



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:53 AM UTC

PDB ID : 8AFI / pdb_00008afi
Title : GABARAP in complex with LIR motif of HsATG3
Authors : Farnung, J.; Benoit, R.M.; Corn, J.E.; Bode, J.W.
Deposited on : 2022-07-18
Resolution : 2.66 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

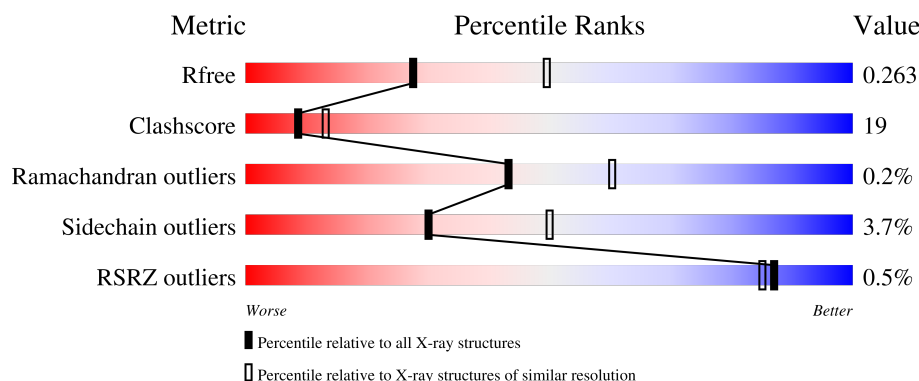
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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.



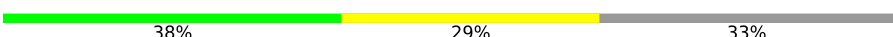
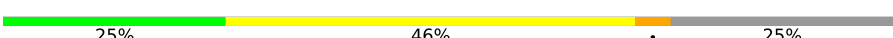
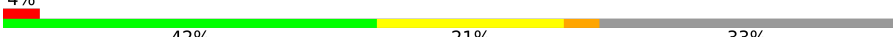
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	115	84% 16%
1	C	115	59% 37% • •
1	E	115	71% 27% •
1	G	115	67% 32% •
1	I	115	71% 27% •

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Mol	Chain	Length	Quality of chain
1	K	115	
1	M	115	
1	O	115	
2	B	24	
2	D	24	
2	F	24	
2	H	24	
2	J	24	
2	L	24	
2	N	24	
2	P	24	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16646 atoms, of which 8089 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 Gamma-aminobutyric acid receptor-associated protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	115	Total	C	H	N	O	S	21	0	0
			1935	633	965	164	172	1			
1	C	114	Total	C	H	N	O	S	21	0	0
			1881	621	930	158	171	1			
1	E	115	Total	C	H	N	O	S	21	0	0
			1935	633	965	164	172	1			
1	G	114	Total	C	H	N	O	S	21	0	0
			1880	624	923	161	171	1			
1	I	115	Total	C	H	N	O	S	21	0	0
			1906	627	944	162	172	1			
1	K	115	Total	C	H	N	O	S	11	0	0
			1897	627	938	159	172	1			
1	M	113	Total	C	H	N	O	S	11	0	0
			1869	622	916	160	170	1			
1	O	115	Total	C	H	N	O	S	21	0	0
			1926	633	956	164	172	1			

- Molecule 2 is a protein called Ubiquitin-like-conjugating enzyme ATG3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	16	Total	C	H	N	O		0	0	0
			213	76	90	17	30				
2	H	8	Total	C	H	N	O		0	0	0
			98	35	41	9	13				
2	B	16	Total	C	H	N	O		0	0	0
			201	72	81	17	31				
2	J	17	Total	C	H	N	O		0	0	0
			198	75	73	18	32				
2	N	9	Total	C	H	N	O		0	0	0
			112	43	44	10	15				
2	P	7	Total	C	H	N	O		0	0	0
			80	32	28	8	12				

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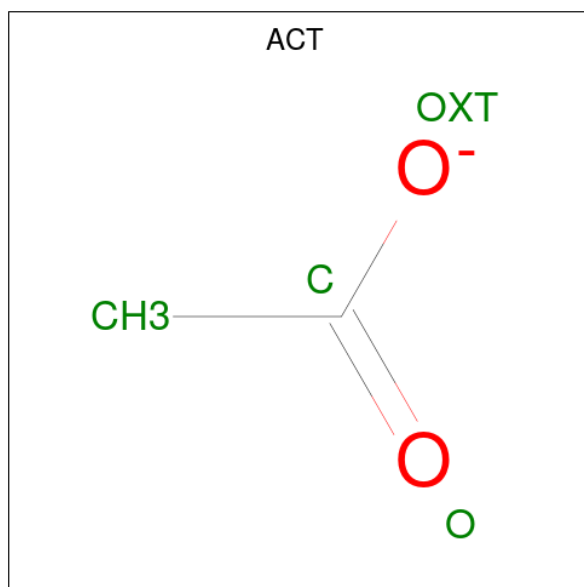
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	H	N	O	0	0	0
			221	83	84	19	35			
2	L	15	Total	C	H	N	O	0	0	0
			150	67	39	16	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	113	GLY	ASN	conflict	UNP C9JNW8
H	113	GLY	ASN	conflict	UNP C9JNW8
B	113	GLY	ASN	conflict	UNP C9JNW8
J	113	GLY	ASN	conflict	UNP C9JNW8
N	113	GLY	ASN	conflict	UNP C9JNW8
P	113	GLY	ASN	conflict	UNP C9JNW8
D	113	GLY	ASN	conflict	UNP C9JNW8
L	113	GLY	ASN	conflict	UNP C9JNW8

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		
4	I	1	Total	C	H	O	0	0
			14	3	8	3		
4	K	1	Total	C	H	O	0	0
			14	3	8	3		
4	M	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	5	Total	H	O	0	0
			7	2	5		
5	C	4	Total	H	O	0	0
			6	2	4		
5	E	5	Total	H	O	0	0
			9	4	5		
5	G	2	Total	O		0	0
			2	2			
5	I	2	Total	O		0	0
			2	2			

