Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:46 am BST

PDB ID	:	4Y1K
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 following versions of software and data (see references ⓘ) were used in the production of this report:

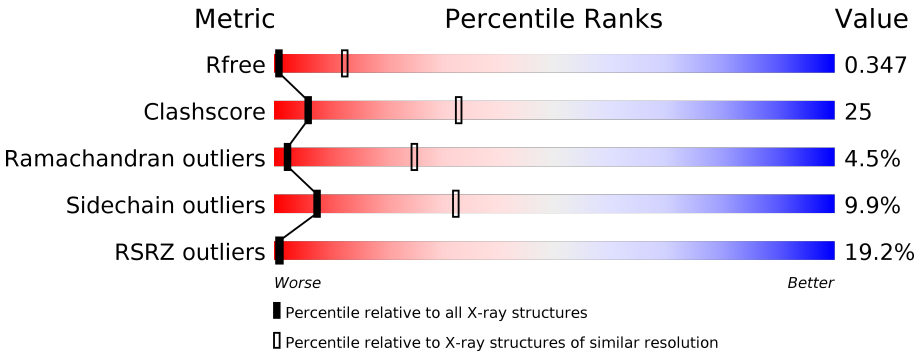
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	12% 46% 43% 7%
1	B	474	10% 47% 45%
1	C	474	12% 48% 42% 6%
1	D	474	27% 44% 45% 7%
1	E	474	26% 46% 46%
1	F	474	24% 41% 50% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLM	A	1001	-	-	-	X

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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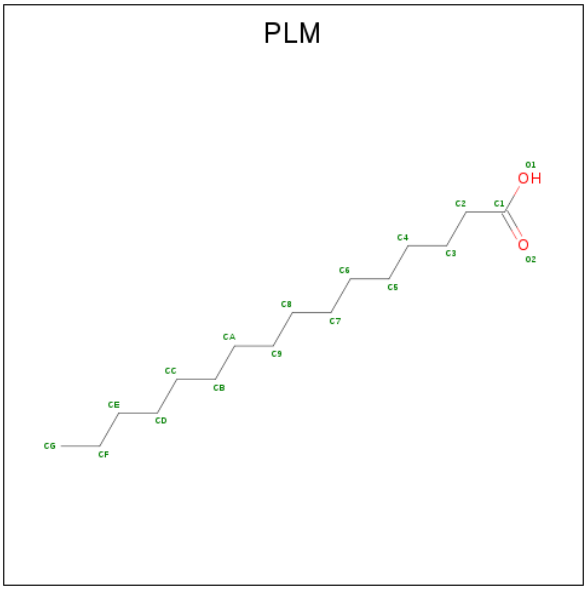
Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP Q51487
D	469	HIS	-	expression tag	UNP Q51487
D	470	HIS	-	expression tag	UNP Q51487
D	471	HIS	-	expression tag	UNP Q51487
D	472	HIS	-	expression tag	UNP Q51487
D	473	HIS	-	expression tag	UNP Q51487
D	474	HIS	-	expression tag	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 (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



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

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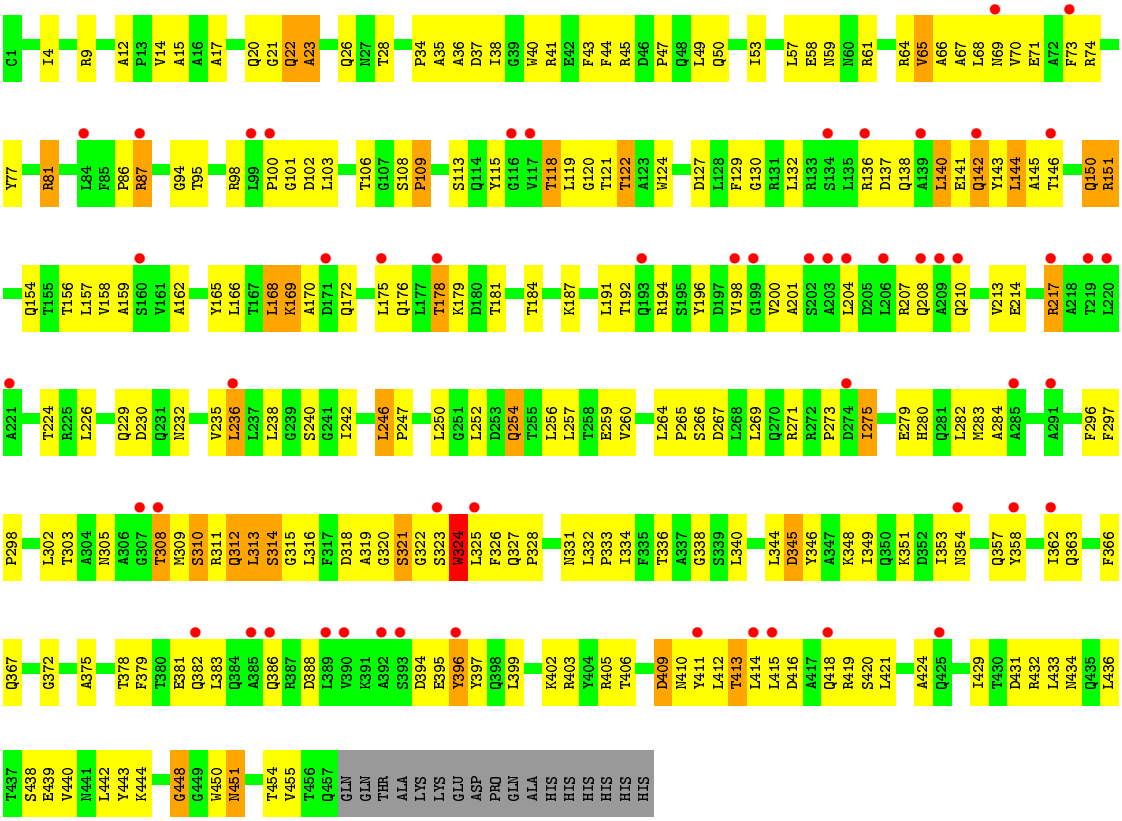
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			17	16	1		

3 Residue-property plots (i)

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

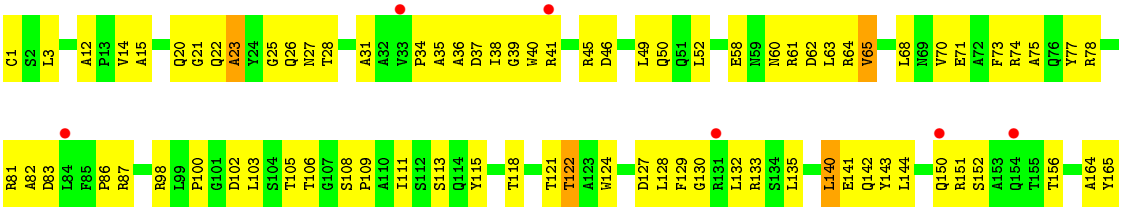
- Molecule 1: Outer membrane protein OprM

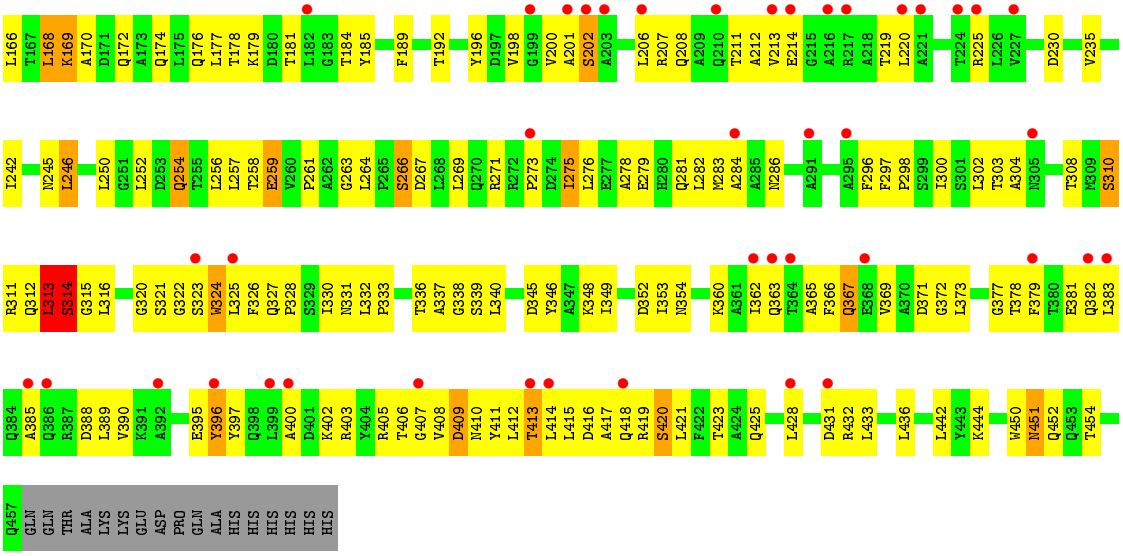
Chain A:



- Molecule 1: Outer membrane protein OprM

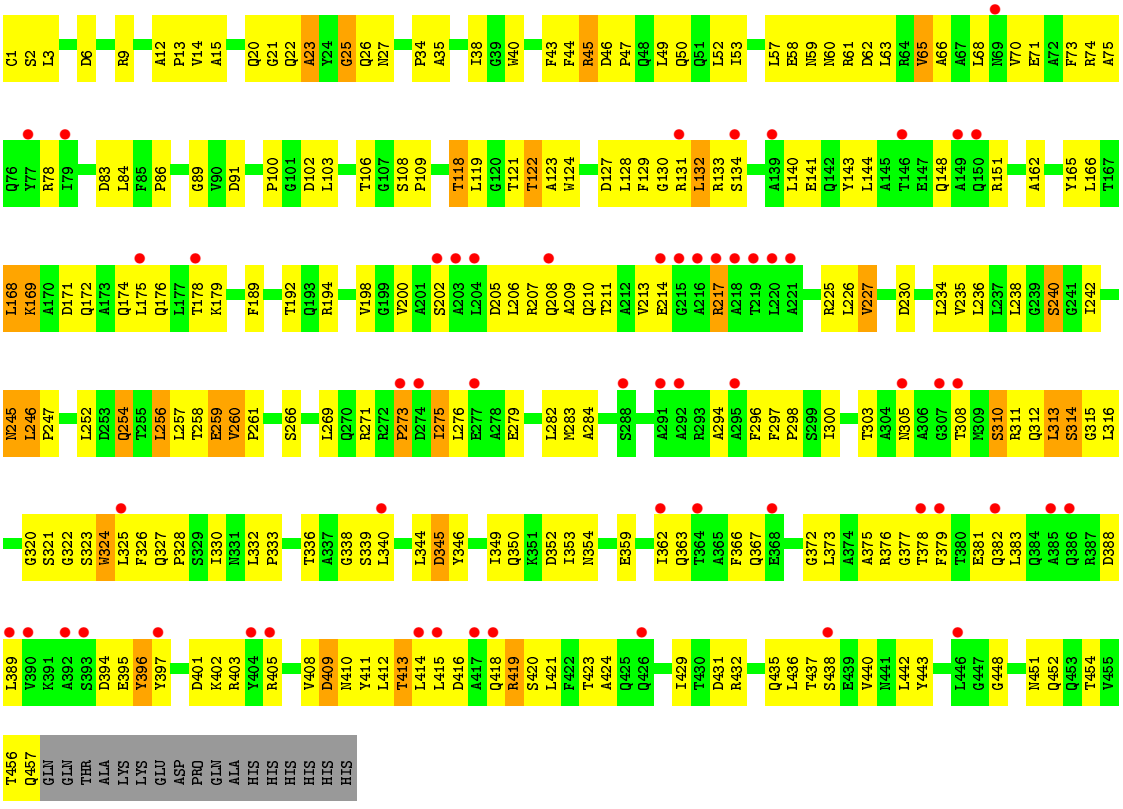
Chain B:





