



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 04:42 PM UTC

PDB ID : 3ECS / pdb_00003ecs
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 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

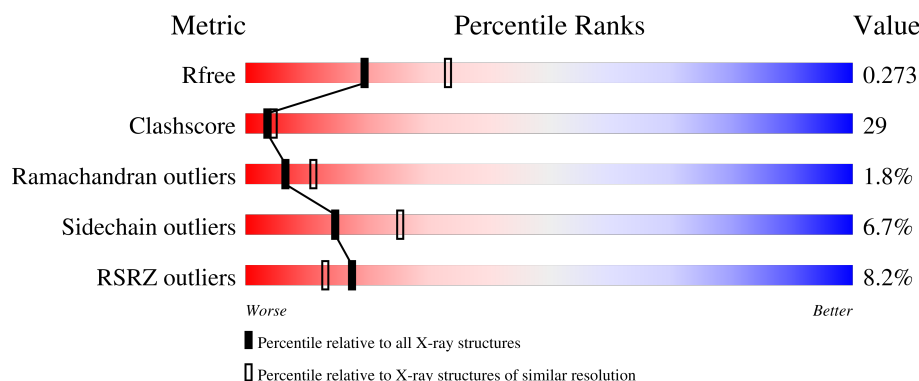
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	315	
1	B	315	
1	C	315	
1	D	315	
1	E	315	

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Mol	Chain	Length	Quality of chain
1	F	315	
1	G	315	
1	H	315	

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

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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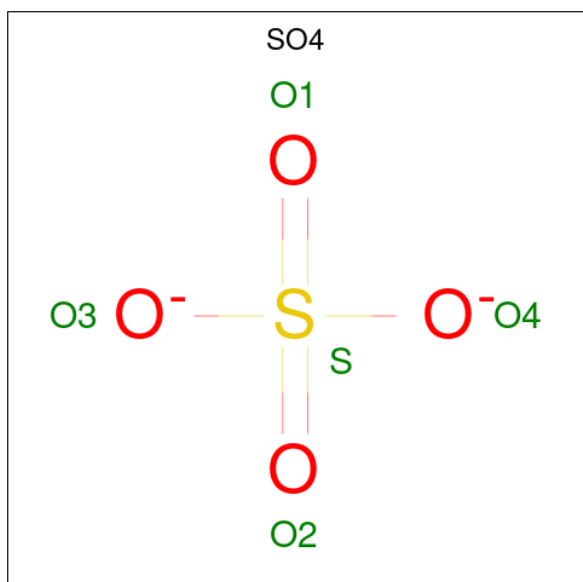
Chain	Residue	Modelled	Actual	Comment	Reference
B	309	GLU	-	expression tag	UNP Q14232
B	310	HIS	-	expression tag	UNP Q14232
B	311	HIS	-	expression tag	UNP Q14232
B	312	HIS	-	expression tag	UNP Q14232
B	313	HIS	-	expression tag	UNP Q14232
B	314	HIS	-	expression tag	UNP Q14232
B	315	HIS	-	expression tag	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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: 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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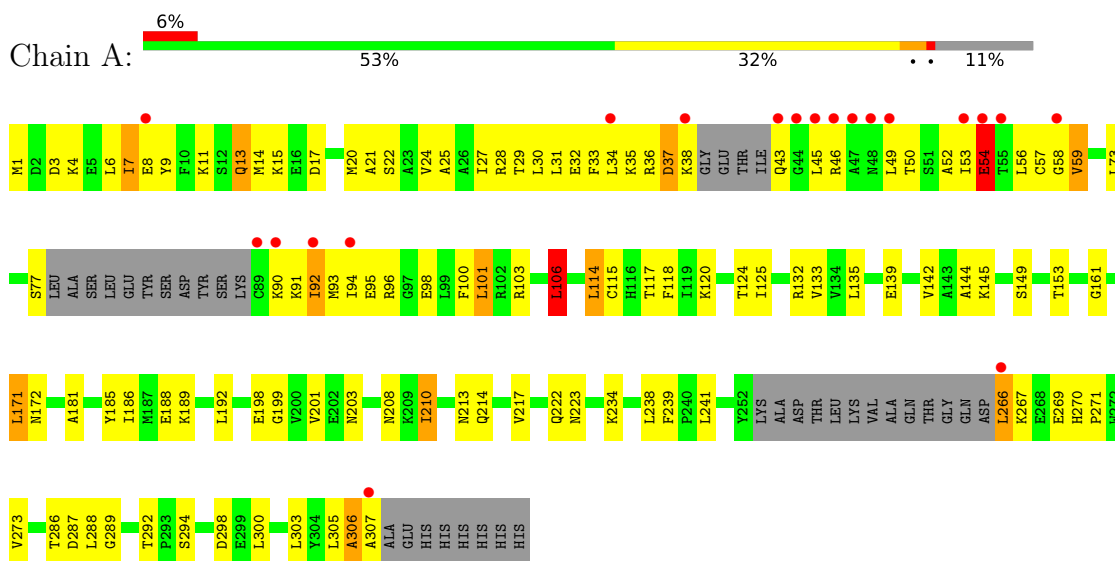
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	15	Total	O	0	0
			15	15		

