



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:57 AM UTC

PDB ID : 4Y1K / pdb_00004y1k
Title : PALMITOYLATED OPRM OUTER MEMBRANE FACTOR
Authors : Monlezun, L.; Phan, G.; Broutin, I.
Deposited on : 2015-02-07
Resolution : 3.80 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:

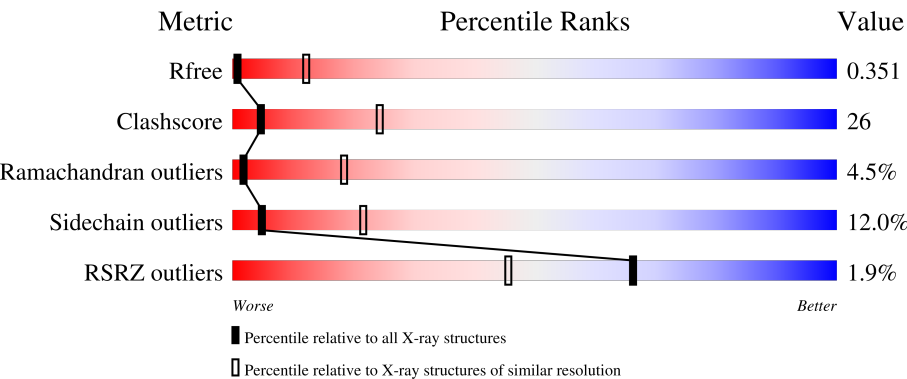
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	474	% 43%44%9% . .
1	B	474	45%45%6% . .
1	C	474	% 45%43%8% .
1	D	474	3% 42%45%9% .
1	E	474	3% 44%46%6% .

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Mol	Chain	Length	Quality of chain
1	F	474	3% 40% 49% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Outer membrane protein OprM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3501	2190	624	684	3			
1	B	457	Total	C	N	O	S	0	0	0
			3501	2190	624	684	3			
1	C	457	Total	C	N	O	S	0	0	0
			3503	2191	624	685	3			
1	D	457	Total	C	N	O	S	0	0	0
			3501	2190	624	684	3			
1	E	456	Total	C	N	O	S	0	0	0
			3492	2185	622	682	3			
1	F	457	Total	C	N	O	S	0	0	0
			3501	2190	624	684	3			

There are 36 discrepancies between the modelled and reference sequences:

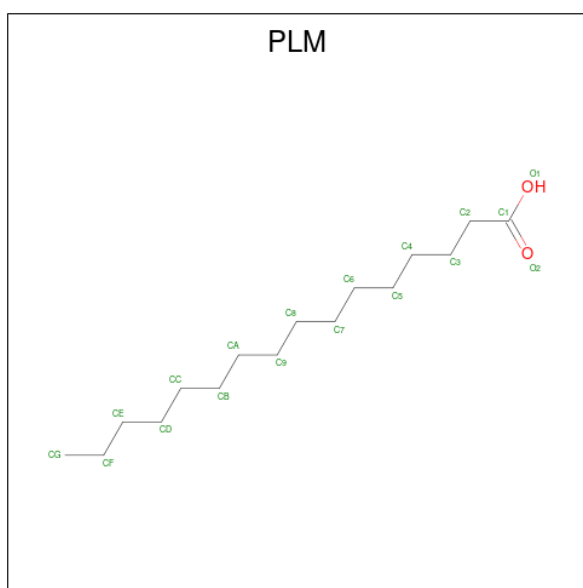
Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP Q51487
A	470	HIS	-	expression tag	UNP Q51487
A	471	HIS	-	expression tag	UNP Q51487
A	472	HIS	-	expression tag	UNP Q51487
A	473	HIS	-	expression tag	UNP Q51487
A	474	HIS	-	expression tag	UNP Q51487
B	469	HIS	-	expression tag	UNP Q51487
B	470	HIS	-	expression tag	UNP Q51487
B	471	HIS	-	expression tag	UNP Q51487
B	472	HIS	-	expression tag	UNP Q51487
B	473	HIS	-	expression tag	UNP Q51487
B	474	HIS	-	expression tag	UNP Q51487
C	469	HIS	-	expression tag	UNP Q51487
C	470	HIS	-	expression tag	UNP Q51487
C	471	HIS	-	expression tag	UNP Q51487
C	472	HIS	-	expression tag	UNP Q51487
C	473	HIS	-	expression tag	UNP Q51487

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Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP Q51487
D	469	HIS	-	expression tag	UNP Q51487
D	470	HIS	-	expression tag	UNP Q51487
D	471	HIS	-	expression tag	UNP Q51487
D	472	HIS	-	expression tag	UNP Q51487
D	473	HIS	-	expression tag	UNP Q51487
D	474	HIS	-	expression tag	UNP Q51487
E	469	HIS	-	expression tag	UNP Q51487
E	470	HIS	-	expression tag	UNP Q51487
E	471	HIS	-	expression tag	UNP Q51487
E	472	HIS	-	expression tag	UNP Q51487
E	473	HIS	-	expression tag	UNP Q51487
E	474	HIS	-	expression tag	UNP Q51487
F	469	HIS	-	expression tag	UNP Q51487
F	470	HIS	-	expression tag	UNP Q51487
F	471	HIS	-	expression tag	UNP Q51487
F	472	HIS	-	expression tag	UNP Q51487
F	473	HIS	-	expression tag	UNP Q51487
F	474	HIS	-	expression tag	UNP Q51487

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		
2	B	1	Total	C	O	0	0
			17	16	1		

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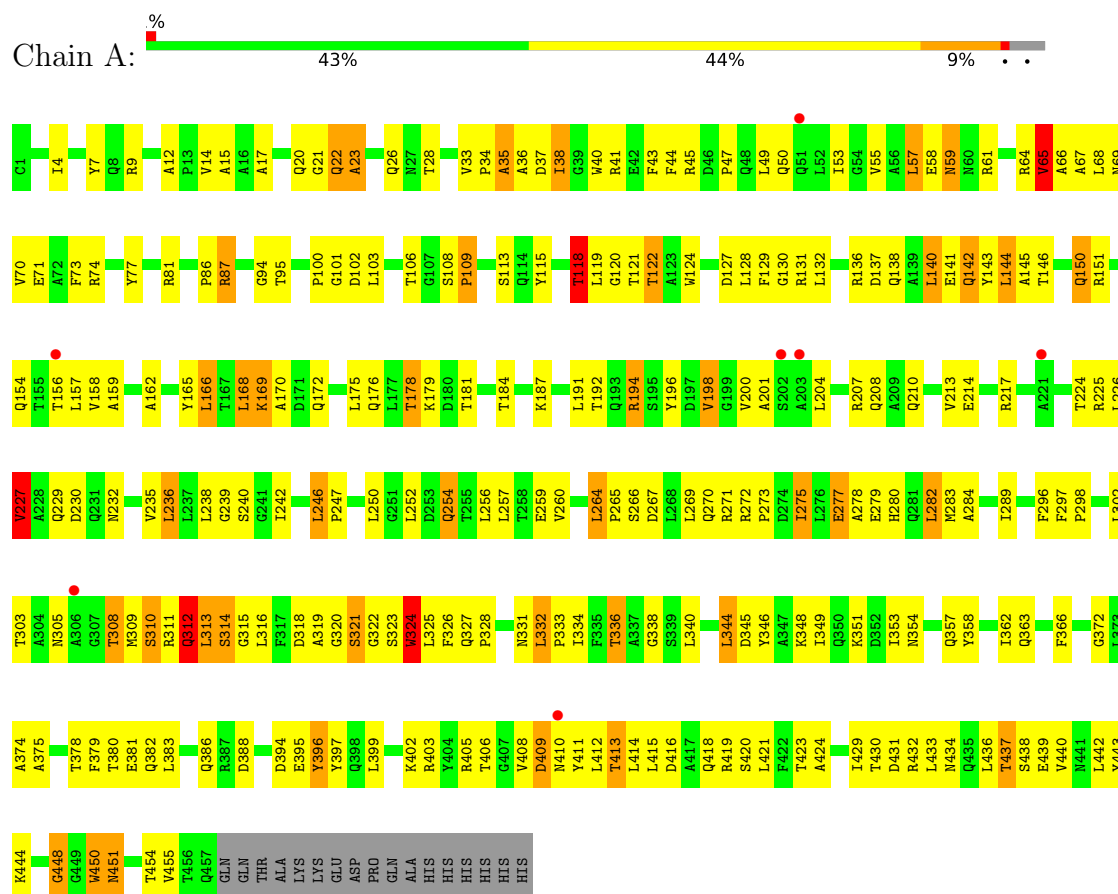
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			17	16	1		

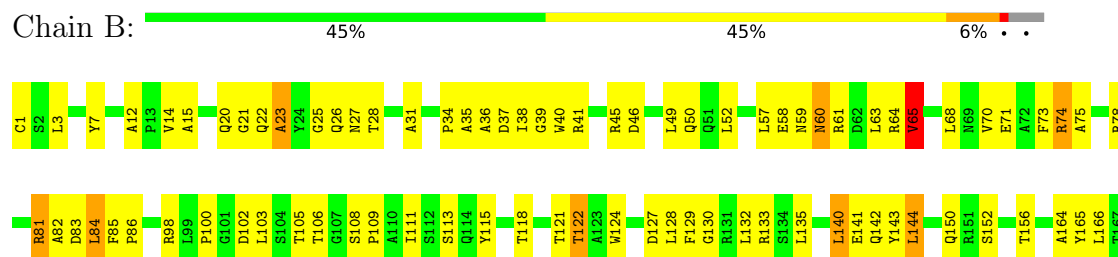
3 Residue-property plots [i](#)

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: Outer membrane protein OprM



• Molecule 1: Outer membrane protein OprM







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.64Å 87.86Å 355.94Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	87.91 – 3.80 87.91 – 3.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (87.91-3.80) 84.4 (87.91-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 3.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.297 , 0.346 0.302 , 0.351	Depositor DCC
R_{free} test set	1992 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 321.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.378 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.339 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	21050	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.23% 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	0.73	0/3557	1.09	22/4838 (0.5%)
1	B	0.76	3/3557 (0.1%)	1.07	13/4838 (0.3%)
1	C	0.75	0/3559	1.08	16/4841 (0.3%)
1	D	0.56	0/3557	1.03	14/4838 (0.3%)
1	E	0.57	0/3548	1.01	9/4826 (0.2%)
1	F	0.56	0/3557	1.02	11/4838 (0.2%)
All	All	0.66	3/21335 (0.0%)	1.05	85/29019 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	HIS	CG-ND1	-7.22	1.30	1.38
1	B	280	HIS	CG-CD2	6.67	1.43	1.35
1	B	280	HIS	ND1-CE1	5.32	1.37	1.32

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	ARG	CA-C-N	8.25	130.15	119.84
1	E	272	ARG	C-N-CA	8.25	130.15	119.84
1	C	272	ARG	CA-C-N	8.08	129.94	119.84
1	C	272	ARG	C-N-CA	8.08	129.94	119.84
1	B	81	ARG	N-CA-C	-7.98	102.17	111.03
1	A	344	LEU	N-CA-C	-7.80	103.38	113.12
1	A	128	LEU	N-CA-C	-7.51	104.08	113.55
1	B	259	GLU	N-CA-C	-7.18	100.38	110.50
1	E	395	GLU	N-CA-C	-7.15	103.17	110.97
1	A	272	ARG	CA-C-N	7.12	128.75	119.84
1	A	272	ARG	C-N-CA	7.12	128.75	119.84
1	C	4	ILE	CB-CA-C	-7.09	103.24	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	ALA	N-CA-C	-7.05	103.53	111.07
1	A	332	LEU	CA-C-N	7.01	127.41	119.83
1	A	332	LEU	C-N-CA	7.01	127.41	119.83
1	A	374	ALA	N-CA-C	-7.00	103.58	111.07
1	E	256	LEU	N-CA-C	6.98	118.97	111.36
1	A	227	VAL	N-CA-C	-6.91	105.11	111.67
1	B	450	TRP	N-CA-C	-6.91	103.20	111.69
1	C	194	ARG	N-CA-C	-6.89	102.61	111.02
1	B	374	ALA	N-CA-C	-6.89	103.46	110.97
1	A	277	GLU	N-CA-C	-6.83	102.69	111.02
1	F	305	ASN	N-CA-C	6.78	118.10	108.74
1	B	74	ARG	N-CA-C	-6.71	104.04	111.36
1	D	174	GLN	N-CA-C	-6.59	104.09	111.28
1	C	259	GLU	N-CA-C	-6.48	101.37	110.50
1	B	59	ASN	N-CA-C	6.43	120.95	112.72
1	C	327	GLN	CA-C-N	6.38	126.57	120.31
1	C	327	GLN	C-N-CA	6.38	126.57	120.31
1	D	297	PHE	CA-C-N	6.28	126.64	119.93
1	D	297	PHE	C-N-CA	6.28	126.64	119.93
1	A	38	ILE	CB-CA-C	-6.24	103.32	111.25
1	C	89	GLY	N-CA-C	6.20	120.42	110.87
1	B	198	VAL	N-CA-C	-6.08	107.20	113.10
1	A	131	ARG	N-CA-C	-6.06	104.59	112.23
1	A	33	VAL	CA-C-N	-6.05	113.72	120.14
1	A	33	VAL	C-N-CA	-6.05	113.72	120.14
1	A	450	TRP	N-CA-C	-5.99	104.32	111.69
1	E	297	PHE	CA-C-N	5.97	127.31	119.84
1	E	297	PHE	C-N-CA	5.97	127.31	119.84
1	F	297	PHE	CA-C-N	5.94	127.27	119.84
1	F	297	PHE	C-N-CA	5.94	127.27	119.84
1	B	272	ARG	CA-C-N	5.91	127.23	119.84
1	B	272	ARG	C-N-CA	5.91	127.23	119.84
1	D	272	ARG	CA-C-N	5.89	127.21	119.84
1	D	272	ARG	C-N-CA	5.89	127.21	119.84
1	D	419	ARG	N-CA-C	-5.80	105.86	113.17
1	A	194	ARG	N-CA-C	-5.79	104.16	111.11
1	C	74	ARG	N-CA-C	-5.79	104.60	111.03
1	C	88	ILE	N-CA-C	5.75	117.61	108.87
1	D	376	ARG	N-CA-C	-5.75	106.91	114.04
1	F	238	LEU	N-CA-C	-5.67	107.36	114.56
1	A	59	ASN	N-CA-C	5.54	120.54	113.18
1	B	277	GLU	N-CA-C	-5.53	104.47	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	LEU	N-CA-C	-5.53	104.90	111.03
1	C	450	TRP	N-CA-C	-5.46	104.86	112.45
1	D	260	VAL	CA-C-N	5.43	125.85	119.99
1	D	260	VAL	C-N-CA	5.43	125.85	119.99
1	E	172	GLN	N-CA-C	-5.42	106.50	113.23
1	D	21	GLY	N-CA-C	5.41	118.37	110.63
1	F	251	GLY	N-CA-C	-5.40	104.43	113.02
1	C	212	ALA	N-CA-C	-5.40	105.04	111.03
1	C	277	GLU	N-CA-C	-5.40	104.43	111.02
1	F	376	ARG	N-CA-C	-5.40	107.24	113.88
1	D	341	ARG	N-CA-C	-5.39	105.30	111.07
1	B	84	LEU	N-CA-C	-5.37	105.99	112.54
1	C	131	ARG	N-CA-C	-5.36	105.47	112.23
1	E	208	GLN	N-CA-C	-5.33	106.46	113.17
1	C	59	ASN	N-CA-C	5.32	120.13	113.43
1	A	118	THR	N-CA-C	5.31	116.07	108.74
1	D	368	GLU	N-CA-C	5.24	116.99	111.28
1	B	60	ASN	N-CA-C	5.23	117.93	110.24
1	B	303	THR	N-CA-C	-5.19	102.07	110.32
1	D	331	ASN	N-CA-C	5.17	117.23	108.02
1	A	312	GLN	N-CA-C	-5.16	102.42	110.42
1	F	70	VAL	N-CA-C	-5.13	105.59	110.42
1	F	410	ASN	N-CA-C	5.10	117.60	109.65
1	F	120	GLY	N-CA-C	5.09	120.43	111.57
1	F	368	GLU	N-CA-C	5.09	117.56	111.71
1	A	239	GLY	N-CA-C	-5.08	108.31	115.32
1	A	35	ALA	N-CA-C	-5.05	105.22	111.33
1	D	304	ALA	N-CA-C	5.05	115.78	107.20
1	E	250	LEU	N-CA-C	5.04	116.61	110.41
1	F	423	THR	N-CA-C	-5.03	107.27	113.41
1	A	336	THR	N-CA-C	-5.03	101.96	109.95

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	3501	0	3475	195	0
1	B	3501	0	3475	182	0
1	C	3503	0	3480	185	0
1	D	3501	0	3476	195	0
1	E	3492	0	3468	196	0
1	F	3501	0	3476	217	0
2	A	17	0	31	0	0
2	B	17	0	31	0	0
2	C	17	0	31	1	0
All	All	21050	0	20943	1082	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 26.