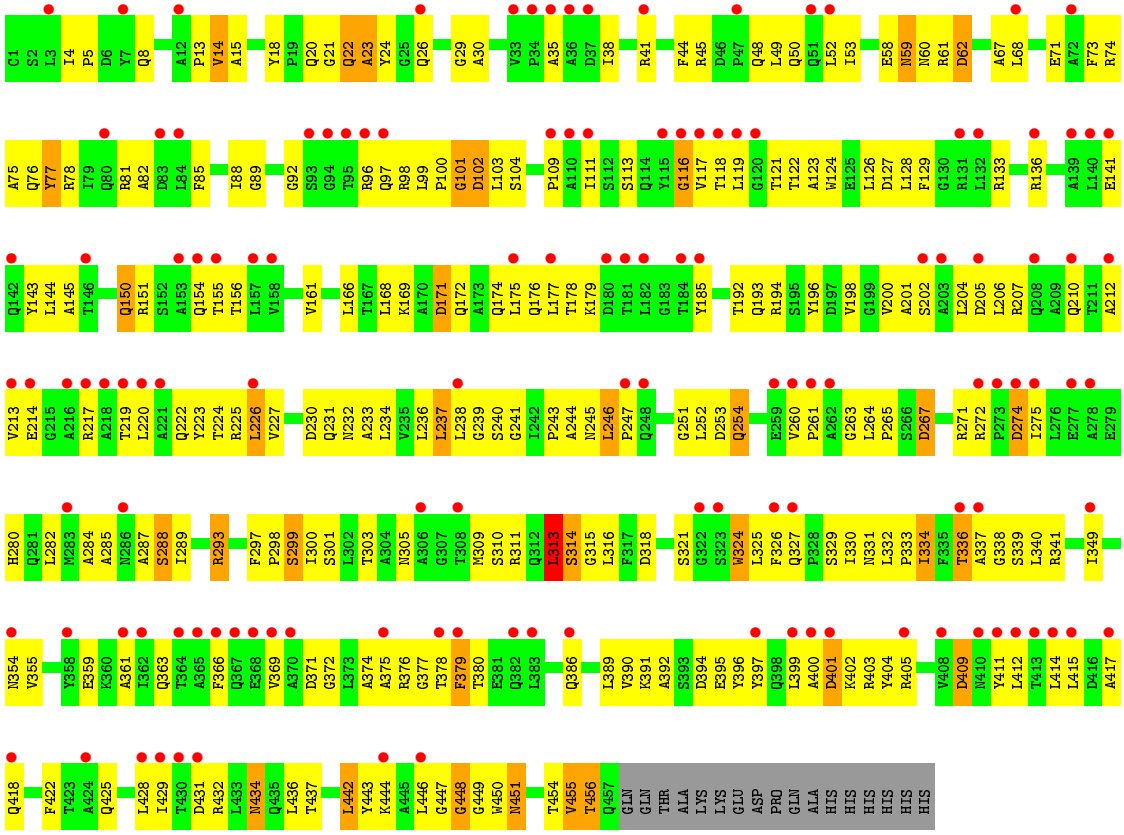
• Molecule 1: Outer membrane protein OprM

Chain C:



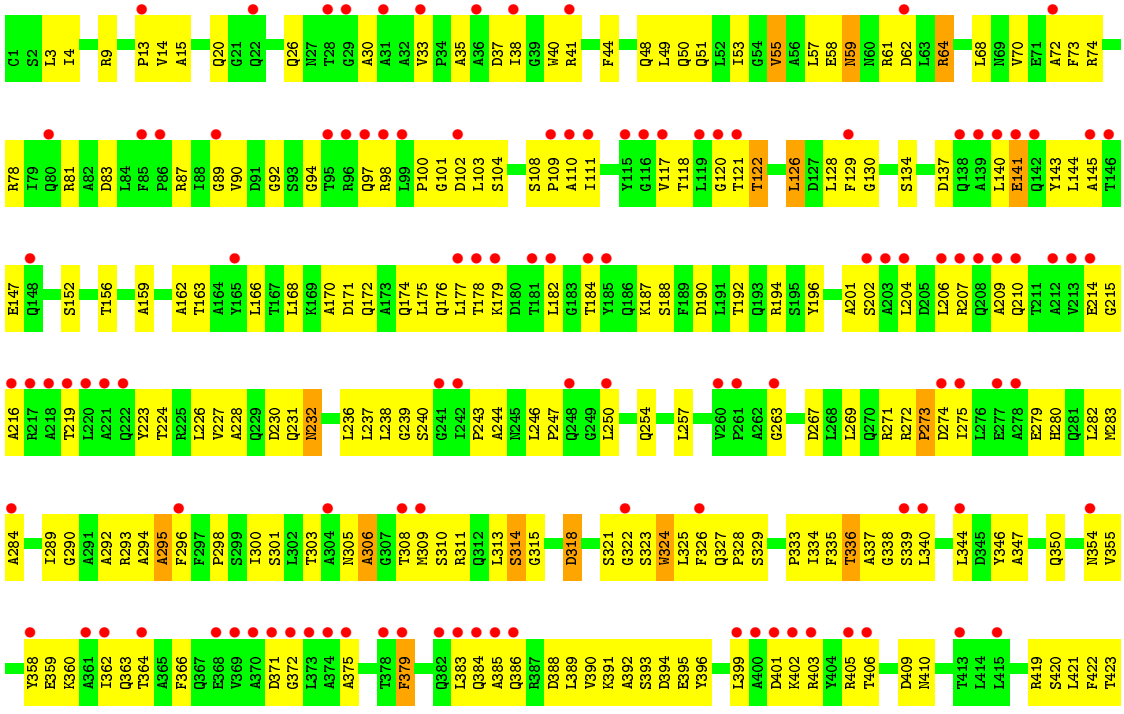
• Molecule 1: Outer membrane protein OprM

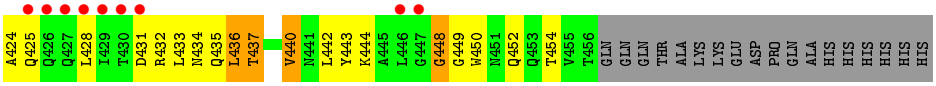
Chain D:



• Molecule 1: Outer membrane protein OprM

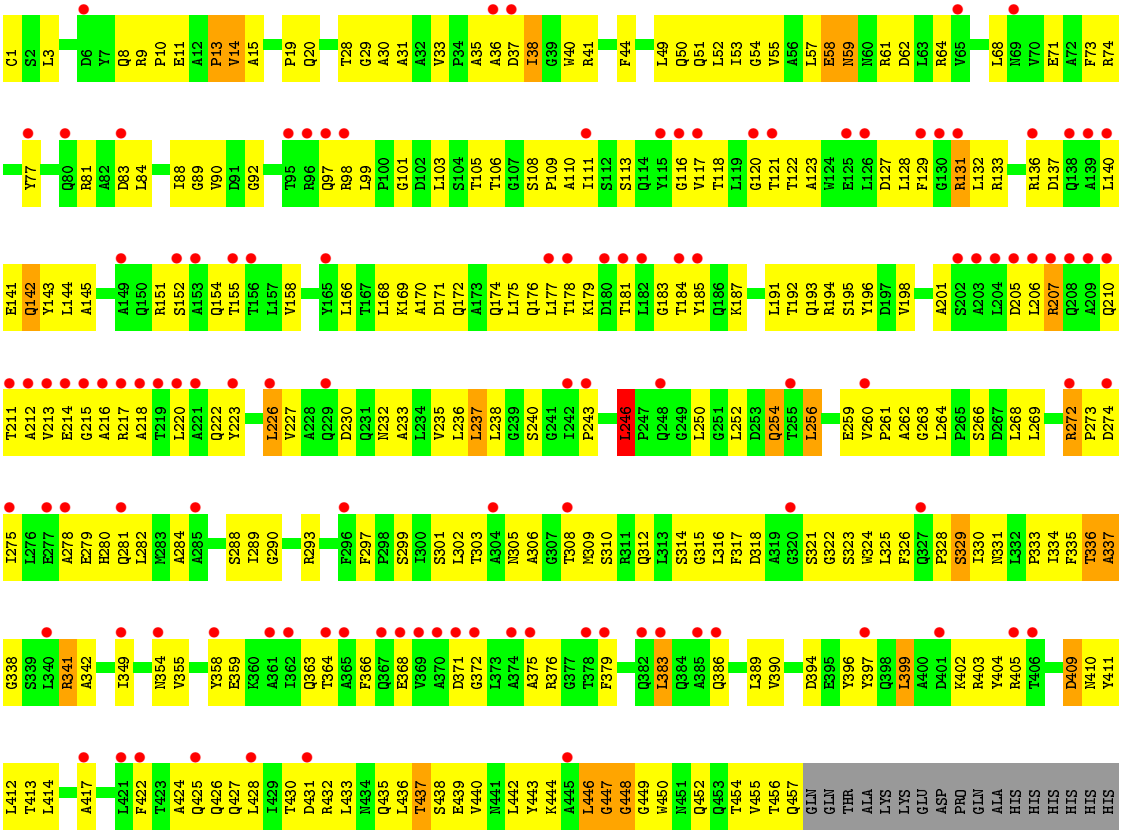
Chain E:





- Molecule 1: Outer membrane protein OprM

Chain F:



4 Data and refinement statistics (i)

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 87.90 – 3.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (87.91-3.80) 84.4 (87.90-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 3.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.297 , 0.346 0.296 , 0.347	Depositor DCC
R_{free} test set	1992 reflections (4.91%)	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)	0.37 , 86.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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	0.86	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/3557	0.73	0/4838
1	B	0.58	0/3557	0.72	0/4838
1	C	0.56	0/3559	0.72	0/4841
1	D	0.43	0/3557	0.63	1/4838 (0.0%)
1	E	0.44	0/3548	0.61	0/4826
1	F	0.43	0/3557	0.63	0/4838
All	All	0.50	0/21335	0.67	1/29019 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	442	LEU	CA-CB-CG	-5.06	103.67	115.30

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	188	0
1	B	3501	0	3475	173	0
1	C	3503	0	3480	173	0
1	D	3501	0	3476	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3492	0	3468	187	0
1	F	3501	0	3476	210	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	1038	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 25.