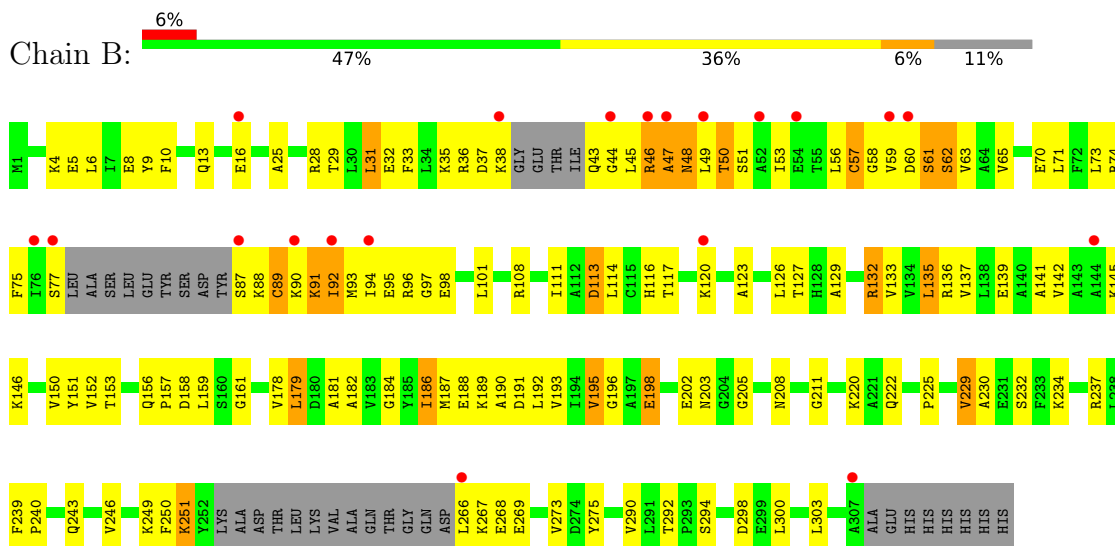
3 Residue-property plots

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

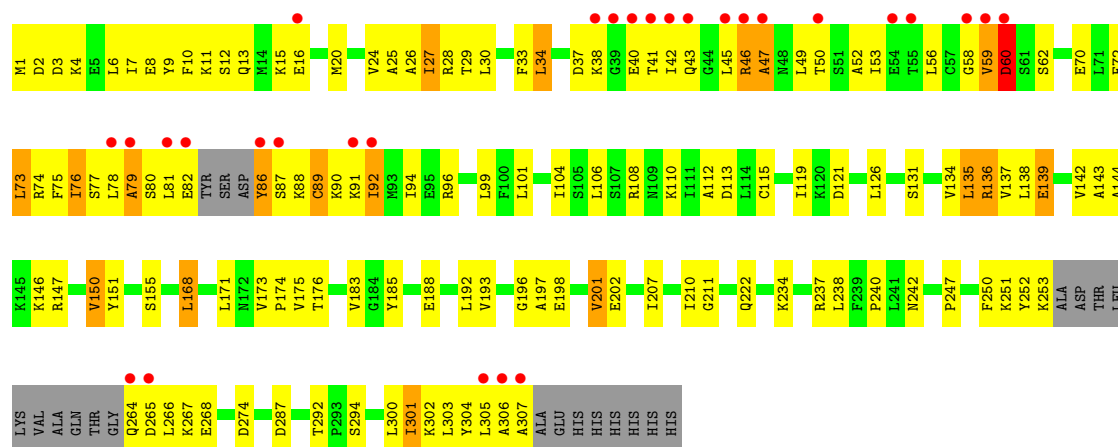


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

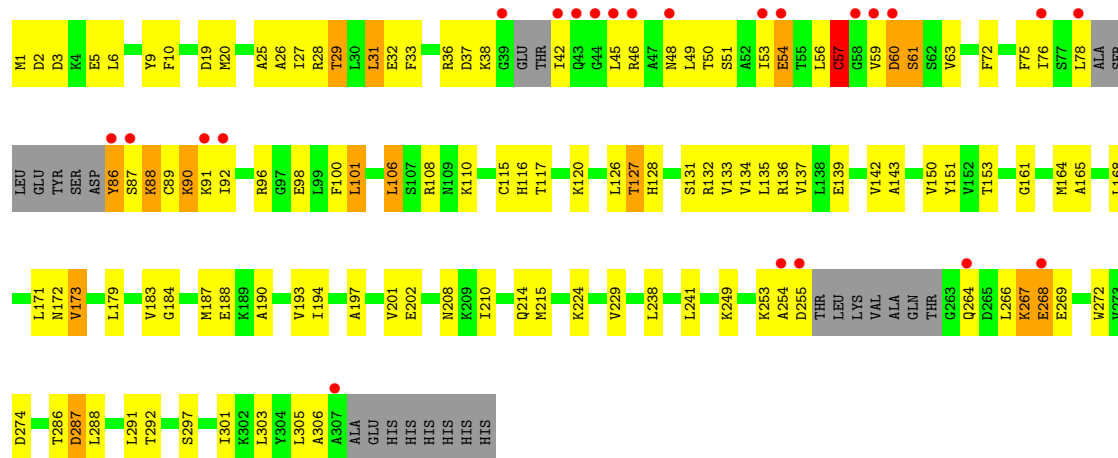


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

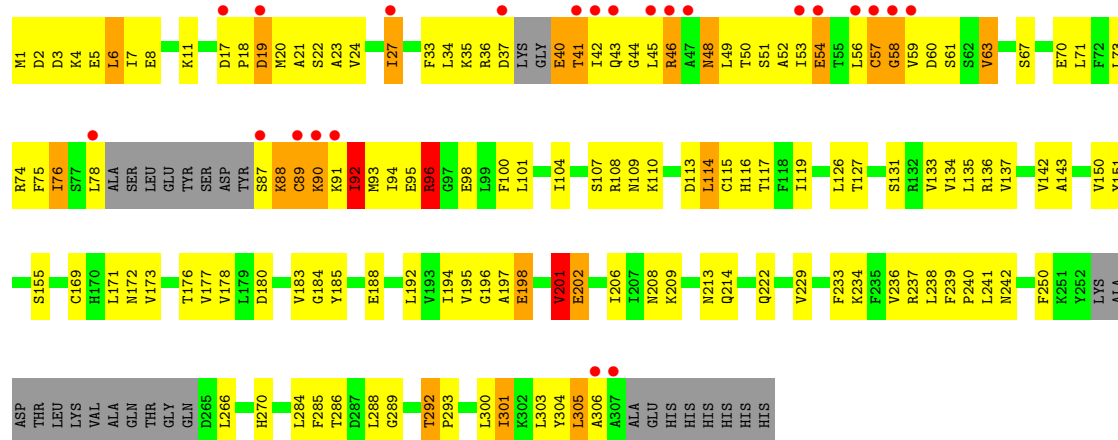




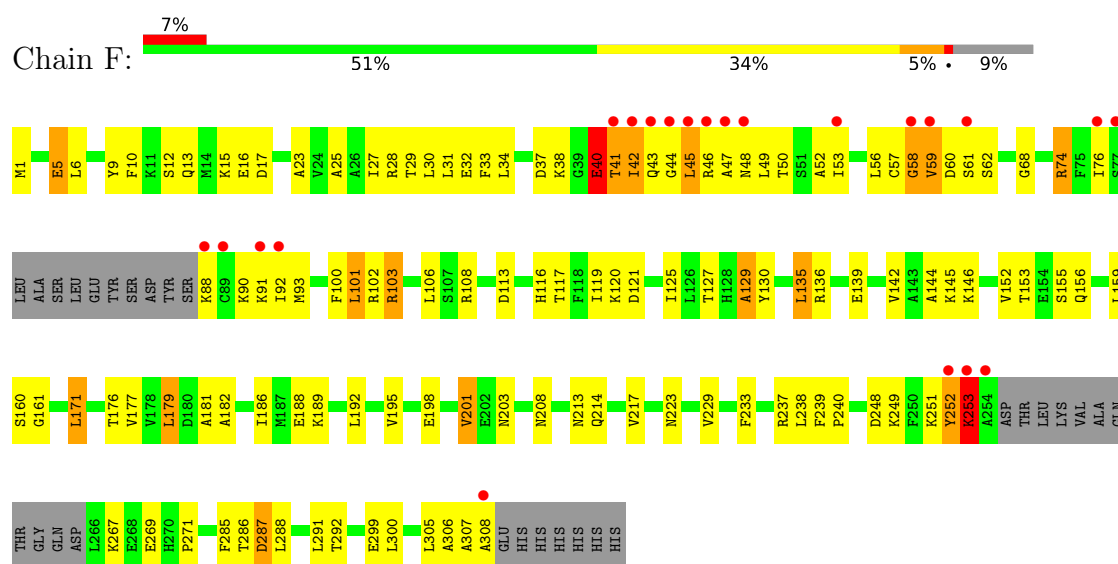
• Molecule 1: Translation initiation factor eIF-2B subunit alpha



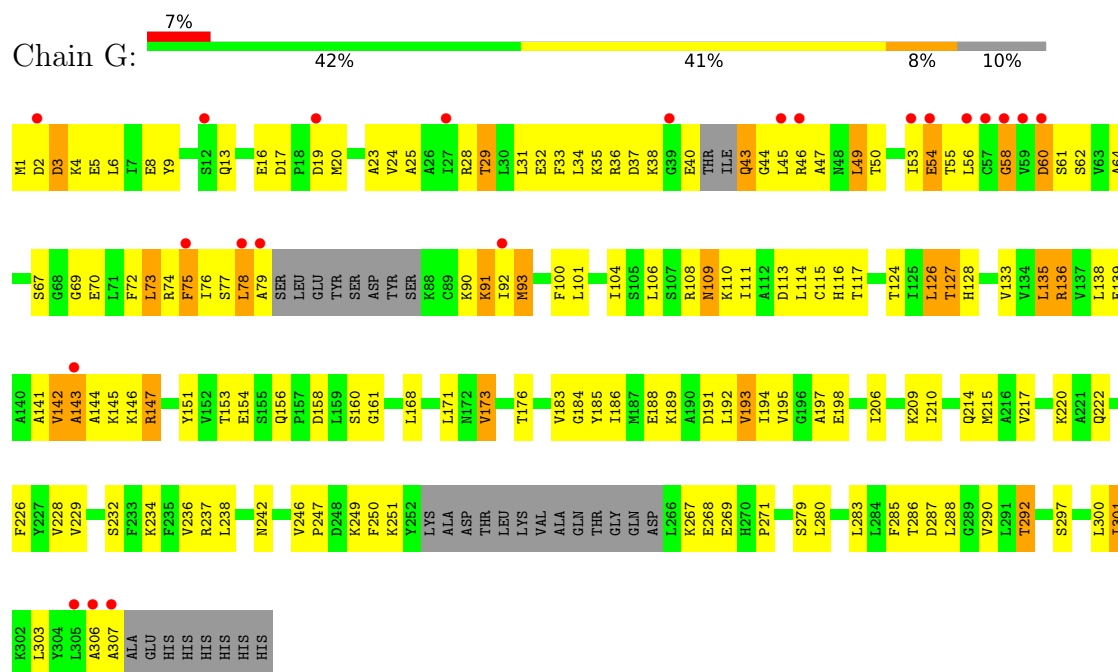
• Molecule 1: Translation initiation factor eIF-2B subunit alpha



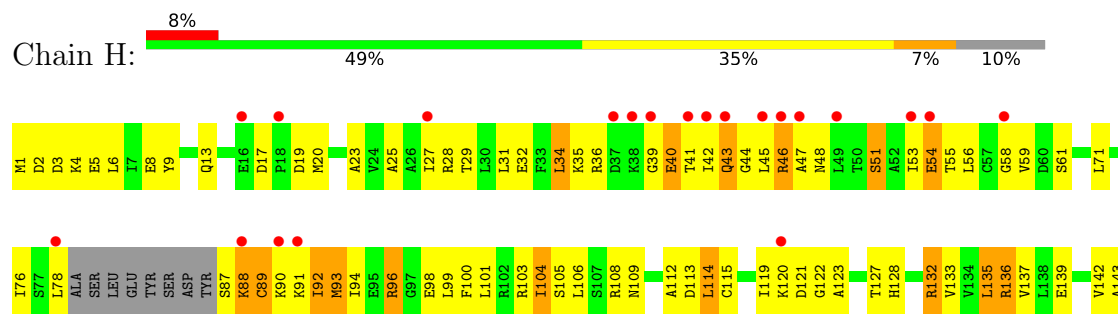
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

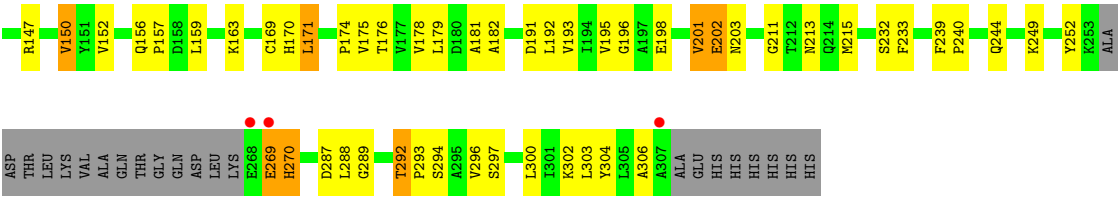


- Molecule 1: Translation initiation factor eIF-2B subunit alpha



- Molecule 1: Translation initiation factor eIF-2B 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	70.89Å 156.39Å 138.44Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.65) 99.2 (50.00-2.65)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.34 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: 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	0.54	0/2191	1.05	10/2945 (0.3%)
1	B	0.53	0/2206	1.03	14/2964 (0.5%)
1	C	0.53	0/2310	1.10	16/3106 (0.5%)
1	D	0.53	0/2282	1.04	8/3066 (0.3%)
1	E	0.51	0/2237	1.07	18/3008 (0.6%)
1	F	0.54	0/2248	1.02	7/3022 (0.2%)
1	G	0.50	0/2226	1.04	11/2991 (0.4%)
1	H	0.48	0/2235	1.14	22/3005 (0.7%)
All	All	0.52	0/17935	1.06	106/24107 (0.4%)

