



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:26 PM UTC

PDB ID : 6SLJ / pdb_00006slj
Title : Structure of the RagAB peptide transporter
Authors : Madej, M.; Ranson, N.A.; White, J.B.R.
Deposited on : 2019-08-20
Resolution : 3.04 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

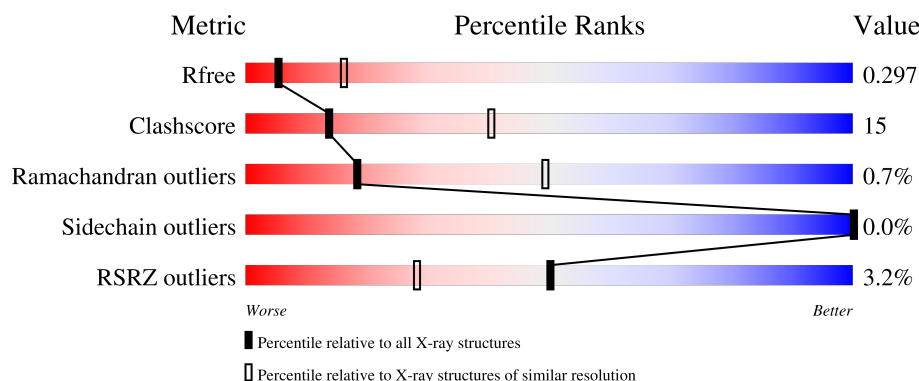
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	997	3% 59% 30% 10%
1	B	997	3% 61% 29% 10%
2	C	488	% 73% 26% .
2	D	488	% 73% 26% .
3	P	13	62% 69% 23% 8%

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Mol	Chain	Length	Quality of chain
4	Q	10	 A horizontal bar chart showing the quality of chain 4 (Q) of length 10. The bar is divided into four segments: red (50%), green (60%), yellow (30%), and orange (10%). The segments are stacked horizontally, with the red segment starting from the left and ending at 50%, the green segment starting at 50% and ending at 60%, the yellow segment starting at 60% and ending at 90%, and the orange segment starting at 90% and ending at 100%. The percentages are labeled above the corresponding segments.

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22178 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 RagA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	900	Total	C	N	O	S	0	3	0
			7069	4482	1183	1372	32			
1	A	898	Total	C	N	O	S	0	0	0
			7035	4459	1177	1367	32			

- Molecule 2 is a protein called Lipoprotein RagB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	482	Total	C	N	O	S	0	0	0
			3842	2440	656	737	9			
2	D	482	Total	C	N	O	S	0	0	0
			3841	2440	656	736	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	502	HIS	-	expression tag	UNP F5H948
C	503	HIS	-	expression tag	UNP F5H948
C	504	HIS	-	expression tag	UNP F5H948
C	505	HIS	-	expression tag	UNP F5H948
C	506	HIS	-	expression tag	UNP F5H948
C	507	HIS	-	expression tag	UNP F5H948
D	502	HIS	-	expression tag	UNP F5H948
D	503	HIS	-	expression tag	UNP F5H948
D	504	HIS	-	expression tag	UNP F5H948
D	505	HIS	-	expression tag	UNP F5H948
D	506	HIS	-	expression tag	UNP F5H948
D	507	HIS	-	expression tag	UNP F5H948

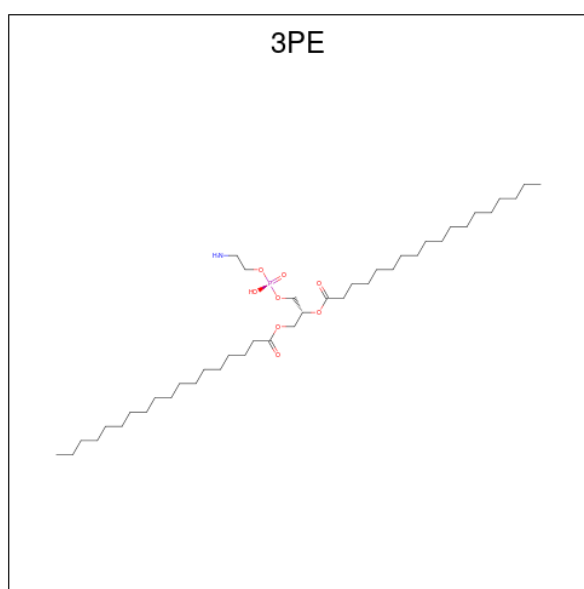
- Molecule 3 is a protein called ALA-SER-THR-THR-GLY-ALA-ASN-SER-GLN-ARG-GLY-SER-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	0	0	0
			82	44	18	20			

- Molecule 4 is a protein called ALA-SER-THR-THR-GLY-ALA-ASN-SER-GLN-ARG.

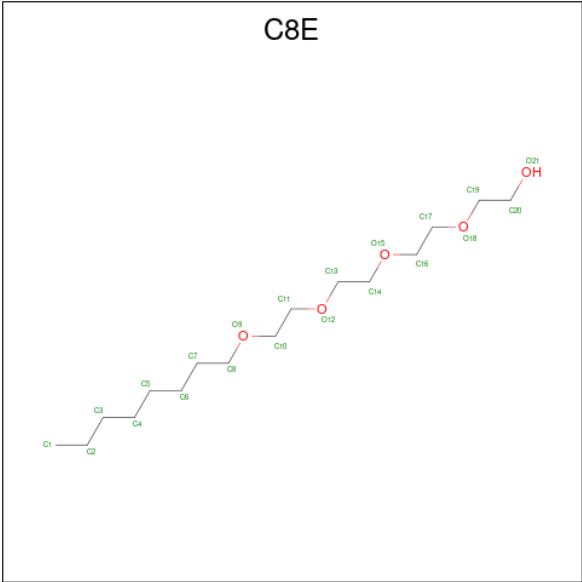
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Q	10	Total	C	N	O	0	0	0
			68	37	15	16			

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



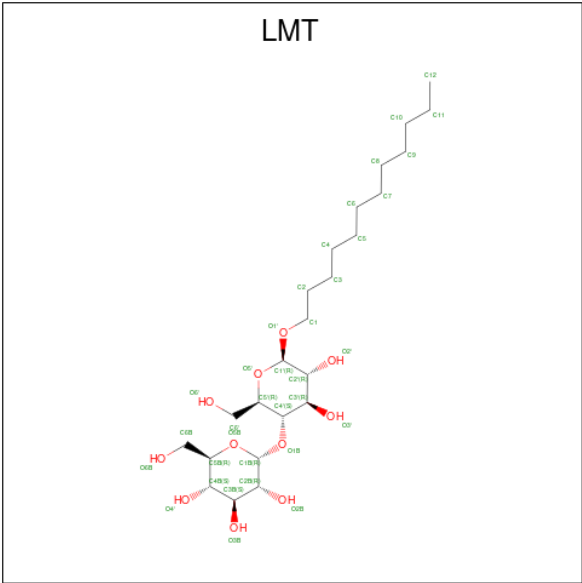
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			34	30	4		
5	A	1	Total	C	O	0	0
			34	30	4		

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			21	16	5		
6	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 7 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



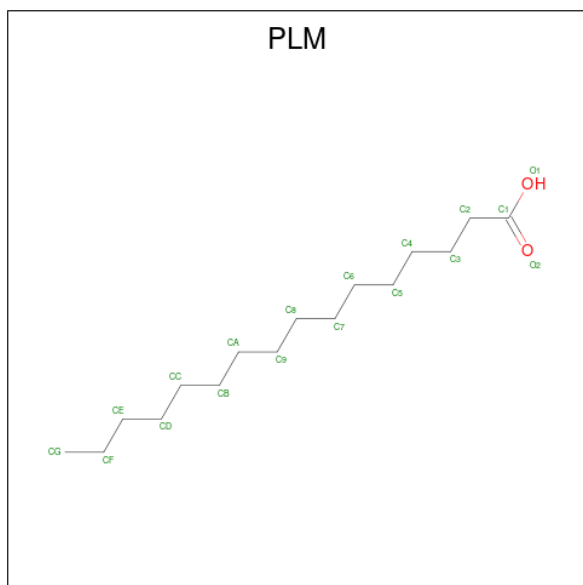
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			28	17	11		
7	A	1	Total	C	O	0	0
			13	12	1		

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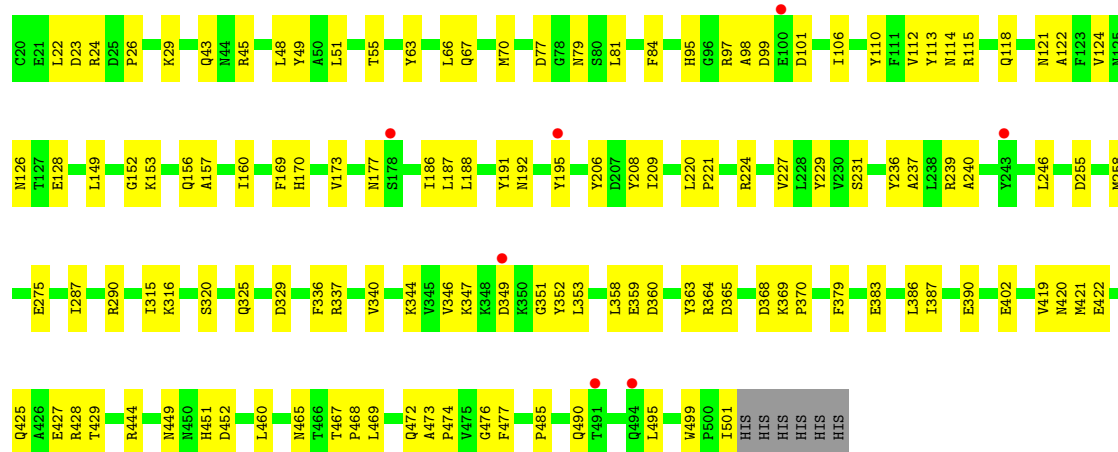
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	12	1		
7	C	1	Total	C	O	0	0
			34	23	11		
7	C	1	Total	C	O	0	0
			13	12	1		

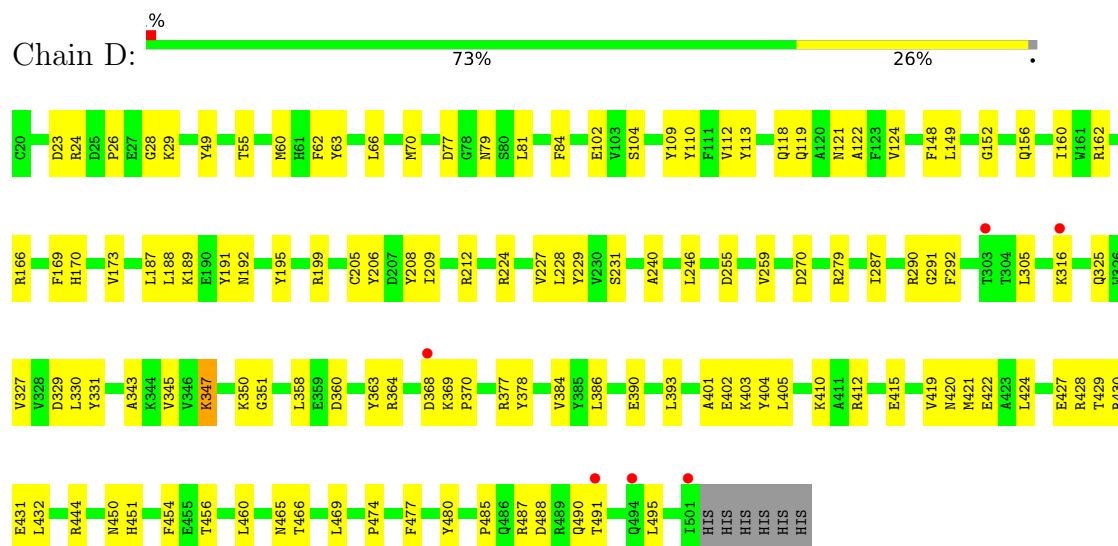
- Molecule 8 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



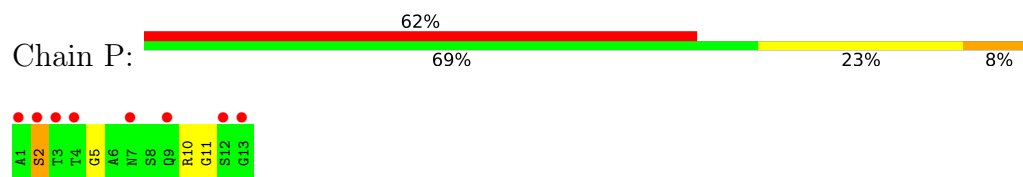
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			14	13	1		
8	D	1	Total	C	O	0	0
			16	15	1		



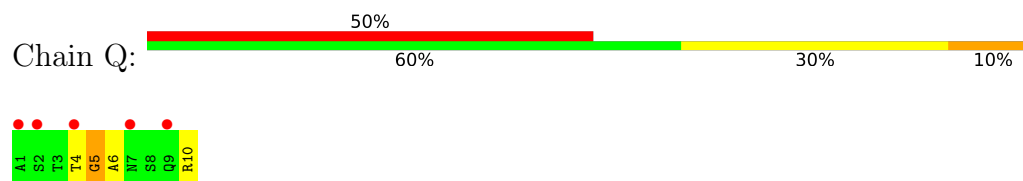
• Molecule 2: Lipoprotein RagB



• Molecule 3: ALA-SER-THR-THR-GLY-ALA-ASN-SER-GLN-ARG-GLY-SER-GLY



• Molecule 4: ALA-SER-THR-THR-GLY-ALA-ASN-SER-GLN-ARG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.60Å 142.02Å 241.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.01 – 3.04 71.01 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.01-3.04) 99.9 (71.01-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.222 , 0.295 0.226 , 0.297	Depositor DCC
R_{free} test set	4357 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.938	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22178	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C8E, 3PE, PLM, LMT

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	0.47	0/7198	0.77	0/9735
1	B	0.47	1/7242 (0.0%)	0.75	0/9794
2	C	0.45	0/3928	0.69	0/5331
2	D	0.44	0/3927	0.70	0/5330
3	P	0.46	0/81	1.02	0/107
4	Q	0.49	0/67	0.84	0/89
All	All	0.46	1/22443 (0.0%)	0.74	0/30386

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	575	ASN	CA-C	-5.02	1.43	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7035	0	6783	249	1
1	B	7069	0	6820	230	1
2	C	3842	0	3739	100	0
2	D	3841	0	3739	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	82	0	77	8	0
4	Q	68	0	66	9	0
5	A	34	0	49	6	0
5	B	34	0	49	2	0
6	A	21	0	34	6	0
6	B	21	0	34	0	0
7	A	26	0	45	2	0
7	B	28	0	28	1	0
7	C	47	0	64	7	0
8	C	14	0	22	3	0
8	D	16	0	26	0	0
All	All	22178	0	21575	636	1

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 15.

