



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 05:15 PM UTC

PDB ID : 2VQI / pdb_00002vqi
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 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

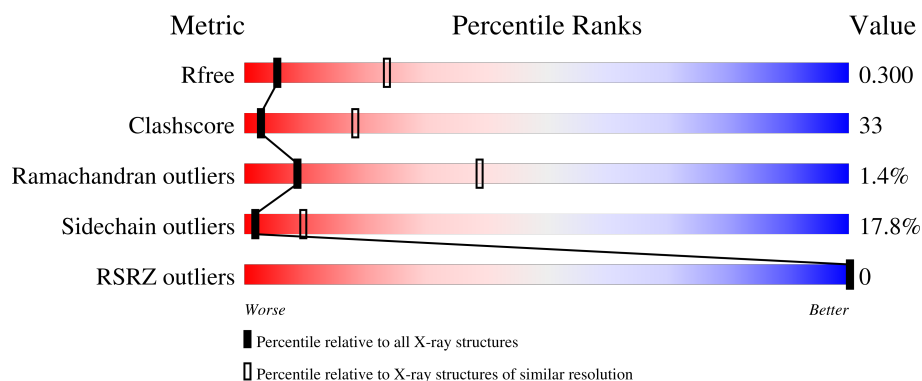
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	515	
1	B	515	

2 Entry composition [i](#)

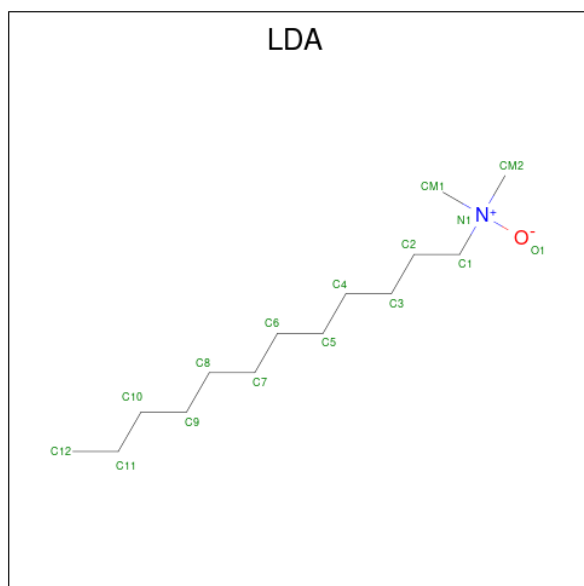
There are 4 unique types of molecules in this entry. The entry contains 7625 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

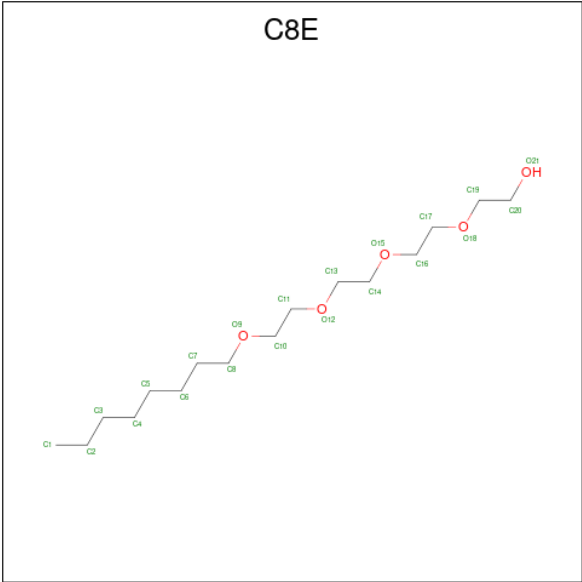
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	Se	0	0	0
			3767	2353	675	731	8			
1	B	477	Total	C	N	O	Se	0	0	0
			3750	2342	674	726	8			

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: 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 (CCD ID: C8E) (formula: $C_{16}H_{34}O_5$).