All (1038) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:177:LEU:HD21	1:E:425:GLN:HB3	1.72	0.72
1:D:396:TYR:HB2	1:E:207:ARG:HB3	1.71	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
1:D:371:ASP:OD1	1:E:232:ASN:ND2	2.16	0.70
1:D:166:LEU:HD13	1:D:436:LEU:HD13	1.72	0.70
1:D:88:ILE:HB	1:F:335:PHE:HB3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:176:GLN:HA	1:C:179:LYS:HG3	1.74	0.69
1:C:35:ALA:HA	1:C:38:ILE:HD12	1.73	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:269:LEU:HD21	1:C:362:ILE:HD11	1.76	0.68
1:C:38:ILE:HA	1:C:454:THR:HG23	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:325:LEU:HD12	1:F:326:PHE:H	1.60	0.66
1:F:59:ASN:O	1:F:61:ARG:NH1	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:ILE:HD11	1:B:362:ILE:HA	1.79	0.64
1:B:39:GLY:H	1:B:454:THR:HG1	1.44	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:E:389:LEU:O	1:E:393:SER:OG	2.04	0.64
1:A:331:ASN:ND2	1:C:91:ASP:OD1	2.30	0.64
1:A:68:LEU:O	1:A:71:GLU:N	2.31	0.63
1:A:9:ARG:NE	1:A:279:GLU:OE2	2.29	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: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
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:C:106:THR:OG1	1:C:108:SER:O	2.16	0.62
1:A:334:ILE:HG12	1:C:89:GLY:HA2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:323:SER:O	1:A:324:TRP:HB3	2.00	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: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:C:395:GLU:C	1:C:397:TYR:H	2.04	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:MET:O	1:B:286:ASN:HB3	2.02	0.59
1:F:184:THR:HA	1:F:187:LYS:HB3	1.85	0.59
1:E:333:PRO:HA	1:F:89:GLY:HA3	1.83	0.59
1:E:334:ILE:HD11	1:F:90:VAL:HG23	1.85	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:B:68:LEU:HD12	1:C:353:ILE:HA	1.84	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:F:250:LEU:HB3	1:F:254:GLN:HG3	1.85	0.58
1:D:336:THR:C	1:D:338:GLY:H	2.06	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:174:GLN:HB3	1:F:223:TYR:CD2	2.39	0.58
1:F:35:ALA:HB3	1:F:446:LEU:HB2	1.85	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: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:D:204:LEU:HD13	1:F:399:LEU:HB3	1.85	0.57
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:170:ALA:HA	1:F:252:LEU:HD11	1.87	0.57
1:F:145:ALA:HB2	1:F:280:HIS:HB3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:222:GLN:HG2	1:F:223:TYR:CD1	2.40	0.56
1:F:33:VAL:HG13	1:F:37:ASP:HB2	1.87	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:C:141:GLU:HG2	1:C:284:ALA:N	2.20	0.56
1:B:181:THR:HA	1:B:184:THR:HB	1.87	0.56
1:B:36:ALA:O	1:B:451:ASN:ND2	2.39	0.56
1:C:102:ASP:N	1:C:102:ASP:OD1	2.34	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: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
1:B:313:LEU:HG	1:B:316:LEU:HD12	1.87	0.56
1:C:225:ARG:C	1:C:227:VAL:H	2.09	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:OD1	1:A:102:ASP:N	2.36	0.56
1:F:171:ASP:OD2	1:F:226:LEU:HB3	2.06	0.56
1:D:100:PRO:HB3	1:F:321:SER:HA	1.88	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:F:236:LEU:C	1:F:238:LEU:H	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:396:TYR:HB2	1:F:207:ARG:HB3	1.89	0.55
1:E:48:GLN:HA	1:E:247:PRO:HD2	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: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:282:LEU:HD13	1:F:354:ASN:C	2.26	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:349:ILE:O	1:C:352:ASP:N	2.40	0.54
1:C:320:GLY:C	1:C:322:GLY:H	2.11	0.54
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:456:THR:OG1	1:C:457:GLN:N	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:395:GLU:C	1:A:397:TYR:H	2.12	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
1:E:118:THR:OG1	1:E:306:ALA:N	2.40	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:C:325:LEU:HD11	1:C:327:GLN:HB2	1.91	0.52
1:F:279:GLU:HB2	1:F:358:TYR:HE1	1.74	0.52
1:F:145:ALA:HB2	1:F:280:HIS:CB	2.39	0.52
1:B:185:TYR:HB3	1:B:213:VAL:HG22	1.92	0.52
1:E:104:SER:OG	1:E:108:SER:O	2.23	0.52
1:E:192:THR:HG23	1:E:201:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:HG1	1:E:306:ALA:H	1.57	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:118:THR:HG1	1:E:306:ALA:N	2.08	0.52
1:E:78:ARG:HG2	1:E:81:ARG:NH2	2.25	0.52
1:E:336:THR:C	1:E:338:GLY:H	2.12	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: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:282:LEU:HD13	1:D:354:ASN:C	2.31	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:236:LEU:C	1:D:238:LEU:H	2.14	0.50
1:F:316:LEU:C	1:F:318:ASP:H	2.14	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: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:C:207:ARG:O	1:C:211:THR:HG23	2.11	0.50
1:B:207:ARG:HB3	1:C:396:TYR:HB2	1.94	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: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
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:336:THR:C	1:F:338:GLY:H	2.14	0.50
1:F:282:LEU:HD13	1:F:355:VAL:N	2.27	0.50
1:A:165:TYR:HD2	1:A:166:LEU:HD23	1.76	0.50
1:A:9:ARG:NE	1:A:358:TYR:OH	2.45	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:176:GLN:OE1	1:B:179:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HB3	1:B:452:GLN:O	2.12	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:324:TRP:CD1	1:C:324:TRP:C	2.85	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:A:320:GLY:C	1:A:322:GLY:H	2.16	0.49
1:C:245:ASN:N	1:C:245:ASN:OD1	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:154:GLN:O	1:A:157:LEU:N	2.45	0.49
1:A:57:LEU:HD21	1:A:154:GLN:HG3	1.93	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
1:C:260:VAL:H	1:C:376:ARG:HH22	1.61	0.49
1:C:49:LEU:HA	1:C:52:LEU:HD12	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:F:44:PHE:HB3	1:F:49:LEU:HD23	1.94	0.49
1:B:156:THR:HG23	1:B:444:LYS:NZ	2.28	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: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: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:B:298:PRO:HA	1:B:331:ASN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HB3	1:B:349:ILE:HD13	1.94	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:138:GLN:NE2	1:A:142:GLN:OE1	2.46	0.48
1:A:49:LEU:HD13	1:A:165:TYR:CD2	2.48	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:E:419:ARG:O	1:E:423:THR:OG1	2.18	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
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:118:THR:OG1	1:E:305:ASN:HB2	2.13	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: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:D:400:ALA:HB2	1:E:204:LEU:HD11	1.95	0.48
1:E:448:GLY:O	1:E:450:TRP:N	2.47	0.48
1:A:395:GLU:C	1:A:397:TYR:N	2.67	0.47
1:A:214:GLU:HG3	1:B:388:ASP:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:PHE:O	1:C:50:GLN:NE2	2.40	0.47
1:D:210:GLN:O	1:D:214:GLU:HG2	2.14	0.47
1:D:113:SER:HB3	1:D:311:ARG:HG3	1.95	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:B:395:GLU:C	1:B:397:TYR:H	2.17	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:E:68:LEU:C	1:E:70:VAL:H	2.18	0.47
1:A:113:SER:O	1:A:311:ARG:HG3	2.14	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
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:C:395:GLU:C	1:C:397:TYR:N	2.68	0.47
1:F:168:LEU:HB2	1:F:230:ASP:HB3	1.95	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: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: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:D:401:ASP:OD2	1:D:402:LYS:HG3	2.15	0.47
1:D:48:GLN:HA	1:D:247:PRO:HB2	1.96	0.47
1:E:168:LEU:HD23	1:E:230:ASP:CB	2.43	0.47
1:E:162:ALA:HB3	1:E:440:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:101:GLY:C	1:D:103:LEU:H	2.18	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:A:298:PRO:HA	1:A:331:ASN:O	2.14	0.47
1:C:320:GLY:C	1:C:322:GLY:N	2.68	0.47
1:C:375:ALA:HB1	1:C:438:SER:HB3	1.97	0.47
1:D:251:GLY:O	1:D:254:GLN:HG2	2.15	0.47
1:D:73:PHE:HB3	1:D:143:TYR:HA	1.96	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:HB3	1:D:45:ARG:HE	1.51	0.46
1:E:145:ALA:HB2	1:E:280:HIS:HB3	1.96	0.46
1:F:101:GLY:C	1:F:103:LEU:H	2.18	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:F:74:ARG:HB2	1:F:143:TYR:CE1	2.50	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:137:ASP:HA	1:F:140:LEU:HB3	1.98	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: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: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:F:68:LEU:O	1:F:71:GLU:N	2.48	0.46
1:A:141:GLU:CG	1:A:283:MET:HB2	2.45	0.46
1:B:192:THR:O	1:B:192:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASP:O	1:B:346:TYR:C	2.53	0.46
1:C:403:ARG:HE	1:C:403:ARG:HB2	1.57	0.46
1:D:133:ARG:O	1:D:136:ARG:HB3	2.15	0.46
1:D:21:GLY:O	1:D:23:ALA:N	2.36	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: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:E:176:GLN:HA	1:E:179:LYS:HD2	1.98	0.46
1:D:232:ASN:ND2	1:F:371:ASP:OD1	2.40	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:264:LEU:O	1:D:267:ASP:HB2	2.14	0.46
1:D:13:PRO:HG2	1:D:363:GLN:CG	2.46	0.46
1:A:379:PHE:O	1:A:383:LEU:HG	2.16	0.46
1:B:324:TRP:CD1	1:B:324:TRP:C	2.89	0.46
1:D:168:LEU:HD23	1:D:230:ASP:CB	2.44	0.46
1:D:156:THR:HG23	1:D:444:LYS:NZ	2.31	0.46
1:D:82:ALA:CB	1:F:337:ALA:HB3	2.46	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:207:ARG:HA	1:A:207:ARG:HD3	1.74	0.45
1:A:324:TRP:CD1	1:A:324:TRP:C	2.89	0.45
1:A:345:ASP:O	1:A:346:TYR:C	2.54	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: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:B:168:LEU:HD23	1:B:230:ASP:CB	2.46	0.45
1:C:235:VAL:HG13	1:C:240:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ALA:O	1:C:377:GLY:HA3	2.16	0.45
1:C:336:THR:O	1:C:338:GLY:N	2.45	0.45
1:E:101:GLY:C	1:E:103:LEU:H	2.18	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:192:THR:HG21	1:C:205:ASP:O	2.17	0.45
