



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:53 PM UTC

PDB ID : 3NVD / pdb_00003nvd
Title : Structure of YBBD in complex with pugnac
Authors : Diederichs, K.
Deposited on : 2010-07-08
Resolution : 1.84 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

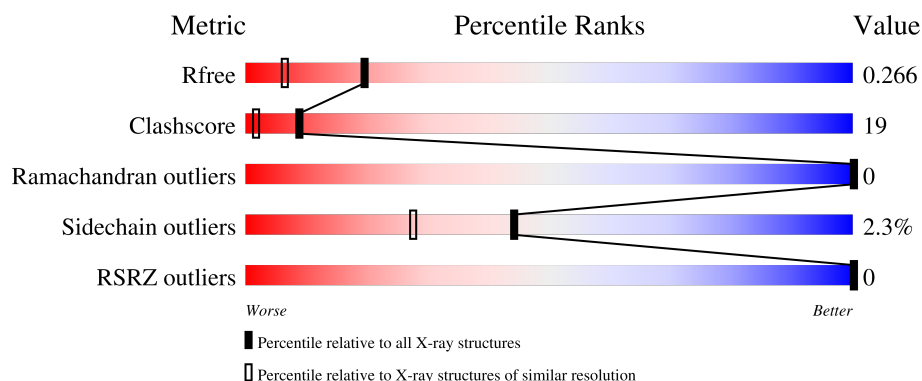
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	642	 67% 27% . .
1	B	642	 70% 24% . .

2 Entry composition [i](#)

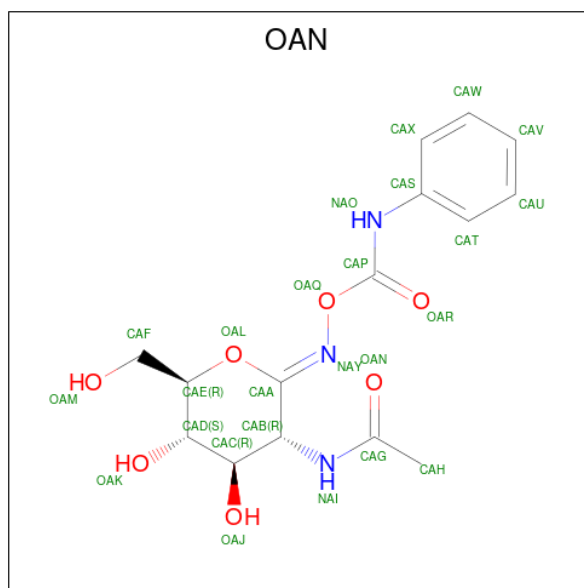
There are 6 unique types of molecules in this entry. The entry contains 20916 atoms, of which 9778 are hydrogens and 0 are deuteriums.

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 Uncharacterized lipoprotein ybbD.

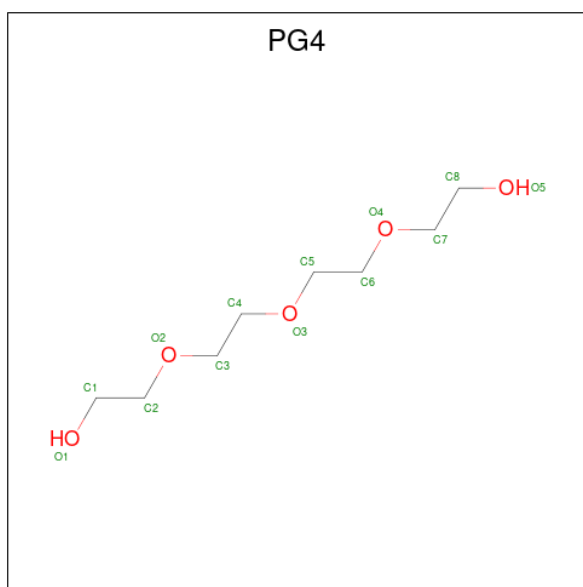
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	617	Total	C	H	N	O	S	7	1	0
			9643	3018	4877	829	900	19			
1	B	617	Total	C	H	N	O	S	5	1	0
			9643	3018	4877	829	900	19			

- Molecule 2 is O-(2-ACETAMIDO-2-DEOXY D-GLUCOPYRANOSYLIDENE) AMINO-N-PHENYLCARBAMATE (CCD ID: OAN) (formula: $C_{15}H_{19}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	15	3	7		
2	B	1	Total	C	N	O	0	0
			25	15	3	7		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