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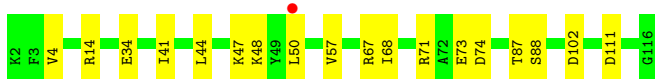
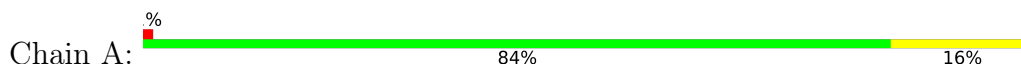
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	3	Total H O 5 2 3	0	0
5	O	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



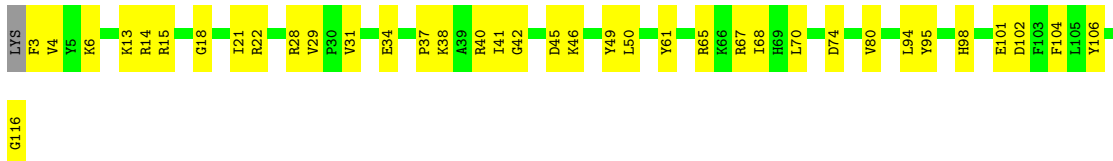
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



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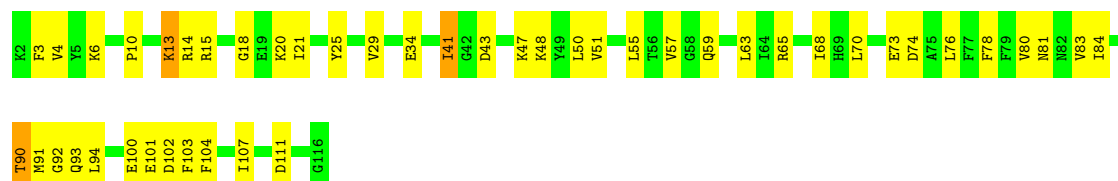


- Molecule 1: Gamma-aminobutyric acid receptor-associated protein

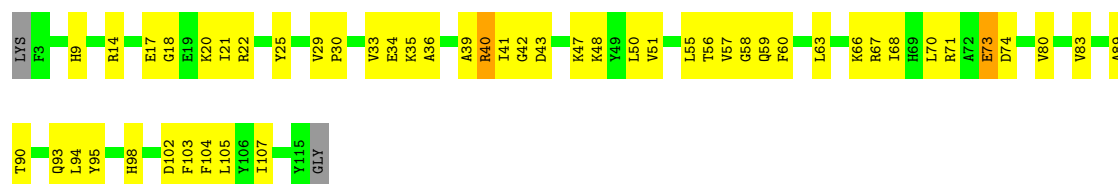




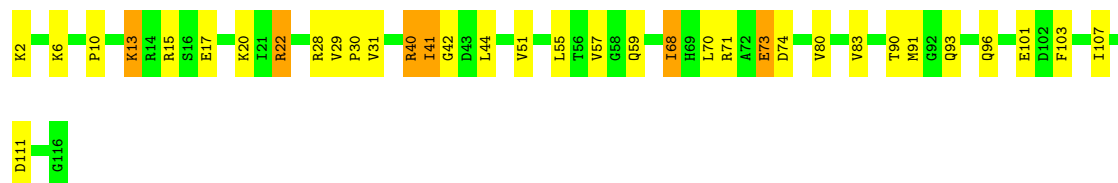
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



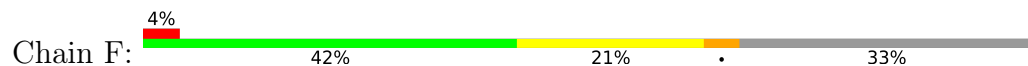
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



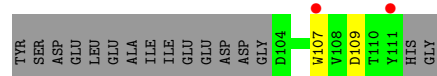
- Molecule 1: Gamma-aminobutyric acid receptor-associated protein



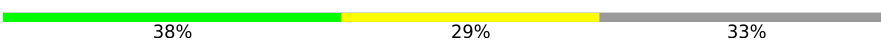
- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3



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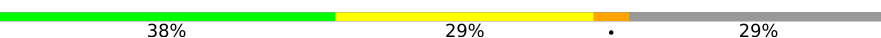


- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3

Chain B: 



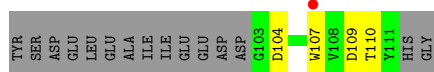
- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3

Chain J: 



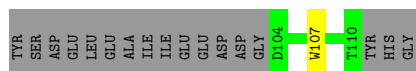
- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3

Chain N: 

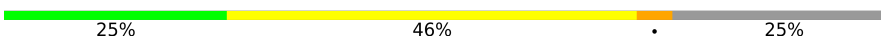


- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3

Chain P: 



- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3

Chain D: 



- Molecule 2: Ubiquitin-like-conjugating enzyme ATG3

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.80Å 63.80Å 73.90Å 64.50° 86.50° 70.30°	Depositor
Resolution (Å)	49.10 – 2.66 49.10 – 2.66	Depositor EDS
% Data completeness (in resolution range)	94.6 (49.10-2.66) 94.7 (49.10-2.66)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.215 , 0.262 0.216 , 0.263	Depositor DCC
R_{free} test set	1369 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 83.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16646	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: GOL, ACT

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	0.56	0/997	0.68	0/1342
1	C	0.47	0/978	0.69	1/1320 (0.1%)
1	E	0.56	0/997	0.71	0/1342
1	G	0.50	0/984	0.68	0/1327
1	I	0.44	0/989	0.67	0/1334
1	K	0.48	0/985	0.72	0/1327
1	M	0.53	1/980 (0.1%)	0.70	2/1322 (0.2%)
1	O	0.52	0/997	0.69	0/1342
2	B	0.40	0/121	0.71	0/164
2	D	0.73	0/138	0.84	0/187
2	F	0.39	0/125	0.66	0/170
2	H	0.33	0/58	0.62	0/79
2	J	0.70	0/126	0.89	0/171
2	L	0.89	1/112 (0.9%)	1.33	4/152 (2.6%)
2	N	0.56	0/70	0.74	0/95
2	P	0.34	0/53	0.78	0/72
All	All	0.52	2/8710 (0.0%)	0.71	7/11746 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	73	GLU	CD-OE2	-5.58	1.14	1.25
2	L	101	ASP	CA-C	-5.25	1.45	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	101	ASP	CA-C-O	-6.98	110.52	120.51
2	L	101	ASP	CA-C-N	5.88	132.77	121.54
2	L	101	ASP	C-N-CA	5.88	132.77	121.54
1	M	40	ARG	NE-CZ-NH2	5.87	124.49	119.20
1	C	67	ARG	NE-CZ-NH1	-5.84	115.66	121.50
2	L	101	ASP	N-CA-C	-5.74	98.57	110.80
1	M	73	GLU	CG-CD-OE1	5.61	131.29	118.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	102	ASP	Sidechain