1:C:86:PRO:HD3	1:C:124:TRP:CZ2	2.51	0.45
1:E:37:ASP:O	1:E:454:THR:HA	2.16	0.45
1:F:144:LEU:HB3	1:F:280:HIS:ND1	2.30	0.45
1:F:122:THR:HA	1:F:303:THR:HG23	1.97	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:O	1:B:406:THR:HG22	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
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:235:VAL:O	1:C:238:LEU:HB2	2.16	0.45
1:C:129:PHE:CD1	1:C:297:PHE:HB3	2.52	0.45
1:C:40:TRP:CZ2	1:C:452:GLN:HG3	2.52	0.45
1:D:234:LEU:O	1:D:238:LEU:HG	2.16	0.45
1:D:74:ARG:HB2	1:D:143:TYR:CE1	2.52	0.45
1:D:92:GLY:HA2	1:D:117:VAL:HG22	1.99	0.45
1:F:127:ASP:OD2	1:F:133:ARG:N	2.49	0.45
1:E:389:LEU:HD13	1:F:211:THR:O	2.16	0.45
1:F:243:PRO:O	1:F:246:LEU:HG	2.16	0.45
1:D:78:ARG:HH12	1:F:341:ARG:NH1	2.15	0.45
1:F:49:LEU:HA	1:F:52:LEU:HD12	1.99	0.45
1:A:229:GLN:HA	1:B:371:ASP:OD1	2.17	0.45
1:C:209:ALA:HA	1:C:411:TYR:OH	2.17	0.45
1:C:65:VAL:HG12	1:C:66:ALA:N	2.31	0.45
1:F:99:LEU:N	1:F:110:ALA:O	2.46	0.45
1:F:424:ALA:O	1:F:428:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:HG11	1:F:449:GLY:HA3	1.98	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: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:379:PHE:O	1:B:383:LEU:HG	2.17	0.45
1:B:74:ARG:HB2	1:B:143:TYR:CE1	2.52	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:176:GLN:OE1	1:A:179:LYS:HD2	2.17	0.44
1:A:74:ARG:HB2	1:A:143:TYR:CE1	2.52	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: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:F:8:GLN:HG2	1:F:8:GLN:H	1.63	0.44
1:A:353:ILE:HA	1:C:68:LEU:HD12	1.99	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:C:345:ASP:O	1:C:346:TYR:C	2.56	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: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:B:196:TYR:C	1:B:198:VAL:H	2.20	0.44
1:B:395:GLU:C	1:B:397:TYR:N	2.71	0.44
1:C:141:GLU:HB3	1:C:284:ALA:HB2	2.00	0.44
1:C:84:LEU:HD23	1:C:132:LEU:HB3	1.99	0.44
1:D:389:LEU:HD22	1:E:215:GLY:CA	2.47	0.44
1:E:41:ARG:HD3	1:E:50:GLN:CD	2.38	0.44
1:F:187:LYS:O	1:F:191:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:158:VAL:HG12	1:A:159:ALA:N	2.33	0.44
1:A:47:PRO:HA	1:A:50:GLN:HB2	1.99	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: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: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: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:40:TRP:CE2	1:B:452:GLN:HA	2.53	0.44
1:C:379:PHE:HB3	1:C:435:GLN:HG3	1.99	0.44
1:E:108:SER:O	1:E:110:ALA:N	2.51	0.44
1:E:97:GLN:O	1:E:111:ILE:HG23	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:395:GLU:O	1:C:397:TYR:N	2.52	0.43
1:C:373:LEU:CD2	1:C:442:LEU:HD21	2.49	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: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:A:94:GLY:O	1:A:95:THR:OG1	2.28	0.43
1:B:23:ALA:O	1:B:377:GLY:HA3	2.19	0.43
1:B:389:LEU:HG	1:B:389:LEU:O	2.18	0.43
1:C:38:ILE:O	1:C:443:TYR:OH	2.22	0.43
1:C:396:TYR:O	1:C:396:TYR:CG	2.72	0.43
1:D:166:LEU:HD13	1:D:436:LEU:CD1	2.46	0.43
1:D:29:GLY:O	1:D:263:GLY:HA2	2.18	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:165:TYR:CD2	1:C:166:LEU:HD23	2.54	0.43
1:C:235:VAL:HA	1:C:238:LEU:HB2	2.01	0.43
1:C:73:PHE:HB3	1:C:143:TYR:HA	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:169:LYS:C	1:D:171:ASP:H	2.21	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:D:99:LEU:HA	1:D:99:LEU:HD23	1.83	0.43
1:E:58:GLU:HG3	1:E:59:ASN:N	2.34	0.43
1:F:41:ARG:HD3	1:F:50:GLN:CD	2.38	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:393:SER:HB3	1:E:421:LEU:HA	2.01	0.43
1:A:181:THR:HA	1:A:184:THR:HB	2.00	0.43
1:A:141:GLU:HG2	1:A:284:ALA:N	2.34	0.43
1:C:411:TYR:CE2	1:C:415:LEU:HD13	2.44	0.43
1:D:363:GLN:HE22	1:E:239:GLY:C	2.22	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:A:137:ASP:O	1:A:138:GLN:C	2.57	0.42
1:B:113:SER:O	1:B:311:ARG:HG3	2.19	0.42
1:B:20:GLN:HG2	1:B:27:ASN:OD1	2.19	0.42
1:B:403:ARG:HE	1:B:403:ARG:HB2	1.59	0.42
1:B:40:TRP:NE1	1:B:452:GLN:HA	2.33	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: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:396:TYR:CG	1:F:396:TYR:O	2.71	0.42
1:F:383:LEU:HD11	1:F:432:ARG:HA	2.01	0.42
1:A:192:THR:O	1:A:192:THR:HG22	2.19	0.42
1:A:41:ARG:HD3	1:A:50:GLN:CD	2.39	0.42
1:D:22:GLN:O	1:D:23:ALA:HB2	2.19	0.42
1:D:394:ASP:HA	1:D:397:TYR:HB3	2.01	0.42
1:D:44:PHE:HB3	1:D:49:LEU:HD23	2.01	0.42
1:E:305:ASN:CG	1:E:325:LEU:HB3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:382:GLN:NE2	1:B:431:ASP:OD2	2.52	0.42
1:A:204:LEU:HD11	1:B:400:ALA:HB2	2.02	0.42
1:D:327:GLN:HA	1:E:94:GLY:O	2.19	0.42
1:D:71:GLU:HB3	1:F:349:ILE:CD1	2.50	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: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:A:68:LEU:O	1:A:70:VAL:N	2.53	0.42
1:B:177:LEU:HD21	1:B:425:GLN:CB	2.49	0.42
1:B:142:GLN:HG3	1:B:284:ALA:CB	2.49	0.42
1:A:419:ARG:NH2	1:B:416:ASP:OD2	2.33	0.42
1:C:320:GLY:O	1:C:322:GLY:N	2.52	0.42
1:D:288:SER:O	1:D:288:SER:OG	2.37	0.42
1:E:303:THR:HB	1:E:327:GLN:HB3	2.01	0.42
1:E:61:ARG:HA	1:E:61:ARG:HD3	1.74	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:169:LYS:HA	1:B:172:GLN:OE1	2.20	0.42
1:B:60:ASN:OD1	1:B:63:LEU:N	2.43	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:305:ASN:CG	1:F:325:LEU:HB3	2.40	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:235:VAL:HG22	1:B:242:ILE:HG13	2.02	0.42
1:B:15:ALA:HB3	1:B:366:PHE:CZ	2.55	0.42
1:B:64:ARG:O	1:B:65:VAL:C	2.58	0.42
1:E:159:ALA:O	1:E:163:THR:HB	2.20	0.42
1:D:24:TYR:OH	1:E:232:ASN:OD1	2.37	0.42
1:A:35:ALA:HA	1:A:38:ILE:CD1	2.49	0.42
1:D:75:ALA:HB1	1:F:342:ALA:O	2.19	0.42
1:F:106:THR:C	1:F:108:SER:H	2.23	0.42
1:F:235:VAL:HG13	1:F:240:SER:O	2.20	0.42
1:D:61:ARG:HE	1:F:359:GLU:CD	2.23	0.42
1:F:268:LEU:HD21	1:F:446:LEU:HD23	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:395:GLU:HB2	1:E:207:ARG:HD2	2.02	0.42
1:D:77:TYR:OH	1:D:81:ARG:NH1	2.53	0.42
1:F:318:ASP:HB2	1:F:321:SER:HB3	2.02	0.42
1:B:264:LEU:O	1:B:267:ASP:HB2	2.20	0.41
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.79	0.41
1:C:14:VAL:HG23	1:C:15:ALA:O	2.19	0.41
1:C:442:LEU:HA	1:C:442:LEU:HD12	1.74	0.41
1:D:264:LEU:HA	1:D:264:LEU:HD23	1.86	0.41
1:E:41:ARG:NH1	1:E:50:GLN:OE1	2.53	0.41
1:D:239:GLY:HA2	1:F:363:GLN:OE1	2.20	0.41
1:A:242:ILE:HG13	1:A:242:ILE:H	1.56	0.41
1:A:320:GLY:C	1:A:322:GLY:N	2.73	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:145:ALA:HB2	1:D:280:HIS:CB	2.43	0.41
1:D:59:ASN:O	1:D:61:ARG:NH1	2.51	0.41
1:F:28:THR:OG1	1:F:29:GLY:N	2.53	0.41
1:A:113:SER:OG	1:A:115:TYR:HE1	2.03	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: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:A:64:ARG:O	1:A:65:VAL:C	2.58	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:156:THR:HG23	1:A:444:LYS:HZ2	1.85	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:HG22	1:C:192:THR:O	2.19	0.41
1:C:389:LEU:O	1:C:389:LEU:HG	2.20	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:372:GLY:CA	1:E:442:LEU:HD22	2.51	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:F:262:ALA:O	1:F:446:LEU:HD22	2.20	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:C:43:PHE:O	1:C:43:PHE:CG	2.73	0.41
1:F:178:THR:HG1	1:F:422:PHE:HZ	1.66	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: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:O	1:A:396:TYR:CG	2.73	0.41
1:B:252:LEU:O	1:B:432:ARG:NE	2.48	0.41
1:D:403:ARG:HB2	1:D:403:ARG:HE	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:185:TYR:CE2	1:F:212:ALA:HB1	2.55	0.41
1:F:118:THR:OG1	1:F:305:ASN:HB2	2.21	0.41
1:A:217:ARG:HB3	1:B:385:ALA:HB1	2.02	0.41
1:A:22:GLN:O	1:A:23:ALA:HB2	2.20	0.41
1:B:189:PHE:HB2	1:B:213:VAL:HG21	2.03	0.41
1:B:20:GLN:HE22	1:B:26:GLN:HA	1.85	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:F:302:LEU:HA	1:F:328:PRO:HA	2.02	0.41
1:A:141:GLU:O	1:A:142:GLN:C	2.59	0.41
1:B:302:LEU:HD11	1:B:304:ALA:HB2	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:LEU:HD21	1:F:154:GLN:CG	2.40	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:129:PHE:CD2	1:B:297:PHE:HD2	2.39	0.41
1:B:113:SER:OG	1:B:311:ARG:O	2.23	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: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:C:68:LEU:O	1:C:71:GLU:N	2.54	0.41
1:E:97:GLN:C	1:E:111:ILE:HG23	2.41	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:77:TYR:CD2	1:A:77:TYR:C	2.93	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: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:D:251:GLY:C	1:D:253:ASP:H	2.23	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: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:A:319:ALA:C	1:A:321:SER:H	2.24	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: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:HA	1:E:182:LEU:HD12	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ARG:HG2	1:F:450:TRP:CZ2	2.56	0.40
1:F:389:LEU:O	1:F:389:LEU:HG	2.22	0.40
1:F:55:VAL:O	1:F:58:GLU:N	2.54	0.40
1:A:313:LEU:O	1:A:315:GLY:N	2.54	0.40
1:A:269:LEU:HD21	1:A:362:ILE:CD1	2.52	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:E:166:LEU:HD13	1:E:436:LEU:HD13	2.02	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:D:82:ALA:HB1	1:F:337:ALA:HB3	2.03	0.40
1:F:41:ARG:HD3	1:F:50:GLN:NE2	2.36	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:HG22	1:A:406:THR:O	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:N	1:B:245:ASN:OD1	2.34	0.40
1:B:365:ALA:O	1:B:369:VAL:HG23	2.21	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 (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	455/474 (96%)	363 (80%)	74 (16%)	18 (4%)	3	28
1	B	455/474 (96%)	368 (81%)	68 (15%)	19 (4%)	3	26
1	C	455/474 (96%)	365 (80%)	67 (15%)	23 (5%)	2	23
1	D	455/474 (96%)	371 (82%)	60 (13%)	24 (5%)	2	23
1	E	454/474 (96%)	380 (84%)	51 (11%)	23 (5%)	2	23
1	F	455/474 (96%)	385 (85%)	54 (12%)	16 (4%)	3	31
All	All	2729/2844 (96%)	2232 (82%)	374 (14%)	123 (4%)	2	25

