



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:40 AM UTC

PDB ID : 5D1W / pdb_00005d1w
Title : Crystal structure of Mycobacterium tuberculosis Rv3249c transcriptional regulator.
Authors : Chou, T.-H.; Delmar, J.; Su, C.-C.; Yu, E.
Deposited on : 2015-08-04
Resolution : 3.59 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

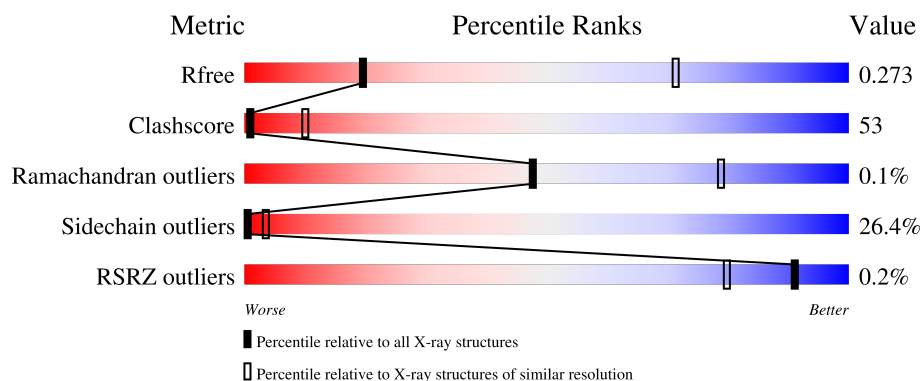
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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.



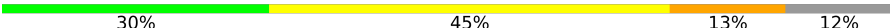
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	

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Mol	Chain	Length	Quality of chain
1	F	217	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (30%), yellow (45%), orange (13%), and grey (12%).

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9108 atoms, of which 124 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 Rv3249c transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1495	942	266	284	3			
1	B	195	Total	C	N	O	S	0	0	0
			1495	942	266	284	3			
1	C	192	Total	C	N	O	S	0	0	0
			1473	929	260	281	3			
1	D	196	Total	C	N	O	S	0	0	0
			1500	946	265	286	3			
1	E	193	Total	C	N	O	S	0	0	0
			1484	935	264	282	3			
1	F	191	Total	C	N	O	S	0	0	0
			1465	923	259	280	3			

There are 36 discrepancies between the modelled and reference sequences:

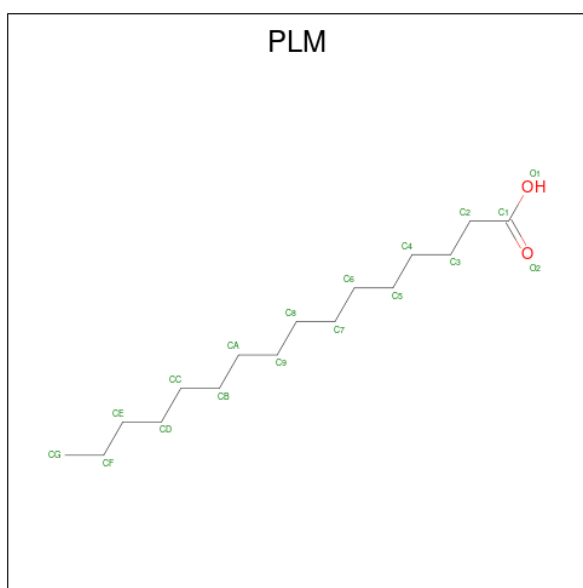
Chain	Residue	Modelled	Actual	Comment	Reference
A	212	HIS	-	expression tag	UNP O05892
A	213	HIS	-	expression tag	UNP O05892
A	214	HIS	-	expression tag	UNP O05892
A	215	HIS	-	expression tag	UNP O05892
A	216	HIS	-	expression tag	UNP O05892
A	217	HIS	-	expression tag	UNP O05892
B	212	HIS	-	expression tag	UNP O05892
B	213	HIS	-	expression tag	UNP O05892
B	214	HIS	-	expression tag	UNP O05892
B	215	HIS	-	expression tag	UNP O05892
B	216	HIS	-	expression tag	UNP O05892
B	217	HIS	-	expression tag	UNP O05892
C	212	HIS	-	expression tag	UNP O05892
C	213	HIS	-	expression tag	UNP O05892
C	214	HIS	-	expression tag	UNP O05892
C	215	HIS	-	expression tag	UNP O05892
C	216	HIS	-	expression tag	UNP O05892

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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	expression tag	UNP O05892
D	212	HIS	-	expression tag	UNP O05892
D	213	HIS	-	expression tag	UNP O05892
D	214	HIS	-	expression tag	UNP O05892
D	215	HIS	-	expression tag	UNP O05892
D	216	HIS	-	expression tag	UNP O05892
D	217	HIS	-	expression tag	UNP O05892
E	212	HIS	-	expression tag	UNP O05892
E	213	HIS	-	expression tag	UNP O05892
E	214	HIS	-	expression tag	UNP O05892
E	215	HIS	-	expression tag	UNP O05892
E	216	HIS	-	expression tag	UNP O05892
E	217	HIS	-	expression tag	UNP O05892
F	212	HIS	-	expression tag	UNP O05892
F	213	HIS	-	expression tag	UNP O05892
F	214	HIS	-	expression tag	UNP O05892
F	215	HIS	-	expression tag	UNP O05892
F	216	HIS	-	expression tag	UNP O05892
F	217	HIS	-	expression tag	UNP O05892

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			49	16	31	2		
2	B	1	Total	C	H	O	0	0
			49	16	31	2		

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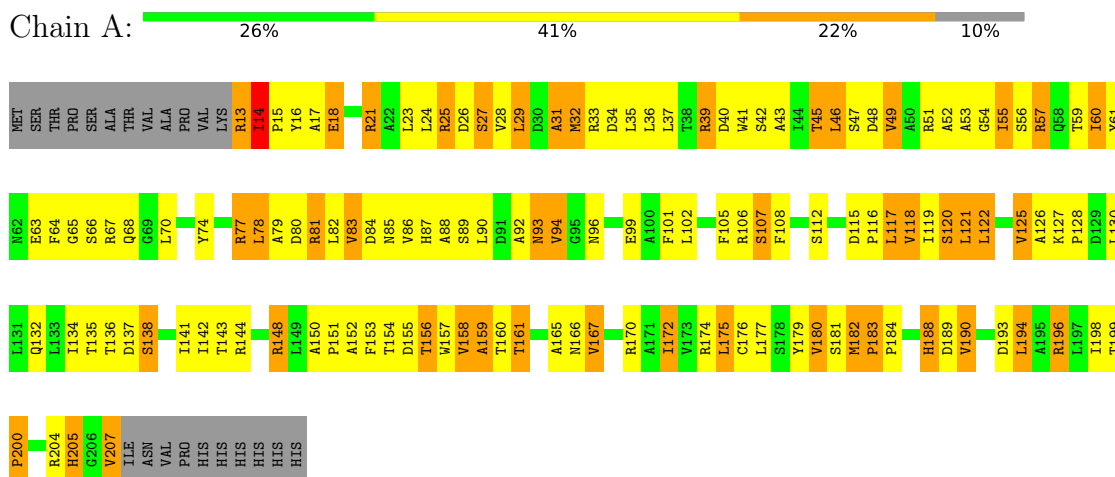
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			49	16	31	2		
2	D	1	Total	C	H	O	0	0
			49	16	31	2		

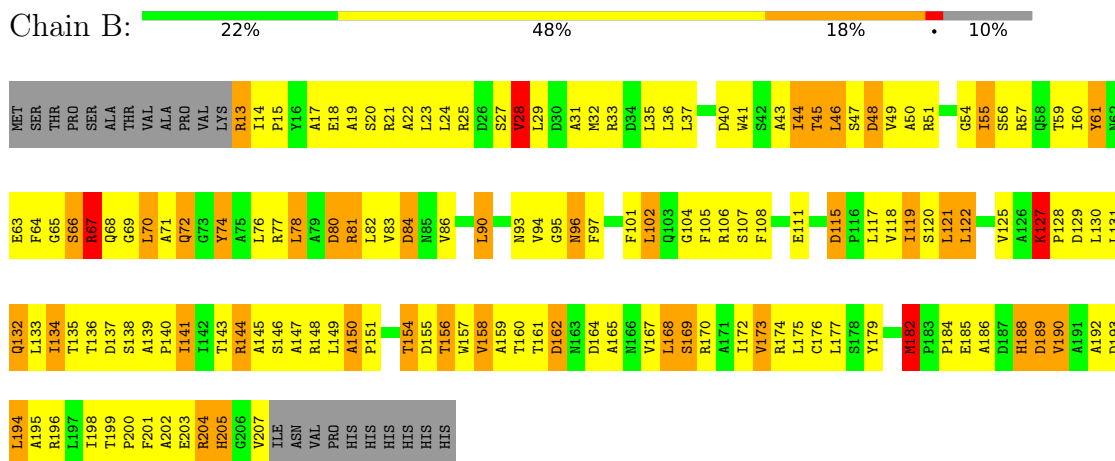
3 Residue-property plots

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: Rv3249c transcriptional regulator

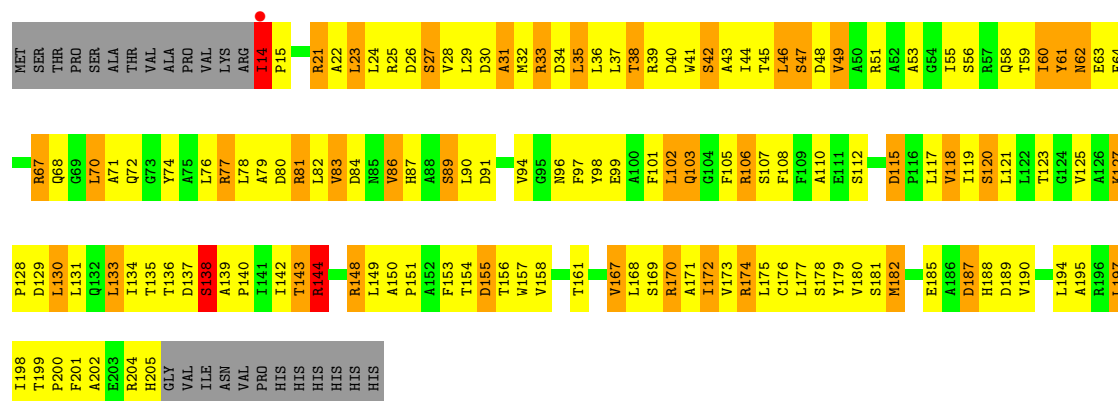


• Molecule 1: Rv3249c transcriptional regulator

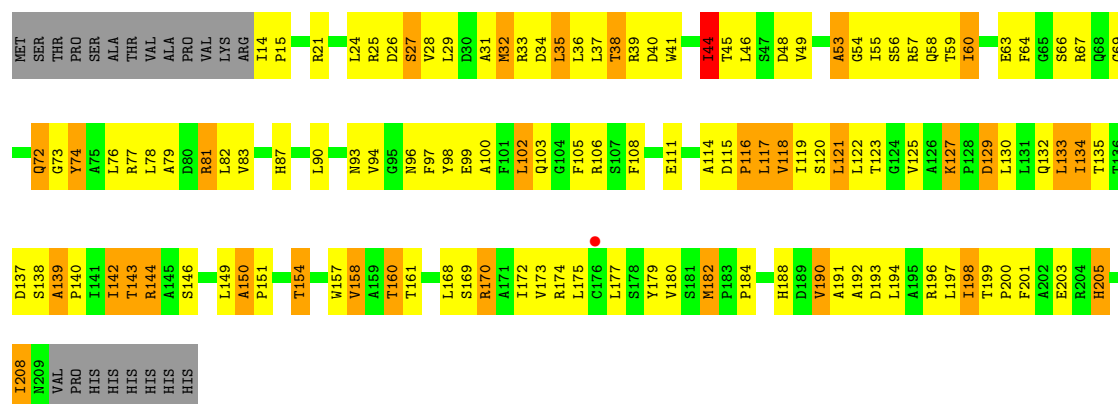


• Molecule 1: Rv3249c transcriptional regulator

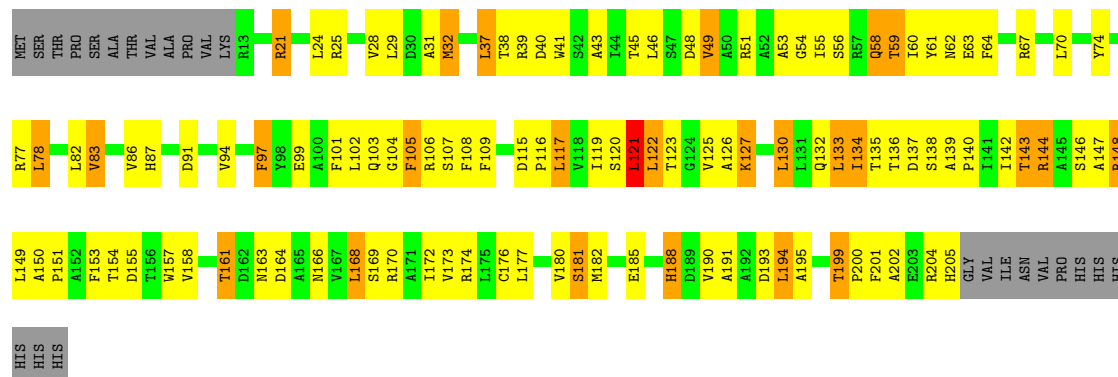




- Molecule 1: Rv3249c transcriptional regulator



- Molecule 1: Rv3249c transcriptional regulator



- Molecule 1: Rv3249c transcriptional regulator





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.05Å 75.49Å 125.36Å 90.00° 121.55° 90.00°	Depositor
Resolution (Å)	39.63 – 3.59 39.63 – 3.59	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.63-3.59) 95.5 (39.63-3.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 3.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.278 0.186 , 0.273	Depositor DCC
R_{free} test set	1082 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	91.8	Xtriage
Anisotropy	0.978	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9108	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: PLM

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	0.89	0/1522	1.42	14/2076 (0.7%)
1	B	0.86	0/1522	1.42	23/2076 (1.1%)
1	C	0.79	0/1500	1.27	11/2047 (0.5%)
1	D	0.80	0/1527	1.30	17/2084 (0.8%)
1	E	0.66	0/1511	1.13	3/2061 (0.1%)
1	F	0.61	0/1492	1.02	3/2035 (0.1%)
All	All	0.78	0/9074	1.27	71/12379 (0.6%)

