2.08	0.54
1:F:179:LEU:HD22	4:G:1078:HOH:O	2.06	0.54
1:F:237:ARG:HG3	1:F:237:ARG:HH11	1.71	0.54
1:G:47:ALA:O	1:G:50:THR:HG22	2.08	0.54
1:C:41:THR:CG2	1:C:45:LEU:HB2	2.38	0.54
1:F:1:MSE:HG3	1:F:5:GLU:CB	2.38	0.54
1:G:32:GLU:O	1:G:36:ARG:HB3	2.08	0.54
1:D:1:MSE:HE3	1:D:36:ARG:NH1	2.23	0.53
1:D:269:GLU:HB2	1:E:178:VAL:HG12	1.90	0.53
1:B:9:TYR:HD2	1:B:29:THR:HG22	1.73	0.53
1:H:46:ARG:C	1:H:48:ASN:H	2.12	0.53
1:A:144:ALA:O	1:A:145:LYS:HB2	2.08	0.53
1:B:113:ASP:OD2	1:D:116:HIS:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ILE:HD11	1:E:101:LEU:CD1	2.38	0.53
1:A:27:ILE:HD13	1:A:100:PHE:HE1	1.73	0.53
1:A:267:LYS:HD3	1:C:175:VAL:O	2.08	0.53
1:A:103:ARG:NH2	1:A:287:ASP:OD2	2.42	0.53
1:A:56:LEU:C	1:A:58:GLY:H	2.12	0.53
1:B:31:LEU:HD22	1:B:35:LYS:NZ	2.23	0.53
1:G:142:VAL:HG13	1:G:143:ALA:N	2.21	0.53
1:D:264:GLN:HE22	1:E:172:ASN:HA	1.72	0.53
1:E:57:CYS:C	1:E:59:VAL:N	2.58	0.53
1:C:10:PHE:O	1:C:13:GLN:HB2	2.08	0.53
1:D:264:GLN:NE2	1:E:172:ASN:HA	2.24	0.53
1:D:264:GLN:OE1	1:E:169:CYS:HA	2.07	0.53
1:H:45:LEU:O	1:H:48:ASN:HB3	2.09	0.53
1:A:203:ASN:HB3	1:A:239:PHE:CZ	2.44	0.53
1:B:178:VAL:HG13	1:B:182:ALA:HB3	1.91	0.53
1:E:192:LEU:N	1:E:192:LEU:HD23	2.23	0.53
1:E:195:VAL:CG1	1:E:196:GLY:N	2.71	0.53
1:G:31:LEU:O	1:G:35:LYS:HG3	2.09	0.53
1:G:32:GLU:OE2	1:G:35:LYS:HD2	2.09	0.53
1:G:20:MSE:HE1	1:G:28:ARG:NE	2.24	0.52
1:H:40:GLU:CG	1:H:88:LYS:HD2	2.38	0.52
1:E:71:LEU:HD23	1:E:304:TYR:HE1	1.75	0.52
1:F:57:CYS:O	1:F:59:VAL:N	2.43	0.52
1:G:43:GLN:C	1:G:45:LEU:N	2.62	0.52
1:A:125:ILE:HG12	1:A:192:LEU:HD21	1.91	0.52
1:B:46:ARG:HH11	1:B:49:LEU:HD11	1.75	0.52
1:A:266:LEU:HD23	1:C:176:THR:OG1	2.09	0.52
1:C:6:LEU:HD22	1:C:53:ILE:CD1	2.34	0.52
1:D:10:PHE:CA	1:D:29:THR:HG21	2.38	0.52
1:E:67:SER:HB3	1:E:236:VAL:HG23	1.89	0.52
1:H:105:SER:C	1:H:106:LEU:HD12	2.30	0.52
1:H:19:ASP:O	1:H:108:ARG:NH2	2.42	0.52
1:H:6:LEU:HD13	1:H:53:ILE:HB	1.90	0.52
1:A:172:ASN:C	1:C:264:GLN:N	2.63	0.52
1:A:210:ILE:HD13	1:A:271:PRO:HG2	1.92	0.52
1:A:31:LEU:HD21	1:A:98:GLU:HG2	1.91	0.52
1:A:30:LEU:HD22	1:A:53:ILE:HD11	1.92	0.52
1:C:42:ILE:HG13	1:C:86:TYR:N	2.25	0.52
1:D:9:TYR:CE1	1:D:32:GLU:HG2	2.44	0.52
1:E:92:ILE:O	1:E:96:ARG:HG2	2.09	0.52
1:C:108:ARG:HD2	1:C:136:ARG:CZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:VAL:HG13	1:D:215:MSE:HE3	1.91	0.52
1:D:264:GLN:OE1	1:E:172:ASN:HA	2.10	0.52
1:A:114:LEU:O	1:A:117:THR:HG22	2.10	0.52
1:D:53:ILE:HG13	1:D:54:GLU:N	2.24	0.52
1:E:3:ASP:O	1:E:7:ILE:HG13	2.10	0.52
1:F:251:LYS:O	1:F:252:TYR:CB	2.58	0.52
1:F:251:LYS:O	1:F:252:TYR:CD1	2.63	0.52
1:B:6:LEU:HD22	1:B:53:ILE:HG13	1.92	0.52
1:H:40:GLU:C	1:H:42:ILE:N	2.59	0.52
1:G:220:LYS:HE3	1:G:279:SER:O	2.09	0.52
1:G:6:LEU:CD1	1:G:53:ILE:HB	2.39	0.52
1:H:104:ILE:O	1:H:104:ILE:HG13	2.09	0.52
1:A:186:ILE:HD11	1:A:189:LYS:HD2	1.91	0.52
1:B:88:LYS:O	1:B:91:LYS:HG2	2.10	0.51
1:C:46:ARG:O	1:C:50:THR:HG22	2.10	0.51
1:D:6:LEU:CD1	1:D:53:ILE:HB	2.41	0.51
1:G:286:THR:HG22	1:G:288:LEU:N	2.21	0.51
1:A:153:THR:O	1:A:161:GLY:HA3	2.10	0.51
1:D:254:ALA:HB3	1:D:272:TRP:CG	2.45	0.51
1:F:108:ARG:CD	1:F:136:ARG:HG3	2.40	0.51
1:B:266:LEU:CD2	1:H:174:PRO:HA	2.40	0.51
1:H:51:SER:C	1:H:53:ILE:H	2.14	0.51
1:A:46:ARG:HB3	1:A:90:LYS:NZ	2.25	0.51
1:D:264:GLN:OE1	1:E:173:VAL:N	2.44	0.51
1:E:1:MSE:HB3	1:E:33:PHE:CD2	2.45	0.51
1:F:23:ALA:HB3	1:F:233:PHE:CE1	2.45	0.51
1:A:199:GLY:HA2	1:A:234:LYS:HB3	1.91	0.51
1:D:91:LYS:HG3	1:D:91:LYS:O	2.09	0.51
1:F:286:THR:CG2	1:F:287:ASP:H	2.22	0.51
1:F:267:LYS:O	1:G:176:THR:HA	2.11	0.51
1:G:269:GLU:HA	4:G:1010:HOH:O	2.10	0.51
1:A:6:LEU:CD1	1:A:53:ILE:HB	2.40	0.51
1:C:78:LEU:C	1:C:80:SER:N	2.61	0.51
1:G:220:LYS:HD2	1:G:280:LEU:HD23	1.92	0.51
1:H:9:TYR:CZ	1:H:32:GLU:HG2	2.45	0.51
1:D:268:GLU:O	1:D:268:GLU:HG2	2.10	0.51
1:G:37:ASP:OD1	1:G:46:ARG:NH1	2.43	0.51
1:H:13:GLN:HG3	1:H:20:MSE:HE1	1.93	0.51
1:H:46:ARG:C	1:H:46:ARG:HD2	2.31	0.51
1:A:117:THR:HG23	1:A:118:PHE:CD1	2.46	0.51
1:B:240:PRO:HG2	1:B:275:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HB3	1:B:48:ASN:CG	2.30	0.51