All (1082) 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:D:177:LEU:HD21	1:D:425:GLN:HB3	1.48	0.95
1:D:372:GLY:HA3	1:D:442:LEU:HD22	1.55	0.88
1:E:210:GLN:HE21	1:E:214:GLU:HG3	1.39	0.87
1:A:81:ARG:HA	1:A:136:ARG:HG3	1.57	0.87
1:E:98:ARG:HA	1:E:111:ILE:HG12	1.55	0.86
1:B:35:ALA:HA	1:B:38:ILE:HD12	1.57	0.86
1:C:122:THR:HA	1:C:303:THR:HG23	1.57	0.85
1:A:412:LEU:HD13	1:B:413:THR:HG23	1.60	0.84
1:D:41:ARG:O	1:D:50:GLN:NE2	2.11	0.83
1:A:275:ILE:HD11	1:A:362:ILE:HA	1.59	0.83
1:D:403:ARG:HG2	1:D:409:ASP:HB2	1.61	0.82
1:F:57:LEU:HD21	1:F:154:GLN:HG3	1.61	0.82
1:D:369:VAL:HA	1:D:442:LEU:HD11	1.62	0.82
1:D:399:LEU:HB3	1:E:204:LEU:HD12	1.61	0.81
1:E:272:ARG:NH1	1:E:274:ASP:OD1	2.12	0.81
1:F:432:ARG:NH1	1:F:435:GLN:OE1	2.13	0.81
1:E:390:VAL:HG21	1:E:428:LEU:HD22	1.63	0.80
1:C:100:PRO:HD2	1:C:103:LEU:HB2	1.64	0.80
1:D:411:TYR:HE2	1:D:415:LEU:HD13	1.46	0.79
1:E:371:ASP:OD1	1:F:232:ASN:ND2	2.15	0.79
1:A:411:TYR:HE2	1:A:415:LEU:HD13	1.48	0.78
1:D:333:PRO:HA	1:E:89:GLY:HA3	1.65	0.78
1:C:275:ILE:HD11	1:C:362:ILE:HA	1.66	0.78
1:B:170:ALA:HA	1:B:252:LEU:HD11	1.64	0.78
1:C:207:ARG:NH1	1:C:210:GLN:OE1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:444:LYS:HA	1:F:448:GLY:HA2	1.65	0.77
1:F:397:TYR:HA	1:F:417:ALA:HB1	1.65	0.77
1:B:314:SER:O	1:B:316:LEU:N	2.16	0.76
1:F:175:LEU:HD22	1:F:227:VAL:HG21	1.67	0.76
1:E:334:ILE:HG12	1:F:89:GLY:HA2	1.67	0.75
1:B:412:LEU:HD13	1:C:413:THR:HG23	1.68	0.75
1:E:324:TRP:CD1	1:F:98:ARG:H	2.05	0.75
1:D:128:LEU:HD22	1:D:300:ILE:HD11	1.69	0.75
1:D:175:LEU:HD22	1:D:227:VAL:HG21	1.68	0.75
1:A:141:GLU:HB3	1:A:284:ALA:HB2	1.67	0.75
1:E:389:LEU:O	1:E:393:SER:OG	2.04	0.74
1:C:168:LEU:HD23	1:C:230:ASP:HB2	1.68	0.74
1:A:41:ARG:O	1:A:50:GLN:NE2	2.21	0.74
1:F:38:ILE:HD12	1:F:260:VAL:HG13	1.70	0.74
1:E:59:ASN:O	1:E:61:ARG:NH1	2.21	0.74
1:A:38:ILE:O	1:A:443:TYR:OH	2.04	0.74
1:F:177:LEU:HD21	1:F:425:GLN:HB3	1.68	0.74
1:B:372:GLY:HA3	1:B:442:LEU:HD13	1.70	0.73
1:E:318:ASP:HB2	1:E:321:SER:HB3	1.69	0.73
1:E:335:PHE:HB3	1:F:88:ILE:HB	1.70	0.73
1:A:122:THR:HA	1:A:303:THR:HG23	1.70	0.73
1:B:411:TYR:HE2	1:B:415:LEU:HD13	1.54	0.73
1:D:20:GLN:NE2	1:D:26:GLN:OE1	2.21	0.73
1:D:89:GLY:HA2	1:F:334:ILE:HG12	1.71	0.73
1:B:336:THR:O	1:B:338:GLY:N	2.21	0.73
1:A:298:PRO:HG3	1:A:332:LEU:HD22	1.70	0.73
1:D:145:ALA:HB2	1:D:280:HIS:HB2	1.71	0.72
1:D:396:TYR:HB2	1:E:207:ARG:HB3	1.71	0.72
1:E:177:LEU:HD21	1:E:425:GLN:HB3	1.72	0.72
1:A:59:ASN:O	1:A:61:ARG:NH1	2.22	0.72
1:C:411:TYR:HE2	1:C:415:LEU:HD13	1.55	0.72
1:F:3:LEU:HB3	1:F:293:ARG:HD3	1.72	0.72
1:A:86:PRO:HB3	1:A:124:TRP:CD2	2.25	0.72
1:E:92:GLY:HA2	1:E:117:VAL:HG22	1.72	0.72
1:A:100:PRO:HD2	1:A:103:LEU:HB2	1.71	0.71
1:D:175:LEU:HG	1:D:179:LYS:HE3	1.72	0.71
1:B:1:CYS:O	1:B:133:ARG:NH1	2.24	0.71
1:C:296:PHE:CE1	1:C:340:LEU:HB3	2.25	0.71
1:B:86:PRO:HB3	1:B:124:TRP:CD2	2.26	0.71
1:B:313:LEU:O	1:B:316:LEU:HG	1.90	0.71
1:E:175:LEU:HD22	1:E:227:VAL:HG21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ASP:OD1	1:E:232:ASN:ND2	2.16	0.70
1:D:88:ILE:HB	1:F:335:PHE:HB3	1.73	0.70
1:D:166:LEU:HD13	1:D:436:LEU:HD13	1.72	0.70
1:B:332:LEU:HD12	1:B:333:PRO:HD2	1.74	0.70
1:C:21:GLY:O	1:C:23:ALA:N	2.24	0.70
1:E:184:THR:HG23	1:E:187:LYS:HE2	1.74	0.70
1:F:168:LEU:HD23	1:F:230:ASP:HB2	1.72	0.70
1:F:144:LEU:HB3	1:F:280:HIS:CE1	2.28	0.69
1:F:262:ALA:HA	1:F:446:LEU:HD13	1.73	0.69
1:C:313:LEU:O	1:C:316:LEU:HG	1.93	0.69
1:C:35:ALA:HA	1:C:38:ILE:HD12	1.73	0.69
1:C:176:GLN:HA	1:C:179:LYS:HG3	1.74	0.69
1:D:168:LEU:HD23	1:D:230:ASP:HB2	1.75	0.69
1:A:413:THR:HG23	1:C:412:LEU:HD13	1.75	0.69
1:C:198:VAL:HG12	1:C:200:VAL:HG23	1.75	0.68
1:D:301:SER:HB3	1:D:329:SER:HB2	1.75	0.68
1:E:168:LEU:HD23	1:E:230:ASP:HB2	1.75	0.68
1:A:254:GLN:O	1:A:432:ARG:NH2	2.26	0.68
1:D:53:ILE:HG12	1:D:161:VAL:HG11	1.76	0.68
1:E:44:PHE:O	1:E:50:GLN:NE2	2.26	0.68
1:E:78:ARG:HG2	1:E:81:ARG:HH21	1.59	0.68
1:C:38:ILE:HA	1:C:454:THR:HG23	1.76	0.68
1:C:269:LEU:HD21	1:C:362:ILE:HD11	1.76	0.68
1:C:372:GLY:HA3	1:C:442:LEU:HD13	1.75	0.67
1:A:12:ALA:HB2	1:A:269:LEU:HD11	1.77	0.67
1:A:141:GLU:HG2	1:A:283:MET:HB2	1.77	0.67
1:F:310:SER:OG	1:F:312:GLN:O	2.10	0.67
1:E:38:ILE:O	1:E:443:TYR:OH	2.13	0.67
1:E:432:ARG:NH1	1:E:435:GLN:OE1	2.27	0.67
1:F:116:GLY:HA3	1:F:309:MET:HG2	1.77	0.66
1:F:316:LEU:O	1:F:318:ASP:N	2.27	0.66
1:A:106:THR:OG1	1:A:108:SER:O	2.13	0.66
1:A:35:ALA:HA	1:A:38:ILE:HD12	1.77	0.66
1:A:349:ILE:HD13	1:C:71:GLU:HB3	1.76	0.66
1:A:310:SER:OG	1:A:312:GLN:O	2.12	0.66
1:E:20:GLN:HE22	1:E:26:GLN:HA	1.61	0.66
1:F:59:ASN:O	1:F:61:ARG:NH1	2.28	0.66
1:F:325:LEU:HD12	1:F:326:PHE:H	1.60	0.66
1:B:106:THR:OG1	1:B:108:SER:O	2.14	0.66
1:D:123:ALA:H	1:D:303:THR:HG23	1.60	0.66
1:A:169:LYS:HA	1:A:172:GLN:OE1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:LEU:HD12	1:E:300:ILE:HG21	1.78	0.66
1:B:298:PRO:HG3	1:B:332:LEU:HD22	1.78	0.65
1:D:390:VAL:HG21	1:D:428:LEU:HD22	1.77	0.65
1:E:282:LEU:HA	1:E:354:ASN:HB3	1.78	0.65
1:A:20:GLN:HE22	1:A:26:GLN:HA	1.60	0.65
1:C:395:GLU:C	1:C:397:TYR:H	2.04	0.65
1:F:233:ALA:O	1:F:237:LEU:HG	1.97	0.65
1:B:325:LEU:HD11	1:B:327:GLN:HB2	1.78	0.65
1:D:144:LEU:HB3	1:D:280:HIS:ND1	2.11	0.65
1:D:397:TYR:HA	1:D:417:ALA:HB1	1.78	0.65
1:A:310:SER:OG	1:A:311:ARG:N	2.30	0.65
1:F:390:VAL:HG21	1:F:428:LEU:HD22	1.77	0.65
1:E:385:ALA:HB3	1:F:218:ALA:HB2	1.79	0.65
1:F:235:VAL:HA	1:F:238:LEU:HD12	1.78	0.65
1:B:34:PRO:HG2	1:B:271:ARG:CZ	2.27	0.65
1:B:282:LEU:HA	1:B:354:ASN:HB3	1.79	0.65
1:B:39:GLY:H	1:B:454:THR:HG1	1.44	0.64
1:B:275:ILE:HD11	1:B:362:ILE:HA	1.79	0.64
1:D:129:PHE:CD1	1:D:297:PHE:HB3	2.33	0.64
1:F:38:ILE:O	1:F:443:TYR:OH	2.09	0.64
1:A:168:LEU:HD23	1:A:230:ASP:HB2	1.77	0.64
1:E:269:LEU:HD21	1:E:362:ILE:HD11	1.79	0.64
1:B:326:PHE:CD2	1:B:328:PRO:HD3	2.33	0.64
1:E:4:ILE:HD11	1:E:134:SER:HA	1.80	0.64
1:F:141:GLU:HB3	1:F:284:ALA:HB2	1.79	0.64
1:A:416:ASP:OD1	1:C:419:ARG:NH1	2.29	0.64
1:D:22:GLN:O	1:E:224:THR:OG1	2.15	0.64
1:A:331:ASN:ND2	1:C:91:ASP:OD1	2.30	0.64
1:A:9:ARG:NE	1:A:279:GLU:OE2	2.29	0.63
1:A:68:LEU:O	1:A:71:GLU:N	2.31	0.63
1:C:23:ALA:HB1	1:C:378:THR:HG23	1.79	0.63
1:E:402:LYS:O	1:E:406:THR:OG1	2.14	0.63
1:D:336:THR:C	1:D:338:GLY:H	2.06	0.63
1:D:359:GLU:OE1	1:E:61:ARG:NE	2.27	0.63
1:F:422:PHE:HA	1:F:425:GLN:HB2	1.79	0.63
1:B:168:LEU:HD23	1:B:230:ASP:HB2	1.79	0.63
1:D:334:ILE:HG12	1:E:89:GLY:HA2	1.81	0.63
1:F:183:GLY:O	1:F:187:LYS:HB2	1.99	0.63
1:B:296:PHE:CE1	1:B:340:LEU:HB3	2.34	0.63
1:F:260:VAL:H	1:F:376:ARG:HH22	1.46	0.63
1:F:402:LYS:HE3	1:F:405:ARG:HH22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:HG2	1:A:409:ASP:HB2	1.81	0.62
1:D:121:THR:HG21	1:D:124:TRP:HB2	1.79	0.62
1:F:92:GLY:HA2	1:F:117:VAL:HG22	1.80	0.62
1:A:207:ARG:HB3	1:B:396:TYR:HB2	1.80	0.62
1:A:334:ILE:HG12	1:C:89:GLY:HA2	1.82	0.62
1:C:106:THR:OG1	1:C:108:SER:O	2.16	0.62
1:B:403:ARG:HG2	1:B:409:ASP:HB2	1.81	0.62
1:B:300:ILE:HG12	1:B:330:ILE:HG23	1.80	0.62
1:A:23:ALA:HB1	1:A:378:THR:HG23	1.81	0.62
1:B:141:GLU:HB3	1:B:284:ALA:HB2	1.81	0.62
1:C:86:PRO:HB3	1:C:124:TRP:CD2	2.34	0.62
1:A:332:LEU:HD12	1:A:333:PRO:HD2	1.81	0.61
1:D:299:SER:HB3	1:D:331:ASN:HB3	1.82	0.61
1:A:70:VAL:HG22	1:A:146:THR:HG22	1.81	0.61
1:E:383:LEU:HD21	1:E:431:ASP:O	2.00	0.61
1:F:123:ALA:H	1:F:303:THR:HG23	1.65	0.61
1:B:254:GLN:O	1:B:432:ARG:NH2	2.32	0.61
1:F:372:GLY:HA3	1:F:442:LEU:HD13	1.81	0.61
1:C:282:LEU:HA	1:C:354:ASN:HB3	1.82	0.61
1:D:321:SER:HA	1:E:100:PRO:HB3	1.83	0.61
1:D:392:ALA:O	1:D:396:TYR:HB3	2.00	0.61
1:F:210:GLN:O	1:F:214:GLU:HG2	2.00	0.61
1:A:37:ASP:OD2	1:A:271:ARG:NH1	2.33	0.61
1:D:176:GLN:HA	1:D:179:LYS:HD2	1.81	0.61
1:F:256:LEU:HD11	1:F:436:LEU:HD13	1.82	0.61
1:B:122:THR:HA	1:B:303:THR:HG23	1.81	0.61
1:C:225:ARG:C	1:C:227:VAL:H	2.09	0.61
1:C:336:THR:HB	1:C:339:SER:HB3	1.81	0.61
1:D:174:GLN:HB3	1:D:223:TYR:CE2	2.36	0.61
1:A:323:SER:O	1:A:324:TRP:HB3	2.00	0.60
1:D:44:PHE:O	1:D:50:GLN:NE2	2.32	0.60
1:C:403:ARG:HG2	1:C:409:ASP:HB2	1.82	0.60
1:E:41:ARG:O	1:E:50:GLN:NE2	2.34	0.60
1:A:326:PHE:CD2	1:A:328:PRO:HD3	2.37	0.60
1:B:198:VAL:HG12	1:B:200:VAL:HG23	1.82	0.60
1:E:236:LEU:O	1:E:238:LEU:N	2.26	0.60
1:E:243:PRO:HD2	1:E:246:LEU:HD21	1.83	0.60
1:C:9:ARG:NE	1:C:279:GLU:OE2	2.35	0.60
1:F:175:LEU:HG	1:F:179:LYS:HE3	1.84	0.60
1:A:296:PHE:CE1	1:A:340:LEU:HB3	2.37	0.59
1:B:208:GLN:HB3	1:B:415:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ILE:HA	1:D:454:THR:HG23	1.84	0.59
1:F:41:ARG:NH1	1:F:50:GLN:OE1	2.34	0.59
1:E:178:THR:HG21	1:E:219:THR:HG22	1.83	0.59
1:F:236:LEU:C	1:F:238:LEU:H	2.10	0.59
1:B:141:GLU:HG2	1:B:284:ALA:N	2.17	0.59
1:E:326:PHE:CD2	1:E:328:PRO:HD3	2.37	0.59
1:E:392:ALA:O	1:E:396:TYR:HB3	2.01	0.59
1:F:282:LEU:HD13	1:F:354:ASN:C	2.26	0.59
1:B:283:MET:O	1:B:286:ASN:HB3	2.02	0.59
1:E:333:PRO:HA	1:F:89:GLY:HA3	1.83	0.59
1:F:184:THR:HA	1:F:187:LYS:HB3	1.85	0.59
1:E:334:ILE:HD11	1:F:90:VAL:HG23	1.85	0.59
1:B:68:LEU:HD12	1:C:353:ILE:HA	1.84	0.59
1:B:402:LYS:HG2	1:B:405:ARG:NH2	2.18	0.59
1:C:13:PRO:O	1:C:363:GLN:NE2	2.36	0.59
1:C:320:GLY:C	1:C:322:GLY:H	2.11	0.59
1:E:175:LEU:HG	1:E:179:LYS:HE3	1.83	0.59
1:E:175:LEU:O	1:E:179:LYS:HG3	2.03	0.59
1:F:282:LEU:HA	1:F:354:ASN:HB3	1.85	0.59
1:D:38:ILE:O	1:D:443:TYR:OH	2.21	0.59
1:E:250:LEU:HB3	1:E:254:GLN:HG3	1.84	0.59
1:A:7:TYR:CD2	1:A:283:MET:HE3	2.38	0.58
1:F:250:LEU:HB3	1:F:254:GLN:HG3	1.85	0.58
1:E:184:THR:HA	1:E:187:LYS:HG2	1.85	0.58
1:B:23:ALA:HB1	1:B:378:THR:HG23	1.85	0.58
1:E:206:LEU:HA	1:E:209:ALA:HB3	1.85	0.58
1:E:73:PHE:HB3	1:E:143:TYR:HA	1.86	0.58
1:A:73:PHE:HB3	1:A:143:TYR:HA	1.85	0.58
1:A:15:ALA:HB3	1:A:366:PHE:CZ	2.38	0.58
1:F:35:ALA:HB3	1:F:446:LEU:HB2	1.85	0.58
1:F:174:GLN:HB3	1:F:223:TYR:CD2	2.39	0.58
1:D:116:GLY:HA3	1:D:309:MET:HG2	1.86	0.57
1:D:325:LEU:HD12	1:D:326:PHE:H	1.69	0.57
1:E:156:THR:HA	1:E:444:LYS:HE3	1.86	0.57
1:F:41:ARG:O	1:F:50:GLN:NE2	2.37	0.57
1:B:310:SER:OG	1:B:312:GLN:O	2.23	0.57
1:C:208:GLN:HB3	1:C:415:LEU:HD22	1.84	0.57
1:D:204:LEU:HD13	1:F:399:LEU:HB3	1.85	0.57
1:D:227:VAL:O	1:D:231:GLN:HG3	2.04	0.57
1:E:289:ILE:O	1:E:293:ARG:HB2	2.04	0.57
1:E:419:ARG:O	1:E:423:THR:OG1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASP:OD2	1:C:130:GLY:HA2	2.05	0.57
1:C:128:LEU:O	1:C:133:ARG:NH2	2.37	0.57
1:E:359:GLU:OE1	1:F:61:ARG:NE	2.32	0.57
1:E:395:GLU:O	1:E:399:LEU:HG	2.05	0.57
1:F:411:TYR:HA	1:F:414:LEU:HB3	1.86	0.57
1:A:336:THR:O	1:A:338:GLY:N	2.36	0.57
1:F:145:ALA:HB2	1:F:280:HIS:HB3	1.85	0.57
1:F:170:ALA:HA	1:F:252:LEU:HD11	1.87	0.57
1:A:198:VAL:HG12	1:A:200:VAL:HG23	1.85	0.57
1:B:279:GLU:O	1:B:282:LEU:HB3	2.05	0.57
1:C:252:LEU:HB3	1:C:432:ARG:HG2	1.86	0.57
1:B:121:THR:HG21	1:B:124:TRP:HB2	1.86	0.57
1:E:293:ARG:HG3	1:E:344:LEU:HD11	1.86	0.57
1:A:264:LEU:O	1:A:267:ASP:HB2	2.05	0.57
1:A:395:GLU:C	1:A:397:TYR:H	2.12	0.57
1:B:325:LEU:HD12	1:B:326:PHE:H	1.69	0.57
1:C:382:GLN:NE2	1:C:431:ASP:OD2	2.38	0.57
1:D:154:GLN:NE2	1:D:449:GLY:O	2.38	0.57
1:B:349:ILE:O	1:B:352:ASP:N	2.38	0.56
1:D:389:LEU:HD22	1:E:215:GLY:HA2	1.86	0.56
1:E:301:SER:HB3	1:E:329:SER:HB2	1.87	0.56
1:F:33:VAL:HG13	1:F:37:ASP:HB2	1.87	0.56
1:F:222:GLN:HG2	1:F:223:TYR:CD1	2.40	0.56
1:A:372:GLY:HA3	1:A:442:LEU:HD13	1.86	0.56
1:E:120:GLY:HA3	1:E:305:ASN:HA	1.84	0.56
1:B:36:ALA:O	1:B:451:ASN:ND2	2.39	0.56
1:B:181:THR:HA	1:B:184:THR:HB	1.87	0.56
1:C:102:ASP:OD1	1:C:102:ASP:N	2.34	0.56
1:C:141:GLU:HG2	1:C:284:ALA:N	2.20	0.56
1:C:326:PHE:CD2	1:C:328:PRO:HD3	2.41	0.56
1:C:346:TYR:CE2	1:C:350:GLN:HG3	2.41	0.56
1:D:282:LEU:HA	1:D:354:ASN:HB3	1.87	0.56
1:E:192:THR:HG22	1:E:206:LEU:HD13	1.88	0.56
1:E:336:THR:C	1:E:338:GLY:H	2.12	0.56
1:B:12:ALA:HB2	1:B:269:LEU:HD11	1.88	0.56
1:E:402:LYS:HG2	1:E:405:ARG:HH22	1.70	0.56
1:F:207:ARG:O	1:F:211:THR:N	2.38	0.56
1:D:391:LYS:O	1:D:394:ASP:N	2.38	0.56
1:E:33:VAL:HG13	1:E:37:ASP:HB2	1.87	0.56
1:A:34:PRO:O	1:A:38:ILE:HG13	2.06	0.56
1:B:100:PRO:HD2	1:B:103:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HG	1:B:316:LEU:HD12	1.87	0.56
1:D:98:ARG:HA	1:D:111:ILE:HG12	1.86	0.56
1:E:308:THR:O	1:E:309:MET:HG3	2.05	0.56
1:A:102:ASP:N	1:A:102:ASP:OD1	2.36	0.56
1:D:100:PRO:HB3	1:F:321:SER:HA	1.88	0.56
1:D:282:LEU:HD13	1:D:354:ASN:C	2.31	0.56
1:F:171:ASP:OD2	1:F:226:LEU:HB3	2.06	0.56
1:A:353:ILE:O	1:A:357:GLN:HG3	2.06	0.56
1:D:422:PHE:HA	1:D:425:GLN:HB2	1.87	0.56
1:E:384:GLN:NE2	1:E:388:ASP:OD1	2.39	0.56
1:F:1:CYS:O	1:F:133:ARG:NH1	2.36	0.56
1:A:38:ILE:HA	1:A:454:THR:HG23	1.88	0.55
1:A:36:ALA:O	1:A:451:ASN:ND2	2.40	0.55
1:D:67:ALA:HA	1:D:150:GLN:OE1	2.06	0.55
1:D:236:LEU:C	1:D:238:LEU:H	2.14	0.55
1:E:48:GLN:HA	1:E:247:PRO:HD2	1.89	0.55
1:E:396:TYR:HB2	1:F:207:ARG:HB3	1.89	0.55
1:B:21:GLY:O	1:B:23:ALA:N	2.39	0.55
1:D:73:PHE:HA	1:D:76:GLN:HB3	1.87	0.55
1:F:316:LEU:C	1:F:318:ASP:H	2.14	0.55
1:E:121:THR:O	1:E:303:THR:HG23	2.07	0.55
1:C:128:LEU:HD21	2:C:1001:PLM:H51	1.89	0.55
1:C:46:ASP:OD2	1:C:165:TYR:OH	2.10	0.55
1:E:372:GLY:HA3	1:E:442:LEU:HD22	1.87	0.55
1:C:314:SER:O	1:C:316:LEU:N	2.34	0.55
1:D:260:VAL:H	1:D:376:ARG:HH22	1.55	0.55
1:E:101:GLY:O	1:E:103:LEU:N	2.39	0.55
1:E:360:LYS:HG3	1:F:62:ASP:OD1	2.07	0.55
1:C:131:ARG:HG3	1:C:294:ALA:HB3	1.89	0.55
1:A:44:PHE:O	1:A:50:GLN:NE2	2.32	0.55
1:C:310:SER:OG	1:C:312:GLN:O	2.23	0.55
1:F:336:THR:C	1:F:338:GLY:H	2.14	0.55
1:A:279:GLU:O	1:A:282:LEU:HB3	2.06	0.54
1:C:300:ILE:HG12	1:C:330:ILE:HG12	1.88	0.54
1:C:432:ARG:CZ	1:C:436:LEU:HD21	2.37	0.54
1:A:34:PRO:HG2	1:A:271:ARG:CZ	2.37	0.54
1:B:71:GLU:HB3	1:C:349:ILE:HD13	1.89	0.54
1:C:7:TYR:CD2	1:C:283:MET:HE3	2.43	0.54
1:C:324:TRP:C	1:C:324:TRP:CD1	2.85	0.54
1:C:349:ILE:O	1:C:352:ASP:N	2.40	0.54
1:A:320:GLY:C	1:A:322:GLY:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLN:O	1:E:55:VAL:HG23	2.06	0.54
1:B:14:VAL:HG23	1:B:15:ALA:O	2.07	0.54
1:C:60:ASN:OD1	1:C:63:LEU:N	2.35	0.54
1:F:269:LEU:HA	1:F:275:ILE:HG21	1.89	0.54
1:D:212:ALA:HB2	1:D:415:LEU:HD11	1.89	0.54
1:B:61:ARG:NE	1:C:359:GLU:OE1	2.39	0.54
1:D:118:THR:OG1	1:D:305:ASN:HB2	2.08	0.54
1:E:15:ALA:HB3	1:E:366:PHE:HZ	1.72	0.54
1:C:20:GLN:HE22	1:C:26:GLN:HA	1.72	0.54
1:C:456:THR:OG1	1:C:457:GLN:N	2.41	0.54
1:E:308:THR:HA	1:E:322:GLY:HA2	1.90	0.53
1:C:34:PRO:O	1:C:38:ILE:HG13	2.08	0.53
1:D:329:SER:HA	1:E:92:GLY:O	2.08	0.53
1:D:185:TYR:HB3	1:D:213:VAL:HG22	1.91	0.53
1:E:386:GLN:O	1:E:390:VAL:HG23	2.09	0.53
1:F:207:ARG:O	1:F:211:THR:HG23	2.07	0.53
1:B:98:ARG:HA	1:B:111:ILE:HG13	1.90	0.53
1:B:178:THR:HG21	1:B:220:LEU:HA	1.90	0.53
1:A:120:GLY:HA3	1:A:305:ASN:HA	1.91	0.53
1:B:128:LEU:O	1:B:133:ARG:NH2	2.41	0.53
1:B:323:SER:O	1:B:324:TRP:HB3	2.09	0.53
1:C:332:LEU:HD12	1:C:333:PRO:HD2	1.91	0.53
1:B:396:TYR:CE2	1:B:417:ALA:HA	2.43	0.53
1:B:451:ASN:ND2	1:B:451:ASN:H	2.07	0.53
1:D:374:ALA:O	1:D:378:THR:OG1	2.26	0.53
1:E:391:LYS:O	1:E:394:ASP:N	2.41	0.53
1:F:29:GLY:O	1:F:263:GLY:HA2	2.09	0.53
1:A:127:ASP:OD2	1:A:130:GLY:HA2	2.08	0.53
1:B:1:CYS:HB2	1:B:129:PHE:HA	1.89	0.53
1:F:194:ARG:O	1:F:198:VAL:HG23	2.08	0.53
1:C:169:LYS:HA	1:C:172:GLN:OE1	2.08	0.53
1:E:403:ARG:O	1:E:409:ASP:HB2	2.08	0.53
1:F:84:LEU:HD11	1:F:136:ARG:HD3	1.91	0.53
1:C:258:THR:HG22	1:C:259:GLU:O	2.09	0.53
1:F:375:ALA:O	1:F:379:PHE:HB2	2.09	0.53
1:F:402:LYS:HG2	1:F:405:ARG:NH2	2.23	0.53
1:D:100:PRO:HG2	1:D:103:LEU:HD12	1.91	0.52
1:D:101:GLY:O	1:D:103:LEU:N	2.43	0.52
1:E:9:ARG:NH2	1:E:279:GLU:OE2	2.42	0.52
1:B:212:ALA:HB2	1:B:415:LEU:HD11	1.92	0.52
1:D:178:THR:HG21	1:D:219:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:OG1	1:E:306:ALA:N	2.40	0.52
1:E:118:THR:HG1	1:E:306:ALA:H	1.57	0.52
1:A:38:ILE:HD12	1:A:260:VAL:HG13	1.91	0.52
1:D:214:GLU:HB2	1:F:389:LEU:HD13	1.90	0.52
1:A:414:LEU:O	1:A:418:GLN:HG3	2.10	0.52
1:B:214:GLU:HG3	1:C:388:ASP:HB3	1.91	0.52
