Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:12 pm BST

PDB ID	:	2VQI
Title	:	Structure of the P pilus usher (PapC) translocation pore
Authors	:	Remaut, H.; Tang, C.; Henderson, N.S.; Pinkner, J.S.; Wang, T.; Hultgren, S.J.; Thanassi, D.G.; Li, H.; Waksman, G.
Deposited on	:	2008-03-16
Resolution	:	3.20 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:

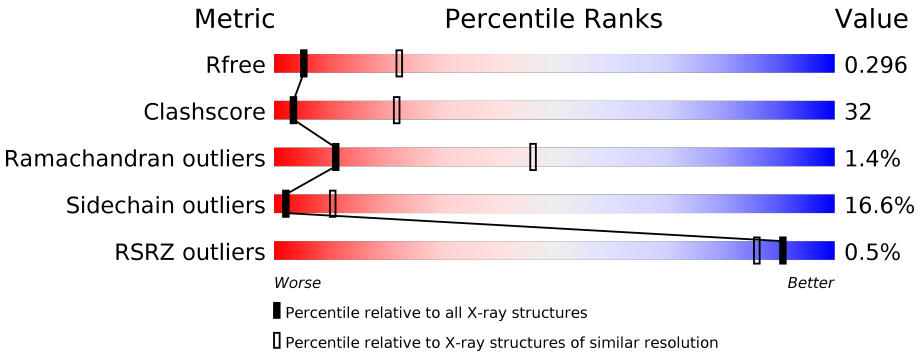
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	515	47% 38% 7% • 7%
1	B	515	% 48% 37% 8% • 7%

2 Entry composition

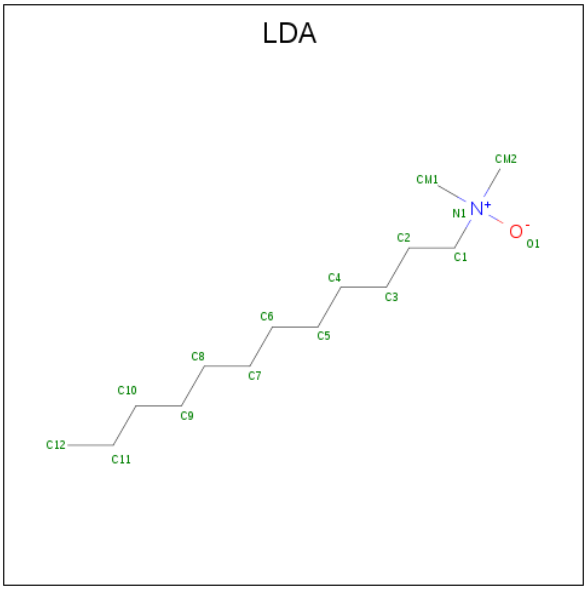
There are 4 unique types of molecules in this entry. The entry contains 7625 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 USHER PROTEIN PAPC.

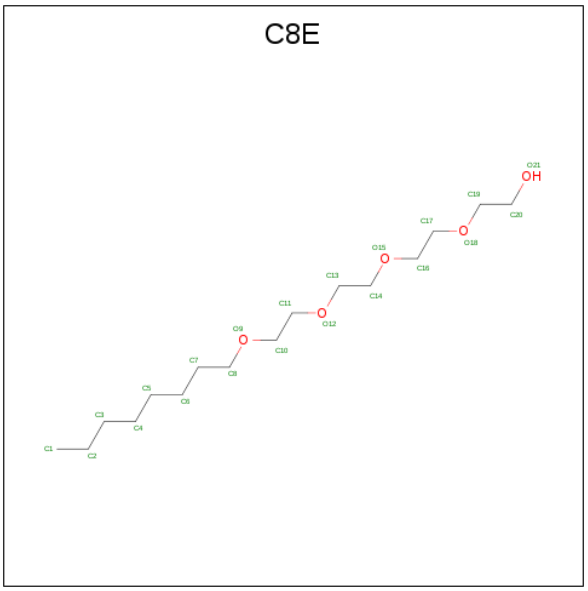
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	Se	0	0	0
			3767	2353	675	731	8			
1	B	477	Total	C	N	O	Se	0	0	0
			3750	2342	674	726	8			

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



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

- Molecule 4 is water.

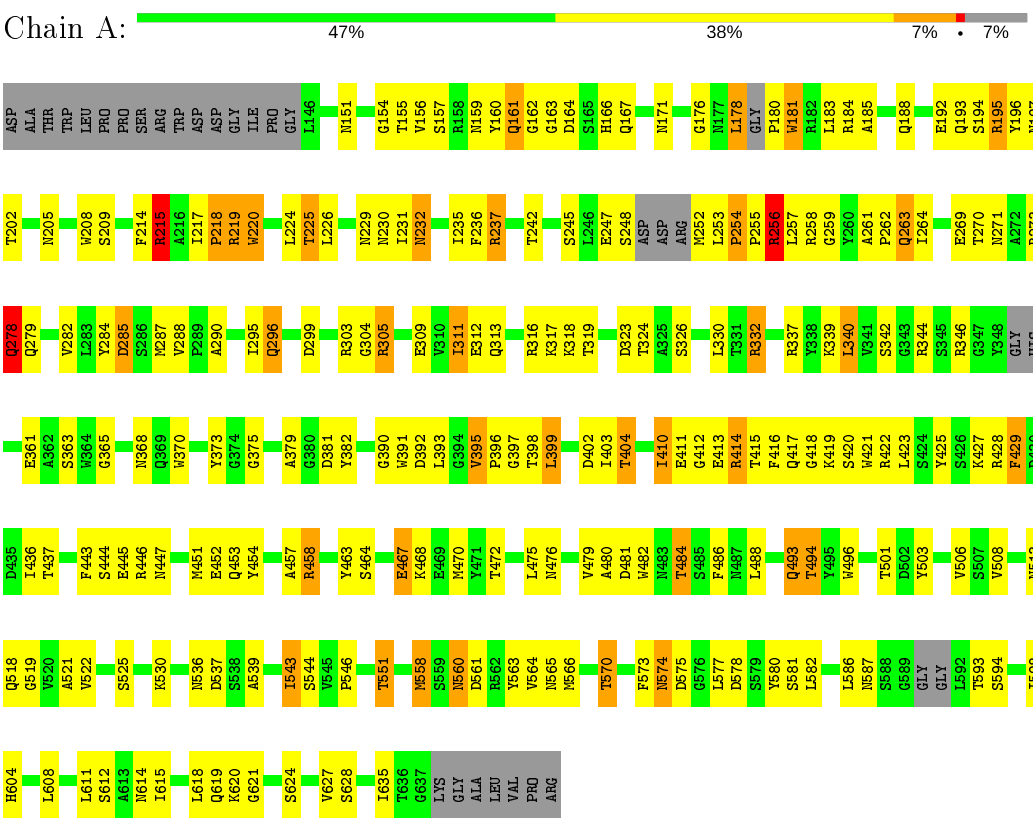
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	15	Total O 15 15	0	0
4	B	19	Total O 19 19	0	0

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.

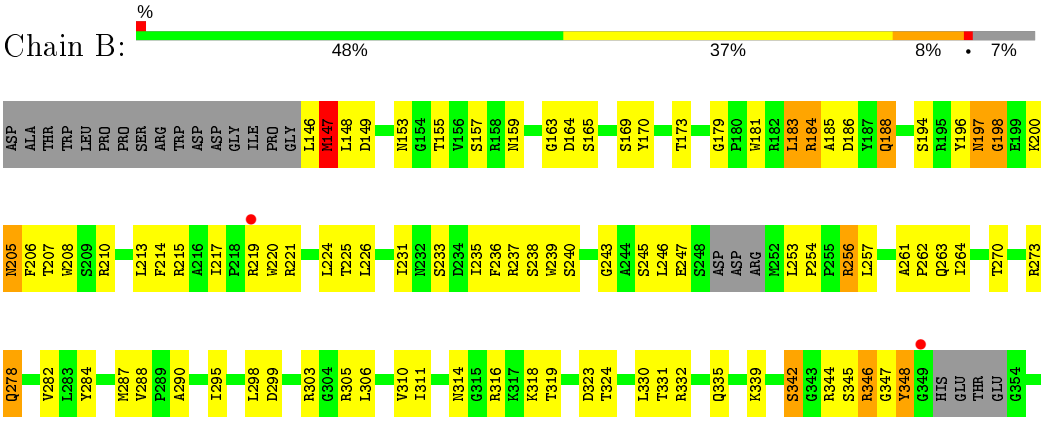
- Molecule 1: OUTER MEMBRANE USHER PROTEIN PAPC