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	970	965	965	23	0
1	C	951	930	930	49	2
1	E	970	965	965	32	0
1	G	957	923	941	35	1
1	I	962	944	943	27	2
1	K	959	938	949	46	0
1	M	953	916	938	54	0
1	O	970	956	965	33	0
2	B	120	81	95	13	0
2	D	137	84	112	24	2
2	F	123	90	98	10	0
2	H	57	41	41	6	1
2	J	125	73	97	12	0
2	L	111	39	89	12	0
2	N	68	44	51	11	0
2	P	52	28	39	1	0
3	A	4	3	3	0	0
3	C	4	3	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	8	8	0	0
4	C	6	8	8	0	0
4	E	6	8	8	0	0
4	G	6	8	8	2	0
4	I	6	8	8	0	0
4	K	6	8	8	1	0
4	M	6	8	8	0	0
5	A	5	2	0	0	0
5	C	4	2	0	0	0
5	E	5	4	0	0	0
5	G	2	0	0	1	0
5	I	2	0	0	0	0
5	M	3	2	0	0	0
5	O	1	0	0	0	0
All	All	8557	8089	8280	314	4

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 19.

All (314) 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:I:41:ILE:HD11	1:I:70:LEU:HD11	1.34	1.06
1:K:15:ARG:NH1	1:K:101:GLU:O	1.90	1.04
1:C:38:LYS:O	1:M:40:ARG:NH1	2.00	0.94
1:G:15:ARG:NH1	1:G:101:GLU:O	2.03	0.91
1:G:41:ILE:HD11	1:G:70:LEU:HD11	1.51	0.91
1:A:71:ARG:NH1	1:A:73:GLU:OE2	2.04	0.91
1:O:15:ARG:NH1	1:O:101:GLU:O	2.05	0.90
1:K:6:LYS:NZ	1:K:100:GLU:OE2	2.06	0.88
1:C:25:TYR:CZ	2:D:98:ILE:HD11	2.12	0.85
1:I:68:ILE:HG23	1:I:70:LEU:HD13	1.60	0.84
1:C:55:LEU:HD21	1:C:63:LEU:HD12	1.62	0.82
2:J:99:GLU:HG3	2:J:102:ASP:OD1	1.80	0.81
1:O:10:PRO:HG2	1:O:13:LYS:HB3	1.63	0.79
1:E:71:ARG:HG3	1:E:73:GLU:H	1.47	0.79
1:C:67:ARG:NH2	2:D:95:GLU:OE2	2.18	0.76
1:M:17:GLU:OE2	1:M:48:LYS:NZ	2.17	0.76
1:E:34:GLU:HG2	1:E:47:LYS:HE3	1.68	0.75
1:C:46:LYS:HE2	2:D:97:ILE:HD11	1.67	0.74
1:A:50:LEU:HG	2:B:107:TRP:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:ASP:OD1	1:E:9:HIS:NE2	2.21	0.73
1:I:31:VAL:HG12	1:I:105:LEU:HB3	1.70	0.73
1:M:80:VAL:O	1:M:83:VAL:HG22	1.89	0.72
1:C:87:THR:HG21	1:O:73:GLU:O	1.90	0.72
1:M:41:ILE:HD11	1:M:70:LEU:CD1	2.20	0.72
2:J:95:GLU:HG3	1:I:67:ARG:HH12	1.55	0.71
2:P:107:TRP:CH2	1:O:30:PRO:HB2	2.27	0.70
1:M:71:ARG:HG2	1:M:74:ASP:OD2	1.92	0.70
1:K:90:THR:HG23	1:K:92:GLY:H	1.57	0.69
2:F:107:TRP:HB3	1:E:50:LEU:HG	1.74	0.69
1:C:22:ARG:HD2	1:C:95:TYR:OH	1.92	0.69
2:D:99:GLU:O	2:D:102:ASP:OD1	2.11	0.69
1:M:90:THR:HG22	1:M:93:GLN:HG3	1.73	0.69
1:C:46:LYS:HZ3	2:D:108:VAL:HG22	1.57	0.69
1:O:31:VAL:HG11	1:O:107:ILE:HD12	1.74	0.68
1:O:42:GLY:O	1:O:68:ILE:HD11	1.93	0.68
1:M:41:ILE:HD11	1:M:70:LEU:HD11	1.76	0.68
1:C:46:LYS:HD3	2:D:108:VAL:CG2	2.26	0.66
1:E:71:ARG:HG3	1:E:73:GLU:N	2.11	0.66
1:G:101:GLU:OE2	1:O:6:LYS:HE2	1.96	0.65
1:M:68:ILE:HG13	1:M:68:ILE:O	1.96	0.65
1:C:46:LYS:CE	2:D:97:ILE:HD11	2.26	0.65
1:I:71:ARG:HG2	1:I:74:ASP:OD2	1.96	0.65
1:M:43:ASP:O	1:M:68:ILE:HD13	1.97	0.65
1:K:80:VAL:O	1:K:81:ASN:HB2	1.96	0.64
1:I:68:ILE:CG2	1:I:70:LEU:HD13	2.27	0.64
2:B:96:ALA:O	2:B:97:ILE:HD13	1.97	0.64
1:G:41:ILE:HD11	1:G:70:LEU:CD1	2.26	0.63
1:O:15:ARG:CZ	1:O:103:PHE:HE1	2.11	0.63
1:K:34:GLU:HG2	1:K:47:LYS:HE3	1.81	0.63
2:B:98:ILE:HG12	2:B:109:ASP:HB2	1.79	0.63
1:O:80:VAL:HG12	1:O:83:VAL:CG2	2.29	0.62
2:L:98:ILE:HG22	2:L:107:TRP:O	2.00	0.61
1:C:54:ASP:OD1	1:C:54:ASP:N	2.33	0.61
1:C:112:GLU:HG3	1:M:40:ARG:NE	2.14	0.61
1:A:71:ARG:HG2	1:A:74:ASP:OD2	2.01	0.60
1:A:71:ARG:HD2	1:A:73:GLU:OE2	2.00	0.60
1:E:62:PHE:HE1	1:E:66:LYS:HE2	1.66	0.60
1:K:73:GLU:HG3	1:M:58:GLY:HA3	1.84	0.60
2:N:107:TRP:CE2	1:M:21:ILE:HD13	2.37	0.60
1:A:4:VAL:HG12	1:A:34:GLU:OE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:17:GLU:HA	1:O:20:LYS:HD2	1.85	0.59
1:O:29:VAL:HG22	1:O:51:VAL:O	2.03	0.59
1:O:41:ILE:HD11	1:O:70:LEU:HD11	1.85	0.59
1:E:71:ARG:HG2	1:E:73:GLU:HB3	1.85	0.59
1:G:21:ILE:HG21	1:G:50:LEU:HD21	1.85	0.59