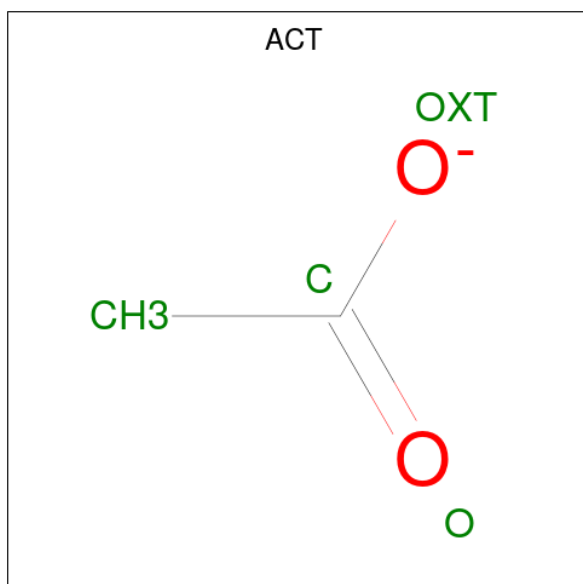


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			23	8	12	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 7 2 3 2	0	0
5	A	1	Total C H O 7 2 3 2	0	0
5	B	1	Total C H O 7 2 3 2	0	0
5	B	1	Total C H O 7 2 3 2	0	0

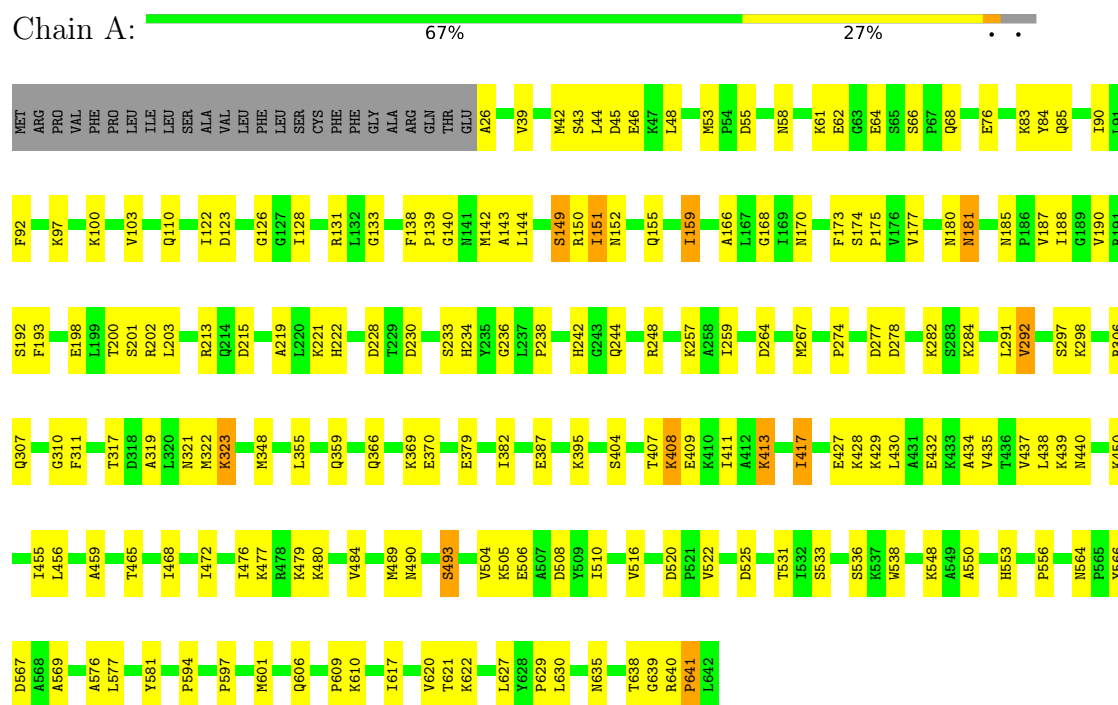
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	769	Total O 769 769	0	0
6	B	758	Total O 758 758	0	0