1:F:253:LYS:HD3	1:F:269:GLU:HA	1.93	0.51
1:G:60:ASP:C	1:G:62:SER:N	2.64	0.51
1:H:133:VAL:O	1:H:137:VAL:HG23	2.10	0.51
1:E:73:LEU:C	1:E:73:LEU:HD23	2.32	0.51
1:G:24:VAL:HG22	1:G:104:ILE:HD12	1.93	0.51
1:G:2:ASP:O	1:G:3:ASP:C	2.50	0.51
1:A:37:ASP:CG	1:A:38:LYS:H	2.14	0.50
1:D:50:THR:HA	1:D:53:ILE:CD1	2.41	0.50
1:E:202:GLU:HB2	1:E:238:LEU:O	2.11	0.50
1:H:195:VAL:HG22	1:H:196:GLY:N	2.26	0.50
1:B:9:TYR:O	1:B:13:GLN:HG2	2.12	0.50
1:C:38:LYS:NZ	1:C:88:LYS:HG2	2.26	0.50
1:F:57:CYS:C	1:F:59:VAL:N	2.63	0.50
1:H:36:ARG:HH11	1:H:36:ARG:HG3	1.76	0.50
1:C:267:LYS:HG3	1:C:268:GLU:H	1.77	0.50
1:G:127:THR:HG22	1:G:128:HIS:H	1.76	0.50
1:A:46:ARG:CB	1:A:90:LYS:NZ	2.74	0.50
1:B:117:THR:HG22	1:B:117:THR:O	2.11	0.50
1:C:4:LYS:HD3	1:C:4:LYS:H	1.77	0.50
1:E:46:ARG:C	1:E:48:ASN:H	2.15	0.50
1:G:72:PHE:HD1	1:G:100:PHE:CD1	2.29	0.50
1:A:139:GLU:O	1:A:142:VAL:HG22	2.12	0.50
1:E:27:ILE:O	1:E:27:ILE:HD12	2.11	0.50
1:F:271:PRO:HG3	1:G:185:TYR:CE2	2.46	0.50
1:F:41:THR:HG23	1:F:42:ILE:N	2.27	0.50
1:H:31:LEU:HD12	1:H:101:LEU:CD1	2.42	0.50
1:H:40:GLU:OE1	1:H:88:LYS:HD2	2.12	0.50
1:B:9:TYR:CE1	1:B:32:GLU:HG2	2.46	0.50
1:D:75:PHE:CD2	1:D:100:PHE:HB2	2.46	0.50
1:G:141:ALA:O	1:G:146:LYS:HB2	2.12	0.50
1:H:203:ASN:HB3	1:H:239:PHE:CE1	2.47	0.50
1:B:101:LEU:HD23	1:B:101:LEU:O	2.11	0.50
1:D:165:ALA:HB1	1:E:266:LEU:HD11	1.94	0.50
1:D:89:CYS:C	1:D:91:LYS:H	2.14	0.50
1:F:59:VAL:HG22	1:F:59:VAL:O	2.11	0.50
1:H:46:ARG:HG2	1:H:46:ARG:NH1	2.24	0.50
1:A:1:MSE:HG3	1:A:36:ARG:NE	2.26	0.50
1:C:237:ARG:O	1:C:238:LEU:HD23	2.12	0.50
1:D:214:GLN:HE21	1:E:183:VAL:N	2.08	0.50
1:E:17:ASP:HB3	1:E:19:ASP:OD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HB	1:B:251:LYS:HE3	1.94	0.49
1:C:192:LEU:N	1:C:192:LEU:HD23	2.27	0.49
1:C:33:PHE:CD1	1:C:53:ILE:HD12	2.47	0.49
1:G:40:GLU:HB2	1:G:43:GLN:HA	1.92	0.49
1:B:179:LEU:HD13	1:H:270:HIS:CD2	2.47	0.49
1:G:267:LYS:CG	1:G:268:GLU:N	2.75	0.49
1:H:78:LEU:HB3	1:H:96:ARG:HH12	1.77	0.49
1:D:78:LEU:CD2	1:D:92:ILE:HD11	2.43	0.49
1:F:57:CYS:C	1:F:59:VAL:H	2.16	0.49
1:G:46:ARG:CZ	1:G:91:LYS:HE3	2.43	0.49
1:E:110:LYS:O	1:E:114:LEU:HB2	2.12	0.49
1:E:50:THR:HA	1:E:53:ILE:HG12	1.93	0.49
1:F:139:GLU:HG3	1:F:171:LEU:HD11	1.94	0.49
1:F:201:VAL:HG12	1:F:203:ASN:H	1.78	0.49
1:A:239:PHE:CE1	1:B:202:GLU:HB3	2.47	0.49
1:E:40:GLU:N	1:E:46:ARG:HH21	2.09	0.49
1:F:12:SER:HA	1:F:15:LYS:HB3	1.94	0.49
1:F:9:TYR:CE1	1:F:32:GLU:HG2	2.47	0.49
1:G:135:LEU:O	1:G:139:GLU:HG3	2.11	0.49
1:C:20:MSE:HE1	1:C:28:ARG:HE	1.77	0.49
1:C:34:LEU:HD13	1:C:94:ILE:CG1	2.42	0.49
1:E:155:SER:HA	1:E:180:ASP:OD2	2.12	0.49
1:G:236:VAL:HG22	1:G:237:ARG:N	2.28	0.49
1:H:120:LYS:HE3	1:H:123:ALA:HB2	1.95	0.49
1:H:78:LEU:HB3	1:H:96:ARG:NH1	2.28	0.49
1:A:208:ASN:O	1:A:273:VAL:HA	2.13	0.49
1:C:47:ALA:CB	4:C:1024:HOH:O	2.56	0.49
1:D:184:GLY:HA3	1:E:213:ASN:HD22	1.78	0.49
1:D:184:GLY:N	1:E:214:GLN:HE21	2.09	0.49
1:F:182:ALA:HA	1:G:210:ILE:HD11	1.93	0.49
1:A:43:GLN:O	1:A:45:LEU:N	2.46	0.49
1:B:10:PHE:HA	1:B:29:THR:HG21	1.94	0.49
1:G:113:ASP:O	1:G:116:HIS:CD2	2.65	0.49
1:H:53:ILE:HA	1:H:56:LEU:HD12	1.93	0.49
1:A:271:PRO:HG3	1:C:185:TYR:CE2	2.48	0.49
1:A:54:GLU:OE1	1:A:73:LEU:HD11	2.12	0.49
1:B:48:ASN:N	1:B:48:ASN:ND2	2.60	0.49
1:C:24:VAL:HG22	1:C:104:ILE:HD11	1.95	0.49
1:D:9:TYR:CD2	1:D:29:THR:HB	2.48	0.49
1:E:42:ILE:HG22	1:E:44:GLY:H	1.78	0.49
1:C:28:ARG:NH1	1:C:28:ARG:HG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ILE:HG12	1:D:45:LEU:CG	2.43	0.49
1:D:56:LEU:C	1:D:56:LEU:HD13	2.33	0.49
1:D:269:GLU:CG	1:E:176:THR:HG21	2.42	0.49
1:E:90:LYS:C	1:E:92:ILE:H	2.14	0.49
1:F:300:LEU:HD23	1:F:300:LEU:C	2.33	0.49
1:F:42:ILE:HG23	1:F:45:LEU:H	1.77	0.49
1:E:300:LEU:HD21	1:E:304:TYR:CE2	2.48	0.48
1:E:70:GLU:HG2	1:E:74:ARG:HE	1.78	0.48
1:C:251:LYS:HG3	1:C:252:TYR:CD1	2.48	0.48
1:D:46:ARG:HH22	1:D:88:LYS:HE3	1.76	0.48
1:E:304:TYR:C	1:E:306:ALA:N	2.66	0.48
1:E:43:GLN:NE2	1:E:43:GLN:O	2.46	0.48
1:F:6:LEU:HD11	1:F:53:ILE:CG2	2.44	0.48
1:F:59:VAL:HG13	1:F:59:VAL:O	2.13	0.48
1:G:206:ILE:HD13	1:G:228:VAL:HG21	1.93	0.48