All (636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:THR:HG23	2:D:316:LYS:HB2	1.50	0.93
1:A:218:ARG:HD3	1:A:663:GLU:HG2	1.48	0.93
1:A:768:ASN:HB3	1:A:771:TRP:HB2	1.52	0.91
1:B:672:LEU:H	1:B:689:THR:HG22	1.37	0.89
3:P:10:ARG:H	3:P:10:ARG:HD3	1.36	0.89
5:A:1101:3PE:H2A2	7:C:603:LMT:H101	1.56	0.87
1:B:440:THR:CG2	2:D:316:LYS:HB2	2.05	0.87
1:A:917:ALA:HA	1:A:927:VAL:HG23	1.57	0.84
1:B:487:THR:HG23	1:B:516:ASP:HB2	1.59	0.84
1:A:698:GLU:HB2	1:A:731:LEU:HD13	1.60	0.84
2:D:79:ASN:HB3	3:P:5:GLY:HA2	1.60	0.84
1:B:749:VAL:HG11	1:B:790:PHE:HB3	1.59	0.83
1:B:947:LEU:HB3	1:B:984:VAL:HG22	1.58	0.83
2:D:427:GLU:OE1	2:D:430:ARG:NH2	2.12	0.83
1:A:711:ALA:HB3	1:A:716:LEU:HB3	1.60	0.82
4:Q:10:ARG:HD3	4:Q:10:ARG:H	1.46	0.81
1:A:618:PHE:O	1:A:623:ARG:NH1	2.13	0.81
1:A:989:GLY:O	1:A:1002:GLN:NE2	2.15	0.80
1:B:768:ASN:HB3	1:B:771:TRP:HB3	1.62	0.80
1:A:758:ASP:HB3	1:A:780:ASN:HD22	1.46	0.80
1:B:171:SER:HA	1:B:730:MET:HE2	1.64	0.80
1:B:579:LEU:HD13	1:A:573:THR:HG22	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ALA:HB3	1:B:716:LEU:HD23	1.62	0.78
1:B:440:THR:HG23	2:D:316:LYS:CB	2.12	0.78
2:D:121:ASN:OD1	2:D:156:GLN:NE2	2.17	0.78
1:A:472:PRO:HG2	1:A:476:LEU:HD21	1.65	0.78
4:Q:4:THR:O	4:Q:6:ALA:N	2.18	0.77
1:B:433:VAL:HG21	1:B:442:PRO:HB2	1.67	0.77
8:C:601:PLM:HA2	7:C:602:LMT:H102	1.65	0.76
1:A:492:SER:OG	1:A:511:GLU:OE2	2.03	0.76
1:B:458:GLU:HB3	1:A:515:ARG:HH12	1.50	0.76
1:B:577:LEU:HD21	1:A:579:LEU:HD12	1.68	0.76
2:C:79:ASN:HB3	4:Q:5:GLY:HA2	1.67	0.75
1:B:730:MET:HE1	1:B:752:MET:HB2	1.67	0.75
1:B:696:SER:H	1:B:748:ASN:HD21	1.33	0.75
1:A:463:ASN:ND2	1:A:485:ASP:OD1	2.20	0.74
1:A:959:PRO:HG2	1:A:962:LEU:HB2	1.69	0.74
1:B:239:ILE:HG23	1:B:1017:PHE:HB2	1.68	0.73
1:A:947:LEU:HB3	1:A:984:VAL:HG22	1.71	0.72
1:A:641:ILE:HD11	1:A:644:SER:HB2	1.72	0.72
1:A:902:GLY:HA3	1:A:930:LEU:HD12	1.72	0.72
1:B:159:THR:HG21	1:B:398:SER:HB3	1.71	0.72
1:B:784:GLN:HB3	1:B:810:PRO:HB3	1.72	0.71
1:B:543:HIS:CE1	5:B:1101:3PE:H331	2.25	0.71
1:A:749:VAL:HG11	1:A:790:PHE:HB3	1.72	0.71
1:B:917:ALA:HA	1:B:927:VAL:HG23	1.72	0.71
1:B:698:GLU:HB2	1:B:731:LEU:HD13	1.73	0.70
1:B:119:SER:OG	1:B:607:ASP:OD2	2.08	0.70
1:A:815:MET:HE1	1:A:941:LEU:HG	1.73	0.70
1:A:171:SER:HA	1:A:730:MET:HE2	1.72	0.70
1:A:135:VAL:HG12	1:A:137:ASN:H	1.57	0.69
1:B:520:SER:HB2	1:B:546:ILE:HD13	1.74	0.69
1:B:901:ASN:O	1:B:910:LYS:HE2	1.92	0.69
1:A:349:ALA:HB2	1:A:373:LEU:HD13	1.74	0.69
1:B:815:MET:HB2	1:B:856:ILE:HD11	1.73	0.69
1:A:166:ILE:HD12	1:A:222:GLY:HA3	1.74	0.69
2:D:55:THR:HG23	2:D:112:VAL:HG23	1.72	0.69
1:A:459:SER:HG	1:A:489:THR:HG1	1.30	0.68
1:B:981:LEU:HA	1:B:1007:LYS:HD3	1.74	0.68
1:B:251:LEU:HD22	1:B:1005:ASN:O	1.94	0.68
1:A:864:ILE:HB	1:A:887:VAL:HG13	1.76	0.67
1:A:623:ARG:NH2	2:C:23:ASP:OD1	2.27	0.67
1:B:135:VAL:HG22	1:B:137:ASN:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:SER:O	1:A:343:GLN:HB2	1.93	0.67
1:B:490:ARG:NH2	1:A:553:ILE:HG13	2.10	0.67
1:B:618:PHE:O	1:B:623:ARG:NH1	2.27	0.67
2:C:79:ASN:HD22	4:Q:5:GLY:HA2	1.60	0.67
2:C:287:ILE:HG21	2:C:290:ARG:HD3	1.78	0.67
1:B:378:ARG:HD3	1:B:384:LYS:HB2	1.76	0.66
1:B:568:LEU:HB2	1:A:582:HIS:HB2	1.78	0.66
1:A:490:ARG:NH2	1:A:511:GLU:OE1	2.22	0.66
1:A:140:ASP:OD1	1:A:979:ARG:NH1	2.29	0.66
2:C:351:GLY:HA3	2:C:460:LEU:HD11	1.77	0.66
1:A:520:SER:HB2	1:A:546:ILE:HD13	1.78	0.65
2:D:60:MET:HE3	2:D:109:TYR:HA	1.78	0.65
1:A:639:LYS:HB3	1:A:640:PHE:HD1	1.60	0.65
1:B:487:THR:CG2	1:B:516:ASP:HB2	2.25	0.65
1:B:898:PHE:HD1	1:B:905:LEU:HD13	1.61	0.65
1:A:672:LEU:HB2	1:A:689:THR:HG22	1.79	0.65
1:A:167:HIS:NE2	1:A:758:ASP:OD2	2.28	0.65
2:D:228:LEU:HD13	2:D:292:PHE:HB2	1.79	0.65
8:C:601:PLM:H31	7:C:603:LMT:H12	1.77	0.65
1:A:538:THR:HB	1:A:597:ASN:HB2	1.78	0.65
1:A:918:TRP:NE1	1:A:923:LYS:HG3	2.11	0.65
1:A:1015:LEU:HD23	1:A:1017:PHE:HZ	1.63	0.64
2:C:186:ILE:HD11	2:C:495:LEU:HD12	1.80	0.64
1:B:239:ILE:HD12	1:B:338:PHE:CE2	2.32	0.64
1:A:274:PHE:O	2:C:465:ASN:ND2	2.31	0.64
1:B:572:LYS:HD2	1:A:680:GLU:O	1.99	0.63
2:D:420:ASN:O	2:D:422:GLU:N	2.31	0.63
1:A:1000:LYS:O	1:A:1002:GLN:N	2.31	0.63
1:A:491:THR:HG22	1:A:512:ARG:HB2	1.80	0.63
1:B:433:VAL:HG21	1:B:442:PRO:CB	2.28	0.63
2:C:474:PRO:HD2	2:C:477:PHE:HB2	1.79	0.63
1:B:461:GLN:OE1	1:B:487:THR:HB	1.99	0.63
1:B:457:SER:HB2	1:B:491:THR:HG22	1.81	0.63
1:B:508:GLU:HB3	1:B:558:LYS:HB3	1.81	0.63
2:C:239:ARG:NE	2:C:255:ASP:OD2	2.25	0.63
2:D:386:LEU:HD13	2:D:428:ARG:HG3	1.79	0.62
1:B:138:ILE:HD12	1:B:197:PRO:HB3	1.79	0.62
1:A:526:GLU:HG3	1:A:540:LEU:HB2	1.82	0.62
1:B:768:ASN:O	1:B:768:ASN:ND2	2.33	0.62
1:B:623:ARG:NH2	2:D:23:ASP:OD1	2.30	0.62
1:A:154:THR:HA	1:A:994:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:HIS:CD2	5:A:1101:3PE:H331	2.36	0.61
2:D:26:PRO:HG2	2:D:29:LYS:HB2	1.83	0.61
1:B:736:MET:HE3	1:B:745:GLN:HB3	1.82	0.61
1:A:797:MET:O	2:C:490:GLN:HG2	2.01	0.61
1:B:611:ARG:NH1	1:B:613:ASP:OD2	2.34	0.60
1:A:603:TRP:CD2	1:A:639:LYS:HG3	2.37	0.60
1:B:573:THR:HG22	1:A:579:LEU:HD11	1.83	0.60
1:A:325:LEU:HD12	1:A:414:VAL:HG12	1.82	0.60
2:C:275:GLU:HG3	2:C:340:VAL:HG13	1.84	0.60
2:D:122:ALA:HB2	2:D:191:TYR:CG	2.37	0.60
1:B:898:PHE:HE1	3:P:5:GLY:HA3	1.66	0.60
1:A:519:LYS:HE3	1:A:547:GLU:OE2	2.01	0.60
1:A:968:VAL:HG13	1:A:969:ILE:HG13	1.83	0.60
2:D:66:LEU:HD13	2:D:81:LEU:HD22	1.83	0.60
1:B:157:ASP:OD1	1:B:159:THR:HG22	2.01	0.60
1:A:603:TRP:CG	1:A:639:LYS:HG3	2.36	0.60
1:B:393:ILE:HG13	6:A:1102:C8E:H41	1.84	0.60
2:C:390:GLU:OE1	2:C:444:ARG:NH2	2.35	0.60
1:B:737:PRO:HB2	1:B:739:ILE:HG12	1.84	0.59
1:B:134:PRO:HB2	1:B:1008:GLN:CD	2.27	0.59
1:B:647:LEU:HD21	1:B:650:LEU:HB2	1.84	0.59
1:B:285:LYS:HG2	1:B:315:PHE:CD2	2.38	0.59
1:B:974:VAL:HG22	1:B:1013:ILE:HG13	1.84	0.59
2:C:51:LEU:HD21	2:C:115:ARG:HG2	1.84	0.59
1:A:639:LYS:HB3	1:A:640:PHE:CD1	2.37	0.59
2:C:451:HIS:HB3	2:C:469:LEU:HD11	1.84	0.59
1:B:134:PRO:HG3	1:B:1010:VAL:HG21	1.86	0.58
1:A:139:MET:HE1	1:A:224:VAL:HG11	1.85	0.58
1:A:896:ARG:NH2	1:A:939:HIS:O	2.36	0.58
2:D:368:ASP:HB3	2:D:369:LYS:HD2	1.85	0.58
1:B:425:ASP:OD1	1:B:427:ASN:N	2.27	0.58
1:B:378:ARG:NH1	1:B:380:ASN:O	2.36	0.58
1:A:251:LEU:HD22	1:A:1005:ASN:O	2.02	0.58
1:A:784:GLN:HB3	1:A:810:PRO:HB3	1.86	0.58
2:C:469:LEU:HD23	2:C:472:GLN:HA	1.85	0.58
1:A:462:ALA:HB2	6:A:1102:C8E:H102	1.85	0.58
1:A:486:ILE:HG12	1:A:517:VAL:HG13	1.84	0.58
2:C:237:ALA:HB1	2:C:379:PHE:CE1	2.39	0.58
2:D:451:HIS:HB3	2:D:469:LEU:HD11	1.86	0.58
1:B:149:MET:HE2	1:B:164:VAL:HG11	1.85	0.58
1:A:546:ILE:HB	1:A:589:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ASP:OD1	1:A:744:SER:HB3	2.03	0.58
1:B:603:TRP:CD2	1:B:639:LYS:HG3	2.39	0.58
1:A:917:ALA:HA	1:A:927:VAL:CG2	2.30	0.57
2:D:405:LEU:HD11	2:D:427:GLU:HG2	1.84	0.57
1:B:261:THR:OG1	1:B:264:GLU:HB2	2.03	0.57
1:B:649:ASP:HB3	1:B:710:GLY:N	2.19	0.57
2:D:390:GLU:HB2	2:D:424:LEU:HD11	1.86	0.57
1:A:451:LYS:HE3	1:A:452:MET:HE2	1.86	0.57
1:B:216:GLY:O	1:B:218:ARG:N	2.36	0.57
1:B:963:PHE:CE2	1:B:971:GLY:HA2	2.40	0.57
1:A:355:ASP:OD2	1:A:367:LYS:HE3	2.04	0.57
1:A:182:VAL:HG22	1:A:226:ILE:HB	1.87	0.57
1:A:416:THR:HB	1:A:908:LEU:HB3	1.85	0.56
1:B:167:HIS:NE2	1:B:758:ASP:OD2	2.30	0.56
1:B:901:ASN:HB2	1:B:934:PRO:HD3	1.88	0.56
5:B:1101:3PE:H222	5:B:1101:3PE:O31	2.05	0.56
1:A:486:ILE:HD12	6:A:1102:C8E:H81	1.87	0.56
1:A:738:TYR:CZ	2:C:98:ALA:HB3	2.41	0.56
1:B:188:SER:O	1:B:192:VAL:HG23	2.06	0.56
1:A:797:MET:HG3	1:A:814:TYR:CD2	2.39	0.56
1:B:614:GLN:HA	1:B:623:ARG:O	2.05	0.56
1:A:382:TRP:O	1:A:471:THR:N	2.36	0.56
1:A:898:PHE:HD1	1:A:905:LEU:HD13	1.69	0.56
1:B:687:ILE:HB	2:D:119:GLN:NE2	2.21	0.56
1:B:573:THR:HG22	1:A:579:LEU:CD1	2.36	0.56
1:A:985:THR:HG21	1:A:992:PRO:HG3	1.88	0.56
1:A:496:MET:HE3	1:A:497:PRO:HD2	1.88	0.56
1:B:751:SER:OG	1:B:787:THR:HB	2.06	0.55
1:B:985:THR:HG21	1:B:992:PRO:HG3	1.87	0.55
1:A:508:GLU:HG2	1:A:558:LYS:HB3	1.87	0.55
2:C:152:GLY:O	2:C:156:GLN:HG3	2.06	0.55
1:B:907:GLN:NE2	2:D:77:ASP:O	2.40	0.55
1:A:893:ASN:HD22	1:A:896:ARG:HD3	1.72	0.55
1:A:918:TRP:HE1	1:A:923:LYS:HG3	1.70	0.55
2:D:70:MET:HE3	2:D:429:THR:HG23	1.89	0.55
1:B:649:ASP:HB3	1:B:710:GLY:H	1.72	0.55
1:B:675:VAL:HG21	1:A:570:GLN:HB3	1.89	0.55
1:A:250:ILE:HG13	1:A:359:MET:HE1	1.89	0.55
1:A:730:MET:HE1	1:A:752:MET:SD	2.47	0.55
1:B:480:ALA:HA	1:B:523:ASN:HB3	1.87	0.55
1:B:855[B]:ARG:NH1	1:B:857:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:HA3	1:A:211:ALA:HB2	1.88	0.54
2:C:236:TYR:CZ	2:C:258:MET:HG2	2.42	0.54
2:D:259:VAL:HG13	2:D:384:VAL:HG11	1.89	0.54
1:B:484:VAL:HG12	1:B:485:ASP:H	1.72	0.54
1:B:672:LEU:H	1:B:689:THR:CG2	2.16	0.54
1:A:823:LYS:HE2	1:A:824:LYS:HG3	1.89	0.54
1:A:830:TRP:CZ3	1:A:848:TYR:HB2	2.42	0.54
2:D:124:VAL:HG13	2:D:149:LEU:HD11	1.89	0.54
1:B:573:THR:O	1:B:573:THR:OG1	2.19	0.54
1:A:508:GLU:HG2	1:A:558:LYS:CB	2.37	0.54
1:A:567:LEU:HD22	2:D:28:GLY:HA3	1.90	0.54
2:C:118:GLN:HE22	2:C:192:ASN:H	1.56	0.54
1:B:228:THR:OG1	1:B:374:ASN:ND2	2.40	0.54
1:A:650:LEU:HD21	1:A:707:LEU:HD21	1.89	0.54
1:B:797:MET:O	2:D:490:GLN:HG2	2.07	0.54
1:A:433:VAL:HG21	1:A:442:PRO:HB2	1.90	0.54
1:A:166:ILE:HG21	1:A:207:LYS:HB3	1.90	0.54
1:B:150:GLN:HA	1:B:865:THR:HG21	1.90	0.54
1:B:440:THR:HG21	2:D:316:LYS:HB2	1.87	0.54
1:A:486:ILE:HG23	1:A:517:VAL:HG22	1.89	0.54
2:C:402:GLU:HA	2:C:419:VAL:HG11	1.90	0.54
1:B:166:ILE:HD12	1:B:222:GLY:HA3	1.90	0.54
1:B:278:ASN:O	1:B:278:ASN:ND2	2.41	0.54
1:B:577:LEU:HD21	1:A:579:LEU:CD1	2.36	0.54