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	MET	CA-C-N	13.04	133.81	120.38
1	A	182	MET	C-N-CA	13.04	133.81	120.38
1	A	57	ARG	N-CA-C	-11.16	98.64	111.03
1	D	139	ALA	CA-C-N	9.76	129.12	118.97
1	D	139	ALA	C-N-CA	9.76	129.12	118.97
1	A	125	VAL	N-CA-C	9.62	120.50	106.85
1	B	115	ASP	CA-C-N	9.53	129.18	119.56
1	B	115	ASP	C-N-CA	9.53	129.18	119.56
1	A	14	ILE	CA-C-N	9.50	131.71	119.84
1	A	14	ILE	C-N-CA	9.50	131.71	119.84
1	B	182	MET	CA-C-N	8.98	129.63	120.38
1	B	182	MET	C-N-CA	8.98	129.63	120.38
1	B	158	VAL	CB-CA-C	-8.49	100.93	111.88
1	D	158	VAL	CB-CA-C	-8.41	100.29	111.81
1	D	150	ALA	CA-C-N	8.04	128.79	119.47
1	D	150	ALA	C-N-CA	8.04	128.79	119.47
1	C	14	ILE	CA-C-N	7.83	128.31	119.93
1	C	14	ILE	C-N-CA	7.83	128.31	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	SER	N-CA-C	-7.63	103.08	113.30
1	D	208	ILE	N-CA-C	7.53	120.28	109.51
1	B	93	ASN	N-CA-C	7.46	122.50	112.88
1	B	150	ALA	CA-C-N	7.32	127.18	119.05
1	B	150	ALA	C-N-CA	7.32	127.18	119.05
1	B	127	LYS	CA-C-N	6.95	127.09	119.87
1	B	127	LYS	C-N-CA	6.95	127.09	119.87
1	B	205	HIS	N-CA-C	6.85	121.65	113.16
1	B	141	ILE	CB-CA-C	-6.75	103.06	111.70
1	C	123	THR	N-CA-C	6.45	121.31	113.38
1	D	44	ILE	CB-CA-C	-6.25	103.40	110.96
1	D	205	HIS	N-CA-C	6.09	120.42	112.92
1	D	123	THR	N-CA-C	6.08	118.82	111.40
1	B	67	ARG	N-CA-C	-6.08	104.77	111.82
1	A	34	ASP	N-CA-C	6.04	120.74	112.04
1	A	159	ALA	N-CA-C	-6.03	101.48	110.23
1	D	34	ASP	N-CA-C	6.02	118.74	111.40
1	D	38	THR	N-CA-C	5.94	120.66	113.17
1	C	31	ALA	CA-C-N	5.91	129.00	120.79
1	C	31	ALA	C-N-CA	5.91	129.00	120.79
1	F	125	VAL	N-CA-C	5.87	116.61	107.28
1	B	162	ASP	N-CA-C	5.85	118.13	111.11
1	F	182	MET	CA-C-N	5.85	126.41	120.38
1	F	182	MET	C-N-CA	5.85	126.41	120.38
1	B	46	LEU	N-CA-C	-5.84	104.55	111.03
1	D	160	THR	N-CA-C	-5.81	100.72	109.95
1	A	158	VAL	CB-CA-C	-5.76	104.45	111.88
1	D	191	ALA	N-CA-C	-5.70	104.98	111.14
1	B	28	VAL	CB-CA-C	-5.69	104.57	112.02
1	A	31	ALA	N-CA-C	-5.68	105.00	111.14
1	D	57	ARG	N-CA-C	-5.68	105.17	111.36
1	D	182	MET	CA-C-N	5.58	126.13	120.38
1	D	182	MET	C-N-CA	5.58	126.13	120.38
1	E	121	LEU	N-CA-C	-5.50	104.98	110.97
1	A	183	PRO	CA-C-N	5.43	125.44	119.90
1	A	183	PRO	C-N-CA	5.43	125.44	119.90
1	A	49	VAL	CB-CA-C	-5.40	104.96	112.04
1	A	205	HIS	N-CA-C	5.40	119.97	113.17
1	C	144	ARG	N-CA-C	5.27	116.71	110.97
1	B	158	VAL	CA-C-N	-5.23	115.46	122.42
1	B	158	VAL	C-N-CA	-5.23	115.46	122.42
1	B	95	GLY	N-CA-C	5.19	120.86	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ALA	CA-C-N	5.15	128.14	120.31
1	B	195	ALA	C-N-CA	5.15	128.14	120.31
1	C	187	ASP	N-CA-C	5.14	118.29	111.30
1	B	80	ASP	N-CA-C	5.11	117.98	111.69
1	E	37	LEU	N-CA-C	-5.10	105.91	111.82
1	E	49	VAL	N-CA-C	5.10	115.76	110.82
1	B	84	ASP	N-CA-C	5.09	119.59	113.17
1	C	115	ASP	CA-C-N	5.07	124.68	119.05
1	C	115	ASP	C-N-CA	5.07	124.68	119.05
1	D	53	ALA	N-CA-C	5.06	119.50	113.23
1	C	189	ASP	N-CA-C	-5.02	99.16	107.99

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	1495	0	1490	174	0
1	B	1495	0	1490	205	0
1	C	1473	0	1465	154	0
1	D	1500	0	1494	158	0
1	E	1484	0	1478	149	0
1	F	1465	0	1455	153	0
2	A	18	31	31	0	0
2	B	18	31	31	4	0
2	C	18	31	31	2	0
2	D	18	31	31	0	0
All	All	8984	124	8996	948	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 53.