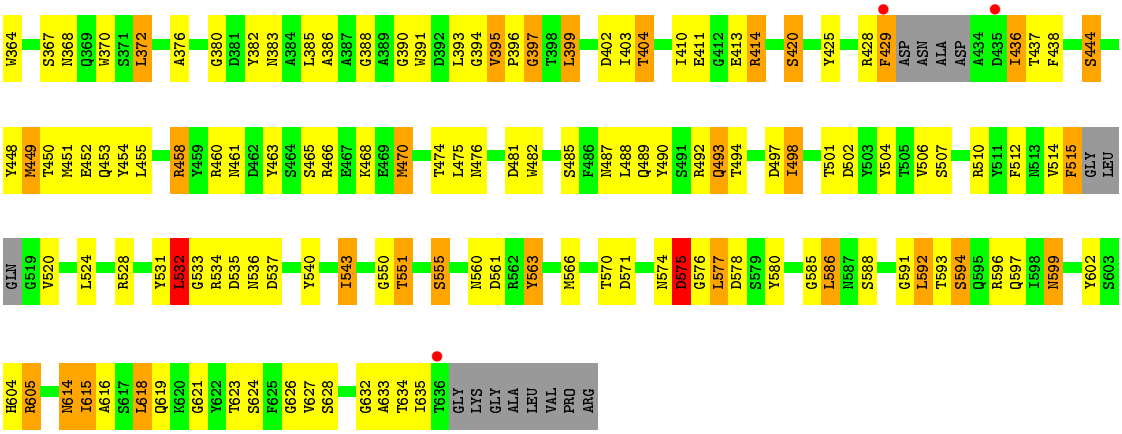
Chain A:



- Molecule 1: OUTER MEMBRANE USHER PROTEIN PAPC

Chain B:




W364 S367 N368 Q369 W370 S371 L372 A376 G380 D381 Y382 N383 A384 L385 A386 A387 G388 A389 G390 W391 D392 L393 G394 V395 P396 G397 T398 L399 D402 I403 T404 I410 E411 G412 E413 R414 S420 Y425 R428 F429 ASP ASN ALA ASP A434 D435 I436 T437 F438 S444
Y448 M449 T450 M451 E452 Q453 Y454 L455 R458 Y459 R460 N461 D462 Y463 S464 S465 R466 E467 K468 E469 M470 T474 L475 N476 D481 W482 S485 F486 N487 L488 Q489 Y490 S491 R492 Q493 T494 D497 I498 T501 D502 Y503 Y504 T505 V506 S507 R510 Y511 F512 N513 V514 F515 GLY LEU
GLN G519 V520 L524 R528 Y531 L532 G533 R534 D535 N536 D537 Y540 I543 G550 T551 S555 N560 D561 R562 Y563 M566 T570 D571 N574 D575 G576 L577 D578 S579 Y580 G585 L586 N587 S588 G591 L592 T593 S594 Q595 R596 Q597 I598 N599 Y602 S603
H604 R605 N614 I615 A616 S617 L618 Q619 R620 G621 Y622 T623 S624 F625 G626 V627 S628 G632 A633 T634 I635 T636 GLY LYS GLY ALA LEU VAL PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.50Å 101.90Å 113.70Å 90.00° 128.20° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-3.20) 99.9 (15.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.259 , 0.296 0.258 , 0.296	Depositor DCC
R_{free} test set	2410 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 13.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7625	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: LDA, C8E

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	0.42	0/3840	0.66	0/5184
1	B	0.52	2/3825 (0.1%)	0.71	1/5167 (0.0%)
All	All	0.47	2/7665 (0.0%)	0.68	1/10351 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	8
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	MSE	CG-SE	13.54	2.41	1.95
1	B	147	MSE	SE-CE	6.98	2.36	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	147	MSE	CG-SE-CE	-6.68	84.21	98.90

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	Peptide
1	A	199	GLU	Peptide
1	A	215	ARG	Sidechain
1	A	218	PRO	Peptide
1	A	278	GLN	Peptide
1	B	179	GLY	Peptide
1	B	219	ARG	Peptide
1	B	345	SER	Peptide
1	B	346	ARG	Peptide
1	B	397	GLY	Peptide
1	B	575	ASP	Peptide
1	B	591	GLY	Peptide
1	B	592	LEU	Peptide

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	3767	0	3590	245	0
1	B	3750	0	3576	225	0
2	A	16	0	31	6	0
2	B	16	0	31	3	0
3	B	42	0	68	6	0
4	A	15	0	0	4	0
4	B	19	0	0	2	0
All	All	7625	0	7296	464	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 32.