1:C:251:LYS:HG3	1:C:252:TYR:CE1	2.48	0.48
1:D:1:MSE:HE3	1:D:36:ARG:CZ	2.42	0.48
1:D:72:PHE:CZ	1:D:76:ILE:HD12	2.47	0.48
1:E:75:PHE:CD2	1:E:100:PHE:HB2	2.48	0.48
1:F:307:ALA:O	1:F:308:ALA:HB2	2.13	0.48
1:H:61:SER:HB2	1:H:249:LYS:O	2.13	0.48
1:A:6:LEU:C	1:A:8:GLU:N	2.66	0.48
1:D:19:ASP:O	1:D:108:ARG:NH2	2.47	0.48
1:A:92:ILE:O	1:A:96:ARG:HG3	2.13	0.48
1:C:210:ILE:HD12	1:C:274:ASP:HB3	1.96	0.48
1:D:202:GLU:HB3	1:F:239:PHE:CE1	2.49	0.48
1:E:70:GLU:HB2	4:E:1173:HOH:O	2.13	0.48
1:F:42:ILE:HD12	1:F:43:GLN:HG2	1.94	0.48
1:F:181:ALA:HA	1:G:214:GLN:NE2	2.28	0.48
1:G:111:ILE:CG2	1:G:229:VAL:HG13	2.43	0.48
1:A:46:ARG:CB	1:A:90:LYS:HZ3	2.27	0.48
1:A:57:CYS:C	1:A:59:VAL:N	2.66	0.48
1:B:73:LEU:O	1:B:73:LEU:HD22	2.14	0.48
1:G:158:ASP:OD1	1:G:160:SER:HB3	2.14	0.48
1:G:38:LYS:HG2	1:G:91:LYS:NZ	2.29	0.48
1:H:28:ARG:CG	1:H:28:ARG:HH11	2.25	0.48
1:B:127:THR:HG23	1:B:152:VAL:HG23	1.95	0.48
1:B:158:ASP:O	1:B:159:LEU:HB2	2.14	0.48
1:B:300:LEU:C	1:B:300:LEU:HD23	2.33	0.48
1:C:300:LEU:O	1:C:303:LEU:HB3	2.13	0.48
1:G:186:ILE:HD11	1:G:189:LYS:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HZ2	1:B:91:LYS:HE3	1.79	0.48
1:E:37:ASP:C	1:E:40:GLU:HG3	2.34	0.48
1:G:147:ARG:HG3	1:G:147:ARG:NH1	2.26	0.48
1:G:186:ILE:CD1	1:G:189:LYS:HD2	2.44	0.48
1:G:45:LEU:O	1:G:49:LEU:HB2	2.14	0.48
1:C:142:VAL:HG23	1:C:143:ALA:N	2.28	0.48
1:D:134:VAL:HG23	1:D:194:ILE:HG22	1.96	0.48
1:D:28:ARG:HG2	1:D:28:ARG:NH1	2.29	0.48
1:G:124:THR:N	1:G:191:ASP:OD2	2.46	0.48
1:G:37:ASP:C	1:G:46:ARG:HH12	2.17	0.48
1:H:40:GLU:HG3	1:H:88:LYS:CD	2.43	0.48
1:F:153:THR:O	1:F:161:GLY:HA3	2.14	0.47
1:G:126:LEU:HB3	1:G:193:VAL:HG12	1.96	0.47
1:G:237:ARG:NH2	1:H:302:LYS:HG3	2.29	0.47
1:F:188:GLU:OE1	1:G:242:ASN:HB2	2.14	0.47
1:H:106:LEU:HD12	1:H:106:LEU:N	2.28	0.47
1:F:113:ASP:HB3	4:F:1065:HOH:O	2.13	0.47
1:H:142:VAL:HG23	1:H:143:ALA:N	2.29	0.47
1:H:42:ILE:HB	1:H:46:ARG:CB	2.43	0.47
1:D:269:GLU:HG2	1:E:176:THR:HG21	1.96	0.47
1:F:44:GLY:O	1:F:48:ASN:ND2	2.47	0.47
1:G:53:ILE:HD12	1:G:53:ILE:C	2.35	0.47
1:B:184:GLY:HA3	1:H:213:ASN:ND2	2.28	0.47
1:C:121:ASP:OD1	1:C:147:ARG:N	2.38	0.47
1:D:108:ARG:HD3	1:D:136:ARG:HG3	1.97	0.47
1:D:31:LEU:HD11	1:D:98:GLU:HG3	1.95	0.47
1:E:113:ASP:O	1:E:116:HIS:HD2	1.98	0.47
1:D:214:GLN:NE2	1:E:184:GLY:H	2.02	0.47
1:F:37:ASP:OD2	1:F:40:GLU:HB2	2.14	0.47
1:G:283:LEU:CD2	1:G:292:THR:HG22	2.45	0.47
1:B:211:GLY:HA2	1:H:181:ALA:O	2.14	0.47
1:H:1:MSE:CE	1:H:32:GLU:HG3	2.38	0.47
1:H:42:ILE:HB	1:H:46:ARG:N	2.29	0.47
1:A:201:VAL:HB	1:A:238:LEU:O	2.14	0.47
1:A:32:GLU:O	1:A:35:LYS:HB2	2.15	0.47
1:B:237:ARG:HG3	1:B:237:ARG:NH1	2.28	0.47
1:C:301:ILE:HD11	1:E:237:ARG:CZ	2.44	0.47
1:H:119:ILE:HG22	1:H:119:ILE:O	2.14	0.47
1:B:5:GLU:HA	1:B:8:GLU:OE1	2.14	0.47
1:C:135:LEU:O	1:C:139:GLU:HG3	2.14	0.47
1:H:113:ASP:C	1:H:115:CYS:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASP:OD2	1:B:294:SER:HB3	2.14	0.47
1:H:304:TYR:C	1:H:306:ALA:N	2.68	0.47
1:A:306:ALA:O	1:A:307:ALA:HB2	2.15	0.47
1:B:71:LEU:CD1	1:B:303:LEU:HD11	2.45	0.47
1:D:25:ALA:O	1:D:29:THR:HG23	2.14	0.47
1:F:91:LYS:HB2	1:F:93:MSE:HG3	1.96	0.47
1:G:142:VAL:C	1:G:144:ALA:N	2.67	0.47
1:H:56:LEU:C	1:H:58:GLY:N	2.68	0.47
1:A:300:LEU:O	1:A:300:LEU:HD23	2.15	0.47
1:A:54:GLU:OE1	1:A:73:LEU:HD21	2.15	0.47
1:C:46:ARG:CG	1:C:46:ARG:HH21	2.27	0.47
1:D:57:CYS:C	1:D:59:VAL:H	2.18	0.47
1:H:27:ILE:HD12	1:H:104:ILE:HD11	1.96	0.47
1:C:50:THR:O	1:C:53:ILE:CG2	2.60	0.47
1:C:75:PHE:HZ	1:C:99:LEU:HD23	1.79	0.47
1:C:9:TYR:CE2	1:C:29:THR:HA	2.50	0.47
1:H:128:HIS:HB2	1:H:215:MSE:HE1	1.95	0.47
1:C:7:ILE:O	1:C:11:LYS:HG3	2.14	0.47
1:C:150:VAL:HG12	1:C:151:TYR:N	2.30	0.47
1:E:208:ASN:O	1:E:209:LYS:C	2.53	0.47
1:G:36:ARG:HG3	1:G:36:ARG:HH11	1.80	0.47
1:C:45:LEU:O	1:C:46:ARG:HB3	2.15	0.46
1:C:3:ASP:O	1:C:6:LEU:HB2	2.15	0.46
1:D:150:VAL:HG12	1:D:151:TYR:N	2.30	0.46
1:D:78:LEU:HD23	1:D:92:ILE:HD11	1.97	0.46
1:F:34:LEU:O	1:F:37:ASP:HB3	2.15	0.46
1:B:195:VAL:HG12	1:B:196:GLY:O	2.15	0.46
1:A:181:ALA:O	1:C:211:GLY:HA2	2.15	0.46
1:C:247:PRO:HD2	1:C:250:PHE:HD1	1.80	0.46
