



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:40 AM UTC

PDB ID : 3FWL / pdb_00003fwl
Title : Crystal Structure of the Full-Length Transglycosylase PBP1b from Escherichia coli
Authors : Sung, M.T.; Lai, Y.T.; Huang, C.Y.; Chou, L.Y.; Wong, C.H.; Ma, C.
Deposited on : 2009-01-19
Resolution : 3.09 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

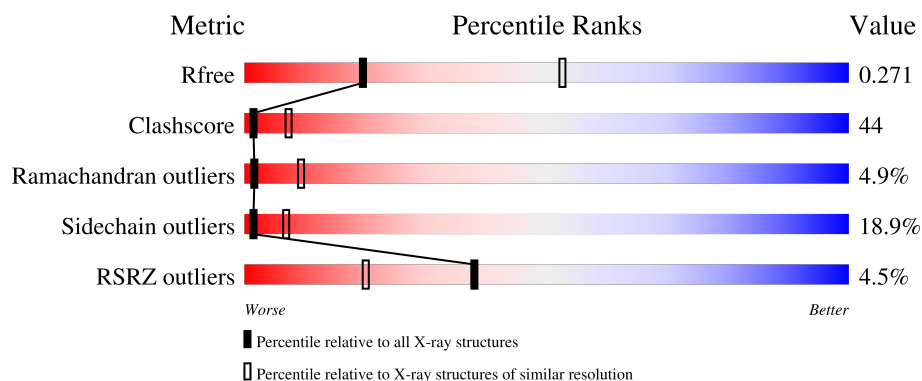
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	751	4% 38% 42% 13% 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5641 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.

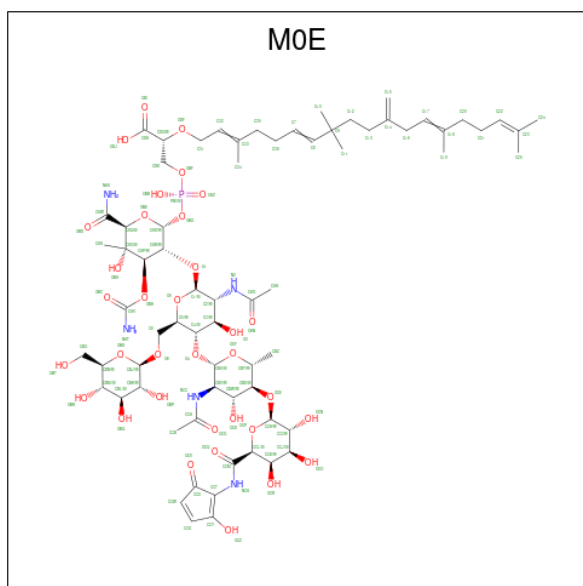
- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	707	5564	3535	974	1029	2	24	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	expression tag	UNP P02919
A	55	SER	-	expression tag	UNP P02919
A	56	HIS	-	expression tag	UNP P02919
A	57	MSE	-	expression tag	UNP P02919

- Molecule 2 is MOENOMYCIN (CCD ID: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).

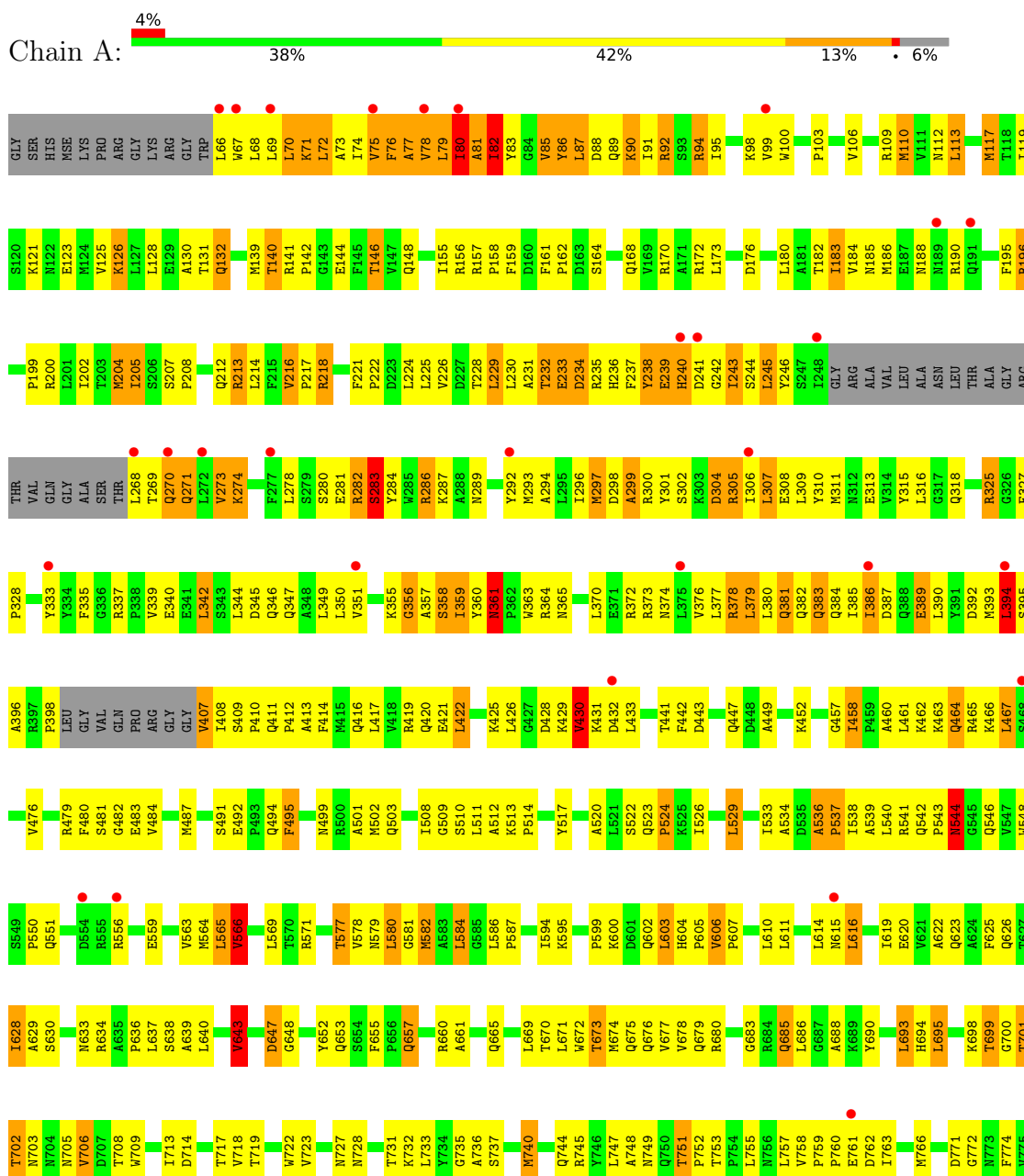


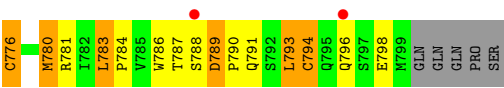
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	77	39	5	32	1	0	0

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: Penicillin-binding protein 1B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	63.24Å 297.00Å 62.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.26 – 3.09 29.26 – 3.09	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.26-3.09) 95.4 (29.26-3.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.11Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.273 0.222 , 0.271	Depositor DCC
R_{free} test set	1112 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5641	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: M0E

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	0.41	0/5653	0.87	8/7632 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	791	GLN	N-CA-C	-8.67	102.41	113.16
1	A	386	ILE	N-CA-C	-7.69	104.86	112.17
1	A	361	ASN	CA-C-N	6.92	128.49	119.84
1	A	361	ASN	C-N-CA	6.92	128.49	119.84
1	A	536	ALA	CA-C-N	6.05	127.40	119.84
1	A	536	ALA	C-N-CA	6.05	127.40	119.84
1	A	184	VAL	N-CA-C	5.71	116.10	108.11
1	A	80	ILE	N-CA-C	-5.38	105.08	110.30

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	5564	0	5610	492	0
2	A	77	0	59	9	0
All	All	5641	0	5669	492	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 44.