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	92	ILE	N-CA-C	-15.23	98.28	112.90
1	C	92	ILE	N-CA-C	-15.04	94.73	113.22
1	D	267	LYS	N-CA-C	-12.88	96.26	112.88
1	H	54	GLU	N-CA-C	-10.44	99.98	111.36
1	E	92	ILE	N-CA-C	-9.30	99.57	112.50
1	B	292	THR	N-CA-C	-9.24	97.54	110.29
1	H	89	CYS	N-CA-C	-8.87	102.45	113.18
1	C	171	LEU	N-CA-C	-8.85	102.03	112.92
1	H	41	THR	N-CA-C	-8.49	102.50	112.86
1	H	47	ALA	N-CA-C	-8.49	102.69	112.87
1	C	292	THR	N-CA-C	-8.07	99.15	110.29
1	C	155	SER	N-CA-C	7.82	120.06	110.91
1	A	292	THR	N-CA-C	-7.78	99.55	110.29
1	C	173	VAL	N-CA-C	-7.78	98.86	107.73
1	F	46	ARG	N-CA-C	-7.78	102.48	110.97
1	F	292	THR	N-CA-C	-7.78	99.94	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	76	ILE	N-CA-C	-7.62	106.06	113.53
1	C	198	GLU	N-CA-C	-7.58	102.36	111.69
1	G	198	GLU	N-CA-C	-7.48	102.81	112.23
1	H	93	MSE	N-CA-C	-7.48	103.21	111.36
1	D	60	ASP	N-CA-C	-7.40	95.05	110.80
1	A	171	LEU	N-CA-C	-7.38	104.31	112.72
1	A	59	VAL	N-CA-C	-7.32	105.41	112.29
1	H	150	VAL	N-CA-C	7.22	119.22	108.46
1	H	59	VAL	N-CA-C	-7.22	102.46	112.50
1	F	171	LEU	N-CA-C	-7.13	102.89	112.94
1	D	115	CYS	N-CA-C	7.11	120.07	111.40
1	E	292	THR	N-CA-C	-6.98	101.28	110.07
1	A	115	CYS	N-CA-C	6.97	120.27	111.69
1	E	198	GLU	N-CA-C	-6.94	104.28	112.89
1	G	292	THR	N-CA-C	-6.73	101.00	110.29
1	C	202	GLU	N-CA-C	6.70	120.91	112.87
1	H	269	GLU	N-CA-C	-6.65	104.91	113.16
1	C	47	ALA	N-CA-C	-6.62	104.46	112.54
1	E	20	MSE	N-CA-C	6.62	119.89	109.96
1	B	92	ILE	N-CA-C	-6.53	102.90	112.04
1	A	114	LEU	N-CA-C	6.51	118.03	111.07
1	B	97	GLY	N-CA-C	-6.47	106.33	114.16
1	G	93	MSE	N-CA-C	-6.38	104.41	111.82
1	H	51	SER	N-CA-C	-6.36	105.65	113.41
1	E	54	GLU	N-CA-C	-6.25	104.57	111.82
1	C	60	ASP	N-CA-C	-6.24	97.51	110.80
1	A	198	GLU	N-CA-C	-6.20	103.83	112.45
1	H	96	ARG	N-CA-C	-6.16	104.65	111.36
1	D	54	GLU	N-CA-C	-6.15	104.57	111.28
1	G	58	GLY	N-CA-C	-6.08	107.98	114.67
1	G	44	GLY	N-CA-C	-6.03	106.27	113.99
1	B	198	GLU	N-CA-C	-6.02	105.01	112.90
1	E	58	GLY	N-CA-C	-6.01	98.93	113.18
1	D	292	THR	N-CA-C	-5.99	102.02	110.29
1	C	115	CYS	N-CA-C	5.94	121.19	113.88
1	G	75	PHE	N-CA-C	5.89	120.09	113.02
1	B	91	LYS	N-CA-C	-5.87	105.30	112.88
1	B	47	ALA	N-CA-C	-5.87	105.97	113.01
1	H	296	VAL	N-CA-C	5.87	116.65	110.72
1	C	150	VAL	N-CA-C	5.86	118.41	108.86
1	H	198	GLU	N-CA-C	-5.85	105.97	113.23
1	D	57	CYS	N-CA-C	-5.80	105.46	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	17	ASP	CA-C-N	5.80	125.66	119.28
1	H	17	ASP	C-N-CA	5.80	125.66	119.28
1	E	171	LEU	N-CA-C	-5.76	105.84	112.92
1	E	202	GLU	N-CA-C	5.69	119.03	111.75
1	F	129	ALA	CB-CA-C	-5.69	109.02	115.79
1	A	270	HIS	N-CA-C	5.63	117.70	109.30
1	H	202	GLU	N-CA-C	5.63	119.25	112.38
1	E	89	CYS	N-CA-C	-5.63	106.31	112.72
1	H	288	LEU	N-CA-C	-5.61	105.78	113.30
1	E	88	LYS	N-CA-C	-5.60	106.77	113.21
1	C	139	GLU	N-CA-C	-5.49	105.19	111.07
1	H	171	LEU	N-CA-C	-5.49	104.84	113.02
1	A	13	GLN	N-CA-C	-5.48	105.31	111.28
1	E	206	ILE	N-CA-C	5.45	116.21	108.42
1	H	252	TYR	N-CA-C	5.45	118.94	110.17
1	E	96	ARG	N-CA-C	-5.41	105.30	111.14
1	A	54	GLU	N-CA-C	-5.39	105.31	111.14
1	H	182	ALA	N-CA-C	5.39	119.84	113.16
1	C	207	ILE	N-CA-C	-5.36	100.67	108.17
1	G	109	ASN	N-CA-C	5.34	116.78	111.07
1	G	115	CYS	N-CA-C	5.33	120.80	113.97
1	D	171	LEU	N-CA-C	-5.30	106.83	113.72
1	B	205	GLY	N-CA-C	-5.30	103.88	112.31
1	G	55	THR	N-CA-C	-5.30	105.59	111.36
1	C	144	ALA	N-CA-C	-5.28	106.69	113.02
1	E	150	VAL	N-CA-C	5.28	116.26	108.45
1	E	133	VAL	N-CA-C	5.27	116.04	110.72
1	E	51	SER	N-CA-C	-5.26	106.81	113.18
1	F	68	GLY	N-CA-C	-5.26	106.39	112.50
1	A	106	LEU	N-CA-C	-5.22	106.86	114.12
1	B	46	ARG	N-CA-C	-5.22	106.76	113.23
1	C	196	GLY	N-CA-C	-5.22	105.42	112.57
1	H	294	SER	N-CA-C	5.21	116.96	111.28
1	B	230	ALA	N-CA-C	5.21	117.00	108.76
1	E	201	VAL	N-CA-C	5.21	115.73	110.05
1	B	129	ALA	CB-CA-C	-5.17	109.64	115.79
1	B	89	CYS	N-CA-C	-5.11	107.00	113.18
1	E	57	CYS	N-CA-C	-5.11	107.33	113.21
1	B	243	GLN	N-CA-C	5.10	117.50	111.33
1	C	168	LEU	N-CA-C	-5.10	105.90	111.82
1	E	185	TYR	N-CA-C	5.10	116.92	111.36
1	B	251	LYS	N-CA-C	5.08	117.94	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	13	GLN	N-CA-C	-5.07	105.45	111.69
1	D	241	LEU	N-CA-C	-5.06	107.49	113.97
1	H	292	THR	N-CA-C	-5.05	103.67	109.93
1	G	54	GLU	N-CA-C	-5.04	105.88	112.23
1	F	287	ASP	N-CA-C	-5.04	107.08	113.18
1	B	57	CYS	N-CA-C	-5.03	105.71	111.14

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	126	0
1	B	2180	0	2265	116	0
1	C	2282	0	2365	148	0
1	D	2255	0	2336	148	0
1	E	2211	0	2291	159	0
1	F	2221	0	2311	131	0
1	G	2200	0	2285	151	0
1	H	2208	0	2293	161	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	28	0	0	3	0
4	H	15	0	0	1	0
All	All	17958	0	18393	1063	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 29.