1:E:2:ASP:O	1:E:6:LEU:HB2	2.15	0.46
1:E:71:LEU:HD12	1:E:233:PHE:HA	1.97	0.46
1:F:127:THR:HG23	1:F:152:VAL:HG23	1.97	0.46
1:G:101:LEU:O	1:G:101:LEU:HD12	2.15	0.46
1:G:43:GLN:C	1:G:43:GLN:OE1	2.53	0.46
1:A:132:ARG:HD2	2:A:501:SO4:O4	2.16	0.46
1:D:27:ILE:CD1	1:D:101:LEU:HG	2.45	0.46
1:E:70:GLU:HG2	1:E:74:ARG:NE	2.31	0.46
1:E:89:CYS:C	1:E:91:LYS:N	2.68	0.46
1:H:42:ILE:HD12	1:H:46:ARG:CG	2.41	0.46
1:H:2:ASP:H	1:H:5:GLU:HB2	1.80	0.46
1:B:70:GLU:O	1:B:74:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:THR:HG22	1:D:287:ASP:N	2.30	0.46
1:G:110:LYS:HD2	1:G:287:ASP:HB2	1.97	0.46
1:H:90:LYS:C	1:H:92:ILE:N	2.67	0.46
1:A:132:ARG:HD2	2:A:501:SO4:O3	2.16	0.46
1:D:133:VAL:HG23	1:D:229:VAL:CG2	2.44	0.46
1:D:142:VAL:HG23	1:D:143:ALA:N	2.30	0.46
1:D:88:LYS:C	1:D:88:LYS:HD3	2.36	0.46
1:H:114:LEU:O	1:H:114:LEU:HD13	2.15	0.46
1:A:214:GLN:OE1	1:C:183:VAL:N	2.49	0.46
1:B:62:SER:CB	1:B:65:VAL:HG23	2.38	0.46
1:C:46:ARG:HG3	1:C:47:ALA:N	2.30	0.46
1:D:254:ALA:O	1:D:255:ASP:HB3	2.15	0.46
1:E:34:LEU:HD22	1:E:94:ILE:CG1	2.46	0.46
1:F:91:LYS:HD3	1:F:91:LYS:H	1.81	0.46
1:H:114:LEU:HD11	1:H:289:GLY:HA2	1.96	0.46
1:C:58:GLY:O	1:C:60:ASP:N	2.48	0.46
1:D:153:THR:O	1:D:161:GLY:HA3	2.16	0.46
1:A:210:ILE:O	1:A:210:ILE:HG23	2.15	0.46
1:D:19:ASP:O	1:D:132:ARG:HD2	2.16	0.46
1:E:46:ARG:HH11	1:E:46:ARG:HG3	1.81	0.46
1:A:33:PHE:CE2	1:A:53:ILE:HG21	2.51	0.46
1:B:186:ILE:CD1	1:B:189:LYS:HD2	2.46	0.46
1:D:131:SER:HB3	1:D:134:VAL:HG12	1.98	0.46
1:E:71:LEU:CD2	1:E:304:TYR:HE1	2.29	0.46
1:F:106:LEU:HB3	1:F:110:LYS:HZ1	1.82	0.45
1:F:60:ASP:O	1:F:62:SER:N	2.49	0.45
1:C:70:GLU:OE2	1:C:74:ARG:HD2	2.16	0.45
1:D:46:ARG:NH2	1:D:91:LYS:HD3	2.32	0.45
1:E:7:ILE:HG22	1:E:11:LYS:HE2	1.97	0.45
1:F:27:ILE:HD13	1:F:100:PHE:HE1	1.80	0.45
1:G:237:ARG:HH22	1:H:302:LYS:HG3	1.81	0.45
1:H:40:GLU:C	1:H:42:ILE:H	2.19	0.45
1:H:51:SER:HA	1:H:54:GLU:HB2	1.98	0.45
1:A:132:ARG:HD2	2:A:501:SO4:S	2.57	0.45
1:B:267:LYS:CG	1:B:268:GLU:H	2.28	0.45
1:B:6:LEU:HD21	1:B:53:ILE:HG23	1.97	0.45
1:D:46:ARG:NH2	1:D:91:LYS:HZ3	2.13	0.45
1:A:188:GLU:CA	1:A:222:GLN:HE22	2.28	0.45
1:B:108:ARG:NH2	1:B:132:ARG:HG3	2.32	0.45
1:D:86:TYR:O	1:D:90:LYS:HG3	2.17	0.45
1:C:294:SER:HB3	1:E:241:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:GLN:OE1	1:G:183:VAL:HB	2.16	0.45
1:H:139:GLU:HG2	1:H:171:LEU:HD11	1.98	0.45
1:A:192:LEU:HD23	1:A:192:LEU:N	2.31	0.45
1:D:214:GLN:NE2	1:E:183:VAL:HB	2.32	0.45
1:D:2:ASP:O	1:D:5:GLU:HB2	2.16	0.45
1:F:177:VAL:HB	1:G:268:GLU:HG2	1.98	0.45
1:G:192:LEU:N	1:G:192:LEU:HD23	2.32	0.45
1:G:126:LEU:HD13	1:G:215:MSE:SE	2.67	0.45
1:G:139:GLU:HG2	1:G:171:LEU:CD1	2.47	0.45
1:G:56:LEU:C	1:G:58:GLY:N	2.69	0.45
1:A:37:ASP:O	1:A:38:LYS:C	2.55	0.45
1:D:20:MSE:CE	1:D:28:ARG:HE	2.30	0.45
1:E:71:LEU:CD1	1:E:233:PHE:HA	2.46	0.45
1:F:10:PHE:CB	1:F:29:THR:HG21	2.46	0.45
1:G:13:GLN:HE22	1:G:28:ARG:HD3	1.82	0.45
1:C:6:LEU:HD21	1:C:33:PHE:CD1	2.50	0.45
1:D:28:ARG:NH1	1:D:101:LEU:HD22	2.31	0.45
1:E:76:ILE:HD12	1:E:93:MSE:HE2	1.99	0.45
1:E:88:LYS:HG3	1:E:88:LYS:O	2.17	0.45
1:G:142:VAL:C	1:G:144:ALA:H	2.20	0.45
1:B:266:LEU:CD2	1:H:175:VAL:H	2.24	0.45
1:H:40:GLU:HA	1:H:42:ILE:CG1	2.41	0.45
1:C:4:LYS:N	1:C:4:LYS:HD3	2.32	0.45
1:D:51:SER:C	1:D:53:ILE:H	2.20	0.45
1:F:108:ARG:HD3	1:F:136:ARG:CG	2.44	0.45
1:F:12:SER:HA	1:F:15:LYS:HB2	1.99	0.45
1:F:286:THR:HG22	1:F:287:ASP:H	1.72	0.45
1:C:136:ARG:NH2	4:C:1116:HOH:O	2.50	0.44
1:F:52:ALA:O	1:F:56:LEU:HG	2.17	0.44
1:G:142:VAL:O	1:G:144:ALA:N	2.49	0.44
1:G:285:PHE:CD2	1:G:290:VAL:HG22	2.53	0.44
1:G:43:GLN:C	1:G:45:LEU:H	2.19	0.44
1:H:3:ASP:CG	1:H:56:LEU:HD13	2.38	0.44
1:E:44:GLY:O	1:E:48:ASN:HB3	2.16	0.44
1:H:51:SER:C	1:H:53:ILE:N	2.70	0.44
1:D:183:VAL:HB	1:E:214:GLN:NE2	2.33	0.44
1:D:188:GLU:OE1	1:E:242:ASN:HB2	2.17	0.44
1:F:135:LEU:HD22	1:F:139:GLU:OE2	2.17	0.44
1:G:25:ALA:O	1:G:29:THR:CG2	2.66	0.44
1:A:94:ILE:HG22	1:A:94:ILE:O	2.17	0.44
1:C:42:ILE:O	1:C:46:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:SER:O	1:D:301:ILE:HG13	2.17	0.44