1:B:822:ASP:HB2	1:B:829:LEU:HD21	1.89	0.54
2:C:26:PRO:HG2	2:C:29:LYS:HB2	1.88	0.54
2:C:122:ALA:HB2	2:C:191:TYR:CG	2.43	0.54
1:A:637:TYR:HA	1:A:641:ILE:HG23	1.90	0.53
2:C:55:THR:HG23	2:C:112:VAL:HG23	1.90	0.53
1:B:242:ASN:O	1:B:334:GLY:HA2	2.08	0.53
1:B:407:MET:HE1	1:B:908:LEU:HD23	1.90	0.53
1:B:770:ASP:OD1	1:B:770:ASP:N	2.41	0.53
1:A:524:THR:HB	1:A:540:LEU:HD11	1.90	0.53
2:D:279:ARG:NH1	2:D:358:LEU:HB3	2.23	0.53
1:B:406:TYR:CD1	3:P:2:SER:HB2	2.43	0.53
1:A:484:VAL:HG22	7:A:1104:LMT:H82	1.90	0.53
1:B:553:ILE:HG13	1:A:490:ARG:NH2	2.23	0.53
1:A:947:LEU:HB3	1:A:984:VAL:CG2	2.38	0.53
2:C:70:MET:CE	2:C:429:THR:HG23	2.39	0.53
1:A:216:GLY:O	1:A:218:ARG:N	2.39	0.53
1:A:382:TRP:HD1	1:A:470:ILE:HG23	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:GLN:HG3	2:D:329:ASP:OD2	2.09	0.53
1:B:898:PHE:CE1	3:P:5:GLY:HA3	2.44	0.53
2:D:102:GLU:OE2	2:D:104:SER:OG	2.19	0.53
1:B:603:TRP:CZ3	1:B:639:LYS:HE3	2.44	0.53
2:C:346:VAL:HG22	2:C:353:LEU:HD23	1.91	0.53
1:B:749:VAL:CG1	1:B:790:PHE:HB3	2.37	0.52
1:A:725:ARG:HB3	1:A:754:ASN:HB2	1.90	0.52
2:D:390:GLU:OE1	2:D:444:ARG:NH2	2.41	0.52
1:B:151:VAL:HG12	1:B:164:VAL:HG13	1.91	0.52
2:D:189:LYS:HE2	2:D:208:TYR:CD1	2.44	0.52
2:C:63:TYR:HB3	2:C:84:PHE:CE1	2.44	0.52
2:D:393:LEU:HG	2:D:401:ALA:HB1	1.91	0.52
7:C:602:LMT:O3'	7:C:602:LMT:H1B	2.09	0.52
1:B:166:ILE:HG21	1:B:207:LYS:HB3	1.92	0.52
1:A:482:ALA:HB1	7:A:1104:LMT:H92	1.92	0.52
1:A:673:VAL:HG11	1:A:685:LEU:HD22	1.92	0.52
4:Q:10:ARG:H	4:Q:10:ARG:CD	2.21	0.52
1:A:667:TYR:CG	2:C:26:PRO:HB3	2.45	0.52
1:A:768:ASN:C	1:A:770:ASP:H	2.17	0.52
1:A:147:ALA:HB1	1:A:758:ASP:HB2	1.92	0.51
1:A:280:THR:HG23	1:A:283:LYS:H	1.74	0.51
1:A:901:ASN:HB3	1:A:934:PRO:HG3	1.90	0.51
2:D:192:ASN:ND2	2:D:195:TYR:HB2	2.25	0.51
1:B:120:GLY:HA3	1:B:211:ALA:HB2	1.92	0.51
1:B:470:ILE:HG22	1:B:472:PRO:HD3	1.91	0.51
1:B:833:PRO:HD3	1:B:852:LEU:HD12	1.92	0.51
1:B:948:ARG:NH2	1:B:991:ASP:OD1	2.39	0.51
1:A:953:LYS:HG3	1:A:977:MET:HG3	1.92	0.51
2:D:152:GLY:O	2:D:156:GLN:HG3	2.11	0.51
1:B:406:TYR:HA	3:P:2:SER:HA	1.94	0.50
1:A:611:ARG:NH1	1:A:613:ASP:OD1	2.44	0.50
1:B:751:SER:HG	1:B:787:THR:HB	1.76	0.50
1:A:783:ARG:NH2	1:A:810:PRO:HD3	2.26	0.50
1:B:495:ARG:NH2	1:B:502:ASP:OD1	2.45	0.50
1:A:901:ASN:O	1:A:910:LYS:HE2	2.12	0.50
1:A:989:GLY:O	1:A:990:PHE:HB2	2.12	0.50
1:B:239:ILE:HD12	1:B:338:PHE:HE2	1.73	0.50
1:B:378:ARG:HH22	1:B:381:GLU:HA	1.75	0.50
1:A:261:THR:OG1	1:A:264:GLU:HB2	2.11	0.50
1:A:898:PHE:CD1	1:A:905:LEU:HD13	2.46	0.50
2:D:166:ARG:NH2	2:D:480:TYR:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ARG:HH21	2:D:370:PRO:HB3	1.76	0.50
1:A:815:MET:CE	1:A:941:LEU:HG	2.40	0.50
2:C:160:ILE:HG22	2:C:209:ILE:HD11	1.94	0.50
1:B:412:PHE:CE2	1:B:416:THR:HG21	2.46	0.50
1:A:170:GLY:C	1:A:752:MET:HE1	2.37	0.50
2:C:67:GLN:HA	2:C:84:PHE:O	2.12	0.50
2:C:224:ARG:NH1	2:C:227:VAL:HG23	2.27	0.50
1:A:323:LYS:O	1:A:361:ARG:NH2	2.45	0.50
2:D:224:ARG:HG3	2:D:231:SER:HB3	1.94	0.50
1:B:611:ARG:HH12	1:B:613:ASP:CG	2.20	0.50
2:D:474:PRO:HD2	2:D:477:PHE:HB2	1.93	0.50
1:A:713:ASN:H	1:A:715:ARG:HG2	1.77	0.49
1:A:901:ASN:HB2	1:A:934:PRO:HD3	1.94	0.49
2:C:95:HIS:O	2:C:106:ILE:HB	2.12	0.49
2:C:501:ILE:HD12	2:C:501:ILE:H	1.76	0.49
1:B:696:SER:OG	1:B:697:TRP:N	2.44	0.49
2:D:169:PHE:HB3	2:D:173:VAL:HG11	1.94	0.49
1:B:206:LEU:HB2	1:B:223:VAL:HG22	1.93	0.49
1:B:345:THR:HA	1:B:376:GLU:O	2.12	0.49
1:A:586:GLU:HG2	1:A:667:TYR:OH	2.12	0.49
2:D:287:ILE:HG21	2:D:290:ARG:HD3	1.94	0.49
2:D:456:THR:HG23	2:D:466:THR:HG22	1.94	0.49
1:A:883:PHE:CE2	1:A:949:LEU:HD13	2.48	0.49
2:C:360:ASP:HB3	2:C:363:TYR:CD2	2.47	0.49
1:B:917:ALA:CB	1:B:930:LEU:HD23	2.42	0.49
1:B:730:MET:CE	1:B:752:MET:HB2	2.41	0.49
2:C:169:PHE:HB3	2:C:173:VAL:HG11	1.95	0.49
1:A:885:TYR:O	1:A:886:ILE:HG13	2.12	0.49
1:B:378:ARG:HH12	1:B:380:ASN:C	2.20	0.49
2:C:420:ASN:O	2:C:422:GLU:N	2.46	0.49
1:B:830:TRP:CH2	1:B:848:TYR:HB2	2.48	0.48
1:B:947:LEU:HB3	1:B:984:VAL:CG2	2.37	0.48
1:B:169:THR:OG1	1:B:861:THR:HG21	2.13	0.48
1:B:565:LEU:HD13	1:A:675:VAL:HG12	1.95	0.48
1:B:730:MET:HE1	1:B:752:MET:SD	2.53	0.48
1:B:734:VAL:HG22	1:B:745:GLN:O	2.13	0.48
2:D:122:ALA:HB2	2:D:191:TYR:HB2	1.95	0.48
2:D:421:MET:HA	2:D:424:LEU:HB3	1.93	0.48
1:B:263:ASP:OD1	1:B:263:ASP:N	2.44	0.48
1:B:355:ASP:OD1	1:B:367:LYS:HE2	2.12	0.48
1:B:528:LYS:HB3	1:B:538:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1101:3PE:H282	7:C:603:LMT:H92	1.95	0.48
1:B:770:ASP:O	1:B:771:TRP:HB2	2.12	0.48
1:A:354:PHE:HB3	1:A:368:ARG:HG2	1.95	0.48
1:A:575:ASN:HB2	2:C:365:ASP:HA	1.94	0.48
2:C:239:ARG:HH21	2:C:255:ASP:CG	2.18	0.48
1:A:218:ARG:HD3	1:A:663:GLU:CG	2.33	0.48
2:C:236:TYR:CE2	2:C:258:MET:HG2	2.49	0.48
1:B:848:TYR:CE2	1:B:935:GLN:HG2	2.49	0.48
1:B:472:PRO:HG2	1:B:476:LEU:HD23	1.94	0.48
2:C:239:ARG:NH2	2:C:255:ASP:OD1	2.40	0.48
2:C:344:LYS:HB2	2:C:352:TYR:CE2	2.48	0.48
1:B:901:ASN:OD1	1:B:904:GLY:N	2.44	0.48
1:A:440:THR:OG1	2:C:316:LYS:HB3	2.14	0.48
2:D:62:PHE:CE1	2:D:305:LEU:HD22	2.49	0.48
2:C:97:ARG:HH21	2:C:99:ASP:CG	2.20	0.48
1:A:882:ASP:O	1:A:950:LYS:N	2.46	0.47
1:B:622:ASN:HB3	1:B:696:SER:HB2	1.96	0.47
1:B:672:LEU:HD22	2:D:29:LYS:HB3	1.95	0.47
1:A:166:ILE:HG13	1:A:178:PRO:HG3	1.95	0.47
2:C:79:ASN:CB	4:Q:5:GLY:HA2	2.41	0.47
1:B:326:PHE:HD2	1:B:359:MET:HE2	1.78	0.47
1:B:795:LYS:HA	1:B:805:TRP:O	2.15	0.47
1:A:778:ASN:HD22	1:A:867:GLY:N	2.12	0.47
1:B:296:TYR:HE2	1:B:310:LEU:HD23	1.79	0.47
1:B:740:SER:C	2:D:118:GLN:HG3	2.39	0.47
1:A:614:GLN:HA	1:A:623:ARG:O	2.15	0.47
2:D:110:TYR:CD2	2:D:485:PRO:HG2	2.49	0.47
1:B:149:MET:CE	1:B:164:VAL:HG11	2.44	0.47
1:B:485:ASP:HB3	1:B:518:SER:HB2	1.96	0.47
1:A:526:GLU:HB2	1:A:540:LEU:HD13	1.95	0.47
1:B:143:GLN:HA	1:B:151:VAL:HG22	1.95	0.47
1:B:203:MET:HE2	1:B:226:ILE:HG12	1.97	0.47
1:B:233:MET:HG2	1:B:342:SER:H	1.80	0.47
1:A:232:LYS:O	1:A:234:SER:N	2.46	0.47
1:A:480:ALA:HA	1:A:523:ASN:HB3	1.96	0.47
1:A:749:VAL:CG1	1:A:790:PHE:HB3	2.42	0.47
1:A:830:TRP:CH2	1:A:848:TYR:HB2	2.49	0.47
1:A:382:TRP:CD1	1:A:470:ILE:HG23	2.50	0.47
2:C:383:GLU:O	2:C:387:ILE:HG13	2.15	0.47
2:D:270:ASP:OD1	2:D:270:ASP:N	2.48	0.47
2:D:369:LYS:HD2	2:D:369:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ALA:CB	1:B:716:LEU:HD23	2.39	0.47
1:A:236:ARG:NH2	1:A:238:ARG:HG3	2.30	0.47
1:A:963:PHE:CE2	1:A:971:GLY:HA2	2.50	0.47
5:A:1101:3PE:H341	8:C:601:PLM:HA1	1.96	0.47
2:C:170:HIS:O	2:C:173:VAL:HG12	2.15	0.47
1:B:537:LEU:HG	1:B:538:THR:N	2.30	0.47
1:B:896:ARG:NE	1:B:900:GLU:OE2	2.41	0.47
1:A:344:GLY:O	1:A:377:SER:HA	2.15	0.47
1:A:345:THR:HA	1:A:376:GLU:O	2.15	0.47
7:B:1103:LMT:H5B	7:B:1103:LMT:H6D	1.97	0.46
1:A:603:TRP:CD1	1:A:639:LYS:HG3	2.50	0.46
1:A:765:ILE:HB	1:A:773:VAL:HB	1.98	0.46
2:D:24:ARG:HA	2:D:24:ARG:HD3	1.79	0.46
2:D:124:VAL:HG21	2:D:156:GLN:OE1	2.15	0.46
1:B:856:ILE:C	1:B:858:LYS:H	2.23	0.46
1:A:157:ASP:OD1	1:A:159:THR:OG1	2.30	0.46
1:A:343:GLN:HB3	1:A:344:GLY:H	1.53	0.46
1:A:982:LEU:HD23	1:A:982:LEU:HA	1.65	0.46
2:C:63:TYR:HB3	2:C:84:PHE:CZ	2.50	0.46
2:D:206:TYR:CZ	2:D:246:LEU:HD11	2.51	0.46
1:A:326:PHE:CD1	1:A:360:ALA:HA	2.50	0.46
2:C:77:ASP:HB2	2:C:320:SER:HB3	1.97	0.46
2:C:173:VAL:HA	2:C:476:GLY:HA2	1.98	0.46
2:D:170:HIS:O	2:D:173:VAL:HG12	2.15	0.46
1:A:180:TYR:O	1:A:181:ILE:HD13	2.16	0.46
2:C:79:ASN:HB3	4:Q:5:GLY:CA	2.43	0.46
2:C:118:GLN:O	2:C:121:ASN:HB2	2.14	0.46
2:C:336:PHE:CD1	2:C:336:PHE:N	2.81	0.46
2:D:160:ILE:HG22	2:D:209:ILE:HD11	1.97	0.46
1:B:981:LEU:HD12	1:B:982:LEU:N	2.31	0.46
1:B:982:LEU:HA	1:B:982:LEU:HD23	1.76	0.46
1:A:768:ASN:C	1:A:770:ASP:N	2.74	0.46
1:A:783:ARG:HH21	1:A:810:PRO:HD3	1.80	0.46
1:B:565:LEU:HD12	1:A:683:MET:HE1	1.98	0.46
1:B:582:HIS:HB2	1:A:568:LEU:HB2	1.97	0.46
1:B:889:LYS:HG2	1:B:944:ALA:HB3	1.98	0.46
1:B:953:LYS:HG3	1:B:977:MET:HG3	1.98	0.46
1:A:201:GLU:N	1:A:227:GLN:O	2.45	0.46
1:A:321:TRP:CZ2	1:A:417:MET:HE2	2.51	0.46
2:D:113:TYR:CE1	2:D:162:ARG:HG3	2.51	0.46
2:D:224:ARG:HD2	2:D:227:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:HA	1:A:526:GLU:O	2.16	0.45
1:A:587:TYR:HB3	1:A:666:ASN:OD1	2.15	0.45
1:A:698:GLU:HG3	1:A:730:MET:HA	1.97	0.45
1:A:866:GLY:HA3	1:A:885:TYR:CZ	2.50	0.45
1:B:812:SER:OG	1:B:855[B]:ARG:NH2	2.49	0.45
1:B:968:VAL:HG13	1:B:969:ILE:HG22	1.97	0.45
1:B:280:THR:O	1:B:284:VAL:HG23	2.16	0.45
2:D:364:ARG:NH2	2:D:370:PRO:HB3	2.31	0.45
1:A:798:LEU:HD21	1:A:805:TRP:CZ2	2.51	0.45
1:A:950:LYS:HA	1:A:950:LYS:HD3	1.64	0.45
1:B:133:LYS:HA	1:B:134:PRO:HD3	1.86	0.45
1:B:648:SER:OG	1:B:712:PHE:O	2.34	0.45
1:B:740:SER:O	2:D:118:GLN:HG3	2.17	0.45
1:A:771:TRP:CE2	1:A:874:TRP:HD1	2.35	0.45
2:C:451:HIS:HE1	2:C:467:THR:O	1.98	0.45
1:B:117:THR:HG22	1:B:211:ALA:HA	1.99	0.45
1:B:276:GLY:H	2:D:465:ASN:CG	2.25	0.45
1:B:425:ASP:OD1	1:B:426:VAL:N	2.50	0.45
1:B:520:SER:CB	1:B:546:ILE:HD13	2.43	0.45
1:A:883:PHE:CZ	1:A:949:LEU:HD13	2.51	0.45
5:A:1101:3PE:H321	7:C:603:LMT:H52	1.98	0.45
1:B:251:LEU:HA	1:B:1007:LYS:HE2	1.98	0.45
1:B:413:GLY:HA2	1:B:416:THR:HG22	1.99	0.45
1:B:453:ARG:NE	1:B:495:ARG:HG3	2.32	0.45
1:A:265:LEU:HD23	1:A:418:PRO:HB3	1.97	0.45
1:A:701:SER:N	1:A:726:THR:O	2.49	0.45
1:A:708:ALA:HB2	1:A:719:GLU:HG3	1.97	0.45
2:C:49:TYR:CE2	2:C:229:TYR:HA	2.52	0.45
2:C:358:LEU:HG	2:C:359:GLU:HG2	1.99	0.45
2:D:240:ALA:HB2	2:D:255:ASP:HB2	1.98	0.45
2:D:327:VAL:O	2:D:330:LEU:HB2	2.17	0.45
1:B:263:ASP:HA	1:B:266:LEU:HB2	1.97	0.45
1:B:458:GLU:HB3	1:A:515:ARG:NH1	2.26	0.45