1:D:391:LYS:O	1:D:395:GLU:HG2	2.10	0.52
1:A:402:LYS:HG2	1:A:405:ARG:NH2	2.25	0.52
1:D:243:PRO:HD2	1:D:246:LEU:HD21	1.92	0.52
1:E:68:LEU:C	1:E:70:VAL:H	2.18	0.52
1:C:325:LEU:HD11	1:C:327:GLN:HB2	1.91	0.52
1:F:145:ALA:HB2	1:F:280:HIS:CB	2.39	0.52
1:F:279:GLU:HB2	1:F:358:TYR:HE1	1.74	0.52
1:B:185:TYR:HB3	1:B:213:VAL:HG22	1.92	0.52
1:E:192:THR:HG23	1:E:201:ALA:HB1	1.92	0.52
1:E:324:TRP:O	1:F:97:GLN:HB2	2.10	0.52
1:A:143:TYR:O	1:A:146:THR:N	2.43	0.52
1:C:59:ASN:O	1:C:61:ARG:NH1	2.43	0.52
1:D:14:VAL:HG23	1:D:15:ALA:H	1.75	0.52
1:E:177:LEU:HD23	1:E:422:PHE:HE1	1.74	0.52
1:E:395:GLU:CB	1:F:207:ARG:HE	2.22	0.52
1:A:415:LEU:HA	1:A:418:GLN:OE1	2.09	0.52
1:B:345:ASP:O	1:B:348:LYS:N	2.42	0.52
1:D:310:SER:OG	1:D:311:ARG:N	2.42	0.52
1:E:78:ARG:HG2	1:E:81:ARG:NH2	2.25	0.52
1:B:395:GLU:C	1:B:397:TYR:H	2.17	0.52
1:A:118:THR:OG1	1:A:119:LEU:N	2.42	0.51
1:B:129:PHE:CD1	1:B:297:PHE:HB3	2.45	0.51
1:C:419:ARG:O	1:C:421:LEU:N	2.43	0.51
1:C:171:ASP:HA	1:C:174:GLN:HB2	1.92	0.51
1:C:429:ILE:O	1:C:432:ARG:HB3	2.10	0.51
1:D:101:GLY:C	1:D:103:LEU:H	2.18	0.51
1:B:326:PHE:HD2	1:B:328:PRO:HD3	1.71	0.51
1:C:421:LEU:O	1:C:424:ALA:N	2.43	0.51
1:D:52:LEU:HD21	1:D:246:LEU:HD22	1.93	0.51
1:D:78:ARG:HG2	1:D:81:ARG:NH2	2.25	0.51
1:E:122:THR:O	1:E:122:THR:OG1	2.29	0.51
1:D:243:PRO:O	1:D:245:ASN:N	2.44	0.51
1:A:14:VAL:HG12	1:A:363:GLN:HG2	1.92	0.51
1:D:402:LYS:HG2	1:D:405:ARG:NH2	2.24	0.51
1:F:74:ARG:HD3	1:F:143:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:O	1:B:211:THR:HG23	2.11	0.51
1:D:175:LEU:O	1:D:179:LYS:HG3	2.11	0.51
1:D:401:ASP:HA	1:D:414:LEU:HD13	1.93	0.51
1:E:118:THR:HG1	1:E:306:ALA:N	2.09	0.51
1:E:152:SER:HA	1:E:273:PRO:HB3	1.92	0.51
1:F:440:VAL:O	1:F:443:TYR:HB3	2.10	0.51
1:B:208:GLN:HG2	1:C:396:TYR:CE1	2.46	0.51
1:A:224:THR:HG22	1:B:23:ALA:HB2	1.92	0.51
1:B:345:ASP:O	1:B:346:TYR:C	2.53	0.51
1:E:166:LEU:HB2	1:E:433:LEU:HD13	1.92	0.51
1:F:37:ASP:O	1:F:454:THR:HA	2.11	0.51
1:A:49:LEU:HD13	1:A:165:TYR:CG	2.46	0.51
1:E:141:GLU:HB3	1:E:284:ALA:HB2	1.93	0.51
1:F:101:GLY:C	1:F:103:LEU:H	2.18	0.51
1:F:213:VAL:O	1:F:217:ARG:HB2	2.11	0.51
1:F:310:SER:HB2	1:F:315:GLY:O	2.11	0.51
1:A:87:ARG:O	1:A:121:THR:HG23	2.10	0.50
1:B:250:LEU:HB3	1:B:254:GLN:HG3	1.93	0.50
1:B:325:LEU:HD12	1:B:326:PHE:N	2.26	0.50
1:C:20:GLN:NE2	1:C:25:GLY:O	2.44	0.50
1:D:174:GLN:HB3	1:D:223:TYR:CD2	2.45	0.50
1:B:70:VAL:O	1:B:73:PHE:N	2.45	0.50
1:C:298:PRO:HD3	1:C:332:LEU:HD13	1.93	0.50
1:A:324:TRP:CD1	1:A:324:TRP:C	2.89	0.50
1:B:98:ARG:H	1:C:324:TRP:CD1	2.29	0.50
1:B:390:VAL:HG21	1:B:428:LEU:HD22	1.93	0.50
1:C:40:TRP:O	1:C:44:PHE:N	2.29	0.50
1:C:75:ALA:HA	1:C:78:ARG:HG3	1.93	0.50
1:E:162:ALA:O	1:E:166:LEU:HG	2.11	0.50
1:A:61:ARG:HB2	1:B:360:LYS:HB2	1.93	0.50
1:A:345:ASP:O	1:A:346:TYR:C	2.54	0.50
1:B:207:ARG:HB3	1:C:396:TYR:HB2	1.94	0.50
1:C:207:ARG:O	1:C:211:THR:HG23	2.11	0.50
1:D:243:PRO:O	1:D:246:LEU:HG	2.12	0.50
1:D:318:ASP:HB2	1:D:321:SER:HB3	1.92	0.50
1:E:101:GLY:C	1:E:103:LEU:H	2.18	0.50
1:E:289:ILE:HA	1:E:347:ALA:HB1	1.92	0.50
1:B:49:LEU:O	1:B:52:LEU:HB2	2.11	0.50
1:D:378:THR:HG21	1:E:224:THR:HG23	1.94	0.50
1:E:424:ALA:O	1:E:428:LEU:HB2	2.12	0.50
1:F:176:GLN:HA	1:F:179:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:O	1:A:316:LEU:HG	2.12	0.50
1:C:12:ALA:HB2	1:C:269:LEU:HD11	1.93	0.50
1:D:118:THR:OG1	1:D:119:LEU:N	2.43	0.50
1:E:171:ASP:OD2	1:E:226:LEU:HB3	2.12	0.50
1:E:296:PHE:CE1	1:E:340:LEU:HB3	2.47	0.50
1:F:278:ALA:HA	1:F:281:GLN:HB2	1.94	0.50
1:A:41:ARG:NH1	1:A:50:GLN:HB3	2.26	0.50
1:C:176:GLN:OE1	1:C:179:LYS:HD2	2.11	0.50
1:C:310:SER:OG	1:C:311:ARG:N	2.45	0.50
1:D:225:ARG:HG2	1:D:226:LEU:HD23	1.94	0.50
1:F:282:LEU:HD13	1:F:355:VAL:N	2.27	0.50
1:A:9:ARG:NE	1:A:358:TYR:OH	2.45	0.50
1:A:165:TYR:HD2	1:A:166:LEU:HD23	1.76	0.50
1:A:395:GLU:C	1:A:397:TYR:N	2.67	0.50
1:C:118:THR:OG1	1:C:119:LEU:N	2.45	0.50
1:E:310:SER:O	1:F:103:LEU:HD21	2.12	0.50
1:A:57:LEU:HD11	1:A:154:GLN:NE2	2.27	0.50
1:B:41:ARG:HB3	1:B:452:GLN:O	2.12	0.50
1:B:176:GLN:OE1	1:B:179:LYS:HD2	2.12	0.50
1:C:320:GLY:C	1:C:322:GLY:N	2.68	0.50
1:E:227:VAL:O	1:E:231:GLN:HG3	2.12	0.50
1:C:279:GLU:O	1:C:282:LEU:HB3	2.12	0.49
1:C:379:PHE:O	1:C:383:LEU:HG	2.12	0.49
1:D:386:GLN:O	1:D:390:VAL:HG23	2.11	0.49
1:C:245:ASN:OD1	1:C:245:ASN:N	2.32	0.49
1:E:196:TYR:HA	1:E:201:ALA:O	2.13	0.49
1:F:432:ARG:O	1:F:436:LEU:HG	2.12	0.49
1:A:419:ARG:NH1	1:B:416:ASP:OD1	2.44	0.49
1:E:228:ALA:O	1:E:232:ASN:ND2	2.45	0.49
1:F:51:GLN:O	1:F:55:VAL:HG23	2.12	0.49
1:D:14:VAL:HG11	1:D:366:PHE:HB2	1.95	0.49
1:F:262:ALA:HA	1:F:446:LEU:CD1	2.41	0.49
1:F:308:THR:HA	1:F:322:GLY:HA2	1.94	0.49
1:A:64:ARG:O	1:A:67:ALA:N	2.37	0.49
1:B:127:ASP:OD2	1:B:130:GLY:HA2	2.11	0.49
1:A:57:LEU:HD21	1:A:154:GLN:HG3	1.93	0.49
1:A:154:GLN:O	1:A:157:LEU:N	2.45	0.49
1:B:324:TRP:CD1	1:B:324:TRP:C	2.89	0.49
1:C:345:ASP:O	1:C:346:TYR:C	2.56	0.49
1:A:156:THR:HG23	1:A:444:LYS:NZ	2.28	0.49
1:B:433:LEU:O	1:B:436:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HA	1:C:52:LEU:HD12	1.94	0.49
1:C:260:VAL:H	1:C:376:ARG:HH22	1.61	0.49
1:F:44:PHE:HB3	1:F:49:LEU:HD23	1.94	0.49
1:F:129:PHE:CD1	1:F:297:PHE:HB3	2.48	0.49
1:F:299:SER:O	1:F:330:ILE:HA	2.12	0.49
1:B:156:THR:HG23	1:B:444:LYS:NZ	2.28	0.49
1:B:395:GLU:C	1:B:397:TYR:N	2.71	0.49
1:C:254:GLN:HB2	1:C:256:LEU:HD23	1.92	0.49
1:D:314:SER:O	1:D:316:LEU:N	2.46	0.49
1:E:41:ARG:HD3	1:E:50:GLN:CD	2.38	0.49
1:E:144:LEU:HB3	1:E:280:HIS:CE1	2.47	0.49
1:F:14:VAL:HG13	1:F:363:GLN:HG2	1.95	0.49
1:F:196:TYR:HA	1:F:201:ALA:O	2.12	0.49
1:F:331:ASN:O	1:F:333:PRO:HD3	2.12	0.49
1:B:31:ALA:HB2	1:B:261:PRO:HB2	1.94	0.49
1:B:196:TYR:C	1:B:198:VAL:H	2.20	0.49
1:B:414:LEU:O	1:B:418:GLN:HG3	2.13	0.49
1:C:397:TYR:O	1:C:401:ASP:HB2	2.12	0.49
1:E:238:LEU:HB2	1:E:240:SER:O	2.13	0.49
1:F:176:GLN:O	1:F:179:LYS:HB2	2.12	0.49
1:F:222:GLN:HE21	1:F:223:TYR:HE1	1.60	0.49
1:A:71:GLU:HB3	1:B:349:ILE:HD13	1.94	0.49
1:B:298:PRO:HA	1:B:331:ASN:O	2.13	0.49
1:D:401:ASP:O	1:D:405:ARG:HG2	2.13	0.49
1:E:130:GLY:O	1:E:134:SER:N	2.46	0.49
1:F:15:ALA:HB3	1:F:366:PHE:HZ	1.77	0.49
1:F:301:SER:O	1:F:329:SER:N	2.46	0.49
1:A:44:PHE:CE2	1:A:162:ALA:HB2	2.48	0.48
1:E:379:PHE:CZ	1:E:434:ASN:HB3	2.48	0.48
1:F:98:ARG:HA	1:F:111:ILE:HG12	1.94	0.48
1:B:258:THR:HG22	1:B:259:GLU:O	2.13	0.48
1:B:320:GLY:O	1:B:322:GLY:N	2.45	0.48
1:D:313:LEU:O	1:D:316:LEU:HG	2.13	0.48
1:E:137:ASP:HA	1:E:140:LEU:HB3	1.93	0.48
1:A:49:LEU:HD13	1:A:165:TYR:CD2	2.48	0.48
1:A:138:GLN:NE2	1:A:142:GLN:OE1	2.46	0.48
1:D:169:LYS:C	1:D:171:ASP:H	2.21	0.48
1:D:207:ARG:NH1	1:D:210:GLN:OE1	2.44	0.48
1:D:324:TRP:O	1:E:97:GLN:HB2	2.13	0.48
1:C:225:ARG:O	1:C:227:VAL:N	2.47	0.48
1:D:97:GLN:HB3	1:F:325:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:HB3	1:A:366:PHE:HZ	1.77	0.48
1:A:21:GLY:O	1:A:23:ALA:N	2.47	0.48
1:A:433:LEU:HD23	1:A:434:ASN:OD1	2.13	0.48
1:B:332:LEU:HD12	1:B:333:PRO:CD	2.42	0.48
1:E:104:SER:OG	1:E:108:SER:O	2.23	0.48
1:E:118:THR:OG1	1:E:305:ASN:HB2	2.13	0.48
1:F:41:ARG:HD3	1:F:50:GLN:CD	2.38	0.48
1:F:308:THR:HG22	1:F:322:GLY:HA2	1.94	0.48
1:A:416:ASP:HA	1:A:419:ARG:HD2	1.95	0.48
1:F:120:GLY:HA3	1:F:305:ASN:CB	2.44	0.48
1:C:332:LEU:HD12	1:C:333:PRO:CD	2.43	0.48
1:E:35:ALA:HA	1:E:38:ILE:HD12	1.96	0.48
1:C:192:THR:O	1:C:206:LEU:HD13	2.14	0.48
1:F:289:ILE:O	1:F:293:ARG:HG2	2.14	0.48
1:A:325:LEU:HD12	1:A:326:PHE:N	2.28	0.48
1:A:419:ARG:O	1:A:421:LEU:N	2.47	0.48
1:B:156:THR:HA	1:B:444:LYS:HE3	1.95	0.48
1:C:165:TYR:HD2	1:C:166:LEU:HD23	1.79	0.48
1:D:400:ALA:HB2	1:E:204:LEU:HD11	1.95	0.48
1:D:412:LEU:HD21	1:F:412:LEU:HD23	1.95	0.48
1:E:170:ALA:O	1:E:174:GLN:HG2	2.14	0.48
1:E:448:GLY:O	1:E:450:TRP:N	2.47	0.48
1:A:214:GLU:HG3	1:B:388:ASP:HB3	1.95	0.47
1:C:44:PHE:O	1:C:50:GLN:NE2	2.40	0.47
1:D:113:SER:HB3	1:D:311:ARG:HG3	1.95	0.47
1:D:210:GLN:O	1:D:214:GLU:HG2	2.14	0.47
1:E:30:ALA:HA	1:E:263:GLY:HA2	1.95	0.47
1:F:64:ARG:O	1:F:68:LEU:HG	2.14	0.47
1:A:382:GLN:NE2	1:A:431:ASP:OD2	2.45	0.47
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.79	0.47
1:D:287:ALA:O	1:D:289:ILE:N	2.38	0.47
1:E:306:ALA:HA	1:E:324:TRP:HA	1.95	0.47
1:F:106:THR:C	1:F:108:SER:H	2.23	0.47
1:C:189:PHE:HB2	1:C:213:VAL:HG21	1.95	0.47
1:D:236:LEU:HG	1:D:237:LEU:HD23	1.95	0.47
1:D:363:GLN:HE22	1:E:239:GLY:C	2.22	0.47
1:A:113:SER:O	1:A:311:ARG:HG3	2.14	0.47
1:A:137:ASP:O	1:A:138:GLN:C	2.57	0.47
1:A:395:GLU:O	1:A:399:LEU:HG	2.14	0.47
1:B:34:PRO:O	1:B:38:ILE:HG13	2.14	0.47
1:C:174:GLN:OE1	1:C:429:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:THR:HG22	1:E:322:GLY:HA2	1.96	0.47
1:E:375:ALA:O	1:E:379:PHE:HB2	2.14	0.47
1:F:129:PHE:CD2	1:F:297:PHE:HD2	2.32	0.47
1:A:378:THR:OG1	1:C:225:ARG:HD3	2.14	0.47
1:A:388:ASP:HB3	1:C:214:GLU:HG3	1.96	0.47
1:B:225:ARG:HD3	1:C:378:THR:OG1	2.14	0.47
1:C:260:VAL:H	1:C:376:ARG:NH2	2.11	0.47
1:D:336:THR:O	1:D:338:GLY:N	2.48	0.47
1:D:432:ARG:O	1:D:436:LEU:HG	2.15	0.47
1:E:128:LEU:HD23	1:E:129:PHE:CZ	2.49	0.47
1:F:84:LEU:CD1	1:F:136:ARG:HD3	2.44	0.47
1:A:235:VAL:O	1:A:238:LEU:HB2	2.15	0.47
1:E:305:ASN:CG	1:E:325:LEU:HB3	2.39	0.47
1:F:168:LEU:HB2	1:F:230:ASP:HB3	1.95	0.47
1:A:41:ARG:HD3	1:A:50:GLN:CD	2.39	0.47
1:A:71:GLU:HB3	1:B:349:ILE:CD1	2.45	0.47
1:B:38:ILE:HA	1:B:454:THR:HG23	1.96	0.47
1:C:15:ALA:HB3	1:C:366:PHE:CZ	2.49	0.47
1:D:151:ARG:HG2	1:D:450:TRP:CE2	2.50	0.47
1:D:401:ASP:OD2	1:D:402:LYS:HG3	2.15	0.47
1:F:181:THR:O	1:F:185:TYR:HB2	2.14	0.47
1:F:193:GLN:OE1	1:F:206:LEU:HD21	2.14	0.47
1:D:48:GLN:HA	1:D:247:PRO:HB2	1.96	0.47
1:E:162:ALA:HB3	1:E:440:VAL:HG11	1.97	0.47
1:E:168:LEU:HD23	1:E:230:ASP:CB	2.43	0.47
1:F:40:TRP:CZ2	1:F:452:GLN:HG3	2.49	0.47
1:A:124:TRP:O	1:A:302:LEU:N	2.48	0.47
1:D:141:GLU:HB3	1:D:284:ALA:HB2	1.97	0.47
1:F:259:GLU:HG2	1:F:376:ARG:NH1	2.30	0.47
1:F:305:ASN:CG	1:F:325:LEU:HB3	2.40	0.47
1:A:298:PRO:HA	1:A:331:ASN:O	2.14	0.47
1:B:64:ARG:O	1:B:65:VAL:C	2.58	0.47
1:C:375:ALA:HB1	1:C:438:SER:HB3	1.97	0.47
1:D:73:PHE:HB3	1:D:143:TYR:HA	1.96	0.47
1:D:251:GLY:O	1:D:254:GLN:HG2	2.15	0.47
1:E:3:LEU:HD12	1:E:294:ALA:HA	1.97	0.47
1:B:37:ASP:OD2	1:B:271:ARG:NH1	2.48	0.46
1:C:175:LEU:O	1:C:178:THR:N	2.48	0.46
1:D:45:ARG:HE	1:D:45:ARG:HB3	1.51	0.46
1:D:61:ARG:HE	1:F:359:GLU:CD	2.23	0.46
1:E:145:ALA:HB2	1:E:280:HIS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ARG:HB2	1:F:143:TYR:CE1	2.50	0.46
1:F:128:LEU:O	1:F:133:ARG:NH2	2.48	0.46
1:F:207:ARG:HD3	1:F:207:ARG:HA	1.66	0.46
1:F:243:PRO:HD2	1:F:246:LEU:HD21	1.96	0.46
1:C:269:LEU:HD21	1:C:362:ILE:CD1	2.45	0.46
1:D:35:ALA:HB3	1:D:446:LEU:HB3	1.97	0.46
1:D:166:LEU:HD13	1:D:436:LEU:HB3	1.97	0.46
1:E:422:PHE:HA	1:E:425:GLN:HB2	1.96	0.46
1:F:3:LEU:O	1:F:290:GLY:HA2	2.15	0.46
1:F:57:LEU:HD23	1:F:57:LEU:HA	1.63	0.46
1:F:137:ASP:HA	1:F:140:LEU:HB3	1.98	0.46
1:A:325:LEU:HD11	1:A:327:GLN:HB2	1.97	0.46
1:B:73:PHE:HB3	1:B:143:TYR:HA	1.96	0.46
1:B:419:ARG:NH1	1:C:416:ASP:OD1	2.45	0.46
1:C:49:LEU:O	1:C:52:LEU:HB2	2.16	0.46
1:E:144:LEU:HD23	1:E:280:HIS:CE1	2.50	0.46
1:F:49:LEU:HD11	1:F:53:ILE:HG13	1.96	0.46
1:D:193:GLN:OE1	1:D:206:LEU:HD21	2.16	0.46
1:D:455:VAL:HG12	1:D:456:THR:H	1.80	0.46
1:F:68:LEU:O	1:F:71:GLU:N	2.48	0.46
1:F:73:PHE:HD2	1:F:142:GLN:O	1.97	0.46
1:F:120:GLY:HA3	1:F:305:ASN:HA	1.98	0.46
1:F:174:GLN:OE1	1:F:426:GLN:HA	2.16	0.46
1:A:141:GLU:CG	1:A:283:MET:HB2	2.45	0.46
1:B:192:THR:HG22	1:B:192:THR:O	2.16	0.46
1:C:403:ARG:HE	1:C:403:ARG:HB2	1.57	0.46
1:D:21:GLY:O	1:D:23:ALA:N	2.36	0.46
1:D:133:ARG:O	1:D:136:ARG:HB3	2.15	0.46
1:D:246:LEU:HG	1:D:246:LEU:H	1.51	0.46
1:E:390:VAL:O	1:E:393:SER:HB2	2.14	0.46
1:A:64:ARG:O	1:A:65:VAL:C	2.58	0.46
1:C:118:THR:OG1	1:C:305:ASN:HB2	2.15	0.46
1:C:373:LEU:HD23	1:C:442:LEU:HD21	1.98	0.46
1:D:232:ASN:ND2	1:F:371:ASP:OD1	2.40	0.46
1:E:176:GLN:HA	1:E:179:LYS:HD2	1.98	0.46
1:F:435:GLN:O	1:F:439:GLU:HG2	2.15	0.46
1:A:118:THR:OG1	1:A:305:ASN:HB2	2.15	0.46
1:B:275:ILE:HG22	1:B:276:LEU:HD23	1.97	0.46
1:A:121:THR:HG22	1:A:122:THR:N	2.30	0.46
1:A:232:ASN:ND2	1:B:371:ASP:OD1	2.30	0.46
1:D:13:PRO:HG2	1:D:363:GLN:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:LEU:O	1:D:267:ASP:HB2	2.14	0.46
1:A:379:PHE:O	1:A:383:LEU:HG	2.16	0.46
1:D:82:ALA:CB	1:F:337:ALA:HB3	2.46	0.46
1:D:156:THR:HG23	1:D:444:LYS:NZ	2.31	0.46
1:D:168:LEU:HD23	1:D:230:ASP:CB	2.44	0.46
1:A:43:PHE:CE2	1:A:44:PHE:HE1	2.33	0.46
1:B:278:ALA:O	1:B:281:GLN:HB2	2.15	0.46
1:D:23:ALA:O	1:D:377:GLY:HA3	2.16	0.46
1:E:145:ALA:HB2	1:E:280:HIS:CB	2.46	0.46
1:E:172:GLN:O	1:E:175:LEU:HB3	2.16	0.46
1:F:174:GLN:HB3	1:F:223:TYR:CE2	2.50	0.46
1:F:432:ARG:CZ	1:F:436:LEU:HD21	2.46	0.46
1:A:141:GLU:O	1:A:142:GLN:C	2.59	0.45
1:A:207:ARG:HA	1:A:207:ARG:HD3	1.74	0.45
1:A:319:ALA:C	1:A:321:SER:H	2.24	0.45
1:B:192:THR:O	1:B:206:LEU:HD13	2.16	0.45
1:C:254:GLN:HB2	1:C:256:LEU:CD2	2.46	0.45
1:C:416:ASP:HA	1:C:419:ARG:HD2	1.98	0.45
1:A:17:ALA:HA	1:A:265:PRO:HG2	1.98	0.45
1:A:279:GLU:O	1:A:283:MET:HG3	2.16	0.45
1:C:395:GLU:C	1:C:397:TYR:N	2.68	0.45
1:D:289:ILE:O	1:D:293:ARG:HG2	2.16	0.45
1:D:298:PRO:HD3	1:D:332:LEU:HD13	1.98	0.45
1:A:77:TYR:CD2	1:A:77:TYR:C	2.93	0.45
1:B:168:LEU:HD23	1:B:230:ASP:CB	2.46	0.45
1:C:23:ALA:O	1:C:377:GLY:HA3	2.16	0.45
1:C:235:VAL:HG13	1:C:240:SER:O	2.16	0.45
1:C:336:THR:O	1:C:338:GLY:N	2.45	0.45
1:E:325:LEU:HD12	1:E:326:PHE:H	1.81	0.45
1:A:252:LEU:HB3	1:A:432:ARG:HG2	1.99	0.45
1:C:86:PRO:HD3	1:C:124:TRP:CZ2	2.51	0.45
1:C:192:THR:HG21	1:C:205:ASP:O	2.17	0.45
1:D:251:GLY:C	1:D:253:ASP:H	2.23	0.45
1:E:37:ASP:O	1:E:454:THR:HA	2.16	0.45
1:F:122:THR:HA	1:F:303:THR:HG23	1.97	0.45
1:F:144:LEU:HB3	1:F:280:HIS:ND1	2.30	0.45
1:A:140:LEU:O	1:A:143:TYR:HB3	2.16	0.45
1:B:102:ASP:OD1	1:B:102:ASP:N	2.49	0.45
1:B:406:THR:HG22	1:B:406:THR:O	2.16	0.45
1:B:419:ARG:O	1:B:421:LEU:N	2.50	0.45
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ASP:OD1	1:D:274:ASP:N	2.34	0.45
1:E:269:LEU:HA	1:E:275:ILE:HG21	1.99	0.45
1:F:131:ARG:HG2	1:F:132:LEU:HD23	1.97	0.45
1:F:236:LEU:O	1:F:238:LEU:N	2.46	0.45
1:A:394:ASP:O	1:A:397:TYR:HB3	2.16	0.45
1:A:429:ILE:O	1:A:432:ARG:HB3	2.16	0.45
1:B:442:LEU:HD12	1:B:442:LEU:HA	1.71	0.45
1:D:285:ALA:O	1:D:289:ILE:HG13	2.16	0.45
1:E:35:ALA:O	1:E:38:ILE:HB	2.16	0.45
1:F:54:GLY:O	1:F:57:LEU:HB2	2.17	0.45
1:C:40:TRP:CZ2	1:C:452:GLN:HG3	2.52	0.45
1:C:129:PHE:CD1	1:C:297:PHE:HB3	2.52	0.45
1:C:235:VAL:O	1:C:238:LEU:HB2	2.16	0.45
1:D:74:ARG:HB2	1:D:143:TYR:CE1	2.52	0.45
1:D:78:ARG:HH12	1:F:341:ARG:NH1	2.15	0.45
1:D:92:GLY:HA2	1:D:117:VAL:HG22	1.99	0.45
1:D:234:LEU:O	1:D:238:LEU:HG	2.16	0.45
1:E:97:GLN:C	1:E:111:ILE:HG23	2.41	0.45
1:E:389:LEU:HD13	1:F:211:THR:O	2.16	0.45
1:F:49:LEU:HA	1:F:52:LEU:HD12	1.99	0.45
1:F:127:ASP:OD2	1:F:133:ARG:N	2.49	0.45
1:F:243:PRO:O	1:F:246:LEU:HG	2.16	0.45
1:A:229:GLN:HA	1:B:371:ASP:OD1	2.17	0.45
1:C:65:VAL:HG12	1:C:66:ALA:N	2.31	0.45
1:C:209:ALA:HA	1:C:411:TYR:OH	2.17	0.45
1:F:99:LEU:N	1:F:110:ALA:O	2.46	0.45
1:F:158:VAL:HG11	1:F:449:GLY:HA3	1.98	0.45
1:F:424:ALA:O	1:F:428:LEU:HB2	2.16	0.45
1:A:252:LEU:O	1:A:432:ARG:NE	2.49	0.45
1:B:402:LYS:HG2	1:B:405:ARG:HH22	1.80	0.45
1:D:349:ILE:HG21	1:E:72:ALA:HB2	1.97	0.45
1:D:360:LYS:C	1:D:362:ILE:H	2.25	0.45
1:E:144:LEU:HD23	1:E:280:HIS:NE2	2.32	0.45
1:F:364:THR:HG22	1:F:368:GLU:OE2	2.17	0.45
1:B:74:ARG:HB2	1:B:143:TYR:CE1	2.52	0.45
1:B:320:GLY:C	1:B:322:GLY:N	2.74	0.45
1:B:379:PHE:O	1:B:383:LEU:HG	2.17	0.45
1:E:190:ASP:O	1:E:194:ARG:HG3	2.17	0.45
1:E:372:GLY:HA3	1:E:442:LEU:HD13	1.99	0.45
1:F:282:LEU:HD21	1:F:355:VAL:HG22	1.99	0.45
1:A:74:ARG:HB2	1:A:143:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:OE1	1:A:179:LYS:HD2	2.17	0.44
1:C:20:GLN:HG2	1:C:27:ASN:OD1	2.17	0.44
1:E:177:LEU:HD23	1:E:422:PHE:CE1	2.52	0.44