All (1063) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:92:ILE:H	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
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:HD23	1:H:78:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:57:CYS:C	1:E:59:VAL:H	1.87	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:H:42:ILE:HD12	1:H:46:ARG:HG2	1.65	0.78
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:B:266:LEU:HD23	1:H:175:VAL:H	1.50	0.76
1:C:6:LEU:CD1	1:C:53:ILE:HG13	2.16	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:D:267:LYS:C	1:D:269:GLU:H	1.94	0.75
1:H:40:GLU:HG3	1:H:88:LYS:HG3	1.67	0.75
1:C:78:LEU:C	1:C:80:SER:H	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:CYS:C	1:A:59:VAL:H	1.97	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:HA	1:F:253:LYS:HE3	1.71	0.71
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:42:ILE:HG12	1:C:43:GLN:N	2.04	0.70
1:H:88:LYS:HZ3	1:H:88:LYS:N	1.89	0.70
1:D:184:GLY:H	1:E:214:GLN:HE21	1.37	0.70
1:D:187:MSE:HE3	1:D:190:ALA:HB3	1.73	0.70
1:H:56:LEU:C	1:H:58:GLY:H	1.99	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:A:43:GLN:C	1:A:45:LEU:H	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:6:LEU:HD11	1:D:53:ILE:HB	1.73	0.69
1:D:193:VAL:HG11	1:D:215:MSE:HE3	1.73	0.69
1:H:89:CYS:O	1:H:92:ILE:HG23	1.92	0.69
1:C:12:SER:HA	1:C:15:LYS:HD3	1.74	0.69
1:H:90:LYS:C	1:H:92:ILE:H	2.01	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:HG2	1:C:28:ARG:HH11	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:E:304:TYR:C	1:E:306:ALA:H	2.00	0.68
1:H:46:ARG:HG2	1:H:46:ARG:HH11	1.59	0.68
1:E:89:CYS:C	1:E:91:LYS:H	2.01	0.68
1:C:301:ILE:O	1:C:305:LEU:HG	1.93	0.68
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: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:B:132:ARG:HG2	2:B:502:SO4:O4	1.95	0.66
1:B:188:GLU:HA	1:B:222:GLN:NE2	2.11	0.66
1:E:1:MSE:HE3	1:E:36:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:H:28:ARG:HG3	1.59	0.66
1:G:297:SER:O	1:G:301:ILE:HG22	1.95	0.66
1:A:46:ARG:HB3	1:A:90:LYS:HZ3	1.61	0.66
1:H:55:THR:HG23	1:H:56:LEU:H	1.61	0.66
1:E:104:ILE:C	1:E:104:ILE:HD12	2.21	0.65
1:H:25:ALA:O	1:H:29:THR:HG23	1.96	0.65
1:B:114:LEU:CD2	1:D:117:THR:HG21	2.26	0.65
1:C:33:PHE:HZ	1:C:49:LEU:HG	1.60	0.65
1:H:113:ASP:C	1:H:115:CYS:H	2.02	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:90:LYS:O	1:H:93:MSE:HG3	1.97	0.65
1:H:201:VAL:CG1	1:H:240:PRO:HD2	2.26	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:B:44:GLY:C	1:B:45:LEU:HD12	2.21	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:A:269:GLU:HG3	1:C:176:THR:HG21	1.79	0.63
1:A:286:THR:HG23	1:A:288:LEU:N	2.13	0.63
1:C:4:LYS:O	1:C:8:GLU:HG3	1.97	0.63
1:A:92:ILE:HD12	1:A:92:ILE:N	2.03	0.63
1:C:60:ASP:C	1:C:62:SER:H	2.07	0.63
1:E:114:LEU:HD11	1:E:289:GLY:HA2	1.80	0.63
1:H:169:CYS:C	1:H:171:LEU:H	2.07	0.63
1:E:87:SER:C	1:E:89:CYS:H	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:ASP:C	1:G:62:SER:H	2.04	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:HD22	1:B:48:ASN:N	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:G:56:LEU:C	1:G:58:GLY:H	2.05	0.62
1:A:43:GLN:C	1:A:45:LEU:N	2.56	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:HB3	1:G:136:ARG:CZ	2.30	0.62
1:A:6:LEU:C	1:A:8:GLU:H	2.06	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
1:E:50:THR:O	1:E:54:GLU:HG3	1.99	0.61
1:F:58:GLY:C	1:F:60:ASP:H	2.08	0.61
1:B:33:PHE:CE1	1:B:53:ILE:HG12	2.35	0.61
1:F:1:MSE:HE2	1:F:5:GLU:C	2.25	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:C:86:TYR:CD1	1:C:87:SER:N	2.69	0.61
1:D:45:LEU:O	1:D:49:LEU:HG	2.00	0.61
1:D:187:MSE:CE	1:D:190:ALA:HB3	2.30	0.61
1:G:92:ILE:C	1:G:92:ILE:HD12	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:ILE:HB	1:H:46:ARG:HB3	1.82	0.61
1:E:57:CYS:C	1:E:59:VAL:N	2.58	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: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:E:56:LEU:C	1:E:58:GLY:H	2.07	0.61
1:F:90:LYS:HD2	1:F:90:LYS:C	2.26	0.60
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:E:78:LEU:HA	1:E:90:LYS:HZ1	1.66	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:176:THR:OG1	1:G:267:LYS:HE3	2.00	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: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:53:ILE:CA	1:F:56:LEU:HD12	2.21	0.59
1:F:108:ARG:HH11	1:F:136:ARG:NH1	1.99	0.59
1:A:45:LEU:O	1:A:49:LEU:HG	2.03	0.59
1:A:46:ARG:CB	1:A:90:LYS:HZ3	2.16	0.59
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:B:87:SER:C	1:B:89:CYS:H	2.10	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