1:A:135:VAL:HG21	1:A:979:ARG:CZ	2.47	0.45
1:A:575:ASN:CB	2:C:365:ASP:HA	2.47	0.45
1:A:730:MET:HE1	1:A:752:MET:HB2	1.99	0.45
1:A:799:PRO:O	1:A:801:THR:HG23	2.16	0.45
2:D:402:GLU:HA	2:D:419:VAL:HG21	1.99	0.45
1:B:417:MET:HE1	1:B:436:MET:SD	2.57	0.44
2:C:206:TYR:CE1	2:C:246:LEU:HD11	2.51	0.44
1:B:259:MET:HE1	1:B:899:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:OE1	1:A:912:LYS:NZ	2.47	0.44
2:D:49:TYR:CE2	2:D:229:TYR:HA	2.52	0.44
1:B:233:MET:HA	1:B:341:GLY:HA3	2.00	0.44
1:A:727:THR:HG22	1:A:730:MET:HB2	1.99	0.44
1:A:823:LYS:HD3	1:A:823:LYS:N	2.32	0.44
1:A:948:ARG:HH21	1:A:993:GLU:HB2	1.82	0.44
1:B:978:ALA:HA	1:B:1008:GLN:O	2.17	0.44
2:C:110:TYR:CD2	2:C:485:PRO:HG2	2.52	0.44
2:D:279:ARG:CZ	2:D:358:LEU:HB3	2.48	0.44
1:B:484:VAL:HG12	1:B:485:ASP:N	2.32	0.44
1:B:815:MET:O	1:B:854:THR:N	2.47	0.44
1:A:597:ASN:ND2	1:A:607:ASP:OD1	2.48	0.44
1:A:698:GLU:OE2	1:A:700:GLN:NE2	2.41	0.44
1:A:738:TYR:HB2	2:C:110:TYR:HE2	1.81	0.44
5:A:1101:3PE:H241	7:C:603:LMT:H41	1.99	0.44
2:C:315:ILE:HD13	2:C:358:LEU:HD11	1.99	0.44
2:D:199:ARG:HG3	2:D:495:LEU:HD12	2.00	0.44
1:B:380:ASN:C	1:B:382:TRP:H	2.25	0.44
1:B:891:MET:HE1	1:B:999:GLY:HA3	1.99	0.44
1:B:627:PHE:HB3	1:B:658:THR:O	2.18	0.44
1:A:752:MET:HB3	1:A:752:MET:HE2	1.67	0.44
2:C:157:ALA:HB1	2:C:209:ILE:HG23	2.00	0.44
1:B:274:PHE:CD1	1:B:906:MET:HB2	2.53	0.44
1:B:591:SER:OG	1:B:613:ASP:OD1	2.36	0.44
1:A:197:PRO:HA	1:A:200:PHE:CD2	2.53	0.44
1:A:789:LEU:HB3	1:A:790:PHE:H	1.63	0.44
2:C:347:LYS:O	2:C:349:ASP:N	2.48	0.44
1:A:142:LEU:O	1:A:143:GLN:C	2.61	0.44
1:A:151:VAL:HG12	1:A:164:VAL:HG13	2.00	0.44
1:A:673:VAL:CG1	1:A:685:LEU:HD22	2.48	0.44
1:A:738:TYR:HB2	2:C:110:TYR:CE2	2.53	0.44
2:D:351:GLY:HA3	2:D:460:LEU:HD21	1.98	0.44
1:B:696:SER:N	1:B:748:ASN:HD21	2.09	0.43
1:B:848:TYR:CD2	1:B:935:GLN:HG2	2.53	0.43
1:B:891:MET:HB3	1:B:891:MET:HE2	1.57	0.43
1:A:199:ASP:HB3	1:A:372:ARG:HD2	1.99	0.43
1:A:534:LYS:O	1:A:600:PHE:HA	2.18	0.43
1:A:662:SER:O	1:A:664:ILE:N	2.51	0.43
1:B:555:ALA:HB2	1:A:555:ALA:HB2	2.00	0.43
1:B:651:ARG:HE	1:B:651:ARG:HB2	1.60	0.43
1:A:292:ALA:HB2	1:A:435:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:SER:HB3	1:A:882:ASP:HA	2.00	0.43
2:D:110:TYR:HE2	2:D:488:ASP:OD2	2.02	0.43
1:A:739:ILE:HA	2:C:114:ASN:OD1	2.18	0.43
2:C:337:ARG:HH22	2:C:427:GLU:CD	2.26	0.43
1:B:220:ALA:O	1:B:725:ARG:NH2	2.49	0.43
1:B:267:ASP:OD2	1:B:271:LYS:NZ	2.39	0.43
1:B:683:MET:HE1	1:A:565:LEU:HD12	2.00	0.43
2:C:48:LEU:HD12	2:C:48:LEU:HA	1.86	0.43
2:C:156:GLN:NE2	2:C:208:TYR:OH	2.51	0.43
2:D:410:LYS:HB2	2:D:415:GLU:HB2	2.00	0.43
2:D:412:ARG:HH21	2:D:431:GLU:CD	2.26	0.43
2:D:450:ASN:HB2	2:D:454:PHE:CZ	2.53	0.43
1:B:241:PHE:HD1	1:B:336:ILE:HD13	1.84	0.43
1:B:574:GLY:C	1:B:576:SER:H	2.26	0.43
1:A:835:GLN:HB3	1:A:843:VAL:HG21	2.00	0.43
2:D:63:TYR:HB3	2:D:84:PHE:CE1	2.54	0.43
2:D:122:ALA:HB2	2:D:191:TYR:CB	2.49	0.43
2:D:403:LYS:HD3	2:D:404:TYR:CE1	2.53	0.43
1:B:568:LEU:HD22	1:A:553:ILE:CD1	2.49	0.43
1:B:791:PHE:N	1:B:791:PHE:CD1	2.86	0.43
1:B:972:ALA:C	1:B:973:ARG:HG3	2.43	0.43
1:B:299:TYR:O	1:B:303:LYS:N	2.48	0.43
2:D:347:LYS:HD2	2:D:350:LYS:HD2	2.01	0.43
1:B:327:LYS:HD2	1:B:328:THR:O	2.19	0.43
1:B:640:PHE:C	1:B:641:ILE:HG13	2.43	0.43
1:A:156:GLY:HA3	1:A:1004:PRO:O	2.19	0.43
2:C:177:ASN:HB2	2:C:499:TRP:O	2.18	0.43
1:A:460:HIS:HB3	6:A:1102:C8E:H131	2.00	0.43
1:A:529:PHE:CZ	1:A:537:LEU:HD13	2.53	0.43
1:A:906:MET:SD	1:A:910:LYS:NZ	2.91	0.43
1:A:974:VAL:HG22	1:A:1013:ILE:HD12	2.00	0.43
2:C:325:GLN:HG3	2:C:329:ASP:OD2	2.19	0.43
1:A:484:VAL:HG12	1:A:485:ASP:H	1.84	0.43
1:A:520:SER:CB	1:A:546:ILE:HD13	2.47	0.43
2:C:452:ASP:OD1	2:C:468:PRO:HA	2.19	0.42
2:D:331:TYR:CE1	2:D:430:ARG:HB3	2.54	0.42
1:A:140:ASP:CG	1:A:979:ARG:HH12	2.27	0.42
1:A:976:LEU:HD13	1:A:976:LEU:HA	1.85	0.42
1:A:300:ASP:HA	1:A:303:LYS:HD2	2.01	0.42
1:A:683:MET:HE3	1:A:685:LEU:HD21	2.01	0.42
1:A:786:ILE:HG21	1:A:789:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ILE:N	1:A:812:SER:O	2.50	0.42
1:A:916:ASN:O	1:A:925:THR:HG21	2.19	0.42
2:C:79:ASN:ND2	4:Q:5:GLY:HA2	2.28	0.42
2:C:240:ALA:HB2	2:C:255:ASP:HB2	2.00	0.42
3:P:10:ARG:HD3	3:P:10:ARG:N	2.19	0.42
1:B:325:LEU:HD12	1:B:414:VAL:HG12	2.01	0.42
1:B:786:ILE:HG21	1:B:789:LEU:CD1	2.49	0.42
1:A:239:ILE:HD13	1:A:239:ILE:HG21	1.75	0.42
2:C:124:VAL:HG21	2:C:156:GLN:OE1	2.19	0.42
2:C:128:GLU:HG3	2:C:149:LEU:HD11	2.00	0.42
1:B:243:ALA:HA	1:B:333:GLN:O	2.18	0.42
1:B:265:LEU:O	1:B:266:LEU:C	2.62	0.42
1:B:464:VAL:HG21	6:A:1102:C8E:H191	2.01	0.42
1:A:412:PHE:O	1:A:416:THR:HG23	2.19	0.42
1:A:622:ASN:HB3	1:A:696:SER:HB2	2.01	0.42
1:A:739:ILE:HA	2:C:114:ASN:CG	2.44	0.42
1:A:936:PHE:HE1	4:Q:6:ALA:CB	2.32	0.42
2:C:122:ALA:O	2:C:126:ASN:ND2	2.52	0.42
1:B:692:ASN:ND2	1:B:747:GLN:HA	2.35	0.42
1:A:203:MET:HE2	1:A:226:ILE:HG12	2.00	0.42
2:C:364:ARG:HH21	2:C:370:PRO:HB3	1.83	0.42
2:D:188:LEU:HD22	2:D:195:TYR:CD2	2.54	0.42
2:D:432:LEU:HD23	2:D:432:LEU:HA	1.78	0.42
1:B:781:TYR:CE1	1:B:863:PRO:HB2	2.55	0.42
1:B:822:ASP:HB3	1:B:825:THR:OG1	2.20	0.42
1:A:412:PHE:CE1	1:A:416:THR:HG21	2.55	0.42
2:C:451:HIS:ND1	2:C:469:LEU:CD1	2.83	0.42
2:D:187:LEU:HD22	2:D:205:CYS:HA	2.01	0.42
2:D:291:GLY:N	2:D:378:TYR:CE2	2.88	0.42
1:A:233:MET:HG3	1:A:342:SER:HA	2.02	0.42
1:A:684:GLY:HA2	2:C:43:GLN:O	2.19	0.42
1:A:795:LYS:HA	1:A:805:TRP:O	2.20	0.42
2:D:287:ILE:HD11	2:D:377:ARG:CZ	2.50	0.42
2:D:343:ALA:O	2:D:345:VAL:HG22	2.19	0.42
1:B:406:TYR:CE1	3:P:2:SER:HB2	2.55	0.42
1:A:786:ILE:O	1:A:807:ILE:O	2.37	0.42
1:A:848:TYR:CG	1:A:935:GLN:HG2	2.55	0.42
2:D:360:ASP:HB3	2:D:363:TYR:CD2	2.55	0.42
1:B:864:ILE:HB	1:B:887:VAL:HG22	2.01	0.42
1:A:734:VAL:HG22	1:A:745:GLN:O	2.19	0.42
2:C:220:LEU:HA	2:C:221:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:LEU:HD11	2:D:208:TYR:CD2	2.55	0.42
1:B:349:ALA:HB2	1:B:373:LEU:HD13	2.01	0.41
1:A:917:ALA:HB1	1:A:928:PRO:O	2.20	0.41
2:C:45:ARG:O	2:C:49:TYR:HD1	2.01	0.41
2:C:97:ARG:NH2	2:C:101:ASP:HB2	2.35	0.41
2:C:122:ALA:N	2:C:191:TYR:HB2	2.35	0.41
2:C:187:LEU:HD12	2:C:187:LEU:HA	1.73	0.41
2:D:110:TYR:CE2	2:D:488:ASP:OD2	2.73	0.41
1:B:182:VAL:HG22	1:B:226:ILE:HB	2.01	0.41
1:B:460:HIS:ND1	1:A:486:ILE:HG21	2.35	0.41
1:B:811:ASN:ND2	1:B:860:VAL:HG21	2.34	0.41
1:A:410:GLY:O	1:A:414:VAL:HG13	2.21	0.41
2:C:22:LEU:HD23	2:C:22:LEU:H	1.85	0.41
1:B:605:TYR:HD2	1:B:633:MET:HE2	1.84	0.41
1:A:252:ASN:HB3	1:A:990:PHE:HA	2.02	0.41
1:A:637:TYR:OH	1:A:643:GLU:HA	2.20	0.41
2:C:337:ARG:NH2	2:C:427:GLU:OE2	2.41	0.41
1:A:124:LYS:HB2	1:A:124:LYS:HE3	1.84	0.41
2:C:55:THR:HG22	2:C:113:TYR:CE1	2.55	0.41
2:C:421:MET:O	2:C:425:GLN:HG3	2.20	0.41
1:B:251:LEU:HD23	1:B:251:LEU:H	1.84	0.41
1:B:416:THR:OG1	1:B:908:LEU:HB3	2.20	0.41
1:B:489:THR:HB	1:B:514:TYR:HB2	2.02	0.41
1:B:768:ASN:HD22	1:B:768:ASN:C	2.22	0.41
1:B:918:TRP:NE1	1:B:923:LYS:HG2	2.35	0.41
1:A:615:SER:O	1:A:623:ARG:HB2	2.20	0.41
2:C:55:THR:HG23	2:C:112:VAL:CG2	2.51	0.41
2:C:66:LEU:HD13	2:C:81:LEU:HD22	2.03	0.41
1:B:646:TRP:CH2	1:B:647:LEU:HD12	2.55	0.41
1:B:721:ASP:O	1:B:757:VAL:HG23	2.21	0.41
1:B:927:VAL:HA	1:B:928:PRO:HD3	1.87	0.41
2:C:24:ARG:HA	2:C:24:ARG:HD3	1.92	0.41
2:D:487:ARG:O	2:D:491:THR:HG22	2.21	0.41
1:B:276:GLY:N	2:D:465:ASN:OD1	2.54	0.41
1:B:289:LEU:HA	1:B:313:VAL:HG11	2.02	0.41
1:B:603:TRP:HD1	1:B:635:ASP:H	1.69	0.41
1:B:664:ILE:CG2	1:B:731:LEU:HD23	2.50	0.41
1:B:738:TYR:CE2	2:D:487:ARG:HB3	2.56	0.41
1:A:407:MET:HE3	1:A:407:MET:O	2.21	0.41
1:A:604:MET:HE2	1:A:604:MET:HB3	1.87	0.41
1:A:1015:LEU:HB3	1:A:1017:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:LEU:HD22	2:C:195:TYR:CD2	2.55	0.41
2:D:122:ALA:HB2	2:D:191:TYR:CD1	2.55	0.41
1:A:206:LEU:HB2	1:A:223:VAL:HG22	2.03	0.41
1:A:678:TYR:CE1	2:C:49:TYR:HB3	2.56	0.41
2:C:449:ASN:HB2	2:C:473:ALA:HB3	2.03	0.41
1:B:139:MET:HE1	1:B:224:VAL:HG11	2.03	0.41
1:B:639:LYS:HD2	1:B:640:PHE:CE1	2.56	0.41
1:B:860:VAL:HG23	1:B:861:THR:N	2.36	0.41
1:A:218:ARG:HD2	1:A:221:ASN:ND2	2.36	0.41
1:A:218:ARG:HD2	1:A:221:ASN:HD22	1.85	0.41
1:A:260:MET:HE2	1:A:915:LEU:CD2	2.51	0.41
1:A:889:LYS:HG2	1:A:944:ALA:HB3	2.02	0.41
2:C:368:ASP:OD2	2:C:369:LYS:HE3	2.21	0.41
1:B:121:SER:HB3	1:B:207:LYS:HG3	2.03	0.41
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.93	0.41
1:B:972:ALA:O	1:B:973:ARG:HG3	2.21	0.40
1:A:433:VAL:CG2	1:A:442:PRO:HB2	2.50	0.40
1:A:674:THR:HB	2:C:29:LYS:HE3	2.02	0.40
2:C:128:GLU:HG2	2:C:149:LEU:HD21	2.03	0.40
1:B:850:ALA:C	1:B:852:LEU:H	2.29	0.40
1:A:149:MET:HE2	1:A:164:VAL:HG11	2.04	0.40
1:A:280:THR:HG22	1:A:283:LYS:HB2	2.04	0.40
1:A:603:TRP:CE2	1:A:639:LYS:HG3	2.56	0.40
1:A:757:VAL:O	1:A:780:ASN:ND2	2.55	0.40
1:A:823:LYS:HD3	1:A:823:LYS:H	1.86	0.40
2:C:149:LEU:O	2:C:153:LYS:HG3	2.21	0.40
1:B:239:ILE:CG2	1:B:1017:PHE:HB2	2.45	0.40
1:A:902:GLY:HA3	1:A:930:LEU:CD1	2.47	0.40
2:C:386:LEU:HD13	2:C:428:ARG:HA	2.04	0.40
1:B:285:LYS:HG2	1:B:315:PHE:CE2	2.57	0.40
1:B:670:GLN:H	1:B:670:GLN:CD	2.24	0.40
1:A:251:LEU:H	1:A:251:LEU:HD23	1.86	0.40
2:D:208:TYR:CZ	2:D:212:ARG:HD2	2.56	0.40
1:B:359:MET:HE3	1:B:359:MET:HB2	1.57	0.40
1:B:490:ARG:NH2	1:B:511:GLU:OE1	2.44	0.40
1:A:214:ILE:HD13	1:A:214:ILE:HG21	1.82	0.40
1:A:462:ALA:CB	6:A:1102:C8E:H82	2.51	0.40
1:A:818:TYR:HE1	1:A:828:GLN:HG2	1.86	0.40
2:C:224:ARG:HG3	2:C:231:SER:HB3	2.04	0.40
2:D:148:PHE:N	2:D:148:PHE:CD1	2.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ASP:OD1	1:A:280:THR:OG1[3_645]	2.05	0.15