1:E:223:TYR:O	1:E:227:VAL:HG23	2.17	0.44
1:F:8:GLN:H	1:F:8:GLN:HG2	1.63	0.44
1:F:264:LEU:HD23	1:F:264:LEU:HA	1.79	0.44
1:F:326:PHE:CD2	1:F:328:PRO:HD3	2.51	0.44
1:A:353:ILE:HA	1:C:68:LEU:HD12	1.99	0.44
1:D:324:TRP:CD1	1:D:324:TRP:C	2.95	0.44
1:E:282:LEU:HD13	1:E:354:ASN:O	2.16	0.44
1:F:192:THR:HG23	1:F:201:ALA:HB1	1.99	0.44
1:A:194:ARG:O	1:A:198:VAL:HB	2.17	0.44
1:B:49:LEU:HB2	1:B:165:TYR:CE2	2.52	0.44
1:D:299:SER:O	1:D:330:ILE:HA	2.17	0.44
1:D:338:GLY:O	1:D:341:ARG:N	2.51	0.44
1:D:451:ASN:OD1	1:D:451:ASN:N	2.50	0.44
1:E:68:LEU:C	1:E:70:VAL:N	2.76	0.44
1:F:171:ASP:O	1:F:175:LEU:HB2	2.17	0.44
1:F:192:THR:HG21	1:F:205:ASP:O	2.17	0.44
1:F:403:ARG:HG2	1:F:409:ASP:HB2	1.99	0.44
1:F:442:LEU:HD12	1:F:442:LEU:HA	1.77	0.44
1:A:187:LYS:O	1:A:191:LEU:HG	2.17	0.44
1:B:140:LEU:O	1:B:143:TYR:HB3	2.17	0.44
1:C:84:LEU:HD23	1:C:132:LEU:HB3	1.99	0.44
1:C:141:GLU:HB3	1:C:284:ALA:HB2	2.00	0.44
1:D:389:LEU:HD22	1:E:215:GLY:CA	2.47	0.44
1:F:187:LYS:O	1:F:191:LEU:HG	2.18	0.44
1:B:246:LEU:H	1:B:246:LEU:HG	1.43	0.44
1:C:131:ARG:O	1:C:134:SER:HB2	2.17	0.44
1:C:323:SER:O	1:C:324:TRP:HB3	2.17	0.44
1:D:206:LEU:HG	1:D:206:LEU:O	2.17	0.44
1:E:336:THR:C	1:E:338:GLY:N	2.75	0.44
1:F:155:THR:HB	1:F:448:GLY:HA3	1.98	0.44
1:F:338:GLY:O	1:F:341:ARG:N	2.50	0.44
1:B:310:SER:OG	1:B:311:ARG:N	2.49	0.44
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.87	0.44
1:B:395:GLU:O	1:B:397:TYR:N	2.51	0.44
1:E:279:GLU:O	1:E:282:LEU:HB3	2.18	0.44
1:E:336:THR:O	1:E:338:GLY:N	2.42	0.44
1:F:260:VAL:O	1:F:376:ARG:NH1	2.51	0.44
1:F:427:GLN:NE2	1:F:431:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HA	1:A:50:GLN:HB2	1.99	0.44
1:A:158:VAL:HG12	1:A:159:ALA:N	2.33	0.44
1:A:225:ARG:C	1:A:227:VAL:H	2.25	0.44
1:C:50:GLN:O	1:C:53:ILE:HB	2.18	0.44
1:D:171:ASP:OD2	1:D:226:LEU:HB3	2.18	0.44
1:D:313:LEU:HD13	1:D:313:LEU:H	1.83	0.44
1:E:310:SER:C	1:F:103:LEU:HD21	2.42	0.44
1:F:279:GLU:HB2	1:F:358:TYR:CE1	2.53	0.44
1:A:86:PRO:HD3	1:A:124:TRP:CZ2	2.53	0.44
1:A:127:ASP:CG	1:A:130:GLY:HA2	2.43	0.44
1:C:148:GLN:HG3	1:C:276:LEU:HB2	1.99	0.44
1:D:18:TYR:CE1	1:D:265:PRO:HD3	2.53	0.44
1:D:282:LEU:HD22	1:D:355:VAL:HA	2.00	0.44
1:E:346:TYR:CE2	1:E:350:GLN:HG3	2.53	0.44
1:E:391:LYS:O	1:E:395:GLU:HG2	2.18	0.44
1:F:15:ALA:HB3	1:F:366:PHE:CZ	2.52	0.44
1:F:390:VAL:O	1:F:394:ASP:HB2	2.18	0.44
1:A:141:GLU:O	1:A:143:TYR:N	2.51	0.44
1:A:169:LYS:O	1:A:172:GLN:HB2	2.17	0.44
1:B:40:TRP:CE2	1:B:452:GLN:HA	2.53	0.44
1:B:129:PHE:CE1	1:B:297:PHE:HB3	2.53	0.44
1:B:196:TYR:HD1	1:B:201:ALA:O	2.00	0.44
1:B:320:GLY:C	1:B:322:GLY:H	2.26	0.44
1:C:379:PHE:HB3	1:C:435:GLN:HG3	1.99	0.44
1:E:97:GLN:O	1:E:111:ILE:HG23	2.17	0.44
1:E:108:SER:O	1:E:110:ALA:N	2.51	0.44
1:F:77:TYR:OH	1:F:81:ARG:NH1	2.49	0.44
1:A:208:GLN:OE1	1:A:411:TYR:HB3	2.17	0.43
1:C:394:ASP:O	1:C:397:TYR:HB3	2.17	0.43
1:D:233:ALA:O	1:D:237:LEU:HG	2.18	0.43
1:D:396:TYR:HB2	1:E:207:ARG:CB	2.44	0.43
1:D:431:ASP:HA	1:D:434:ASN:HB2	1.99	0.43
1:E:291:ALA:C	1:E:293:ARG:H	2.26	0.43
1:E:402:LYS:HG2	1:E:405:ARG:NH2	2.32	0.43
1:A:196:TYR:HD1	1:A:201:ALA:O	2.00	0.43
1:A:309:MET:HG3	1:A:323:SER:HB3	2.00	0.43
1:C:174:GLN:HG2	1:C:429:ILE:HG21	2.00	0.43
1:D:397:TYR:O	1:D:401:ASP:HB3	2.18	0.43
1:E:59:ASN:HB3	1:E:238:LEU:O	2.19	0.43
1:A:118:THR:HG1	1:A:305:ASN:HB2	1.84	0.43
1:C:194:ARG:O	1:C:198:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ALA:O	1:D:379:PHE:HB2	2.18	0.43
1:E:64:ARG:O	1:E:68:LEU:HG	2.19	0.43
1:F:13:PRO:O	1:F:363:GLN:NE2	2.50	0.43
1:F:31:ALA:HB2	1:F:261:PRO:HB2	2.01	0.43
1:F:250:LEU:HD22	1:F:254:GLN:CD	2.43	0.43
1:B:177:LEU:HD21	1:B:425:GLN:HB3	1.99	0.43
1:B:336:THR:OG1	1:B:339:SER:HB3	2.17	0.43
1:C:242:ILE:HG22	1:C:246:LEU:HD21	2.01	0.43
1:C:373:LEU:CD2	1:C:442:LEU:HD21	2.49	0.43
1:C:395:GLU:O	1:C:397:TYR:N	2.52	0.43
1:D:236:LEU:O	1:D:238:LEU:N	2.51	0.43
1:F:309:MET:HG3	1:F:323:SER:OG	2.18	0.43
1:F:404:TYR:HD1	1:F:410:ASN:HA	1.83	0.43
1:E:40:TRP:CD1	1:E:452:GLN:HA	2.53	0.43
1:A:94:GLY:O	1:A:95:THR:OG1	2.28	0.43
1:A:207:ARG:NH1	1:A:210:GLN:OE1	2.51	0.43
1:A:325:LEU:HD12	1:A:326:PHE:H	1.82	0.43
1:B:23:ALA:O	1:B:377:GLY:HA3	2.19	0.43
1:B:389:LEU:O	1:B:389:LEU:HG	2.18	0.43
1:C:38:ILE:O	1:C:443:TYR:OH	2.22	0.43
1:C:396:TYR:CG	1:C:396:TYR:O	2.72	0.43
1:D:29:GLY:O	1:D:263:GLY:HA2	2.18	0.43
1:D:166:LEU:HD13	1:D:436:LEU:CD1	2.46	0.43
1:D:272:ARG:HD3	1:D:275:ILE:HG13	2.00	0.43
1:D:313:LEU:HD13	1:D:313:LEU:N	2.34	0.43
1:A:395:GLU:O	1:A:397:TYR:N	2.52	0.43
1:B:39:GLY:HA2	1:B:451:ASN:O	2.19	0.43
1:C:73:PHE:HB3	1:C:143:TYR:HA	2.01	0.43
1:C:165:TYR:CD2	1:C:166:LEU:HD23	2.54	0.43
1:C:225:ARG:C	1:C:227:VAL:N	2.72	0.43
1:C:235:VAL:HA	1:C:238:LEU:HB2	2.01	0.43
1:C:313:LEU:O	1:C:314:SER:C	2.62	0.43
1:D:168:LEU:O	1:D:172:GLN:HG3	2.18	0.43
1:D:282:LEU:HB2	1:D:354:ASN:O	2.19	0.43
1:A:40:TRP:H	1:A:40:TRP:CD1	2.35	0.43
1:A:141:GLU:HG3	1:A:280:HIS:HB3	2.00	0.43
1:A:175:LEU:O	1:A:178:THR:N	2.52	0.43
1:B:164:ALA:O	1:B:168:LEU:HB2	2.18	0.43
1:B:396:TYR:O	1:B:396:TYR:CG	2.72	0.43
1:B:416:ASP:HA	1:B:419:ARG:HD2	2.00	0.43
1:C:8:GLN:O	1:C:9:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD23	1:D:99:LEU:HA	1.83	0.43
1:D:192:THR:HG23	1:D:201:ALA:HB1	2.00	0.43
1:D:331:ASN:HA	1:E:90:VAL:O	2.19	0.43
1:E:58:GLU:HG3	1:E:59:ASN:N	2.34	0.43
1:F:36:ALA:HB2	1:F:447:GLY:HA3	1.99	0.43
1:A:213:VAL:HG12	1:A:214:GLU:OE2	2.17	0.43
1:A:444:LYS:O	1:A:448:GLY:N	2.49	0.43
1:B:225:ARG:HD2	1:C:375:ALA:HA	2.00	0.43
1:C:47:PRO:HA	1:C:50:GLN:HB2	2.00	0.43
1:D:60:ASN:OD1	1:D:62:ASP:N	2.52	0.43
1:E:74:ARG:HB2	1:E:143:TYR:CE1	2.53	0.43
1:E:388:ASP:HB3	1:F:214:GLU:CD	2.43	0.43
1:E:393:SER:HB3	1:E:421:LEU:HA	2.01	0.43
1:A:141:GLU:HG2	1:A:284:ALA:N	2.34	0.43
1:A:181:THR:HA	1:A:184:THR:HB	2.00	0.43
1:C:411:TYR:CE2	1:C:415:LEU:HD13	2.44	0.43
1:D:151:ARG:HG2	1:D:450:TRP:CD2	2.53	0.43
1:F:172:GLN:O	1:F:175:LEU:HB3	2.19	0.43
1:A:129:PHE:CD1	1:A:297:PHE:HB3	2.54	0.42
1:B:7:TYR:CD2	1:B:283:MET:HE3	2.54	0.42
1:B:20:GLN:HG2	1:B:27:ASN:OD1	2.19	0.42
1:B:40:TRP:NE1	1:B:452:GLN:HA	2.33	0.42
1:B:113:SER:O	1:B:311:ARG:HG3	2.19	0.42
1:B:403:ARG:HE	1:B:403:ARG:HB2	1.59	0.42
1:C:316:LEU:O	1:C:321:SER:OG	2.33	0.42
1:C:419:ARG:C	1:C:421:LEU:N	2.77	0.42
1:C:440:VAL:O	1:C:443:TYR:HB3	2.19	0.42
1:D:155:THR:HB	1:D:448:GLY:HA3	2.01	0.42
1:B:84:LEU:C	1:B:85:PHE:HD1	2.26	0.42
1:D:196:TYR:HA	1:D:201:ALA:O	2.20	0.42
1:E:272:ARG:HA	1:E:273:PRO:HD2	1.81	0.42
1:F:383:LEU:HD11	1:F:432:ARG:HA	2.01	0.42
1:F:396:TYR:O	1:F:396:TYR:CG	2.71	0.42
1:A:192:THR:O	1:A:192:THR:HG22	2.19	0.42
1:A:320:GLY:C	1:A:322:GLY:N	2.73	0.42
1:D:22:GLN:O	1:D:23:ALA:HB2	2.19	0.42
1:D:44:PHE:HB3	1:D:49:LEU:HD23	2.01	0.42
1:D:394:ASP:HA	1:D:397:TYR:HB3	2.01	0.42
1:D:428:LEU:C	1:D:430:THR:H	2.28	0.42
1:F:49:LEU:O	1:F:52:LEU:N	2.52	0.42
1:A:40:TRP:CE3	1:A:53:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD11	1:B:400:ALA:HB2	2.02	0.42
1:B:382:GLN:NE2	1:B:431:ASP:OD2	2.52	0.42
1:D:71:GLU:HB3	1:F:349:ILE:CD1	2.50	0.42
1:D:327:GLN:HA	1:E:94:GLY:O	2.19	0.42
1:A:165:TYR:CD2	1:A:166:LEU:HD23	2.54	0.42
1:B:34:PRO:HD2	1:B:37:ASP:OD2	2.19	0.42
1:C:256:LEU:C	1:C:257:LEU:HD23	2.44	0.42
1:D:14:VAL:HG23	1:D:15:ALA:N	2.34	0.42
1:E:44:PHE:HB3	1:E:49:LEU:HD23	2.00	0.42
1:E:291:ALA:C	1:E:293:ARG:N	2.78	0.42
1:A:68:LEU:O	1:A:70:VAL:N	2.53	0.42
1:A:419:ARG:NH2	1:B:416:ASP:OD2	2.33	0.42
1:B:142:GLN:HG3	1:B:284:ALA:CB	2.49	0.42
1:B:177:LEU:HD21	1:B:425:GLN:CB	2.49	0.42
1:C:320:GLY:O	1:C:322:GLY:N	2.52	0.42
1:E:61:ARG:HD3	1:E:61:ARG:HA	1.74	0.42
1:E:303:THR:HB	1:E:327:GLN:HB3	2.01	0.42
1:F:211:THR:O	1:F:215:GLY:N	2.46	0.42
1:A:141:GLU:O	1:A:144:LEU:N	2.52	0.42
1:A:236:LEU:HD22	1:B:367:GLN:HG3	2.01	0.42
1:B:60:ASN:OD1	1:B:63:LEU:N	2.43	0.42
1:B:169:LYS:HA	1:B:172:GLN:OE1	2.20	0.42
1:D:192:THR:HG21	1:D:205:ASP:O	2.19	0.42
1:E:83:ASP:OD1	1:E:87:ARG:NH1	2.52	0.42
1:F:386:GLN:HG3	1:F:428:LEU:HD13	2.01	0.42
1:B:14:VAL:HG12	1:B:363:GLN:HG2	2.00	0.42
1:B:15:ALA:HB3	1:B:366:PHE:CZ	2.55	0.42
1:B:235:VAL:HG22	1:B:242:ILE:HG13	2.02	0.42
1:D:24:TYR:OH	1:E:232:ASN:OD1	2.37	0.42
1:E:159:ALA:O	1:E:163:THR:HB	2.20	0.42
1:A:35:ALA:HA	1:A:38:ILE:CD1	2.49	0.42
1:C:436:LEU:O	1:C:437:THR:C	2.63	0.42
1:D:75:ALA:HB1	1:F:342:ALA:O	2.19	0.42
1:F:235:VAL:HG13	1:F:240:SER:O	2.20	0.42
1:F:268:LEU:HD21	1:F:446:LEU:HD23	2.01	0.42
1:F:272:ARG:HH11	1:F:274:ASP:CG	2.28	0.42
1:A:66:ALA:O	1:A:150:GLN:HG3	2.20	0.42
1:A:170:ALA:HA	1:A:252:LEU:HD11	2.01	0.42
1:B:46:ASP:O	1:B:50:GLN:HG3	2.20	0.42
1:C:271:ARG:O	1:C:273:PRO:HD3	2.20	0.42
1:C:325:LEU:HD12	1:C:326:PHE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TYR:OH	1:D:81:ARG:NH1	2.53	0.42
1:D:287:ALA:C	1:D:289:ILE:H	2.25	0.42
1:D:395:GLU:HB2	1:E:207:ARG:HD2	2.02	0.42
1:F:318:ASP:HB2	1:F:321:SER:HB3	2.02	0.42
1:B:225:ARG:C	1:B:227:VAL:H	2.27	0.41
1:B:264:LEU:O	1:B:267:ASP:HB2	2.20	0.41
1:B:313:LEU:O	1:B:314:SER:C	2.62	0.41
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.79	0.41
1:C:14:VAL:HG23	1:C:15:ALA:O	2.19	0.41
1:C:442:LEU:HD12	1:C:442:LEU:HA	1.74	0.41
1:D:101:GLY:C	1:D:103:LEU:N	2.78	0.41
1:D:239:GLY:HA2	1:F:363:GLN:OE1	2.20	0.41
1:D:264:LEU:HD23	1:D:264:LEU:HA	1.86	0.41
1:E:41:ARG:NH1	1:E:50:GLN:OE1	2.53	0.41
1:E:236:LEU:C	1:E:238:LEU:H	2.20	0.41
1:A:242:ILE:H	1:A:242:ILE:HG13	1.56	0.41
1:B:141:GLU:O	1:B:144:LEU:N	2.54	0.41
1:C:414:LEU:O	1:C:418:GLN:HG3	2.20	0.41
1:D:59:ASN:O	1:D:61:ARG:NH1	2.51	0.41
1:D:145:ALA:HB2	1:D:280:HIS:CB	2.43	0.41
1:F:28:THR:OG1	1:F:29:GLY:N	2.53	0.41
1:A:23:ALA:HB1	1:A:378:THR:CG2	2.48	0.41
1:A:68:LEU:HD12	1:B:353:ILE:HA	2.03	0.41
1:A:113:SER:OG	1:A:115:TYR:HE1	2.03	0.41
1:D:234:LEU:HG	1:D:238:LEU:HD11	2.01	0.41
1:E:20:GLN:NE2	1:E:26:GLN:OE1	2.53	0.41
1:E:393:SER:HB3	1:E:420:SER:O	2.20	0.41
1:F:166:LEU:HB2	1:F:433:LEU:HD13	2.02	0.41
1:F:425:GLN:O	1:F:428:LEU:HB3	2.20	0.41
1:A:61:ARG:O	1:A:64:ARG:N	2.53	0.41
1:B:75:ALA:O	1:B:78:ARG:HB2	2.20	0.41
1:C:296:PHE:HE1	1:C:340:LEU:HB3	1.77	0.41
1:D:194:ARG:O	1:D:198:VAL:HG23	2.21	0.41
1:D:240:SER:OG	1:D:241:GLY:N	2.54	0.41
1:F:158:VAL:HG21	1:F:449:GLY:HA3	2.01	0.41
1:A:386:GLN:HE22	1:A:424:ALA:HA	1.86	0.41
1:B:165:TYR:CD2	1:B:166:LEU:HD23	2.56	0.41
1:C:140:LEU:O	1:C:143:TYR:HB3	2.20	0.41
1:C:192:THR:O	1:C:192:THR:HG22	2.19	0.41
1:C:389:LEU:O	1:C:389:LEU:HG	2.20	0.41
1:C:419:ARG:C	1:C:421:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:GLY:O	1:D:340:LEU:N	2.54	0.41
1:E:293:ARG:C	1:E:295:ALA:N	2.78	0.41
1:E:372:GLY:CA	1:E:442:LEU:HD22	2.51	0.41
1:F:262:ALA:O	1:F:446:LEU:HD22	2.20	0.41
1:F:272:ARG:HA	1:F:273:PRO:HD3	1.92	0.41
1:F:427:GLN:HA	1:F:430:THR:HB	2.02	0.41
1:A:308:THR:HB	1:A:321:SER:OG	2.20	0.41
1:C:269:LEU:HA	1:C:269:LEU:HD23	1.62	0.41
1:F:178:THR:HG23	1:F:422:PHE:CZ	2.55	0.41
1:F:282:LEU:HD22	1:F:355:VAL:HA	2.02	0.41
1:A:210:GLN:O	1:A:214:GLU:HG2	2.21	0.41
1:A:433:LEU:O	1:A:436:LEU:N	2.54	0.41
1:A:440:VAL:O	1:A:443:TYR:HB3	2.20	0.41
1:C:43:PHE:O	1:C:43:PHE:CG	2.73	0.41
1:C:45:ARG:NE	1:C:45:ARG:HA	2.31	0.41
1:D:35:ALA:O	1:D:38:ILE:HB	2.21	0.41
1:F:166:LEU:CB	1:F:433:LEU:HD13	2.50	0.41
1:A:282:LEU:HA	1:A:354:ASN:HB3	2.02	0.41
1:A:396:TYR:CG	1:A:396:TYR:O	2.73	0.41
1:B:252:LEU:O	1:B:432:ARG:NE	2.48	0.41
1:B:419:ARG:C	1:B:421:LEU:N	2.79	0.41
1:D:403:ARG:HE	1:D:403:ARG:HB2	1.69	0.41
1:E:98:ARG:CA	1:E:111:ILE:HG12	2.38	0.41
1:E:355:VAL:O	1:E:358:TYR:HB3	2.20	0.41
1:E:362:ILE:HG22	1:E:363:GLN:N	2.35	0.41
1:F:9:ARG:HA	1:F:10:PRO:HD3	1.90	0.41
1:F:118:THR:OG1	1:F:305:ASN:HB2	2.21	0.41
1:F:185:TYR:CE2	1:F:212:ALA:HB1	2.55	0.41
1:A:22:GLN:O	1:A:23:ALA:HB2	2.20	0.41
1:A:217:ARG:HB3	1:B:385:ALA:HB1	2.02	0.41
1:A:277:GLU:O	1:A:278:ALA:C	2.64	0.41
1:B:20:GLN:HE22	1:B:26:GLN:HA	1.85	0.41
1:B:189:PHE:HB2	1:B:213:VAL:HG21	2.03	0.41
1:B:302:LEU:HD11	1:B:304:ALA:HB2	2.02	0.41
1:B:326:PHE:CE2	1:B:328:PRO:HD3	2.56	0.41
1:C:44:PHE:CZ	1:C:162:ALA:HB2	2.55	0.41
1:C:75:ALA:O	1:C:78:ARG:HB2	2.21	0.41
1:C:141:GLU:OE2	1:C:283:MET:HB3	2.21	0.41
1:E:141:GLU:HG2	1:E:283:MET:HB2	2.02	0.41
1:F:57:LEU:HD21	1:F:154:GLN:CG	2.40	0.41
1:F:106:THR:C	1:F:108:SER:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:LEU:HA	1:F:328:PRO:HA	2.02	0.41
1:F:336:THR:C	1:F:338:GLY:N	2.79	0.41
1:F:338:GLY:C	1:F:340:LEU:N	2.79	0.41
1:F:413:THR:O	1:F:417:ALA:HB2	2.21	0.41
1:F:437:THR:HG22	1:F:438:SER:N	2.35	0.41
1:A:254:GLN:HB2	1:A:256:LEU:CD2	2.51	0.41
1:A:375:ALA:HB1	1:A:438:SER:HB3	2.02	0.41
1:B:71:GLU:HB3	1:C:349:ILE:CD1	2.51	0.41
1:B:81:ARG:O	1:B:83:ASP:N	2.54	0.41
1:B:113:SER:OG	1:B:311:ARG:O	2.23	0.41
1:B:129:PHE:CD2	1:B:297:PHE:HD2	2.39	0.41
1:C:68:LEU:O	1:C:71:GLU:N	2.54	0.41
1:C:83:ASP:HB3	1:C:132:LEU:CD1	2.51	0.41
1:C:260:VAL:HG12	1:C:261:PRO:HD2	2.03	0.41
1:E:3:LEU:HD12	1:E:294:ALA:N	2.36	0.41
1:E:292:ALA:O	1:E:295:ALA:HB3	2.21	0.41
1:E:450:TRP:HA	1:E:450:TRP:CE3	2.56	0.41
1:A:68:LEU:C	1:A:70:VAL:N	2.79	0.40
1:C:129:PHE:CD2	1:C:297:PHE:HD2	2.40	0.40
1:C:402:LYS:HG2	1:C:405:ARG:NH2	2.36	0.40
1:D:4:ILE:HA	1:D:5:PRO:HD3	1.81	0.40
1:D:82:ALA:O	1:D:85:PHE:HB2	2.21	0.40
1:D:128:LEU:HD23	1:D:129:PHE:CE1	2.55	0.40
1:D:185:TYR:OH	1:D:418:GLN:HB3	2.21	0.40
1:E:144:LEU:HB3	1:E:280:HIS:ND1	2.35	0.40
1:A:151:ARG:HG2	1:A:450:TRP:HB2	2.04	0.40
1:A:246:LEU:H	1:A:246:LEU:HG	1.61	0.40
1:B:219:THR:O	1:B:219:THR:HG22	2.21	0.40
1:B:242:ILE:HG22	1:B:246:LEU:HD21	2.03	0.40
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.86	0.40
1:C:307:GLY:O	1:C:323:SER:OG	2.25	0.40
1:D:141:GLU:HG2	1:D:284:ALA:N	2.36	0.40
1:D:260:VAL:HA	1:D:261:PRO:HD3	1.97	0.40
1:D:404:TYR:CD2	1:D:414:LEU:HD22	2.56	0.40
1:E:182:LEU:HD12	1:E:182:LEU:HA	1.79	0.40
1:F:404:TYR:CZ	1:F:411:TYR:HD1	2.39	0.40
1:A:101:GLY:HA2	1:A:109:PRO:HD3	2.02	0.40
1:A:145:ALA:HB2	1:A:280:HIS:HB2	2.03	0.40
1:A:270:GLN:C	1:A:271:ARG:HG3	2.47	0.40
1:A:348:LYS:O	1:A:351:LYS:HB3	2.21	0.40
1:A:396:TYR:HB2	1:C:207:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLN:HA	1:B:174:GLN:OE1	2.21	0.40
1:C:208:GLN:OE1	1:C:411:TYR:HB3	2.20	0.40
1:E:4:ILE:HG12	1:E:290:GLY:HA3	2.03	0.40
1:F:55:VAL:O	1:F:58:GLU:N	2.54	0.40
1:F:151:ARG:HG2	1:F:450:TRP:CZ2	2.56	0.40
1:F:389:LEU:HG	1:F:389:LEU:O	2.22	0.40
1:A:269:LEU:HD21	1:A:362:ILE:CD1	2.52	0.40
1:A:313:LEU:O	1:A:315:GLY:N	2.54	0.40
1:A:436:LEU:O	1:A:437:THR:C	2.64	0.40
1:B:419:ARG:C	1:B:421:LEU:H	2.28	0.40
1:C:298:PRO:CD	1:C:332:LEU:HD13	2.50	0.40
1:D:68:LEU:O	1:D:71:GLU:N	2.55	0.40
1:D:82:ALA:HB1	1:F:337:ALA:HB3	2.03	0.40
1:E:166:LEU:HD13	1:E:436:LEU:HD13	2.02	0.40
1:F:41:ARG:HD3	1:F:50:GLN:NE2	2.36	0.40
1:F:184:THR:HA	1:F:187:LYS:CB	2.49	0.40
1:F:222:GLN:HG2	1:F:223:TYR:CE1	2.56	0.40
1:A:235:VAL:HG13	1:A:240:SER:O	2.21	0.40
1:A:315:GLY:HA2	1:A:318:ASP:OD1	2.21	0.40
1:A:406:THR:O	1:A:406:THR:HG22	2.20	0.40
1:A:442:LEU:HD12	1:A:442:LEU:HA	1.83	0.40
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.82	0.40
1:B:245:ASN:OD1	1:B:245:ASN:N	2.34	0.40
1:B:365:ALA:O	1:B:369:VAL:HG23	2.21	0.40
1:C:21:GLY:C	1:C:23:ALA:H	2.27	0.40
1:C:121:THR:HG22	1:C:122:THR:N	2.36	0.40
1:C:189:PHE:CB	1:C:213:VAL:HG21	2.51	0.40
1:C:234:LEU:HD12	1:C:234:LEU:HA	1.86	0.40
1:D:89:GLY:O	1:D:119:LEU:HD12	2.21	0.40
1:E:168:LEU:HB2	1:E:230:ASP:HB3	2.04	0.40
1:E:333:PRO:O	1:E:334:ILE:HD13	2.22	0.40
1:F:268:LEU:HD22	1:F:446:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/474 (96%)	363 (80%)	74 (16%)	18 (4%)	2	20
1	B	455/474 (96%)	368 (81%)	68 (15%)	19 (4%)	2	19
1	C	455/474 (96%)	365 (80%)	67 (15%)	23 (5%)	1	17
1	D	455/474 (96%)	371 (82%)	60 (13%)	24 (5%)	1	16
1	E	454/474 (96%)	380 (84%)	51 (11%)	23 (5%)	1	17
1	F	455/474 (96%)	385 (85%)	54 (12%)	16 (4%)	3	23
All	All	2729/2844 (96%)	2232 (82%)	374 (14%)	123 (4%)	2	18