1:E:34:LEU:O	1:E:34:LEU:HD23	2.17	0.44
1:F:10:PHE:HB2	1:F:29:THR:HG21	1.98	0.44
1:F:41:THR:HG23	1:F:42:ILE:H	1.81	0.44
1:H:100:PHE:O	1:H:103:ARG:HB2	2.17	0.44
1:C:11:LYS:O	1:C:15:LYS:HG3	2.17	0.44
1:D:131:SER:HB3	1:D:134:VAL:CG1	2.48	0.44
1:H:99:LEU:HD11	1:H:103:ARG:HH12	1.79	0.44
1:C:41:THR:CG2	1:C:42:ILE:H	2.21	0.44
1:E:301:ILE:C	1:E:301:ILE:HD12	2.37	0.44
1:H:135:LEU:O	1:H:139:GLU:HG3	2.17	0.44
1:E:45:LEU:HA	1:E:48:ASN:HD22	1.83	0.44
1:E:96:ARG:CG	1:E:96:ARG:HH11	2.30	0.44
1:F:129:ALA:HB2	1:F:155:SER:OG	2.18	0.44
1:G:133:VAL:CG1	1:G:229:VAL:CG1	2.94	0.44
1:G:267:LYS:CG	1:G:268:GLU:H	2.30	0.44
1:H:127:THR:HG23	1:H:152:VAL:HG23	1.99	0.44
1:B:63:VAL:HG22	1:B:250:PHE:CD1	2.53	0.44
1:E:270:HIS:HB3	4:E:1077:HOH:O	2.18	0.44
1:F:30:LEU:HD22	1:F:53:ILE:CD1	2.48	0.44
1:B:266:LEU:HB3	1:H:175:VAL:O	2.18	0.44
1:H:128:HIS:HB2	1:H:215:MSE:CE	2.47	0.44
1:C:24:VAL:HG22	1:C:104:ILE:CD1	2.48	0.43
1:F:237:ARG:HG3	1:F:237:ARG:NH1	2.33	0.43
1:B:90:LYS:O	1:B:93:MSE:HG2	2.18	0.43
1:C:300:LEU:C	1:C:300:LEU:HD23	2.39	0.43
1:C:72:PHE:CZ	1:C:76:ILE:HD12	2.52	0.43
1:D:134:VAL:HG13	1:D:164:MSE:CE	2.47	0.43
1:D:57:CYS:C	1:D:59:VAL:N	2.72	0.43
1:E:90:LYS:HG3	1:E:90:LYS:O	2.18	0.43
1:G:17:ASP:HB3	1:G:19:ASP:OD1	2.17	0.43
1:B:203:ASN:HB3	1:B:239:PHE:CE1	2.53	0.43
1:D:253:LYS:HE3	1:D:253:LYS:HB2	1.81	0.43
1:E:2:ASP:HB3	1:E:5:GLU:OE1	2.18	0.43
1:G:72:PHE:HB2	1:G:100:PHE:CE1	2.52	0.43
1:D:10:PHE:HE1	1:D:26:ALA:N	2.17	0.43
1:E:119:ILE:HD11	1:E:137:VAL:CG1	2.46	0.43
1:G:139:GLU:HA	1:G:142:VAL:CG1	2.49	0.43
1:H:120:LYS:NZ	1:H:191:ASP:HB3	2.33	0.43
1:B:181:ALA:O	1:H:211:GLY:HA2	2.19	0.43
1:C:74:ARG:NH2	1:E:305:LEU:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:LEU:HD23	1:E:34:LEU:C	2.39	0.43
1:F:6:LEU:HD21	1:F:33:PHE:HD2	1.82	0.43
1:H:42:ILE:C	1:H:44:GLY:N	2.70	0.43
1:A:28:ARG:HH21	1:A:101:LEU:HD21	1.83	0.43
1:A:214:GLN:OE1	1:C:183:VAL:HB	2.18	0.43
1:A:49:LEU:O	1:A:53:ILE:HG23	2.18	0.43
1:E:53:ILE:HG22	1:E:56:LEU:CD1	2.45	0.43
1:F:213:ASN:HD22	1:G:184:GLY:HA3	1.83	0.43
1:H:120:LYS:HE3	1:H:120:LYS:HB2	1.82	0.43
1:B:92:ILE:HG23	1:B:95:GLU:OE1	2.19	0.43
1:D:45:LEU:HB3	1:D:49:LEU:HD11	2.01	0.43
1:B:111:ILE:HG21	1:B:229:VAL:HG22	2.00	0.43
1:B:208:ASN:O	1:B:273:VAL:HA	2.19	0.43
1:E:34:LEU:HD22	1:E:94:ILE:HG12	2.01	0.43
1:F:38:LYS:HD2	1:F:38:LYS:HA	1.88	0.43
1:H:42:ILE:CB	1:H:46:ARG:HB3	2.48	0.43
1:A:305:LEU:O	1:A:306:ALA:C	2.55	0.43
1:A:9:TYR:CD2	1:A:29:THR:HA	2.54	0.43
1:D:42:ILE:HG12	1:D:45:LEU:HD12	2.01	0.43
1:G:133:VAL:HG11	1:G:229:VAL:HG12	2.01	0.43
1:G:61:SER:HB2	1:G:249:LYS:O	2.18	0.43
1:H:55:THR:CG2	1:H:56:LEU:N	2.81	0.43
1:C:27:ILE:HD11	1:C:101:LEU:HG	2.01	0.43
1:G:1:MSE:HE1	1:G:9:TYR:HB2	2.01	0.43
1:B:179:LEU:HD22	1:H:270:HIS:HD2	1.84	0.43
1:H:36:ARG:HH11	1:H:36:ARG:CG	2.32	0.43
1:D:187:MSE:O	1:D:187:MSE:HE3	2.19	0.42
1:F:42:ILE:CD1	1:F:43:GLN:HG2	2.49	0.42
1:G:168:LEU:HB3	1:G:173:VAL:HG22	1.99	0.42
1:G:238:LEU:HD11	1:G:250:PHE:HE1	1.83	0.42
1:G:283:LEU:HD23	1:G:292:THR:HG22	2.01	0.42
1:G:69:GLY:O	1:G:73:LEU:HB2	2.18	0.42
1:H:23:ALA:HB3	1:H:233:PHE:CE1	2.54	0.42
1:B:28:ARG:CG	1:B:101:LEU:HD11	2.49	0.42
1:B:133:VAL:HG11	1:B:229:VAL:HG13	1.99	0.42
1:C:301:ILE:HG13	1:C:302:LYS:N	2.32	0.42
1:D:168:LEU:O	1:D:173:VAL:HG13	2.19	0.42
1:G:197:ALA:O	1:G:234:LYS:HD3	2.19	0.42
1:G:79:ALA:CB	1:G:90:LYS:HG3	2.49	0.42
1:B:142:VAL:O	1:B:145:LYS:N	2.47	0.42
1:C:131:SER:OG	1:C:134:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ALA:O	1:C:234:LYS:HD3	2.18	0.42
1:E:36:ARG:O	1:E:36:ARG:HG2	2.18	0.42
1:F:42:ILE:CG2	1:F:45:LEU:HB2	2.45	0.42
1:G:16:GLU:HG2	1:G:16:GLU:O	2.18	0.42
1:A:59:VAL:HG22	1:A:59:VAL:O	2.19	0.42
1:C:89:CYS:O	1:C:92:ILE:HG13	2.20	0.42
1:E:109:ASN:ND2	1:E:136:ARG:HH21	2.17	0.42
1:G:110:LYS:O	1:G:114:LEU:HG	2.20	0.42
1:H:4:LYS:HB3	1:H:4:LYS:HE2	1.71	0.42
1:D:266:LEU:O	1:E:177:VAL:N	2.42	0.42
1:D:42:ILE:HG12	1:D:45:LEU:HG	2.01	0.42
1:D:89:CYS:O	1:D:91:LYS:N	2.53	0.42
1:G:153:THR:O	1:G:161:GLY:HA3	2.20	0.42
1:G:58:GLY:C	1:G:60:ASP:N	2.73	0.42