All (464) 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:395:VAL:HB	1:B:429:PHE:CE1	1.67	1.28
1:B:181:TRP:CZ3	1:B:215:ARG:HB3	1.70	1.27
1:B:147:MSE:CE	1:B:147:MSE:SE	2.36	1.23
1:A:180:PRO:O	1:A:215:ARG:HB2	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:HH21	1:A:318:LYS:NZ	1.41	1.19
1:B:147:MSE:SE	1:B:147:MSE:CG	2.41	1.19
1:B:394:GLY:O	1:B:395:VAL:HG13	1.44	1.17
1:B:394:GLY:C	1:B:395:VAL:HG13	1.73	1.07
1:A:256:ARG:HB2	1:A:256:ARG:HH11	1.16	1.07
1:A:403:ILE:HD12	1:A:421:TRP:CD1	1.90	1.06
1:B:574:ASN:O	1:B:575:ASP:HB2	1.47	1.05
1:B:395:VAL:N	1:B:396:PRO:HD2	1.72	1.04
1:A:342:SER:HB2	2:A:1638:LDA:H12	1.33	1.03
1:B:436:ILE:HD13	1:B:436:ILE:H	1.20	1.03
1:A:365:GLY:HA3	4:A:2006:HOH:O	1.59	1.03
1:B:510:ARG:HH12	3:B:1637:C8E:H191	1.23	1.02
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.23	1.00
1:A:522:VAL:HG22	1:A:543:ILE:HG22	1.39	1.00
1:B:394:GLY:C	1:B:396:PRO:CD	2.30	1.00
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.24	0.98
1:A:403:ILE:HD12	1:A:421:TRP:HD1	1.28	0.97
1:A:551:THR:HG23	1:A:570:THR:HG23	1.47	0.96
1:B:577:LEU:HB3	1:B:605:ARG:O	1.64	0.96
1:B:395:VAL:N	1:B:396:PRO:CD	2.31	0.93
1:B:551:THR:HG23	1:B:570:THR:HG23	1.48	0.93
1:B:577:LEU:HD13	1:B:577:LEU:N	1.82	0.93
1:B:394:GLY:C	1:B:396:PRO:HD2	1.89	0.92
1:A:264:ILE:HD11	1:A:295:ILE:HD12	1.52	0.91
1:A:413:GLU:O	1:A:414:ARG:HB2	1.69	0.90
1:B:264:ILE:HD11	1:B:306:LEU:HD12	1.52	0.90
1:A:316:ARG:NH2	1:A:318:LYS:NZ	2.20	0.89
1:B:394:GLY:O	1:B:396:PRO:HD3	1.73	0.88
1:B:577:LEU:N	1:B:577:LEU:CD1	2.37	0.88
1:B:394:GLY:C	1:B:395:VAL:CG1	2.41	0.87
1:B:184:ARG:HH11	1:B:184:ARG:HG3	1.36	0.87
1:B:395:VAL:HB	1:B:429:PHE:HE1	1.06	0.87
1:B:181:TRP:CZ3	1:B:215:ARG:CB	2.58	0.87
1:B:181:TRP:CE3	1:B:215:ARG:CB	2.58	0.86
1:A:342:SER:CB	2:A:1638:LDA:H12	2.04	0.86
1:A:402:ASP:C	1:A:403:ILE:HD13	1.96	0.86
1:B:534:ARG:HG3	1:B:535:ASP:H	1.40	0.86
1:A:254:PRO:HG2	1:A:257:LEU:HD12	1.56	0.85
1:B:181:TRP:CE3	1:B:215:ARG:HB3	2.11	0.85
1:B:394:GLY:C	1:B:396:PRO:HD3	1.97	0.85
1:A:271:ASN:ND2	1:A:599:ASN:HD21	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:N	1:A:396:PRO:HD2	1.92	0.85
1:A:316:ARG:HH21	1:A:318:LYS:HZ2	1.24	0.83
1:B:253:LEU:HD12	1:B:257:LEU:HD23	1.60	0.83
1:A:217:ILE:CG2	1:A:218:PRO:HD2	2.08	0.83
1:A:342:SER:HB3	2:A:1638:LDA:H41	1.60	0.83
1:B:253:LEU:HB2	1:B:254:PRO:HD2	1.59	0.83
1:B:510:ARG:NH1	3:B:1637:C8E:H191	1.95	0.81
1:A:217:ILE:HG23	1:A:218:PRO:HD2	1.61	0.81
1:A:256:ARG:CB	1:A:256:ARG:HH11	1.93	0.81
1:A:196:TYR:HD2	1:A:197:ASN:H	1.26	0.81
1:B:395:VAL:CB	1:B:429:PHE:HE1	1.90	0.81
1:A:486:PHE:HD1	1:A:508:VAL:HG22	1.47	0.80
1:A:515:PHE:C	1:A:517:LEU:N	2.36	0.80
1:A:395:VAL:HG12	1:A:429:PHE:CE1	2.17	0.80
1:A:463:TYR:CG	1:B:592:LEU:HD11	2.17	0.79
1:A:482:TRP:O	1:A:484:THR:HG22	1.82	0.79
1:B:596:ARG:H	1:B:619:GLN:HB3	1.48	0.79
1:B:214:PHE:HB2	1:B:225:THR:HG22	1.62	0.78
1:A:253:LEU:HB3	1:A:254:PRO:HD2	1.64	0.78
1:A:316:ARG:HH21	1:A:318:LYS:HZ3	1.28	0.78
1:B:413:GLU:O	1:B:414:ARG:HB2	1.82	0.78
1:B:534:ARG:HG3	1:B:535:ASP:N	1.99	0.78
1:B:577:LEU:HD13	1:B:577:LEU:H	1.45	0.78
1:A:395:VAL:N	1:A:396:PRO:CD	2.47	0.77
1:A:219:ARG:HG3	1:A:219:ARG:NH1	1.98	0.77
1:B:618:LEU:HB3	1:B:621:GLY:HA3	1.65	0.77
1:B:181:TRP:CE3	1:B:215:ARG:HB2	2.20	0.76
1:B:436:ILE:H	1:B:436:ILE:CD1	1.95	0.76
1:A:256:ARG:NH1	1:A:256:ARG:HB2	1.99	0.76
1:B:184:ARG:CG	1:B:184:ARG:HH11	1.98	0.76
1:B:316:ARG:HD3	4:B:2004:HOH:O	1.85	0.76
1:B:436:ILE:HD13	1:B:436:ILE:N	2.00	0.75
1:B:181:TRP:HZ3	1:B:215:ARG:HB3	1.48	0.75
1:A:340:LEU:HG	1:A:340:LEU:O	1.85	0.75
3:B:1637:C8E:O9	3:B:1637:C8E:C13	2.35	0.75
1:A:332:ARG:HG3	1:A:332:ARG:NH1	1.91	0.74
1:B:510:ARG:HH12	3:B:1637:C8E:C19	2.00	0.74
1:B:183:LEU:HB2	1:B:213:LEU:HD23	1.69	0.74
1:A:254:PRO:HG2	1:A:257:LEU:CD1	2.18	0.74
1:B:394:GLY:O	1:B:395:VAL:CG1	2.30	0.73
1:A:271:ASN:ND2	1:A:599:ASN:ND2	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:SER:HA	1:B:498:ILE:HD11	1.70	0.73
1:B:217:ILE:HG22	1:B:220:TRP:H	1.54	0.73
1:B:576:GLY:H	1:B:577:LEU:HD13	1.53	0.73
1:A:235:ILE:HG12	1:A:361:GLU:OE2	1.89	0.73
1:B:149:ASP:HB2	1:B:173:THR:HG23	1.70	0.72
1:A:429:PHE:CD2	1:A:429:PHE:N	2.55	0.72
1:A:194:SER:O	1:A:200:LYS:HA	1.90	0.72
1:B:148:LEU:HB3	1:B:633:ALA:HB3	1.71	0.71
1:A:196:TYR:OH	1:B:460:ARG:NH1	2.21	0.71
1:A:275:VAL:HB	1:A:285:ASP:HB2	1.73	0.70
1:A:403:ILE:CD1	1:A:421:TRP:HD1	2.04	0.70
1:B:498:ILE:H	1:B:498:ILE:HD13	1.57	0.70
1:B:287:MSE:HE3	1:B:614:ASN:HD22	1.56	0.69
1:A:418:GLY:HA2	1:A:445:GLU:OE1	1.92	0.69
1:B:146:LEU:HD12	1:B:635:ILE:CD1	2.22	0.69
1:A:635:ILE:HG13	1:A:635:ILE:O	1.92	0.68
1:A:395:VAL:H	1:A:396:PRO:HD2	1.58	0.68
1:B:395:VAL:HB	1:B:429:PHE:CZ	2.27	0.68
1:A:427:LYS:HB3	1:A:437:THR:CG2	2.23	0.68
1:B:515:PHE:CD2	1:B:515:PHE:C	2.67	0.67
1:A:220:TRP:N	1:A:220:TRP:CD1	2.62	0.67
1:A:309:GLU:OE2	1:A:317:LYS:HD3	1.93	0.67
1:A:417:GLN:O	1:A:447:ASN:HB2	1.95	0.67
1:B:615:ILE:C	1:B:615:ILE:HD13	2.15	0.67
1:A:379:ALA:HB3	1:A:382:TYR:O	1.95	0.67
1:B:386:ALA:HB2	1:B:404:THR:HB	1.77	0.67
1:A:395:VAL:HG12	1:A:429:PHE:HE1	1.58	0.66
1:B:376:ALA:HB2	1:B:385:LEU:HD12	1.77	0.66
1:B:504:TYR:HB3	1:B:528:ARG:HG2	1.77	0.66
1:B:214:PHE:CB	1:B:225:THR:HG22	2.26	0.66