All (492) 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:A:487:MSE:HE1	1:A:502:MSE:SE	2.13	0.99
1:A:700:GLY:HA3	1:A:709:TRP:HB2	1.45	0.97
1:A:90:LYS:HZ3	1:A:91:ILE:H	0.98	0.94
1:A:77:ALA:HA	1:A:80:ILE:HD11	1.51	0.93
1:A:271:GLN:H	1:A:271:GLN:HE21	1.13	0.92
1:A:606:VAL:HG23	1:A:607:PRO:HD2	1.53	0.91
1:A:417:LEU:HA	1:A:502:MSE:HE1	1.49	0.90
1:A:282:ARG:H	1:A:282:ARG:HD3	1.37	0.89
1:A:430:VAL:HA	1:A:433:LEU:HD12	1.54	0.89
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.38	0.87
1:A:382:GLN:HA	1:A:383:GLN:HB3	1.56	0.87
1:A:146:THR:HG22	1:A:148:GLN:HE22	1.36	0.87
1:A:132:GLN:HA	1:A:132:GLN:HE21	1.40	0.86
1:A:90:LYS:NZ	1:A:91:ILE:H	1.72	0.85
1:A:304:ASP:O	1:A:307:LEU:HD22	1.76	0.85
1:A:776:CYS:HB3	1:A:793:LEU:HD21	1.57	0.85
1:A:110:MSE:HG3	1:A:199:PRO:HG3	1.59	0.84
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.43	0.84
1:A:283:SER:OG	1:A:284:TYR:HA	1.79	0.83
1:A:90:LYS:HZ3	1:A:91:ILE:N	1.75	0.83
1:A:283:SER:CB	1:A:284:TYR:HA	2.08	0.83
1:A:188:ASN:OD1	1:A:190:ARG:HB2	1.79	0.82
1:A:224:LEU:HD12	1:A:224:LEU:H	1.47	0.79
1:A:556:ARG:HA	1:A:556:ARG:NE	1.96	0.79
1:A:441:THR:HG23	1:A:484:VAL:O	1.81	0.79
1:A:370:LEU:HD21	1:A:373:ARG:HH21	1.48	0.79
1:A:363:TRP:NE1	1:A:398:PRO:HD3	1.98	0.79
1:A:623:GLN:HE22	1:A:637:LEU:H	1.31	0.79
1:A:586:LEU:HD13	1:A:605:PRO:O	1.83	0.78
1:A:78:VAL:HG23	1:A:79:LEU:HD23	1.65	0.78
1:A:344:LEU:HA	1:A:347:GLN:HB3	1.65	0.78
1:A:393:MSE:HE2	1:A:393:MSE:HA	1.66	0.77
1:A:236:HIS:CD2	1:A:237:PHE:H	2.03	0.77
1:A:281:GLU:HB3	1:A:282:ARG:HD3	1.66	0.76
1:A:92:ARG:HG3	1:A:92:ARG:NH1	1.97	0.76
1:A:282:ARG:H	1:A:282:ARG:CD	1.99	0.75
1:A:70:LEU:HD22	1:A:71:LYS:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:HG	1:A:566:VAL:HG13	1.69	0.75
1:A:274:LYS:HA	1:A:278:LEU:HD12	1.67	0.75
1:A:85:VAL:O	1:A:89:GLN:HG2	1.88	0.74
1:A:569:LEU:HD23	1:A:673:THR:HG21	1.68	0.74
1:A:196:ARG:CG	1:A:196:ARG:HH11	2.01	0.74
1:A:520:ALA:O	1:A:523:GLN:HG2	1.88	0.74
1:A:75:VAL:O	1:A:79:LEU:HD21	1.88	0.73
1:A:442:PHE:CE1	1:A:447:GLN:HG3	2.23	0.73
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.52	0.72
1:A:271:GLN:H	1:A:271:GLN:NE2	1.88	0.72
1:A:87:LEU:HD11	1:A:292:TYR:HE2	1.53	0.72
1:A:441:THR:OG1	1:A:483:GLU:HB3	1.89	0.72
1:A:447:GLN:HE21	1:A:487:MSE:H	1.38	0.72
1:A:761:GLU:CD	1:A:761:GLU:H	1.98	0.71
1:A:564:MSE:HE2	1:A:772:GLY:HA3	1.72	0.71
1:A:87:LEU:C	1:A:90:LYS:HZ1	1.98	0.71
1:A:293:MSE:HA	1:A:296:ILE:HD12	1.71	0.71
1:A:82:ILE:O	1:A:85:VAL:HG12	1.91	0.70
1:A:225:LEU:HD13	1:A:347:GLN:HG3	1.72	0.70
1:A:318:GLN:NE2	2:A:901:M0E:HCL	2.06	0.70
1:A:780:MSE:HE3	1:A:781:ARG:HB2	1.72	0.70
1:A:628:ILE:HD11	1:A:671:LEU:HG	1.73	0.70
1:A:359:ILE:HG23	2:A:901:M0E:HCB1	1.74	0.70
1:A:487:MSE:HE3	1:A:501:ALA:HB3	1.72	0.70
1:A:110:MSE:CG	1:A:199:PRO:HG3	2.21	0.70
1:A:286:ARG:HG2	1:A:286:ARG:NH1	2.01	0.70
1:A:523:GLN:HB2	1:A:524:PRO:HA	1.72	0.70
1:A:690:TYR:HB3	1:A:693:LEU:HD22	1.73	0.70
1:A:229:LEU:HD12	1:A:311:MSE:HE3	1.73	0.70
1:A:229:LEU:O	1:A:232:THR:HG23	1.92	0.69
1:A:370:LEU:HD13	1:A:374:ASN:HD21	1.58	0.69
1:A:126:LYS:HE3	1:A:126:LYS:HA	1.76	0.68
1:A:702:THR:HG21	1:A:706:VAL:HG22	1.76	0.68
1:A:109:ARG:HG2	1:A:442:PHE:O	1.93	0.68
1:A:793:LEU:C	1:A:793:LEU:HD23	2.19	0.68
1:A:442:PHE:CZ	1:A:447:GLN:HG3	2.29	0.68
1:A:69:LEU:O	1:A:73:ALA:HB2	1.94	0.67
1:A:72:LEU:HA	1:A:75:VAL:HG12	1.75	0.67
1:A:389:GLU:CD	1:A:389:GLU:H	2.03	0.67
1:A:180:LEU:HD21	1:A:183:ILE:HD11	1.78	0.66
1:A:271:GLN:HE21	1:A:271:GLN:N	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MSE:HE2	1:A:499:ASN:OD1	1.95	0.66
1:A:556:ARG:NE	1:A:556:ARG:CA	2.57	0.66
1:A:774:PHE:HB2	1:A:796:GLN:HG3	1.78	0.66
1:A:776:CYS:HA	1:A:793:LEU:HG	1.76	0.66
1:A:67:TRP:CG	1:A:68:LEU:H	2.11	0.66
1:A:447:GLN:NE2	1:A:487:MSE:H	1.93	0.66
1:A:581:GLY:HA3	1:A:610:LEU:HD21	1.78	0.66
1:A:523:GLN:OE1	1:A:523:GLN:HA	1.93	0.66
1:A:373:ARG:O	1:A:377:LEU:HD13	1.96	0.66
1:A:92:ARG:NE	1:A:300:ARG:HE	1.94	0.66
1:A:524:PRO:HG3	1:A:786:TRP:CD2	2.31	0.66
1:A:776:CYS:HA	1:A:793:LEU:CG	2.25	0.66
1:A:70:LEU:HD13	1:A:70:LEU:H	1.60	0.65
1:A:695:LEU:H	1:A:695:LEU:HD22	1.60	0.65
1:A:68:LEU:HA	1:A:71:LYS:HG3	1.77	0.65
1:A:373:ARG:O	1:A:373:ARG:HD2	1.97	0.65
1:A:499:ASN:C	1:A:499:ASN:HD22	2.03	0.65
1:A:603:LEU:H	1:A:603:LEU:HD22	1.61	0.65
1:A:713:ILE:HG12	1:A:718:VAL:HG22	1.79	0.64