All (948) 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:B:168:LEU:HD12	1:B:172:ILE:HD11	1.29	1.14
1:B:45:THR:H	1:B:48:ASP:HB2	1.07	1.13
1:D:32:MET:HE2	1:D:74:TYR:CD2	1.84	1.12
1:B:151:PRO:HA	1:B:154:THR:HG22	1.31	1.11
1:A:13:ARG:HD2	1:A:14:ILE:HG12	1.31	1.08
1:F:29:LEU:HD12	1:F:77:ARG:HD2	1.33	1.08
1:E:193:ASP:HB3	1:F:167:VAL:HG11	1.36	1.08
1:A:29:LEU:HB2	1:A:77:ARG:HH12	1.16	1.07
1:B:179:TYR:CE1	1:B:190:VAL:HG11	1.90	1.07
1:C:151:PRO:HA	1:C:154:THR:HG22	1.38	1.05
1:B:179:TYR:HE1	1:B:190:VAL:HG11	1.17	1.05
1:A:32:MET:CE	1:A:70:LEU:HG	1.89	1.02
1:B:127:LYS:HD2	1:B:130:LEU:HD12	1.36	1.02
1:C:134:ILE:HG22	1:C:177:LEU:HD11	1.38	1.02
1:D:151:PRO:HA	1:D:154:THR:HG23	1.42	1.01
1:E:28:VAL:HG12	1:E:29:LEU:HD23	1.42	0.97
1:D:32:MET:HE2	1:D:74:TYR:HD2	1.22	0.97
1:E:83:VAL:HG11	1:E:148:ARG:HG2	1.46	0.97
1:A:120:SER:O	1:A:127:LYS:NZ	2.00	0.95
1:D:149:LEU:HD23	1:D:169:SER:HB2	1.46	0.95
1:A:48:ASP:HA	1:A:51:ARG:HH12	1.32	0.94
1:A:151:PRO:HA	1:A:154:THR:HG22	1.50	0.93
1:C:179:TYR:CE1	1:C:190:VAL:HG11	2.04	0.93
1:B:168:LEU:CD1	1:B:172:ILE:HD11	1.98	0.92
1:B:35:LEU:HD12	1:B:49:VAL:HG12	1.47	0.92
1:B:168:LEU:HD12	1:B:172:ILE:CD1	2.00	0.92
1:F:119:ILE:HD12	1:F:123:THR:HG23	1.50	0.92
1:B:45:THR:N	1:B:48:ASP:HB2	1.85	0.91
1:B:45:THR:H	1:B:48:ASP:CB	1.82	0.91
1:B:121:LEU:HD11	1:B:134:ILE:CD1	2.00	0.91
1:E:39:ARG:HH22	1:E:43:ALA:HB1	1.33	0.90
1:A:29:LEU:HD21	1:A:64:PHE:CZ	2.07	0.90
1:E:182:MET:HB3	1:F:174:ARG:HH22	1.37	0.89
1:E:121:LEU:HD21	1:E:130:LEU:HD12	1.51	0.88
1:F:150:ALA:HB3	1:F:151:PRO:HD3	1.53	0.88
1:A:175:LEU:HD12	1:A:194:LEU:HD21	1.56	0.88
1:E:39:ARG:NH2	1:E:43:ALA:HB1	1.89	0.87
1:A:179:TYR:HD1	1:A:184:PRO:HD3	1.38	0.86
1:E:168:LEU:O	1:E:172:ILE:HG13	1.74	0.86
1:E:97:PHE:CZ	1:E:158:VAL:HG13	2.11	0.86
1:D:168:LEU:HD11	1:D:172:ILE:HD11	1.57	0.85
1:A:29:LEU:HB2	1:A:77:ARG:NH1	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:HA	1:A:51:ARG:NH1	1.91	0.85
1:D:35:LEU:HD12	1:D:35:LEU:H	1.40	0.85
1:B:35:LEU:CD1	1:B:49:VAL:HG12	2.06	0.85
1:F:142:ILE:HG23	1:F:143:THR:HG23	1.58	0.84
1:D:105:PHE:HE2	1:D:198:ILE:HD11	1.43	0.84
1:A:175:LEU:CD2	1:B:175:LEU:HG	2.08	0.84
1:E:97:PHE:HZ	1:E:158:VAL:HG13	1.42	0.83
1:E:121:LEU:HD21	1:E:130:LEU:CD1	2.08	0.83
1:E:32:MET:HE3	1:E:74:TYR:HD2	1.43	0.81
1:B:46:LEU:HD23	1:B:70:LEU:HD23	1.60	0.81
1:A:13:ARG:CD	1:A:14:ILE:HG12	2.10	0.81
1:C:167:VAL:HG22	1:D:193:ASP:HB3	1.61	0.81
1:A:32:MET:HE3	1:A:70:LEU:HG	1.60	0.81
1:A:160:THR:CG2	1:A:165:ALA:HB2	2.10	0.80
1:E:32:MET:CE	1:E:74:TYR:HB2	2.12	0.80
1:F:86:VAL:HG11	1:F:149:LEU:HD11	1.62	0.80
1:A:46:LEU:HD23	1:A:61:TYR:CZ	2.17	0.79
1:C:29:LEU:HB2	1:C:77:ARG:HH12	1.45	0.79
1:C:45:THR:HG22	1:C:47:SER:H	1.48	0.79
1:F:32:MET:HE2	1:F:74:TYR:CD2	2.17	0.79
1:B:32:MET:HA	1:B:35:LEU:HB2	1.65	0.79
1:D:168:LEU:CD1	1:D:172:ILE:HD11	2.12	0.79
1:A:46:LEU:HD23	1:A:61:TYR:CE1	2.18	0.78
1:A:80:ASP:HB3	1:A:148:ARG:NH2	1.99	0.78
1:E:58:GLN:O	1:E:62:ASN:ND2	2.16	0.78
1:F:158:VAL:HG12	1:F:160:THR:HG23	1.66	0.78
1:C:185:GLU:OE2	1:C:185:GLU:N	2.16	0.78
1:F:32:MET:SD	1:F:70:LEU:HD11	2.22	0.78
1:B:54:GLY:C	1:B:55:ILE:HD12	2.09	0.78
1:B:90:LEU:HD13	1:B:156:THR:HG21	1.64	0.78
1:E:97:PHE:CE2	1:E:202:ALA:HB1	2.19	0.78
1:F:34:ASP:HA	1:F:37:LEU:HD12	1.65	0.77
1:C:45:THR:HB	1:C:48:ASP:H	1.49	0.77
1:A:28:VAL:O	1:A:31:ALA:N	2.17	0.77
1:D:105:PHE:CE2	1:D:198:ILE:HD11	2.20	0.77
1:F:31:ALA:HB2	1:F:53:ALA:HB2	1.66	0.77
1:D:96:ASN:OD1	1:D:99:GLU:HB2	1.84	0.76
1:C:97:PHE:CE1	1:C:202:ALA:HB1	2.19	0.76
1:D:120:SER:O	1:D:127:LYS:NZ	2.16	0.76
1:D:55:ILE:HG22	1:D:56:SER:O	1.85	0.76
1:E:148:ARG:O	1:E:151:PRO:HD2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:HE3	1:E:74:TYR:CD2	2.21	0.76
1:C:32:MET:HE2	1:C:74:TYR:CD2	2.20	0.76
1:B:80:ASP:HA	1:B:83:VAL:HG12	1.65	0.75
1:D:38:THR:HG23	1:D:39:ARG:HG3	1.69	0.75
1:A:45:THR:HB	1:A:48:ASP:H	1.52	0.75
1:C:174:ARG:NH2	1:D:182:MET:HG3	2.02	0.75
1:D:53:ALA:CB	1:D:55:ILE:HG12	2.16	0.75
1:A:138:SER:HB3	1:A:142:ILE:HD12	1.69	0.75
1:F:94:VAL:HG13	1:F:157:TRP:CD2	2.22	0.74
1:F:94:VAL:HG22	1:F:157:TRP:CD1	2.21	0.74
1:F:94:VAL:HG22	1:F:157:TRP:NE1	2.02	0.74
1:B:140:PRO:HA	1:B:143:THR:HG22	1.68	0.74
1:C:105:PHE:CE1	1:C:194:LEU:HD13	2.22	0.73
1:C:172:ILE:HD11	1:C:198:ILE:HD13	1.70	0.73
1:C:174:ARG:HH22	1:D:182:MET:HG3	1.52	0.73
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.69	0.73
1:D:102:LEU:HD23	1:D:192:ALA:HA	1.71	0.73
1:B:102:LEU:HD11	1:B:106:ARG:NE	2.03	0.73
1:D:36:LEU:HD13	1:D:117:LEU:HD23	1.71	0.73
1:F:190:VAL:HG12	1:F:194:LEU:HD11	1.70	0.73
1:A:170:ARG:HD3	1:B:188:HIS:HE1	1.53	0.73
1:D:132:GLN:HG3	1:D:137:ASP:OD2	1.89	0.73
1:B:76:LEU:HD12	1:B:76:LEU:H	1.54	0.72
1:E:127:LYS:HB3	1:E:130:LEU:HB2	1.71	0.72
1:A:93:ASN:OD1	1:A:93:ASN:N	2.22	0.72
1:B:204:ARG:HG3	1:B:205:HIS:ND1	2.04	0.72
1:F:83:VAL:HG11	1:F:148:ARG:HD3	1.71	0.72
1:F:121:LEU:HD11	1:F:134:ILE:HD11	1.70	0.72
1:C:39:ARG:HD2	1:C:43:ALA:CB	2.19	0.72
1:C:175:LEU:O	1:C:178:SER:OG	2.03	0.72
1:E:149:LEU:HD21	1:E:153:PHE:HE2	1.55	0.72
1:F:109:PHE:CE2	1:F:191:ALA:HB2	2.25	0.72
1:D:150:ALA:HB3	1:D:151:PRO:HD3	1.72	0.72
1:E:185:GLU:O	1:E:188:HIS:HB2	1.90	0.72
1:B:185:GLU:OE1	1:B:185:GLU:N	2.14	0.71
1:D:45:THR:H	1:D:48:ASP:HB2	1.55	0.71
1:B:94:VAL:HA	1:B:157:TRP:CE2	2.26	0.71
1:F:46:LEU:HD12	1:F:61:TYR:CE1	2.24	0.71
1:A:175:LEU:HD23	1:B:175:LEU:HG	1.70	0.71
1:D:169:SER:O	1:D:173:VAL:HG23	1.91	0.71
1:E:139:ALA:O	1:E:143:THR:OG1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:O	1:B:60:ILE:HG22	1.91	0.71
1:B:102:LEU:HD13	1:B:106:ARG:HG3	1.72	0.70
1:D:74:TYR:HD1	1:D:74:TYR:C	1.99	0.70
1:E:182:MET:HB2	1:F:174:ARG:HH12	1.56	0.70
1:A:160:THR:HG22	1:A:165:ALA:HB2	1.72	0.70
1:F:142:ILE:HD12	1:F:173:VAL:CG1	2.21	0.70
1:A:142:ILE:HD11	1:B:182:MET:SD	2.31	0.70
1:A:166:ASN:HB3	1:A:170:ARG:HH21	1.54	0.70
1:D:25:ARG:CG	1:D:63:GLU:HG3	2.21	0.70
1:E:41:TRP:O	1:E:67:ARG:NH2	2.25	0.70
1:B:159:ALA:O	1:B:207:VAL:HG12	1.92	0.69
1:A:55:ILE:HG22	1:A:56:SER:N	2.07	0.69
1:B:40:ASP:OD1	1:B:127:LYS:NZ	2.24	0.69
1:D:77:ARG:NH1	1:D:81:ARG:HH22	1.90	0.69
1:B:28:VAL:O	1:B:31:ALA:HB3	1.93	0.69
1:E:168:LEU:HD11	1:E:172:ILE:HD11	1.73	0.69
1:A:199:THR:HB	1:A:200:PRO:HD3	1.75	0.69
1:B:66:SER:OG	1:B:69:GLY:N	2.25	0.69
1:B:72:GLN:O	1:B:72:GLN:HG3	1.91	0.69
1:A:55:ILE:HG22	1:A:56:SER:H	1.57	0.69
1:C:151:PRO:HA	1:C:154:THR:CG2	2.21	0.69
1:E:28:VAL:HG11	1:E:60:ILE:HD11	1.75	0.69
1:E:169:SER:O	1:E:173:VAL:HG23	1.93	0.68
1:F:90:LEU:CD2	1:F:100:ALA:HB1	2.24	0.68
1:E:45:THR:HG22	1:E:46:LEU:H	1.57	0.68
1:C:33:ARG:O	1:C:37:LEU:HD12	1.93	0.68
1:E:46:LEU:HD22	1:E:60:ILE:HG23	1.75	0.68
1:B:104:GLY:HA3	2:B:301:PLM:O2	1.92	0.68
1:D:29:LEU:HB3	1:D:77:ARG:HH21	1.59	0.68
1:E:177:LEU:O	1:E:180:VAL:HB	1.92	0.68
1:C:29:LEU:CB	1:C:77:ARG:HH12	2.07	0.68
1:D:83:VAL:CG2	1:D:149:LEU:HB2	2.24	0.68
1:A:121:LEU:HD23	1:A:122:LEU:HD23	1.74	0.68
1:B:121:LEU:HB3	1:B:122:LEU:HD23	1.75	0.68
1:C:32:MET:HE1	1:C:71:ALA:HA	1.74	0.68
1:C:68:GLN:OE1	1:C:133:LEU:HD12	1.93	0.68
1:E:83:VAL:HG23	1:E:149:LEU:HD13	1.76	0.68
1:B:43:ALA:C	1:B:44:ILE:HD13	2.18	0.68
1:B:47:SER:HB3	1:B:57:ARG:CG	2.24	0.68
1:B:94:VAL:HA	1:B:157:TRP:NE1	2.09	0.68
1:D:66:SER:O	1:D:69:GLY:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:LEU:CD1	1:F:134:ILE:HD11	2.24	0.67
1:A:150:ALA:HB3	1:A:151:PRO:HD3	1.76	0.67
1:A:35:LEU:HD11	1:A:52:ALA:CB	2.24	0.67
1:F:120:SER:O	1:F:127:LYS:NZ	2.22	0.67
1:C:21:ARG:HG3	1:C:22:ALA:N	2.07	0.67
1:D:74:TYR:C	1:D:74:TYR:CD1	2.73	0.67
1:A:55:ILE:CG2	1:A:59:THR:HB	2.25	0.67
1:B:108:PHE:CZ	1:B:176:CYS:HB3	2.30	0.67
1:D:32:MET:CE	1:D:74:TYR:HD2	2.04	0.67
1:E:83:VAL:CG1	1:E:148:ARG:HG2	2.21	0.67
1:D:76:LEU:O	1:D:79:ALA:HB3	1.95	0.67
1:D:54:GLY:C	1:D:55:ILE:HD13	2.19	0.67
1:A:199:THR:HB	1:A:200:PRO:CD	2.25	0.67
1:B:45:THR:HB	1:B:48:ASP:H	1.60	0.67
1:E:168:LEU:HD22	1:E:201:PHE:CD2	2.30	0.67
1:A:13:ARG:HD2	1:A:14:ILE:CG1	2.18	0.66
1:D:25:ARG:HG2	1:D:63:GLU:HG3	1.78	0.66
1:D:133:LEU:HD12	1:D:133:LEU:O	1.96	0.66
1:B:55:ILE:HG22	1:B:56:SER:N	2.11	0.66
1:B:179:TYR:CE1	1:B:190:VAL:CG1	2.75	0.66
1:F:121:LEU:CD2	1:F:130:LEU:HD13	2.25	0.66
1:D:83:VAL:HG23	1:D:149:LEU:HB2	1.78	0.66
1:F:15:PRO:HB2	1:F:18:GLU:HG2	1.76	0.66
1:B:188:HIS:CD2	1:B:188:HIS:H	2.10	0.66
1:D:60:ILE:HG22	1:D:64:PHE:HD2	1.60	0.66
1:A:39:ARG:HG3	1:A:40:ASP:N	2.11	0.66
1:B:199:THR:HB	1:B:200:PRO:HD3	1.78	0.66
1:D:45:THR:HG22	1:D:46:LEU:H	1.60	0.65
1:E:29:LEU:HD21	1:E:64:PHE:CZ	2.31	0.65
1:A:33:ARG:O	1:A:33:ARG:HG3	1.96	0.65
1:D:53:ALA:HB1	1:D:55:ILE:HG12	1.79	0.65
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.59	0.65
1:E:46:LEU:HD22	1:E:60:ILE:CG2	2.27	0.65
1:F:119:ILE:CD1	1:F:123:THR:HG23	2.25	0.65
1:A:175:LEU:HD21	1:B:175:LEU:HG	1.79	0.65
1:E:83:VAL:CG2	1:E:149:LEU:HB2	2.27	0.65
1:F:80:ASP:HA	1:F:83:VAL:HG12	1.79	0.65
1:F:90:LEU:HD11	1:F:153:PHE:CE1	2.32	0.65
1:F:102:LEU:HD11	1:F:106:ARG:HE	1.62	0.65
1:B:76:LEU:HD12	1:B:76:LEU:N	2.11	0.65
1:B:32:MET:HE2	1:B:36:LEU:HD11	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:THR:HG23	1:C:155:ASP:OD1	1.96	0.64
1:F:55:ILE:HG22	1:F:59:THR:HB	1.78	0.64
1:B:128:PRO:O	1:B:132:GLN:NE2	2.29	0.64
1:C:23:LEU:O	1:C:27:SER:HB3	1.96	0.64
1:A:40:ASP:O	1:A:43:ALA:N	2.28	0.64
1:B:186:ALA:HB3	1:B:188:HIS:CD2	2.33	0.64
1:C:201:PHE:CD1	1:D:197:LEU:HA	2.32	0.64
1:D:77:ARG:HD2	1:D:81:ARG:NH1	2.11	0.64
1:E:97:PHE:HE1	1:E:158:VAL:HG22	1.62	0.64
1:B:179:TYR:HD1	1:B:184:PRO:HG3	1.63	0.64
1:D:55:ILE:CG2	1:D:59:THR:HB	2.28	0.64
1:B:76:LEU:HD23	1:B:144:ARG:HD2	1.79	0.64
1:C:78:LEU:HD13	2:C:301:PLM:HE1	1.78	0.64
1:B:97:PHE:HD1	1:B:101:PHE:HE2	1.46	0.64
1:E:168:LEU:HD22	1:E:201:PHE:HD2	1.63	0.64
1:A:54:GLY:C	1:A:55:ILE:HD12	2.21	0.64
1:B:165:ALA:O	1:B:169:SER:HB2	1.98	0.64
1:F:31:ALA:CB	1:F:53:ALA:HB2	2.28	0.64
1:B:70:LEU:HD12	1:B:70:LEU:O	1.97	0.64
1:B:151:PRO:HA	1:B:154:THR:CG2	2.20	0.63
1:E:125:VAL:HG12	1:E:126:ALA:N	2.13	0.63
1:B:168:LEU:HD22	1:B:201:PHE:CD2	2.33	0.63
1:A:166:ASN:CB	1:A:170:ARG:HH21	2.11	0.63
1:C:39:ARG:HD2	1:C:43:ALA:HB1	1.78	0.63
1:F:90:LEU:HD22	1:F:100:ALA:HB1	1.78	0.63
1:E:25:ARG:NE	1:E:63:GLU:OE1	2.32	0.63
1:A:179:TYR:CE2	1:B:174:ARG:HD3	2.33	0.63
1:F:135:THR:OG1	1:F:136:THR:N	2.30	0.63
1:A:37:LEU:O	1:A:37:LEU:HD23	1.99	0.62
1:B:90:LEU:CD1	1:B:156:THR:HG21	2.29	0.62
1:B:150:ALA:HB3	1:B:151:PRO:HD3	1.80	0.62
1:A:32:MET:HE2	1:A:70:LEU:HD23	1.80	0.62
1:A:115:ASP:OD2	1:A:117:LEU:N	2.30	0.62
1:D:158:VAL:HG12	1:D:160:THR:CG2	2.29	0.62
1:E:74:TYR:HD1	1:E:74:TYR:O	1.82	0.62
1:A:46:LEU:CD2	1:A:61:TYR:CE1	2.82	0.62
1:B:97:PHE:CE1	1:B:202:ALA:HB1	2.34	0.62
1:F:121:LEU:HD23	1:F:130:LEU:HD13	1.81	0.62
1:A:29:LEU:HD21	1:A:64:PHE:CE1	2.35	0.62
1:A:32:MET:CE	1:A:70:LEU:CG	2.72	0.62
1:A:135:THR:OG1	1:A:136:THR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD1	1:A:194:LEU:HD21	2.29	0.62
1:B:47:SER:HB3	1:B:57:ARG:HD3	1.80	0.62
1:D:24:LEU:HD21	1:D:59:THR:HG22	1.81	0.61
1:E:168:LEU:O	1:E:168:LEU:HD12	1.99	0.61
1:E:188:HIS:CD2	1:F:170:ARG:HH12	2.18	0.61
1:A:108:PHE:CZ	1:A:176:CYS:HB3	2.35	0.61
1:A:190:VAL:HG13	1:A:194:LEU:HD12	1.82	0.61
1:F:109:PHE:HE2	1:F:191:ALA:HB2	1.64	0.61
1:C:118:VAL:O	1:C:121:LEU:HB3	2.00	0.61
1:C:102:LEU:HD22	1:C:102:LEU:O	2.00	0.61
1:E:83:VAL:HG21	1:E:149:LEU:HB2	1.82	0.61
1:A:32:MET:HE2	1:A:70:LEU:CD2	2.29	0.61
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.65	0.61
1:B:185:GLU:H	1:B:185:GLU:CD	2.07	0.61
1:F:182:MET:SD	1:F:183:PRO:HD2	2.40	0.61
1:A:152:ALA:O	1:A:156:THR:HG23	2.00	0.61
1:B:33:ARG:O	1:B:37:LEU:HD13	2.01	0.61
1:E:38:THR:C	1:E:39:ARG:HG3	2.24	0.61
1:E:45:THR:O	1:E:49:VAL:HG23	2.00	0.61
1:F:97:PHE:CE1	1:F:158:VAL:HG13	2.36	0.61
1:A:80:ASP:HB3	1:A:148:ARG:HH21	1.63	0.61
1:E:29:LEU:HB2	1:E:77:ARG:HH11	1.66	0.61
1:E:132:GLN:HG3	1:E:136:THR:HB	1.83	0.61
1:B:46:LEU:CD2	1:B:70:LEU:HD23	2.30	0.60
1:D:45:THR:N	1:D:48:ASP:HB2	2.16	0.60
1:D:199:THR:HB	1:D:200:PRO:HD3	1.83	0.60
1:A:96:ASN:OD1	1:A:99:GLU:HB2	2.01	0.60
1:A:159:ALA:HB1	1:A:207:VAL:H	1.65	0.60
1:C:153:PHE:O	1:C:158:VAL:HB	2.00	0.60
1:E:40:ASP:OD1	1:E:120:SER:OG	2.18	0.60
1:B:77:ARG:O	1:B:80:ASP:N	2.35	0.60
1:D:53:ALA:HB3	1:D:55:ILE:HG12	1.83	0.60
1:D:149:LEU:O	1:D:149:LEU:HG	2.01	0.60
1:A:112:SER:O	1:A:118:VAL:HG11	2.01	0.60
1:A:118:VAL:HG12	1:A:119:ILE:N	2.16	0.60
1:B:127:LYS:O	1:B:131:LEU:HG	2.01	0.60
1:E:168:LEU:CD1	1:E:172:ILE:HD11	2.31	0.60
1:B:41:TRP:CZ2	1:B:67:ARG:HG2	2.36	0.60
1:F:24:LEU:O	1:F:24:LEU:HD12	2.00	0.60
1:A:39:ARG:HG3	1:A:40:ASP:H	1.64	0.60
1:F:44:ILE:HG23	1:F:48:ASP:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD21	1:A:41:TRP:HB2	1.84	0.60
1:E:121:LEU:N	1:E:121:LEU:HD23	2.16	0.60
1:F:29:LEU:CD1	1:F:77:ARG:HD2	2.22	0.60
1:D:83:VAL:HG23	1:D:149:LEU:CD1	2.32	0.60
1:B:55:ILE:HD12	1:B:55:ILE:N	2.17	0.59
1:C:204:ARG:HG2	1:C:205:HIS:CE1	2.37	0.59
1:B:45:THR:OG1	1:B:48:ASP:OD2	2.20	0.59
1:F:127:LYS:HB3	1:F:130:LEU:HB2	1.84	0.59
1:B:55:ILE:HG22	1:B:56:SER:H	1.66	0.59
1:E:116:PRO:HA	1:E:119:ILE:HD12	1.84	0.59
1:A:32:MET:HE2	1:A:70:LEU:HG	1.81	0.59
1:A:55:ILE:HD12	1:A:55:ILE:N	2.18	0.59
1:D:97:PHE:HE1	1:D:158:VAL:HG22	1.68	0.59
1:F:107:SER:O	1:F:111:GLU:HB2	2.03	0.59
1:C:170:ARG:O	1:C:174:ARG:HB2	2.02	0.59
1:D:45:THR:HG22	1:D:46:LEU:N	2.16	0.59
1:E:150:ALA:HB3	1:E:151:PRO:HD3	1.85	0.59
1:D:41:TRP:NE1	1:D:67:ARG:HH21	2.01	0.59
1:D:44:ILE:HD13	1:D:44:ILE:N	2.18	0.59
1:F:90:LEU:HD11	1:F:153:PHE:HE1	1.67	0.59
1:F:94:VAL:HG13	1:F:157:TRP:CE2	2.38	0.59
1:A:181:SER:O	1:A:183:PRO:HD3	2.03	0.58
1:B:36:LEU:CD1	1:B:117:LEU:HD23	2.33	0.58
1:C:45:THR:HG22	1:C:47:SER:N	2.17	0.58
1:C:139:ALA:N	1:C:140:PRO:HD2	2.18	0.58
1:B:135:THR:OG1	1:B:136:THR:N	2.31	0.58
1:A:94:VAL:HG13	1:A:157:TRP:CD1	2.38	0.58
1:B:32:MET:SD	1:B:74:TYR:HD2	2.26	0.58
1:B:133:LEU:O	1:B:138:SER:HA	2.03	0.58
1:A:101:PHE:HE1	1:A:153:PHE:HE1	1.50	0.58