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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	0.59
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:F:92:ILE:C	1:F:92:ILE:HD12	2.27	0.59
1:H:42:ILE:O	1:H:43:GLN:C	2.45	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:C:50:THR:C	1:C:53:ILE:HG22	2.27	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:D:92:ILE:C	1:D:92:ILE:HD12	2.28	0.59
1:A:90:LYS:HG3	1:A:93:MSE:SE	2.53	0.59
1:A:124:THR:HG21	1:A:189:LYS:O	2.03	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:56:LEU:O	1:D:59:VAL:HG23	2.03	0.58
1:D:214:GLN:HE22	1:E:183:VAL:H	1.51	0.58
1:C:59:VAL:HG23	1:C:59:VAL:O	2.02	0.58
1:C:188:GLU:HA	1:C:222:GLN:HE22	1.68	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:HH11	1:D:28:ARG:HG2	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:H:46:ARG:C	1:H:48:ASN:H	2.12	0.58
1:A:46:ARG:HD2	1:A:46:ARG:N	2.19	0.58
1:B:59:VAL:HG13	1:B:59:VAL:O	2.02	0.58
1:B:187:MSE:CE	1:B:190:ALA:HB3	2.33	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: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:HG3	1:G:108:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:56:LEU:C	1:A:58:GLY:H	2.12	0.57
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:20:MSE:CE	1:C:28:ARG:HE	2.17	0.57
1:C:201:VAL:CG1	1:C:240:PRO:HD2	2.34	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:D:50:THR:HA	1:D:53:ILE:HD11	1.85	0.57
1:G:43:GLN:C	1:G:45:LEU:N	2.62	0.57
1:H:31:LEU:HD11	1:H:98:GLU:HG2	1.86	0.57
1:H:105:SER:C	1:H:106:LEU:HD12	2.30	0.57
1:A:172:ASN:C	1:C:264:GLN:N	2.63	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:86:TYR:HD1	1:C:87:SER:N	2.02	0.57
1:C:139:GLU:O	1:C:142:VAL:HG22	2.03	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:A:53:ILE:HA	1:A:56:LEU:HD12	1.86	0.56
1:B:38:LYS:HZ3	1:B:91:LYS:HE3	1.68	0.56
1:G:45:LEU:CD2	1:G:49:LEU:HD12	2.35	0.56
1:H:40:GLU:C	1:H:42:ILE:N	2.59	0.56
1:H:232:SER:N	1:H:287:ASP:OD1	2.38	0.56
1:A:1:MSE:HG3	1:A:36:ARG:CG	2.35	0.56
1:A:7:ILE:O	1:A:7:ILE:HG22	2.05	0.56
1:B:43:GLN:HG2	1:B:44:GLY:N	2.19	0.56
1:B:135:LEU:O	1:B:139:GLU:HG3	2.04	0.56
1:E:4:LYS:O	1:E:8:GLU:HG3	2.04	0.56
1:E:201:VAL:HG11	1:E:240:PRO:HD2	1.86	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: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:1:MSE:HG3	1:F:5:GLU:HB3	1.87	0.56
1:H:46:ARG:C	1:H:46:ARG:HD2	2.31	0.56
1:H:51:SER:C	1:H:53:ILE:H	2.14	0.56
1:E:27:ILE:HD11	1:E:101:LEU:HD13	1.87	0.56
1:F:144:ALA:O	1:F:145:LYS:HB2	2.04	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:B:45:LEU:HB3	1:B:48:ASN:CG	2.30	0.56
1:H:150:VAL:O	1:H:175:VAL:HA	2.06	0.56
1:G:60:ASP:C	1:G:62:SER:N	2.64	0.55
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:A:37:ASP:CG	1:A:38:LYS:H	2.14	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:73:LEU:C	1:E:73:LEU:HD23	2.32	0.55
1:E:76:ILE:HG13	1:E:76:ILE:O	2.05	0.55
1:G:2:ASP:O	1:G:3:ASP:C	2.50	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:C:294:SER:HB2	1:E:239:PHE:CD2	2.41	0.55
1:D:266:LEU:HB3	1:D:268:GLU:HB2	1.89	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:D:267:LYS:C	1:D:269:GLU:N	2.59	0.55
1:F:125:ILE:HG12	1:F:192:LEU:HD21	1.87	0.55
1:G:54:GLU:OE1	1:G:73:LEU:HD12	2.07	0.55
1:G:246:VAL:HB	1:G:251:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:GLU:HB2	1:C:90:LYS:NZ	2.22	0.54
1:C:252:TYR:O	1:C:253:LYS:HB2	2.07	0.54
1:D:89:CYS:C	1:D:91:LYS:H	2.14	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: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:D:78:LEU:HB3	1:D:96:ARG:HH12	1.73	0.54
1:D:133:VAL:CG2	1:D:229:VAL:HG23	2.38	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:F:57:CYS:C	1:F:59:VAL:H	2.16	0.54
1:H:192:LEU:N	1:H:192:LEU:HD23	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:A:266:LEU:HD13	1:C:174:PRO:HB3	1.89	0.54
1:B:153:THR:O	1:B:161:GLY:HA3	2.08	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:HH11	1:F:237:ARG:HG3	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:56:LEU:HD13	1:D:56:LEU:C	2.33	0.53
1:D:269:GLU:HB2	1:E:178:VAL:HG12	1.90	0.53
1:E:90:LYS:C	1:E:92:ILE:H	2.14	0.53
1:F:300:LEU:C	1:F:300:LEU:HD23	2.33	0.53
1:E:304:TYR:C	1:E:306:ALA:N	2.66	0.53
1:B:9:TYR:HD2	1:B:29:THR:HG22	1.73	0.53
1:F:57:CYS:C	1:F:59:VAL:N	2.63	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:6:LEU:C	1:A:8:GLU:N	2.66	0.53
1:E:46:ARG:C	1:E:48:ASN:H	2.15	0.53
1:A:27:ILE:HD13	1:A:100:PHE:HE1	1.73	0.53
1:A:103:ARG:NH2	1:A:287:ASP:OD2	2.42	0.53
1:A:267:LYS:HD3	1:C:175:VAL:O	2.08	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: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:B:300:LEU:HD23	1:B:300:LEU:C	2.33	0.53
1:E:37:ASP:C	1:E:40:GLU:HG3	2.34	0.53
1:E:192:LEU:N	1:E:192:LEU:HD23	2.23	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:37:ASP:C	1:G:46:ARG:HH12	2.17	0.52
1:A:125:ILE:HG12	1:A:192:LEU:HD21	1.91	0.52
1:A:266:LEU:HD23	1:C:176:THR:OG1	2.09	0.52
1:B:46:ARG:HH11	1:B:49:LEU:HD11	1.75	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:6:LEU:HD13	1:H:53:ILE:HB	1.90	0.52
1:H:19:ASP:O	1:H:108:ARG:NH2	2.42	0.52
1:A:30:LEU:HD22	1:A:53:ILE:HD11	1.92	0.52
1:A:31:LEU:HD21	1:A:98:GLU:HG2	1.91	0.52
1:A:210:ILE:HD13	1:A:271:PRO:HG2	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:E:195:VAL:CG1	1:E:196:GLY:N	2.71	0.52
1:G:53:ILE:HD12	1:G:53:ILE:C	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HD2	1:C:136:ARG:CZ	2.40	0.52
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:113:ASP:C	1:H:115:CYS:N	2.68	0.52
1:G:6:LEU:CD1	1:G:53:ILE:HB	2.39	0.52
1:G:220:LYS:HE3	1:G:279:SER:O	2.09	0.52
1:H:56:LEU:C	1:H:58:GLY:N	2.68	0.52
1:A:186:ILE:HD11	1:A:189:LYS:HD2	1.91	0.52
1:H:104:ILE:HG13	1:H:104:ILE:O	2.09	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:B:266:LEU:CD2	1:H:174:PRO:HA	2.40	0.51
1:D:57:CYS:C	1:D:59:VAL:H	2.18	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: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:E:208:ASN:O	1:E:209:LYS:C	2.53	0.51
1:H:90:LYS:C	1:H:92:ILE:N	2.67	0.51
1:F:23:ALA:HB3	1:F:233:PHE:CE1	2.45	0.51
1:A:57:CYS:C	1:A:59:VAL:N	2.66	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:267:LYS:O	1:G:176:THR:HA	2.11	0.51
1:F:286:THR:CG2	1:F:287:ASP:H	2.22	0.51
1:G:43:GLN:C	1:G:43:GLN:OE1	2.53	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:88:LYS:HD3	1:D:88:LYS:C	2.36	0.51
1:F:253:LYS:HD3	1:F:269:GLU:HA	1.93	0.51
1:C:78:LEU:C	1:C:80:SER:N	2.61	0.51
1:H:133:VAL:O	1:H:137:VAL:HG23	2.10	0.51
1:G:24:VAL:HG22	1:G:104:ILE:HD12	1.93	0.51
1:D:50:THR:HA	1:D:53:ILE:CD1	2.41	0.50
1:D:268:GLU:O	1:D:268:GLU:HG2	2.10	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:H:36:ARG:HG3	1:H:36:ARG:HH11	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:H	1:C:4:LYS:HD3	1.77	0.50
1:G:72:PHE:HD1	1:G:100:PHE:CD1	2.29	0.50
1:H:40:GLU:C	1:H:42:ILE:H	2.19	0.50
1:H:304:TYR:C	1:H:306:ALA:N	2.68	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:41:THR:HG23	1:F:42:ILE:N	2.27	0.50
1:F:271:PRO:HG3	1:G:185:TYR:CE2	2.46	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:G:142:VAL:C	1:G:144:ALA:H	2.20	0.50
1:H:203:ASN:HB3	1:H:239:PHE:CE1	2.47	0.50
1:B:101:LEU:O	1:B:101:LEU:HD23	2.11	0.50
1:D:165:ALA:HB1	1:E:266:LEU:HD11	1.94	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:33:PHE:CD1	1:C:53:ILE:HD12	2.47	0.49
1:C:192:LEU:N	1:C:192:LEU:HD23	2.27	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:56:LEU:C	1:G:58:GLY:N	2.69	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:51:SER:C	1:D:53:ILE:H	2.20	0.49
1:D:78:LEU:CD2	1:D:92:ILE:HD11	2.43	0.49
1:G:46:ARG:CZ	1:G:91:LYS:HE3	2.43	0.49
1:E:50:THR:HA	1:E:53:ILE:HG12	1.93	0.49
1:E:110:LYS:O	1:E:114:LEU:HB2	2.12	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:46:ARG:HB3	1:A:90:LYS:NZ	2.25	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:9:TYR:CE1	1:F:32:GLU:HG2	2.47	0.49
1:F:12:SER:HA	1:F:15:LYS:HB3	1.94	0.49
1:G:135:LEU:O	1:G:139:GLU:HG3	2.11	0.49
1:H:3:ASP:CG	1:H:56:LEU:HD13	2.38	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:H:78:LEU:HB3	1:H:96:ARG:NH1	2.28	0.49
1:H:120:LYS:HE3	1:H:123:ALA:HB2	1.95	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:54:GLU:OE1	1:A:73:LEU:HD11	2.12	0.49
1:A:271:PRO:HG3	1:C:185:TYR:CE2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ARG:HG2	1:C:28:ARG:NH1	2.28	0.49
1:D:42:ILE:HG12	1:D:45:LEU:CG	2.43	0.49
1:D:269:GLU:CG	1:E:176:THR:HG21	2.42	0.49
1:E:301:ILE:C	1:E:301:ILE:HD12	2.37	0.49
1:F:42:ILE:HG23	1:F:45:LEU:H	1.77	0.49
1:G:43:GLN:C	1:G:45:LEU:H	2.19	0.49
1:E:70:GLU:HG2	1:E:74:ARG:HE	1.78	0.48
1:E:300:LEU:HD21	1:E:304:TYR:CE2	2.48	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:43:GLN:O	1:E:43:GLN:NE2	2.46	0.48
1:F:6:LEU:HD11	1:F:53:ILE:CG2	2.44	0.48
1:F:59:VAL:O	1:F:59:VAL:HG13	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:D:19:ASP:O	1:D:108:ARG:NH2	2.47	0.48
1:G:142:VAL:C	1:G:144:ALA:N	2.67	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:C:300:LEU:HD23	1:C:300:LEU:C	2.39	0.48
1:D:57:CYS:C	1:D:59:VAL:N	2.72	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:B:73:LEU:HD22	1:B:73:LEU:O	2.14	0.48
1:G:38:LYS:HG2	1:G:91:LYS:NZ	2.29	0.48
1:G:158:ASP:OD1	1:G:160:SER:HB3	2.14	0.48
1:H:28:ARG:HH11	1:H:28:ARG:CG	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:C:300:LEU:O	1:C:303:LEU:HB3	2.13	0.48
1:E:34:LEU:C	1:E:34:LEU:HD23	2.39	0.48
1:G:186:ILE:HD11	1:G:189:LYS:HD2	1.94	0.48
1:H:51:SER:C	1:H:53:ILE:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:O	1:A:38:LYS:C	2.55	0.48
1:G:45:LEU:O	1:G:49:LEU:HB2	2.14	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:H:42:ILE:C	1:H:44:GLY:N	2.70	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:G:236:VAL:HG22	1:G:237:ARG:N	2.28	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: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:F:188:GLU:OE1	1:G:242:ASN:HB2	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:H:106:LEU:HD12	1:H:106:LEU:N	2.28	0.47
1:A:305:LEU:O	1:A:306:ALA:C	2.55	0.47
1:F:113:ASP:HB3	4:F:1065:HOH:O	2.13	0.47
1:H:42:ILE:HB	1:H:46:ARG:CB	2.43	0.47
1:H:142:VAL:HG23	1:H:143:ALA:N	2.29	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:B:184:GLY:HA3	1:H:213:ASN:ND2	2.28	0.47
1:B:211:GLY:HA2	1:H:181:ALA:O	2.14	0.47
1:C:121:ASP:OD1	1:C:147:ARG:N	2.38	0.47
1:D:31:LEU:HD11	1:D:98:GLU:HG3	1.95	0.47
1:D:108:ARG:HD3	1:D:136:ARG:HG3	1.97	0.47
1:D:214:GLN:NE2	1:E:184:GLY:H	2.02	0.47
1:E:56:LEU:C	1:E:58:GLY:N	2.73	0.47
1:E:113:ASP:O	1:E:116:HIS:HD2	1.98	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: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:32:GLU:O	1:A:35:LYS:HB2	2.15	0.47
1:A:201:VAL:HB	1:A:238:LEU:O	2.14	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:O	1:H:119:ILE:HG22	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