1:A:88:ASP:HB3	1:A:300:ARG:HH22	1.61	0.64
1:A:655:PHE:O	1:A:657:GLN:HG3	1.96	0.64
1:A:90:LYS:HZ3	1:A:90:LYS:N	1.94	0.64
1:A:533:ILE:HD11	1:A:565:LEU:HD22	1.78	0.64
1:A:83:TYR:O	1:A:87:LEU:HD12	1.98	0.64
1:A:67:TRP:CG	1:A:68:LEU:N	2.64	0.64
1:A:196:ARG:HG2	1:A:196:ARG:NH1	2.13	0.64
1:A:670:THR:O	1:A:674:MSE:HG3	1.97	0.64
1:A:389:GLU:CD	1:A:389:GLU:N	2.56	0.64
1:A:218:ARG:HD3	1:A:307:LEU:HD21	1.80	0.63
1:A:92:ARG:HH11	1:A:92:ARG:CG	2.08	0.63
1:A:325:ARG:HH11	1:A:325:ARG:CG	2.11	0.63
1:A:776:CYS:HA	1:A:793:LEU:CD1	2.28	0.63
1:A:481:SER:OG	1:A:483:GLU:HG3	1.99	0.62
1:A:77:ALA:HA	1:A:80:ILE:CD1	2.27	0.62
1:A:110:MSE:HE1	1:A:162:PRO:HD3	1.81	0.62
1:A:580:LEU:HD22	1:A:584:LEU:HD22	1.82	0.62
1:A:786:TRP:CD1	1:A:786:TRP:C	2.78	0.62
1:A:204:MSE:HB2	1:A:212:GLN:HE22	1.65	0.61
1:A:117:MSE:HE2	1:A:119:ILE:CG2	2.30	0.61
1:A:538:ILE:HB	1:A:550:PRO:HG2	1.81	0.61
1:A:457:GLY:HA2	1:A:745:ARG:HE	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ARG:HA	1:A:556:ARG:CZ	2.30	0.61
1:A:761:GLU:O	1:A:762:ASP:HB2	2.00	0.61
1:A:208:PRO:HD3	1:A:431:LYS:HE2	1.81	0.61
1:A:67:TRP:HB2	1:A:70:LEU:HD11	1.82	0.61
1:A:90:LYS:NZ	1:A:90:LYS:H	1.98	0.61
1:A:236:HIS:CE1	1:A:269:THR:HG21	2.35	0.61
1:A:457:GLY:HA2	1:A:745:ARG:NE	2.16	0.61
1:A:523:GLN:HG3	1:A:526:ILE:HB	1.82	0.61
1:A:517:TYR:HD1	1:A:565:LEU:CD1	2.14	0.61
1:A:467:LEU:HD21	1:A:732:LYS:HB2	1.83	0.60
1:A:204:MSE:HB2	1:A:212:GLN:NE2	2.16	0.60
1:A:594:ILE:HG23	1:A:600:LYS:HD3	1.82	0.60
1:A:103:PRO:HB2	1:A:204:MSE:HE3	1.84	0.60
1:A:77:ALA:O	1:A:79:LEU:N	2.33	0.60
1:A:349:LEU:HD13	1:A:373:ARG:HB2	1.84	0.60
1:A:776:CYS:CB	1:A:793:LEU:HD21	2.31	0.60
1:A:286:ARG:HH12	2:A:901:M0E:HDK2	1.67	0.60
1:A:224:LEU:O	1:A:228:THR:HG22	2.01	0.59
1:A:103:PRO:HG3	1:A:207:SER:HB2	1.83	0.59
1:A:226:VAL:HA	1:A:311:MSE:HE1	1.84	0.59
1:A:236:HIS:CG	1:A:237:PHE:H	2.17	0.59
1:A:508:ILE:HG21	1:A:616:LEU:HD22	1.84	0.59
1:A:72:LEU:HD23	1:A:73:ALA:N	2.17	0.59
1:A:307:LEU:HD23	1:A:308:GLU:N	2.17	0.59
1:A:318:GLN:CD	2:A:901:M0E:HCL	2.27	0.59
1:A:702:THR:CG2	1:A:703:ASN:N	2.66	0.59
1:A:278:LEU:HG	1:A:293:MSE:HE1	1.82	0.59
1:A:685:GLN:HB3	1:A:740:MSE:HE2	1.84	0.59
1:A:582:MSE:HA	1:A:582:MSE:CE	2.33	0.59
1:A:72:LEU:O	1:A:76:PHE:N	2.35	0.59
1:A:243:ILE:HD12	1:A:244:SER:N	2.18	0.59
1:A:665:GLN:HG3	1:A:763:ILE:HD11	1.85	0.59
1:A:606:VAL:HG23	1:A:607:PRO:CD	2.32	0.58
1:A:325:ARG:HH11	1:A:325:ARG:HG2	1.67	0.58
1:A:714:ASP:HB2	1:A:753:THR:O	2.03	0.58
1:A:543:PRO:C	1:A:544:ASN:HD22	2.12	0.58
1:A:141:ARG:HB2	1:A:142:PRO:CD	2.33	0.58
1:A:170:ARG:HD3	1:A:186:MSE:HB2	1.86	0.58
1:A:482:GLY:O	1:A:637:LEU:HA	2.04	0.58
1:A:542:GLN:HB2	1:A:546:GLN:O	2.04	0.58
1:A:94:ARG:HG2	1:A:94:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:HG2	1:A:325:ARG:NH1	2.19	0.57
1:A:302:SER:O	1:A:306:ILE:HG12	2.04	0.57
1:A:411:GLN:N	1:A:412:PRO:HD3	2.18	0.57
1:A:381:GLN:HB2	1:A:382:GLN:OE1	2.05	0.57
1:A:499:ASN:C	1:A:499:ASN:ND2	2.62	0.57
1:A:327:PHE:CE1	1:A:350:LEU:HB3	2.39	0.57
1:A:370:LEU:CD1	1:A:374:ASN:HD21	2.18	0.57
1:A:216:VAL:HG13	1:A:328:PRO:HB3	1.87	0.56
1:A:335:PHE:CE2	1:A:346:GLN:HB3	2.40	0.56
1:A:582:MSE:HA	1:A:582:MSE:HE2	1.87	0.56
1:A:669:LEU:HD21	1:A:784:PRO:O	2.05	0.56
1:A:776:CYS:HA	1:A:793:LEU:HD11	1.87	0.56
1:A:594:ILE:HG12	1:A:600:LYS:HZ2	1.70	0.56
1:A:90:LYS:NZ	1:A:90:LYS:N	2.53	0.56
1:A:273:VAL:HB	1:A:293:MSE:HE3	1.86	0.56
1:A:541:ARG:O	1:A:541:ARG:HG2	2.05	0.56
1:A:92:ARG:HE	1:A:300:ARG:HE	1.54	0.56
1:A:72:LEU:HD11	1:A:76:PHE:CE2	2.40	0.55
1:A:92:ARG:HH21	1:A:300:ARG:HD2	1.71	0.55
1:A:359:ILE:HD12	2:A:901:M0E:HCB1	1.88	0.55
1:A:372:ARG:O	1:A:376:VAL:HG22	2.07	0.55
1:A:564:MSE:CE	1:A:772:GLY:HA3	2.35	0.55
1:A:356:GLY:O	1:A:359:ILE:HD13	2.06	0.55
1:A:736:ALA:O	1:A:740:MSE:HB2	2.06	0.55
1:A:386:ILE:HG22	1:A:386:ILE:O	2.07	0.55
1:A:376:VAL:HG23	1:A:377:LEU:H	1.72	0.55
1:A:731:THR:O	1:A:732:LYS:HB2	2.07	0.55
1:A:87:LEU:HD11	1:A:292:TYR:CE2	2.39	0.54
1:A:316:LEU:HA	1:A:357:ALA:CB	2.37	0.54
1:A:673:THR:O	1:A:676:GLN:HB2	2.07	0.54
1:A:693:LEU:HB3	1:A:695:LEU:HD13	1.90	0.54
1:A:68:LEU:CD1	1:A:71:LYS:HD2	2.38	0.54
1:A:131:THR:O	1:A:132:GLN:HB2	2.08	0.54
1:A:110:MSE:HE2	1:A:161:PHE:CD1	2.43	0.54
1:A:327:PHE:HE1	1:A:350:LEU:HB3	1.71	0.54
1:A:619:ILE:O	1:A:622:ALA:HB3	2.07	0.54
1:A:578:VAL:HA	1:A:610:LEU:HD23	1.90	0.54