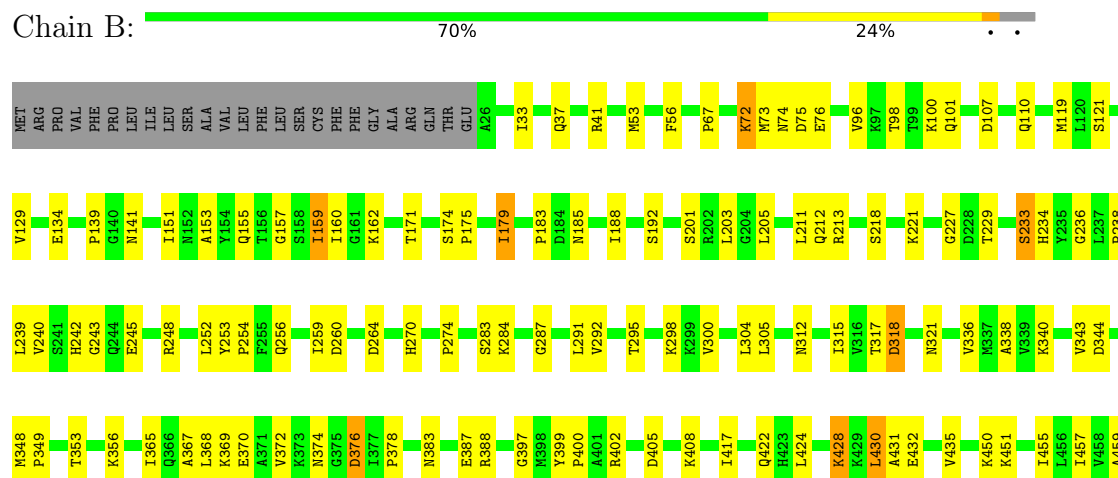
3 Residue-property plots

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: Uncharacterized lipoprotein ybbD



• Molecule 1: Uncharacterized lipoprotein ybbD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.47Å 73.21Å 83.79Å 79.83° 69.45° 88.22°	Depositor
Resolution (Å)	48.55 – 1.84 48.55 – 1.84	Depositor EDS
% Data completeness (in resolution range)	93.6 (48.55-1.84) 85.8 (48.55-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.187 , 0.246 0.204 , 0.266	Depositor DCC
R_{free} test set	5235 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.187 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20916	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: OAN, PG4, ACT, NA

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	1.02	5/4853 (0.1%)	1.07	12/6552 (0.2%)
1	B	1.01	8/4853 (0.2%)	1.07	6/6552 (0.1%)
All	All	1.01	13/9706 (0.1%)	1.07	18/13104 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	596	ILE	CA-CB	7.24	1.58	1.54
1	B	295	THR	CA-CB	6.42	1.63	1.53
1	A	177	VAL	CA-CB	6.14	1.60	1.54
1	A	317	THR	CA-CB	6.10	1.63	1.53
1	B	179	ILE	CA-CB	5.80	1.61	1.54
1	B	531	THR	CA-CB	5.64	1.63	1.53
1	A	292	VAL	CA-C	5.59	1.59	1.52
1	A	437	VAL	CA-C	-5.57	1.45	1.52
1	B	96	VAL	CA-CB	5.44	1.61	1.54
1	B	596	ILE	CA-C	5.42	1.57	1.52
1	A	382	ILE	CA-CB	5.37	1.60	1.54
1	B	188	ILE	CA-CB	5.17	1.61	1.54
1	B	435	VAL	CA-CB	5.07	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLY	N-CA-C	-7.12	103.72	112.33
1	A	151	ILE	CB-CA-C	-6.28	102.09	112.26
1	A	617	ILE	CB-CA-C	-6.20	104.06	111.18
1	B	129	VAL	CB-CA-C	-6.01	105.16	111.23
1	B	141	ASN	N-CA-C	5.91	117.40	111.07
1	A	617	ILE	CA-C-N	5.79	126.08	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	617	ILE	C-N-CA	5.79	126.08	119.83
1	A	39	VAL	N-CA-C	5.78	115.96	110.53
1	B	284	LYS	N-CA-C	-5.76	104.97	112.23
1	A	627	LEU	N-CA-C	-5.64	106.44	113.55
1	B	417	ILE	CB-CA-C	-5.55	106.99	111.71
1	A	193	PHE	N-CA-C	5.54	117.31	111.28
1	A	159	ILE	N-CA-C	5.47	115.67	110.53
1	A	382	ILE	N-CA-C	-5.40	105.45	110.53
1	B	318	ASP	N-CA-C	-5.30	103.49	110.33
1	A	417	ILE	CB-CA-C	-5.30	105.46	111.55
1	A	259	ILE	N-CA-C	-5.22	105.62	110.53
1	B	159	ILE	N-CA-C	5.01	115.74	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4766	4877	4888	185	2
1	B	4766	4877	4888	173	2
2	A	25	0	18	7	0
2	B	25	0	18	5	0
3	A	11	12	12	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	8	6	6	1	0
5	B	8	6	6	0	0
6	A	769	0	0	105	6
6	B	758	0	0	104	7
All	All	11138	9778	9836	362	9

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 19.