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

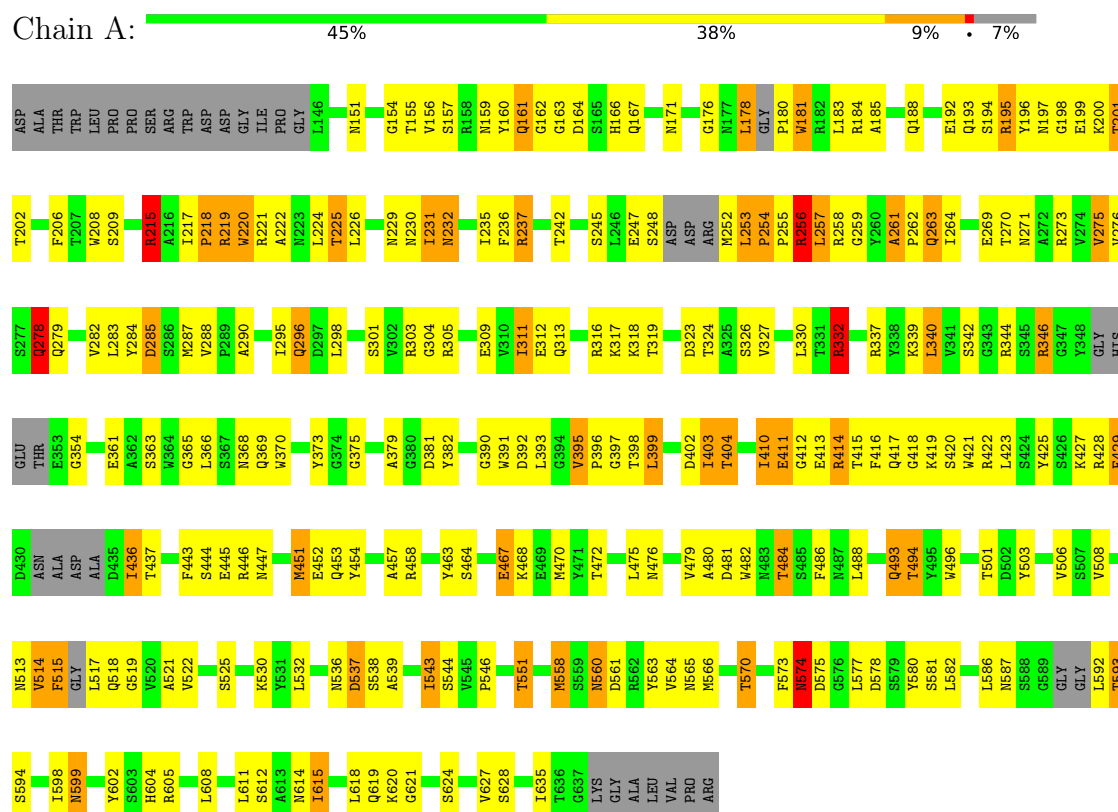
- Molecule 4 is water.

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

3 Residue-property plots

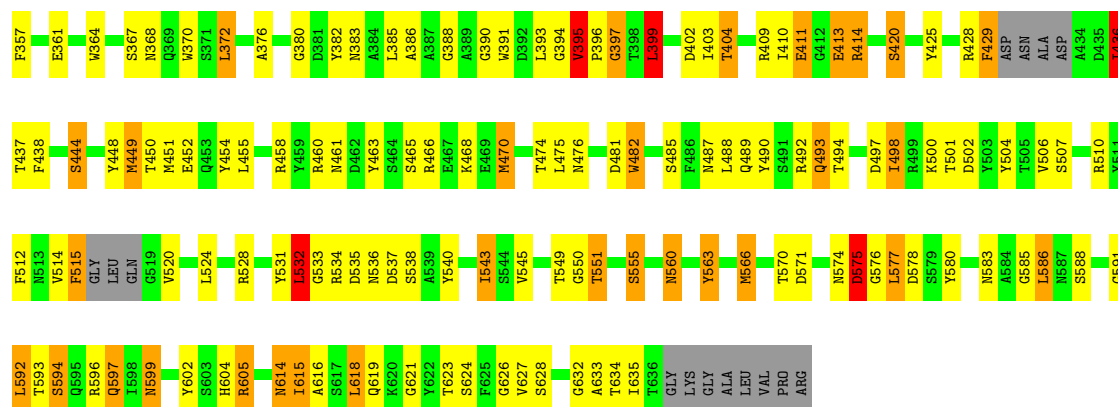
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: OUTER MEMBRANE USHER PROTEIN PAPC



• Molecule 1: OUTER MEMBRANE USHER PROTEIN PAPC





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.259 , 0.296 0.264 , 0.300	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)	0.24 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C8E, LDA

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	0.51	0/3840	0.95	16/5184 (0.3%)
1	B	0.63	2/3825 (0.1%)	1.02	20/5167 (0.4%)
All	All	0.57	2/7665 (0.0%)	0.99	36/10351 (0.3%)

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	15.35	2.41	1.95
1	B	147	MSE	SE-CE	13.72	2.36	1.95