1:A:113:LEU:HD23	1:A:173:LEU:HD21	1.90	0.54
1:A:132:GLN:HE21	1:A:132:GLN:CA	2.17	0.54
1:A:204:MSE:HE1	1:A:213:ARG:O	2.08	0.54
1:A:363:TRP:CE2	1:A:398:PRO:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:HG22	1:A:719:THR:HG23	1.89	0.54
1:A:780:MSE:CE	1:A:781:ARG:HB2	2.37	0.54
1:A:68:LEU:C	1:A:70:LEU:H	2.16	0.54
1:A:270:GLN:HE21	1:A:270:GLN:C	2.15	0.54
1:A:271:GLN:NE2	1:A:271:GLN:N	2.53	0.54
1:A:236:HIS:CD2	1:A:239:GLU:N	2.77	0.53
1:A:86:TYR:CG	1:A:87:LEU:N	2.76	0.53
1:A:599:PRO:HB2	1:A:602:GLN:HG2	1.90	0.53
1:A:625:PHE:HA	1:A:628:ILE:HG23	1.90	0.53
1:A:643:VAL:CG1	1:A:652:TYR:HB3	2.38	0.53
1:A:196:ARG:HH11	1:A:196:ARG:CB	2.20	0.53
1:A:77:ALA:CA	1:A:80:ILE:HD11	2.33	0.53
1:A:333:TYR:CE1	1:A:363:TRP:HH2	2.27	0.53
1:A:421:GLU:HG2	1:A:425:LYS:HD2	1.90	0.53
1:A:196:ARG:HH11	1:A:196:ARG:HB3	1.74	0.53
1:A:302:SER:OG	1:A:305:ARG:HB3	2.08	0.52
1:A:307:LEU:HD23	1:A:307:LEU:C	2.34	0.52
1:A:529:LEU:O	1:A:566:VAL:HG22	2.09	0.52
1:A:340:GLU:O	1:A:340:GLU:HG2	2.09	0.52
1:A:68:LEU:HD13	1:A:71:LYS:HD2	1.90	0.52
1:A:81:ALA:O	1:A:83:TYR:N	2.42	0.52
1:A:499:ASN:ND2	1:A:501:ALA:H	2.07	0.52
1:A:140:THR:HG23	1:A:141:ARG:HG2	1.90	0.52
1:A:200:ARG:O	1:A:202:ILE:HD12	2.09	0.52
1:A:68:LEU:O	1:A:72:LEU:HB3	2.10	0.52
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.23	0.52
1:A:674:MSE:HE3	1:A:698:LYS:HB2	1.91	0.52
1:A:86:TYR:C	1:A:88:ASP:H	2.18	0.52
1:A:305:ARG:HH21	1:A:309:LEU:HD21	1.75	0.52
1:A:347:GLN:O	1:A:351:VAL:HG23	2.10	0.52
1:A:508:ILE:HG23	1:A:614:LEU:O	2.10	0.52
1:A:72:LEU:HD21	1:A:76:PHE:HD2	1.75	0.52
1:A:78:VAL:CG2	1:A:79:LEU:HD23	2.36	0.52
1:A:328:PRO:HA	1:A:339:VAL:HB	1.92	0.52
1:A:683:GLY:HA2	1:A:740:MSE:HE1	1.92	0.51
1:A:582:MSE:HE3	1:A:610:LEU:HD22	1.92	0.51
1:A:452:LYS:HD3	1:A:749:ASN:CG	2.35	0.51
1:A:693:LEU:HD21	1:A:752:PRO:HG2	1.93	0.51
1:A:793:LEU:C	1:A:793:LEU:CD2	2.84	0.51
1:A:407:VAL:HB	1:A:410:PRO:HG3	1.93	0.51
1:A:110:MSE:HE3	1:A:159:PHE:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLN:CD	1:A:381:GLN:H	2.18	0.51
1:A:176:ASP:C	1:A:176:ASP:OD1	2.54	0.51
1:A:690:TYR:OH	1:A:748:ALA:HB2	2.11	0.51
1:A:393:MSE:HA	1:A:393:MSE:CE	2.40	0.51
1:A:517:TYR:HD1	1:A:565:LEU:HD13	1.76	0.51
1:A:289:ASN:O	1:A:293:MSE:HB2	2.11	0.50
1:A:460:ALA:HA	1:A:463:LYS:HE2	1.93	0.50
1:A:99:VAL:HG13	1:A:100:TRP:CE3	2.47	0.50
1:A:443:ASP:C	1:A:443:ASP:OD2	2.53	0.50
1:A:629:ALA:HB2	1:A:713:ILE:HD13	1.92	0.50
1:A:172:ARG:NH1	1:A:186:MSE:HE3	2.27	0.50
1:A:600:LYS:NZ	1:A:603:LEU:HD23	2.27	0.50
1:A:623:GLN:NE2	1:A:637:LEU:H	2.05	0.50
1:A:67:TRP:CE3	1:A:70:LEU:HD21	2.47	0.50
1:A:358:SER:HB2	2:A:901:M0E:OCG	2.11	0.50
1:A:428:ASP:OD1	1:A:428:ASP:N	2.44	0.50
1:A:675:GLN:O	1:A:678:VAL:HG12	2.12	0.49
1:A:146:THR:CG2	1:A:148:GLN:HE22	2.14	0.49
1:A:304:ASP:O	1:A:306:ILE:N	2.46	0.49
1:A:88:ASP:HB3	1:A:300:ARG:NH2	2.26	0.49
1:A:113:LEU:HB3	1:A:183:ILE:CD1	2.43	0.49
1:A:243:ILE:HD12	1:A:244:SER:H	1.76	0.49
1:A:407:VAL:CG1	1:A:410:PRO:HG3	2.42	0.49
1:A:72:LEU:O	1:A:76:PHE:HB2	2.13	0.49
1:A:230:LEU:C	1:A:232:THR:H	2.21	0.49
1:A:693:LEU:HB3	1:A:695:LEU:CD1	2.42	0.49
1:A:283:SER:HB3	1:A:284:TYR:CD1	2.48	0.49
1:A:705:ASN:O	1:A:731:THR:HG23	2.13	0.49
1:A:360:TYR:CZ	1:A:372:ARG:HG3	2.47	0.49
1:A:376:VAL:O	1:A:379:LEU:HB2	2.12	0.49
1:A:464:GLN:HE21	1:A:465:ARG:HH12	1.59	0.49
1:A:87:LEU:C	1:A:90:LYS:NZ	2.68	0.49
1:A:542:GLN:HE21	1:A:548:TRP:N	2.10	0.49
1:A:185:ASN:HB3	1:A:188:ASN:OD1	2.12	0.49
1:A:213:ARG:HH11	1:A:313:GLU:HA	1.77	0.49
1:A:494:GLN:O	1:A:495:PHE:HB2	2.13	0.49
1:A:709:TRP:CZ3	1:A:722:TRP:HB2	2.48	0.49
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.68	0.48
1:A:202:ILE:HD12	1:A:202:ILE:N	2.28	0.48
1:A:441:THR:CG2	1:A:639:ALA:HA	2.43	0.48
1:A:487:MSE:HE1	1:A:502:MSE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:CZ	1:A:87:LEU:HG	2.48	0.48
1:A:283:SER:CB	1:A:284:TYR:CA	2.88	0.48
1:A:793:LEU:HD22	1:A:794:CYS:SG	2.53	0.48
1:A:117:MSE:HE2	1:A:119:ILE:HG21	1.95	0.48
1:A:88:ASP:CB	1:A:300:ARG:HH22	2.26	0.48
1:A:224:LEU:HB2	1:A:347:GLN:OE1	2.12	0.48
1:A:315:TYR:CE2	1:A:357:ALA:HB3	2.49	0.48
1:A:325:ARG:CG	1:A:325:ARG:NH1	2.74	0.48
1:A:327:PHE:N	1:A:328:PRO:HD2	2.29	0.48
1:A:595:LYS:O	1:A:634:ARG:HD3	2.14	0.48
1:A:90:LYS:H	1:A:90:LYS:HZ2	1.60	0.47
1:A:370:LEU:HD13	1:A:374:ASN:ND2	2.27	0.47