All (362) 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:46:GLU:HB2	6:A:1492:HOH:O	1.41	1.20
1:A:152:ASN:HA	6:A:1305:HOH:O	1.64	0.97
1:A:348:MET:SD	6:A:1140:HOH:O	2.22	0.96
1:A:144:LEU:HG	6:A:1400:HOH:O	1.69	0.93
1:A:55:ASP:HB3	6:A:1140:HOH:O	1.71	0.91
1:A:43:SER:N	6:A:1492:HOH:O	2.04	0.89
1:A:274:PRO:O	6:A:1123:HOH:O	1.92	0.87
1:A:505:LYS:HD3	1:A:553:HIS:CE1	2.10	0.87
1:A:188:ILE:HG12	6:A:1338:HOH:O	1.75	0.86
1:A:516:VAL:HG21	6:A:1503:HOH:O	1.74	0.86
1:A:407:THR:HG23	6:A:1163:HOH:O	1.76	0.85
1:A:200:THR:OG1	6:A:1508:HOH:O	1.95	0.85
1:B:139:PRO:HD3	6:B:1412:HOH:O	1.76	0.84
1:A:149:SER:O	6:A:1452:HOH:O	1.94	0.83
1:B:494:GLN:HB3	6:B:1356:HOH:O	1.79	0.83
1:B:75:ASP:OD1	6:B:1046:HOH:O	1.97	0.82
1:A:159:ILE:HD12	6:A:1151:HOH:O	1.78	0.82
6:A:851:HOH:O	1:B:151:ILE:HD12	1.78	0.82
1:A:92:PHE:CE2	6:A:1513:HOH:O	2.31	0.82
1:B:388:ARG:HB2	6:B:1277:HOH:O	1.80	0.82
1:B:516:VAL:HG13	6:B:1360:HOH:O	1.79	0.82
1:B:192:SER:CB	6:B:1271:HOH:O	2.29	0.81
1:A:459:ALA:HB3	1:A:465:THR:HG23	1.63	0.80
1:B:157:GLY:HA2	6:B:1483:HOH:O	1.81	0.80
1:B:623:PRO:HA	6:B:725:HOH:O	1.80	0.79
1:A:277:ASP:C	6:A:1123:HOH:O	2.27	0.78
1:A:140:GLY:O	6:A:1400:HOH:O	2.01	0.78
1:A:310:GLY:HA2	6:A:1339:HOH:O	1.82	0.78
1:A:533:SER:HB3	6:A:1126:HOH:O	1.83	0.77
1:A:567:ASP:N	6:A:1503:HOH:O	2.16	0.77
1:A:43:SER:O	6:A:1492:HOH:O	2.02	0.77
1:B:259:ILE:HG22	6:B:1498:HOH:O	1.83	0.77
1:B:400:PRO:O	6:B:1164:HOH:O	2.00	0.77
1:A:53:MET:HG2	6:A:959:HOH:O	1.84	0.77
1:A:90:ILE:HG22	6:A:959:HOH:O	1.83	0.77
1:B:514:SER:OG	6:B:1360:HOH:O	2.03	0.76
1:B:495:VAL:O	6:B:1356:HOH:O	2.04	0.76
1:B:397:GLY:O	6:B:1164:HOH:O	2.04	0.75
1:A:100:LYS:HG3	1:A:411:ILE:HG21	1.67	0.75
3:A:647:PG4:O4	6:A:1259:HOH:O	2.05	0.74
1:B:374:ASN:HB3	1:B:376:ASP:OD1	1.86	0.74
1:A:103:VAL:HG12	6:A:1163:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HE3	6:A:1330:HOH:O	1.88	0.73
1:B:240:VAL:O	6:B:1060:HOH:O	2.07	0.73
1:A:639:GLY:CA	6:A:1216:HOH:O	2.36	0.72
1:A:150:ARG:NH2	1:A:202:ARG:HD3	2.03	0.72
1:B:157:GLY:O	6:B:1483:HOH:O	2.08	0.72
3:A:647:PG4:C7	6:A:1259:HOH:O	2.37	0.71
1:B:353:THR:HB	6:B:1395:HOH:O	1.90	0.71
1:A:531:THR:HG22	3:A:647:PG4:H22	1.72	0.70
1:B:153:ALA:HB2	6:B:1238:HOH:O	1.89	0.70
1:A:282:LYS:O	6:A:1176:HOH:O	2.08	0.70
1:B:259:ILE:CG2	6:B:1498:HOH:O	2.38	0.70
1:B:388:ARG:CB	6:B:1277:HOH:O	2.38	0.70
1:B:388:ARG:HD2	6:B:1277:HOH:O	1.91	0.70
1:B:552:GLN:NE2	6:B:753:HOH:O	2.24	0.69
1:A:640:ARG:HA	6:A:895:HOH:O	1.93	0.69