1:A:161:THR:HG23	1:A:205:HIS:O	2.04	0.58
1:C:94:VAL:HG22	1:C:157:TRP:NE1	2.19	0.58
1:E:193:ASP:CB	1:F:167:VAL:HG11	2.24	0.58
1:A:36:LEU:CD2	1:A:41:TRP:HB2	2.33	0.58
1:A:188:HIS:CD2	1:B:170:ARG:HH11	2.21	0.58
1:C:135:THR:OG1	1:C:136:THR:N	2.36	0.58
1:F:49:VAL:HG21	1:F:70:LEU:HD21	1.86	0.58
1:F:75:ALA:O	1:F:78:LEU:N	2.34	0.58
1:D:29:LEU:CB	1:D:77:ARG:NH2	2.66	0.58
1:E:83:VAL:HG13	1:E:148:ARG:HD2	1.86	0.58
1:F:125:VAL:O	1:F:127:LYS:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:SER:HB3	1:B:57:ARG:HG3	1.86	0.58
1:B:156:THR:HG23	1:B:157:TRP:N	2.19	0.58
1:C:94:VAL:HG13	1:C:157:TRP:CG	2.39	0.58
1:D:78:LEU:HD23	1:D:78:LEU:O	2.04	0.58
1:A:132:GLN:O	1:A:132:GLN:HG3	2.04	0.58
1:D:117:LEU:O	1:D:120:SER:N	2.36	0.58
1:E:195:ALA:O	1:E:199:THR:OG1	2.21	0.58
1:B:21:ARG:HA	1:B:24:LEU:HB3	1.85	0.57
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.69	0.57
1:C:29:LEU:HD12	1:C:77:ARG:NH1	2.19	0.57
1:A:190:VAL:CG1	1:A:194:LEU:HD12	2.34	0.57
1:B:41:TRP:CZ2	1:B:71:ALA:HB2	2.39	0.57
1:B:117:LEU:O	1:B:120:SER:HB3	2.04	0.57
1:B:189:ASP:OD1	1:B:192:ALA:HB2	2.03	0.57
1:C:39:ARG:HD2	1:C:43:ALA:HB3	1.85	0.57
1:D:118:VAL:HG22	1:D:180:VAL:HG12	1.87	0.57
1:D:158:VAL:HG12	1:D:160:THR:HG22	1.86	0.57
1:E:182:MET:CB	1:F:174:ARG:HH12	2.17	0.57
1:A:61:TYR:O	1:A:65:GLY:HA2	2.04	0.57
1:C:67:ARG:HD2	1:C:67:ARG:C	2.29	0.57
1:A:81:ARG:HG2	1:A:81:ARG:NH1	2.20	0.57
1:C:175:LEU:HD13	1:C:194:LEU:HD21	1.86	0.57
1:D:32:MET:HE2	1:D:74:TYR:CG	2.38	0.57
1:E:78:LEU:HD11	1:E:115:ASP:CG	2.30	0.57
1:F:186:ALA:HB3	1:F:188:HIS:CE1	2.40	0.57
1:C:74:TYR:CD1	1:C:74:TYR:C	2.83	0.57
1:C:175:LEU:HD21	1:D:175:LEU:HG	1.87	0.57
1:B:21:ARG:O	1:B:24:LEU:HB3	2.04	0.57
1:B:173:VAL:HG13	2:B:301:PLM:H71	1.86	0.57
1:E:139:ALA:HB2	1:F:182:MET:CE	2.35	0.57
1:F:133:LEU:HD11	1:F:141:ILE:HD11	1.85	0.57
1:B:97:PHE:HD1	1:B:101:PHE:CE2	2.23	0.57
1:C:32:MET:HE2	1:C:74:TYR:CG	2.40	0.57
1:A:55:ILE:HG22	1:A:59:THR:HB	1.86	0.57
1:A:179:TYR:CD1	1:A:184:PRO:HD3	2.30	0.57
1:E:121:LEU:HD11	1:E:130:LEU:HD12	1.87	0.57
1:F:151:PRO:HA	1:F:154:THR:CG2	2.35	0.57
1:F:190:VAL:HG12	1:F:194:LEU:CD1	2.36	0.56
1:C:96:ASN:ND2	1:C:99:GLU:HG3	2.19	0.56
1:D:106:ARG:HG2	1:D:106:ARG:HH11	1.70	0.56
1:E:149:LEU:HG	1:E:149:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD13	1:C:49:VAL:HG23	1.88	0.56
1:A:32:MET:HE2	1:A:70:LEU:CG	2.35	0.56
1:A:179:TYR:CE1	1:A:190:VAL:HG11	2.40	0.56
1:C:179:TYR:HE1	1:C:190:VAL:HG11	1.64	0.56
1:D:24:LEU:HD21	1:D:59:THR:CG2	2.35	0.56
1:C:156:THR:HG23	1:C:158:VAL:H	1.70	0.56
1:E:109:PHE:HZ	1:E:194:LEU:CD1	2.19	0.56
1:D:32:MET:HA	1:D:35:LEU:CD1	2.35	0.56
1:F:142:ILE:HD12	1:F:173:VAL:HG11	1.87	0.56
1:A:79:ALA:O	1:A:83:VAL:HG13	2.06	0.55
1:D:93:ASN:ND2	1:D:103:GLN:OE1	2.39	0.55
1:B:189:ASP:O	1:B:192:ALA:HB3	2.06	0.55
1:C:60:ILE:HG22	1:C:61:TYR:N	2.21	0.55
1:C:172:ILE:HD11	1:C:198:ILE:CD1	2.35	0.55
1:C:94:VAL:HG13	1:C:157:TRP:CD2	2.41	0.55
1:E:139:ALA:N	1:E:140:PRO:HD2	2.20	0.55
1:D:38:THR:C	1:D:39:ARG:HG3	2.32	0.55
1:D:83:VAL:HG23	1:D:149:LEU:HD13	1.88	0.55
1:B:15:PRO:O	1:B:18:GLU:HB3	2.07	0.55
1:B:83:VAL:CG2	1:B:149:LEU:HB2	2.36	0.55
1:C:168:LEU:HD12	1:C:201:PHE:CD2	2.42	0.55
1:E:45:THR:H	1:E:48:ASP:HB2	1.71	0.55
1:E:29:LEU:HD23	1:E:29:LEU:N	2.20	0.55
1:B:44:ILE:O	1:B:67:ARG:HD2	2.06	0.55
1:B:45:THR:HB	1:B:48:ASP:N	2.22	0.55
1:B:188:HIS:H	1:B:188:HIS:HD2	1.52	0.55
1:E:142:ILE:HA	1:E:173:VAL:HG11	1.87	0.55
1:F:70:LEU:HD12	1:F:70:LEU:O	2.07	0.55
1:A:154:THR:HG23	1:A:155:ASP:OD1	2.07	0.55
1:A:188:HIS:CD2	1:B:170:ARG:NH1	2.74	0.55
1:B:96:ASN:N	1:B:96:ASN:OD1	2.40	0.55
1:F:133:LEU:CD1	1:F:141:ILE:HD11	2.37	0.55
1:B:94:VAL:HG22	1:B:157:TRP:CD1	2.42	0.55
1:B:102:LEU:HD13	1:B:102:LEU:C	2.31	0.55
1:A:157:TRP:HE3	1:A:157:TRP:O	1.90	0.54
1:B:47:SER:HB3	1:B:57:ARG:CD	2.37	0.54
1:F:168:LEU:O	1:F:172:ILE:HG13	2.07	0.54
1:B:102:LEU:CD1	1:B:106:ARG:HG3	2.37	0.54
1:F:24:LEU:HD12	1:F:24:LEU:C	2.32	0.54
1:F:55:ILE:CG2	1:F:59:THR:HB	2.38	0.54
1:B:21:ARG:HG3	1:B:22:ALA:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:O	1:C:38:THR:HG23	2.07	0.54
1:E:109:PHE:CZ	1:E:194:LEU:CD1	2.91	0.54
1:F:115:ASP:OD1	1:F:117:LEU:N	2.40	0.54
1:A:196:ARG:HH22	1:B:164:ASP:CG	2.16	0.54
1:C:28:VAL:CG1	1:C:60:ILE:HD11	2.38	0.54
1:C:182:MET:HB2	1:D:174:ARG:HH12	1.73	0.54
1:F:37:LEU:HD23	1:F:116:PRO:HG3	1.90	0.54
1:A:160:THR:HG21	1:A:165:ALA:HB2	1.90	0.54
1:E:28:VAL:CG1	1:E:60:ILE:HD11	2.38	0.54
1:C:91:ASP:HA	1:C:157:TRP:HE1	1.73	0.54
1:D:28:VAL:O	1:D:31:ALA:HB3	2.08	0.54
1:C:199:THR:HB	1:C:200:PRO:HD3	1.90	0.54
1:F:83:VAL:HG21	1:F:148:ARG:HB3	1.89	0.54
1:E:48:ASP:OD1	1:E:51:ARG:NH2	2.38	0.54
1:C:78:LEU:O	1:C:82:LEU:HD12	2.08	0.53
1:C:175:LEU:CD1	1:C:194:LEU:HD21	2.38	0.53
1:E:45:THR:HG22	1:E:46:LEU:N	2.23	0.53
1:B:23:LEU:O	1:B:23:LEU:HD12	2.09	0.53
1:C:26:ASP:OD1	1:C:26:ASP:N	2.42	0.53
1:C:28:VAL:O	1:C:31:ALA:HB3	2.09	0.53
1:E:54:GLY:C	1:E:55:ILE:HD12	2.33	0.53
1:E:108:PHE:CZ	1:E:176:CYS:HB3	2.43	0.53
1:C:45:THR:HG22	1:C:46:LEU:N	2.24	0.53
1:A:53:ALA:HB3	1:A:55:ILE:HD13	1.90	0.53
1:B:140:PRO:O	1:B:143:THR:HG22	2.08	0.53
1:F:102:LEU:HD11	1:F:106:ARG:NE	2.23	0.53
1:F:144:ARG:HH12	1:F:148:ARG:NE	2.06	0.53
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.24	0.53
1:E:102:LEU:HD13	1:E:102:LEU:C	2.34	0.53
1:F:169:SER:O	1:F:173:VAL:HG23	2.09	0.53
1:F:184:PRO:HB3	1:F:190:VAL:CG2	2.39	0.53
1:B:121:LEU:HD11	1:B:134:ILE:HD11	1.87	0.53
1:C:167:VAL:HG22	1:D:193:ASP:CB	2.35	0.53
1:F:57:ARG:O	1:F:60:ILE:HG22	2.09	0.53
1:F:193:ASP:O	1:F:196:ARG:HB3	2.09	0.53
1:B:179:TYR:CD1	1:B:184:PRO:HG3	2.44	0.53
1:D:58:GLN:O	1:D:58:GLN:HG3	2.08	0.53
1:F:29:LEU:HD21	1:F:64:PHE:CZ	2.44	0.53
1:A:45:THR:HG22	1:A:46:LEU:N	2.24	0.52
1:F:86:VAL:HG11	1:F:149:LEU:CD1	2.38	0.52
1:B:151:PRO:CA	1:B:154:THR:HG22	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASN:HB2	1:C:99:GLU:HB2	1.91	0.52
1:D:28:VAL:HG11	1:D:64:PHE:CE2	2.43	0.52
1:F:97:PHE:HD2	1:F:203:GLU:HG3	1.74	0.52
1:A:204:ARG:HH22	1:B:203:GLU:HB2	1.75	0.52
1:C:41:TRP:HA	1:C:44:ILE:HG12	1.91	0.52
1:E:139:ALA:HB2	1:F:182:MET:HE2	1.91	0.52
1:F:139:ALA:HB3	1:F:140:PRO:CD	2.40	0.52
1:E:142:ILE:O	1:E:146:SER:HB3	2.09	0.52
1:B:108:PHE:CD1	1:B:108:PHE:C	2.88	0.52
1:B:121:LEU:HD11	1:B:134:ILE:HD13	1.85	0.52
1:C:128:PRO:HA	1:C:131:LEU:HD12	1.92	0.52
1:A:105:PHE:HZ	1:A:172:ILE:HD13	1.74	0.52
1:E:31:ALA:CB	1:E:53:ALA:HB2	2.40	0.52
1:B:144:ARG:CG	1:B:145:ALA:N	2.71	0.52
1:E:29:LEU:HB2	1:E:77:ARG:NH1	2.25	0.52
1:C:28:VAL:HG13	1:C:60:ILE:HD11	1.92	0.52
1:C:61:TYR:CD1	1:C:61:TYR:C	2.88	0.52
1:F:175:LEU:CD1	1:F:194:LEU:HD22	2.40	0.52
1:A:28:VAL:CG1	1:A:60:ILE:HD11	2.39	0.52
1:A:156:THR:OG1	1:A:157:TRP:N	2.41	0.52
1:B:46:LEU:CD1	1:B:61:TYR:HB2	2.40	0.52
1:B:55:ILE:CG2	1:B:56:SER:H	2.23	0.52
1:A:83:VAL:O	1:A:86:VAL:HG12	2.09	0.52
1:C:41:TRP:CD1	1:C:130:LEU:HD21	2.45	0.52
1:E:32:MET:HE3	1:E:74:TYR:HB2	1.90	0.52
1:C:174:ARG:NH1	1:D:179:TYR:CD1	2.78	0.51
1:E:53:ALA:HB3	1:E:55:ILE:HD13	1.93	0.51
1:E:122:LEU:HD23	1:E:122:LEU:N	2.25	0.51
1:E:191:ALA:O	1:E:194:LEU:HB2	2.09	0.51
1:A:157:TRP:O	1:A:157:TRP:CE3	2.62	0.51
1:A:175:LEU:HD12	1:A:194:LEU:CD2	2.36	0.51
1:C:55:ILE:HG22	1:C:56:SER:N	2.25	0.51
1:C:149:LEU:HD12	1:C:149:LEU:O	2.09	0.51
1:D:36:LEU:CD1	1:D:117:LEU:HD23	2.38	0.51
1:D:150:ALA:N	1:D:151:PRO:HD2	2.25	0.51
1:E:138:SER:O	1:E:142:ILE:HG12	2.09	0.51
1:A:182:MET:SD	1:B:139:ALA:HB2	2.51	0.51
1:E:154:THR:HG23	1:E:155:ASP:OD1	2.11	0.51
1:F:150:ALA:CB	1:F:151:PRO:HD3	2.33	0.51
1:E:161:THR:HG23	1:E:164:ASP:HB2	1.92	0.51
1:A:107:SER:OG	1:A:108:PHE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:PHE:HZ	1:E:194:LEU:HD11	1.76	0.51
1:F:29:LEU:HB2	1:F:77:ARG:NH1	2.26	0.51
1:F:34:ASP:HA	1:F:37:LEU:CD1	2.38	0.51
1:F:142:ILE:HG23	1:F:143:THR:N	2.26	0.51
1:C:133:LEU:O	1:C:138:SER:HA	2.10	0.51
1:B:107:SER:O	1:B:111:GLU:HB2	2.11	0.51
1:D:25:ARG:HG3	1:D:63:GLU:CG	2.41	0.51
1:A:85:ASN:O	1:A:88:ALA:HB3	2.11	0.51
1:D:25:ARG:CG	1:D:63:GLU:CG	2.88	0.51
1:D:102:LEU:CD2	1:D:192:ALA:HA	2.40	0.51
1:E:163:ASN:O	1:E:166:ASN:HB2	2.10	0.51
1:B:24:LEU:O	1:B:27:SER:HB2	2.10	0.51
1:E:177:LEU:O	1:E:177:LEU:HD12	2.10	0.51
1:F:109:PHE:CD2	1:F:191:ALA:HB2	2.46	0.51
1:A:141:ILE:H	1:A:141:ILE:HD12	1.76	0.50
1:C:58:GLN:O	1:C:62:ASN:HB2	2.11	0.50
1:D:102:LEU:O	1:D:102:LEU:HD13	2.11	0.50
1:F:175:LEU:O	1:F:178:SER:OG	2.28	0.50
1:F:186:ALA:HB3	1:F:188:HIS:ND1	2.26	0.50
1:C:33:ARG:HG3	1:C:37:LEU:HD11	1.92	0.50
1:C:181:SER:HB2	1:D:135:THR:CG2	2.41	0.50
1:C:197:LEU:HD12	1:C:197:LEU:O	2.10	0.50
1:F:21:ARG:O	1:F:24:LEU:N	2.45	0.50
1:B:13:ARG:C	1:B:13:ARG:HD2	2.36	0.50
1:C:24:LEU:O	1:C:28:VAL:HG23	2.12	0.50
1:D:97:PHE:HE1	1:D:158:VAL:CG2	2.24	0.50
1:A:172:ILE:HG22	1:A:172:ILE:O	2.11	0.50
1:B:44:ILE:HD13	1:B:44:ILE:N	2.26	0.50
1:B:45:THR:HG22	1:B:46:LEU:H	1.76	0.50
1:B:173:VAL:HG12	2:B:301:PLM:H91	1.93	0.50
1:C:120:SER:O	1:C:127:LYS:NZ	2.43	0.50
1:D:83:VAL:HG21	1:D:149:LEU:HB2	1.93	0.50
1:F:127:LYS:O	1:F:131:LEU:HG	2.12	0.50
1:C:181:SER:HB2	1:D:135:THR:HG22	1.94	0.50
1:E:28:VAL:HG12	1:E:29:LEU:CD2	2.27	0.50
1:B:83:VAL:CG1	1:B:148:ARG:HH11	2.25	0.50
1:F:119:ILE:HD12	1:F:123:THR:CG2	2.35	0.50
1:B:132:GLN:O	1:B:137:ASP:HB2	2.11	0.50
1:F:29:LEU:HD13	1:F:74:TYR:HA	1.94	0.50
1:F:150:ALA:O	1:F:154:THR:HG22	2.12	0.50
1:C:198:ILE:HG22	1:D:197:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ASP:CG	1:F:148:ARG:HH12	2.20	0.49
1:F:136:THR:HG22	1:F:137:ASP:CG	2.37	0.49
1:F:138:SER:O	1:F:142:ILE:HG22	2.12	0.49
1:B:70:LEU:HD12	1:B:70:LEU:C	2.37	0.49
1:D:150:ALA:HB3	1:D:151:PRO:CD	2.42	0.49
1:F:142:ILE:HD11	1:F:174:ARG:HG3	1.93	0.49
1:E:204:ARG:HG3	1:E:205:HIS:CE1	2.47	0.49
1:A:29:LEU:HD12	1:A:77:ARG:NH1	2.27	0.49
1:E:102:LEU:HD11	1:E:106:ARG:HE	1.76	0.49
1:F:28:VAL:O	1:F:31:ALA:HB3	2.13	0.49
1:B:64:PHE:CD2	1:B:70:LEU:HB2	2.48	0.49
1:B:97:PHE:CE1	1:B:158:VAL:HG13	2.47	0.49
1:C:32:MET:HE2	1:C:74:TYR:CB	2.41	0.49
1:E:121:LEU:CD2	1:E:130:LEU:HD12	2.33	0.49
1:F:144:ARG:HH12	1:F:148:ARG:HE	1.59	0.49
1:D:37:LEU:CD2	1:D:116:PRO:HG3	2.43	0.49
1:D:197:LEU:O	1:D:197:LEU:HD12	2.12	0.49
1:A:29:LEU:HD12	1:A:77:ARG:HH11	1.77	0.49
1:E:97:PHE:CE2	1:E:202:ALA:CB	2.93	0.49
1:E:125:VAL:CG1	1:E:126:ALA:N	2.76	0.49
1:C:41:TRP:CH2	1:C:67:ARG:HD3	2.47	0.49
1:C:96:ASN:HD22	1:C:99:GLU:HG3	1.78	0.49
1:D:102:LEU:O	1:D:106:ARG:HG3	2.12	0.49
1:D:97:PHE:CE1	1:D:158:VAL:HG22	2.48	0.48
1:E:40:ASP:O	1:E:43:ALA:HB3	2.12	0.48
1:E:41:TRP:CD1	1:E:130:LEU:HD23	2.48	0.48
1:B:117:LEU:O	1:B:117:LEU:HD13	2.14	0.48
1:C:79:ALA:HB2	2:C:301:PLM:HB2	1.95	0.48
1:D:151:PRO:CA	1:D:154:THR:HG23	2.28	0.48
1:D:201:PHE:CE1	1:D:205:HIS:ND1	2.81	0.48
1:F:105:PHE:CB	1:F:191:ALA:HB1	2.43	0.48
1:B:55:ILE:CG2	1:B:56:SER:N	2.74	0.48
1:B:115:ASP:O	1:B:119:ILE:HG13	2.13	0.48
1:D:27:SER:O	1:D:31:ALA:HB2	2.13	0.48
1:D:118:VAL:CG2	1:D:180:VAL:CG1	2.91	0.48
1:E:97:PHE:CE1	1:E:158:VAL:HG13	2.48	0.48
1:A:180:VAL:HG12	1:A:181:SER:N	2.29	0.48
1:D:102:LEU:HD13	1:D:102:LEU:C	2.39	0.48
1:F:131:LEU:N	1:F:131:LEU:HD23	2.28	0.48
1:E:191:ALA:HA	1:E:194:LEU:HD12	1.95	0.48
1:F:83:VAL:HG13	1:F:148:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG11	1:A:60:ILE:HD11	1.94	0.48
1:B:82:LEU:HD21	1:B:111:GLU:HG2	1.94	0.48
1:F:112:SER:O	1:F:118:VAL:HG21	2.13	0.48
1:D:28:VAL:CG1	1:D:64:PHE:CE2	2.97	0.48
1:D:97:PHE:HB3	1:D:199:THR:HG23	1.95	0.48
1:D:149:LEU:HD23	1:D:169:SER:CB	2.31	0.48
1:E:193:ASP:OD2	1:F:167:VAL:HG21	2.14	0.48
1:F:136:THR:HG22	1:F:137:ASP:OD2	2.14	0.48
1:C:72:GLN:HA	1:C:133:LEU:HD21	1.95	0.48
1:E:102:LEU:HD21	1:E:106:ARG:HE	1.79	0.48
1:F:105:PHE:HB3	1:F:191:ALA:CB	2.43	0.48
1:A:55:ILE:CG2	1:A:56:SER:N	2.76	0.48
1:B:36:LEU:HD13	1:B:117:LEU:HD23	1.96	0.48
1:B:49:VAL:HG23	1:B:50:ALA:N	2.29	0.48
1:B:186:ALA:HB3	1:B:188:HIS:NE2	2.29	0.48
1:C:98:TYR:CD1	1:C:195:ALA:HB1	2.49	0.48
1:E:134:ILE:HG23	1:E:177:LEU:HD11	1.96	0.48
1:F:90:LEU:HD23	1:F:100:ALA:HB1	1.95	0.48
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.75	0.47
1:B:169:SER:O	1:B:173:VAL:HG23	2.14	0.47
1:A:66:SER:OG	1:A:68:GLN:N	2.47	0.47
1:D:29:LEU:CB	1:D:77:ARG:HH21	2.25	0.47
1:F:139:ALA:O	1:F:142:ILE:HG22	2.15	0.47
1:A:170:ARG:HD3	1:B:188:HIS:CE1	2.42	0.47
1:B:168:LEU:HD22	1:B:201:PHE:CE2	2.49	0.47
1:C:33:ARG:CG	1:C:34:ASP:N	2.77	0.47
1:F:107:SER:O	1:F:111:GLU:N	2.47	0.47
1:F:74:TYR:CD1	1:F:74:TYR:C	2.92	0.47
1:F:134:ILE:HG22	1:F:177:LEU:CD1	2.45	0.47
1:E:32:MET:CE	1:E:74:TYR:HD2	2.22	0.47
1:F:94:VAL:HG12	1:F:95:GLY:N	2.30	0.47
1:C:197:LEU:HD12	1:C:197:LEU:C	2.39	0.47
1:D:29:LEU:HB2	1:D:77:ARG:NH2	2.30	0.47
1:D:32:MET:HA	1:D:35:LEU:HD11	1.96	0.47
1:F:46:LEU:HD12	1:F:61:TYR:CD1	2.49	0.47
1:D:77:ARG:HD2	1:D:81:ARG:HH12	1.79	0.47
1:E:55:ILE:HG22	1:E:56:SER:N	2.30	0.47
1:F:119:ILE:HD13	1:F:119:ILE:HA	1.61	0.47
1:F:133:LEU:HD13	1:F:133:LEU:O	2.14	0.47
1:A:170:ARG:NH1	1:B:188:HIS:ND1	2.62	0.47
1:B:154:THR:HG23	1:B:155:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:VAL:HG23	1:E:149:LEU:HB2	1.95	0.47
1:A:35:LEU:HD11	1:A:52:ALA:HB1	1.97	0.47
1:A:116:PRO:O	1:A:120:SER:HB3	2.15	0.47
1:B:121:LEU:HB3	1:B:122:LEU:CD2	2.44	0.47
1:C:168:LEU:HD23	1:C:168:LEU:O	2.15	0.47
1:F:142:ILE:HD12	1:F:173:VAL:HG12	1.97	0.47
1:F:189:ASP:O	1:F:192:ALA:HB3	2.15	0.47
1:A:35:LEU:HD12	1:A:35:LEU:N	2.30	0.47
1:C:45:THR:HG21	1:C:47:SER:HB2	1.96	0.47
1:F:55:ILE:HG22	1:F:56:SER:N	2.29	0.47
1:A:84:ASP:CG	1:A:148:ARG:HH12	2.22	0.46
1:A:108:PHE:CZ	1:A:176:CYS:CB	2.98	0.46
1:B:74:TYR:CD1	1:B:74:TYR:C	2.92	0.46
1:A:138:SER:HB3	1:A:142:ILE:CD1	2.43	0.46
1:C:29:LEU:HD12	1:C:77:ARG:HH12	1.79	0.46
1:C:86:VAL:HG12	1:C:87:HIS:N	2.29	0.46
1:F:50:ALA:O	1:F:54:GLY:N	2.48	0.46
1:A:167:VAL:HG22	1:B:193:ASP:HB3	1.96	0.46
1:B:120:SER:O	1:B:127:LYS:HE3	2.14	0.46
1:C:84:ASP:OD2	1:C:148:ARG:NH1	2.48	0.46
1:E:101:PHE:O	1:E:105:PHE:HB2	2.15	0.46
1:E:149:LEU:CD2	1:E:153:PHE:HE2	2.26	0.46
1:F:105:PHE:HZ	1:F:172:ILE:HD13	1.81	0.46