1:B:566:MSE:HE2	1:B:585:GLY:HA3	1.77	0.66
1:A:479:VAL:C	1:A:481:ASP:H	2.00	0.65
1:A:410:ILE:HD11	1:A:416:PHE:HE1	1.60	0.65
1:B:256:ARG:HA	1:B:428:ARG:NH2	2.12	0.64
1:A:514:VAL:C	1:A:515:PHE:HD1	2.00	0.64
1:A:395:VAL:H	1:A:396:PRO:CD	2.10	0.63
1:B:278:GLN:NE2	1:B:305:ARG:O	2.32	0.63
1:B:514:VAL:O	1:B:514:VAL:HG13	1.98	0.63
1:B:420:SER:OG	1:B:444:SER:HB3	1.98	0.63
1:A:271:ASN:HD21	1:A:599:ASN:HD21	1.47	0.63
1:A:580:TYR:CD1	1:A:602:TYR:HB2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD12	1:B:635:ILE:HD11	1.81	0.62
1:B:264:ILE:HD11	1:B:306:LEU:CD1	2.25	0.62
1:A:332:ARG:CG	1:A:332:ARG:HH11	2.05	0.62
1:A:235:ILE:HD11	1:A:361:GLU:HB2	1.81	0.62
1:A:232:ASN:H	1:A:232:ASN:HD22	1.47	0.62
1:A:342:SER:HB2	2:A:1638:LDA:C1	2.22	0.61
1:A:425:TYR:OH	1:A:427:LYS:HB2	2.01	0.61
1:B:217:ILE:HG21	1:B:220:TRP:HB2	1.83	0.61
1:B:393:LEU:HB2	1:B:396:PRO:HG2	1.82	0.61
1:A:503:TYR:OH	1:A:530:LYS:HE2	1.99	0.61
1:B:449:MSE:HE2	1:B:466:ARG:NH1	2.16	0.61
1:A:403:ILE:HD13	1:A:403:ILE:N	2.13	0.61
1:A:414:ARG:HH21	1:A:416:PHE:HE2	1.47	0.61
1:A:159:ASN:HB3	1:A:161:GLN:HG2	1.83	0.61
1:A:253:LEU:CB	1:A:254:PRO:HD2	2.30	0.61
1:B:498:ILE:HD13	1:B:498:ILE:N	2.16	0.60
1:A:458:ARG:C	1:A:458:ARG:HD3	2.22	0.60
1:B:184:ARG:CG	1:B:184:ARG:NH1	2.62	0.60
1:A:514:VAL:C	1:A:515:PHE:CD1	2.75	0.60
1:A:312:GLU:HG3	1:A:318:LYS:HE2	1.84	0.60
1:B:449:MSE:HE2	1:B:466:ARG:HH12	1.67	0.60
1:B:270:THR:C	1:B:290:ALA:HB2	2.23	0.59
1:B:243:GLY:HA3	1:B:342:SER:O	2.02	0.59
1:A:570:THR:HB	1:A:581:SER:HB3	1.84	0.59
1:A:580:TYR:HD1	1:A:602:TYR:HB2	1.65	0.59
1:A:235:ILE:HD13	1:A:361:GLU:HG3	1.85	0.59
1:B:402:ASP:OD1	1:B:402:ASP:N	2.35	0.59
1:A:416:PHE:HB3	1:A:447:ASN:HB3	1.85	0.59
1:A:468:LYS:HG3	1:A:496:TRP:CE2	2.37	0.59
1:B:256:ARG:HA	1:B:428:ARG:CZ	2.33	0.58
1:B:437:THR:HA	1:B:474:THR:O	2.03	0.58
1:A:337:ARG:HB2	1:A:363:SER:HB3	1.84	0.58
1:A:468:LYS:HB3	1:A:494:THR:OG1	2.03	0.58
1:A:419:LYS:HG3	1:A:421:TRP:CH2	2.39	0.58
1:B:246:LEU:HB2	2:B:1639:LDA:H91	1.86	0.58
1:A:414:ARG:HG2	1:A:415:THR:H	1.69	0.58
1:A:410:ILE:HD11	1:A:416:PHE:CE1	2.38	0.58
1:B:615:ILE:HD13	1:B:616:ALA:N	2.19	0.57
1:A:218:PRO:HB2	1:A:219:ARG:HG2	1.87	0.57
1:A:316:ARG:HH22	1:A:536:ASN:HD21	1.52	0.57
1:A:252:MSE:HA	1:A:258:ARG:NH2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:NH1	1:A:256:ARG:CB	2.63	0.57
1:B:287:MSE:HE3	1:B:614:ASN:ND2	2.19	0.57
1:A:262:PRO:HB3	1:A:324:THR:HG22	1.87	0.57
1:A:463:TYR:CD1	1:B:592:LEU:HD11	2.40	0.57
1:B:550:GLY:HA2	1:B:571:ASP:HA	1.85	0.57
1:A:330:LEU:CD2	1:A:390:GLY:HA3	2.34	0.56
1:B:348:TYR:CE1	1:B:455:LEU:HD13	2.39	0.56
1:B:488:LEU:C	1:B:488:LEU:HD23	2.24	0.56
1:B:531:TYR:CD2	1:B:532:LEU:HD22	2.41	0.56
1:A:402:ASP:O	1:A:403:ILE:HD13	2.06	0.56
1:B:574:ASN:O	1:B:575:ASP:CB	2.34	0.56
1:A:392:ASP:OD1	1:A:393:LEU:N	2.38	0.56
1:B:254:PRO:HD3	1:B:332:ARG:NH1	2.20	0.56
1:A:413:GLU:O	1:A:414:ARG:CB	2.48	0.56
1:A:577:LEU:HD23	4:A:2014:HOH:O	2.05	0.56
1:B:391:TRP:HE3	1:B:399:LEU:HD23	1.71	0.55
1:B:368:ASN:CB	1:B:370:TRP:HE3	2.18	0.55
1:A:217:ILE:HG22	1:A:218:PRO:HD2	1.88	0.55
1:A:264:ILE:O	1:A:264:ILE:HG13	2.06	0.55
1:A:181:TRP:CE3	1:A:215:ARG:HB3	2.42	0.55
1:A:413:GLU:OE1	1:B:592:LEU:HD22	2.06	0.55
1:B:342:SER:HB3	2:B:1639:LDA:H61	1.88	0.55
1:B:476:ASN:ND2	1:B:487:ASN:ND2	2.56	0.54
1:A:470:MSE:HE3	1:A:472:THR:HG22	1.90	0.54
1:A:468:LYS:HG3	1:A:496:TRP:CZ2	2.42	0.54
1:B:287:MSE:CE	1:B:614:ASN:HD22	2.20	0.54
1:B:284:TYR:CD2	1:B:295:ILE:HD13	2.42	0.54
1:A:420:SER:HB3	1:A:444:SER:CB	2.37	0.54
1:B:376:ALA:HB2	1:B:385:LEU:CD1	2.37	0.54
1:B:159:ASN:HB2	1:B:163:GLY:H	1.73	0.54
1:B:386:ALA:CB	1:B:404:THR:HB	2.38	0.53
1:A:219:ARG:CG	1:A:219:ARG:NH1	2.66	0.53
1:B:231:ILE:HD11	1:B:238:SER:HA	1.90	0.53
1:B:451:MSE:O	1:B:455:LEU:HG	2.09	0.53
1:A:521:ALA:HB3	1:A:544:SER:OG	2.08	0.53
1:A:255:PRO:HA	1:A:258:ARG:HE	1.72	0.53
1:A:181:TRP:HA	1:A:181:TRP:CE3	2.43	0.53
1:A:479:VAL:C	1:A:481:ASP:N	2.62	0.53
1:B:184:ARG:NH1	1:B:186:ASP:OD1	2.42	0.53
1:A:515:PHE:CD1	1:A:515:PHE:N	2.77	0.52
1:A:519:GLY:O	1:A:546:PRO:HD3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:TRP:CD1	1:A:392:ASP:N	2.78	0.52
4:A:2002:HOH:O	1:B:348:TYR:HA	2.09	0.52
1:A:427:LYS:HB3	1:A:437:THR:HG23	1.91	0.52
1:A:311:ILE:HG13	1:A:311:ILE:O	2.10	0.52
1:B:393:LEU:CB	1:B:396:PRO:HG2	2.38	0.52
1:B:146:LEU:CD1	1:B:635:ILE:HD11	2.39	0.52
1:A:156:VAL:HG22	1:A:166:HIS:HD2	1.74	0.52
1:A:419:LYS:HG2	1:A:445:GLU:CD	2.30	0.52
1:A:271:ASN:O	1:A:313:GLN:HG3	2.10	0.52
1:B:157:SER:HB3	1:B:624:SER:HB3	1.91	0.52
1:A:373:TYR:CE2	1:A:402:ASP:OD1	2.62	0.52
1:A:160:TYR:HE2	1:B:461:ASN:HB2	1.75	0.52
1:A:160:TYR:CE2	1:B:461:ASN:HB2	2.45	0.52
1:A:342:SER:CB	2:A:1638:LDA:H41	2.36	0.51
1:A:501:THR:HG23	1:A:501:THR:O	2.10	0.51
1:A:330:LEU:HD21	1:A:390:GLY:HA3	1.93	0.51
1:A:573:PHE:CE1	1:A:578:ASP:HB2	2.46	0.51
1:B:347:GLY:C	1:B:348:TYR:CG	2.84	0.51
1:A:264:ILE:HD13	1:A:276:VAL:HG22	1.92	0.51
1:A:395:VAL:C	1:A:397:GLY:H	2.13	0.51
1:A:156:VAL:HG22	1:A:166:HIS:CD2	2.46	0.51
1:B:157:SER:CB	1:B:624:SER:HB3	2.40	0.51
1:B:599:ASN:OD1	1:B:599:ASN:C	2.48	0.51
1:B:146:LEU:HD12	1:B:635:ILE:HG13	1.91	0.51
1:A:271:ASN:HD21	1:A:599:ASN:ND2	2.04	0.51