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
1	E	313	LEU
1	F	13	PRO
1	F	30	ALA
1	F	317	PHE

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Mol	Chain	Res	Type
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
1	E	244	ALA
1	E	295	ALA
1	E	315	GLY
1	E	339	SER

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Mol	Chain	Res	Type
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
1	F	337	ALA
1	B	25	GLY
1	C	25	GLY
1	D	447	GLY

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Mol	Chain	Res	Type
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 (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	359/375 (96%)	320 (89%)	39 (11%)	6 29
1	B	359/375 (96%)	319 (89%)	40 (11%)	6 29
1	C	360/375 (96%)	321 (89%)	39 (11%)	6 30
1	D	359/375 (96%)	322 (90%)	37 (10%)	7 31
1	E	358/375 (96%)	333 (93%)	25 (7%)	15 46
1	F	359/375 (96%)	325 (90%)	34 (10%)	8 34
All	All	2154/2250 (96%)	1940 (90%)	214 (10%)	8 32

All (214) 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	58	GLU
1	A	81	ARG
1	A	87	ARG
1	A	98	ARG
1	A	118	THR
1	A	122	THR

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Mol	Chain	Res	Type
1	A	132	LEU
1	A	140	LEU
1	A	144	LEU
1	A	150	GLN
1	A	151	ARG
1	A	168	LEU
1	A	169	LYS
1	A	178	THR
1	A	217	ARG
1	A	246	LEU
1	A	250	LEU
1	A	257	LEU
1	A	259	GLU
1	A	266	SER
1	A	275	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	345	ASP
1	A	367	GLN
1	A	381	GLU
1	A	409	ASP
1	A	410	ASN
1	A	413	THR
1	A	439	GLU
1	A	451	ASN
1	A	455	VAL
1	B	3	LEU
1	B	28	THR
1	B	45	ARG
1	B	58	GLU
1	B	62	ASP
1	B	77	TYR
1	B	87	ARG
1	B	105	THR
1	B	115	TYR
1	B	118	THR
1	B	122	THR
1	B	132	LEU

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Mol	Chain	Res	Type
1	B	140	LEU
1	B	150	GLN
1	B	151	ARG
1	B	152	SER
1	B	168	LEU
1	B	169	LYS
1	B	202	SER
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	313	LEU
1	B	314	SER
1	B	324	TRP
1	B	367	GLN
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	450	TRP
1	B	451	ASN
1	C	1	CYS
1	C	2	SER
1	C	3	LEU
1	C	6	ASP
1	C	45	ARG
1	C	57	LEU
1	C	58	GLU
1	C	62	ASP
1	C	74	ARG
1	C	118	THR
1	C	122	THR
1	C	132	LEU
1	C	151	ARG
1	C	168	LEU

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Mol	Chain	Res	Type
1	C	169	LYS
1	C	217	ARG
1	C	227	VAL
1	C	240	SER
1	C	245	ASN
1	C	246	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	308	THR
1	C	310	SER
1	C	324	TRP
1	C	344	LEU
1	C	345	ASP
1	C	367	GLN
1	C	381	GLU
1	C	408	VAL
1	C	409	ASP
1	C	410	ASN
1	C	413	THR
1	C	423	THR
1	C	451	ASN
1	D	8	GLN
1	D	58	GLU
1	D	59	ASN
1	D	62	ASP
1	D	77	TYR
1	D	96	ARG
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	200	VAL
1	D	217	ARG
1	D	220	LEU
1	D	222	GLN
1	D	224	THR

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Mol	Chain	Res	Type
1	D	226	LEU
1	D	246	LEU
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	401	ASP
1	D	409	ASP
1	D	434	ASN
1	D	437	THR
1	D	451	ASN
1	D	455	VAL
1	E	53	ILE
1	E	57	LEU
1	E	59	ASN
1	E	62	ASP
1	E	64	ARG
1	E	122	THR
1	E	141	GLU
1	E	147	GLU
1	E	188	SER
1	E	202	SER
1	E	232	ASN
1	E	257	LEU
1	E	267	ASP
1	E	271	ARG
1	E	311	ARG
1	E	314	SER
1	E	323	SER
1	E	324	TRP
1	E	336	THR
1	E	364	THR
1	E	379	PHE
1	E	401	ASP

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Mol	Chain	Res	Type
1	E	410	ASN
1	E	437	THR
1	E	440	VAL
1	F	11	GLU
1	F	20	GLN
1	F	58	GLU
1	F	59	ASN
1	F	83	ASP
1	F	105	THR
1	F	113	SER
1	F	121	THR
1	F	131	ARG
1	F	142	GLN
1	F	152	SER
1	F	169	LYS
1	F	195	SER
1	F	207	ARG
1	F	220	LEU
1	F	226	LEU
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	341	ARG
1	F	383	LEU
1	F	399	LEU
1	F	409	ASP
1	F	437	THR
1	F	446	LEU
1	F	455	VAL
1	F	457	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN

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Mol	Chain	Res	Type
1	A	154	GLN
1	A	451	ASN
1	B	193	GLN
1	B	210	GLN
1	B	451	ASN
1	C	350	GLN
1	D	357	GLN
1	E	20	GLN
1	E	210	GLN
1	F	51	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 carbohydrates 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	B	1001	1	16,16,17	0.51	0	15,15,17	0.96	0
2	PLM	A	1001	1	16,16,17	1.56	3 (18%)	15,15,17	1.10	2 (13%)
2	PLM	C	1001	1	16,16,17	0.39	0	15,15,17	1.08	1 (6%)

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	1001	1	-	9/13/14/15	-
2	PLM	A	1001	1	-	7/13/14/15	-
2	PLM	C	1001	1	-	7/13/14/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PLM	C3-C2	4.75	1.71	1.52
2	A	1001	PLM	C5-C4	-2.39	1.38	1.51
2	A	1001	PLM	C7-C6	2.11	1.63	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	PLM	O2-C1-C2	-2.30	111.76	126.89
2	C	1001	PLM	O2-C1-C2	-2.10	113.09	126.89
2	A	1001	PLM	C3-C2-C1	2.06	123.41	114.26

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	A	1001	PLM	C2-C3-C4-C5
2	B	1001	PLM	CC-CD-CE-CF
2	B	1001	PLM	C2-C3-C4-C5
2	C	1001	PLM	C2-C3-C4-C5
2	B	1001	PLM	C8-C9-CA-CB
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	C3-C4-C5-C6
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

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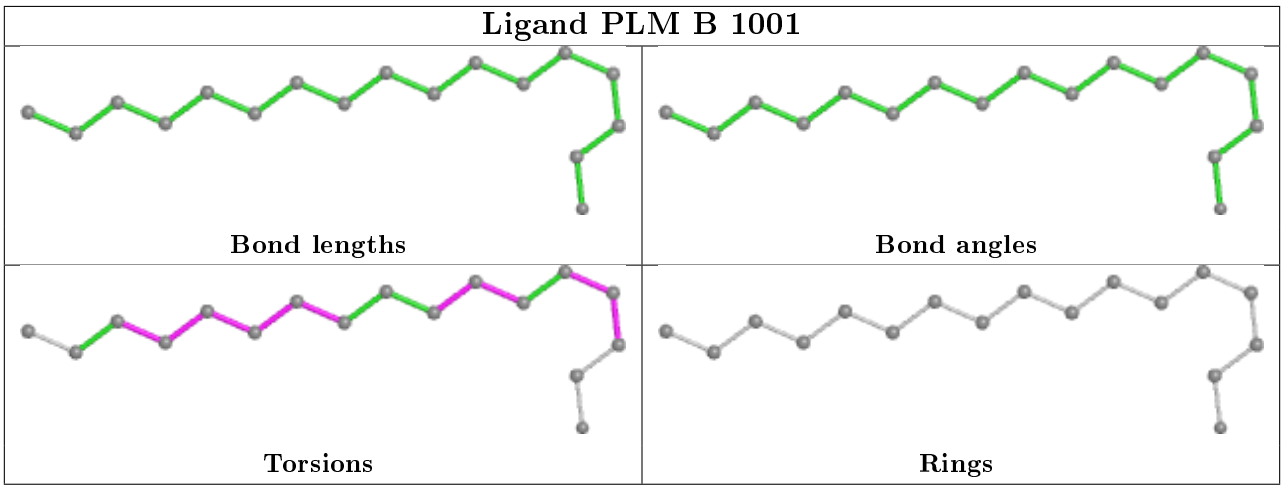
Mol	Chain	Res	Type	Atoms
2	B	1001	PLM	C9-CA-CB-CC
2	B	1001	PLM	C5-C6-C7-C8
2	C	1001	PLM	CB-CC-CD-CE
2	A	1001	PLM	C6-C7-C8-C9
2	C	1001	PLM	C6-C7-C8-C9
2	B	1001	PLM	C1-C2-C3-C4
2	B	1001	PLM	CA-CB-CC-CD
2	C	1001	PLM	C7-C8-C9-CA