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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: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:A:54:GLU:OE1	1:A:73:LEU:HD21	2.15	0.47
1:A:300:LEU:HD23	1:A:300:LEU:O	2.15	0.47
1:B:93:MSE:O	1:B:94:ILE:C	2.58	0.47
1:C:46:ARG:HH21	1:C:46:ARG:CG	2.27	0.47
1:H:27:ILE:HD12	1:H:104:ILE:HD11	1.96	0.47
1:C:9:TYR:CE2	1:C:29:THR:HA	2.50	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:F:15:LYS:C	1:F:17:ASP:H	2.23	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:F:47:ALA:C	1:F:50:THR:HG22	2.39	0.47
1:G:36:ARG:HG3	1:G:36:ARG:HH11	1.80	0.47
1:C:3:ASP:O	1:C:6:LEU:HB2	2.15	0.46
1:C:45:LEU:O	1:C:46:ARG:HB3	2.15	0.46
1:D:78:LEU:HD23	1:D:92:ILE:HD11	1.97	0.46
1:D:150:VAL:HG12	1:D:151:TYR:N	2.30	0.46
1:F:34:LEU:O	1:F:37:ASP:HB3	2.15	0.46
1:A:181:ALA:O	1:C:211:GLY:HA2	2.15	0.46
1:B:195:VAL:HG12	1:B:196:GLY:O	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:90:LYS:C	1:G:92:ILE:H	2.23	0.46
1:G:101:LEU:HD12	1:G:101:LEU:O	2.15	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:G:58:GLY:C	1:G:60:ASP:N	2.73	0.46
1:H:2:ASP:H	1:H:5:GLU:HB2	1.80	0.46
1:H:42:ILE:HD12	1:H:46:ARG:CG	2.41	0.46
1:H:87:SER:C	1:H:88:LYS:HZ3	2.24	0.46
1:B:70:GLU:O	1:B:74:ARG:HG3	2.15	0.46
1:D:286:THR:HG22	1:D:287:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:LYS:HD2	1:G:287:ASP:HB2	1.97	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:H:114:LEU:HD13	1:H:114:LEU:O	2.15	0.46
1:A:8:GLU:O	1:A:9:TYR:C	2.59	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:B:46:ARG:C	1:B:48:ASN:H	2.24	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:D:33:PHE:CD1	1:D:33:PHE:C	2.93	0.46
1:E:46:ARG:HG3	1:E:46:ARG:HH11	1.81	0.46
1:A:33:PHE:CE2	1:A:53:ILE:HG21	2.51	0.46
1:B:60:ASP:O	1:B:61:SER:C	2.58	0.46
1:B:186:ILE:CD1	1:B:189:LYS:HD2	2.46	0.46
1:F:74:ARG:C	1:F:76:ILE:H	2.24	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: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:HG12	2.41	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:A:185:TYR:C	1:A:185:TYR:CD2	2.93	0.45
1:C:306:ALA:O	1:C:307:ALA:C	2.59	0.45
1:F:251:LYS:C	1:F:252:TYR:HD1	2.25	0.45
1:H:169:CYS:C	1:H:171:LEU:N	2.73	0.45
1:B:6:LEU:HD21	1:B:53:ILE:HG23	1.97	0.45
1:B:267:LYS:CG	1:B:268:GLU:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:294:SER:HB3	1:E:241:LEU:HD11	1.99	0.45
1:D:86:TYR:O	1:D:90:LYS:HG3	2.17	0.45
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:2:ASP:O	1:D:5:GLU:HB2	2.16	0.45
1:D:214:GLN:NE2	1:E:183:VAL:HB	2.32	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:D:92:ILE:C	1:D:92:ILE:CD1	2.89	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:D:20:MSE:CE	1:D:28:ARG:HE	2.30	0.45
1:D:46:ARG:NH2	1:D:91:LYS:HZ2	2.14	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:F:34:LEU:C	1:F:34:LEU:HD23	2.41	0.45
1:G:13:GLN:HE22	1:G:28:ARG:HD3	1.82	0.45
1:H:45:LEU:HD13	1:H:45:LEU:C	2.41	0.45
1:B:266:LEU:CD2	1:H:175:VAL:H	2.24	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:O	1:E:88:LYS:HG3	2.17	0.45
1:H:40:GLU:HA	1:H:42:ILE:CG1	2.41	0.45
1:C:4:LYS:HD3	1:C:4:LYS:N	2.32	0.45
1:F:12:SER:HA	1:F:15:LYS:HB2	1.99	0.45
1:F:108:ARG:HD3	1:F:136:ARG:CG	2.44	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:D:264:GLN:CD	1:E:172:ASN:HA	2.42	0.44
1:E:58:GLY:C	1:E:60:ASP:H	2.23	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:B:48:ASN:N	1:B:48:ASN:ND2	2.60	0.44
1:B:51:SER:C	1:B:53:ILE:H	2.24	0.44
1:E:44:GLY:O	1:E:48:ASN:HB3	2.16	0.44
1:D:183:VAL:HB	1:E:214:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLU:OE1	1:E:242:ASN:HB2	2.17	0.44
1:E:107:SER:O	1:E:108:ARG:C	2.60	0.44
1:F:90:LYS:C	1:F:90:LYS:CD	2.91	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:C:42:ILE:O	1:C:46:ARG:HG2	2.18	0.44
1:D:297:SER:O	1:D:301:ILE:HG13	2.17	0.44
1:E:34:LEU:HD23	1:E:34:LEU:O	2.17	0.44
1:E:48:ASN:CG	1:E:49:LEU:N	2.72	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:E:33:PHE:CD1	1:E:33:PHE:C	2.96	0.44
1:G:92:ILE:C	1:G:92:ILE:CD1	2.89	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:D:78:LEU:C	1:D:78:LEU:HD12	2.42	0.44
1:F:33:PHE:CD1	1:F:33:PHE:C	2.96	0.44
1:H:135:LEU:O	1:H:139:GLU:HG3	2.17	0.44
1:B:87:SER:C	1:B:89:CYS:N	2.75	0.44
1:E:45:LEU:HA	1:E:48:ASN:HD22	1.83	0.44
1:E:96:ARG:HH11	1:E:96:ARG:CG	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:B:266:LEU:HB3	1:H:175:VAL:O	2.18	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:H:128:HIS:HB2	1:H:215:MSE:CE	2.47	0.44
1:A:300:LEU:HD23	1:A:300:LEU:C	2.43	0.43
1:C:24:VAL:HG22	1:C:104:ILE:CD1	2.48	0.43
1:C:86:TYR:CD1	1:C:86:TYR:C	2.96	0.43
1:F:88:LYS:C	1:F:90:LYS:N	2.74	0.43
1:F:237:ARG:HG3	1:F:237:ARG:NH1	2.33	0.43
1:G:269:GLU:C	1:G:271:PRO:HD3	2.43	0.43
1:H:304:TYR:C	1:H:306:ALA:H	2.25	0.43
1:B:90:LYS:O	1:B:93:MSE:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:46:ARG:C	1:E:48:ASN:N	2.73	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:B:181:ALA:O	1:H:211:GLY:HA2	2.19	0.43
1:C:60:ASP:C	1:C:62:SER:N	2.72	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:C:74:ARG:NH2	1:E:305:LEU:HD13	2.34	0.43
1:E:2:ASP:CG	1:E:3:ASP:N	2.75	0.43
1:F:6:LEU:HD21	1:F:33:PHE:HD2	1.82	0.43
1:A:28:ARG:HH21	1:A:101:LEU:HD21	1.83	0.43
1:A:49:LEU:O	1:A:53:ILE:HG23	2.18	0.43
1:A:94:ILE:O	1:A:94:ILE:HG22	2.17	0.43
1:A:214:GLN:OE1	1:C:183:VAL:HB	2.18	0.43
1:E:53:ILE:HG22	1:E:56:LEU:CD1	2.45	0.43
1:F:37:ASP:O	1:F:37:ASP:CG	2.61	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:46:ARG:C	1:B:48:ASN:N	2.76	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:A:30:LEU:O	1:A:31:LEU:C	2.62	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: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:61:SER:HB2	1:G:249:LYS:O	2.18	0.43
1:G:133:VAL:HG11	1:G:229:VAL:HG12	2.01	0.43
1:G:209:LYS:O	1:G:210:ILE:C	2.62	0.43
1:H:55:THR:CG2	1:H:56:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:THR:O	1:H:293:PRO:C	2.61	0.43
1:B:57:CYS:O	1:B:58:GLY:C	2.62	0.43
1:B:179:LEU:HD22	1:H:270:HIS:HD2	1.84	0.43
1:C:27:ILE:HD11	1:C:101:LEU:HG	2.01	0.43
1:C:38:LYS:HZ1	1:C:88:LYS:HG2	1.83	0.43
1:E:292:THR:O	1:E:293:PRO:C	2.62	0.43
1:G:1:MSE:HE1	1:G:9:TYR:HB2	2.01	0.43
1:H:36:ARG:HH11	1:H:36:ARG:CG	2.32	0.43
1:D:187:MSE:HE3	1:D:187:MSE:O	2.19	0.42
1:F:42:ILE:CD1	1:F:43:GLN:HG2	2.49	0.42
1:F:248:ASP:O	1:F:249:LYS:C	2.62	0.42
1:G:69:GLY:O	1:G:73:LEU:HB2	2.18	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:H:23:ALA:HB3	1:H:233:PHE:CE1	2.54	0.42
1:A:56:LEU:C	1:A:58:GLY:N	2.75	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:D:168:LEU:O	1:D:173:VAL:HG13	2.19	0.42
1:G:79:ALA:CB	1:G:90:LYS:HG3	2.49	0.42
1:G:197:ALA:O	1:G:234:LYS:HD3	2.19	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
1:C:197:ALA:O	1:C:234:LYS:HD3	2.18	0.42
1:D:46:ARG:NH2	1:D:91:LYS:HZ3	2.16	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:O	1:G:16:GLU:HG2	2.18	0.42
1:A:17:ASP:C	1:A:17:ASP:OD1	2.61	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:HE2	1:H:4:LYS:HB3	1.71	0.42
1:C:82:GLU:HB2	1:C:90:LYS:HZ1	1.83	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:D:266:LEU:O	1:E:177:VAL:N	2.42	0.42
1:G:153:THR:O	1:G:161:GLY:HA3	2.20	0.42
1:B:113:ASP:HA	1:B:116:HIS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:PHE:C	1:C:33:PHE:CD2	2.97	0.42
1:D:49:LEU:C	1:D:51:SER:H	2.26	0.42
1:D:305:LEU:O	1:D:306:ALA:C	2.62	0.42
1:E:301:ILE:O	1:E:305:LEU:HG	2.19	0.42
1:F:58:GLY:C	1:F:60:ASP:N	2.78	0.42
1:G:90:LYS:O	1:G:93:MSE:HG3	2.20	0.42
1:H:114:LEU:O	1:H:114:LEU:HD22	2.20	0.42
1:B:156:GLN:HB3	1:B:157:PRO:HA	2.01	0.42
1:C:77:SER:O	1:C:78:LEU:HD23	2.20	0.42
1:C:119:ILE:O	1:C:146:LYS:HD3	2.20	0.42
1:C:301:ILE:HG13	1:C:302:LYS:N	2.32	0.42
1:F:130:TYR:HB2	1:F:160:SER:HB2	2.01	0.42
1:G:300:LEU:C	1:G:300:LEU:HD23	2.44	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:H:103:ARG:C	1:H:105:SER:H	2.26	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:D:91:LYS:O	1:D:91:LYS:CG	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: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:89:CYS:C	1:D:91:LYS:N	2.78	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:F:15:LYS:C	1:F:17:ASP:N	2.78	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
1:H:203:ASN:HB3	1:H:239:PHE:CZ	2.55	0.42
1:C:46:ARG:CG	1:C:46:ARG:NH2	2.82	0.42
1:C:138:LEU:HD12	1:C:168:LEU:HD21	2.02	0.42
1:G:232:SER:C	1:G:234:LYS:H	2.28	0.42
1:B:150:VAL:HG12	1:B:151:TYR:N	2.35	0.41
1:E:17:ASP:HB3	1:E:19:ASP:CG	2.45	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:G:301:ILE:C	1:G:303:LEU:H	2.27	0.41
1:A:9:TYR:CE2	1:A:32:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LYS:HE2	1:C:287:ASP:O	2.21	0.41
1:D:42:ILE:CD1	1:D:45:LEU:HG	2.50	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:E:303:LEU:C	1:E:303:LEU:HD23	2.46	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:HA	1:C:38:LYS:HD2	1.95	0.41
1:C:266:LEU:C	1:C:266:LEU:HD23	2.44	0.41
1:F:32:GLU:O	1:F:33:PHE:C	2.64	0.41
1:G:70:GLU:HG2	1:G:74:ARG:HD2	2.03	0.41
1:C:78:LEU:HD12	1:C:96:ARG:NE	2.36	0.41
1:C:142:VAL:CG2	1:C:143:ALA:N	2.83	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:28:ARG:NH1	1:H:28:ARG:CG	2.81	0.41
1:H:135:LEU:HD22	1:H:139:GLU:HG3	2.01	0.41
1:C:238:LEU:HD11	1:C:250:PHE:CE1	2.56	0.41
1:G:9:TYR:CE2	1:G:29:THR:HA	2.56	0.41
1:G:246:VAL:HA	1:G:247:PRO:HD3	1.95	0.41
1:H:87:SER:C	1:H:88:LYS:NZ	2.79	0.41
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.87	0.41
1:D:28:ARG:NH1	1:D:101:LEU:CD2	2.84	0.41
1:F:44:GLY:C	1:F:48:ASN:ND2	2.79	0.41
1:F:201:VAL:CG1	1:F:240:PRO:HD2	2.45	0.41
1:F:305:LEU:O	1:F:306:ALA:C	2.62	0.41
1:A:6:LEU:HD21	1:A:33:PHE:CD2	2.49	0.41
1:A:6:LEU:O	1:A:8:GLU:N	2.52	0.41
1:A:33:PHE:O	1:A:36:ARG:HB2	2.21	0.41
1:A:188:GLU:HA	1:A:222:GLN:NE2	2.32	0.41
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.87	0.41
1:B:32:GLU:CG	1:B:36:ARG:NH1	2.84	0.41
1:B:132:ARG:HG2	1:B:132:ARG:H	1.57	0.41
1:C:41:THR:HG21	1:C:45:LEU:HD12	2.03	0.41
1:C:242:ASN:OD1	1:C:242:ASN:C	2.64	0.41
1:D:48:ASN:HA	1:D:51:SER:HB3	2.02	0.41
1:E:21:ALA:O	1:E:22:SER:C	2.63	0.41
1:E:52:ALA:O	1:E:56:LEU:HG	2.21	0.41
1:E:126:LEU:HD12	1:E:151:TYR:O	2.20	0.41
1:F:186:ILE:CD1	1:F:189:LYS:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:PHE:O	1:G:37:ASP:HB2	2.21	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:G:286:THR:C	1:G:288:LEU:N	2.78	0.41
1:H:109:ASN:HD21	1:H:136:ARG:HE	1.69	0.41
1:A:14:MSE:HE3	1:A:22:SER:HA	2.02	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:G:301:ILE:C	1:G:303:LEU:N	2.77	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:C:86:TYR:HD1	1:C:86:TYR:C	2.28	0.40
1:D:142:VAL:CG2	1:D:143:ALA:N	2.84	0.40
1:G:144:ALA:O	1:G:145:LYS:HB2	2.20	0.40
1:G:214:GLN:H	1:G:214:GLN:HG2	1.72	0.40
1:H:3:ASP:O	1:H:4:LYS:C	2.64	0.40
1:H:43:GLN:HE22	1:H:87:SER:N	2.19	0.40
1:A:46:ARG:HB2	1:A:90:LYS:NZ	2.35	0.40
1:A:139:GLU:HG3	1:A:171:LEU:HD13	2.02	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:HA	1:G:31:LEU:HD23	1.82	0.40
1:G:35:LYS:C	1:G:37:ASP:N	2.79	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:E:40:GLU:O	1:E:41:THR:O	2.39	0.40
1:F:49:LEU:HD12	1:F:49:LEU:HA	1.88	0.40
1:G:78:LEU:HD21	1:G:307:ALA:C	2.45	0.40
1:A:6:LEU:HD13	1:A:53:ILE:HB	2.02	0.40
1:A:45:LEU:HD12	1:A:46:ARG:CZ	2.51	0.40
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.87	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:63:VAL:HG13	1:E:250:PHE:CG	2.57	0.40
1:E:197:ALA:O	1:E:234:LYS:HD3	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:C	1:A:36:ARG:H	2.29	0.40
1:B:37:ASP:OD2	1:B:46:ARG:HD2	2.21	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:232:SER:C	1:B:234:LYS:H	2.29	0.40
1:E:142:VAL:CG2	1:E:143:ALA:N	2.84	0.40
1:F:217:VAL:HG12	1:G:217:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/315 (86%)	251 (93%)	16 (6%)	4 (2%)	8	13
1	B	273/315 (87%)	252 (92%)	18 (7%)	3 (1%)	11	19
1	C	288/315 (91%)	264 (92%)	19 (7%)	5 (2%)	7	12
1	D	283/315 (90%)	258 (91%)	19 (7%)	6 (2%)	5	9
1	E	277/315 (88%)	254 (92%)	19 (7%)	4 (1%)	9	14
1	F	281/315 (89%)	257 (92%)	16 (6%)	8 (3%)	4	6
1	G	276/315 (88%)	254 (92%)	19 (7%)	3 (1%)	11	19
1	H	279/315 (89%)	253 (91%)	19 (7%)	7 (2%)	4	7
All	All	2228/2520 (88%)	2043 (92%)	145 (6%)	40 (2%)	6	11