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	ALA
1	A	69	ASN
1	A	314	SER
1	B	22	GLN
1	B	23	ALA
1	B	266	SER
1	B	314	SER
1	B	315	GLY
1	B	337	ALA
1	C	22	GLN
1	C	23	ALA
1	C	65	VAL
1	C	254	GLN
1	C	313	LEU
1	C	314	SER
1	C	448	GLY
1	D	23	ALA
1	D	30	ALA
1	D	127	ASP
1	D	244	ALA
1	D	254	GLN
1	D	456	THR
1	E	109	PRO
1	E	237	LEU
1	E	273	PRO

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Mol	Chain	Res	Type
1	E	313	LEU
1	F	13	PRO
1	F	30	ALA
1	F	317	PHE
1	F	456	THR
1	A	313	LEU
1	A	396	TYR
1	A	420	SER
1	A	448	GLY
1	B	313	LEU
1	B	321	SER
1	B	396	TYR
1	B	420	SER
1	C	226	LEU
1	C	315	GLY
1	C	396	TYR
1	C	420	SER
1	D	22	GLN
1	D	101	GLY
1	D	102	ASP
1	D	202	SER
1	D	237	LEU
1	D	337	ALA
1	E	102	ASP
1	E	126	LEU
1	E	314	SER
1	E	448	GLY
1	E	449	GLY
1	F	14	VAL
1	F	237	LEU
1	F	306	ALA
1	F	448	GLY
1	A	65	VAL
1	A	254	GLN
1	A	324	TRP
1	B	254	GLN
1	C	123	ALA
1	C	321	SER
1	D	14	VAL
1	D	313	LEU
1	E	55	VAL
1	E	216	ALA