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	PRO	CA-C-N	8.81	128.45	118.85
1	B	254	PRO	C-N-CA	8.81	128.45	118.85
1	B	436	ILE	N-CA-C	8.24	120.45	108.58
1	B	238	SER	N-CA-C	8.23	120.53	110.41
1	B	549	THR	N-CA-C	-7.36	104.15	113.72
1	A	369	GLN	N-CA-C	-7.05	104.77	113.15
1	A	538	SER	N-CA-C	7.04	121.06	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	GLU	N-CA-C	7.01	120.54	110.24
1	A	298	LEU	N-CA-C	6.96	120.58	110.28
1	A	574	ASN	N-CA-C	-6.92	104.14	112.58
1	B	583	ASN	N-CA-C	6.69	120.07	109.50
1	A	605	ARG	N-CA-C	6.69	117.97	108.54
1	B	147	MSE	CG-SE-CE	-6.69	84.21	98.92
1	B	173	THR	N-CA-C	6.19	118.54	108.26
1	A	253	LEU	N-CA-C	-6.16	102.59	108.13
1	B	482	TRP	N-CA-C	-6.11	103.42	113.50
1	A	221	ARG	N-CA-C	-6.10	104.43	112.24
1	A	327	VAL	N-CA-C	5.81	115.29	108.96
1	B	500	LYS	N-CA-C	5.80	118.42	110.24
1	B	197	ASN	N-CA-C	5.62	119.64	112.34
1	B	342	SER	N-CA-C	5.61	116.93	108.46
1	A	301	SER	N-CA-C	5.48	119.67	112.92
1	A	261	ALA	CA-C-N	5.48	126.69	119.84
1	A	261	ALA	C-N-CA	5.48	126.69	119.84
1	B	597	GLN	N-CA-C	5.40	118.20	109.40
1	A	332	ARG	CA-C-N	5.26	126.41	119.84
1	A	332	ARG	C-N-CA	5.26	126.41	119.84
1	B	320	PHE	N-CA-C	5.24	116.25	108.86
1	A	537	ASP	N-CA-C	5.24	117.26	107.99
1	A	366	LEU	N-CA-C	-5.22	103.64	110.53
1	B	327	VAL	CA-C-N	5.14	126.26	119.84
1	B	327	VAL	C-N-CA	5.14	126.26	119.84
1	B	545	VAL	N-CA-C	5.10	113.06	107.60
1	B	399	LEU	N-CA-C	5.09	116.81	109.07
1	B	409	ARG	CB-CG-CD	5.06	122.94	111.30
1	B	538	SER	N-CA-C	5.06	116.67	109.14

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

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Mol	Chain	Res	Type	Group
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	255	0
1	B	3750	0	3576	229	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	478	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 33.