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	894/997 (90%)	817 (91%)	71 (8%)	6 (1%)	18	49
1	B	899/997 (90%)	821 (91%)	70 (8%)	8 (1%)	14	44
2	C	480/488 (98%)	453 (94%)	27 (6%)	0	100	100
2	D	480/488 (98%)	449 (94%)	30 (6%)	1 (0%)	43	73
3	P	11/13 (85%)	7 (64%)	2 (18%)	2 (18%)	0	0
4	Q	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	1
All	All	2772/2993 (93%)	2552 (92%)	202 (7%)	18 (1%)	18	53

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	771	TRP
1	A	343	GLN
1	A	771	TRP
1	A	1001	ASN
3	P	2	SER
4	Q	5	GLY
1	B	532	ASP
1	B	342	SER
1	A	990	PHE
1	B	766	TYR
2	D	347	LYS
1	A	173	GLY

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Mol	Chain	Res	Type
1	A	218	ARG
1	B	666	ASN
1	B	664	ILE
1	B	173	GLY
3	P	11	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	751/832 (90%)	751 (100%)	0	100	100
1	B	755/832 (91%)	753 (100%)	2 (0%)	86	88
2	C	402/408 (98%)	402 (100%)	0	100	100
2	D	402/408 (98%)	402 (100%)	0	100	100
3	P	8/8 (100%)	8 (100%)	0	100	100
4	Q	7/7 (100%)	7 (100%)	0	100	100
All	All	2325/2495 (93%)	2323 (100%)	2 (0%)	100	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	728[A]	ASN
1	B	728[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	278	ASN
1	B	463	ASN
1	B	543	HIS
1	B	612	ASN
1	B	666	ASN
1	B	748	ASN