1:B:387:GLU:OE1	6:B:779:HOH:O	2.10	0.69
1:B:353:THR:O	6:B:1395:HOH:O	2.10	0.69
1:A:228:ASP:OD2	1:A:242:HIS:NE2	2.25	0.69
1:A:64:GLU:HB3	6:A:1184:HOH:O	1.93	0.68
1:A:221:LYS:HB3	1:A:267:MET:HB3	1.75	0.68
1:A:123:ASP:OD2	6:A:1513:HOH:O	2.12	0.68
1:B:542:PHE:CB	6:B:1469:HOH:O	2.43	0.67
1:A:366:GLN:O	1:A:370:GLU:HG2	1.95	0.66
1:A:244:GLN:O	1:A:248:ARG:HG3	1.95	0.66
1:B:495:VAL:HG22	1:B:534:ASP:O	1.95	0.66
1:B:240:VAL:C	6:B:1060:HOH:O	2.39	0.65
1:A:92:PHE:HE1	6:A:1140:HOH:O	1.78	0.65
1:A:323:LYS:O	6:A:1268:HOH:O	2.14	0.65
1:A:322:MET:HA	2:A:646:OAN:HAX	1.79	0.65
1:B:495:VAL:HG22	1:B:534:ASP:C	2.21	0.65
1:A:620:VAL:HB	6:A:1445:HOH:O	1.95	0.64
1:B:192:SER:HB3	6:B:1271:HOH:O	1.90	0.64
1:B:374:ASN:HB3	6:B:1113:HOH:O	1.98	0.64
1:B:321:ASN:HD21	2:B:646:OAN:CAW	2.09	0.64
1:A:215:ASP:OD1	6:A:1037:HOH:O	2.14	0.64
1:A:306:ARG:HG2	6:A:800:HOH:O	1.97	0.63
1:A:151:ILE:HG13	1:A:152:ASN:N	2.12	0.63
1:A:479:LYS:HA	6:A:1520:HOH:O	1.98	0.63
1:A:122:ILE:HD11	1:A:131:ARG:HB2	1.80	0.63
1:B:506:GLU:OE1	6:B:711:HOH:O	2.15	0.62
1:A:200:THR:CG2	6:A:1508:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:PRO:HD2	6:B:1060:HOH:O	1.98	0.62
1:B:356:LYS:HE3	6:B:1023:HOH:O	1.99	0.62
1:B:53:MET:HE1	1:B:119:MET:HE2	1.82	0.62
1:B:203:LEU:HD22	6:B:1238:HOH:O	2.01	0.61
1:B:367:ALA:O	6:B:732:HOH:O	2.16	0.61
1:A:144:LEU:CG	6:A:1400:HOH:O	2.37	0.61
1:A:480:LYS:HD2	6:A:1099:HOH:O	2.00	0.61
1:B:259:ILE:HB	6:B:1498:HOH:O	2.00	0.61
1:B:139:PRO:HG3	1:B:430:LEU:HG	1.84	0.60
1:B:179:ILE:O	1:B:227:GLY:HA3	2.01	0.60
1:B:528:ILE:HG23	6:B:1388:HOH:O	2.01	0.60
1:B:542:PHE:HB2	6:B:1469:HOH:O	1.99	0.60
2:B:646:OAN:HAX	2:B:646:OAN:OAR	2.00	0.60
1:A:468:ILE:O	1:A:472:ILE:HG13	2.01	0.60
1:A:144:LEU:CD1	6:A:1400:HOH:O	2.50	0.59
1:A:278:ASP:OD1	5:A:644:ACT:O	2.20	0.59
1:A:621:THR:HG23	6:A:1445:HOH:O	2.02	0.59
1:B:497:LYS:NZ	6:B:1126:HOH:O	2.24	0.59
1:B:183:PRO:HD2	6:B:1294:HOH:O	2.02	0.59
1:A:150:ARG:CZ	1:A:202:ARG:HD3	2.32	0.59
1:B:378:PRO:HG2	6:B:1337:HOH:O	2.03	0.59
1:A:298:LYS:NZ	6:A:1213:HOH:O	2.36	0.59
1:A:85:GLN:NE2	6:A:976:HOH:O	2.35	0.59
1:A:639:GLY:HA2	6:A:1216:HOH:O	2.02	0.59
1:B:638:THR:OG1	1:B:640:ARG:HG2	2.02	0.59
1:A:322:MET:HA	2:A:646:OAN:CAX	2.33	0.58
1:A:278:ASP:N	6:A:1123:HOH:O	2.33	0.58
1:A:319:ALA:HB1	1:A:321:ASN:OD1	2.03	0.58
1:A:307:GLN:HA	6:A:1339:HOH:O	2.03	0.58
1:B:344:ASP:CG	6:B:1277:HOH:O	2.46	0.58
1:B:107:ASP:O	6:B:773:HOH:O	2.17	0.58
1:B:388:ARG:CD	6:B:1277:HOH:O	2.51	0.58
1:A:92:PHE:CD2	6:A:1513:HOH:O	2.54	0.58