All (478) 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:SE	1:B:147:MSE:CE	2.36	1.23
1:A:180:PRO:O	1:A:215:ARG:HB2	1.40	1.20
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	1.12
1:A:256:ARG:HH11	1:A:256:ARG:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:GLY:C	1:B:396:PRO:CD	2.30	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: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:B:394:GLY:C	1:B:396:PRO:HD2	1.89	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:N	1:B:577:LEU:HD13	1.82	0.93
1:B:394:GLY:C	1:B:395:VAL:CG1	2.41	0.92
1:A:264:ILE:HD11	1:A:295:ILE:HD12	1.52	0.91
1:A:402:ASP:C	1:A:403:ILE:HD13	1.96	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:B:394:GLY:C	1:B:396:PRO:HD3	1.97	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:184:ARG:HG3	1:B:184:ARG:HH11	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: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:A:271:ASN:ND2	1:A:599:ASN:HD21	1.74	0.85
1:A:395:VAL:N	1:A:396:PRO:HD2	1.92	0.85
1:A:515:PHE:C	1:A:517:LEU:N	2.36	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:256:ARG:CB	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: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:HB2	1:A:256:ARG:NH1	1.99	0.76
1:B:184:ARG:HH11	1:B:184:ARG:CG	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:C13	3:B:1637:C8E:O9	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
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:N	1:A:429:PHE:CD2	2.55	0.72
1:B:515:PHE:C	1:B:515:PHE:CD2	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:SER:O	1:A:200:LYS:HA	1.90	0.72
1:B:615:ILE:C	1:B:615:ILE:HD13	2.15	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:A:479:VAL:C	1:A:481:ASP:H	2.00	0.70
1:A:514:VAL:C	1:A:515:PHE:HD1	2.00	0.70
1:B:498:ILE:HD13	1:B:498:ILE:H	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:A:220:TRP:CD1	1:A:220:TRP:N	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: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:410:ILE:HD11	1:A:416:PHE:HE1	1.60	0.65
1:A:458:ARG:HD3	1:A:458:ARG:C	2.22	0.65
1:B:270:THR:C	1:B:290:ALA:HB2	2.23	0.64
1:A:514:VAL:C	1:A:515:PHE:CD1	2.75	0.64
1:B:256:ARG:HA	1:B:428:ARG:NH2	2.12	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
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:HH11	1:A:332:ARG:CG	2.05	0.62
1:A:235:ILE:HD11	1:A:361:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:ARG:HH21	1:A:416:PHE:HE2	1.47	0.61
1:B:488:LEU:C	1:B:488:LEU:HD23	2.24	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:B:184:ARG:CG	1:B:184:ARG:NH1	2.62	0.60
1:A:403:ILE:HD13	1:A:403:ILE:N	2.13	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: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:410:ILE:HD11	1:A:416:PHE:CE1	2.38	0.58
1:A:414:ARG:HG2	1:A:415:THR:H	1.69	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
1:A:256:ARG:CB	1:A:256:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:TYR:CE1	1:B:455:LEU:HD13	2.39	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:A:419:LYS:HG2	1:A:445:GLU:CD	2.30	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:B:347:GLY:C	1:B:348:TYR:CG	2.84	0.56
1:A:413:GLU:O	1:A:414:ARG:CB	2.48	0.56
1:B:599:ASN:OD1	1:B:599:ASN:C	2.48	0.56
1:A:395:VAL:C	1:A:397:GLY:H	2.13	0.56
1:A:577:LEU:HD23	4:A:2014:HOH:O	2.05	0.56
1:A:411:GLU:C	1:A:413:GLU:H	2.14	0.55
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:231:ILE:HD12	1:B:231:ILE:C	2.32	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:NH1	1:A:219:ARG:CG	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:237:ARG:HH22	1:A:467:GLU:CD	2.16	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:368:ASN:C	1:A:370:TRP:H	2.15	0.53
1:A:181:TRP:CE3	1:A:181:TRP:HA	2.43	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:146:LEU:CD1	1:B:635:ILE:HD11	2.39	0.52
1:B:393:LEU:CB	1:B:396:PRO:HG2	2.38	0.52
1:A:156:VAL:HG22	1:A:166:HIS:HD2	1.74	0.52
1:A:479:VAL:C	1:A:481:ASP:N	2.62	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:235:ILE:HG12	1:A:361:GLU:CD	2.35	0.52
1:A:160:TYR:CE2	1:B:461:ASN:HB2	2.45	0.52
1:A:411:GLU:C	1:A:413:GLU:N	2.66	0.52
1:A:342:SER:CB	2:A:1638:LDA:H41	2.36	0.51
1:A:501:THR:O	1:A:501:THR:HG23	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:A:264:ILE:HD13	1:A:276:VAL:HG22	1.92	0.51
1:A:156:VAL:HG22	1:A:166:HIS:CD2	2.46	0.51
1:B:146:LEU:HD12	1:B:635:ILE:HG13	1.91	0.51
1:B:157:SER:CB	1:B:624:SER:HB3	2.40	0.51
1:B:206:PHE:CD1	1:B:206:PHE:C	2.89	0.51
1:A:224:LEU:HD23	1:A:224:LEU:C	2.35	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:A:231:ILE:C	1:A:231:ILE:HD12	2.35	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:B:368:ASN:HB3	1:B:370:TRP:HE3	1.76	0.51
1:A:326:SER:HB2	1:A:422:ARG:HH21	1.74	0.50
1:A:393:LEU:HB2	1:A:397:GLY:O	2.11	0.50
1:B:206:PHE:CD1	1:B:207:THR:N	2.78	0.50
1:B:224:LEU:C	1:B:224:LEU:HD23	2.36	0.50
1:B:586:LEU:HD22	1:B:594:SER:HB2	1.92	0.50
1:A:463:TYR:CD1	1:B:592:LEU:CD1	2.94	0.50
1:B:403:ILE:HD12	1:B:403:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:O	1:A:202:THR:HA	2.11	0.50
1:A:253:LEU:O	1:A:254:PRO:C	2.54	0.50
1:A:279:GLN:HE22	1:A:452:GLU:CD	2.19	0.50
1:A:403:ILE:CD1	1:A:421:TRP:CD1	2.79	0.50
1:A:419:LYS:HG2	1:A:445:GLU:OE1	2.12	0.50
1:B:458:ARG:C	1:B:458:ARG:HD3	2.37	0.50
1:A:188:GLN:OE1	1:A:282:VAL:HG23	2.11	0.49