1:B:113:ASP:HA	1:B:116:HIS:HD2	1.85	0.42
1:B:93:MSE:O	1:B:94:ILE:C	2.58	0.42
1:E:301:ILE:O	1:E:305:LEU:HG	2.19	0.42
1:G:90:LYS:O	1:G:93:MSE:HG3	2.20	0.42
1:H:114:LEU:HD22	1:H:114:LEU:O	2.20	0.42
1:B:156:GLN:HB3	1:B:157:PRO:HA	2.01	0.42
1:B:60:ASP:O	1:B:61:SER:C	2.58	0.42
1:C:119:ILE:O	1:C:146:LYS:HD3	2.20	0.42
1:C:77:SER:O	1:C:78:LEU:HD23	2.20	0.42
1:D:46:ARG:NH2	1:D:91:LYS:HZ2	2.17	0.42
1:F:130:TYR:HB2	1:F:160:SER:HB2	2.01	0.42
1:F:15:LYS:C	1:F:17:ASP:H	2.23	0.42
1:H:28:ARG:HH11	1:H:101:LEU:HD22	1.81	0.42
1:H:55:THR:CG2	1:H:56:LEU:H	2.29	0.42
1:A:13:GLN:NE2	1:A:28:ARG:HD2	2.34	0.42
1:B:192:LEU:HB3	1:B:225:PRO:HG2	2.02	0.42
1:C:82:GLU:HB2	1:C:90:LYS:HZ3	1.84	0.42
1:D:91:LYS:CG	1:D:91:LYS:O	2.67	0.42
1:E:41:THR:OG1	1:E:42:ILE:N	2.53	0.42
1:F:116:HIS:CD2	1:F:117:THR:N	2.87	0.42
1:F:47:ALA:C	1:F:50:THR:HG22	2.39	0.42
1:H:112:ALA:HA	1:H:137:VAL:HG22	2.02	0.42
1:C:33:PHE:O	1:C:37:ASP:CB	2.64	0.42
1:D:286:THR:CG2	1:D:287:ASP:N	2.83	0.42
1:E:301:ILE:HD12	1:E:301:ILE:O	2.19	0.42
1:G:133:VAL:HG12	1:G:229:VAL:HG12	1.96	0.42
1:H:201:VAL:CG1	1:H:202:GLU:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:ASN:HB3	1:H:239:PHE:CZ	2.55	0.42
1:A:46:ARG:HB2	1:A:90:LYS:HZ2	1.85	0.42
1:C:138:LEU:HD12	1:C:168:LEU:HD21	2.02	0.42
1:C:46:ARG:NH2	1:C:46:ARG:CG	2.82	0.42
1:G:90:LYS:C	1:G:92:ILE:H	2.23	0.42
1:B:150:VAL:HG12	1:B:151:TYR:N	2.35	0.41
1:E:46:ARG:C	1:E:48:ASN:N	2.73	0.41
1:D:201:VAL:HB	1:D:238:LEU:O	2.20	0.41
1:E:142:VAL:HG23	1:E:143:ALA:N	2.35	0.41
1:G:75:PHE:CE1	1:G:306:ALA:HB3	2.55	0.41
1:H:48:ASN:O	1:H:51:SER:HB2	2.19	0.41
1:A:9:TYR:CE2	1:A:32:GLU:HB2	2.56	0.41
1:A:8:GLU:O	1:A:9:TYR:C	2.59	0.41
1:B:46:ARG:C	1:B:48:ASN:H	2.24	0.41
1:C:110:LYS:HE2	1:C:287:ASP:O	2.21	0.41
1:D:128:HIS:HA	1:D:153:THR:OG1	2.20	0.41
1:D:286:THR:HG22	1:D:288:LEU:N	2.09	0.41
1:D:42:ILE:CD1	1:D:45:LEU:HG	2.50	0.41
1:H:122:GLY:N	1:H:147:ARG:O	2.50	0.41
1:B:47:ALA:O	1:B:50:THR:HG22	2.21	0.41
1:C:38:LYS:HD2	1:C:38:LYS:HA	1.95	0.41
1:G:70:GLU:HG2	1:G:74:ARG:HD2	2.03	0.41
1:C:142:VAL:CG2	1:C:143:ALA:N	2.83	0.41
1:C:78:LEU:HD12	1:C:96:ARG:NE	2.36	0.41
1:D:33:PHE:C	1:D:33:PHE:CD1	2.93	0.41
1:E:17:ASP:HA	1:E:18:PRO:HD2	1.92	0.41
1:E:23:ALA:HB3	1:E:233:PHE:CE1	2.56	0.41
1:G:67:SER:HB3	1:G:236:VAL:HB	2.01	0.41
1:H:135:LEU:HD22	1:H:139:GLU:HG3	2.01	0.41
1:H:28:ARG:CG	1:H:28:ARG:NH1	2.81	0.41
1:A:6:LEU:O	1:A:8:GLU:N	2.52	0.41
1:C:238:LEU:HD11	1:C:250:PHE:CE1	2.56	0.41
1:F:88:LYS:C	1:F:90:LYS:N	2.74	0.41
1:G:246:VAL:HA	1:G:247:PRO:HD3	1.95	0.41
1:G:9:TYR:CE2	1:G:29:THR:HA	2.56	0.41
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.87	0.41
1:C:60:ASP:C	1:C:62:SER:N	2.72	0.41
1:D:28:ARG:NH1	1:D:101:LEU:CD2	2.84	0.41
1:F:201:VAL:CG1	1:F:240:PRO:HD2	2.45	0.41
1:F:74:ARG:C	1:F:76:ILE:H	2.24	0.41
1:A:188:GLU:HA	1:A:222:GLN:NE2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD21	1:A:33:PHE:CD2	2.49	0.41
1:B:32:GLU:CG	1:B:36:ARG:NH1	2.84	0.41
1:C:41:THR:HG21	1:C:45:LEU:HD12	2.03	0.41
1:E:126:LEU:HD12	1:E:151:TYR:O	2.20	0.41
1:E:52:ALA:O	1:E:56:LEU:HG	2.21	0.41
1:F:186:ILE:CD1	1:F:189:LYS:HD2	2.51	0.41
1:G:139:GLU:HA	1:G:142:VAL:HG12	2.03	0.41
1:G:151:TYR:CD1	1:G:176:THR:HB	2.56	0.41
1:G:154:GLU:OE2	1:G:156:GLN:NE2	2.51	0.41
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.87	0.41
1:A:33:PHE:O	1:A:36:ARG:HB2	2.21	0.41
1:B:132:ARG:H	1:B:132:ARG:HG2	1.57	0.41
1:D:48:ASN:HA	1:D:51:SER:HB3	2.02	0.41
1:G:33:PHE:O	1:G:37:ASP:HB2	2.21	0.41
1:H:109:ASN:HD21	1:H:136:ARG:HE	1.69	0.41
1:H:169:CYS:C	1:H:171:LEU:N	2.73	0.41
1:H:40:GLU:C	1:H:42:ILE:HG12	2.41	0.41
1:A:14:MSE:HE3	1:A:22:SER:HA	2.02	0.41
1:A:185:TYR:C	1:A:185:TYR:CD2	2.93	0.41
1:C:306:ALA:O	1:C:307:ALA:C	2.59	0.41
1:C:41:THR:HG21	1:C:45:LEU:CD1	2.51	0.41
1:G:136:ARG:CZ	1:G:136:ARG:CB	2.98	0.41
1:A:133:VAL:HG23	2:A:501:SO4:O2	2.21	0.40
1:C:2:ASP:OD1	1:C:3:ASP:N	2.54	0.40
1:D:142:VAL:CG2	1:D:143:ALA:N	2.84	0.40
1:F:251:LYS:C	1:F:252:TYR:HD1	2.25	0.40
1:G:144:ALA:O	1:G:145:LYS:HB2	2.20	0.40
1:G:214:GLN:HG2	1:G:214:GLN:H	1.72	0.40