1:A:66:SER:O	6:A:1184:HOH:O	2.17	0.57
1:B:56:PHE:CE2	6:B:953:HOH:O	2.52	0.57
1:B:160:ILE:HB	6:B:1483:HOH:O	2.05	0.57
1:A:440:ASN:O	6:A:745:HOH:O	2.17	0.57
1:B:185:ASN:HA	1:B:229:THR:O	2.05	0.57
1:B:213:ARG:HD2	1:B:213:ARG:O	2.03	0.57
1:B:192:SER:OG	6:B:1271:HOH:O	2.17	0.57
1:A:168:GLY:C	6:A:1312:HOH:O	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:VAL:HG13	1:A:510:ILE:HD13	1.87	0.57
1:B:292:VAL:HG12	6:B:1157:HOH:O	2.04	0.57
1:A:505:LYS:HD3	1:A:553:HIS:NE2	2.19	0.57
1:B:430:LEU:HD12	1:B:430:LEU:O	2.05	0.56
1:B:312:ASN:ND2	6:B:938:HOH:O	2.37	0.56
1:A:639:GLY:N	6:A:1216:HOH:O	2.37	0.56
1:B:245:GLU:CG	6:B:1484:HOH:O	2.54	0.56
1:A:140:GLY:C	6:A:1400:HOH:O	2.46	0.56
1:B:505:LYS:HG2	1:B:553:HIS:CE1	2.41	0.55
1:B:259:ILE:CB	6:B:1498:HOH:O	2.53	0.55
1:A:26:ALA:N	1:B:637:LYS:HZ1	2.04	0.55
1:A:151:ILE:HD11	6:A:842:HOH:O	2.05	0.55
1:A:435:VAL:HB	1:A:609:PRO:HB3	1.89	0.55
1:B:253:TYR:HB3	1:B:254:PRO:HD3	1.87	0.55
1:B:298:LYS:HE3	6:B:1471:HOH:O	2.05	0.55
1:A:213:ARG:NH2	6:A:1107:HOH:O	2.40	0.54
1:A:455:ILE:HD12	1:A:484:VAL:HG21	1.88	0.54
1:A:459:ALA:HB3	1:A:465:THR:CG2	2.35	0.54
1:B:424:LEU:HD13	6:B:869:HOH:O	2.06	0.54
1:B:405:ASP:N	6:B:1111:HOH:O	2.40	0.54
1:A:150:ARG:HA	1:A:203:LEU:HD23	1.90	0.54
1:B:256:GLN:NE2	6:B:1498:HOH:O	2.36	0.54
1:B:174:SER:OG	1:B:175:PRO:HA	2.08	0.53
1:B:192:SER:C	6:B:1271:HOH:O	2.50	0.53
1:A:236:GLY:O	1:A:238:PRO:HD3	2.07	0.53
1:A:635:ASN:CG	1:A:638:THR:HG22	2.33	0.53
1:B:515:TYR:N	6:B:1360:HOH:O	2.41	0.53
1:B:56:PHE:CZ	6:B:953:HOH:O	2.62	0.53
1:B:542:PHE:CD2	6:B:1469:HOH:O	2.61	0.53
1:B:596:ILE:O	1:B:600:VAL:HG23	2.09	0.53
1:B:422:GLN:CA	6:B:787:HOH:O	2.57	0.53
1:A:100:LYS:HA	1:A:411:ILE:HG23	1.89	0.53
1:B:528:ILE:HA	6:B:1388:HOH:O	2.08	0.53
1:A:155:GLN:HB3	6:A:1305:HOH:O	2.09	0.53
1:A:307:GLN:CA	6:A:1339:HOH:O	2.56	0.53
1:A:322:MET:CA	2:A:646:OAN:HAX	2.39	0.53
1:B:72:LYS:HG3	6:B:1352:HOH:O	2.08	0.53
1:B:270:HIS:NE2	1:B:318:ASP:HB3	2.24	0.53
1:A:45:ASP:OD1	1:A:369:LYS:HE3	2.10	0.52
1:B:499:GLU:O	1:B:503:GLN:HG3	2.10	0.52
1:B:635:ASN:HB2	1:B:642:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASN:HB3	1:A:566:TYR:CD2	2.44	0.52
1:A:629:PRO:HD3	6:A:1101:HOH:O	2.10	0.52
1:B:260:ASP:N	6:B:1498:HOH:O	2.43	0.52
1:B:502:LYS:HA	1:B:505:LYS:HD3	1.92	0.52
1:A:103:VAL:CG1	6:A:1163:HOH:O	2.51	0.52
1:B:517:VAL:HG13	6:B:1299:HOH:O	2.09	0.52
1:B:428:LYS:HD3	1:B:432:GLU:CD	2.35	0.52
1:A:230:ASP:C	1:A:230:ASP:OD1	2.51	0.52