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Mol	Chain	Res	Type
1	E	244	ALA
1	E	295	ALA
1	E	315	GLY
1	E	339	SER
1	E	436	LEU
1	A	109	PRO
1	A	142	GLN
1	A	236	LEU
1	A	321	SER
1	B	109	PRO
1	B	263	GLY
1	C	202	SER
1	C	217	ARG
1	C	236	LEU
1	C	419	ARG
1	C	437	THR
1	D	109	PRO
1	D	252	LEU
1	D	361	ALA
1	D	448	GLY
1	E	298	PRO
1	E	337	ALA
1	F	216	ALA
1	F	246	LEU
1	F	254	GLN
1	A	226	LEU
1	A	247	PRO
1	B	82	ALA
1	B	407	GLY
1	C	109	PRO
1	C	247	PRO
1	C	273	PRO
1	D	315	GLY
1	E	318	ASP
1	F	38	ILE
1	F	109	PRO
1	A	273	PRO
1	B	202	SER
1	D	288	SER
1	D	339	SER
1	E	306	ALA
1	E	437	THR

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Mol	Chain	Res	Type
1	F	337	ALA
1	B	25	GLY
1	C	25	GLY
1	D	447	GLY
1	F	447	GLY
1	B	65	VAL
1	B	273	PRO
1	E	13	PRO
1	F	19	PRO
1	C	70	VAL
1	D	116	GLY
1	E	14	VAL
1	D	429	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/375 (96%)	313 (87%)	46 (13%)	4	21
1	B	359/375 (96%)	317 (88%)	42 (12%)	5	22
1	C	360/375 (96%)	311 (86%)	49 (14%)	3	18
1	D	359/375 (96%)	316 (88%)	43 (12%)	5	21
1	E	358/375 (96%)	321 (90%)	37 (10%)	7	27
1	F	359/375 (96%)	317 (88%)	42 (12%)	5	22
All	All	2154/2250 (96%)	1895 (88%)	259 (12%)	5	21