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	SER
1	C	46	ARG
1	C	265	ASP

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	227 (96%)	10 (4%)	26	45
1	B	239/260 (92%)	223 (93%)	16 (7%)	15	25
1	C	250/260 (96%)	236 (94%)	14 (6%)	19	32
1	D	246/260 (95%)	228 (93%)	18 (7%)	13	22
1	E	243/260 (94%)	226 (93%)	17 (7%)	14	24
1	F	242/260 (93%)	225 (93%)	17 (7%)	14	24
1	G	240/260 (92%)	220 (92%)	20 (8%)	10	18
1	H	242/260 (93%)	225 (93%)	17 (7%)	14	24
All	All	1939/2080 (93%)	1810 (93%)	129 (7%)	15	25

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	92	ILE
1	A	101	LEU
1	A	106	LEU
1	A	120	LYS
1	A	135	LEU
1	A	149	SER
1	A	223	ASN
1	A	266	LEU
1	A	303	LEU
1	B	31	LEU
1	B	48	ASN
1	B	50	THR
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	193	VAL
1	B	195	VAL

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Mol	Chain	Res	Type
1	B	220	LYS
1	B	229	VAL
1	B	249	LYS
1	C	27	ILE
1	C	34	LEU
1	C	73	LEU
1	C	76	ILE
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	193	VAL
1	C	201	VAL
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
1	D	287	ASP
1	D	291	LEU
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

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Mol	Chain	Res	Type
1	E	92	ILE
1	E	96	ARG
1	E	98	GLU
1	E	114	LEU
1	E	117	THR
1	E	135	LEU
1	E	198	GLU
1	E	201	VAL
1	E	284	LEU
1	E	301	ILE
1	F	5	GLU
1	F	31	LEU
1	F	40	GLU
1	F	42	ILE
1	F	45	LEU
1	F	74	ARG
1	F	101	LEU
1	F	103	ARG
1	F	120	LYS
1	F	121	ASP
1	F	135	LEU
1	F	142	VAL
1	F	179	LEU
1	F	195	VAL
1	F	201	VAL
1	F	223	ASN
1	F	253	LYS
1	G	29	THR
1	G	34	LEU
1	G	43	GLN
1	G	49	LEU
1	G	60	ASP
1	G	73	LEU
1	G	78	LEU
1	G	106	LEU
1	G	109	ASN
1	G	117	THR
1	G	126	LEU
1	G	127	THR
1	G	135	LEU
1	G	136	ARG
1	G	142	VAL