1:A:564:VAL:HG22	1:A:587:ASN:OD1	2.11	0.51
1:B:253:LEU:CD1	1:B:257:LEU:HD23	2.37	0.51
1:B:148:LEU:O	1:B:632:GLY:HA2	2.10	0.51
1:A:264:ILE:CG1	1:A:295:ILE:HB	2.40	0.51
1:A:269:GLU:OE1	1:A:318:LYS:NZ	2.44	0.51
1:A:443:PHE:HA	1:A:468:LYS:O	2.11	0.51
1:A:411:GLU:C	1:A:413:GLU:H	2.14	0.51
1:B:368:ASN:HB3	1:B:370:TRP:HE3	1.76	0.51
1:A:393:LEU:HB2	1:A:397:GLY:O	2.11	0.50
1:A:326:SER:HB2	1:A:422:ARG:HH21	1.74	0.50
1:B:206:PHE:CD1	1:B:207:THR:N	2.78	0.50
1:B:586:LEU:HD22	1:B:594:SER:HB2	1.92	0.50
1:B:403:ILE:HD12	1:B:403:ILE:N	2.27	0.50
1:A:463:TYR:CD1	1:B:592:LEU:CD1	2.94	0.50
1:A:192:GLU:O	1:A:202:THR:HA	2.11	0.50
1:A:403:ILE:CD1	1:A:421:TRP:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:HG2	1:A:445:GLU:OE1	2.12	0.50
1:A:515:PHE:N	1:A:515:PHE:HD1	2.10	0.50
1:A:188:GLN:OE1	1:A:282:VAL:HG23	2.11	0.49
1:B:235:ILE:HG23	1:B:236:PHE:CD1	2.47	0.49
1:B:465:SER:HA	1:B:498:ILE:CD1	2.41	0.49
1:A:176:GLY:N	1:A:183:LEU:HB3	2.27	0.49
1:A:215:ARG:HG3	1:A:215:ARG:O	2.12	0.49
1:A:411:GLU:O	1:A:413:GLU:N	2.45	0.49
1:B:466:ARG:HG2	1:B:497:ASP:OD1	2.12	0.49
1:A:368:ASN:C	1:A:370:TRP:H	2.15	0.49
1:B:580:TYR:CE1	1:B:602:TYR:HB2	2.47	0.49
1:A:344:ARG:HB3	1:A:354:GLY:O	2.12	0.49
1:B:263:GLN:HE22	1:B:487:ASN:HD21	1.59	0.49
1:A:263:GLN:CG	1:A:296:GLN:HB3	2.42	0.49
1:A:521:ALA:O	1:A:543:ILE:HA	2.12	0.49
1:B:231:ILE:HD12	1:B:231:ILE:C	2.32	0.49
1:B:382:TYR:CE2	1:B:451:MSE:HG2	2.47	0.49
1:A:232:ASN:N	1:A:232:ASN:HD22	2.09	0.49
1:A:264:ILE:HD13	1:A:276:VAL:CG2	2.42	0.49
1:A:514:VAL:HG12	1:A:515:PHE:CE1	2.47	0.49
1:A:570:THR:CB	1:A:581:SER:HB3	2.42	0.49
1:B:146:LEU:HD12	1:B:635:ILE:CG1	2.43	0.48
1:A:181:TRP:CZ3	1:A:215:ARG:HB3	2.48	0.48
1:A:611:LEU:HD23	1:A:612:SER:N	2.28	0.48
1:B:493:GLN:HB3	1:B:501:THR:HG22	1.95	0.48
1:A:458:ARG:HD3	1:A:458:ARG:O	2.14	0.48
1:A:275:VAL:HA	1:A:284:TYR:O	2.13	0.48
1:A:413:GLU:HG2	1:A:463:TYR:OH	2.14	0.48
1:B:330:LEU:HD21	1:B:390:GLY:HA3	1.96	0.48
1:A:180:PRO:O	1:A:215:ARG:CB	2.35	0.48
1:A:573:PHE:CD1	1:A:578:ASP:HB2	2.48	0.48
1:B:217:ILE:HG21	1:B:220:TRP:CB	2.42	0.48
1:A:411:GLU:C	1:A:413:GLU:N	2.66	0.48
1:B:388:GLY:HA3	1:B:402:ASP:HB3	1.96	0.48
1:B:531:TYR:CD2	1:B:532:LEU:CD2	2.97	0.48
1:A:198:GLY:HA3	1:B:205:ASN:HD22	1.79	0.48
1:B:264:ILE:HD12	1:B:276:VAL:HG11	1.96	0.48
1:A:242:THR:OG1	1:A:346:ARG:HD2	2.14	0.48
1:A:427:LYS:HB3	1:A:437:THR:HG22	1.96	0.48
1:A:237:ARG:HH22	1:A:467:GLU:CD	2.16	0.48
1:B:395:VAL:HG23	1:B:395:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLY:H	1:A:183:LEU:HB3	1.78	0.47
1:B:514:VAL:O	1:B:514:VAL:CG1	2.62	0.47
1:A:543:ILE:HD13	1:A:543:ILE:H	1.79	0.47
1:A:257:LEU:HD22	1:A:330:LEU:HB2	1.95	0.47
1:A:429:PHE:N	1:A:429:PHE:HD2	2.07	0.47
1:B:217:ILE:CG2	1:B:220:TRP:HB2	2.43	0.47
1:B:391:TRP:CE3	1:B:399:LEU:HD23	2.49	0.47
1:B:580:TYR:CD1	1:B:602:TYR:HB2	2.48	0.47
1:A:164:ASP:HB2	1:A:195:ARG:HH12	1.79	0.47
1:B:240:SER:HB2	1:B:346:ARG:NH1	2.29	0.47
1:B:397:GLY:HA3	1:B:425:TYR:CE1	2.49	0.47
1:B:170:TYR:OH	1:B:206:PHE:HD2	1.98	0.47
1:B:231:ILE:CG1	1:B:238:SER:HA	2.45	0.47
1:A:193:GLN:HA	1:A:201:THR:O	2.14	0.47
1:A:218:PRO:HG2	1:A:219:ARG:CG	2.45	0.47
1:A:479:VAL:O	1:A:481:ASP:N	2.47	0.47
1:A:235:ILE:HG12	1:A:361:GLU:CD	2.35	0.47
1:A:365:GLY:CA	4:A:2006:HOH:O	2.37	0.47
1:B:153:ASN:HB2	1:B:169:SER:OG	2.15	0.47
1:B:185:ALA:HB1	1:B:208:TRP:CZ3	2.50	0.47
1:B:437:THR:OG1	1:B:475:LEU:HD23	2.14	0.47
1:A:159:ASN:HB2	1:A:163:GLY:H	1.79	0.47
1:A:578:ASP:OD1	1:A:604:HIS:ND1	2.48	0.47
1:B:256:ARG:HA	1:B:428:ARG:NH1	2.30	0.47
1:A:373:TYR:OH	1:A:402:ASP:OD1	2.27	0.47
1:A:235:ILE:CD1	1:A:375:GLY:HA3	2.44	0.47
1:B:448:TYR:O	1:B:466:ARG:NH2	2.48	0.47
1:B:488:LEU:HD23	1:B:489:GLN:N	2.30	0.47
1:B:512:PHE:N	1:B:520:VAL:O	2.41	0.47
1:A:468:LYS:HE3	1:A:496:TRP:CZ3	2.49	0.46
1:A:514:VAL:HB	1:A:515:PHE:HD1	1.80	0.46
1:B:410:ILE:CD1	1:B:454:TYR:CE1	2.98	0.46
1:A:224:LEU:C	1:A:224:LEU:HD23	2.35	0.46
1:A:278:GLN:NE2	1:A:305:ARG:O	2.49	0.46
1:B:206:PHE:CD1	1:B:206:PHE:C	2.89	0.46
1:B:460:ARG:HG2	1:B:460:ARG:HH11	1.80	0.46
1:A:231:ILE:HD12	1:A:231:ILE:C	2.35	0.46
1:A:224:LEU:HD23	1:A:225:THR:N	2.31	0.46
1:A:391:TRP:HD1	1:A:392:ASP:N	2.13	0.46
1:A:420:SER:HB3	1:A:444:SER:HB3	1.96	0.46
1:A:486:PHE:CD1	1:A:508:VAL:HG22	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:MSE:CE	1:B:597:GLN:OE1	2.63	0.46
1:B:634:THR:O	1:B:634:THR:HG23	2.15	0.46
1:A:264:ILE:HG12	1:A:295:ILE:HB	1.97	0.46
1:A:436:ILE:HD11	1:A:476:ASN:HB2	1.97	0.46
1:A:410:ILE:CD1	1:A:416:PHE:HE1	2.27	0.46
1:B:224:LEU:C	1:B:224:LEU:HD23	2.36	0.46
1:B:514:VAL:HG12	1:B:520:VAL:HG21	1.98	0.46
1:B:481:ASP:O	1:B:482:TRP:CD1	2.69	0.46
1:A:253:LEU:O	1:A:254:PRO:C	2.54	0.45
1:A:279:GLN:HE22	1:A:452:GLU:CD	2.19	0.45
1:B:257:LEU:HD11	1:B:330:LEU:HB2	1.98	0.45
1:B:364:TRP:HE3	1:B:372:LEU:O	1.98	0.45
1:B:458:ARG:C	1:B:458:ARG:HD3	2.37	0.45
1:B:196:TYR:CG	1:B:197:ASN:N	2.84	0.45
1:B:311:ILE:HD12	1:B:311:ILE:N	2.31	0.45
1:B:188:GLN:OE1	1:B:282:VAL:HG23	2.16	0.45
1:B:262:PRO:HB3	1:B:324:THR:HB	1.99	0.45
1:B:543:ILE:HD13	1:B:543:ILE:N	2.31	0.45
1:A:419:LYS:N	1:A:445:GLU:OE1	2.50	0.45
1:B:536:ASN:HA	1:B:560:ASN:OD1	2.17	0.45
1:A:263:GLN:HG3	1:A:296:GLN:HB3	1.98	0.45
1:A:404:THR:O	1:A:419:LYS:HA	2.16	0.45