1:H:43:GLN:HE22	1:H:87:SER:N	2.19	0.40
1:A:139:GLU:HG3	1:A:171:LEU:HD13	2.02	0.40
1:A:46:ARG:HB2	1:A:90:LYS:NZ	2.35	0.40
1:B:191:ASP:HB2	1:B:192:LEU:HD23	2.03	0.40
1:C:112:ALA:HA	1:C:137:VAL:HG22	2.03	0.40
1:F:156:GLN:NE2	1:F:159:LEU:HD21	2.36	0.40
1:F:286:THR:HG22	1:F:288:LEU:N	2.26	0.40
1:G:31:LEU:HD23	1:G:31:LEU:HA	1.82	0.40
1:G:60:ASP:O	1:G:62:SER:N	2.54	0.40
1:C:33:PHE:CZ	1:C:49:LEU:HG	2.48	0.40
1:D:92:ILE:C	1:D:92:ILE:CD1	2.89	0.40
1:E:40:GLU:O	1:E:41:THR:O	2.39	0.40
1:F:49:LEU:HA	1:F:49:LEU:HD12	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HA	1:A:106:LEU:HD12	1.87	0.40
1:A:45:LEU:HD12	1:A:46:ARG:CZ	2.51	0.40
1:A:6:LEU:HD13	1:A:53:ILE:HB	2.02	0.40
1:D:49:LEU:O	1:D:53:ILE:HG23	2.21	0.40
1:E:24:VAL:HG22	1:E:104:ILE:HD13	2.03	0.40
1:E:197:ALA:O	1:E:234:LYS:HD3	2.22	0.40
1:E:63:VAL:HG13	1:E:250:PHE:CG	2.57	0.40
1:F:251:LYS:HD3	1:G:185:TYR:OH	2.21	0.40
1:G:193:VAL:CG2	1:G:226:PHE:CD1	3.05	0.40
1:H:195:VAL:HG22	1:H:196:GLY:H	1.85	0.40
1:B:114:LEU:HD22	1:B:290:VAL:HG23	2.04	0.40
1:B:123:ALA:HA	1:B:191:ASP:OD2	2.21	0.40
1:B:37:ASP:OD2	1:B:46:ARG:HD2	2.21	0.40
1:B:51:SER:C	1:B:53:ILE:H	2.24	0.40
1:E:142:VAL:CG2	1:E:143:ALA:N	2.84	0.40
1:F:34:LEU:C	1:F:34:LEU:HD23	2.41	0.40
1:F:217:VAL:HG12	1:G:217:VAL:HG12	2.03	0.40
1:H:45:LEU:HD13	1:H:45:LEU:C	2.41	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	271/315 (86%)	251 (93%)	16 (6%)	4 (2%)	10 15
1	B	273/315 (87%)	252 (92%)	18 (7%)	3 (1%)	14 21
1	C	288/315 (91%)	264 (92%)	19 (7%)	5 (2%)	9 13
1	D	283/315 (90%)	258 (91%)	19 (7%)	6 (2%)	7 10
1	E	277/315 (88%)	254 (92%)	19 (7%)	4 (1%)	11 16
1	F	281/315 (89%)	257 (92%)	16 (6%)	8 (3%)	5 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	276/315 (88%)	254 (92%)	19 (7%)	3 (1%)	14 21
1	H	279/315 (89%)	253 (91%)	19 (7%)	7 (2%)	5 7
All	All	2228/2520 (88%)	2043 (92%)	145 (6%)	40 (2%)	8 12

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	SER
1	C	46	ARG
1	C	265	ASP
1	D	61	SER
1	D	88	LYS
1	D	268	GLU
1	E	41	THR
1	F	252	TYR
1	H	40	GLU
1	D	90	LYS
1	F	59	VAL
1	F	61	SER
1	H	104	ILE
1	C	60	ASP
1	D	60	ASP
1	E	305	LEU
1	G	3	ASP
1	H	43	GLN
1	C	59	VAL
1	D	37	ASP
1	F	16	GLU
1	F	58	GLY
1	F	253	LYS
1	G	91	LYS
1	H	170	HIS
1	A	306	ALA
1	B	62	SER
1	C	79	ALA
1	E	90	LYS
1	G	143	ALA
1	A	37	ASP
1	B	75	PHE
1	F	40	GLU
1	F	41	THR

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Mol	Chain	Res	Type
1	H	76	ILE
1	H	270	HIS
1	A	7	ILE
1	E	76	ILE
1	A	210	ILE
1	H	39	GLY

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	237/260 (91%)	228 (96%)	9 (4%)	33 49
1	B	239/260 (92%)	224 (94%)	15 (6%)	18 28
1	C	250/260 (96%)	238 (95%)	12 (5%)	25 39
1	D	246/260 (95%)	229 (93%)	17 (7%)	15 24
1	E	243/260 (94%)	229 (94%)	14 (6%)	20 31
1	F	242/260 (93%)	228 (94%)	14 (6%)	20 31
1	G	240/260 (92%)	225 (94%)	15 (6%)	18 28
1	H	242/260 (93%)	228 (94%)	14 (6%)	20 31
All	All	1939/2080 (93%)	1829 (94%)	110 (6%)	20 31

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	103	ARG
1	A	106	LEU
1	A	120	LYS
1	A	132	ARG
1	A	135	LEU
1	A	149	SER
1	A	266	LEU
1	A	303	LEU

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Mol	Chain	Res	Type
1	B	31	LEU
1	B	48	ASN
1	B	50	THR
1	B	103	ARG
1	B	113	ASP
1	B	120	LYS
1	B	126	LEU
1	B	132	ARG
1	B	135	LEU
1	B	136	ARG
1	B	179	LEU
1	B	186	ILE
1	B	229	VAL
1	B	249	LYS
1	B	252	TYR
1	C	34	LEU
1	C	46	ARG
1	C	73	LEU
1	C	86	TYR
1	C	89	CYS
1	C	106	LEU
1	C	113	ASP
1	C	126	LEU
1	C	135	LEU
1	C	136	ARG
1	C	239	PHE
1	C	301	ILE
1	D	29	THR
1	D	31	LEU
1	D	38	LYS
1	D	57	CYS
1	D	63	VAL
1	D	86	TYR
1	D	101	LEU
1	D	106	LEU
1	D	120	LYS
1	D	126	LEU
1	D	127	THR
1	D	135	LEU
1	D	172	ASN
1	D	173	VAL
1	D	179	LEU

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Mol	Chain	Res	Type
1	D	287	ASP
1	D	303	LEU
1	E	6	LEU
1	E	19	ASP
1	E	27	ILE
1	E	40	GLU
1	E	46	ARG
1	E	48	ASN
1	E	63	VAL
1	E	92	ILE
1	E	96	ARG
1	E	114	LEU
1	E	117	THR
1	E	135	LEU
1	E	284	LEU
1	E	301	ILE
1	F	31	LEU
1	F	40	GLU
1	F	45	LEU
1	F	74	ARG
1	F	90	LYS
1	F	91	LYS
1	F	101	LEU
1	F	103	ARG
1	F	116	HIS
1	F	121	ASP