1:A:619:GLN:C	1:A:621:GLY:N	2.69	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: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: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:382:TYR:CE2	1:B:451:MSE:HG2	2.47	0.49
1:A:232:ASN:HD22	1:A:232:ASN:N	2.09	0.49
1:A:264:ILE:HD13	1:A:276:VAL:CG2	2.42	0.49
1:A:488:LEU:C	1:A:488:LEU:HD13	2.38	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:A:515:PHE:HD1	1:A:515:PHE:N	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:HB3	1:A:437:THR:HG22	1.96	0.48
1:B:395:VAL:HG23	1:B:395:VAL:O	2.13	0.48
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:A:270:THR:C	1:A:290:ALA:HB2	2.39	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:B:438:PHE:C	1:B:438:PHE:CD2	2.92	0.47
1:A:159:ASN:HB2	1:A:163:GLY:H	1.79	0.47
1:A:365:GLY:CA	4:A:2006:HOH:O	2.37	0.47
1:A:578:ASP:OD1	1:A:604:HIS:ND1	2.48	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:256:ARG:HA	1:B:428:ARG:NH1	2.30	0.47
1:B:437:THR:OG1	1:B:475:LEU:HD23	2.14	0.47
1:A:208:TRP:O	1:A:209:SER:C	2.58	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:278:GLN:NE2	1:A:305:ARG:O	2.49	0.46
1:B:460:ARG:HG2	1:B:460:ARG:HH11	1.80	0.46
1:A:493:GLN:HE21	1:A:493:GLN:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:CD1	1:A:508:VAL:HG22	2.38	0.46
1:B:566:MSE:CE	1:B:597:GLN:OE1	2.63	0.46
1:B:634:THR:HG23	1:B:634:THR:O	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:B:395:VAL:C	1:B:397:GLY:H	2.24	0.46
1:A:410:ILE:CD1	1:A:416:PHE:HE1	2.27	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:B:357:PHE:CD1	1:B:357:PHE:C	2.94	0.45
1:B:578:ASP:CG	1:B:604:HIS:HD1	2.24	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:196:TYR:CG	1:B:197:ASN:N	2.84	0.45
1:B:311:ILE:N	1:B:311:ILE:HD12	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:N	1:B:543:ILE:HD13	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:B:402:ASP:C	1:B:403:ILE:HD12	2.41	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:619:GLN:C	1:B:621:GLY:N	2.73	0.45
1:A:615:ILE:HD13	1:A:615:ILE:C	2.41	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:237:ARG:NH2	1:A:467:GLU:OE1	2.50	0.45
1:A:454:TYR:O	1:A:457:ALA:HB3	2.16	0.45
1:B:262:PRO:O	1:B:298:LEU:HD12	2.17	0.45
3:B:1637:C8E:O9	3:B:1637:C8E:H132	2.14	0.45
1:A:178:LEU:HD23	1:A:178:LEU:HA	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:232:ASN:CG	1:A:232:ASN:O	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:THR:HA	1:B:626:GLY:HA2	1.99	0.44
1:A:225:THR:CG2	1:A:245:SER:OG	2.66	0.44
1:A:592:LEU:O	1:A:593:THR:C	2.61	0.44
1:A:196:TYR:O	1:A:197:ASN:C	2.61	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:HE3	1:B:470:MSE:O	2.18	0.44
1:B:615:ILE:C	1:B:615:ILE:CD1	2.85	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:HG2	1:A:184:ARG:HH11	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:HE2	1:A:470:MSE:O	2.18	0.43
1:A:229:ASN:CG	1:A:230:ASN:H	2.25	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:A:368:ASN:C	1:A:370:TRP:N	2.76	0.43
1:B:532:LEU:C	1:B:532:LEU:HD23	2.44	0.43
1:B:623:THR:HG23	1:B:623:THR:O	2.19	0.43
1:A:157:SER:HB3	1:A:624:SER:HB2	2.01	0.43
1:A:399:LEU:HD12	1:A:425:TYR:CD1	2.54	0.43
1:A:543:ILE:HD13	1:A:543:ILE:N	2.33	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:220:TRP:C	1:A:222:ALA:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:TYR:HD2	1:B:588:SER:HG	1.65	0.42
1:B:586:LEU:CD2	1:B:594:SER:HB2	2.49	0.42
1:A:382:TYR:CE2	1:A:451:MSE:HG2	2.55	0.42
1:B:532:LEU:HD22	1:B:532:LEU:H	1.83	0.42
1:A:261:ALA:HA	1:A:262:PRO:HD3	1.79	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
1:B:240:SER:HB2	1:B:346:ARG:HH12	1.85	0.42
1:B:310:VAL:HB	1:B:318:LYS:HB2	2.00	0.42
1:A:463:TYR:CD2	1:B:592:LEU:HD11	2.54	0.42
1:B:507:SER:HA	1:B:524:LEU:O	2.19	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:275:VAL:HG13	1:A:309:GLU:HB3	2.02	0.42
1:A:574:ASN:HD22	1:A:574:ASN:N	2.18	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: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:206:PHE:CD1	1:A:206:PHE:C	2.98	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	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:HD23	1:B:592:LEU:HA	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: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:A:373:TYR:OH	1:A:402:ASP:OD1	2.27	0.41
1:B:575:ASP:HB3	1:B:576:GLY:H	1.65	0.41
1:A:573:PHE:O	1:A:574:ASN:HB2	2.20	0.41
1:B:316:ARG:CD	4:B:2004:HOH:O	2.55	0.41
1:A:154:GLY:HA2	1:A:167:GLN:O	2.19	0.41
1:A:262:PRO:CB	1:A:324:THR:HG22	2.50	0.41
2:A:1638:LDA:H12	2:A:1638:LDA:H41	1.85	0.41
1:B:261:ALA:HA	1:B:262:PRO:HD3	1.81	0.41
1:B:488:LEU:C	1:B:488:LEU:CD2	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:PHE:C	1:B:515:PHE:HD2	2.25	0.41
1:B:575:ASP:HB3	1:B:577:LEU:HD13	2.03	0.41
1:A:215:ARG:O	1:A:215:ARG:HG3	2.12	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
1:A:564:VAL:C	1:A:565:ASN:HD22	2.29	0.40
1:B:273:ARG:HA	1:B:287:MSE:HA	2.03	0.40
1:A:255:PRO:C	1:A:257:LEU:H	2.29	0.40
3:B:1637:C8E:O9	3:B:1637:C8E:H131	2.16	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:298:LEU:O	1:B:299:ASP:C	2.64	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%)	8	37
1	B	467/515 (91%)	424 (91%)	37 (8%)	6 (1%)	9	40
All	All	930/1030 (90%)	840 (90%)	77 (8%)	13 (1%)	9	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	ARG
1	B	395	VAL