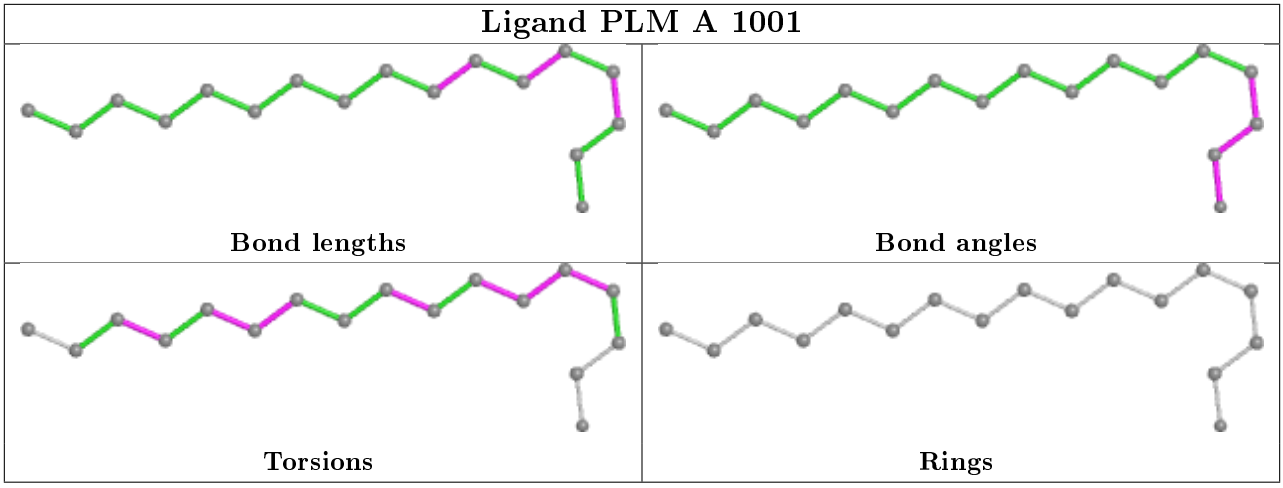
There are no ring outliers.

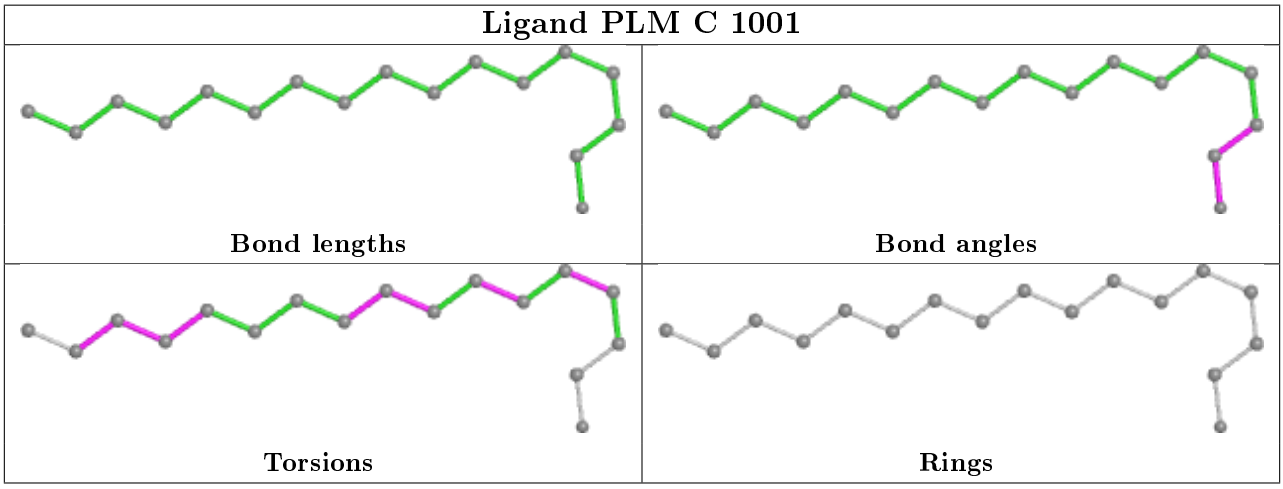
1 monomer is involved in 1 short contact:

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 then 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	457/474 (96%)	0.83	55 (12%)	4 4	57, 72, 105, 105	0
1	B	457/474 (96%)	0.81	48 (10%)	6 5	54, 69, 102, 102	0
1	C	457/474 (96%)	0.86	57 (12%)	3 4	54, 69, 102, 102	0
1	D	457/474 (96%)	1.31	129 (28%)	0 0	81, 121, 121, 121	0
1	E	456/474 (96%)	1.44	124 (27%)	0 0	109, 120, 120, 120	0
1	F	457/474 (96%)	1.30	113 (24%)	0 0	79, 119, 119, 119	0
All	All	2741/2844 (96%)	1.09	526 (19%)	1 1	54, 105, 121, 121	0