1:I:80:VAL:O	1:I:83:VAL:HG22	2.03	0.59
1:K:65:ARG:HH11	1:K:76:LEU:HB3	1.68	0.59
1:C:46:LYS:CD	2:D:108:VAL:CG2	2.80	0.58
1:O:40:ARG:HG3	1:O:111:ASP:OD2	2.03	0.57
1:M:51:VAL:HG11	1:M:60:PHE:CE1	2.39	0.57
1:C:55:LEU:HD21	1:C:63:LEU:CD1	2.34	0.57
2:N:107:TRP:NE1	1:M:21:ILE:HD13	2.19	0.57
1:G:61:TYR:HB3	4:G:201:GOL:O3	2.04	0.57
2:J:99:GLU:HG3	2:J:102:ASP:CG	2.28	0.57
2:L:98:ILE:HD11	1:K:25:TYR:CZ	2.39	0.57
1:C:90:THR:OG1	1:C:93:GLN:HG3	2.05	0.57
1:G:40:ARG:O	1:G:40:ARG:HG3	2.04	0.57
1:G:101:GLU:OE2	1:O:6:LYS:CE	2.52	0.57
1:M:18:GLY:HA2	1:M:104:PHE:HE1	1.70	0.57
1:K:91:MET:HE2	1:K:94:LEU:HD12	1.87	0.56
1:M:57:VAL:HG23	1:M:89:ALA:O	2.04	0.56
1:K:65:ARG:HG3	1:K:76:LEU:HD23	1.86	0.56
1:O:44:LEU:HG	1:O:68:ILE:HD12	1.87	0.56
2:J:104:ASP:OD1	2:J:104:ASP:O	2.24	0.56
1:M:55:LEU:HD11	1:M:59:GLN:HB3	1.88	0.56
1:G:65:ARG:CZ	1:G:70:LEU:HD23	2.36	0.56
2:H:109:ASP:OD1	1:G:28:ARG:NH1	2.39	0.55
1:K:59:GLN:CG	1:M:73:GLU:OE2	2.54	0.55
1:G:41:ILE:HG13	1:G:42:GLY:H	1.71	0.55
1:O:41:ILE:HD13	1:O:111:ASP:HB3	1.89	0.55
1:C:71:ARG:NH1	1:C:73:GLU:OE2	2.40	0.55
2:H:107:TRP:CZ2	1:G:104:PHE:HE1	2.24	0.55
1:G:80:VAL:HG23	1:G:106:TYR:O	2.07	0.55
1:A:71:ARG:HD2	1:A:73:GLU:CG	2.37	0.55
1:E:38:LYS:HD2	1:E:116:GLY:HA2	1.88	0.55
2:J:95:GLU:N	2:J:95:GLU:OE1	2.40	0.54
2:D:108:VAL:O	2:D:110:THR:HG23	2.07	0.54
1:O:57:VAL:HA	1:O:91:MET:HE3	1.88	0.54
1:K:57:VAL:HG22	1:K:91:MET:CE	2.38	0.54
1:K:59:GLN:HG2	1:M:73:GLU:OE2	2.06	0.54
1:C:42:GLY:O	1:C:68:ILE:HD11	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:LYS:HG2	1:K:14:ARG:CZ	2.38	0.54
1:M:90:THR:HG22	1:M:93:GLN:CG	2.37	0.54
1:G:29:VAL:HG21	1:G:95:TYR:HB2	1.89	0.54
1:M:95:TYR:OH	1:M:103:PHE:O	2.14	0.54
1:E:34:GLU:CG	1:E:47:LYS:HE3	2.37	0.54
1:E:45:ASP:OD1	1:E:45:ASP:N	2.40	0.54
1:O:80:VAL:HG12	1:O:83:VAL:HG23	1.89	0.54
1:A:71:ARG:HD2	1:A:73:GLU:CD	2.33	0.54
1:E:29:VAL:HG13	1:E:95:TYR:CD1	2.43	0.54
1:E:29:VAL:HG11	1:E:95:TYR:HB2	1.89	0.54
1:C:67:ARG:HH12	2:D:95:GLU:CD	2.16	0.54
2:N:110:THR:HG22	1:M:67:ARG:HH21	1.72	0.54
1:K:65:ARG:NH2	1:K:74:ASP:O	2.27	0.54
1:A:71:ARG:HE	1:A:74:ASP:CG	2.16	0.53
2:J:107:TRP:NE1	1:I:21:ILE:HD11	2.23	0.53
2:N:110:THR:HG22	1:M:67:ARG:NH2	2.22	0.53
1:C:25:TYR:CE2	2:D:98:ILE:HD11	2.43	0.53
1:C:55:LEU:HD11	1:C:59:GLN:HB3	1.88	0.53
1:G:41:ILE:CD1	1:G:70:LEU:HD11	2.30	0.53
1:I:14:ARG:NH1	1:I:102:ASP:OD2	2.41	0.53
1:M:34:GLU:HG2	1:M:47:LYS:HD2	1.91	0.53
1:M:41:ILE:HG13	1:M:42:GLY:N	2.24	0.53
1:A:71:ARG:CZ	1:A:73:GLU:OE2	2.57	0.53
2:D:93:GLU:HG3	2:D:94:LEU:H	1.74	0.53
1:K:43:ASP:O	1:K:68:ILE:HD13	2.09	0.53
1:K:93:GLN:HG3	1:O:96:GLN:HB3	1.90	0.53
2:F:99:GLU:OE2	1:E:25:TYR:HE2	1.92	0.52
1:I:57:VAL:HG22	1:I:94:LEU:HD12	1.90	0.52
1:C:80:VAL:HG11	1:C:94:LEU:HD11	1.90	0.52
1:M:94:LEU:HD12	1:M:98:HIS:CD2	2.44	0.52
1:A:57:VAL:HB	1:A:87:THR:HA	1.92	0.52
2:N:107:TRP:CZ2	1:M:21:ILE:HD13	2.44	0.52
1:K:90:THR:HG23	1:K:92:GLY:N	2.22	0.52
1:M:41:ILE:HG13	1:M:42:GLY:H	1.74	0.52
1:K:55:LEU:HD11	1:K:59:GLN:HB3	1.91	0.52
2:N:107:TRP:HE1	1:M:21:ILE:CD1	2.23	0.52
1:K:90:THR:HG22	1:K:93:GLN:H	1.75	0.51
2:D:93:GLU:C	2:D:94:LEU:HG	2.36	0.51
1:C:112:GLU:HG3	1:M:40:ARG:CZ	2.40	0.51
1:C:46:LYS:NZ	2:D:97:ILE:HD11	2.26	0.51
1:O:55:LEU:HD11	1:O:59:GLN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:68:ILE:HG13	1:K:68:ILE:O	2.10	0.51
2:F:107:TRP:CH2	1:E:30:PRO:HB2	2.46	0.50
1:G:101:GLU:HG2	1:O:6:LYS:NZ	2.26	0.50
1:I:80:VAL:HG22	1:I:107:ILE:HG12	1.91	0.50
1:G:41:ILE:HG13	1:G:42:GLY:N	2.27	0.50
1:K:10:PRO:HD2	1:K:13:LYS:CE	2.41	0.50
1:C:95:TYR:HA	1:C:105:LEU:HD22	1.94	0.50
1:C:67:ARG:CZ	2:D:95:GLU:OE2	2.59	0.50