1:A:479:ARG:H	1:A:717:THR:HA	1.79	0.47
1:A:315:TYR:HE1	1:A:318:GLN:NE2	2.12	0.47
1:A:327:PHE:N	1:A:328:PRO:CD	2.78	0.47
1:A:339:VAL:HA	1:A:342:LEU:CD2	2.45	0.47
1:A:117:MSE:HE2	1:A:119:ILE:HG22	1.96	0.47
1:A:517:TYR:CD1	1:A:565:LEU:HD13	2.49	0.47
1:A:70:LEU:HD13	1:A:70:LEU:N	2.30	0.47
1:A:110:MSE:HE3	1:A:159:PHE:CE2	2.49	0.47
1:A:236:HIS:HD2	1:A:239:GLU:N	2.13	0.47
1:A:239:GLU:HB2	1:A:240:HIS:H	1.45	0.47
1:A:449:ALA:HA	1:A:749:ASN:HB3	1.96	0.47
1:A:487:MSE:CE	1:A:502:MSE:HB2	2.44	0.47
1:A:239:GLU:C	1:A:240:HIS:CG	2.92	0.47
1:A:702:THR:HG23	1:A:703:ASN:N	2.30	0.47
1:A:119:ILE:HG13	1:A:123:GLU:HB3	1.97	0.47
1:A:235:ARG:C	1:A:235:ARG:HE	2.22	0.47
1:A:236:HIS:CD2	1:A:238:TYR:N	2.83	0.47
1:A:727:ASN:C	1:A:728:ASN:HD22	2.22	0.47
1:A:74:ILE:HG13	1:A:75:VAL:N	2.28	0.47
1:A:294:ALA:O	1:A:297:MSE:HB3	2.14	0.47
1:A:517:TYR:HD1	1:A:565:LEU:HD11	1.79	0.47
1:A:513:LYS:O	1:A:517:TYR:HD2	1.99	0.46
1:A:204:MSE:HE3	1:A:204:MSE:HB3	1.80	0.46
1:A:342:LEU:HB3	1:A:347:GLN:HB2	1.98	0.46
1:A:364:ARG:HG2	1:A:365:ASN:ND2	2.30	0.46
1:A:747:LEU:HD12	1:A:747:LEU:HA	1.68	0.46
1:A:82:ILE:HG22	1:A:83:TYR:N	2.30	0.46
1:A:112:ASN:HD21	1:A:196:ARG:NH1	2.13	0.46
1:A:509:GLY:HA3	1:A:701:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:HIS:HD2	1:A:238:TYR:H	1.64	0.46
1:A:441:THR:HG21	1:A:639:ALA:HA	1.97	0.46
1:A:581:GLY:CA	1:A:610:LEU:HD21	2.45	0.46
1:A:755:LEU:HD11	1:A:757:LEU:CD1	2.45	0.46
1:A:286:ARG:HH11	1:A:286:ARG:CG	2.17	0.46
1:A:382:GLN:CA	1:A:383:GLN:HB3	2.38	0.46
1:A:511:LEU:HD22	1:A:709:TRP:CB	2.45	0.46
1:A:80:ILE:H	1:A:80:ILE:HG13	1.40	0.46
1:A:130:ALA:O	1:A:200:ARG:HD3	2.15	0.46
1:A:315:TYR:CE1	1:A:318:GLN:NE2	2.84	0.46
1:A:67:TRP:O	1:A:68:LEU:HB3	2.16	0.46
1:A:242:GLY:O	1:A:245:LEU:HD13	2.15	0.46
1:A:299:ALA:C	1:A:301:TYR:H	2.23	0.46
1:A:156:ARG:HG3	1:A:195:PHE:CZ	2.50	0.46
1:A:68:LEU:C	1:A:70:LEU:N	2.73	0.46
1:A:271:GLN:NE2	1:A:310:TYR:HE1	2.14	0.46
1:A:361:ASN:OD1	1:A:363:TRP:HE3	1.99	0.46
1:A:582:MSE:HE3	1:A:610:LEU:CD2	2.46	0.46
1:A:731:THR:OG1	1:A:733:LEU:HB2	2.16	0.46
1:A:755:LEU:HD11	1:A:757:LEU:HD13	1.98	0.46
1:A:76:PHE:C	1:A:77:ALA:O	2.59	0.46
1:A:520:ALA:HB2	1:A:584:LEU:HD21	1.98	0.45
1:A:615:ASN:C	1:A:616:LEU:HD13	2.41	0.45
1:A:75:VAL:O	1:A:75:VAL:HG13	2.16	0.45
1:A:241:ASP:O	1:A:242:GLY:C	2.60	0.45
1:A:349:LEU:HB2	1:A:373:ARG:CG	2.46	0.45
1:A:541:ARG:O	1:A:541:ARG:CG	2.64	0.45
1:A:67:TRP:C	1:A:69:LEU:H	2.24	0.45
1:A:83:TYR:CD2	1:A:83:TYR:C	2.94	0.45
1:A:385:ILE:HG13	1:A:385:ILE:O	2.16	0.45
1:A:221:PHE:HA	1:A:222:PRO:HD2	1.81	0.45
1:A:335:PHE:O	1:A:337:ARG:HG3	2.16	0.45
1:A:349:LEU:HB2	1:A:373:ARG:HG2	1.99	0.45
1:A:106:VAL:HG21	1:A:205:ILE:HD12	1.98	0.45
1:A:304:ASP:O	1:A:305:ARG:C	2.60	0.45
1:A:121:LYS:O	1:A:125:VAL:HG23	2.17	0.45
1:A:214:LEU:O	1:A:328:PRO:HB2	2.17	0.45
1:A:430:VAL:C	1:A:432:ASP:N	2.75	0.45
1:A:70:LEU:HD22	1:A:71:LYS:H	1.75	0.45
1:A:72:LEU:HA	1:A:75:VAL:CG1	2.44	0.45
1:A:236:HIS:HD2	1:A:239:GLU:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:GLY:C	1:A:740:MSE:HE1	2.42	0.45
1:A:464:GLN:NE2	1:A:465:ARG:HH12	2.15	0.45
1:A:464:GLN:HE21	1:A:465:ARG:NH1	2.15	0.44
1:A:619:ILE:HG23	1:A:620:GLU:N	2.31	0.44
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.44
1:A:383:GLN:HG3	1:A:384:GLN:HB2	1.99	0.44
1:A:422:LEU:HD22	1:A:640:LEU:HD21	1.99	0.44
1:A:569:LEU:HD23	1:A:673:THR:CG2	2.43	0.44
1:A:679:GLN:HG3	1:A:680:ARG:N	2.33	0.44
1:A:776:CYS:CA	1:A:793:LEU:HG	2.45	0.44
1:A:78:VAL:HG23	1:A:79:LEU:N	2.32	0.44
1:A:238:TYR:HA	1:A:298:ASP:OD2	2.18	0.44
1:A:282:ARG:HD3	1:A:282:ARG:N	2.18	0.44
1:A:702:THR:HG23	1:A:703:ASN:H	1.82	0.44
1:A:158:PRO:HG3	1:A:168:GLN:HB3	2.00	0.44
1:A:511:LEU:HD22	1:A:709:TRP:HB3	2.00	0.44
1:A:536:ALA:HB1	1:A:537:PRO:HD2	1.98	0.44
1:A:394:LEU:O	1:A:395:SER:HB3	2.16	0.44
1:A:761:GLU:CD	1:A:761:GLU:N	2.70	0.44
1:A:274:LYS:HZ2	2:A:901:M0E:PBI	2.40	0.44
1:A:685:GLN:HB3	1:A:740:MSE:CE	2.46	0.44
1:A:735:GLY:C	1:A:737:SER:H	2.26	0.44
1:A:487:MSE:HE3	1:A:501:ALA:CB	2.47	0.44
1:A:131:THR:O	1:A:132:GLN:CB	2.65	0.44
1:A:236:HIS:HD2	1:A:238:TYR:N	2.16	0.43
1:A:603:LEU:HD22	1:A:603:LEU:N	2.28	0.43
1:A:683:GLY:HA2	1:A:740:MSE:CE	2.48	0.43
1:A:87:LEU:HA	1:A:90:LYS:NZ	2.32	0.43
1:A:407:VAL:HG11	1:A:410:PRO:HG3	2.00	0.43
1:A:458:ILE:HD13	1:A:491:SER:HB2	1.99	0.43