1	F	135	LEU
1	F	142	VAL
1	F	223	ASN
1	F	253	LYS
1	G	29	THR
1	G	32	GLU
1	G	34	LEU
1	G	49	LEU
1	G	60	ASP
1	G	73	LEU
1	G	78	LEU
1	G	126	LEU
1	G	127	THR
1	G	135	LEU
1	G	136	ARG
1	G	147	ARG

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Mol	Chain	Res	Type
1	G	169	CYS
1	G	239	PHE
1	G	301	ILE
1	H	34	LEU
1	H	36	ARG
1	H	46	ARG
1	H	71	LEU
1	H	90	LYS
1	H	114	LEU
1	H	132	ARG
1	H	135	LEU
1	H	136	ARG
1	H	157	PRO
1	H	193	VAL
1	H	244	GLN
1	H	300	LEU
1	H	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	208	ASN
1	A	222	GLN
1	B	116	HIS
1	B	172	ASN
1	B	208	ASN
1	B	222	GLN
1	C	208	ASN
1	C	222	GLN
1	C	244	GLN
1	C	264	GLN
1	D	48	ASN
1	D	208	ASN
1	D	213	ASN
1	D	214	GLN
1	E	48	ASN
1	E	109	ASN
1	E	116	HIS
1	E	208	ASN
1	E	213	ASN
1	E	214	GLN

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Mol	Chain	Res	Type
1	E	222	GLN
1	E	244	GLN
1	F	48	ASN
1	F	109	ASN
1	F	116	HIS
1	F	208	ASN
1	F	213	ASN
1	F	222	GLN
1	F	244	GLN
1	G	13	GLN
1	G	116	HIS
1	G	208	ASN
1	G	213	ASN
1	G	222	GLN
1	H	109	ASN
1	H	208	ASN
1	H	213	ASN
1	H	244	GLN
1	H	270	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
2	SO4	H	508	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	E	505	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	F	506	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	C	503	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	F	510	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	G	507	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	D	504	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	A	509	-	4,4,4	0.24	0	6,6,6	0.10	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	508	SO4	1	0
2	A	501	SO4	4	0
2	B	502	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	272/315 (86%)	-0.19	12 (4%)	34	31	12, 34, 93, 112	0
1	B	274/315 (86%)	-0.09	15 (5%)	25	21	17, 40, 103, 118	0
1	C	287/315 (91%)	-0.24	8 (2%)	53	49	20, 41, 85, 107	0
1	D	284/315 (90%)	-0.19	7 (2%)	57	53	19, 41, 83, 117	0
1	E	278/315 (88%)	-0.11	7 (2%)	57	53	20, 46, 88, 113	0
1	F	280/315 (88%)	-0.31	2 (0%)	87	87	18, 36, 82, 97	0
1	G	277/315 (87%)	-0.12	1 (0%)	92	93	23, 46, 88, 97	0
1	H	278/315 (88%)	-0.08	12 (4%)	35	31	21, 49, 95, 120	0
All	All	2230/2520 (88%)	-0.17	64 (2%)	51	48	12, 41, 89, 120	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	45	LEU	6.4
1	D	86	TYR	6.0
1	A	266	LEU	5.5
1	H	41	THR	5.1
1	C	45	LEU	4.3
1	A	43	GLN	4.3
1	B	89	CYS	4.3
1	H	43	GLN	3.8
1	D	254	ALA	3.8
1	D	78	LEU	3.7
1	A	90	LYS	3.7
1	A	34	LEU	3.6
1	H	39	GLY	3.6
1	B	43	GLN	3.6
1	A	8	GLU	3.5
1	B	90	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	255	ASP	3.5
1	E	42	ILE	3.5
1	H	42	ILE	3.4
1	E	53	ILE	3.4
1	B	95	GLU	3.3
1	B	87	SER	3.3
1	D	268	GLU	3.3
1	C	86	TYR	3.2
1	C	38	LYS	3.2
1	A	37	ASP	3.1
1	H	46	ARG	3.1
1	B	46	ARG	3.1
1	C	43	GLN	3.0
1	A	12	SER	2.9
1	C	264	GLN	2.9
1	A	33	PHE	2.8
1	B	6	LEU	2.7
1	A	53	ILE	2.7
1	C	40	GLU	2.7
1	E	266	LEU	2.7
1	A	38	LYS	2.7
1	B	92	ILE	2.6
1	E	267	LYS	2.6
1	A	5	GLU	2.6
1	B	96	ARG	2.6
1	E	37	ASP	2.6
1	H	48	ASN	2.5
1	A	36	ARG	2.5
1	H	87	SER	2.5
1	B	45	LEU	2.5
1	C	265	ASP	2.5
1	F	253	LYS	2.5
1	D	46	ARG	2.5
1	C	16	GLU	2.4
1	B	5	GLU	2.4
1	B	33	PHE	2.4
1	H	40	GLU	2.3
1	D	92	ILE	2.3
1	H	53	ILE	2.3
1	E	17	ASP	2.3
1	B	77	SER	2.3
1	B	47	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	53	ILE	2.2
1	H	147	ARG	2.2
1	F	254	ALA	2.2
1	H	33	PHE	2.1
1	E	87	SER	2.1
1	B	3	ASP	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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	601	1/1	0.95	0.31	54,54,54,54	0
2	SO4	A	509	5/5	0.96	0.14	76,80,80,81	0
2	SO4	A	501	5/5	0.97	0.16	44,47,49,51	0
2	SO4	F	510	5/5	0.97	0.10	72,74,75,77	0
2	SO4	G	507	5/5	0.97	0.20	51,55,57,59	0
2	SO4	B	502	5/5	0.98	0.14	45,45,47,52	0
2	SO4	F	506	5/5	0.98	0.12	52,53,55,56	0
2	SO4	C	503	5/5	0.98	0.12	56,59,60,60	0
2	SO4	D	504	5/5	0.98	0.15	53,54,56,57	0
2	SO4	H	508	5/5	0.98	0.13	67,68,72,73	0
2	SO4	E	505	5/5	0.99	0.12	58,58,62,64	0

6.5 Other polymers (i)

There are no such residues in this entry.