1:B:32:MET:CE	1:B:36:LEU:HD11	2.45	0.46
1:C:78:LEU:O	1:C:78:LEU:HD23	2.16	0.46
1:C:83:VAL:O	1:C:86:VAL:HB	2.15	0.46
1:C:89:SER:HB2	1:C:103:GLN:HB3	1.98	0.46
1:E:102:LEU:CD1	1:E:106:ARG:HE	2.28	0.46
1:F:175:LEU:HD13	1:F:194:LEU:HD22	1.96	0.46
1:A:35:LEU:HD21	1:A:48:ASP:O	2.16	0.46
1:A:177:LEU:HA	1:A:177:LEU:HD12	1.43	0.46
1:D:29:LEU:HB3	1:D:77:ARG:NH2	2.24	0.46
1:D:35:LEU:HD12	1:D:35:LEU:N	2.17	0.46
1:D:60:ILE:H	1:D:60:ILE:HG12	1.62	0.46
1:F:175:LEU:HD11	1:F:194:LEU:CD2	2.46	0.46
1:B:132:GLN:HE21	1:B:132:GLN:HB2	1.48	0.46
1:C:107:SER:O	1:C:110:ALA:HB3	2.16	0.46
1:D:94:VAL:HA	1:D:157:TRP:CE2	2.50	0.46
1:A:74:TYR:CD1	1:A:74:TYR:C	2.94	0.46
1:C:36:LEU:C	1:C:38:THR:N	2.74	0.46
1:D:38:THR:O	1:D:39:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ALA:C	1:E:55:ILE:HD12	2.41	0.46
1:E:55:ILE:CG2	1:E:59:THR:HG21	2.46	0.46
1:F:33:ARG:O	1:F:33:ARG:HG3	2.14	0.46
1:F:45:THR:HB	1:F:47:SER:H	1.81	0.46
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.30	0.46
1:A:196:ARG:NH1	1:B:205:HIS:CD2	2.84	0.46
1:B:44:ILE:HG23	1:B:49:VAL:HG13	1.96	0.46
1:B:77:ARG:HG2	1:B:78:LEU:N	2.29	0.46
1:A:160:THR:HG22	1:A:161:THR:O	2.16	0.45
1:A:179:TYR:HE1	1:A:190:VAL:HG21	1.80	0.45
1:D:45:THR:HB	1:D:48:ASP:H	1.79	0.45
1:D:121:LEU:HB3	1:D:122:LEU:HD23	1.98	0.45
1:E:135:THR:OG1	1:F:131:LEU:HD13	2.16	0.45
1:E:190:VAL:O	1:E:194:LEU:HD12	2.16	0.45
1:F:119:ILE:HD13	1:F:122:LEU:CD2	2.45	0.45
1:B:134:ILE:C	1:B:138:SER:HB3	2.41	0.45
1:B:201:PHE:HE1	1:B:205:HIS:CG	2.34	0.45
1:C:91:ASP:O	1:C:94:VAL:HG23	2.17	0.45
1:D:97:PHE:CE1	1:D:158:VAL:HG13	2.51	0.45
1:E:168:LEU:HD12	1:E:172:ILE:HG13	1.97	0.45
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.81	0.45
1:C:81:ARG:O	1:C:81:ARG:HG3	2.15	0.45
1:D:29:LEU:HD21	1:D:64:PHE:CZ	2.51	0.45
1:E:29:LEU:HD21	1:E:64:PHE:CE2	2.50	0.45
1:E:180:VAL:HG12	1:E:181:SER:N	2.31	0.45
1:A:24:LEU:HD21	1:A:59:THR:CG2	2.46	0.45
1:C:96:ASN:HD22	1:C:99:GLU:CG	2.30	0.45
1:E:91:ASP:HA	1:E:157:TRP:HE1	1.81	0.45
1:F:32:MET:SD	1:F:70:LEU:CD1	2.99	0.45
1:F:119:ILE:HD13	1:F:122:LEU:HD22	1.98	0.45
1:F:127:LYS:HZ1	1:F:130:LEU:CD1	2.30	0.45
1:F:151:PRO:HA	1:F:154:THR:HG23	1.97	0.45
1:A:152:ALA:O	1:A:156:THR:CG2	2.65	0.45
1:B:14:ILE:HB	1:B:19:ALA:HB2	1.98	0.45
1:C:78:LEU:HD11	1:C:115:ASP:OD2	2.16	0.45
1:C:121:LEU:HD21	1:C:180:VAL:HG12	1.99	0.45
1:D:177:LEU:HA	1:D:180:VAL:HG23	1.99	0.45
1:D:28:VAL:CG1	1:D:64:PHE:HE2	2.29	0.45
1:A:90:LEU:O	1:A:157:TRP:NE1	2.38	0.45
1:A:182:MET:HB2	1:B:135:THR:O	2.17	0.45
1:B:156:THR:HG23	1:B:158:VAL:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ARG:HD3	1:C:144:ARG:C	2.41	0.45
1:E:127:LYS:HE3	1:E:127:LYS:HB2	1.65	0.45
1:E:164:ASP:HB3	1:E:201:PHE:HZ	1.80	0.45
1:B:47:SER:CB	1:B:57:ARG:HD3	2.47	0.45
1:B:151:PRO:O	1:B:154:THR:N	2.49	0.45
1:D:74:TYR:HD1	1:D:74:TYR:O	1.99	0.45
1:E:41:TRP:CD1	1:E:130:LEU:CD2	3.00	0.45
1:E:133:LEU:HD13	1:E:133:LEU:HA	1.76	0.45
1:B:74:TYR:HD1	1:B:74:TYR:O	2.00	0.45
1:B:84:ASP:OD2	1:B:148:ARG:NH1	2.50	0.45
1:F:151:PRO:O	1:F:155:ASP:N	2.41	0.45
1:A:89:SER:HA	1:A:92:ALA:CB	2.47	0.45
1:F:26:ASP:O	1:F:30:ASP:HB2	2.17	0.45
1:F:122:LEU:HD13	1:F:122:LEU:H	1.82	0.45
1:A:14:ILE:HA	1:A:15:PRO:HD3	1.75	0.44
1:D:79:ALA:O	1:D:83:VAL:HG12	2.17	0.44
1:B:13:ARG:CZ	1:B:15:PRO:HG3	2.47	0.44
1:B:90:LEU:HD21	1:B:158:VAL:CG2	2.47	0.44
1:C:55:ILE:HG22	1:C:56:SER:O	2.17	0.44
1:E:164:ASP:HB3	1:E:201:PHE:CZ	2.52	0.44
1:C:68:GLN:O	1:C:71:ALA:HB3	2.17	0.44
1:F:50:ALA:O	1:F:53:ALA:N	2.49	0.44
1:F:175:LEU:HD21	1:F:179:TYR:HE2	1.82	0.44
1:B:45:THR:CA	1:B:48:ASP:HB2	2.46	0.44
1:B:49:VAL:C	1:B:51:ARG:N	2.74	0.44
1:B:90:LEU:HD21	1:B:158:VAL:HG21	1.98	0.44
1:C:41:TRP:CZ2	1:C:71:ALA:HB2	2.53	0.44
1:C:112:SER:O	1:C:118:VAL:HG11	2.18	0.44
1:C:188:HIS:CE1	1:D:170:ARG:HH11	2.34	0.44
1:D:45:THR:H	1:D:48:ASP:CB	2.28	0.44
1:E:102:LEU:O	1:E:106:ARG:HG3	2.17	0.44
1:F:132:GLN:HG2	1:F:137:ASP:OD2	2.17	0.44
1:A:64:PHE:CD2	1:A:70:LEU:HD12	2.52	0.44
1:B:97:PHE:HE1	1:B:158:VAL:HG13	1.83	0.44
1:B:147:ALA:O	1:B:151:PRO:HD3	2.18	0.44
1:C:32:MET:SD	1:C:70:LEU:HD11	2.58	0.44
1:D:32:MET:HE2	1:D:74:TYR:CB	2.48	0.44
1:E:127:LYS:CB	1:E:130:LEU:HB2	2.45	0.44
1:C:25:ARG:CZ	1:C:64:PHE:HE1	2.31	0.44
1:C:102:LEU:HD11	1:C:106:ARG:NH2	2.32	0.44
1:C:135:THR:O	1:C:138:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LEU:HD11	1:E:115:ASP:OD1	2.18	0.44
1:A:57:ARG:O	1:A:59:THR:N	2.51	0.44
1:C:55:ILE:CG2	1:C:56:SER:N	2.80	0.44
1:F:50:ALA:HB1	1:F:55:ILE:O	2.17	0.44
1:F:79:ALA:O	1:F:83:VAL:HG12	2.18	0.44
1:C:194:LEU:HA	1:C:194:LEU:HD23	1.59	0.44
1:D:111:GLU:O	1:D:114:ALA:HB3	2.17	0.44
1:D:129:ASP:OD1	1:D:129:ASP:N	2.35	0.44
1:F:144:ARG:NH1	1:F:148:ARG:HD2	2.33	0.44
1:A:53:ALA:CB	1:A:55:ILE:HD13	2.47	0.43
1:B:84:ASP:OD2	1:B:148:ARG:NH2	2.51	0.43
1:B:105:PHE:CE2	1:B:198:ILE:HD11	2.53	0.43
1:D:78:LEU:HD11	1:D:115:ASP:CG	2.43	0.43
1:D:108:PHE:CD1	1:D:108:PHE:C	2.93	0.43
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.54	0.43
1:F:83:VAL:HG23	1:F:149:LEU:HD13	2.00	0.43
1:A:46:LEU:HG	1:A:60:ILE:HG21	2.00	0.43
1:A:121:LEU:HD23	1:A:122:LEU:CD2	2.45	0.43
1:B:29:LEU:HD23	1:B:29:LEU:N	2.32	0.43
1:D:78:LEU:HD23	1:D:82:LEU:HG	1.99	0.43
1:F:136:THR:HG22	1:F:137:ASP:N	2.33	0.43
1:A:25:ARG:CZ	1:A:63:GLU:OE1	2.66	0.43
1:A:126:ALA:O	1:A:128:PRO:HD3	2.17	0.43
1:B:61:TYR:HD1	1:B:65:GLY:HA2	1.83	0.43
1:D:127:LYS:HE2	1:D:127:LYS:HB2	1.36	0.43
1:E:46:LEU:HA	1:E:46:LEU:HD23	1.62	0.43
1:F:134:ILE:HG22	1:F:177:LEU:HD11	2.00	0.43
1:A:174:ARG:NH1	1:B:182:MET:O	2.49	0.43
1:A:190:VAL:HG13	1:A:194:LEU:CD1	2.48	0.43
1:B:49:VAL:O	1:B:51:ARG:N	2.51	0.43
1:B:83:VAL:HG23	1:B:149:LEU:HB2	1.99	0.43
1:B:132:GLN:HG2	1:B:137:ASP:OD1	2.19	0.43
1:B:133:LEU:O	1:B:138:SER:CA	2.65	0.43
1:B:168:LEU:HD13	1:B:168:LEU:HA	1.78	0.43
1:B:185:GLU:HG2	1:B:186:ALA:N	2.33	0.43
1:C:21:ARG:O	1:C:24:LEU:N	2.52	0.43
1:D:102:LEU:HD11	1:D:106:ARG:NE	2.34	0.43
1:E:32:MET:CE	1:E:74:TYR:CD2	2.99	0.43
1:E:32:MET:SD	1:E:70:LEU:CD2	3.07	0.43
1:A:24:LEU:C	1:A:24:LEU:HD12	2.41	0.43
1:A:157:TRP:CE3	1:A:157:TRP:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LEU:CD2	1:C:180:VAL:HG12	2.47	0.43
1:E:56:SER:HB3	1:E:59:THR:HB	1.99	0.43
1:A:170:ARG:CD	1:B:188:HIS:HE1	2.27	0.43
1:E:104:GLY:O	1:E:107:SER:HB3	2.18	0.43
1:B:78:LEU:HA	1:B:78:LEU:HD23	1.51	0.43
1:B:188:HIS:CD2	1:B:188:HIS:N	2.82	0.43
1:C:33:ARG:HG3	1:C:37:LEU:CD1	2.49	0.43
1:C:36:LEU:C	1:C:38:THR:H	2.25	0.43
1:E:31:ALA:HB3	1:E:53:ALA:HB2	1.99	0.43
1:E:32:MET:HE3	1:E:74:TYR:CB	2.49	0.43
1:B:184:PRO:HA	1:B:185:GLU:OE1	2.19	0.43
1:D:102:LEU:HD11	1:D:106:ARG:HE	1.84	0.43
1:E:102:LEU:CD2	1:E:106:ARG:HE	2.32	0.43
1:A:21:ARG:HD2	1:A:63:GLU:OE2	2.19	0.43
1:A:57:ARG:NH1	1:A:61:TYR:OH	2.52	0.43
1:B:29:LEU:HA	1:B:32:MET:HG2	2.01	0.43
1:B:134:ILE:HG22	1:B:177:LEU:HD11	2.00	0.43
1:B:190:VAL:O	1:B:194:LEU:HB2	2.19	0.43
1:C:172:ILE:CD1	1:C:198:ILE:HD13	2.44	0.43
1:C:179:TYR:CE1	1:C:190:VAL:CG1	2.91	0.43
1:D:72:GLN:O	1:D:76:LEU:HB2	2.19	0.43
1:D:97:PHE:O	1:D:100:ALA:HB3	2.19	0.43
1:E:32:MET:HE2	1:E:74:TYR:HB2	1.95	0.43
1:B:102:LEU:C	1:B:102:LEU:CD1	2.92	0.43
1:D:76:LEU:HD22	1:D:144:ARG:HH11	1.84	0.43
1:D:118:VAL:O	1:D:122:LEU:HG	2.19	0.43
1:D:146:SER:HA	1:D:173:VAL:HG21	2.01	0.43
1:D:175:LEU:HD13	1:D:194:LEU:HD21	2.01	0.43
1:E:94:VAL:HG22	1:E:157:TRP:CD1	2.53	0.43
1:F:176:CYS:O	1:F:180:VAL:HG23	2.18	0.43
1:B:122:LEU:CD2	1:B:122:LEU:N	2.81	0.42
1:C:32:MET:HG2	1:C:74:TYR:CD2	2.54	0.42
1:C:169:SER:C	1:C:171:ALA:N	2.76	0.42
1:E:21:ARG:O	1:E:24:LEU:HB3	2.19	0.42
1:E:170:ARG:O	1:E:174:ARG:HG3	2.19	0.42
1:B:74:TYR:C	1:B:74:TYR:HD1	2.27	0.42
1:F:28:VAL:HG12	1:F:64:PHE:HE2	1.84	0.42
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.58	0.42
1:C:105:PHE:CD1	1:C:194:LEU:HD13	2.53	0.42
1:C:168:LEU:O	1:C:172:ILE:HG13	2.19	0.42
1:E:135:THR:OG1	1:E:136:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PRO:HA	1:B:143:THR:CG2	2.42	0.42
1:E:147:ALA:O	1:E:151:PRO:HD3	2.18	0.42
1:F:125:VAL:O	1:F:125:VAL:HG13	2.19	0.42
1:A:15:PRO:HD2	1:A:18:GLU:CB	2.49	0.42
1:B:60:ILE:HG23	1:B:61:TYR:N	2.34	0.42
1:B:74:TYR:CD1	1:B:74:TYR:O	2.72	0.42
1:B:77:ARG:HG3	1:B:81:ARG:HE	1.83	0.42
1:E:21:ARG:HG3	1:E:63:GLU:OE2	2.19	0.42
1:F:151:PRO:HA	1:F:154:THR:HG22	2.02	0.42
1:A:16:TYR:O	1:A:17:ALA:C	2.62	0.42
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.33	0.42
1:A:89:SER:HA	1:A:92:ALA:HB3	2.01	0.42
1:A:193:ASP:HB3	1:B:167:VAL:HG13	2.00	0.42
1:C:14:ILE:HB	1:C:15:PRO:HD3	2.02	0.42
1:C:71:ALA:O	1:C:74:TYR:HB3	2.20	0.42
1:C:77:ARG:HA	1:C:80:ASP:HB2	2.02	0.42
1:C:83:VAL:HB	1:C:149:LEU:HB2	2.02	0.42
1:E:39:ARG:CZ	1:E:43:ALA:HB1	2.47	0.42
1:E:99:GLU:OE1	1:E:99:GLU:HA	2.19	0.42
1:A:46:LEU:HG	1:A:60:ILE:CG2	2.49	0.42
1:B:57:ARG:HB2	1:B:57:ARG:CZ	2.49	0.42
1:C:101:PHE:O	1:C:105:PHE:HD2	2.03	0.42
1:D:14:ILE:HA	1:D:15:PRO:HD3	1.85	0.42
1:D:28:VAL:HG11	1:D:64:PHE:HE2	1.82	0.42
1:D:40:ASP:OD1	1:D:120:SER:OG	2.37	0.42
1:C:31:ALA:HB2	1:C:53:ALA:HB2	2.01	0.42
1:D:140:PRO:O	1:D:144:ARG:HB2	2.20	0.42
1:A:118:VAL:CG1	1:A:119:ILE:N	2.82	0.42
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.24	0.42
1:C:32:MET:HE2	1:C:74:TYR:HB2	2.00	0.42
1:E:83:VAL:HG11	1:E:148:ARG:CG	2.34	0.42
1:F:68:GLN:NE2	1:F:133:LEU:HD23	2.35	0.42
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.70	0.41
1:A:125:VAL:HG13	1:A:125:VAL:O	2.20	0.41
1:A:177:LEU:HG	1:B:182:MET:HE1	2.01	0.41
1:B:201:PHE:CD1	1:B:201:PHE:C	2.95	0.41
1:C:41:TRP:CZ2	1:C:67:ARG:CD	3.02	0.41
1:F:108:PHE:CZ	1:F:176:CYS:HB3	2.55	0.41
1:A:142:ILE:O	1:A:143:THR:C	2.63	0.41
1:D:142:ILE:O	1:D:143:THR:C	2.63	0.41
1:E:204:ARG:HA	1:E:204:ARG:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:CG1	1:A:87:HIS:N	2.83	0.41
1:A:153:PHE:O	1:A:158:VAL:O	2.37	0.41
1:A:175:LEU:HD22	1:A:175:LEU:HA	1.82	0.41
1:C:108:PHE:CZ	1:C:176:CYS:HB3	2.54	0.41
1:C:170:ARG:HE	1:C:170:ARG:HB2	1.45	0.41
1:D:168:LEU:HD11	1:D:198:ILE:HG21	2.02	0.41
1:B:105:PHE:CZ	1:B:194:LEU:HD13	2.55	0.41
1:C:27:SER:OG	1:C:28:VAL:N	2.53	0.41
1:C:40:ASP:O	1:C:42:SER:N	2.53	0.41
1:C:142:ILE:O	1:C:143:THR:C	2.63	0.41
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.81	0.41
1:E:29:LEU:C	1:E:77:ARG:HH12	2.27	0.41
1:F:28:VAL:CG1	1:F:64:PHE:HE2	2.32	0.41
1:C:35:LEU:CD1	1:C:49:VAL:HG23	2.50	0.41
1:C:82:LEU:HD22	1:C:108:PHE:HD2	1.85	0.41
1:C:94:VAL:HG13	1:C:157:TRP:CD1	2.55	0.41
1:D:44:ILE:CG2	1:D:49:VAL:HG23	2.50	0.41
1:D:122:LEU:HD23	1:D:122:LEU:N	2.34	0.41
1:B:61:TYR:O	1:B:61:TYR:CD1	2.74	0.41
1:B:169:SER:O	1:B:173:VAL:CG2	2.69	0.41
1:C:86:VAL:CG1	1:C:87:HIS:N	2.83	0.41
1:D:184:PRO:HB3	1:D:190:VAL:HG21	2.03	0.41
1:A:166:ASN:O	1:A:167:VAL:C	2.64	0.41
1:A:180:VAL:CG1	1:A:181:SER:N	2.83	0.41
1:B:25:ARG:O	1:B:28:VAL:HG23	2.21	0.41
1:C:167:VAL:CG2	1:D:193:ASP:OD2	2.69	0.41
1:D:46:LEU:HD23	1:D:46:LEU:HA	1.85	0.41
1:E:122:LEU:HD11	1:E:180:VAL:O	2.21	0.41
1:E:199:THR:HB	1:E:200:PRO:HD3	2.03	0.41
1:C:134:ILE:HG22	1:C:177:LEU:CD1	2.29	0.41
1:D:60:ILE:HG22	1:D:64:PHE:CD2	2.49	0.41
1:D:130:LEU:HD23	1:D:133:LEU:HD23	2.03	0.41
1:D:199:THR:O	1:D:203:GLU:HG3	2.20	0.41
1:F:105:PHE:HB2	1:F:191:ALA:HB1	2.01	0.41
1:A:23:LEU:O	1:A:27:SER:HB2	2.21	0.41
1:A:24:LEU:HD21	1:A:59:THR:HG22	2.03	0.41
1:A:39:ARG:HG3	1:A:43:ALA:HB3	2.02	0.41
1:A:55:ILE:N	1:A:55:ILE:CD1	2.84	0.41
1:A:67:ARG:NH1	1:A:67:ARG:HG2	2.36	0.41
1:A:78:LEU:CD2	1:A:82:LEU:HG	2.50	0.41
1:B:17:ALA:O	1:B:20:SER:OG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HG11	1:B:149:LEU:HD11	2.03	0.41
1:C:185:GLU:H	1:C:185:GLU:CD	2.25	0.41
1:D:118:VAL:HG22	1:D:180:VAL:CG1	2.48	0.41
1:D:139:ALA:HB3	1:D:140:PRO:CD	2.50	0.41
1:D:198:ILE:H	1:D:198:ILE:HG12	1.72	0.41
1:E:121:LEU:N	1:E:121:LEU:CD2	2.81	0.41
1:E:144:ARG:O	1:E:148:ARG:HB3	2.21	0.41
1:F:102:LEU:HD12	1:F:106:ARG:HG3	2.03	0.41
1:F:150:ALA:HB3	1:F:151:PRO:CD	2.38	0.41
1:F:182:MET:HA	1:F:183:PRO:HD3	1.82	0.41
1:F:185:GLU:H	1:F:185:GLU:HG3	1.38	0.41
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.79	0.41
1:B:199:THR:O	1:B:203:GLU:HG2	2.21	0.41
1:B:201:PHE:CE1	1:B:205:HIS:HB2	2.55	0.41
1:D:78:LEU:CD1	1:D:115:ASP:CG	2.93	0.41
1:D:134:ILE:C	1:D:138:SER:HB3	2.46	0.41
1:D:150:ALA:N	1:D:151:PRO:CD	2.83	0.41
1:A:101:PHE:CG	1:A:198:ILE:HD11	2.56	0.40
1:C:199:THR:N	1:C:200:PRO:CD	2.84	0.40
1:D:73:GLY:HA2	1:D:76:LEU:HB2	2.02	0.40
1:D:87:HIS:HA	1:D:90:LEU:HB3	2.03	0.40
1:D:197:LEU:HD12	1:D:197:LEU:C	2.46	0.40
1:A:55:ILE:HG21	1:A:59:THR:HB	2.00	0.40
1:A:179:TYR:CE2	1:B:174:ARG:CD	3.03	0.40
1:E:60:ILE:O	1:E:64:PHE:HB2	2.21	0.40
1:A:86:VAL:HG13	1:A:87:HIS:N	2.36	0.40
1:A:190:VAL:CG1	1:A:194:LEU:CD1	2.98	0.40
1:B:55:ILE:HG22	1:B:59:THR:OG1	2.21	0.40
1:C:134:ILE:HD12	1:C:181:SER:HB3	2.03	0.40
1:D:60:ILE:HD12	1:D:60:ILE:HG21	1.81	0.40
1:E:82:LEU:HA	1:E:82:LEU:HD23	1.82	0.40
1:A:81:ARG:HH11	1:A:81:ARG:CG	2.31	0.40
1:A:105:PHE:O	1:A:106:ARG:C	2.65	0.40
1:B:46:LEU:HD13	1:B:61:TYR:HB2	2.04	0.40
1:B:198:ILE:H	1:B:198:ILE:HG12	1.75	0.40
1:C:41:TRP:O	1:C:41:TRP:CG	2.74	0.40
1:C:101:PHE:HE1	1:C:153:PHE:CE1	2.39	0.40
1:E:125:VAL:HG12	1:E:126:ALA:H	1.85	0.40
1:F:144:ARG:O	1:F:148:ARG:HB2	2.22	0.40
1:B:108:PHE:HE2	2:B:301:PLM:H81	1.87	0.40
1:C:41:TRP:NE1	1:C:130:LEU:HD21	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ALA:CB	1:C:151:PRO:HD3	2.47	0.40
1:C:188:HIS:CE1	1:D:170:ARG:NH1	2.90	0.40
1:D:98:TYR:CD2	1:D:98:TYR:C	3.00	0.40
1:E:117:LEU:O	1:E:117:LEU:HD22	2.21	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	193/217 (89%)	171 (89%)	21 (11%)	1 (0%)	24	57
1	B	193/217 (89%)	177 (92%)	16 (8%)	0	100	100
1	C	190/217 (88%)	172 (90%)	18 (10%)	0	100	100
1	D	194/217 (89%)	184 (95%)	10 (5%)	0	100	100
1	E	191/217 (88%)	181 (95%)	10 (5%)	0	100	100
1	F	189/217 (87%)	179 (95%)	10 (5%)	0	100	100
All	All	1150/1302 (88%)	1064 (92%)	85 (7%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	LEU