1:A:359:ILE:CD1	2:A:901:M0E:HCB1	2.47	0.43
1:A:600:LYS:HZ1	1:A:603:LEU:HD23	1.84	0.43
1:A:333:TYR:CE1	1:A:363:TRP:CH2	3.06	0.43
1:A:594:ILE:HD11	1:A:600:LYS:HZ3	1.84	0.43
1:A:88:ASP:O	1:A:300:ARG:NH2	2.52	0.43
1:A:131:THR:O	1:A:131:THR:HG22	2.18	0.43
1:A:600:LYS:HB3	1:A:600:LYS:HE3	1.76	0.43
1:A:304:ASP:C	1:A:307:LEU:HD22	2.42	0.43
1:A:414:PHE:CE2	1:A:442:PHE:HB2	2.54	0.43
1:A:240:HIS:HB2	1:A:241:ASP:H	1.73	0.42
1:A:282:ARG:CD	1:A:282:ARG:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ALA:HB3	1:A:579:ASN:OD1	2.19	0.42
1:A:79:LEU:HD23	1:A:79:LEU:H	1.85	0.42
1:A:222:PRO:HG2	1:A:225:LEU:CB	2.50	0.42
1:A:565:LEU:O	1:A:566:VAL:C	2.61	0.42
1:A:205:ILE:O	1:A:205:ILE:HG22	2.19	0.42
1:A:225:LEU:N	1:A:347:GLN:OE1	2.52	0.42
1:A:269:THR:O	1:A:270:GLN:C	2.62	0.42
1:A:616:LEU:HD13	1:A:616:LEU:N	2.35	0.42
1:A:693:LEU:O	1:A:694:HIS:C	2.61	0.42
1:A:766:MSE:HE3	1:A:790:PRO:HB3	2.01	0.42
1:A:88:ASP:OD1	1:A:296:ILE:HD13	2.18	0.42
1:A:361:ASN:OD1	1:A:363:TRP:CE3	2.73	0.42
1:A:595:LYS:HB3	1:A:661:ALA:HB1	2.01	0.42
1:A:653:GLN:HG2	1:A:655:PHE:CZ	2.55	0.42
1:A:758:VAL:HA	1:A:759:PRO:HD3	1.74	0.42
1:A:140:THR:HG22	1:A:144:GLU:OE1	2.20	0.42
1:A:586:LEU:N	1:A:587:PRO:CD	2.82	0.42
1:A:286:ARG:O	1:A:287:LYS:C	2.62	0.42
1:A:462:LYS:O	1:A:466:LYS:N	2.52	0.42
1:A:72:LEU:HD21	1:A:76:PHE:CD2	2.53	0.42
1:A:665:GLN:CD	1:A:665:GLN:H	2.27	0.42
1:A:113:LEU:HB3	1:A:183:ILE:HD11	2.02	0.42
1:A:599:PRO:HB2	1:A:602:GLN:CG	2.48	0.42
1:A:759:PRO:HA	1:A:760:PRO:HD3	1.97	0.42
1:A:431:LYS:HA	1:A:431:LYS:HD2	1.86	0.42
1:A:672:TRP:CH2	1:A:783:LEU:HD12	2.55	0.42
1:A:363:TRP:CD1	1:A:398:PRO:HD3	2.53	0.42
1:A:70:LEU:HA	1:A:73:ALA:HB3	2.02	0.41
1:A:77:ALA:O	1:A:78:VAL:HG22	2.20	0.41
1:A:225:LEU:HG	1:A:311:MSE:HE2	2.00	0.41
1:A:286:ARG:NH1	2:A:901:M0E:HDK2	2.34	0.41
1:A:539:ALA:HA	1:A:548:TRP:O	2.18	0.41
1:A:619:ILE:HD12	1:A:637:LEU:HD23	2.02	0.41
1:A:633:ASN:HD22	1:A:660:ARG:HA	1.85	0.41
1:A:94:ARG:CG	1:A:94:ARG:NH1	2.82	0.41
1:A:698:LYS:NZ	1:A:699:THR:HG22	2.35	0.41
1:A:327:PHE:O	1:A:328:PRO:C	2.62	0.41
1:A:407:VAL:CB	1:A:410:PRO:HG3	2.50	0.41
1:A:533:ILE:CD1	1:A:565:LEU:HD22	2.48	0.41
1:A:580:LEU:CD2	1:A:584:LEU:HD22	2.50	0.41
1:A:619:ILE:CD1	1:A:637:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:GLN:NE2	1:A:630:SER:HB3	2.35	0.41
1:A:218:ARG:HD3	1:A:307:LEU:CD2	2.47	0.41
1:A:345:ASP:HB2	1:A:393:MSE:SE	2.70	0.41
1:A:479:ARG:HD3	1:A:480:PHE:CE2	2.55	0.41
1:A:674:MSE:O	1:A:677:VAL:HB	2.19	0.41
1:A:229:LEU:HD11	1:A:310:TYR:CE2	2.56	0.41
1:A:513:LYS:N	1:A:514:PRO:CD	2.84	0.41
1:A:556:ARG:NE	1:A:556:ARG:N	2.68	0.41
1:A:586:LEU:HB2	1:A:587:PRO:HD3	2.03	0.41
1:A:604:HIS:HA	1:A:605:PRO:HD3	1.84	0.41
1:A:270:GLN:C	1:A:270:GLN:NE2	2.78	0.41
1:A:94:ARG:HD2	1:A:95:ILE:HD12	2.03	0.41
1:A:383:GLN:HG3	1:A:384:GLN:N	2.35	0.41
1:A:510:SER:C	1:A:512:ALA:N	2.77	0.41
1:A:280:SER:HA	1:A:281:GLU:HA	1.71	0.41
1:A:674:MSE:HA	1:A:677:VAL:HG23	2.02	0.41
1:A:77:ALA:HA	1:A:80:ILE:CG1	2.49	0.41
1:A:85:VAL:O	1:A:88:ASP:HB2	2.21	0.41
1:A:85:VAL:HG22	1:A:89:GLN:HE21	1.85	0.41
1:A:132:GLN:HB2	1:A:157:ARG:NH2	2.36	0.41
1:A:139:MSE:SE	1:A:155:ILE:HG13	2.71	0.41
1:A:218:ARG:NH2	1:A:226:VAL:HG21	2.36	0.41
1:A:307:LEU:HA	1:A:310:TYR:HB3	2.03	0.41
1:A:708:THR:OG1	1:A:723:VAL:HB	2.21	0.41
1:A:87:LEU:HD22	1:A:87:LEU:O	2.21	0.41
1:A:392:ASP:O	1:A:393:MSE:HG2	2.21	0.41
1:A:510:SER:C	1:A:512:ALA:H	2.29	0.41
1:A:524:PRO:HD3	1:A:786:TRP:CZ3	2.56	0.41
1:A:686:LEU:C	1:A:688:ALA:N	2.77	0.41
1:A:218:ARG:HA	1:A:218:ARG:HD2	1.86	0.40
1:A:233:GLU:O	1:A:234:ASP:C	2.64	0.40
1:A:305:ARG:O	1:A:306:ILE:C	2.64	0.40
1:A:345:ASP:OD2	1:A:346:GLN:HG3	2.22	0.40
1:A:408:ILE:HG23	1:A:409:SER:H	1.87	0.40
1:A:417:LEU:O	1:A:420:GLN:HB3	2.21	0.40
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.92	0.40
1:A:623:GLN:HE22	1:A:636:PRO:HA	1.86	0.40
1:A:292:TYR:O	1:A:296:ILE:HG13	2.21	0.40
1:A:364:ARG:O	1:A:365:ASN:CG	2.64	0.40
1:A:685:GLN:CB	1:A:740:MSE:HE2	2.51	0.40
1:A:751:THR:HA	1:A:752:PRO:HD3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:O	1:A:325:ARG:HG2	2.21	0.40
1:A:315:TYR:CD2	1:A:357:ALA:HB3	2.57	0.40
1:A:386:ILE:O	1:A:386:ILE:CG2	2.68	0.40
1:A:513:LYS:HD3	1:A:577:THR:OG1	2.22	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	701/751 (93%)	563 (80%)	104 (15%)	34 (5%)	1 9