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	28	THR
1	A	45	ARG
1	A	55	VAL
1	A	57	LEU

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Mol	Chain	Res	Type
1	A	58	GLU
1	A	65	VAL
1	A	87	ARG
1	A	118	THR
1	A	122	THR
1	A	132	LEU
1	A	140	LEU
1	A	144	LEU
1	A	150	GLN
1	A	166	LEU
1	A	168	LEU
1	A	169	LYS
1	A	178	THR
1	A	198	VAL
1	A	227	VAL
1	A	246	LEU
1	A	250	LEU
1	A	257	LEU
1	A	259	GLU
1	A	264	LEU
1	A	266	SER
1	A	275	ILE
1	A	289	ILE
1	A	308	THR
1	A	310	SER
1	A	312	GLN
1	A	314	SER
1	A	324	TRP
1	A	344	LEU
1	A	380	THR
1	A	381	GLU
1	A	408	VAL
1	A	409	ASP
1	A	410	ASN
1	A	413	THR
1	A	423	THR
1	A	430	THR
1	A	437	THR
1	A	439	GLU
1	A	451	ASN
1	A	455	VAL
1	B	3	LEU

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Mol	Chain	Res	Type
1	B	28	THR
1	B	45	ARG
1	B	57	LEU
1	B	58	GLU
1	B	65	VAL
1	B	105	THR
1	B	115	TYR
1	B	118	THR
1	B	122	THR
1	B	132	LEU
1	B	140	LEU
1	B	144	LEU
1	B	150	GLN
1	B	152	SER
1	B	168	LEU
1	B	169	LYS
1	B	202	SER
1	B	227	VAL
1	B	245	ASN
1	B	246	LEU
1	B	256	LEU
1	B	257	LEU
1	B	259	GLU
1	B	266	SER
1	B	275	ILE
1	B	308	THR
1	B	310	SER
1	B	314	SER
1	B	324	TRP
1	B	330	ILE
1	B	364	THR
1	B	381	GLU
1	B	408	VAL
1	B	409	ASP
1	B	410	ASN
1	B	413	THR
1	B	420	SER
1	B	423	THR
1	B	437	THR
1	B	451	ASN
1	B	455	VAL
1	C	1	CYS

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Mol	Chain	Res	Type
1	C	2	SER
1	C	3	LEU
1	C	6	ASP
1	C	28	THR
1	C	45	ARG
1	C	57	LEU
1	C	58	GLU
1	C	65	VAL
1	C	71	GLU
1	C	74	ARG
1	C	105	THR
1	C	118	THR
1	C	122	THR
1	C	132	LEU
1	C	140	LEU
1	C	147	GLU
1	C	150	GLN
1	C	166	LEU
1	C	167	THR
1	C	168	LEU
1	C	169	LYS
1	C	198	VAL
1	C	217	ARG
1	C	227	VAL
1	C	240	SER
1	C	245	ASN
1	C	246	LEU
1	C	250	LEU
1	C	256	LEU
1	C	257	LEU
1	C	259	GLU
1	C	260	VAL
1	C	266	SER
1	C	275	ILE
1	C	281	GLN
1	C	308	THR
1	C	310	SER
1	C	344	LEU
1	C	345	ASP
1	C	364	THR
1	C	381	GLU
1	C	408	VAL

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Mol	Chain	Res	Type
1	C	409	ASP
1	C	410	ASN
1	C	413	THR
1	C	423	THR
1	C	430	THR
1	C	455	VAL
1	D	8	GLN
1	D	22	GLN
1	D	53	ILE
1	D	58	GLU
1	D	59	ASN
1	D	62	ASP
1	D	70	VAL
1	D	102	ASP
1	D	104	SER
1	D	122	THR
1	D	126	LEU
1	D	150	GLN
1	D	171	ASP
1	D	198	VAL
1	D	200	VAL
1	D	217	ARG
1	D	219	THR
1	D	222	GLN
1	D	224	THR
1	D	226	LEU
1	D	246	LEU
1	D	259	GLU
1	D	267	ASP
1	D	271	ARG
1	D	274	ASP
1	D	293	ARG
1	D	299	SER
1	D	313	LEU
1	D	314	SER
1	D	324	TRP
1	D	334	ILE
1	D	336	THR
1	D	379	PHE
1	D	380	THR
1	D	399	LEU
1	D	401	ASP

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Mol	Chain	Res	Type
1	D	408	VAL
1	D	409	ASP
1	D	429	ILE
1	D	434	ASN
1	D	437	THR
1	D	451	ASN
1	D	455	VAL
1	E	1	CYS
1	E	53	ILE
1	E	57	LEU
1	E	59	ASN
1	E	64	ARG
1	E	95	THR
1	E	122	THR
1	E	140	LEU
1	E	141	GLU
1	E	146	THR
1	E	147	GLU
1	E	163	THR
1	E	168	LEU
1	E	177	LEU
1	E	188	SER
1	E	200	VAL
1	E	202	SER
1	E	204	LEU
1	E	213	VAL
1	E	220	LEU
1	E	232	ASN
1	E	257	LEU
1	E	267	ASP
1	E	311	ARG
1	E	314	SER
1	E	323	SER
1	E	324	TRP
1	E	336	THR
1	E	349	ILE
1	E	364	THR
1	E	401	ASP
1	E	410	ASN
1	E	430	THR
1	E	437	THR
1	E	440	VAL

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Mol	Chain	Res	Type
1	E	444	LYS
1	E	455	VAL
1	F	11	GLU
1	F	14	VAL
1	F	20	GLN
1	F	33	VAL
1	F	53	ILE
1	F	58	GLU
1	F	63	LEU
1	F	65	VAL
1	F	83	ASP
1	F	105	THR
1	F	113	SER
1	F	121	THR
1	F	131	ARG
1	F	144	LEU
1	F	152	SER
1	F	168	LEU
1	F	169	LYS
1	F	177	LEU
1	F	195	SER
1	F	206	LEU
1	F	207	ARG
1	F	220	LEU
1	F	226	LEU
1	F	242	ILE
1	F	246	LEU
1	F	256	LEU
1	F	266	SER
1	F	272	ARG
1	F	274	ASP
1	F	288	SER
1	F	314	SER
1	F	324	TRP
1	F	329	SER
1	F	336	THR
1	F	383	LEU
1	F	399	LEU
1	F	408	VAL
1	F	409	ASP
1	F	437	THR
1	F	446	LEU

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Mol	Chain	Res	Type
1	F	455	VAL
1	F	457	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	76	GLN
1	A	193	GLN
1	A	286	ASN
1	A	350	GLN
1	A	357	GLN
1	A	363	GLN
1	A	367	GLN
1	A	426	GLN
1	A	451	ASN
1	B	59	ASN
1	B	76	GLN
1	B	150	GLN
1	B	193	GLN
1	B	398	GLN
1	B	426	GLN
1	B	451	ASN
1	C	59	ASN
1	C	76	GLN
1	C	138	GLN
1	C	154	GLN
1	C	193	GLN
1	C	254	GLN
1	C	350	GLN
1	C	357	GLN
1	C	435	GLN
1	D	176	GLN
1	D	254	GLN
1	D	386	GLN
1	D	425	GLN
1	E	20	GLN
1	E	76	GLN
1	E	172	GLN
1	E	210	GLN
1	E	245	ASN
1	E	270	GLN