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/176 (89%)	109 (70%)	47 (30%)	0	2
1	B	156/176 (89%)	110 (70%)	46 (30%)	0	2
1	C	154/176 (88%)	100 (65%)	54 (35%)	0	1
1	D	157/176 (89%)	124 (79%)	33 (21%)	1	7
1	E	155/176 (88%)	124 (80%)	31 (20%)	1	8
1	F	153/176 (87%)	118 (77%)	35 (23%)	1	6
All	All	931/1056 (88%)	685 (74%)	246 (26%)	0	3

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	ILE
1	A	18	GLU
1	A	21	ARG
1	A	25	ARG
1	A	26	ASP
1	A	27	SER
1	A	29	LEU
1	A	32	MET
1	A	39	ARG
1	A	42	SER
1	A	45	THR
1	A	46	LEU
1	A	47	SER
1	A	49	VAL
1	A	55	ILE
1	A	60	ILE
1	A	77	ARG
1	A	78	LEU
1	A	81	ARG
1	A	83	VAL
1	A	93	ASN
1	A	94	VAL
1	A	102	LEU
1	A	107	SER
1	A	117	LEU
1	A	118	VAL
1	A	120	SER

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Mol	Chain	Res	Type
1	A	121	LEU
1	A	134	ILE
1	A	137	ASP
1	A	138	SER
1	A	144	ARG
1	A	148	ARG
1	A	156	THR
1	A	161	THR
1	A	167	VAL
1	A	172	ILE
1	A	175	LEU
1	A	180	VAL
1	A	188	HIS
1	A	189	ASP
1	A	190	VAL
1	A	194	LEU
1	A	196	ARG
1	A	200	PRO
1	A	207	VAL
1	B	13	ARG
1	B	28	VAL
1	B	44	ILE
1	B	45	THR
1	B	48	ASP
1	B	55	ILE
1	B	61	TYR
1	B	63	GLU
1	B	66	SER
1	B	67	ARG
1	B	68	GLN
1	B	70	LEU
1	B	72	GLN
1	B	74	TYR
1	B	78	LEU
1	B	81	ARG
1	B	90	LEU
1	B	96	ASN
1	B	102	LEU
1	B	118	VAL
1	B	119	ILE
1	B	121	LEU
1	B	122	LEU