1:A:619:GLN:C	1:A:621:GLY:N	2.69	0.45
1:B:514:VAL:O	1:B:515:PHE:HB3	2.16	0.45
1:A:525:SER:O	1:A:539:ALA:HA	2.17	0.45
1:A:573:PHE:N	1:A:573:PHE:CD2	2.84	0.45
1:B:368:ASN:HB2	1:B:370:TRP:HE3	1.82	0.45
1:A:235:ILE:CD1	1:A:361:GLU:HG3	2.47	0.45
1:A:454:TYR:O	1:A:457:ALA:HB3	2.16	0.45
1:A:237:ARG:NH2	1:A:467:GLU:OE1	2.50	0.45
3:B:1637:C8E:O9	3:B:1637:C8E:H132	2.14	0.45
1:B:262:PRO:O	1:B:298:LEU:HD12	2.17	0.45
1:B:615:ILE:CD1	1:B:615:ILE:C	2.85	0.45
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.79	0.44
1:B:231:ILE:HG13	1:B:238:SER:HA	1.99	0.44
1:A:185:ALA:HB1	1:A:208:TRP:CZ3	2.51	0.44
1:A:488:LEU:HD13	1:A:488:LEU:C	2.38	0.44
1:B:577:LEU:O	1:B:605:ARG:N	2.50	0.44
1:A:373:TYR:CZ	1:A:402:ASP:OD1	2.71	0.44
1:A:551:THR:HG23	1:A:570:THR:CG2	2.33	0.44
1:B:155:THR:HA	1:B:626:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:CG2	1:A:245:SER:OG	2.66	0.44
1:A:202:THR:O	1:B:201:THR:HA	2.17	0.44
1:B:217:ILE:CG2	1:B:220:TRP:CB	2.96	0.44
1:A:627:VAL:HG12	1:A:628:SER:N	2.32	0.44
1:B:470:MSE:O	1:B:470:MSE:HE3	2.18	0.44
1:B:197:ASN:HD22	1:B:198:GLY:N	2.15	0.44
1:A:159:ASN:HB2	1:A:163:GLY:N	2.32	0.44
1:A:235:ILE:HG13	1:A:236:PHE:CD1	2.53	0.44
1:B:231:ILE:CD1	1:B:238:SER:HA	2.48	0.44
1:B:380:GLY:O	1:B:383:ASN:ND2	2.51	0.44
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.83	0.43
1:A:316:ARG:NH2	1:A:318:LYS:HZ3	2.05	0.43
1:A:253:LEU:O	1:A:258:ARG:CZ	2.66	0.43
1:A:513:ASN:OD1	1:A:518:GLN:HA	2.18	0.43
1:A:259:GLY:HA3	1:A:303:ARG:NH2	2.33	0.43
1:A:470:MSE:O	1:A:470:MSE:HE2	2.18	0.43
1:B:413:GLU:HG3	1:B:463:TYR:OH	2.18	0.43
1:A:225:THR:HG23	1:A:245:SER:OG	2.18	0.43
1:A:304:GLY:O	1:A:324:THR:HG23	2.19	0.43
1:B:623:THR:HG23	1:B:623:THR:O	2.19	0.43
1:A:399:LEU:HD12	1:A:425:TYR:CD1	2.54	0.43
1:A:543:ILE:N	1:A:543:ILE:HD13	2.33	0.43
1:A:157:SER:HB3	1:A:624:SER:HB2	2.01	0.43
1:B:194:SER:O	1:B:200:LYS:HA	2.18	0.43
1:B:237:ARG:HD2	1:B:450:THR:HG21	2.01	0.43
1:B:314:ASN:HD21	1:B:316:ARG:HD2	1.83	0.43
1:B:330:LEU:CD2	1:B:390:GLY:HA3	2.47	0.43
1:B:540:TYR:CE2	1:B:555:SER:HB3	2.54	0.43
1:A:316:ARG:NH2	1:A:318:LYS:HZ2	1.98	0.43
1:B:368:ASN:CB	1:B:370:TRP:CE3	3.00	0.43
1:B:490:TYR:OH	1:B:492:ARG:HD2	2.19	0.43
1:B:224:LEU:CD1	2:B:1639:LDA:H123	2.49	0.42
1:B:233:SER:HB3	1:B:236:PHE:O	2.19	0.42
1:B:586:LEU:CD2	1:B:594:SER:HB2	2.49	0.42
1:A:270:THR:C	1:A:290:ALA:HB2	2.39	0.42
1:A:382:TYR:CE2	1:A:451:MSE:HG2	2.55	0.42
1:B:532:LEU:H	1:B:532:LEU:HD22	1.83	0.42
1:A:261:ALA:HA	1:A:262:PRO:HD3	1.79	0.42
1:B:438:PHE:CD2	1:B:438:PHE:C	2.92	0.42
1:A:273:ARG:HA	1:A:287:MSE:HA	2.02	0.42
1:B:231:ILE:HG12	1:B:239:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:SER:HB2	1:B:346:ARG:HH12	1.85	0.42
1:B:563:TYR:HD2	1:B:588:SER:HG	1.66	0.42
1:B:310:VAL:HB	1:B:318:LYS:HB2	2.00	0.42
1:B:507:SER:HA	1:B:524:LEU:O	2.19	0.42
1:A:463:TYR:CD2	1:B:592:LEU:HD11	2.54	0.42
1:B:627:VAL:HG12	1:B:628:SER:N	2.34	0.42
1:B:410:ILE:CD1	1:B:454:TYR:HE1	2.32	0.42
1:A:208:TRP:O	1:A:209:SER:C	2.58	0.42
1:A:275:VAL:HG13	1:A:309:GLU:HB3	2.02	0.42
1:A:574:ASN:N	1:A:574:ASN:HD22	2.18	0.42
1:A:573:PHE:O	1:A:574:ASN:HB2	2.20	0.42
1:B:348:TYR:OH	1:B:452:GLU:OE2	2.38	0.42
1:B:531:TYR:O	1:B:533:GLY:N	2.48	0.42
1:A:151:ASN:HB3	1:A:171:ASN:O	2.19	0.41
1:A:493:GLN:C	1:A:493:GLN:HE21	2.23	0.41
1:A:514:VAL:HG12	1:A:515:PHE:HE1	1.85	0.41
1:A:619:GLN:O	1:A:621:GLY:N	2.53	0.41
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.57	0.41
1:A:470:MSE:CE	1:A:472:THR:HG22	2.49	0.41
1:B:253:LEU:CB	1:B:254:PRO:HD2	2.35	0.41
1:B:592:LEU:HA	1:B:592:LEU:HD23	1.77	0.41
1:A:381:ASP:HB2	1:A:454:TYR:OH	2.19	0.41
1:B:256:ARG:HA	1:B:428:ARG:HH22	1.84	0.41
1:B:395:VAL:C	1:B:397:GLY:H	2.24	0.41
1:A:235:ILE:HG13	1:A:236:PHE:N	2.35	0.41
1:A:558:MSE:HE3	1:A:560:ASN:O	2.20	0.41
1:B:368:ASN:HB3	1:B:370:TRP:CE3	2.54	0.41
1:B:410:ILE:HD12	1:B:410:ILE:HG23	1.85	0.41
1:B:468:LYS:HB3	1:B:494:THR:HG23	2.01	0.41
1:B:575:ASP:HB3	1:B:576:GLY:H	1.65	0.41
1:B:316:ARG:CD	4:B:2004:HOH:O	2.55	0.41
1:A:262:PRO:CB	1:A:324:THR:HG22	2.50	0.41
1:B:357:PHE:CD1	1:B:357:PHE:C	2.94	0.41
1:B:578:ASP:CG	1:B:604:HIS:HD1	2.24	0.41
2:A:1638:LDA:H41	2:A:1638:LDA:H12	1.85	0.41
1:A:154:GLY:HA2	1:A:167:GLN:O	2.19	0.41
1:B:261:ALA:HA	1:B:262:PRO:HD3	1.81	0.41
1:B:575:ASP:HB3	1:B:577:LEU:HD13	2.03	0.41
1:B:619:GLN:C	1:B:621:GLY:N	2.73	0.40
1:A:403:ILE:CD1	1:A:403:ILE:N	2.83	0.40
1:A:463:TYR:CD1	1:A:463:TYR:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HA	1:B:287:MSE:HA	2.03	0.40
3:B:1637:C8E:O9	3:B:1637:C8E:H131	2.16	0.40
1:B:402:ASP:C	1:B:403:ILE:HD12	2.41	0.40
1:A:229:ASN:OD1	1:A:230:ASN:N	2.51	0.40
1:A:247:GLU:HB3	1:A:339:LYS:HG2	2.03	0.40
1:B:247:GLU:CG	1:B:339:LYS:HG2	2.52	0.40
1:A:425:TYR:CZ	1:A:427:LYS:HB2	2.57	0.40
1:B:497:ASP:OD2	1:B:498:ILE:HD12	2.21	0.40
1:B:504:TYR:OH	1:B:506:VAL:HG21	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/515 (90%)	416 (90%)	40 (9%)	7 (2%)	10	44
1	B	467/515 (91%)	424 (91%)	37 (8%)	6 (1%)	12	47
All	All	930/1030 (90%)	840 (90%)	77 (8%)	13 (1%)	11	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	ARG
1	B	395	VAL
1	B	414	ARG
1	B	575	ASP
1	A	480	ALA
1	A	256	ARG
1	B	198	GLY
1	B	411	GLU
1	B	532	LEU