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Mol	Chain	Res	Type
1	B	811	ASN
1	B	835	GLN
1	A	150	GLN
1	A	198	ASN
1	A	258	ASN
1	A	269	GLN
1	A	395	ASN
1	A	499	ASN
1	A	523	ASN
1	A	543	HIS
1	A	570	GLN
1	A	597	ASN
1	A	612	ASN
1	A	614	GLN
1	A	780	ASN
1	A	794	ASN
1	A	811	ASN
1	A	893	ASN
1	A	894	ASN
2	C	117	ASN
2	C	118	GLN
2	C	156	GLN
2	C	394	GLN
2	D	156	GLN
2	D	450	ASN
2	D	486	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

11 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
6	C8E	A	1102	-	20,20,20	0.56	0	19,19,19	0.52	0
6	C8E	B	1102	-	20,20,20	0.62	0	19,19,19	0.61	0
7	LMT	C	602	-	35,35,36	1.21	4 (11%)	46,46,47	1.16	3 (6%)
7	LMT	A	1103	-	12,12,36	0.36	0	11,11,47	0.80	0
8	PLM	C	601	2	12,13,17	0.80	0	11,12,17	0.49	0
7	LMT	C	603	-	12,12,36	0.16	0	11,11,47	0.74	0
5	3PE	A	1101	-	33,33,50	1.17	4 (12%)	35,35,55	1.41	6 (17%)
5	3PE	B	1101	-	33,33,50	1.13	3 (9%)	35,35,55	1.88	5 (14%)
7	LMT	B	1103	-	29,29,36	1.14	1 (3%)	40,40,47	0.98	2 (5%)
7	LMT	A	1104	-	12,12,36	0.17	0	11,11,47	0.58	0
8	PLM	D	601	-	14,15,17	0.92	0	13,14,17	0.61	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
6	C8E	A	1102	-	-	9/18/18/18	-
6	C8E	B	1102	-	-	8/18/18/18	-
7	LMT	C	602	-	-	11/20/60/61	0/2/2/2
7	LMT	A	1103	-	-	7/10/10/61	-
8	PLM	C	601	2	-	7/11/11/15	-
7	LMT	C	603	-	-	4/10/10/61	-
5	3PE	A	1101	-	-	13/34/34/54	-
5	3PE	B	1101	-	-	17/34/34/54	-
7	LMT	B	1103	-	-	8/14/54/61	0/2/2/2
7	LMT	A	1104	-	-	8/10/10/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PLM	D	601	-	-	6/13/13/15	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1101	3PE	O21-C2	-3.79	1.40	1.47
5	B	1101	3PE	O21-C21	3.11	1.43	1.34
7	C	602	LMT	O3'-C3'	-2.95	1.35	1.43
7	B	1103	LMT	O3'-C3'	-2.56	1.36	1.43
5	A	1101	3PE	O21-C21	2.52	1.41	1.34
5	B	1101	3PE	O31-C31	2.48	1.40	1.33
5	A	1101	3PE	O31-C31	2.46	1.40	1.33
5	B	1101	3PE	O31-C3	-2.45	1.39	1.45
5	A	1101	3PE	O31-C3	-2.28	1.40	1.45
7	C	602	LMT	O2'-C2'	-2.27	1.37	1.43
7	C	602	LMT	O3B-C3B	-2.20	1.37	1.43
7	C	602	LMT	O4'-C4B	-2.15	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	3PE	O21-C21-C22	6.55	125.64	111.48
5	B	1101	3PE	C2-O21-C21	5.99	126.42	117.78
5	A	1101	3PE	O21-C21-C22	4.78	121.82	111.48
7	C	602	LMT	C3'-C4'-C5'	-3.82	102.46	110.93
5	A	1101	3PE	O31-C31-C32	3.19	121.55	111.83
5	B	1101	3PE	O21-C2-C3	2.98	113.06	106.21
5	B	1101	3PE	O31-C31-C32	2.96	120.85	111.83
5	A	1101	3PE	O21-C2-C3	2.81	112.68	106.21
5	A	1101	3PE	C1-C2-C3	-2.70	105.11	112.69
7	C	602	LMT	O5B-C5B-C4B	2.69	114.55	109.70
5	B	1101	3PE	O22-C21-C22	-2.41	114.35	123.78
5	A	1101	3PE	O31-C31-O32	-2.14	118.28	123.63
7	B	1103	LMT	C3'-C4'-C5'	-2.12	106.22	110.93
7	B	1103	LMT	C1'-O5'-C5'	-2.06	109.69	113.72
7	C	602	LMT	O1B-C1B-C2B	2.01	113.04	108.09
5	A	1101	3PE	O21-C21-O22	-2.01	119.01	123.70

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	3PE	C3-C2-O21-C21
5	B	1101	3PE	O22-C21-O21-C2
5	A	1101	3PE	C22-C21-O21-C2
8	D	601	PLM	O2-C1-C2-C3
5	A	1101	3PE	O22-C21-O21-C2
5	B	1101	3PE	C22-C21-O21-C2
7	C	602	LMT	C4B-C5B-C6B-O6B
7	C	602	LMT	O5'-C5'-C6'-O6'
7	B	1103	LMT	O5'-C1'-O1'-C1
7	B	1103	LMT	O5B-C5B-C6B-O6B
7	C	602	LMT	O5B-C5B-C6B-O6B
8	D	601	PLM	C3-C4-C5-C6
6	B	1102	C8E	O18-C19-C20-O21
5	A	1101	3PE	C32-C31-O31-C3
7	B	1103	LMT	C4B-C5B-C6B-O6B
7	B	1103	LMT	C2'-C1'-O1'-C1
6	A	1102	C8E	O12-C13-C14-O15
6	B	1102	C8E	O12-C13-C14-O15
7	B	1103	LMT	O5'-C5'-C6'-O6'
5	A	1101	3PE	O32-C31-O31-C3
7	C	602	LMT	C4'-C5'-C6'-O6'
7	C	602	LMT	C5'-C4'-O1B-C1B
6	A	1102	C8E	O18-C19-C20-O21
7	C	602	LMT	C3'-C4'-O1B-C1B
5	A	1101	3PE	C21-C22-C23-C24
8	C	601	PLM	C5-C6-C7-C8
7	A	1103	LMT	C2-C1-O1'-C1'
8	C	601	PLM	C6-C7-C8-C9
6	A	1102	C8E	O15-C16-C17-O18
5	B	1101	3PE	C37-C38-C39-C3A
7	A	1104	LMT	C4-C5-C6-C7
7	A	1103	LMT	C4-C5-C6-C7
5	B	1101	3PE	C29-C2A-C2B-C2C
7	C	602	LMT	C4-C5-C6-C7
5	B	1101	3PE	C2A-C2B-C2C-C2D
6	A	1102	C8E	C5-C6-C7-C8
7	A	1103	LMT	C3-C4-C5-C6
8	C	601	PLM	C2-C3-C4-C5
5	A	1101	3PE	C24-C25-C26-C27
7	A	1104	LMT	C6-C7-C8-C9
7	A	1104	LMT	C7-C8-C9-C10
8	C	601	PLM	C3-C4-C5-C6
7	C	603	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	C	601	PLM	C4-C5-C6-C7
8	D	601	PLM	C4-C5-C6-C7
7	C	603	LMT	C11-C10-C9-C8
5	B	1101	3PE	C1-C2-O21-C21
6	A	1102	C8E	C2-C3-C4-C5
7	A	1103	LMT	C1-C2-C3-C4
5	B	1101	3PE	C36-C37-C38-C39
5	B	1101	3PE	C2C-C2D-C2E-C2F
8	D	601	PLM	C5-C6-C7-C8
7	B	1103	LMT	O5B-C1B-O1B-C4'
8	D	601	PLM	CB-CC-CD-CE
6	B	1102	C8E	C1-C2-C3-C4
7	C	602	LMT	C5-C6-C7-C8
5	A	1101	3PE	C1-C2-C3-O31
7	A	1104	LMT	C5-C6-C7-C8
5	B	1101	3PE	C39-C3A-C3B-C3C
5	A	1101	3PE	C38-C39-C3A-C3B
5	A	1101	3PE	O21-C2-C3-O31
7	C	602	LMT	C3-C4-C5-C6
7	A	1103	LMT	C2-C3-C4-C5
5	B	1101	3PE	C33-C34-C35-C36
7	A	1104	LMT	C9-C10-C11-C12
5	B	1101	3PE	C28-C29-C2A-C2B
7	A	1103	LMT	C7-C8-C9-C10
6	A	1102	C8E	C17-C16-O15-C14
6	B	1102	C8E	C10-C11-O12-C13
6	B	1102	C8E	C16-C17-O18-C19
8	D	601	PLM	C6-C7-C8-C9
5	A	1101	3PE	C2B-C2C-C2D-C2E
7	A	1104	LMT	C11-C10-C9-C8
6	B	1102	C8E	C20-C19-O18-C17
7	C	602	LMT	C2-C3-C4-C5
5	B	1101	3PE	C34-C35-C36-C37
5	B	1101	3PE	C38-C39-C3A-C3B
5	A	1101	3PE	C3-C2-O21-C21
7	B	1103	LMT	C2B-C1B-O1B-C4'
6	B	1102	C8E	C11-C10-O9-C8
7	A	1103	LMT	C6-C7-C8-C9
5	B	1101	3PE	C31-C32-C33-C34
7	A	1104	LMT	C1-C2-C3-C4
7	C	602	LMT	C7-C8-C9-C10
6	A	1102	C8E	C10-C11-O12-C13

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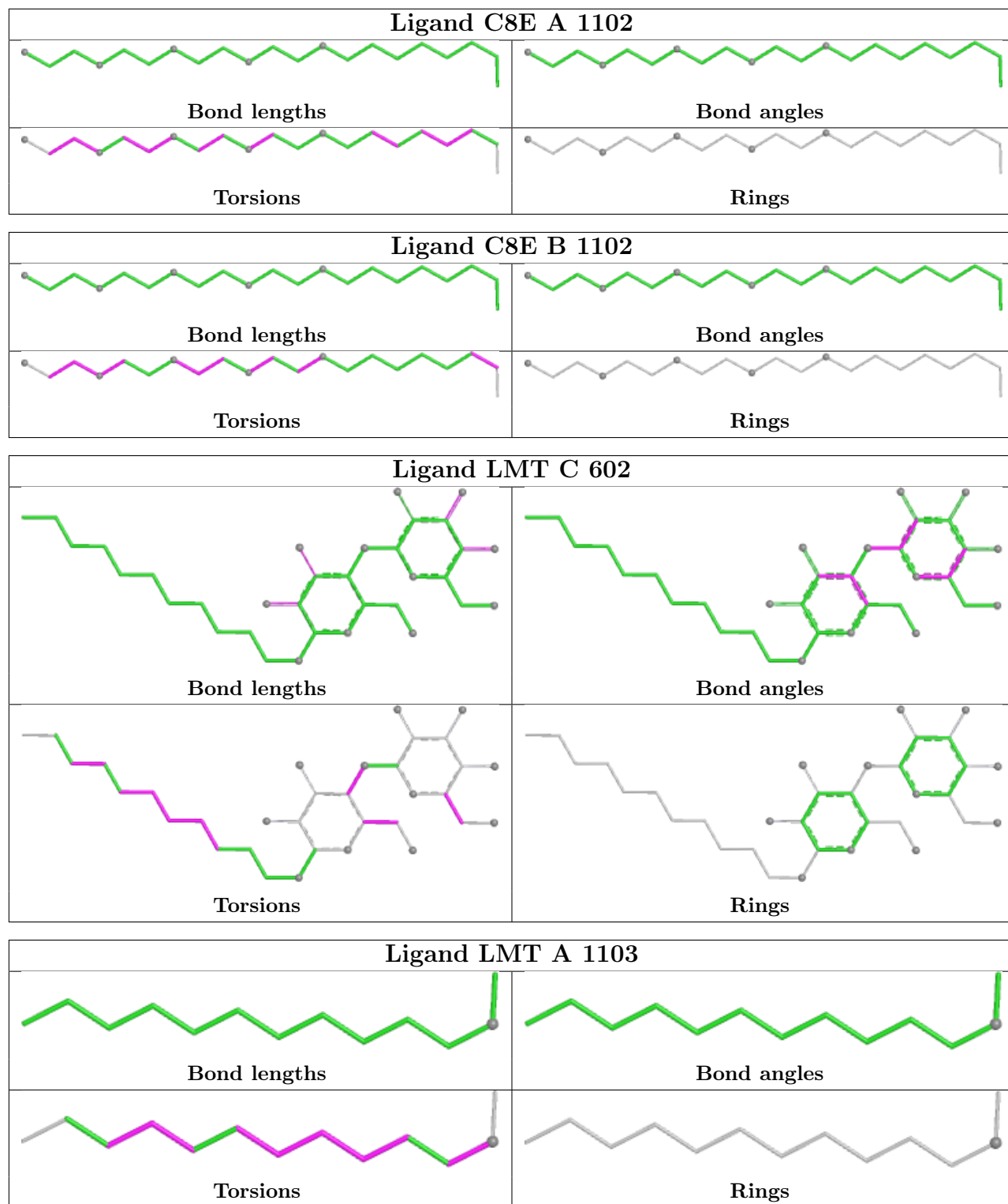
Mol	Chain	Res	Type	Atoms
8	C	601	PLM	C7-C8-C9-CA
6	A	1102	C8E	C20-C19-O18-C17
6	B	1102	C8E	C13-C14-O15-C16
5	A	1101	3PE	C37-C38-C39-C3A
8	C	601	PLM	CA-CB-CC-CD
7	C	603	LMT	C7-C8-C9-C10
7	B	1103	LMT	C5'-C4'-O1B-C1B
5	A	1101	3PE	C33-C34-C35-C36
6	A	1102	C8E	C3-C4-C5-C6
7	C	603	LMT	C6-C7-C8-C9
5	B	1101	3PE	O31-C31-C32-C33
7	A	1104	LMT	C2-C3-C4-C5
5	B	1101	3PE	O32-C31-C32-C33