All (526) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	203	ALA	18.0
1	F	210	GLN	16.4
1	E	219	THR	13.5
1	D	261	PRO	10.6
1	A	202	SER	10.5
1	F	208	GLN	10.5
1	F	382	GLN	10.5
1	F	204	LEU	10.4
1	E	203	ALA	10.1
1	E	216	ALA	9.5
1	F	216	ALA	9.4
1	F	214	GLU	9.3
1	F	209	ALA	9.3
1	F	212	ALA	9.0
1	D	417	ALA	8.9
1	A	203	ALA	8.6
1	E	213	VAL	8.3
1	D	418	GLN	8.3
1	B	202	SER	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	382	GLN	8.2
1	E	430	THR	8.2
1	E	181	THR	7.8
1	D	110	ALA	7.7
1	E	382	GLN	7.6
1	E	383	LEU	7.6
1	E	386	GLN	7.4
1	F	120	GLY	7.3
1	D	368	GLU	7.2
1	F	383	LEU	7.1
1	E	212	ALA	7.0
1	E	308	THR	7.0
1	E	372	GLY	7.0
1	E	385	ALA	6.9
1	F	218	ALA	6.8
1	F	116	GLY	6.8
1	D	365	ALA	6.8
1	F	211	THR	6.8
1	D	35	ALA	6.7
1	D	386	GLN	6.6
1	D	415	LEU	6.6
1	E	182	LEU	6.5
1	E	218	ALA	6.3
1	F	215	GLY	6.3
1	D	203	ALA	6.3
1	D	401	ASP	6.3
1	F	213	VAL	6.3
1	D	217	ARG	6.3
1	D	109	PRO	6.2
1	D	181	THR	6.2
1	C	204	LEU	6.2
1	F	219	THR	6.2
1	D	260	VAL	6.1
1	E	209	ALA	6.1
1	D	413	THR	6.0
1	E	371	ASP	5.9
1	D	364	THR	5.9
1	D	220	LEU	5.7
1	F	379	PHE	5.6
1	B	418	GLN	5.6
1	E	184	THR	5.6
1	D	142	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	28	THR	5.5
1	E	139	ALA	5.5
1	E	210	GLN	5.4
1	D	216	ALA	5.4
1	F	368	GLU	5.4
1	E	248	GLN	5.4
1	B	217	ARG	5.4
1	E	138	GLN	5.3
1	E	202	SER	5.3
1	F	178	THR	5.3
1	B	383	LEU	5.3
1	E	368	GLU	5.3
1	A	204	LEU	5.3
1	A	221	ALA	5.2
1	F	181	THR	5.2
1	D	180	ASP	5.2
1	E	428	LEU	5.2
1	E	429	ILE	5.2
1	C	393	SER	5.1
1	D	369	VAL	5.1
1	E	217	ARG	5.1
1	F	364	THR	5.0
1	F	386	GLN	5.0
1	D	83	ASP	5.0
1	F	37	ASP	5.0
1	C	202	SER	4.9
1	E	220	LEU	4.9
1	F	111	ILE	4.9
1	D	97	GLN	4.9
1	C	217	ARG	4.9
1	D	286	ASN	4.9
1	E	111	ILE	4.9
1	A	385	ALA	4.8
1	E	241	GLY	4.8
1	A	393	SER	4.8
1	E	369	VAL	4.8
1	C	386	GLN	4.8
1	A	396	TYR	4.8
1	C	382	GLN	4.7
1	E	322	GLY	4.7
1	F	202	SER	4.7
1	F	156	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	217	ARG	4.7
1	A	386	GLN	4.7
1	E	354	ASN	4.7
1	F	117	VAL	4.6
1	D	272	ARG	4.6
1	E	120	GLY	4.6
1	A	389	LEU	4.6
1	E	242	ILE	4.6
1	F	207	ARG	4.6
1	F	354	ASN	4.5
1	E	185	TYR	4.5
1	E	400	ALA	4.5
1	A	175	LEU	4.5
1	D	139	ALA	4.5
1	D	218	ALA	4.5
1	E	406	THR	4.5
1	E	72	ALA	4.4
1	A	178	THR	4.4
1	F	153	ALA	4.4
1	B	214	GLU	4.4
1	B	291	ALA	4.3
1	A	415	LEU	4.3
1	D	379	PHE	4.3
1	D	414	LEU	4.3
1	E	97	GLN	4.3
1	C	389	LEU	4.3
1	E	33	VAL	4.3
1	B	386	GLN	4.3
1	F	320	GLY	4.3
1	B	382	GLN	4.3
1	D	277	GLU	4.2
1	E	261	PRO	4.2
1	D	399	LEU	4.2
1	B	220	LEU	4.2
1	A	220	LEU	4.2
1	C	203	ALA	4.2
1	F	115	TYR	4.2
1	F	370	ALA	4.1
1	B	392	ALA	4.1
1	D	34	PRO	4.1
1	E	86	PRO	4.1
1	D	411	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	115	TYR	4.1
1	C	218	ALA	4.1
1	E	274	ASP	4.1
1	D	412	LEU	4.1
1	E	178	THR	4.1
1	E	204	LEU	4.0
1	E	260	VAL	4.0
1	E	206	LEU	4.0
1	D	208	GLN	4.0
1	E	207	ARG	4.0
1	E	379	PHE	4.0
1	F	372	GLY	3.9
1	E	375	ALA	3.9
1	B	203	ALA	3.9
1	E	278	ALA	3.9
1	F	130	GLY	3.9
1	D	431	ASP	3.9
1	F	371	ASP	3.9
1	C	178	THR	3.8
1	E	141	GLU	3.8
1	E	431	ASP	3.8
1	D	221	ALA	3.8
1	F	378	THR	3.8
1	B	206	LEU	3.8
1	E	96	ARG	3.8
1	D	115	TYR	3.8
1	E	309	MET	3.8
1	C	308	THR	3.8
1	F	36	ALA	3.8
1	D	33	VAL	3.7
1	D	400	ALA	3.7
1	D	185	TYR	3.7
1	D	36	ALA	3.7
1	B	385	ALA	3.7
1	E	378	THR	3.7
1	D	140	LEU	3.7
1	E	140	LEU	3.7
1	D	84	LEU	3.7
1	D	132	LEU	3.7
1	C	208	GLN	3.7
1	D	383	LEU	3.7
1	D	117	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	80	GLN	3.7
1	E	401	ASP	3.7
1	D	446	LEU	3.7
1	E	179	LYS	3.6
1	F	155	THR	3.6
1	F	272	ARG	3.6
1	D	94	GLY	3.6
1	D	397	TYR	3.6
1	F	97	GLN	3.6
1	D	111	ILE	3.6
1	F	243	PRO	3.6
1	D	146	THR	3.6
1	D	184	THR	3.6
1	D	202	SER	3.6
1	C	379	PHE	3.6
1	E	405	ARG	3.5
1	F	406	THR	3.5
1	D	430	THR	3.5
1	C	214	GLU	3.5
1	F	138	GLN	3.5
1	D	131	ARG	3.5
1	F	274	ASP	3.5
1	B	84	LEU	3.5
1	E	370	ALA	3.5
1	D	219	THR	3.4
1	F	221	ALA	3.4
1	B	396	TYR	3.4
1	A	418	GLN	3.4
1	E	358	TYR	3.4
1	E	110	ALA	3.4
1	F	428	LEU	3.4
1	B	295	ALA	3.4
1	E	214	GLU	3.4
1	B	413	THR	3.4
1	F	185	TYR	3.4
1	C	150	GLN	3.4
1	D	213	VAL	3.4
1	D	408	VAL	3.3
1	D	51	GLN	3.3
1	E	415	LEU	3.3
1	F	275	ILE	3.3
1	D	428	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	41	ARG	3.3
1	C	438	SER	3.3
1	D	362	ILE	3.3
1	C	216	ALA	3.3
1	E	80	GLN	3.3
1	E	373	LEU	3.3
1	E	296	PHE	3.3
1	F	140	LEU	3.3
1	E	277	GLU	3.3
1	E	31	ALA	3.3
1	E	148	GLN	3.3
1	E	399	LEU	3.3
1	A	217	ARG	3.3
1	C	390	VAL	3.3
1	D	238	LEU	3.2
1	F	401	ASP	3.2
1	F	165	TYR	3.2
1	F	417	ALA	3.2
1	D	405	ARG	3.2
1	E	413	THR	3.2
1	A	198	VAL	3.2
1	F	422	PHE	3.2
1	E	117	VAL	3.2
1	C	215	GLY	3.2
1	E	339	SER	3.2
1	E	374	ALA	3.2
1	B	323	SER	3.1
1	D	26	GLN	3.1
1	B	379	PHE	3.1
1	E	403	ARG	3.1
1	B	431	ASP	3.1
1	F	405	ARG	3.1
1	D	120	GLY	3.1
1	B	400	ALA	3.1
1	D	429	ILE	3.1
1	E	95	THR	3.1
1	F	340	LEU	3.1
1	F	278	ALA	3.1
1	F	358	TYR	3.1
1	A	382	GLN	3.1
1	E	142	GLN	3.1
1	C	277	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	93	SER	3.1
1	B	325	LEU	3.1
1	E	129	PHE	3.1
1	F	96	ARG	3.1
1	A	236	LEU	3.1
1	F	129	PHE	3.1
1	E	29	GLY	3.0
1	E	121	THR	3.0
1	A	308	THR	3.0
1	B	364	THR	3.0
1	E	208	GLN	3.0
1	B	362	ILE	3.0
1	E	165	TYR	3.0
1	F	308	THR	3.0
1	D	80	GLN	3.0
1	F	229	GLN	3.0
1	F	277	GLU	3.0
1	E	340	LEU	3.0
1	E	326	PHE	3.0
1	D	96	ARG	2.9
1	F	369	VAL	2.9
1	F	6	ASP	2.9
1	C	273	PRO	2.9
1	C	415	LEU	2.9
1	D	367	GLN	2.9
1	E	89	GLY	2.9
1	D	52	LEU	2.9
1	D	182	LEU	2.9
1	E	221	ALA	2.9
1	F	95	THR	2.9
1	D	275	ILE	2.9
1	D	337	ALA	2.9
1	E	109	PRO	2.8
1	B	221	ALA	2.8
1	F	367	GLN	2.8
1	D	322	GLY	2.8
1	B	150	GLN	2.8
1	E	284	ALA	2.8
1	F	365	ALA	2.8
1	A	199	GLY	2.8
1	E	98	ARG	2.8
1	D	68	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLN	2.8
1	A	206	LEU	2.8
1	D	247	PRO	2.8
1	D	95	THR	2.8
1	D	370	ALA	2.8
1	E	145	ALA	2.8
1	C	414	LEU	2.8
1	D	119	LEU	2.8
1	D	323	SER	2.8
1	F	375	ALA	2.8
1	D	274	ASP	2.7
1	C	131	ARG	2.7
1	E	362	ILE	2.7
1	D	7	TYR	2.7
1	F	361	ALA	2.7
1	E	85	PHE	2.7
1	D	12	ALA	2.7
1	D	336	THR	2.7
1	A	354	ASN	2.7
1	E	177	LEU	2.7
1	B	210	GLN	2.7
1	D	248	GLN	2.7
1	F	131	ARG	2.7
1	D	410	ASN	2.7
1	C	288	SER	2.7
1	D	214	GLU	2.7
1	F	126	LEU	2.6
1	A	219	THR	2.6
1	B	201	ALA	2.6
1	F	180	ASP	2.6
1	F	385	ALA	2.6
1	B	368	GLU	2.6
1	A	307	GLY	2.6
1	F	223	TYR	2.6
1	D	308	THR	2.6
1	F	242	ILE	2.6
1	F	220	LEU	2.6
1	A	142	GLN	2.6
1	F	304	ALA	2.6
1	A	425	GLN	2.6
1	F	182	LEU	2.6
1	D	157	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	425	GLN	2.6
1	F	285	ALA	2.6
1	F	421	LEU	2.5
1	E	119	LEU	2.5
1	B	216	ALA	2.5
1	C	219	THR	2.5
1	D	47	PRO	2.5
1	D	153	ALA	2.5
1	E	222	GLN	2.5
1	A	325	LEU	2.5
1	C	69	ASN	2.5
1	E	146	THR	2.5
1	D	262	ALA	2.5
1	B	224	THR	2.5
1	C	378	THR	2.5
1	F	177	LEU	2.5
1	D	158	VAL	2.5
1	C	368	GLU	2.5
1	A	291	ALA	2.5
1	A	146	THR	2.5
1	A	208	GLN	2.5
1	E	263	GLY	2.5
1	D	210	GLN	2.5
1	D	378	THR	2.5
1	F	296	PHE	2.5
1	E	446	LEU	2.5
1	B	273	PRO	2.4
1	D	205	ASP	2.4
1	C	221	ALA	2.4
1	F	136	ARG	2.4
1	D	259	GLU	2.4
1	E	384	GLN	2.4
1	D	37	ASP	2.4
1	A	414	LEU	2.4
1	B	182	LEU	2.4
1	E	102	ASP	2.4
1	F	205	ASP	2.4
1	B	33	VAL	2.4
1	F	248	GLN	2.4
1	D	366	PHE	2.4
1	F	260	VAL	2.4
1	C	292	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	184	THR	2.4
1	F	98	ARG	2.4
1	A	362	ILE	2.4
1	F	255	THR	2.4
1	A	171	ASP	2.4
1	A	100	PRO	2.4
1	F	362	ILE	2.4
1	E	361	ALA	2.4
1	A	134	SER	2.4
1	C	417	ALA	2.3
1	C	404	TYR	2.3
1	D	358	TYR	2.3
1	E	447	GLY	2.3
1	F	69	ASN	2.3
1	C	418	GLN	2.3
1	F	65	VAL	2.3
1	A	274	ASP	2.3
1	B	41	ARG	2.3
1	D	278	ALA	2.3
1	A	117	VAL	2.3
1	F	121	THR	2.3
1	C	139	ALA	2.3
1	D	349	ILE	2.3
1	D	375	ALA	2.3
1	F	281	GLN	2.3
1	E	250	LEU	2.3
1	A	69	ASN	2.3
1	B	414	LEU	2.3
1	C	220	LEU	2.3
1	C	364	THR	2.3
1	E	13	PRO	2.2
1	C	325	LEU	2.2
1	F	206	LEU	2.2
1	C	340	LEU	2.2
1	D	361	ALA	2.2
1	D	326	PHE	2.2
1	C	146	THR	2.2
1	D	444	LYS	2.2
1	A	139	ALA	2.2
1	D	3	LEU	2.2
1	D	141	GLU	2.2
1	D	283	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	349	ILE	2.2
1	C	307	GLY	2.2
1	A	209	ALA	2.2
1	E	275	ILE	2.2
1	F	83	ASP	2.2
1	F	327	GLN	2.2
1	B	407	GLY	2.2
1	D	116	GLY	2.2
1	D	72	ALA	2.2
1	E	402	LYS	2.2
1	E	427	GLN	2.2
1	C	274	ASP	2.2
1	A	210	GLN	2.2
1	C	149	ALA	2.2
1	E	38	ILE	2.2
1	E	116	GLY	2.2
1	B	284	ALA	2.2
1	D	424	ALA	2.2
1	F	149	ALA	2.2
1	F	445	ALA	2.2
1	B	154	GLN	2.2
1	B	363	GLN	2.2
1	C	175	LEU	2.2
1	B	225	ARG	2.2
1	C	385	ALA	2.2
1	C	77	TYR	2.2
1	E	36	ALA	2.2
1	C	405	ARG	2.2
1	C	305	ASN	2.2
1	C	446	LEU	2.2
1	A	73	PHE	2.2
1	D	212	ALA	2.2
1	A	323	SER	2.2
1	E	425	GLN	2.2
1	E	304	ALA	2.1
1	B	305	ASN	2.1
1	A	116	GLY	2.1
1	C	392	ALA	2.1
1	A	84	LEU	2.1
1	D	306	ALA	2.1
1	D	177	LEU	2.1
1	F	226	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	TYR	2.1
1	A	99	LEU	2.1
1	A	136	ARG	2.1
1	B	213	VAL	2.1
1	D	175	LEU	2.1
1	F	139	ALA	2.1
1	F	77	TYR	2.1
1	D	354	ASN	2.1
1	A	390	VAL	2.1
1	A	358	TYR	2.1
1	C	134	SER	2.1
1	C	362	ILE	2.1
1	D	118	THR	2.1
1	D	273	PRO	2.1
1	D	226	LEU	2.1
1	C	397	TYR	2.1
1	B	227	VAL	2.1
1	E	22	GLN	2.1
1	E	344	LEU	2.1
1	A	392	ALA	2.0
1	C	79	ILE	2.0
1	C	291	ALA	2.0
1	D	41	ARG	2.0
1	B	428	LEU	2.0
1	E	99	LEU	2.0
1	C	426	GLN	2.0
1	E	426	GLN	2.0
1	A	87	ARG	2.0
1	A	285	ALA	2.0
1	C	295	ALA	2.0
1	F	374	ALA	2.0
1	B	399	LEU	2.0
1	D	155	THR	2.0
1	E	364	THR	2.0
1	B	131	ARG	2.0
1	D	136	ARG	2.0
1	F	397	TYR	2.0
1	E	62	ASP	2.0
1	A	160	SER	2.0
1	F	152	SER	2.0
1	F	125	GLU	2.0
1	D	154	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	327	GLN	2.0
1	B	199	GLY	2.0
1	F	431	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