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Mol	Chain	Res	Type
1	B	125	VAL
1	B	127	LYS
1	B	129	ASP
1	B	132	GLN
1	B	134	ILE
1	B	141	ILE
1	B	144	ARG
1	B	146	SER
1	B	154	THR
1	B	156	THR
1	B	160	THR
1	B	161	THR
1	B	162	ASP
1	B	168	LEU
1	B	169	SER
1	B	173	VAL
1	B	182	MET
1	B	188	HIS
1	B	189	ASP
1	B	190	VAL
1	B	194	LEU
1	B	196	ARG
1	B	204	ARG
1	C	14	ILE
1	C	21	ARG
1	C	23	LEU
1	C	27	SER
1	C	30	ASP
1	C	33	ARG
1	C	35	LEU
1	C	38	THR
1	C	42	SER
1	C	46	LEU
1	C	47	SER
1	C	49	VAL
1	C	51	ARG
1	C	59	THR
1	C	60	ILE
1	C	61	TYR
1	C	62	ASN
1	C	63	GLU
1	C	67	ARG

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Mol	Chain	Res	Type
1	C	70	LEU
1	C	76	LEU
1	C	77	ARG
1	C	81	ARG
1	C	83	VAL
1	C	86	VAL
1	C	89	SER
1	C	90	LEU
1	C	102	LEU
1	C	103	GLN
1	C	106	ARG
1	C	117	LEU
1	C	118	VAL
1	C	119	ILE
1	C	120	SER
1	C	125	VAL
1	C	127	LYS
1	C	129	ASP
1	C	130	LEU
1	C	133	LEU
1	C	137	ASP
1	C	138	SER
1	C	143	THR
1	C	144	ARG
1	C	148	ARG
1	C	155	ASP
1	C	161	THR
1	C	167	VAL
1	C	170	ARG
1	C	172	ILE
1	C	173	VAL
1	C	174	ARG
1	C	182	MET
1	C	187	ASP
1	C	197	LEU
1	D	21	ARG
1	D	26	ASP
1	D	27	SER
1	D	32	MET
1	D	33	ARG
1	D	35	LEU
1	D	44	ILE

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Mol	Chain	Res	Type
1	D	60	ILE
1	D	72	GLN
1	D	74	TYR
1	D	81	ARG
1	D	102	LEU
1	D	116	PRO
1	D	117	LEU
1	D	118	VAL
1	D	119	ILE
1	D	121	LEU
1	D	125	VAL
1	D	127	LYS
1	D	129	ASP
1	D	133	LEU
1	D	134	ILE
1	D	142	ILE
1	D	143	THR
1	D	144	ARG
1	D	154	THR
1	D	161	THR
1	D	170	ARG
1	D	188	HIS
1	D	190	VAL
1	D	196	ARG
1	D	198	ILE
1	D	208	ILE
1	E	21	ARG
1	E	32	MET
1	E	37	LEU
1	E	58	GLN
1	E	59	THR
1	E	61	TYR
1	E	78	LEU
1	E	83	VAL
1	E	86	VAL
1	E	87	HIS
1	E	97	PHE
1	E	103	GLN
1	E	105	PHE
1	E	117	LEU
1	E	121	LEU
1	E	122	LEU

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Mol	Chain	Res	Type
1	E	123	THR
1	E	127	LYS
1	E	130	LEU
1	E	133	LEU
1	E	134	ILE
1	E	137	ASP
1	E	143	THR
1	E	144	ARG
1	E	148	ARG
1	E	161	THR
1	E	168	LEU
1	E	181	SER
1	E	188	HIS
1	E	194	LEU
1	E	199	THR
1	F	20	SER
1	F	24	LEU
1	F	26	ASP
1	F	30	ASP
1	F	33	ARG
1	F	37	LEU
1	F	39	ARG
1	F	45	THR
1	F	62	ASN
1	F	78	LEU
1	F	86	VAL
1	F	96	ASN
1	F	103	GLN
1	F	117	LEU
1	F	118	VAL
1	F	119	ILE
1	F	120	SER
1	F	121	LEU
1	F	122	LEU
1	F	123	THR
1	F	127	LYS
1	F	129	ASP
1	F	130	LEU
1	F	131	LEU
1	F	133	LEU
1	F	134	ILE
1	F	136	THR

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Mol	Chain	Res	Type
1	F	144	ARG
1	F	167	VAL
1	F	172	ILE
1	F	177	LEU
1	F	181	SER
1	F	185	GLU
1	F	198	ILE
1	F	199	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	HIS
1	B	62	ASN
1	B	132	GLN
1	B	188	HIS
1	C	72	GLN
1	C	96	ASN
1	C	166	ASN
1	D	72	GLN
1	D	93	ASN
1	E	72	GLN
1	E	103	GLN
1	E	205	HIS
1	F	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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
2	PLM	B	301	-	17,17,17	0.59	0	17,17,17	1.47	5 (29%)
2	PLM	A	301	-	17,17,17	0.70	1 (5%)	17,17,17	1.17	1 (5%)
2	PLM	C	301	-	17,17,17	0.63	0	17,17,17	0.95	0
2	PLM	D	301	-	17,17,17	0.55	0	17,17,17	1.37	3 (17%)

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
2	PLM	B	301	-	-	5/15/15/15	-
2	PLM	A	301	-	-	7/15/15/15	-
2	PLM	C	301	-	-	4/15/15/15	-
2	PLM	D	301	-	-	7/15/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PLM	O2-C1	2.02	1.28	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	PLM	C3-C2-C1	2.58	121.24	114.51
2	B	301	PLM	O1-C1-C2	2.51	121.95	114.00
2	B	301	PLM	C9-C8-C7	2.40	126.48	114.37
2	A	301	PLM	C3-C2-C1	2.37	120.70	114.51
2	B	301	PLM	O1-C1-O2	-2.37	117.24	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	PLM	O1-C1-C2	2.35	121.44	114.00
2	D	301	PLM	O1-C1-O2	-2.31	117.39	123.33
2	B	301	PLM	C4-C3-C2	2.14	120.99	113.13
2	B	301	PLM	C3-C2-C1	2.04	119.82	114.51

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	PLM	CC-CD-CE-CF
2	A	301	PLM	C2-C3-C4-C5
2	D	301	PLM	CA-CB-CC-CD
2	D	301	PLM	C6-C7-C8-C9
2	D	301	PLM	C5-C6-C7-C8
2	B	301	PLM	C5-C6-C7-C8
2	D	301	PLM	CC-CD-CE-CF
2	A	301	PLM	C6-C7-C8-C9
2	C	301	PLM	C6-C7-C8-C9
2	C	301	PLM	C5-C6-C7-C8
2	A	301	PLM	C8-C9-CA-CB
2	D	301	PLM	C9-CA-CB-CC
2	C	301	PLM	C2-C3-C4-C5
2	A	301	PLM	C4-C5-C6-C7
2	A	301	PLM	CD-CE-CF-CG
2	A	301	PLM	O2-C1-C2-C3
2	A	301	PLM	O1-C1-C2-C3
2	D	301	PLM	O1-C1-C2-C3
2	D	301	PLM	O2-C1-C2-C3
2	B	301	PLM	O1-C1-C2-C3
2	B	301	PLM	C7-C8-C9-CA
2	B	301	PLM	C6-C7-C8-C9
2	B	301	PLM	O2-C1-C2-C3