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Mol	Chain	Res	Type
1	E	386	GLN
1	E	452	GLN
1	F	51	GLN
1	F	229	GLN
1	F	382	GLN
1	F	425	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	C	1001	1	15,16,17	0.36	0	14,15,17	1.03	0
2	PLM	B	1001	1	15,16,17	0.53	0	14,15,17	0.94	0
2	PLM	A	1001	1	15,16,17	1.66	3 (20%)	14,15,17	0.89	0

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	C	1001	1	-	7/14/14/15	-
2	PLM	B	1001	1	-	9/14/14/15	-
2	PLM	A	1001	1	-	7/14/14/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PLM	C3-C2	4.49	1.71	1.52
2	A	1001	PLM	C5-C4	-2.74	1.38	1.51
2	A	1001	PLM	C7-C6	2.35	1.63	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

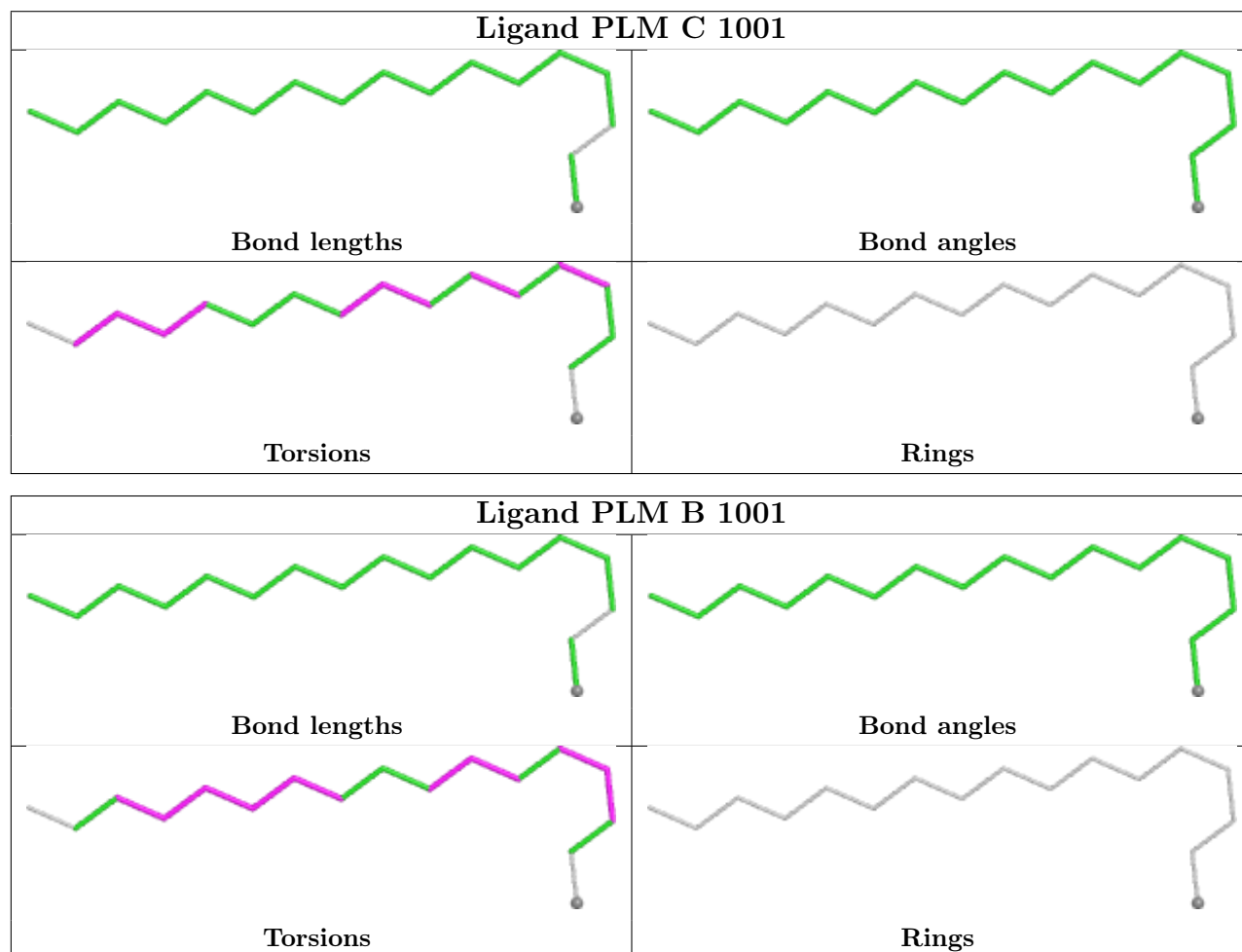
Mol	Chain	Res	Type	Atoms
2	A	1001	PLM	C4-C5-C6-C7
2	A	1001	PLM	CA-CB-CC-CD
2	B	1001	PLM	C2-C3-C4-C5
2	C	1001	PLM	C2-C3-C4-C5
2	A	1001	PLM	C2-C3-C4-C5
2	B	1001	PLM	C8-C9-CA-CB
2	B	1001	PLM	CC-CD-CE-CF
2	A	1001	PLM	C3-C4-C5-C6
2	A	1001	PLM	CC-CD-CE-CF
2	B	1001	PLM	C4-C5-C6-C7
2	B	1001	PLM	CB-CC-CD-CE
2	A	1001	PLM	C9-CA-CB-CC
2	C	1001	PLM	CD-CE-CF-CG
2	C	1001	PLM	CC-CD-CE-CF
2	C	1001	PLM	C4-C5-C6-C7
2	B	1001	PLM	C9-CA-CB-CC
2	B	1001	PLM	C5-C6-C7-C8
2	C	1001	PLM	CB-CC-CD-CE
2	A	1001	PLM	C6-C7-C8-C9
2	C	1001	PLM	C6-C7-C8-C9
2	B	1001	PLM	C1-C2-C3-C4
2	B	1001	PLM	CA-CB-CC-CD
2	C	1001	PLM	C7-C8-C9-CA

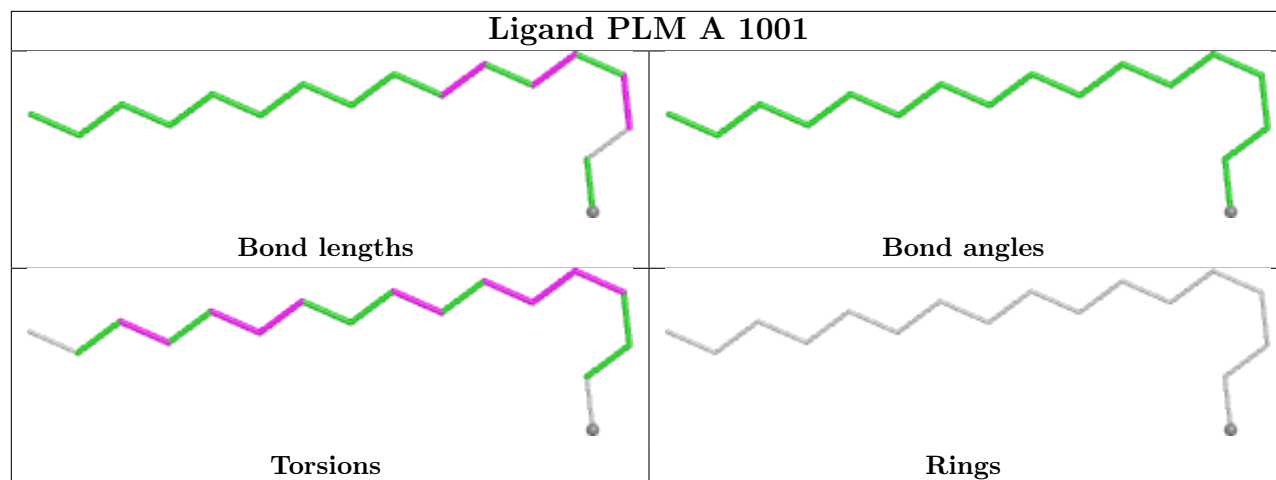
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	PLM	1	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 ⓘ

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	457/474 (96%)	-0.35	7 (1%)	72 50	57, 72, 105, 105	0
1	B	457/474 (96%)	-0.42	1 (0%)	91 81	54, 69, 102, 102	0
1	C	457/474 (96%)	-0.41	6 (1%)	75 53	54, 69, 102, 102	0
1	D	457/474 (96%)	-0.01	14 (3%)	51 35	81, 121, 121, 121	0
1	E	456/474 (96%)	0.02	13 (2%)	53 37	109, 120, 120, 120	0
1	F	457/474 (96%)	0.01	12 (2%)	57 39	79, 119, 119, 119	0
All	All	2741/2844 (96%)	-0.19	53 (1%)	66 45	54, 105, 121, 121	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ALA	5.5
1	E	368	GLU	5.0
1	D	260	VAL	4.7
1	F	156	THR	4.7
1	A	202	SER	4.5
1	E	400	ALA	4.0
1	D	261	PRO	4.0
1	F	425	GLN	3.9
1	E	117	VAL	3.8
1	E	62	ASP	3.5
1	C	230	ASP	3.5
1	E	403	ARG	3.4
1	D	83	ASP	3.4
1	D	116	GLY	3.2
1	A	306	ALA	3.2
1	F	83	ASP	3.2
1	D	286	ASN	3.2
1	E	203	ALA	3.0
1	F	203	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	132	LEU	2.9
1	F	153	ALA	2.9
1	F	210	GLN	2.9
1	F	214	GLU	2.8
1	D	430	THR	2.8
1	D	405	ARG	2.8
1	A	156	THR	2.8
1	E	306	ALA	2.7
1	D	110	ALA	2.7
1	F	155	THR	2.6
1	D	322	GLY	2.5
1	C	453	GLN	2.5
1	F	138	GLN	2.5
1	A	51	GLN	2.5
1	B	295	ALA	2.5
1	D	262	ALA	2.4
1	C	405	ARG	2.4
1	D	382	GLN	2.4
1	C	306	ALA	2.4
1	C	11	GLU	2.3
1	A	410	ASN	2.3
1	F	149	ALA	2.3
1	F	452	GLN	2.3
1	D	410	ASN	2.2
1	E	216	ALA	2.2
1	E	225	ARG	2.2
1	E	242	ILE	2.2
1	E	218	ALA	2.1
1	E	188	SER	2.1
1	C	307	GLY	2.1
1	A	221	ALA	2.1
1	D	386	GLN	2.1
1	E	221	ALA	2.0
1	F	202	SER	2.0

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

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

6.3 Carbohydrates [i](#)

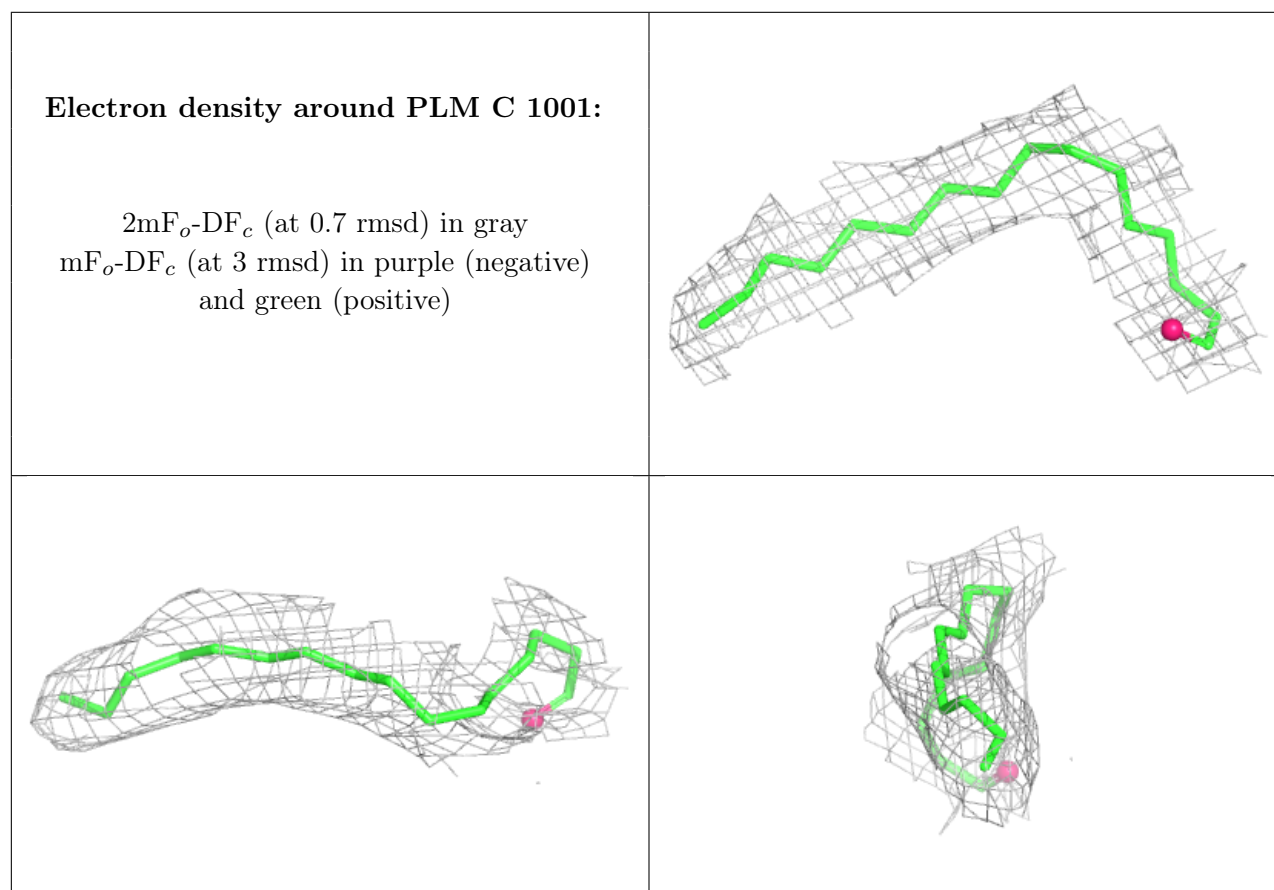
There are no oligosaccharides in this entry.

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.

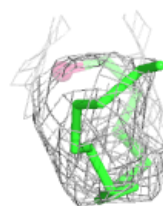
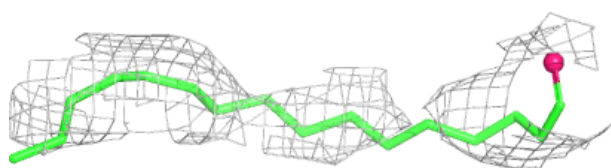
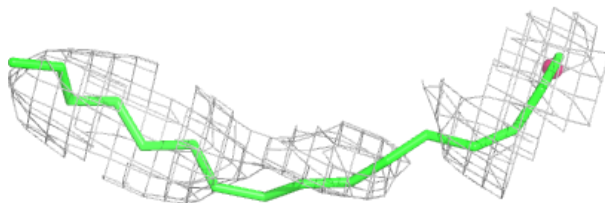
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLM	C	1001	17/18	0.96	0.07	58,58,58,58	0
2	PLM	B	1001	17/18	0.97	0.09	72,72,72,72	0
2	PLM	A	1001	17/18	0.98	0.08	72,72,76,76	0

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.

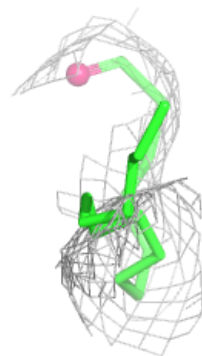
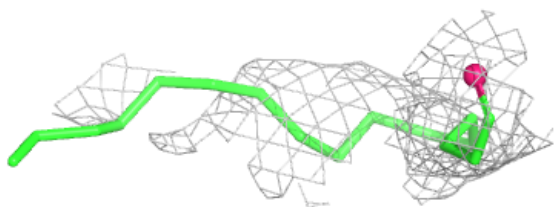
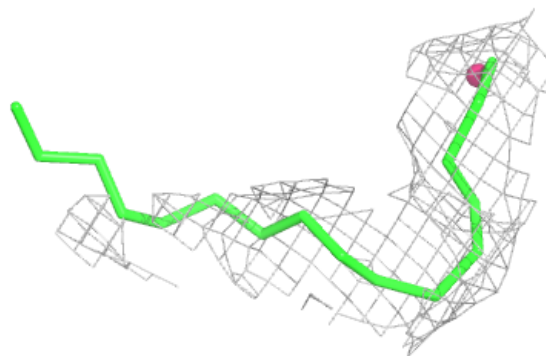


Electron density around PLM B 1001:

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

**Electron density around PLM A 1001:**

$2mF_o-DF_c$ (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.