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	ARG
1	A	430	VAL
1	A	495	PHE
1	A	566	VAL
1	A	647	ASP
1	A	77	ALA
1	A	81	ALA
1	A	238	TYR
1	A	299	ALA
1	A	378	ARG
1	A	383	GLN
1	A	394	LEU
1	A	429	LYS
1	A	643	VAL
1	A	140	THR
1	A	164	SER
1	A	231	ALA

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Mol	Chain	Res	Type
1	A	467	LEU
1	A	544	ASN
1	A	648	GLY
1	A	78	VAL
1	A	240	HIS
1	A	283	SER
1	A	297	MSE
1	A	396	ALA
1	A	234	ASP
1	A	274	LYS
1	A	356	GLY
1	A	82	ILE
1	A	361	ASN
1	A	380	LEU
1	A	789	ASP
1	A	217	PRO
1	A	537	PRO

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	599/605 (99%)	486 (81%)	113 (19%)	1 7

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	71	LYS
1	A	72	LEU
1	A	75	VAL
1	A	76	PHE
1	A	79	LEU
1	A	80	ILE
1	A	82	ILE
1	A	85	VAL

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Mol	Chain	Res	Type
1	A	86	TYR
1	A	87	LEU
1	A	90	LYS
1	A	92	ARG
1	A	94	ARG
1	A	98	LYS
1	A	110	MSE
1	A	113	LEU
1	A	117	MSE
1	A	126	LYS
1	A	128	LEU
1	A	132	GLN
1	A	146	THR
1	A	182	THR
1	A	183	ILE
1	A	196	ARG
1	A	204	MSE
1	A	205	ILE
1	A	213	ARG
1	A	216	VAL
1	A	218	ARG
1	A	229	LEU
1	A	232	THR
1	A	233	GLU
1	A	239	GLU
1	A	243	ILE
1	A	245	LEU
1	A	246	TYR
1	A	268	LEU
1	A	270	GLN
1	A	271	GLN
1	A	273	VAL
1	A	282	ARG
1	A	283	SER
1	A	286	ARG
1	A	304	ASP
1	A	307	LEU
1	A	325	ARG
1	A	342	LEU
1	A	355	LYS
1	A	358	SER
1	A	359	ILE

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Mol	Chain	Res	Type
1	A	378	ARG
1	A	379	LEU
1	A	381	GLN
1	A	387	ASP
1	A	389	GLU
1	A	390	LEU
1	A	394	LEU
1	A	407	VAL
1	A	419	ARG
1	A	422	LEU
1	A	426	LEU
1	A	430	VAL
1	A	458	ILE
1	A	461	LEU
1	A	464	GLN
1	A	492	GLU
1	A	503	GLN
1	A	522	SER
1	A	524	PRO
1	A	529	LEU
1	A	540	LEU
1	A	544	ASN
1	A	551	GLN
1	A	559	GLU
1	A	563	VAL
1	A	565	LEU
1	A	566	VAL
1	A	571	ARG
1	A	577	THR
1	A	580	LEU
1	A	582	MSE
1	A	584	LEU
1	A	603	LEU
1	A	606	VAL
1	A	611	LEU
1	A	616	LEU
1	A	628	ILE
1	A	638	SER
1	A	643	VAL
1	A	647	ASP
1	A	657	GLN
1	A	673	THR

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Mol	Chain	Res	Type
1	A	685	GLN
1	A	693	LEU
1	A	695	LEU
1	A	699	THR
1	A	701	THR
1	A	702	THR
1	A	706	VAL
1	A	740	MSE
1	A	744	GLN
1	A	751	THR
1	A	771	ASP
1	A	776	CYS
1	A	780	MSE
1	A	783	LEU
1	A	787	THR
1	A	788	SER
1	A	789	ASP
1	A	793	LEU
1	A	794	CYS
1	A	798	GLU

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	112	ASN
1	A	132	GLN
1	A	148	GLN
1	A	179	HIS
1	A	191	GLN
1	A	209	ASN
1	A	236	HIS
1	A	270	GLN
1	A	271	GLN
1	A	289	ASN
1	A	318	GLN
1	A	322	ASN
1	A	365	ASN
1	A	374	ASN
1	A	383	GLN
1	A	384	GLN
1	A	420	GLN

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Mol	Chain	Res	Type
1	A	423	GLN
1	A	447	GLN
1	A	464	GLN
1	A	494	GLN
1	A	499	ASN
1	A	542	GLN
1	A	544	ASN
1	A	615	ASN
1	A	623	GLN
1	A	626	GLN
1	A	633	ASN
1	A	685	GLN
1	A	728	ASN
1	A	796	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

1 ligand is 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	M0E	A	901	-	79,81,114	1.04	3 (3%)	112,122,166	1.33	15 (13%)

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	M0E	A	901	-	-	15/52/158/206	0/5/5/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	M0E	OBH-CAV	5.41	1.46	1.35
2	A	901	M0E	OCQ-CCM	5.32	1.33	1.23
2	A	901	M0E	CCM-NCS	-2.56	1.26	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	M0E	OBH-CAV-NAT	5.39	119.27	110.92
2	A	901	M0E	CBU-CBV-NCC	-3.87	104.43	110.92
2	A	901	M0E	C3-C2-N2	-3.53	104.12	110.62
2	A	901	M0E	C1-O1-CAR	-3.37	109.98	117.98
2	A	901	M0E	CCH-OCE-CBX	-3.24	110.30	117.98
2	A	901	M0E	C1-C2-N2	-3.07	105.76	110.92
2	A	901	M0E	OBH-CAV-OBC	-3.02	118.45	123.06
2	A	901	M0E	ODJ-CDH-CDG	2.75	118.56	112.74
2	A	901	M0E	CBW-CBV-NCC	-2.72	105.60	110.62
2	A	901	M0E	OBS-CBN-CBM	2.44	114.09	109.70
2	A	901	M0E	CBL-CBM-CBN	2.39	114.56	110.23
2	A	901	M0E	CAQ-CAW-NAU	-2.26	116.01	117.34
2	A	901	M0E	OBD-CAW-CAQ	2.20	120.52	118.93
2	A	901	M0E	CBU-O4-C4	-2.18	112.82	117.98
2	A	901	M0E	OBC-CAV-NAT	-2.09	122.28	125.58