1:M:36:ALA:HB3	1:M:39:ALA:HB2	1.92	0.50
1:C:59:GLN:O	1:C:63:LEU:HG	2.12	0.49
1:C:80:VAL:O	1:C:83:VAL:HG22	2.12	0.49
1:K:10:PRO:HD2	1:K:13:LYS:HE2	1.94	0.49
2:J:95:GLU:O	2:J:95:GLU:HG2	2.11	0.49
1:M:25:TYR:CG	1:M:50:LEU:HD21	2.47	0.49
1:E:14:ARG:NH1	1:E:102:ASP:OD2	2.45	0.49
1:O:71:ARG:HG2	1:O:73:GLU:H	1.78	0.49
1:A:88:SER:HB2	1:E:90:THR:HG21	1.94	0.49
1:C:22:ARG:HD2	1:C:95:TYR:CZ	2.47	0.49
2:L:110:THR:HG21	1:K:63:LEU:HD21	1.94	0.49
2:F:97:ILE:HG12	1:E:46:LYS:NZ	2.28	0.48
1:G:21:ILE:CG2	1:G:50:LEU:HD21	2.43	0.48
1:G:65:ARG:NH2	1:G:74:ASP:O	2.39	0.48
1:M:43:ASP:O	1:M:68:ILE:CD1	2.61	0.48
1:C:38:LYS:CB	1:M:40:ARG:NH1	2.77	0.48
1:G:98:HIS:O	5:G:301:HOH:O	2.20	0.48
1:A:34:GLU:HG2	1:A:47:LYS:HD2	1.95	0.48
2:F:104:ASP:OD1	1:E:9:HIS:CE1	2.66	0.48
1:E:102:ASP:O	1:E:103:PHE:HB2	2.12	0.48
1:M:18:GLY:HA2	1:M:104:PHE:CE1	2.47	0.48
1:C:38:LYS:C	1:M:40:ARG:NH1	2.71	0.48
1:E:68:ILE:HG13	1:E:70:LEU:HD13	1.95	0.48
1:O:71:ARG:HD3	1:O:73:GLU:CG	2.44	0.48
2:L:98:ILE:HG21	1:K:50:LEU:HD12	1.96	0.48
1:E:80:VAL:O	1:E:81:ASN:HB2	2.13	0.48
1:O:22:ARG:NH2	1:O:28:ARG:O	2.46	0.48
1:C:46:LYS:HD2	2:D:108:VAL:HG21	1.96	0.48
2:J:98:ILE:CG2	2:J:99:GLU:N	2.76	0.48
1:M:40:ARG:O	1:M:40:ARG:HG3	2.14	0.48
1:K:18:GLY:HA2	1:K:104:PHE:CE1	2.49	0.47
1:K:91:MET:HE2	1:K:91:MET:HA	1.95	0.47
1:A:50:LEU:CG	2:B:107:TRP:HB3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:107:TRP:HE1	1:M:21:ILE:HD11	1.79	0.47
1:K:65:ARG:HH11	1:K:76:LEU:CB	2.27	0.47
2:D:97:ILE:HG22	2:D:98:ILE:N	2.29	0.47
1:A:44:LEU:HD13	1:A:68:ILE:HG23	1.95	0.47
2:L:97:ILE:HG22	2:L:100:GLU:HB2	1.95	0.47
2:L:107:TRP:NE1	1:K:21:ILE:HD11	2.28	0.47
1:K:3:PHE:HE1	4:K:201:GOL:H2	1.79	0.47
1:E:73:GLU:O	1:I:87:THR:HB	2.15	0.47
1:I:31:VAL:HG12	1:I:105:LEU:HD23	1.97	0.47
1:O:70:LEU:HG	1:O:74:ASP:HB2	1.97	0.47
1:A:41:ILE:HG23	1:A:111:ASP:HB3	1.97	0.47
1:C:56:THR:HG23	1:C:59:GLN:OE1	2.15	0.47
1:A:48:LYS:HZ3	2:B:107:TRP:CG	2.33	0.47
1:A:14:ARG:NH1	1:A:102:ASP:OD2	2.45	0.47
1:G:38:LYS:N	1:G:116:GLY:O	2.48	0.47
1:C:58:GLY:CA	1:C:87:THR:CG2	2.93	0.47
1:C:17:GLU:OE2	2:D:102:ASP:OD2	2.33	0.47
1:G:18:GLY:O	1:G:22:ARG:HG2	2.15	0.47
1:E:55:LEU:HD11	1:E:59:GLN:HB3	1.96	0.46
1:G:4:VAL:HG12	1:G:34:GLU:CD	2.39	0.46
2:H:107:TRP:CZ2	1:G:104:PHE:CE1	3.04	0.46
1:K:18:GLY:HA3	1:K:103:PHE:HB2	1.97	0.46
1:M:14:ARG:NH1	1:M:102:ASP:OD2	2.48	0.46
1:M:33:VAL:O	1:M:47:LYS:HG2	2.15	0.46
1:C:15:ARG:NH1	1:C:101:GLU:O	2.49	0.46
2:N:107:TRP:NE1	1:M:21:ILE:CD1	2.78	0.46
1:K:59:GLN:HG3	1:M:73:GLU:OE2	2.16	0.46
1:M:90:THR:CG2	1:M:93:GLN:HG3	2.41	0.46
2:J:99:GLU:CG	2:J:102:ASP:OD1	2.59	0.46
2:L:101:ASP:O	2:L:102:ASP:CG	2.59	0.46
1:K:51:VAL:HG13	1:K:55:LEU:HD22	1.96	0.46
1:M:63:LEU:O	1:M:67:ARG:HG3	2.15	0.46
1:E:71:ARG:HG3	1:E:72:ALA:N	2.31	0.46
1:A:4:VAL:HG12	1:A:34:GLU:CD	2.41	0.45
1:C:60:PHE:HA	1:C:63:LEU:HD12	1.98	0.45
1:M:80:VAL:HG22	1:M:107:ILE:HG12	1.98	0.45
2:H:107:TRP:NE1	1:G:21:ILE:HD11	2.31	0.45
1:E:30:PRO:HA	1:E:50:LEU:HD23	1.98	0.45
1:K:41:ILE:HD13	1:K:111:ASP:HB3	1.97	0.45
1:I:102:ASP:O	1:I:103:PHE:HB2	2.15	0.45
1:A:48:LYS:HE2	2:B:107:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HG	1:C:74:ASP:HB2	1.99	0.45
1:M:95:TYR:HA	1:M:105:LEU:HD22	1.98	0.45
1:E:50:LEU:HD23	1:E:50:LEU:HA	1.80	0.45
2:J:100:GLU:HG3	2:J:101:ASP:N	2.32	0.45
2:D:104:ASP:O	2:D:104:ASP:CG	2.60	0.45
1:O:31:VAL:CG1	1:O:107:ILE:HD12	2.44	0.45
1:E:71:ARG:CG	1:E:73:GLU:HB3	2.46	0.45
1:I:6:LYS:HG3	1:I:106:TYR:CE2	2.52	0.45
2:D:95:GLU:OE2	2:D:108:VAL:CG1	2.65	0.45
1:M:30:PRO:HD2	1:M:95:TYR:CE2	2.52	0.45
1:M:35:LYS:HG2	1:M:39:ALA:HB3	1.99	0.44