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/414 (96%)	323 (82%)	73 (18%)	1	9
1	B	392/414 (95%)	325 (83%)	67 (17%)	2	11
All	All	788/828 (95%)	648 (82%)	140 (18%)	2	10

All (140) 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	215	ARG
1	A	219	ARG
1	A	220	TRP
1	A	225	THR
1	A	226	LEU
1	A	231	ILE

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Mol	Chain	Res	Type
1	A	232	ASN
1	A	237	ARG
1	A	248	SER
1	A	256	ARG
1	A	257	LEU
1	A	263	GLN
1	A	275	VAL
1	A	278	GLN
1	A	283	LEU
1	A	285	ASP
1	A	288	VAL
1	A	296	GLN
1	A	311	ILE
1	A	319	THR
1	A	323	ASP
1	A	332	ARG
1	A	340	LEU
1	A	346	ARG
1	A	395	VAL
1	A	398	THR
1	A	399	LEU
1	A	403	ILE
1	A	404	THR
1	A	410	ILE
1	A	423	LEU
1	A	428	ARG
1	A	429	PHE
1	A	436	ILE
1	A	446	ARG
1	A	451	MSE
1	A	453	GLN
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	514	VAL
1	A	515	PHE
1	A	532	LEU
1	A	537	ASP

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Mol	Chain	Res	Type
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	566	MSE
1	A	570	THR
1	A	574	ASN
1	A	575	ASP
1	A	582	LEU
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	165	SER
1	B	182	ARG
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	237	ARG
1	B	245	SER
1	B	256	ARG
1	B	263	GLN
1	B	275	VAL
1	B	278	GLN
1	B	288	VAL
1	B	299	ASP
1	B	303	ARG
1	B	319	THR

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Mol	Chain	Res	Type
1	B	328	PRO
1	B	331	THR
1	B	335	GLN
1	B	339	LYS
1	B	342	SER
1	B	344	ARG
1	B	356	VAL
1	B	361	GLU
1	B	367	SER
1	B	372	LEU
1	B	395	VAL
1	B	399	LEU
1	B	404	THR
1	B	411	GLU
1	B	413	GLU
1	B	420	SER
1	B	429	PHE
1	B	436	ILE
1	B	444	SER
1	B	449	MSE
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	560	ASN
1	B	563	TYR
1	B	566	MSE
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

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Mol	Chain	Res	Type
1	B	615	ILE
1	B	618	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	166	HIS
1	A	167	GLN
1	A	230	ASN
1	A	232	ASN
1	A	278	GLN
1	A	279	GLN
1	A	313	GLN
1	A	489	GLN
1	A	493	GLN
1	A	536	ASN
1	A	560	ASN
1	A	565	ASN
1	A	597	GLN
1	A	599	ASN
1	B	151	ASN
1	B	171	ASN
1	B	197	ASN
1	B	205	ASN
1	B	278	GLN
1	B	314	ASN
1	B	335	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	C8E	B	1637	-	20,20,20	0.38	0	19,19,19	0.39	0
3	C8E	B	1638	-	20,20,20	0.38	0	19,19,19	0.39	0
2	LDA	A	1638	-	13,15,15	2.49	2 (15%)	14,17,17	0.52	0
2	LDA	B	1639	-	13,15,15	2.49	2 (15%)	14,17,17	0.52	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
3	C8E	B	1637	-	-	9/18/18/18	-
3	C8E	B	1638	-	-	10/18/18/18	-
2	LDA	A	1638	-	-	10/13/13/13	-
2	LDA	B	1639	-	-	4/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1638	LDA	O1-N1	-6.85	1.25	1.42
2	B	1639	LDA	O1-N1	-6.84	1.25	1.42
2	A	1638	LDA	C1-N1	-5.76	1.45	1.51
2	B	1639	LDA	C1-N1	-5.75	1.45	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (33) 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	1637	C8E	O12-C13-C14-O15
3	B	1638	C8E	O12-C13-C14-O15
3	B	1638	C8E	C5-C6-C7-C8
2	A	1638	LDA	C4-C5-C6-C7
2	A	1638	LDA	C5-C6-C7-C8
2	B	1639	LDA	C1-C2-C3-C4
2	B	1639	LDA	C2-C3-C4-C5
3	B	1637	C8E	O9-C10-C11-O12
3	B	1638	C8E	O18-C19-C20-O21
2	B	1639	LDA	C6-C7-C8-C9
2	A	1638	LDA	C2-C3-C4-C5
3	B	1638	C8E	C1-C2-C3-C4
3	B	1637	C8E	C5-C6-C7-C8
3	B	1637	C8E	C3-C4-C5-C6
2	A	1638	LDA	C9-C10-C11-C12
2	B	1639	LDA	C3-C4-C5-C6
3	B	1637	C8E	C14-C13-O12-C11
3	B	1638	C8E	C14-C13-O12-C11
3	B	1637	C8E	C13-C14-O15-C16
3	B	1638	C8E	C7-C8-O9-C10
3	B	1638	C8E	C20-C19-O18-C17
2	A	1638	LDA	C6-C7-C8-C9
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	1637	C8E	C7-C8-O9-C10
3	B	1638	C8E	O15-C16-C17-O18

There are no ring outliers.