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	M0E	ODF-CDG-CDK-OBF

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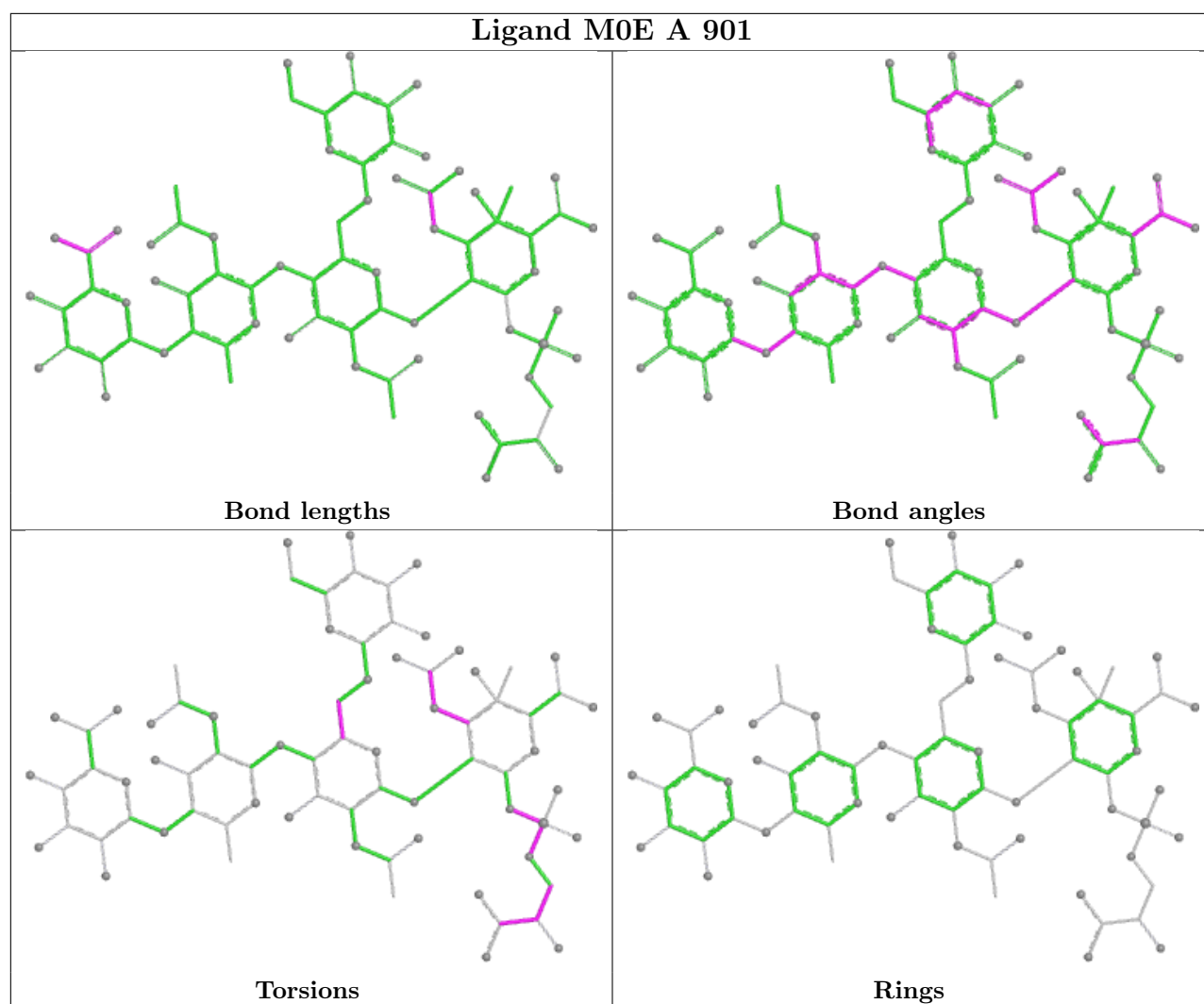
Mol	Chain	Res	Type	Atoms
2	A	901	M0E	CDK-OBF-PBI-OBB
2	A	901	M0E	CDK-OBF-PBI-OBG
2	A	901	M0E	CAX-OBG-PBI-OBF
2	A	901	M0E	CAX-OBG-PBI-OBB
2	A	901	M0E	CAR-CAP-OBH-CAV
2	A	901	M0E	OBC-CAV-OBH-CAP
2	A	901	M0E	NAT-CAV-OBH-CAP
2	A	901	M0E	O5-C5-C6-O6
2	A	901	M0E	C4-C5-C6-O6
2	A	901	M0E	CDH-CDG-CDK-OBF
2	A	901	M0E	CAO-CAP-OBH-CAV
2	A	901	M0E	ODF-CDG-CDH-ODI
2	A	901	M0E	ODF-CDG-CDH-ODJ
2	A	901	M0E	CDK-CDG-CDH-ODI

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	M0E	9	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	683/751 (90%)	0.34	31 (4%) 38 20	46, 79, 162, 228	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	LEU	4.9
1	A	191	GLN	3.5
1	A	333	TYR	3.5
1	A	66	LEU	3.4
1	A	272	LEU	3.3
1	A	78	VAL	3.0
1	A	241	ASP	3.0
1	A	248	ILE	2.9
1	A	270	GLN	2.9
1	A	554	ASP	2.9
1	A	761	GLU	2.7
1	A	67	TRP	2.7
1	A	351	VAL	2.7
1	A	394	LEU	2.7
1	A	292	TYR	2.7
1	A	240	HIS	2.6
1	A	468	SER	2.6
1	A	615	ASN	2.5
1	A	556	ARG	2.3
1	A	788	SER	2.3
1	A	69	LEU	2.3
1	A	99	VAL	2.3
1	A	75	VAL	2.2
1	A	189	ASN	2.2
1	A	80	ILE	2.2
1	A	432	ASP	2.2
1	A	375	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	386	ILE	2.1
1	A	277	PHE	2.1
1	A	306	ILE	2.0
1	A	796	GLN	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](#)

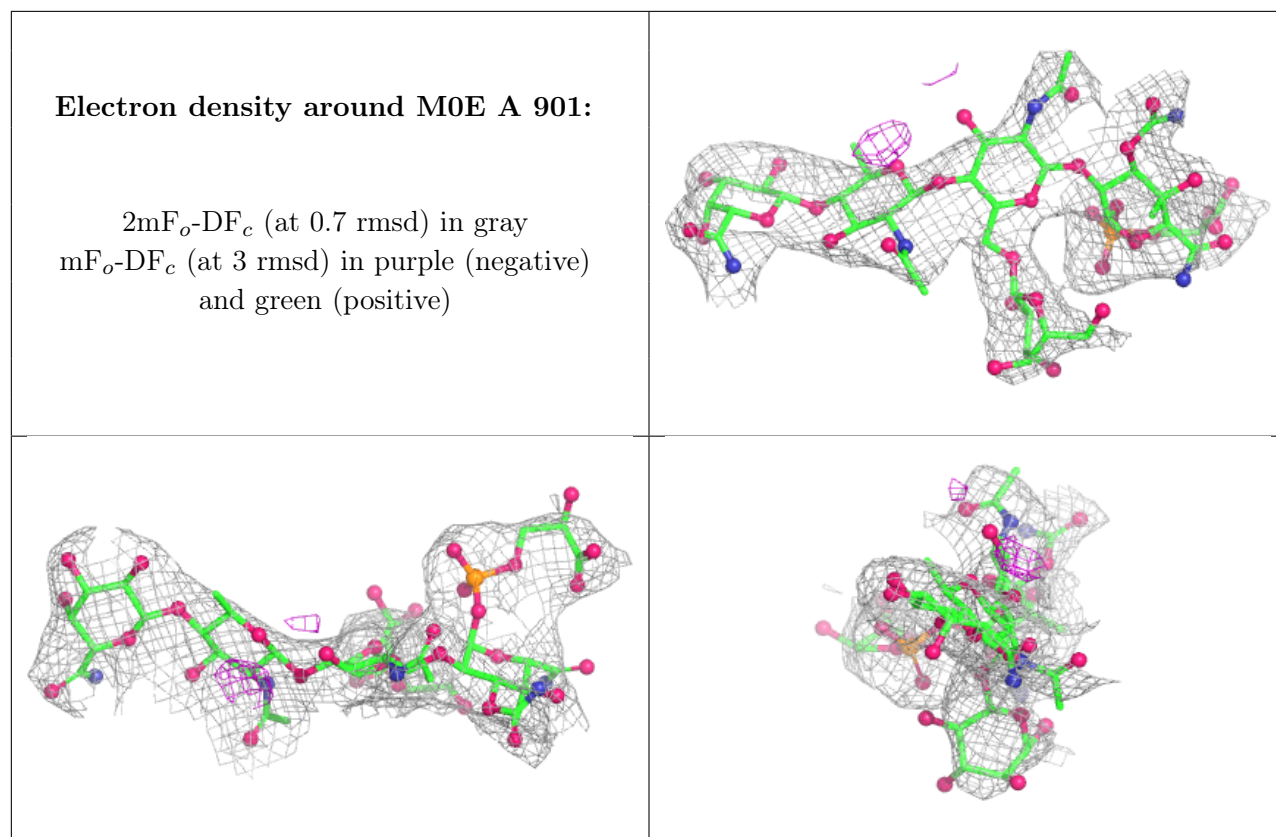
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	M0E	A	901	77/109	0.87	0.11	94,150,165,168	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.