1:O:90:THR:HG23	1:O:93:GLN:H	1.82	0.44
1:A:67:ARG:NH1	2:B:95:GLU:OE2	2.48	0.44
1:I:31:VAL:CG1	1:I:105:LEU:HD23	2.47	0.44
1:I:57:VAL:CG2	1:I:94:LEU:HD12	2.47	0.44
2:B:96:ALA:C	2:B:97:ILE:HD13	2.43	0.44
1:M:56:THR:HA	1:M:90:THR:HA	1.98	0.44
1:K:65:ARG:CZ	1:K:70:LEU:HD23	2.48	0.44
2:N:104:ASP:OD2	1:M:9:HIS:CE1	2.70	0.44
1:K:78:PHE:O	1:K:84:ILE:HA	2.18	0.44
2:F:98:ILE:HG13	2:F:109:ASP:HB2	2.00	0.43
1:C:21:ILE:HD11	2:D:107:TRP:NE1	2.32	0.43
1:C:32:ILE:HA	1:C:47:LYS:O	2.17	0.43
2:L:107:TRP:CE3	1:K:48:LYS:HB3	2.54	0.43
2:F:98:ILE:CD1	2:F:109:ASP:OD2	2.66	0.43
2:J:107:TRP:CE2	1:I:48:LYS:HE2	2.53	0.43
1:K:91:MET:CE	1:K:94:LEU:HD12	2.48	0.43
1:O:71:ARG:NE	1:O:73:GLU:HB3	2.33	0.43
1:A:48:LYS:HZ3	2:B:107:TRP:CD1	2.37	0.43
1:C:94:LEU:HD12	1:C:98:HIS:ND1	2.33	0.43
2:F:104:ASP:OD2	1:E:48:LYS:HE3	2.18	0.43
1:I:71:ARG:HG3	1:I:73:GLU:HG2	2.01	0.43
1:G:31:VAL:HG22	1:G:49:TYR:O	2.19	0.43
1:C:61:TYR:CE1	1:C:76:LEU:HB3	2.53	0.43
1:A:71:ARG:HD2	1:A:73:GLU:HG2	1.99	0.42
1:C:41:ILE:HG23	1:C:42:GLY:N	2.34	0.42
1:C:46:LYS:CD	2:D:108:VAL:HG22	2.48	0.42
1:K:4:VAL:CG1	1:K:47:LYS:HZ2	2.32	0.42
2:H:107:TRP:CE2	1:G:21:ILE:HD13	2.54	0.42
1:O:80:VAL:HG12	1:O:83:VAL:HG22	2.01	0.42
2:N:107:TRP:CH2	1:M:30:PRO:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:42:GLY:C	1:O:68:ILE:HD11	2.44	0.42
1:O:83:VAL:HG23	1:O:83:VAL:O	2.20	0.42
2:B:98:ILE:CG1	2:B:109:ASP:HB2	2.46	0.42
1:G:37:PRO:HB2	1:G:116:GLY:O	2.19	0.42
1:G:65:ARG:HD2	4:G:201:GOL:H12	2.02	0.42
1:I:43:ASP:O	1:I:68:ILE:CD1	2.67	0.42
1:K:65:ARG:HG3	1:K:76:LEU:CD2	2.48	0.42
1:M:22:ARG:HD3	1:M:95:TYR:OH	2.20	0.42
1:A:48:LYS:HE2	2:B:107:TRP:CE2	2.55	0.42
1:C:38:LYS:HG3	1:C:116:GLY:C	2.45	0.42
2:J:99:GLU:O	2:J:102:ASP:OD2	2.38	0.42
2:L:100:GLU:O	2:L:101:ASP:CB	2.68	0.42
1:E:87:THR:HG21	1:I:77:PHE:HE1	1.85	0.42
1:K:102:ASP:O	1:K:103:PHE:HB2	2.18	0.41
1:I:71:ARG:CZ	1:I:73:GLU:OE2	2.69	0.41
1:K:51:VAL:HG11	1:K:91:MET:HG3	2.02	0.41
1:M:41:ILE:HD11	1:M:70:LEU:HD13	1.98	0.41
1:G:68:ILE:CD1	1:G:70:LEU:HD13	2.51	0.41
1:I:23:LYS:HD3	1:I:23:LYS:HA	1.94	0.41
1:I:55:LEU:HD11	1:I:59:GLN:HB3	2.01	0.41
1:O:2:LYS:HD2	1:O:2:LYS:HA	1.88	0.41
1:C:46:LYS:HD2	2:D:108:VAL:CG2	2.50	0.41
2:B:102:ASP:OD1	2:B:102:ASP:C	2.64	0.41
1:G:14:ARG:NH1	1:G:102:ASP:OD2	2.54	0.41
1:G:45:ASP:N	1:G:45:ASP:OD1	2.52	0.41
1:I:94:LEU:HD23	1:I:98:HIS:ND1	2.36	0.41
1:K:4:VAL:CG1	1:K:47:LYS:NZ	2.84	0.41
1:C:71:ARG:CZ	1:C:73:GLU:OE2	2.69	0.41
2:B:102:ASP:OD1	2:B:102:ASP:O	2.39	0.41
1:I:38:LYS:HD2	1:I:116:GLY:HA3	2.03	0.41
1:K:80:VAL:HG22	1:K:107:ILE:HG12	2.02	0.41
2:L:98:ILE:C	2:L:100:GLU:N	2.79	0.41
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.80	0.40
2:F:107:TRP:CB	1:E:50:LEU:HG	2.48	0.40
2:N:109:ASP:CG	2:N:110:THR:N	2.78	0.40
2:L:107:TRP:CE3	1:K:50:LEU:HG	2.56	0.40
1:C:28:ARG:HG2	1:C:52:PRO:HA	2.03	0.40
2:D:97:ILE:CG2	2:D:98:ILE:N	2.84	0.40
1:E:66:LYS:HD3	1:E:66:LYS:HA	1.91	0.40
1:G:94:LEU:HD12	1:G:94:LEU:HA	1.91	0.40
1:C:80:VAL:O	1:C:80:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:97:ILE:HD13	2:L:97:ILE:HA	1.81	0.40
1:E:57:VAL:HG21	1:E:86:PRO:O	2.21	0.40
1:M:29:VAL:HG22	1:M:51:VAL:HG23	2.03	0.40
1:G:3:PHE:HB2	1:G:6:LYS:HE2	2.03	0.40
1:K:51:VAL:HG13	1:K:55:LEU:CD2	2.52	0.40
1:O:44:LEU:CD2	1:O:68:ILE:HD12	2.51	0.40
2:H:107:TRP:CE3	1:G:50:LEU:HG	2.56	0.40
1:I:45:ASP:OD1	1:I:45:ASP:N	2.54	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LYS:HZ3	1:I:8:GLU:OE2[1_564]	1.23	0.37
1:C:13:LYS:NZ	1:I:8:GLU:OE2[1_564]	2.01	0.19
2:D:101:ASP:OD1	1:G:67:ARG:NH1[1_564]	2.07	0.13
2:H:109:ASP:H	2:D:97:ILE:O[1_546]	1.52	0.08