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Mol	Chain	Res	Type
1	A	254	PRO
1	A	593	THR
1	A	412	GLY
1	A	620	LYS

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	396/414 (96%)	327 (83%)	69 (17%)	2 10
1	B	392/414 (95%)	330 (84%)	62 (16%)	2 12
All	All	788/828 (95%)	657 (83%)	131 (17%)	2 10

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	THR
1	A	161	GLN
1	A	178	LEU
1	A	181	TRP
1	A	195	ARG
1	A	201	THR
1	A	205	ASN
1	A	214	PHE
1	A	215	ARG
1	A	219	ARG
1	A	220	TRP
1	A	225	THR
1	A	226	LEU
1	A	232	ASN
1	A	237	ARG
1	A	248	SER
1	A	256	ARG
1	A	263	GLN
1	A	278	GLN

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Mol	Chain	Res	Type
1	A	285	ASP
1	A	288	VAL
1	A	296	GLN
1	A	299	ASP
1	A	305	ARG
1	A	311	ILE
1	A	319	THR
1	A	323	ASP
1	A	332	ARG
1	A	340	LEU
1	A	395	VAL
1	A	398	THR
1	A	399	LEU
1	A	404	THR
1	A	410	ILE
1	A	423	LEU
1	A	428	ARG
1	A	429	PHE
1	A	446	ARG
1	A	453	GLN
1	A	458	ARG
1	A	464	SER
1	A	467	GLU
1	A	475	LEU
1	A	484	THR
1	A	493	GLN
1	A	494	THR
1	A	506	VAL
1	A	515	PHE
1	A	537	ASP
1	A	543	ILE
1	A	551	THR
1	A	558	MSE
1	A	560	ASN
1	A	561	ASP
1	A	563	TYR
1	A	565	ASN
1	A	566	MSE
1	A	570	THR
1	A	574	ASN
1	A	575	ASP
1	A	582	LEU

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Mol	Chain	Res	Type
1	A	586	LEU
1	A	594	SER
1	A	598	ILE
1	A	599	ASN
1	A	608	LEU
1	A	614	ASN
1	A	615	ILE
1	A	618	LEU
1	B	147	MSE
1	B	164	ASP
1	B	165	SER
1	B	183	LEU
1	B	184	ARG
1	B	188	GLN
1	B	197	ASN
1	B	202	THR
1	B	203	ASN
1	B	205	ASN
1	B	210	ARG
1	B	221	ARG
1	B	226	LEU
1	B	245	SER
1	B	256	ARG
1	B	275	VAL
1	B	278	GLN
1	B	288	VAL
1	B	299	ASP
1	B	303	ARG
1	B	319	THR
1	B	323	ASP
1	B	331	THR
1	B	335	GLN
1	B	342	SER
1	B	344	ARG
1	B	348	TYR
1	B	361	GLU
1	B	367	SER
1	B	372	LEU
1	B	399	LEU
1	B	404	THR
1	B	420	SER
1	B	429	PHE

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Mol	Chain	Res	Type
1	B	436	ILE
1	B	444	SER
1	B	449	MSE
1	B	453	GLN
1	B	458	ARG
1	B	470	MSE
1	B	485	SER
1	B	493	GLN
1	B	498	ILE
1	B	502	ASP
1	B	515	PHE
1	B	532	LEU
1	B	537	ASP
1	B	543	ILE
1	B	551	THR
1	B	555	SER
1	B	561	ASP
1	B	563	TYR
1	B	575	ASP
1	B	577	LEU
1	B	586	LEU
1	B	593	THR
1	B	594	SER
1	B	599	ASN
1	B	605	ARG
1	B	614	ASN
1	B	615	ILE
1	B	618	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	166	HIS
1	A	167	GLN
1	A	232	ASN
1	A	278	GLN
1	A	279	GLN
1	A	493	GLN
1	A	536	ASN
1	A	565	ASN
1	A	597	GLN

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Mol	Chain	Res	Type
1	A	599	ASN
1	B	151	ASN
1	B	197	ASN
1	B	205	ASN
1	B	278	GLN
1	B	314	ASN
1	B	335	GLN
1	B	369	GLN
1	B	476	ASN
1	B	487	ASN
1	B	493	GLN
1	B	595	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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LDA	A	1638	-	12,15,15	2.09	1 (8%)	14,17,17	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LDA	B	1639	-	12,15,15	2.08	1 (8%)	14,17,17	0.52	0
3	C8E	B	1638	-	20,20,20	0.38	0	19,19,19	0.39	0
3	C8E	B	1637	-	20,20,20	0.37	0	19,19,19	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	A	1638	-	-	10/13/13/13	-
2	LDA	B	1639	-	-	4/13/13/13	-
3	C8E	B	1638	-	-	10/18/18/18	-
3	C8E	B	1637	-	-	8/18/18/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1638	LDA	O1-N1	-7.18	1.25	1.42
2	B	1639	LDA	O1-N1	-7.17	1.25	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1638	LDA	C2-C1-N1-O1
2	A	1638	LDA	C2-C1-N1-CM1
2	A	1638	LDA	C2-C1-N1-CM2
3	B	1638	C8E	C4-C5-C6-C7
3	B	1637	C8E	C10-C11-O12-C13
3	B	1638	C8E	O12-C13-C14-O15
3	B	1637	C8E	O12-C13-C14-O15
2	A	1638	LDA	C4-C5-C6-C7
2	A	1638	LDA	C5-C6-C7-C8
3	B	1638	C8E	C5-C6-C7-C8
2	B	1639	LDA	C2-C3-C4-C5
2	B	1639	LDA	C1-C2-C3-C4
2	B	1639	LDA	C6-C7-C8-C9
3	B	1637	C8E	O9-C10-C11-O12