3 monomers are involved in 15 short contacts:

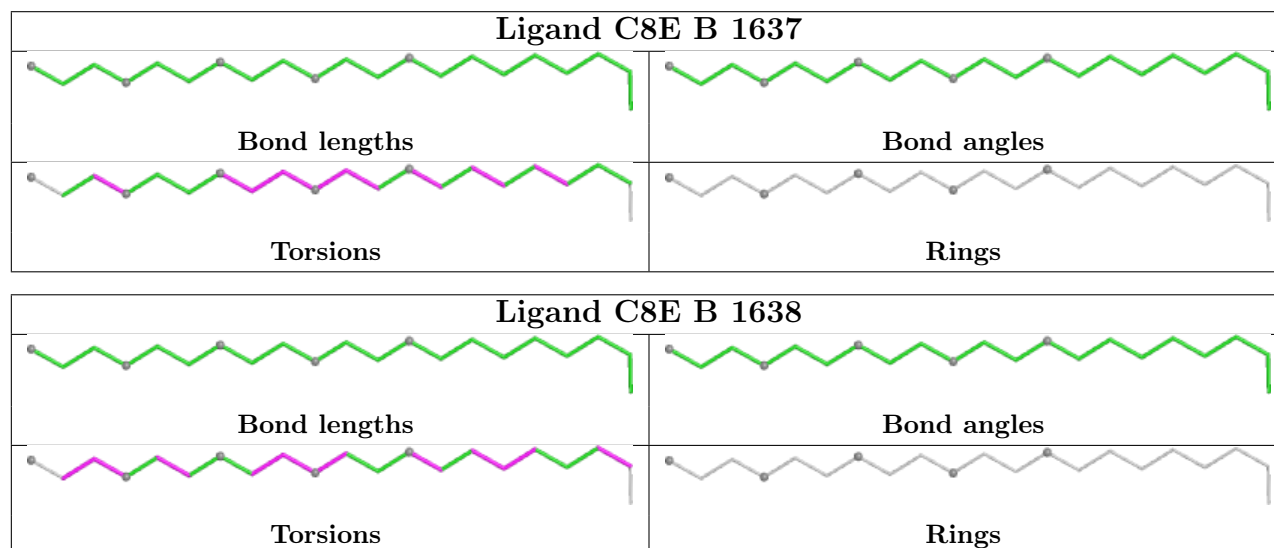
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1637	C8E	6	0
2	A	1638	LDA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1639	LDA	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	469/515 (91%)	-1.60	0 100 100	18, 46, 75, 87	33 (7%)
1	B	469/515 (91%)	-1.59	0 100 100	18, 46, 75, 91	32 (6%)
All	All	938/1030 (91%)	-1.59	0 100 100	18, 46, 75, 91	65 (6%)

There are no RSRZ outliers to report.

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.

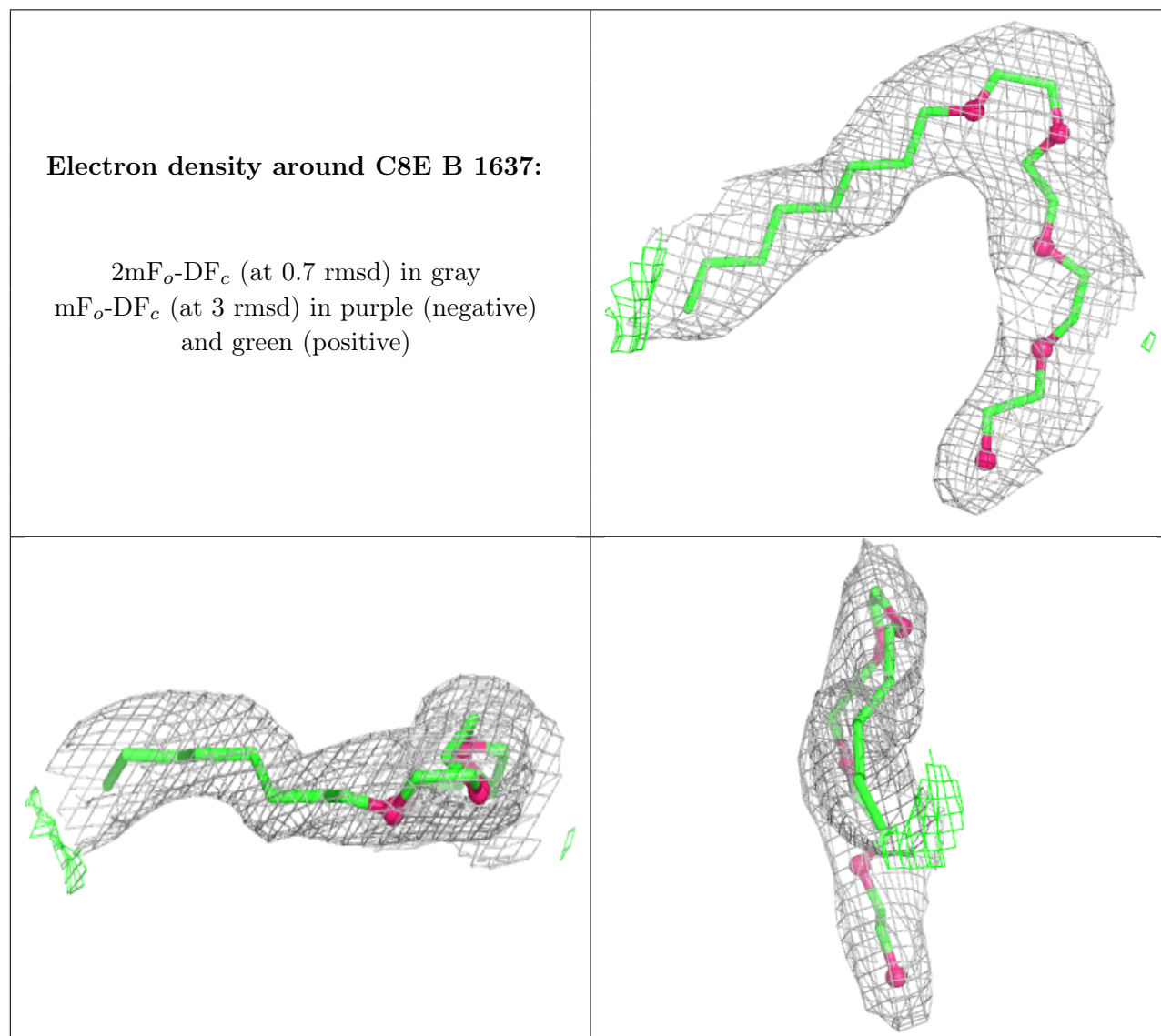
6.4 Ligands [i](#)