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	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	C	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
1	G	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	I	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	K	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
1	M	111/115 (96%)	109 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
2	B	14/24 (58%)	13 (93%)	1 (7%)	0	100	100
2	D	16/24 (67%)	14 (88%)	2 (12%)	0	100	100
2	F	14/24 (58%)	11 (79%)	3 (21%)	0	100	100
2	H	6/24 (25%)	4 (67%)	2 (33%)	0	100	100
2	J	15/24 (62%)	13 (87%)	2 (13%)	0	100	100
2	L	13/24 (54%)	10 (77%)	1 (8%)	2 (15%)	0	0
2	N	7/24 (29%)	5 (71%)	2 (29%)	0	100	100
2	P	5/24 (21%)	5 (100%)	0	0	100	100
All	All	990/1112 (89%)	959 (97%)	29 (3%)	2 (0%)	43	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	101	ASP
2	L	102	ASP

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	104/104 (100%)	104 (100%)	0	100	100
1	C	101/104 (97%)	94 (93%)	7 (7%)	14	24
1	E	104/104 (100%)	100 (96%)	4 (4%)	29	49
1	G	102/104 (98%)	100 (98%)	2 (2%)	48	69
1	I	102/104 (98%)	99 (97%)	3 (3%)	37	58
1	K	102/104 (98%)	96 (94%)	6 (6%)	18	30
1	M	102/104 (98%)	100 (98%)	2 (2%)	48	69
1	O	104/104 (100%)	98 (94%)	6 (6%)	18	31
2	B	12/19 (63%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	14/19 (74%)	13 (93%)	1 (7%)	13	23
2	F	12/19 (63%)	11 (92%)	1 (8%)	10	18
2	H	5/19 (26%)	5 (100%)	0	100	100
2	J	12/19 (63%)	12 (100%)	0	100	100
2	L	11/19 (58%)	10 (91%)	1 (9%)	9	14
2	N	6/19 (32%)	6 (100%)	0	100	100
2	P	5/19 (26%)	5 (100%)	0	100	100
All	All	898/984 (91%)	865 (96%)	33 (4%)	30	50