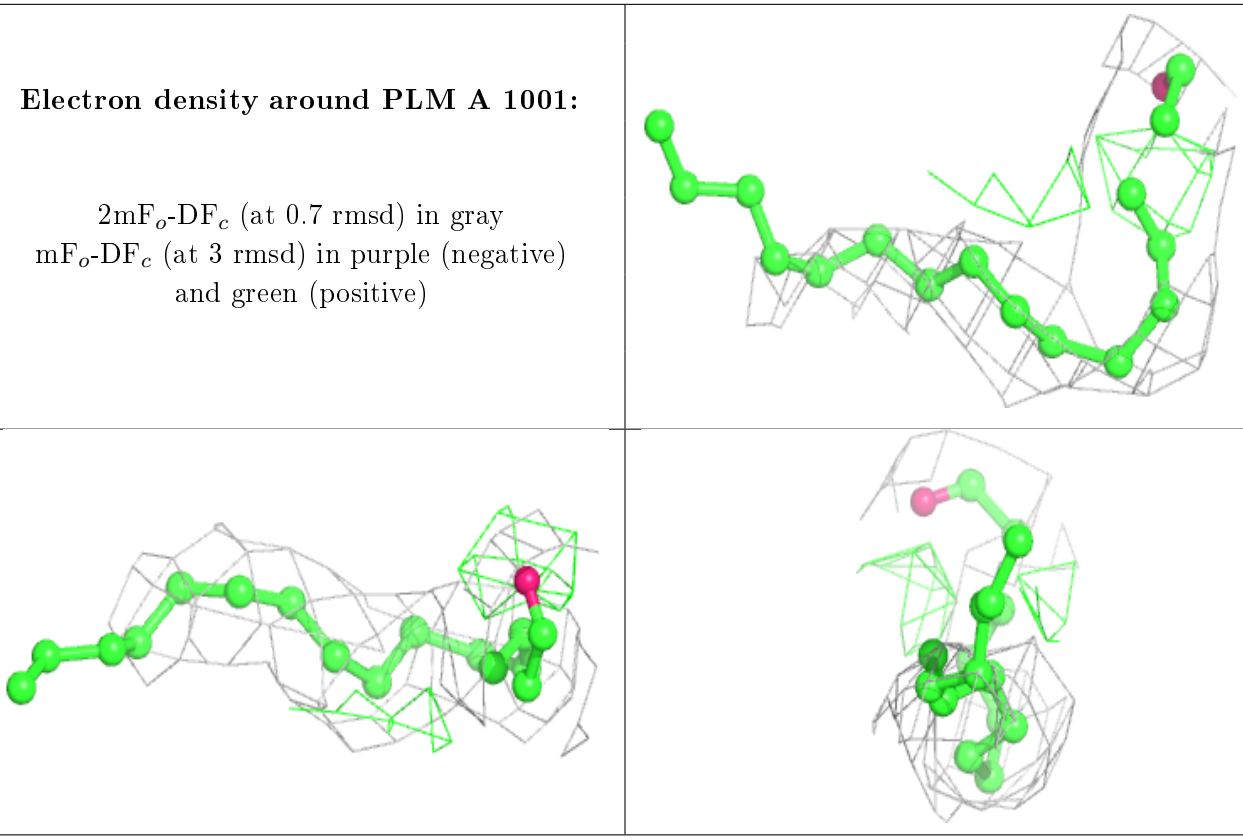
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLM	A	1001	17/18	0.65	0.44	72,72,76,76	0
2	PLM	B	1001	17/18	0.77	0.37	72,72,72,72	0
2	PLM	C	1001	17/18	0.80	0.30	58,58,58,58	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.

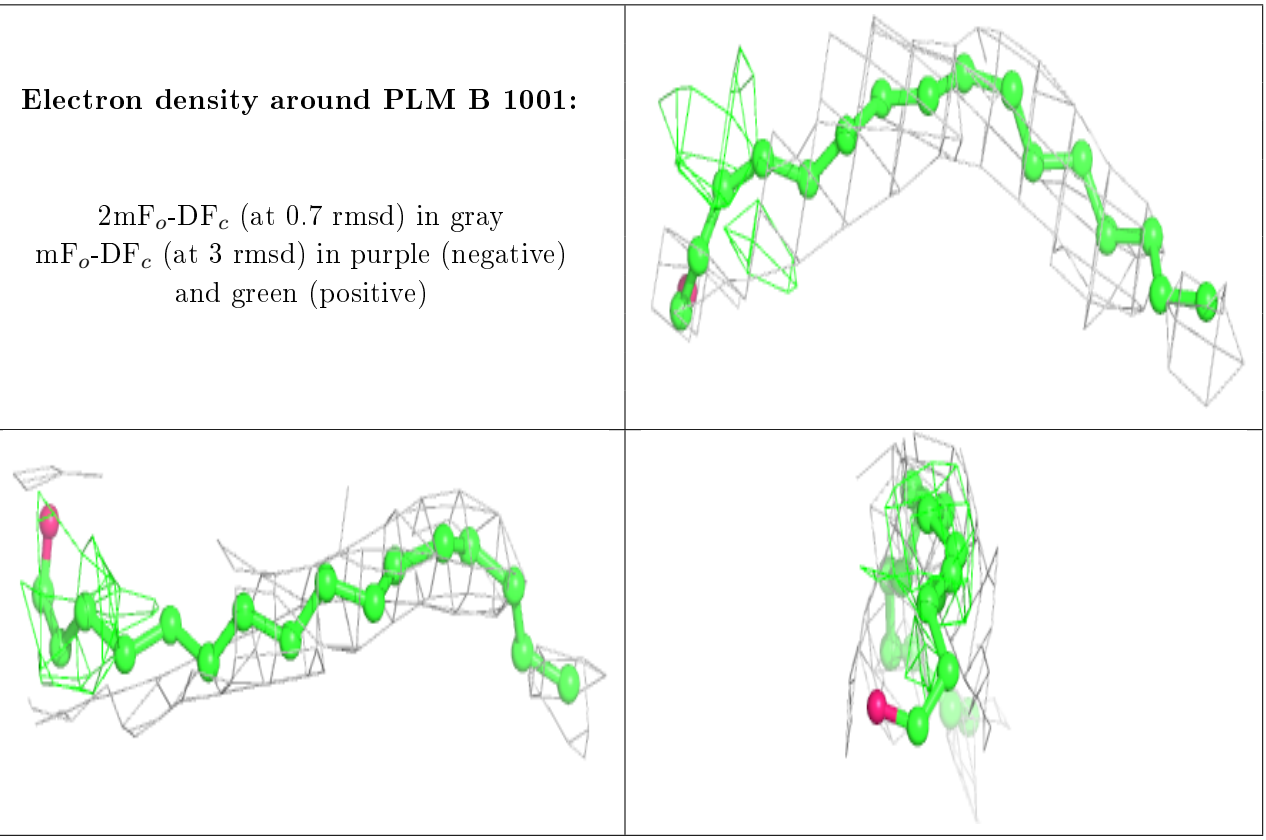
Electron density around PLM A 1001:

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



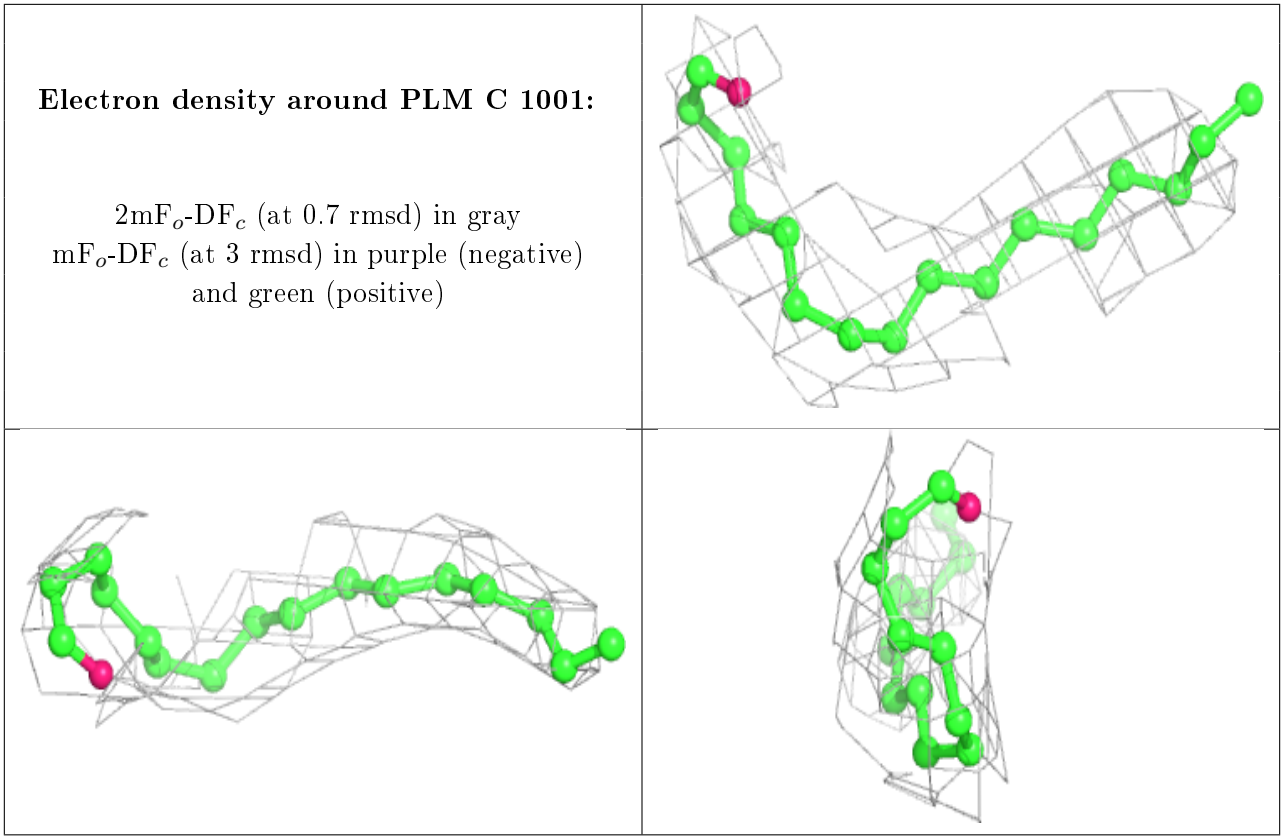
Electron density around PLM B 1001:

$2mF_o$-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 C 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

There are no such residues in this entry.