1:B:336:VAL:CG1	1:B:340:LYS:HE3	2.40	0.52
1:A:92:PHE:CE1	6:A:1140:HOH:O	2.53	0.51
1:A:493:SER:H	1:A:538:TRP:CG	2.29	0.51
1:A:198:GLU:HB3	1:A:202:ARG:HH21	1.75	0.51
1:A:456:LEU:HD11	1:A:489:MET:HE3	1.92	0.51
1:A:306:ARG:O	6:A:1339:HOH:O	2.19	0.51
1:B:542:PHE:CG	6:B:1469:HOH:O	2.54	0.51
1:A:387:GLU:OE2	6:A:1200:HOH:O	2.18	0.50
1:B:159:ILE:HA	1:B:162:LYS:HD2	1.93	0.50
1:A:476:ILE:HA	6:A:1520:HOH:O	2.10	0.50
1:B:157:GLY:CA	6:B:1483:HOH:O	2.51	0.50
1:B:67:PRO:HG3	6:B:1395:HOH:O	2.11	0.50
1:A:506:GLU:HA	6:A:970:HOH:O	2.10	0.50
1:A:638:THR:CG2	1:A:640:ARG:HG2	2.41	0.50
1:B:242:HIS:CG	6:B:1447:HOH:O	2.65	0.50
1:B:517:VAL:CG1	6:B:1299:HOH:O	2.59	0.50
1:A:140:GLY:HA3	6:A:835:HOH:O	2.12	0.50
1:A:138:PHE:HB3	1:A:139:PRO:HD2	1.94	0.49
1:B:201:SER:HA	1:B:254:PRO:HB3	1.93	0.49
1:B:283:SER:O	1:B:287:GLY:HA2	2.11	0.49
1:A:277:ASP:N	6:A:1123:HOH:O	2.45	0.49
1:A:459:ALA:O	1:A:490:ASN:HA	2.12	0.49
1:B:121:SER:HA	1:B:171:THR:O	2.11	0.49
1:B:495:VAL:O	1:B:497:LYS:HD3	2.12	0.49
1:B:495:VAL:HG13	6:B:1076:HOH:O	2.12	0.49
1:A:142:MET:HG2	1:A:581:TYR:CD1	2.47	0.49
1:A:307:GLN:C	6:A:1339:HOH:O	2.55	0.49
1:A:428:LYS:O	1:A:432:GLU:HG3	2.13	0.49
1:B:402:ARG:HG3	6:B:1164:HOH:O	2.13	0.49
1:A:150:ARG:HA	1:A:203:LEU:CD2	2.42	0.49
1:A:525:ASP:HA	6:A:1411:HOH:O	2.13	0.49
1:A:522:VAL:HA	6:A:1052:HOH:O	2.13	0.49
1:B:528:ILE:HG12	6:B:1388:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASP:CA	6:A:1503:HOH:O	2.60	0.49
1:B:242:HIS:CE1	6:B:1447:HOH:O	2.66	0.49
1:B:635:ASN:HB3	1:B:638:THR:HG23	1.95	0.49
1:B:520:ASP:HA	6:B:982:HOH:O	2.13	0.49
1:A:379:GLU:HB2	6:A:1479:HOH:O	2.12	0.48
1:B:291:LEU:HD21	6:B:1270:HOH:O	2.12	0.48
1:A:201:SER:HB3	6:A:1310:HOH:O	2.13	0.48
1:A:144:LEU:HD12	6:A:1400:HOH:O	2.13	0.48
1:B:234:HIS:NE2	2:B:646:OAN:OAQ	2.47	0.48
1:A:128:ILE:HD13	1:A:190:VAL:CG2	2.44	0.48
1:A:274:PRO:C	6:A:1123:HOH:O	2.48	0.48
1:A:110:GLN:OE1	1:A:110:GLN:HA	2.14	0.48
1:B:239:LEU:HD12	6:B:1060:HOH:O	2.14	0.48
1:B:243:GLY:N	6:B:714:HOH:O	2.45	0.48
1:B:538:TRP:CE3	1:B:539:ALA:HA	2.49	0.48
1:B:564:ASN:ND2	6:B:1282:HOH:O	2.46	0.48
1:A:187:VAL:HG13	6:A:1338:HOH:O	2.12	0.48
1:A:408:LYS:HD2	6:A:1453:HOH:O	2.14	0.48
1:B:300:VAL:O	1:B:304:LEU:HB3	2.14	0.48
3:A:647:PG4:C6	6:A:1259:HOH:O	2.60	0.48
1:A:321:ASN:HD21	2:A:646:OAN:HAO	1.61	0.47
1:B:253:TYR:N	6:B:1340:HOH:O	2.47	0.47
1:A:44:LEU:O	1:A:48:LEU:HG	2.14	0.47
1:B:399:TYR:HD1	1:B:400:PRO:HA	1.79	0.47
1:A:606:GLN:OE1	6:A:1099:HOH:O	2.20	0.47
1:A:404:SER:HA	6:A:1167:HOH:O	2.14	0.47