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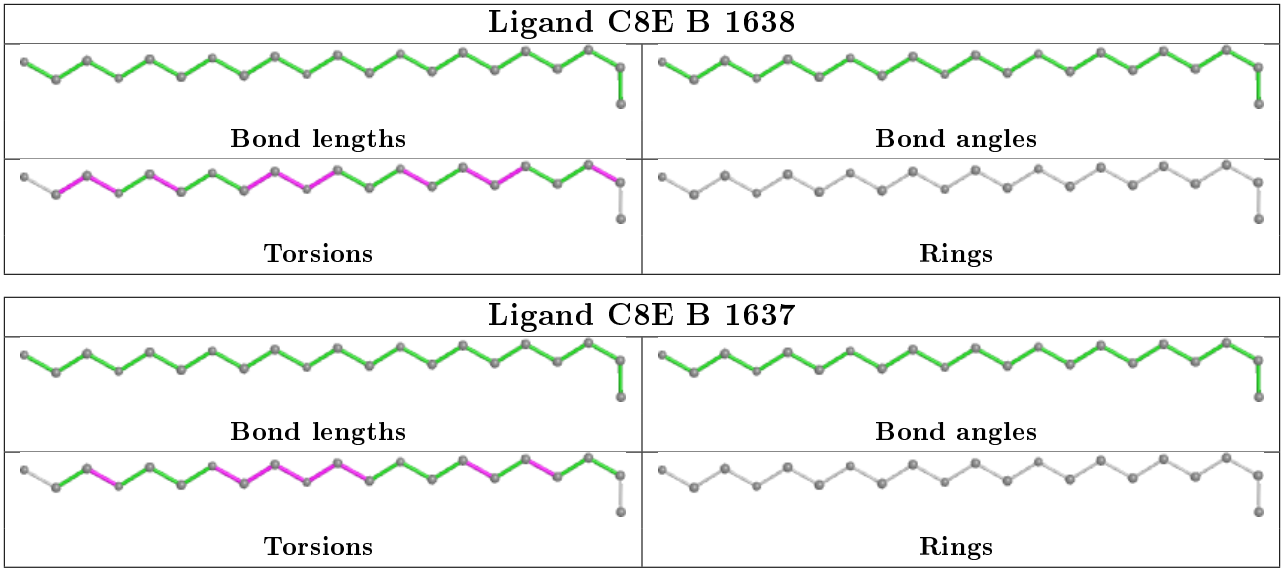
Mol	Chain	Res	Type	Atoms
2	A	1638	LDA	C2-C3-C4-C5
3	B	1638	C8E	O18-C19-C20-O21
3	B	1638	C8E	C1-C2-C3-C4
3	B	1637	C8E	C3-C4-C5-C6
2	A	1638	LDA	C9-C10-C11-C12
3	B	1637	C8E	C5-C6-C7-C8
2	B	1639	LDA	C3-C4-C5-C6
3	B	1637	C8E	C14-C13-O12-C11
3	B	1637	C8E	C13-C14-O15-C16
3	B	1638	C8E	C14-C13-O12-C11
3	B	1638	C8E	C7-C8-O9-C10
2	A	1638	LDA	C6-C7-C8-C9
3	B	1638	C8E	C20-C19-O18-C17
3	B	1637	C8E	C20-C19-O18-C17
2	A	1638	LDA	C11-C10-C9-C8
3	B	1638	C8E	C10-C11-O12-C13
2	A	1638	LDA	C1-C2-C3-C4
3	B	1638	C8E	O15-C16-C17-O18

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1638	LDA	6	0
2	B	1639	LDA	3	0
3	B	1637	C8E	6	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	469/515 (91%)	-0.36	0 100 100	18, 47, 75, 87	33 (7%)
1	B	469/515 (91%)	-0.36	5 (1%) 80 69	21, 47, 75, 91	32 (6%)
All	All	938/1030 (91%)	-0.36	5 (0%) 91 86	18, 47, 75, 91	65 (6%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	636	THR	2.9
1	B	429	PHE	2.8
1	B	349	GLY	2.6
1	B	219	ARG	2.5
1	B	435	ASP	2.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

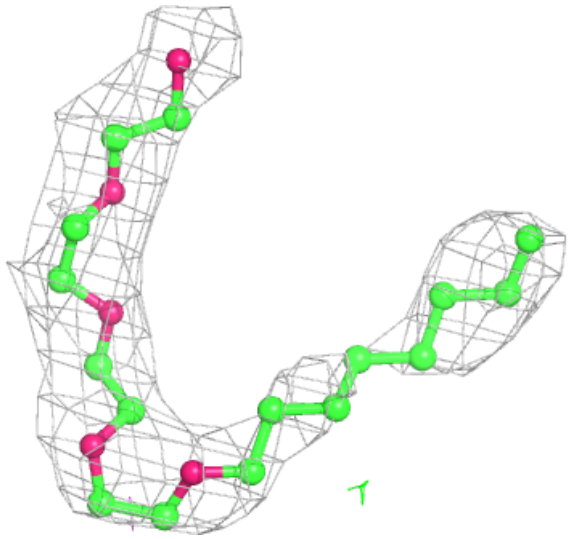
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

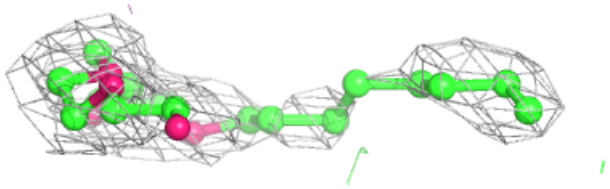
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C8E	B	1637	21/21	0.78	0.34	77,83,86,86	0
2	LDA	B	1639	16/16	0.82	0.28	54,57,70,70	0
3	C8E	B	1638	21/21	0.85	0.30	81,90,93,94	0
2	LDA	A	1638	16/16	0.89	0.27	78,83,89,90	0

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 C8E B 1637:

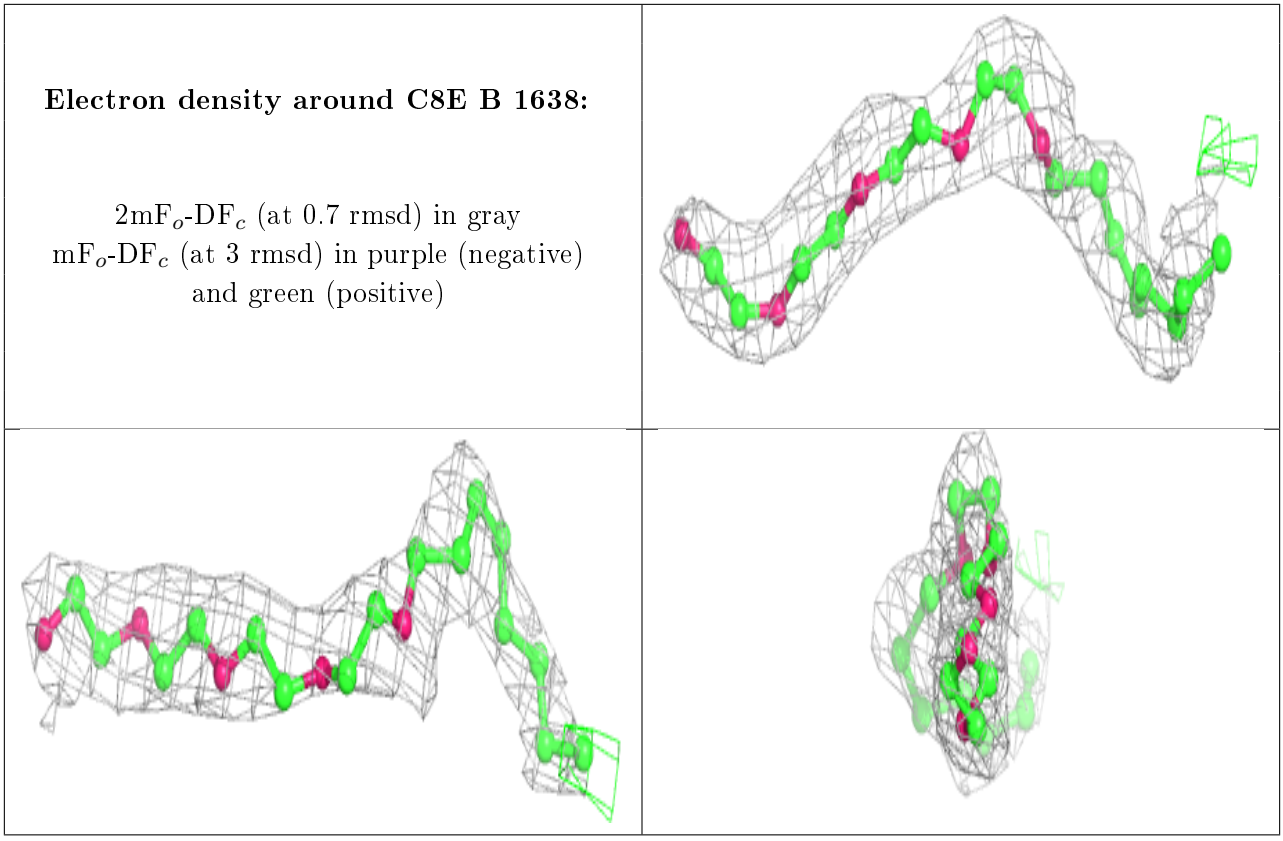
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around C8E B 1638:

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



6.5 Other polymers (i)

There are no such residues in this entry.