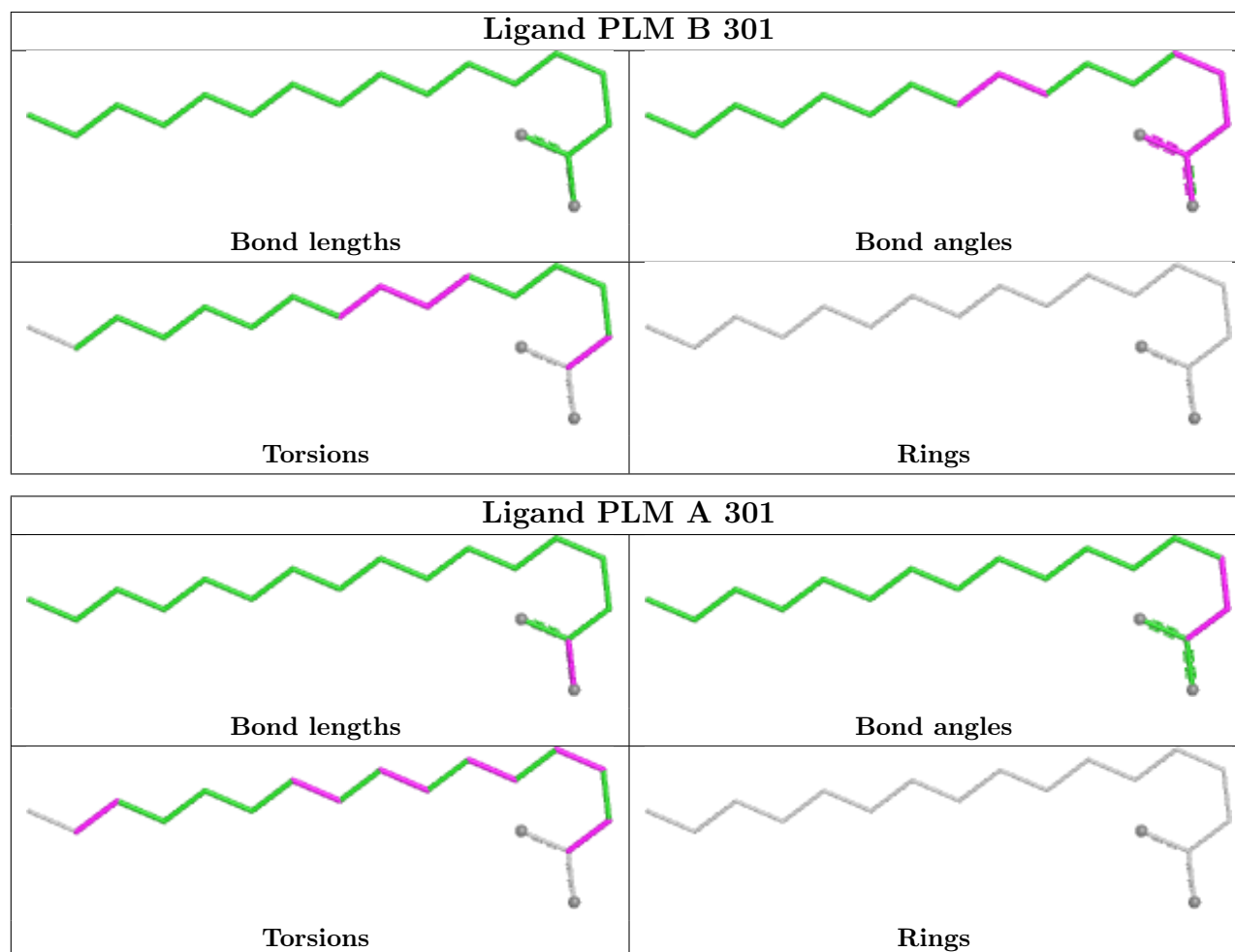
There are no ring outliers.

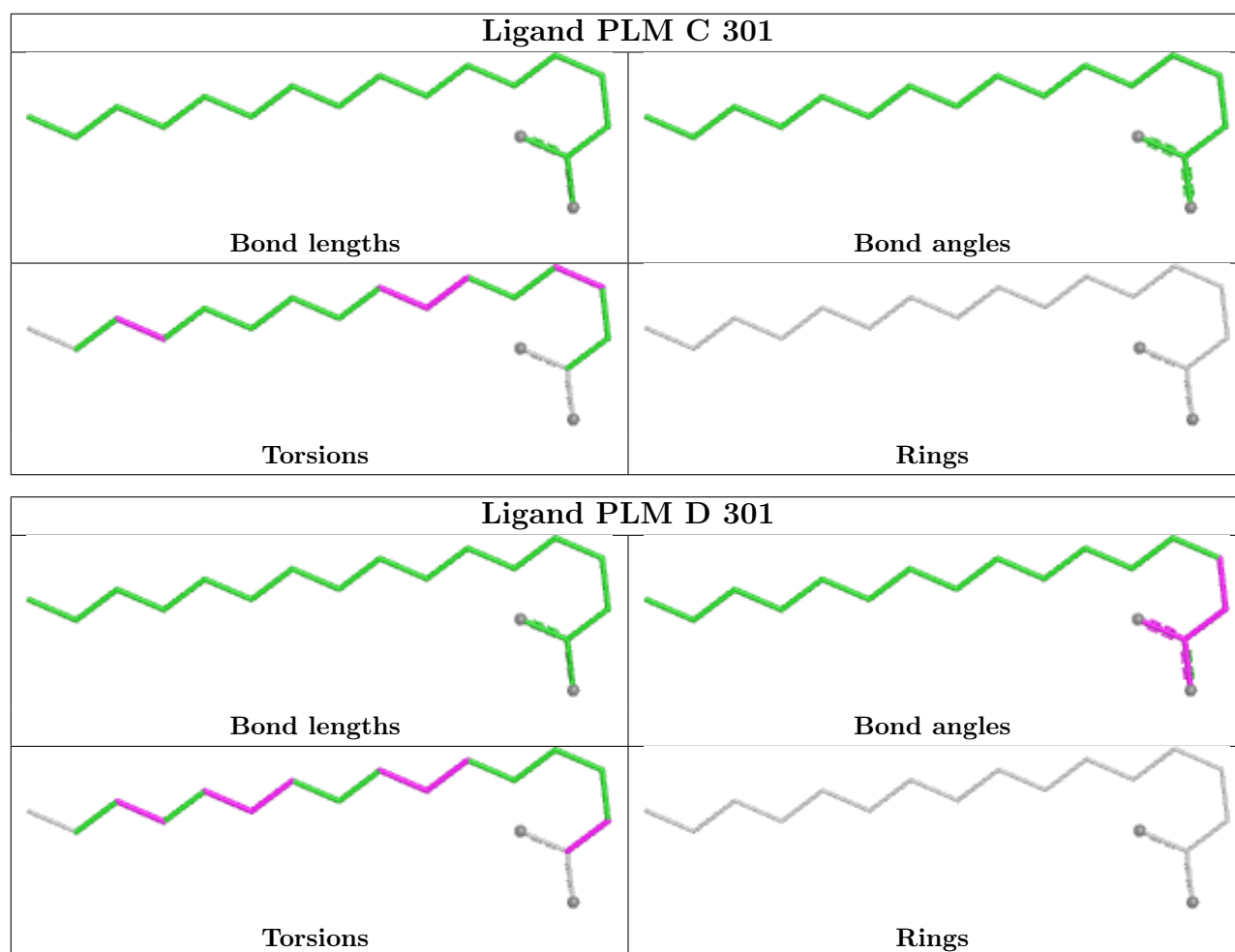
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PLM	4	0
2	C	301	PLM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	195/217 (89%)	-0.76	0	100	100	13, 27, 47, 91	0
1	B	195/217 (89%)	-0.72	0	100	100	16, 36, 60, 79	0
1	C	192/217 (88%)	-0.68	1 (0%)	87	66	21, 42, 76, 85	0
1	D	196/217 (90%)	-0.72	1 (0%)	87	66	19, 35, 66, 89	0
1	E	193/217 (88%)	-0.60	0	100	100	44, 88, 136, 144	0
1	F	191/217 (88%)	-0.64	0	100	100	48, 89, 134, 144	0
All	All	1162/1302 (89%)	-0.69	2 (0%)	91	80	13, 47, 127, 144	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	ILE	2.2
1	D	176	CYS	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](#)

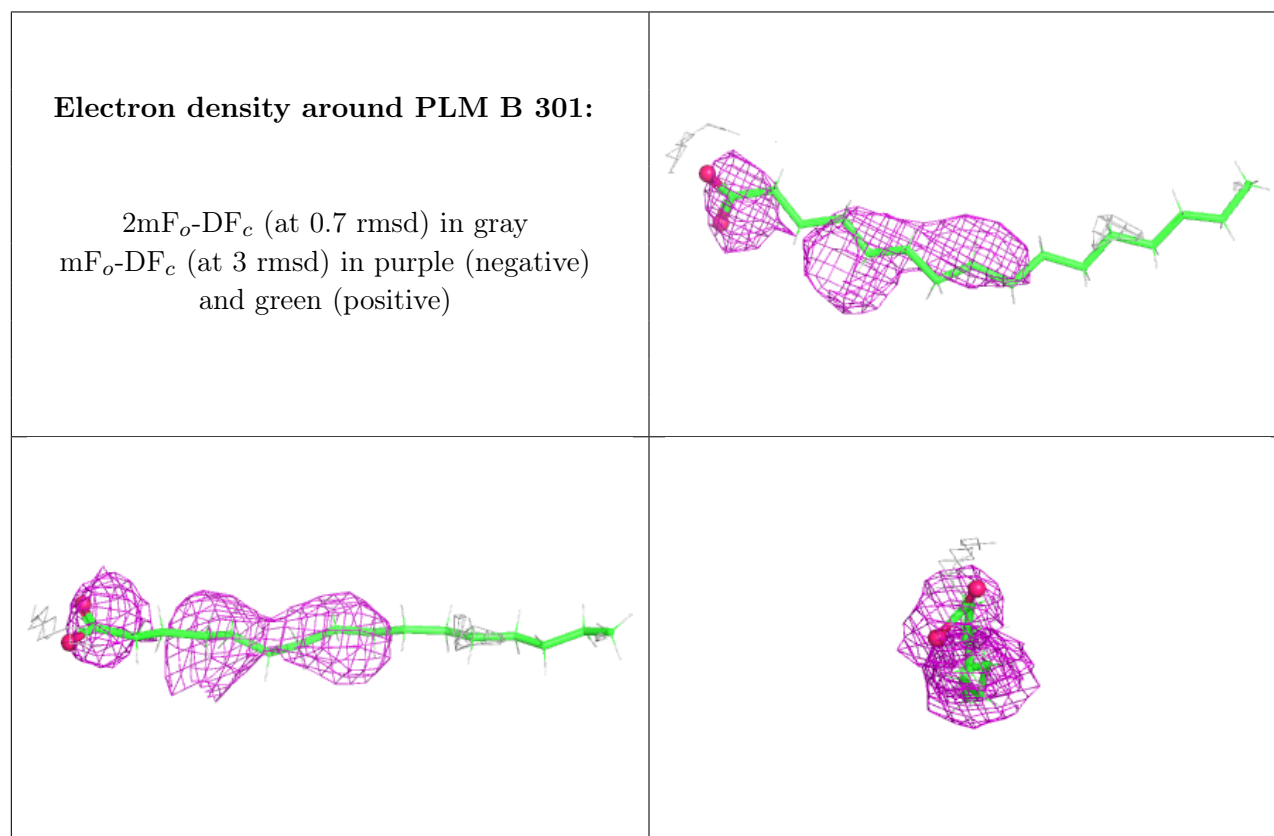
There are no oligosaccharides in this entry.

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.

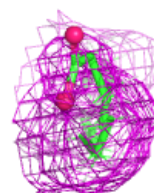
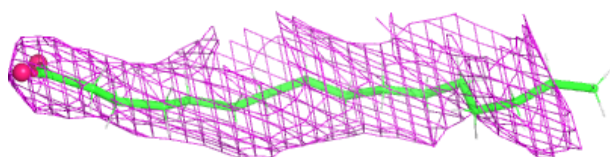
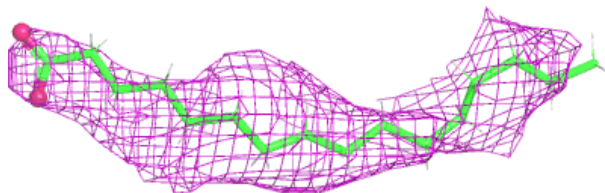
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLM	B	301	18/18	0.84	0.41	13,23,38,39	0
2	PLM	C	301	18/18	0.84	0.72	18,37,70,76	0
2	PLM	D	301	18/18	0.89	0.34	15,23,52,56	0
2	PLM	A	301	18/18	0.90	0.24	10,16,40,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

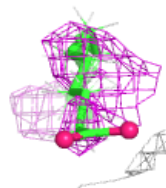
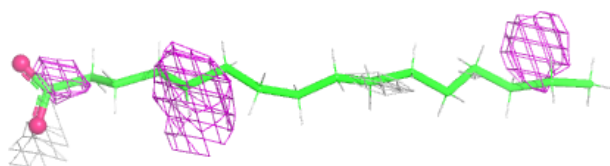
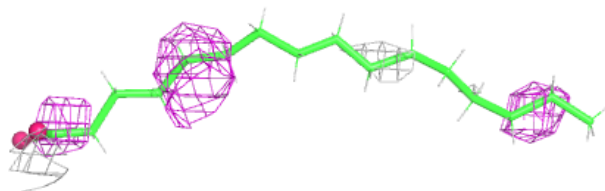


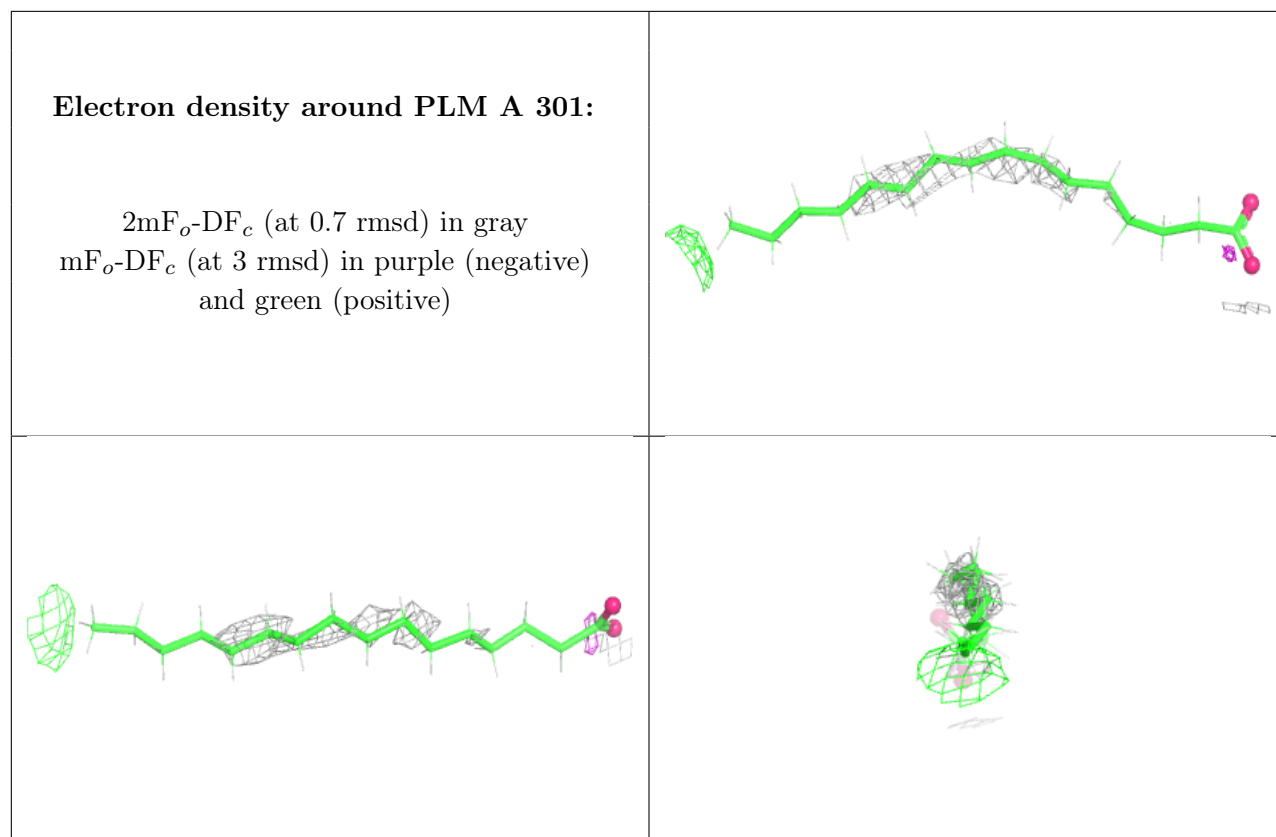
Electron density around PLM C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PLM D 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.