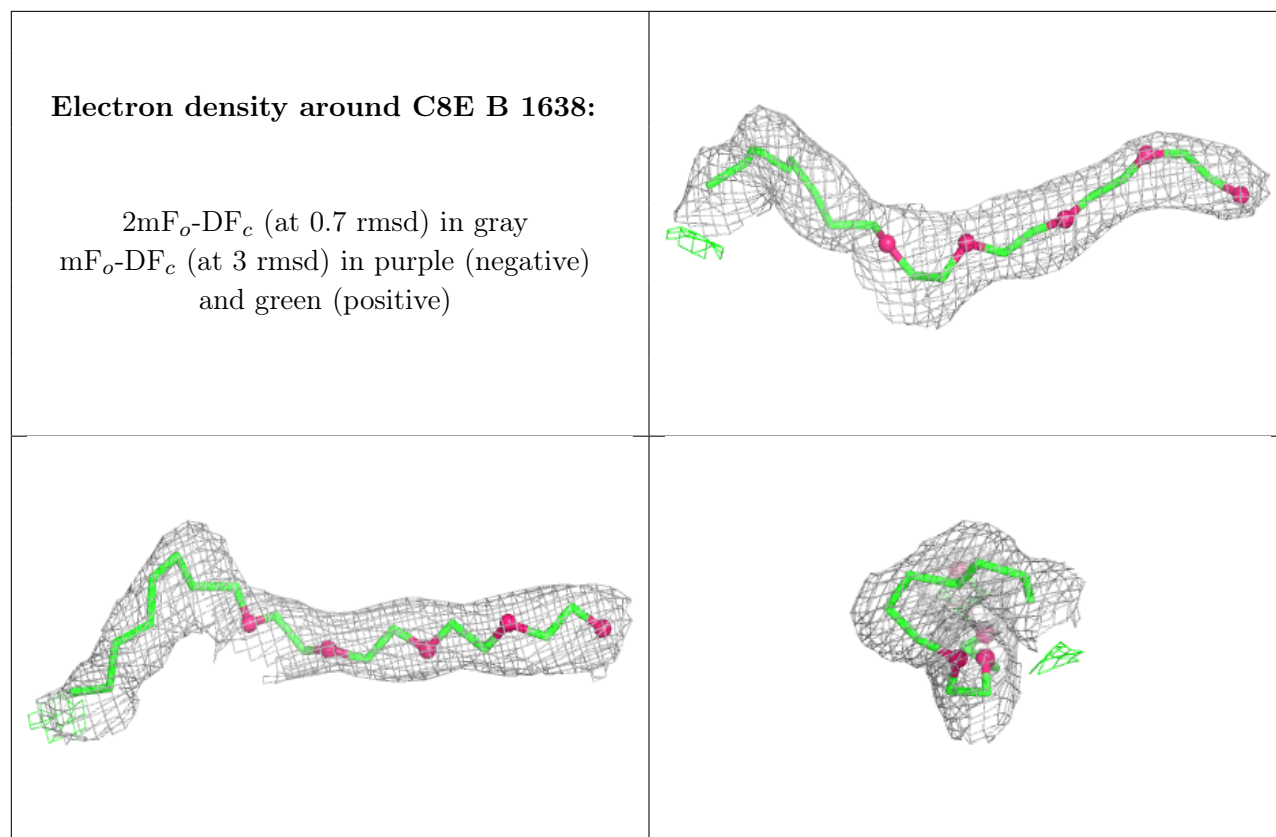
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	C8E	B	1637	21/21	0.98	0.04	77,83,86,86	0
2	LDA	A	1638	16/16	0.99	0.04	78,83,89,90	0
3	C8E	B	1638	21/21	0.99	0.04	81,90,93,94	0
2	LDA	B	1639	16/16	1.00	0.04	54,57,70,70	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.