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	VAL
1	C	29	VAL
1	C	41	ILE
1	C	45	ASP
1	C	51	VAL
1	C	54	ASP
1	C	88	SER
2	F	98	ILE
2	D	94	LEU
2	L	97	ILE
1	E	41	ILE
1	E	48	LYS
1	E	68	ILE
1	E	83	VAL
1	G	13	LYS
1	G	46	LYS
1	I	29	VAL
1	I	70	LEU
1	I	94	LEU
1	K	13	LYS
1	K	20	LYS
1	K	29	VAL
1	K	41	ILE
1	K	83	VAL
1	K	90	THR
1	M	20	LYS
1	M	66	LYS
1	O	13	LYS

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Mol	Chain	Res	Type
1	O	22	ARG
1	O	40	ARG
1	O	41	ILE
1	O	68	ILE
1	O	73	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	C	9	HIS
1	E	96	GLN
1	M	9	HIS
1	M	81	ASN
1	M	98	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](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	C	201	-	3,3,3	1.09	0	3,3,3	1.36	0
4	GOL	G	201	-	5,5,5	0.82	0	5,5,5	0.92	0
4	GOL	E	201	-	5,5,5	0.59	0	5,5,5	0.70	0
3	ACT	A	201	-	3,3,3	1.12	0	3,3,3	1.50	0
4	GOL	I	201	-	5,5,5	0.74	0	5,5,5	1.11	0
4	GOL	K	201	-	5,5,5	1.03	0	5,5,5	0.86	0
4	GOL	C	202	-	5,5,5	0.92	0	5,5,5	0.74	0
4	GOL	M	201	-	5,5,5	0.65	0	5,5,5	1.14	0
4	GOL	A	202	-	5,5,5	0.96	0	5,5,5	1.27	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	201	-	-	2/4/4/4	-
4	GOL	E	201	-	-	2/4/4/4	-
4	GOL	I	201	-	-	2/4/4/4	-
4	GOL	K	201	-	-	2/4/4/4	-
4	GOL	C	202	-	-	2/4/4/4	-
4	GOL	M	201	-	-	0/4/4/4	-
4	GOL	A	202	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	202	GOL	C3-C2-C1	-2.13	103.98	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	GOL	C1-C2-C3-O3
4	E	201	GOL	O2-C2-C3-O3
4	G	201	GOL	C1-C2-C3-O3
4	K	201	GOL	O1-C1-C2-C3
4	C	202	GOL	O1-C1-C2-C3
4	I	201	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	G	201	GOL	O2-C2-C3-O3
4	I	201	GOL	O1-C1-C2-O2
4	C	202	GOL	O1-C1-C2-O2
4	K	201	GOL	O1-C1-C2-O2
4	A	202	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	201	GOL	2	0
4	K	201	GOL	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, 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	115/115 (100%)	-0.31	1 (0%) 81 78	44, 74, 110, 119	3 (2%)
1	C	114/115 (99%)	-0.19	0 100 100	53, 92, 126, 139	3 (2%)
1	E	115/115 (100%)	-0.21	0 100 100	49, 77, 114, 139	3 (2%)
1	G	114/115 (99%)	-0.19	0 100 100	62, 96, 129, 148	3 (2%)
1	I	115/115 (100%)	-0.28	0 100 100	51, 83, 122, 133	3 (2%)
1	K	115/115 (100%)	-0.02	0 100 100	68, 105, 134, 152	2 (1%)
1	M	113/115 (98%)	-0.07	0 100 100	57, 101, 131, 152	2 (1%)
1	O	115/115 (100%)	0.10	0 100 100	77, 122, 146, 156	3 (2%)
2	B	16/24 (66%)	0.14	0 100 100	90, 121, 149, 157	0
2	D	18/24 (75%)	0.31	0 100 100	97, 133, 160, 169	0
2	F	16/24 (66%)	0.40	1 (6%) 26 19	96, 128, 150, 154	0
2	H	8/24 (33%)	1.15	2 (25%) 2 1	101, 109, 143, 144	0
2	J	17/24 (70%)	0.19	0 100 100	93, 119, 173, 186	0
2	L	15/24 (62%)	0.24	0 100 100	104, 122, 145, 146	0
2	N	9/24 (37%)	0.97	1 (11%) 10 8	139, 144, 152, 153	0
2	P	7/24 (29%)	0.56	0 100 100	125, 128, 148, 150	0
All	All	1022/1112 (91%)	-0.09	5 (0%) 87 85	44, 98, 142, 186	22 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	111	TYR	2.8
2	N	107	TRP	2.3
1	A	50	LEU	2.2
2	F	96	ALA	2.1
2	H	107	TRP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	201	4/4	0.69	0.17	103,103,124,124	0
4	GOL	C	202	6/6	0.69	0.09	98,119,121,121	0
3	ACT	C	201	4/4	0.81	0.10	69,70,84,84	0
4	GOL	A	202	6/6	0.82	0.14	73,89,91,91	0
4	GOL	I	201	6/6	0.84	0.13	67,81,91,93	0
4	GOL	G	201	6/6	0.86	0.11	83,101,105,106	0
4	GOL	E	201	6/6	0.88	0.10	67,81,83,83	0
4	GOL	K	201	6/6	0.89	0.08	72,87,90,91	0
4	GOL	M	201	6/6	0.89	0.09	76,92,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.