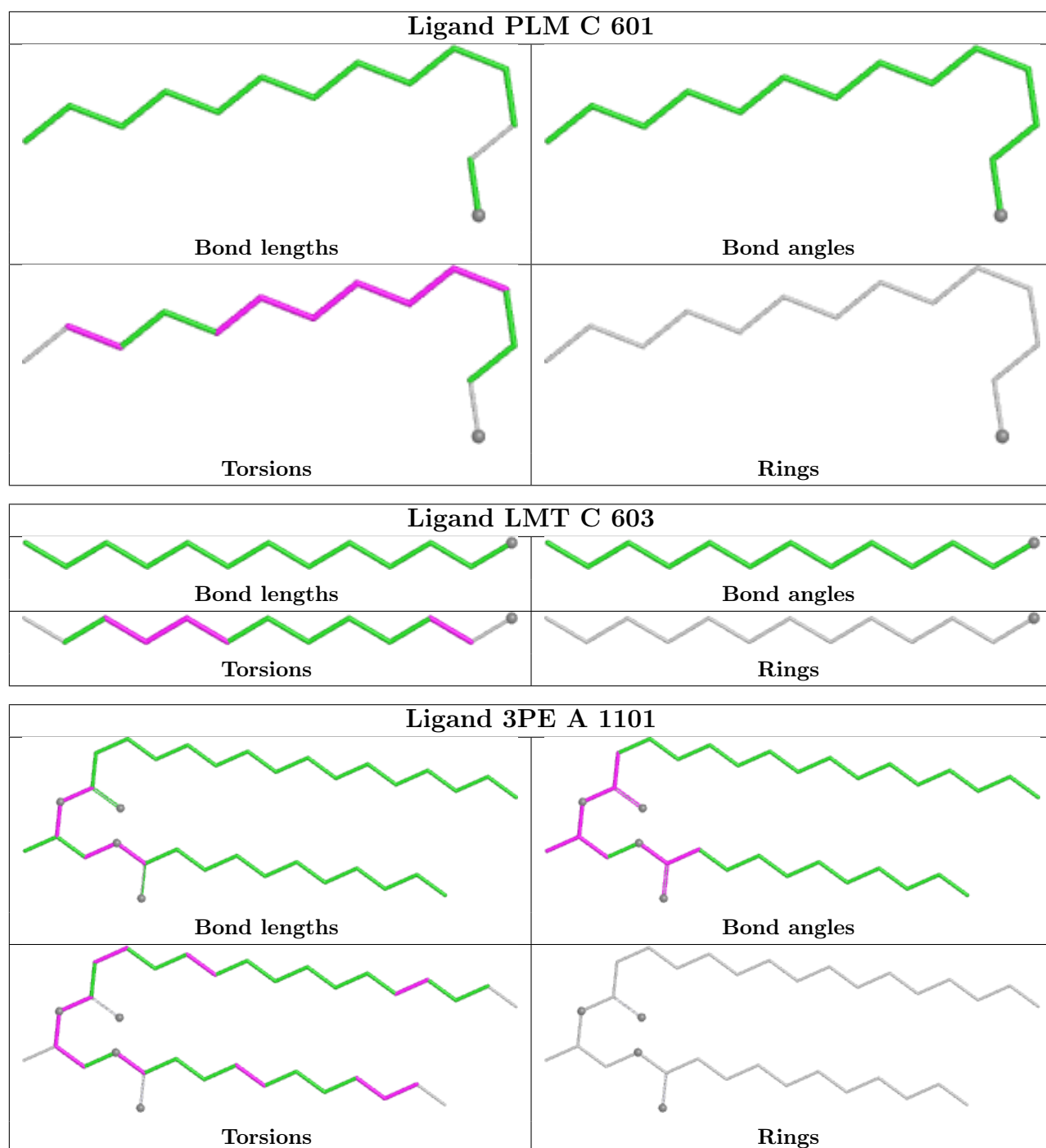
There are no ring outliers.

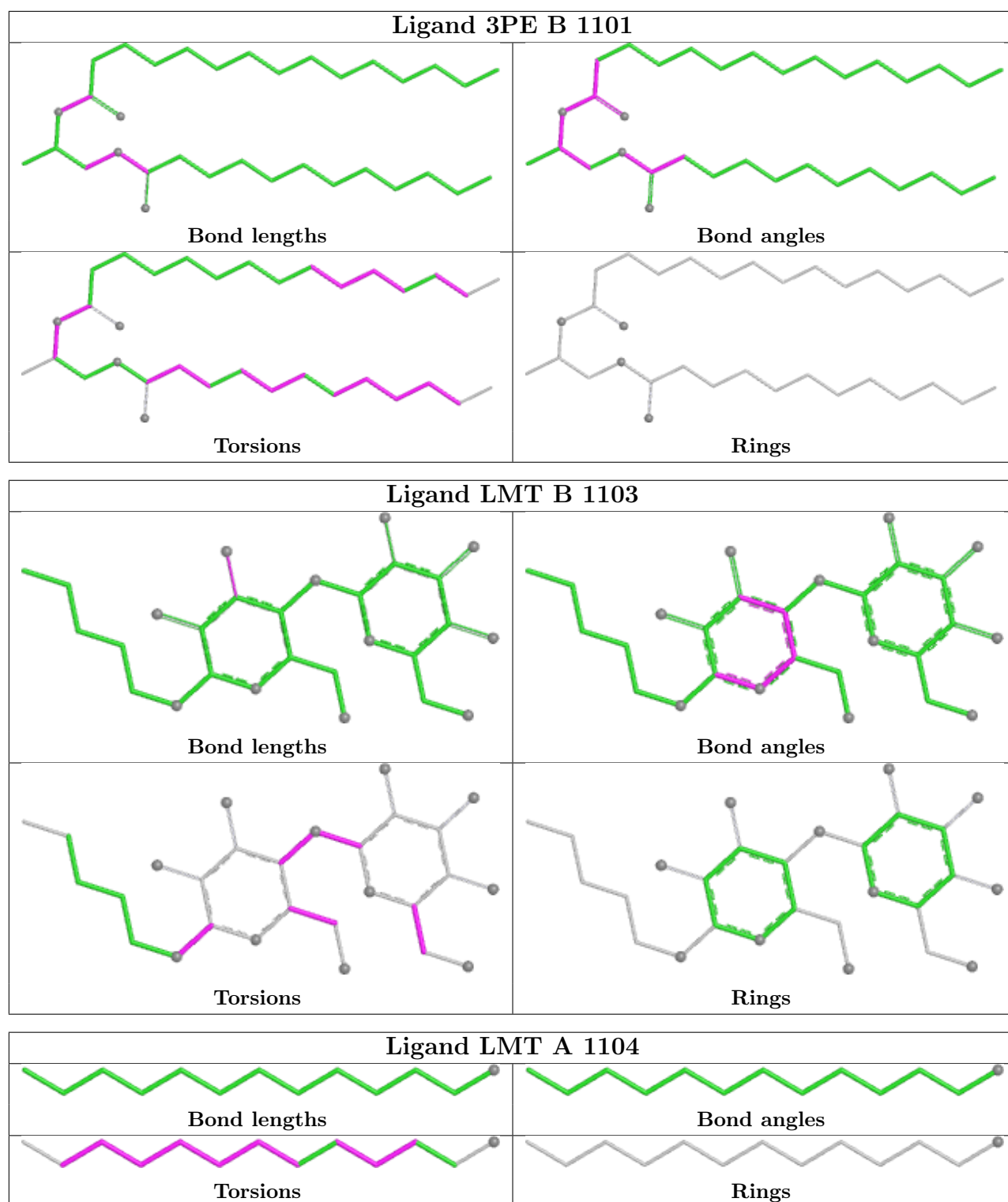
8 monomers are involved in 20 short contacts:

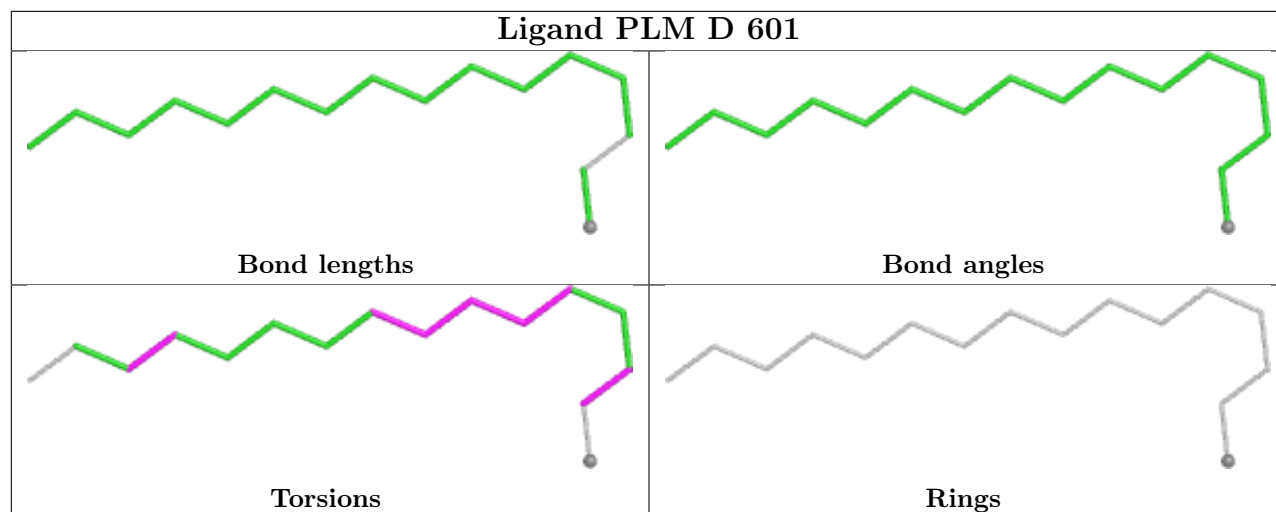
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1102	C8E	6	0
7	C	602	LMT	2	0
8	C	601	PLM	3	0
7	C	603	LMT	5	0
5	A	1101	3PE	6	0
5	B	1101	3PE	2	0
7	B	1103	LMT	1	0
7	A	1104	LMT	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	898/997 (90%)	0.31	32 (3%)	46 25	19, 40, 69, 94	0
1	B	900/997 (90%)	0.33	31 (3%)	48 27	19, 40, 76, 108	3 (0%)
2	C	482/488 (98%)	0.15	7 (1%)	72 48	21, 38, 58, 73	0
2	D	482/488 (98%)	0.02	6 (1%)	76 54	21, 35, 54, 72	0
3	P	13/13 (100%)	2.11	8 (61%)	0 0	50, 62, 96, 117	0
4	Q	10/10 (100%)	1.56	5 (50%)	0 0	54, 61, 66, 68	0
All	All	2785/2993 (93%)	0.25	89 (3%)	50 28	19, 39, 67, 117	3 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	SER	6.9
1	B	115	LEU	5.9
1	A	116	SER	5.9
2	D	501	ILE	5.7
1	A	691	GLY	4.7
2	C	178	SER	4.5
2	D	368	ASP	4.2
2	C	494	GLN	4.1
1	A	774	TYR	4.1
1	B	235	GLU	4.0
1	B	117	THR	4.0
1	B	603	TRP	4.0
1	B	215	TYR	4.0
1	B	126	SER	3.6
1	A	640	PHE	3.5
1	A	835	GLN	3.4
1	A	115	LEU	3.4
1	B	771	TRP	3.3
2	C	100	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	959	PRO	3.2
3	P	3	THR	3.2
1	A	641	ILE	3.2
1	B	960	ASN	3.2
1	A	253	THR	3.1
1	A	531	ILE	3.1
2	D	316	LYS	3.0
1	A	249	GLN	3.0
1	A	688	SER	3.0
1	B	184	GLY	3.0
1	B	966	GLN	2.9
1	B	382	TRP	2.9
1	A	128	GLU	2.9
1	B	481	GLN	2.9
1	A	645	ASN	2.9
1	A	638	ASN	2.8
2	D	494	GLN	2.8
3	P	1	ALA	2.8
2	D	491	THR	2.8
1	B	874	TRP	2.8
1	B	689	THR	2.8
1	B	238	ARG	2.7
3	P	4	THR	2.7
2	C	243	TYR	2.7
1	A	215	TYR	2.7
1	A	712	PHE	2.7
1	A	689	THR	2.7
1	A	369	TYR	2.7
3	P	12	SER	2.7
1	B	774	TYR	2.6
1	B	357	GLU	2.6
1	A	722	PHE	2.6
3	P	2	SER	2.6
1	A	132	GLU	2.6
1	A	211	ALA	2.5
1	A	1005	ASN	2.5
2	C	491	THR	2.5
2	C	195	TYR	2.5
1	A	235	GLU	2.5
4	Q	7	ASN	2.5
4	Q	9	GLN	2.5
2	C	349	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	13	GLY	2.4
1	B	638	ASN	2.3
1	B	836	VAL	2.3
1	A	307	GLY	2.3
3	P	7	ASN	2.2
1	B	705	PHE	2.2
4	Q	2	SER	2.2
2	D	303	THR	2.2
1	B	597	ASN	2.2
1	A	427	ASN	2.2
1	A	834	GLY	2.1
1	B	607	ASP	2.1
1	B	688	SER	2.1
1	A	859	SER	2.1
1	B	713	ASN	2.1
1	B	964	ALA	2.1
1	A	642	GLN	2.1
3	P	9	GLN	2.1
4	Q	1	ALA	2.1
1	B	508	GLU	2.1
1	B	485	ASP	2.1
1	B	925	THR	2.1
1	A	131	ALA	2.1
1	A	926	ASP	2.1
1	A	117	THR	2.0
1	A	246	GLY	2.0
4	Q	4	THR	2.0
1	B	128	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