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Mol	Chain	Res	Type
1	G	147	ARG
1	G	173	VAL
1	G	193	VAL
1	G	195	VAL
1	G	301	ILE
1	H	34	LEU
1	H	46	ARG
1	H	71	LEU
1	H	88	LYS
1	H	114	LEU
1	H	132	ARG
1	H	135	LEU
1	H	136	ARG
1	H	157	PRO
1	H	163	LYS
1	H	178	VAL
1	H	179	LEU
1	H	193	VAL
1	H	201	VAL
1	H	244	GLN
1	H	300	LEU
1	H	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	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

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Mol	Chain	Res	Type
1	E	116	HIS
1	E	213	ASN
1	E	214	GLN
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	507	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	F	510	-	4,4,4	0.40	0	6,6,6	0.13	0
2	SO4	A	501	-	4,4,4	0.38	0	6,6,6	0.15	0
2	SO4	E	505	-	4,4,4	0.35	0	6,6,6	0.15	0
2	SO4	H	508	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	A	509	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	B	502	-	4,4,4	0.34	0	6,6,6	0.18	0
2	SO4	F	506	-	4,4,4	0.36	0	6,6,6	0.23	0
2	SO4	C	503	-	4,4,4	0.37	0	6,6,6	0.12	0
2	SO4	D	504	-	4,4,4	0.33	0	6,6,6	0.09	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	A	501	SO4	4	0
2	H	508	SO4	1	0
2	B	502	SO4	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 ⓘ

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, 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	272/315 (86%)	0.06	20 (7%) 20 15	12, 34, 93, 112	0
1	B	274/315 (86%)	0.23	20 (7%) 21 15	17, 40, 103, 118	0
1	C	287/315 (91%)	0.21	29 (10%) 12 10	20, 41, 85, 107	0
1	D	284/315 (90%)	0.22	23 (8%) 18 13	19, 41, 83, 117	0
1	E	278/315 (88%)	0.35	23 (8%) 17 12	20, 46, 88, 113	0
1	F	280/315 (88%)	0.15	22 (7%) 18 14	18, 36, 82, 97	0
1	G	277/315 (87%)	0.41	22 (7%) 18 14	23, 46, 88, 97	0
1	H	278/315 (88%)	0.37	24 (8%) 16 12	21, 49, 95, 120	0
All	All	2230/2520 (88%)	0.25	183 (8%) 17 13	12, 41, 89, 120	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	307	ALA	5.5
1	F	254	ALA	5.2
1	E	307	ALA	5.0
1	A	90	LYS	4.8
1	D	59	VAL	4.6
1	C	45	LEU	4.5
1	C	264	GLN	4.5
1	E	54	GLU	4.5
1	E	78	LEU	4.3
1	C	81	LEU	4.3
1	A	45	LEU	4.2
1	F	89	CYS	4.2
1	A	266	LEU	4.2
1	D	254	ALA	4.1
1	C	307	ALA	4.0
1	D	86	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	61	SER	3.9
1	D	45	LEU	3.8
1	A	34	LEU	3.7
1	F	47	ALA	3.7
1	A	89	CYS	3.7
1	A	43	GLN	3.6
1	D	39	GLY	3.6
1	D	58	GLY	3.6
1	F	42	ILE	3.6
1	G	75	PHE	3.6
1	D	43	GLN	3.6
1	F	58	GLY	3.5
1	C	43	GLN	3.5
1	H	58	GLY	3.5
1	C	54	GLU	3.5
1	F	253	LYS	3.5
1	G	92	ILE	3.5
1	E	57	CYS	3.5
1	G	143	ALA	3.5
1	E	45	LEU	3.4
1	D	268	GLU	3.4
1	D	307	ALA	3.4
1	H	45	LEU	3.4
1	D	54	GLU	3.4
1	H	47	ALA	3.4
1	H	268	GLU	3.3
1	C	39	GLY	3.3
1	C	38	LYS	3.3
1	E	53	ILE	3.3
1	B	92	ILE	3.3
1	D	53	ILE	3.3
1	F	46	ARG	3.3
1	G	58	GLY	3.3
1	E	59	VAL	3.3
1	F	53	ILE	3.3
1	C	265	ASP	3.3
1	H	49	LEU	3.2
1	B	47	ALA	3.2
1	D	42	ILE	3.2
1	E	306	ALA	3.2
1	C	306	ALA	3.2
1	C	78	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLU	3.1
1	C	40	GLU	3.1
1	H	53	ILE	3.1
1	F	48	ASN	3.1
1	E	17	ASP	3.1
1	H	54	GLU	3.1
1	H	88	LYS	3.1
1	D	44	GLY	3.0
1	A	47	ALA	3.0
1	F	308	ALA	3.0
1	C	82	GLU	3.0
1	E	42	ILE	3.0
1	G	53	ILE	3.0
1	B	52	ALA	3.0
1	F	41	THR	2.9
1	D	46	ARG	2.9
1	B	87	SER	2.9
1	E	43	GLN	2.9
1	A	53	ILE	2.9
1	C	58	GLY	2.9
1	E	58	GLY	2.9
1	G	54	GLU	2.9
1	H	43	GLN	2.9
1	C	86	TYR	2.8
1	E	41	THR	2.8
1	D	91	LYS	2.8
1	C	92	ILE	2.8
1	C	47	ALA	2.8
1	C	79	ALA	2.8
1	D	76	ILE	2.7
1	A	54	GLU	2.7
1	D	255	ASP	2.7
1	D	87	SER	2.7
1	B	94	ILE	2.7
1	A	46	ARG	2.7
1	B	77	SER	2.7
1	G	46	ARG	2.7
1	A	38	LYS	2.7
1	C	46	ARG	2.7
1	B	16	GLU	2.7
1	B	59	VAL	2.7
1	F	59	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	78	LEU	2.6
1	A	58	GLY	2.6
1	E	90	LYS	2.6
1	H	37	ASP	2.6
1	H	39	GLY	2.6
1	G	59	VAL	2.6
1	C	41	THR	2.5
1	C	50	THR	2.5
1	D	92	ILE	2.5
1	B	307	ALA	2.5
1	G	306	ALA	2.5
1	D	48	ASN	2.5
1	B	266	LEU	2.5
1	H	38	LYS	2.5
1	C	59	VAL	2.5
1	G	79	ALA	2.5
1	A	94	ILE	2.5
1	B	144	ALA	2.5
1	B	90	LYS	2.5
1	F	76	ILE	2.5
1	G	56	LEU	2.5
1	E	37	ASP	2.5
1	F	88	LYS	2.4
1	H	91	LYS	2.4
1	G	45	LEU	2.4
1	C	91	LYS	2.4
1	E	91	LYS	2.4
1	A	55	THR	2.4
1	F	91	LYS	2.4
1	C	16	GLU	2.4
1	D	60	ASP	2.4
1	A	92	ILE	2.4
1	A	44	GLY	2.4
1	D	264	GLN	2.4
1	C	60	ASP	2.3
1	G	60	ASP	2.3
1	E	46	ARG	2.3
1	B	49	LEU	2.3
1	G	78	LEU	2.3
1	G	305	LEU	2.3
1	E	19	ASP	2.3
1	G	19	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	46	ARG	2.3
1	E	56	LEU	2.3
1	G	27	ILE	2.3
1	H	120	LYS	2.3
1	G	2	ASP	2.3
1	B	44	GLY	2.3
1	E	47	ALA	2.3
1	A	49	LEU	2.3
1	H	78	LEU	2.3
1	E	27	ILE	2.2
1	F	92	ILE	2.2
1	F	43	GLN	2.2
1	H	42	ILE	2.2
1	H	41	THR	2.2
1	C	87	SER	2.2
1	C	55	THR	2.2
1	G	57	CYS	2.2
1	H	16	GLU	2.2
1	G	12	SER	2.2
1	H	269	GLU	2.2
1	B	46	ARG	2.2
1	B	38	LYS	2.2
1	F	44	GLY	2.2
1	B	60	ASP	2.2
1	F	77	SER	2.2
1	H	90	LYS	2.1
1	A	307	ALA	2.1
1	F	45	LEU	2.1
1	E	87	SER	2.1
1	C	305	LEU	2.1
1	A	48	ASN	2.1
1	H	307	ALA	2.1
1	B	120	LYS	2.1
1	B	76	ILE	2.1
1	H	27	ILE	2.1
1	H	18	PRO	2.0
1	C	42	ILE	2.0
1	E	89	CYS	2.0
1	F	252	TYR	2.0
1	A	8	GLU	2.0
1	G	39	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	SO4	F	510	5/5	0.91	0.10	72,74,75,77	0
2	SO4	A	509	5/5	0.92	0.09	76,80,80,81	0
2	SO4	G	507	5/5	0.93	0.09	51,55,57,59	0
2	SO4	H	508	5/5	0.93	0.11	67,68,72,73	0
2	SO4	A	501	5/5	0.94	0.10	44,47,49,51	0
3	CL	A	601	1/1	0.94	0.22	54,54,54,54	0
2	SO4	B	502	5/5	0.95	0.08	45,45,47,52	0
2	SO4	C	503	5/5	0.96	0.07	56,59,60,60	0
2	SO4	E	505	5/5	0.96	0.08	58,58,62,64	0
2	SO4	D	504	5/5	0.97	0.08	53,54,56,57	0
2	SO4	F	506	5/5	0.97	0.07	52,53,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.