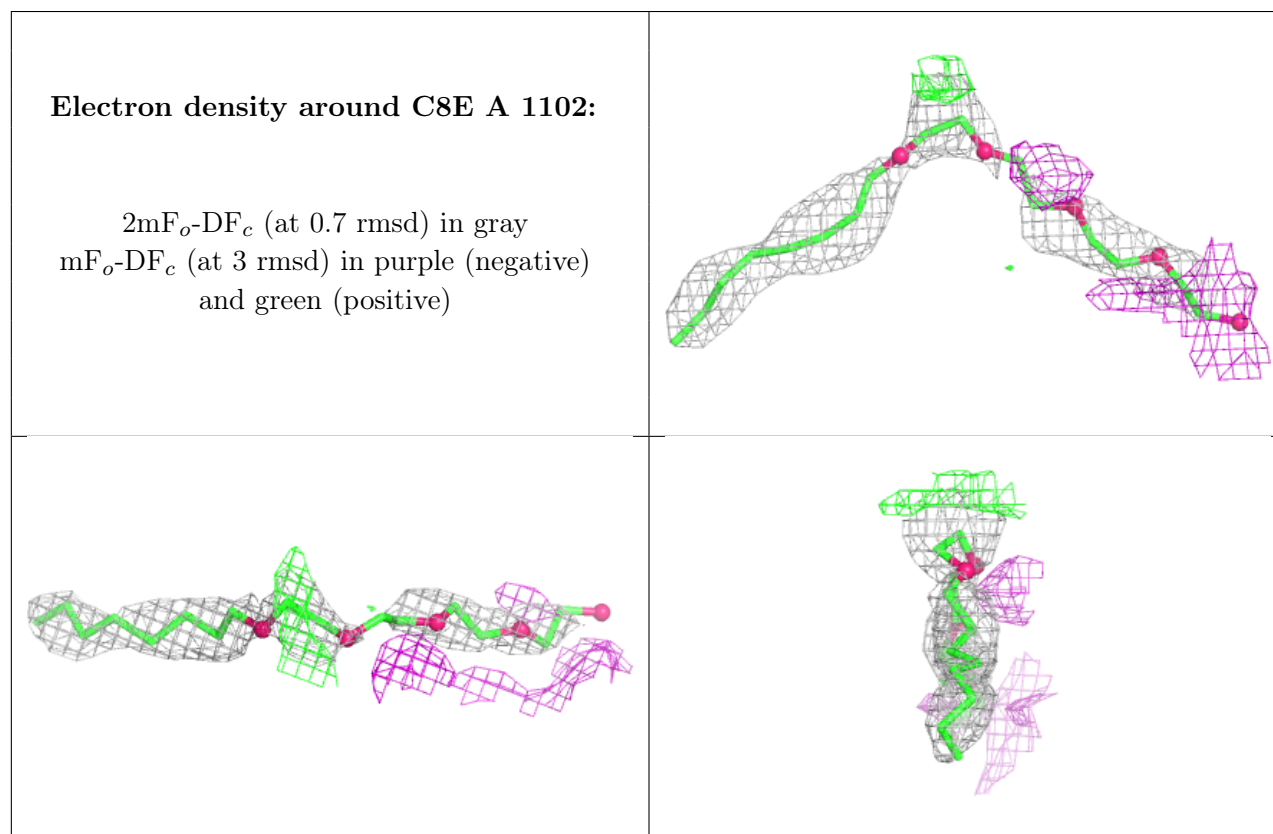
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

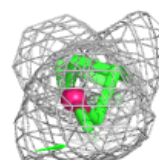
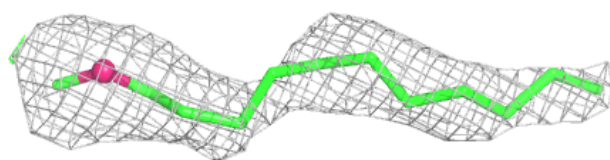
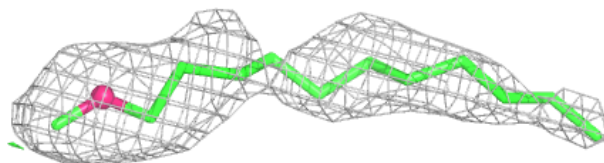
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	C8E	A	1102	21/21	0.78	0.24	19,34,60,62	0
7	LMT	A	1103	13/35	0.82	0.26	37,42,58,63	0
6	C8E	B	1102	21/21	0.85	0.20	24,36,44,49	0
7	LMT	B	1103	28/35	0.86	0.14	26,54,70,88	0
7	LMT	A	1104	13/35	0.88	0.19	7,19,62,63	0
7	LMT	C	602	34/35	0.88	0.12	33,48,65,71	0
8	PLM	C	601	14/18	0.89	0.13	7,20,43,51	0
5	3PE	A	1101	34/51	0.90	0.16	24,38,56,64	0
7	LMT	C	603	13/35	0.90	0.16	24,34,46,49	0
5	3PE	B	1101	34/51	0.90	0.14	7,29,39,41	0
8	PLM	D	601	16/18	0.90	0.15	17,37,47,47	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.

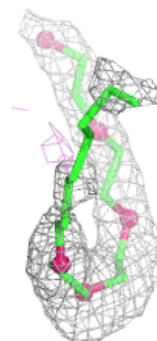
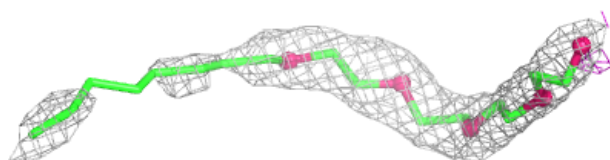
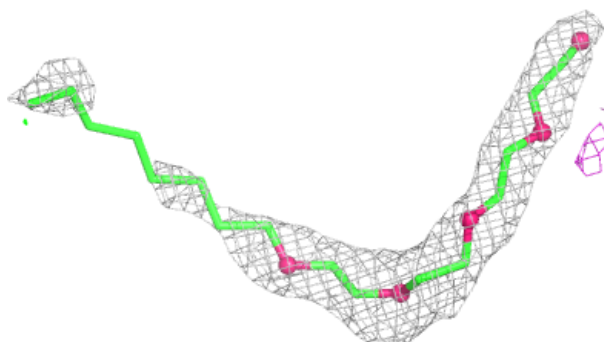


Electron density around LMT A 1103:

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

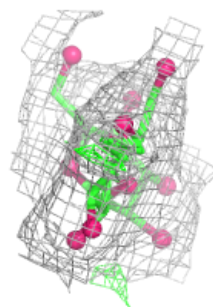
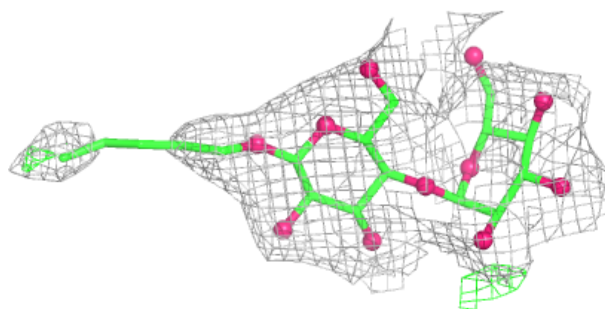
**Electron density around C8E B 1102:**

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

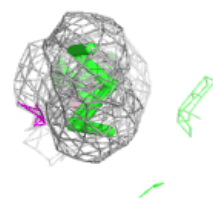
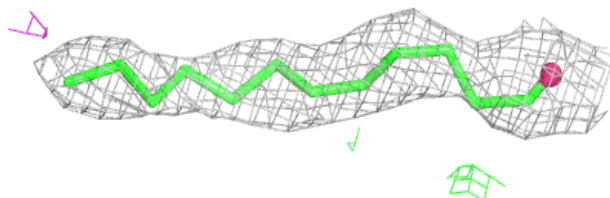
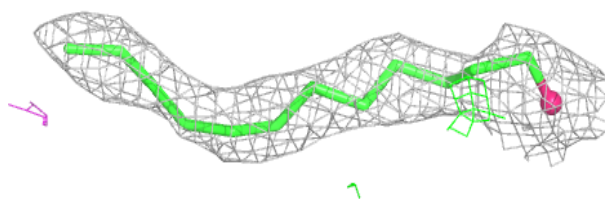


Electron density around LMT B 1103:

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

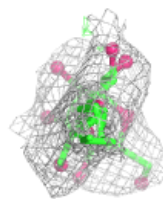
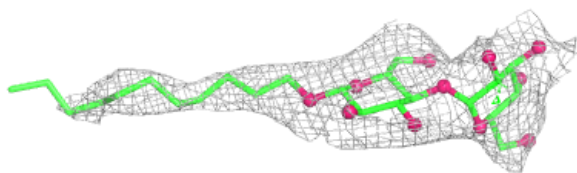
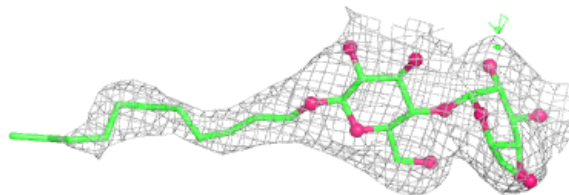
**Electron density around LMT A 1104:**

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

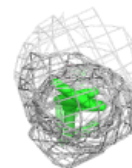
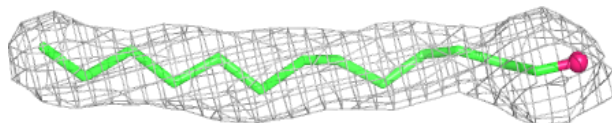
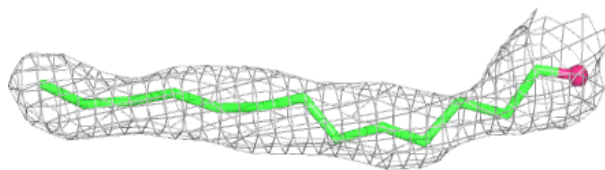


Electron density around LMT C 602:

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

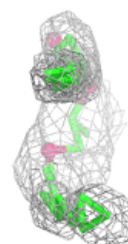
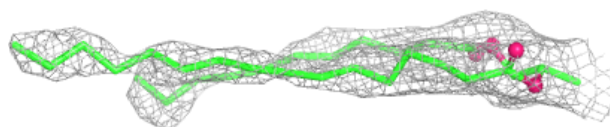
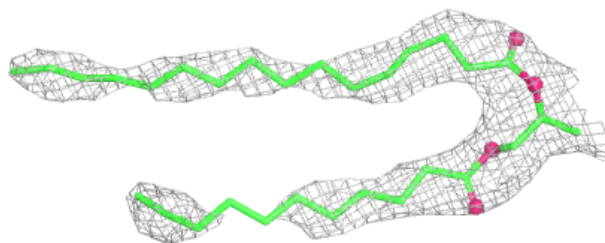
**Electron density around PLM C 601:**

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

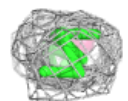
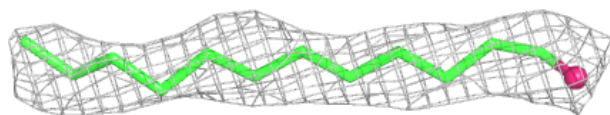
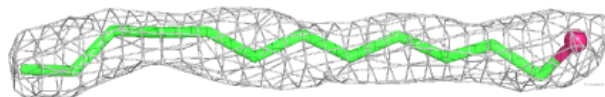


Electron density around 3PE A 1101:

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

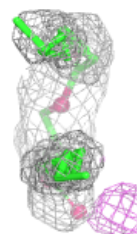
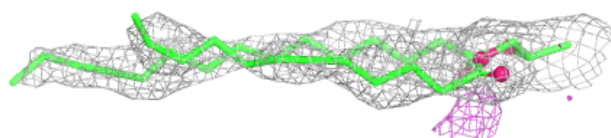
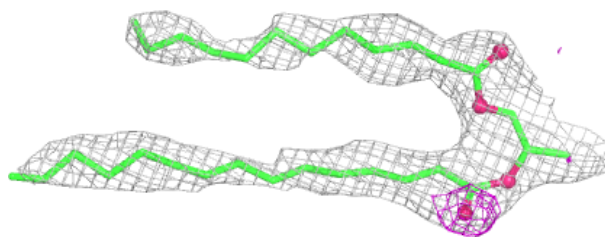
**Electron density around LMT C 603:**

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

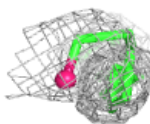
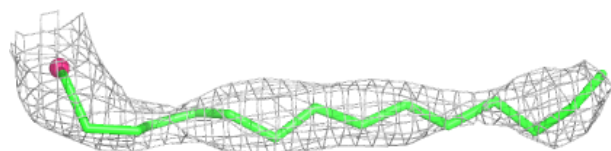
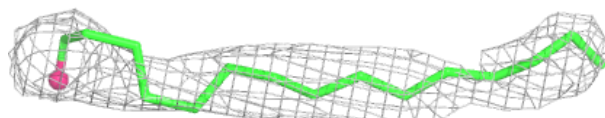


Electron density around 3PE B 1101:

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

**Electron density around PLM D 601:**

$2mF_o-DF_c$ (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.