1:A:359:GLN:HG3	6:A:1280:HOH:O	2.14	0.47
1:A:630:LEU:HD23	1:A:630:LEU:C	2.40	0.47
1:A:635:ASN:OD1	1:A:638:THR:HG22	2.14	0.47
1:B:365:ILE:HG21	6:B:1189:HOH:O	2.13	0.47
1:B:376:ASP:OD1	1:B:376:ASP:N	2.47	0.47
1:A:174:SER:OG	1:A:175:PRO:HA	2.15	0.47
1:B:450:LYS:HG2	6:B:1324:HOH:O	2.15	0.47
1:B:455:ILE:HD12	1:B:484:VAL:HG21	1.97	0.47
1:A:200:THR:HG23	6:A:1508:HOH:O	2.11	0.47
1:A:322:MET:HA	2:A:646:OAN:CAW	2.45	0.46
1:B:98:THR:OG1	1:B:101:GLN:HB2	2.14	0.46
1:A:450:LYS:HB2	6:A:1086:HOH:O	2.15	0.46
1:A:635:ASN:HB3	1:A:638:THR:CG2	2.45	0.46
1:B:248:ARG:HA	1:B:252:LEU:HD12	1.98	0.46
1:A:139:PRO:HB2	1:A:143:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HB2	6:B:1268:HOH:O	2.15	0.46
1:B:211:LEU:CD2	6:B:1483:HOH:O	2.63	0.46
1:B:533:SER:C	6:B:1007:HOH:O	2.59	0.46
1:A:439:LYS:O	1:A:576:ALA:HA	2.16	0.46
1:B:298:LYS:NZ	6:B:761:HOH:O	2.48	0.46
1:B:383:ASN:O	1:B:387:GLU:HG3	2.15	0.46
1:B:428:LYS:C	1:B:428:LYS:CD	2.89	0.46
1:A:413:LYS:O	1:A:417:ILE:HG13	2.16	0.46
1:B:582:GLY:HA3	1:B:595:ASN:CG	2.41	0.46
1:A:321:ASN:HD21	2:A:646:OAN:CAS	2.28	0.46
1:A:366:GLN:OE1	1:A:370:GLU:OE2	2.34	0.46
1:B:212:GLN:HE21	1:B:264:ASP:CG	2.23	0.46
1:B:233:SER:HA	1:B:236:GLY:O	2.16	0.46
1:A:233:SER:HA	1:A:236:GLY:O	2.16	0.46
1:A:292:VAL:HG12	6:A:1056:HOH:O	2.16	0.46
1:A:43:SER:CA	6:A:1492:HOH:O	2.60	0.46
1:A:306:ARG:HD3	1:A:311:PHE:O	2.16	0.46
1:A:510:ILE:CD1	1:A:550:ALA:HB2	2.46	0.46
1:A:83:LYS:HE2	1:A:84:TYR:CZ	2.51	0.45
1:A:533:SER:HA	3:A:647:PG4:C8	2.47	0.45
1:B:73:MET:HE2	1:B:73:MET:HA	1.98	0.45
1:A:520:ASP:OD1	1:A:520:ASP:O	2.35	0.45
1:B:522:VAL:O	6:B:1388:HOH:O	2.21	0.45
1:A:264:ASP:OD1	1:A:395:LYS:HE3	2.16	0.45
1:B:234:HIS:HD2	2:B:646:OAN:HAO	1.65	0.45
1:B:317:THR:C	1:B:318:ASP:O	2.58	0.45
1:A:427:GLU:HG3	1:A:594:PRO:HG3	1.99	0.45
1:B:134:GLU:HB2	6:B:919:HOH:O	2.16	0.45
1:B:523:VAL:HB	6:B:1388:HOH:O	2.16	0.45
1:A:409:GLU:HG2	6:A:825:HOH:O	2.17	0.44
1:A:508:ASP:O	1:A:556:PRO:HD2	2.16	0.44
1:B:431:ALA:N	6:B:1412:HOH:O	2.48	0.44
1:A:504:VAL:HG13	1:A:510:ILE:CD1	2.47	0.44
1:B:74:ASN:OD1	1:B:76:GLU:HB2	2.18	0.44
1:A:42:MET:HB3	6:A:1492:HOH:O	2.16	0.44
1:B:239:LEU:CD1	6:B:1060:HOH:O	2.65	0.44
1:B:240:VAL:HA	6:B:933:HOH:O	2.16	0.44
1:B:459:ALA:HB3	1:B:465:THR:HG23	2.00	0.44
1:B:470:GLN:HG3	1:B:586:TYR:CE1	2.52	0.44
1:A:166:ALA:HB2	6:A:1303:HOH:O	2.17	0.44
1:B:213:ARG:HB3	6:B:1241:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:O	1:A:133:GLY:HA3	2.18	0.44
1:B:270:HIS:CE1	1:B:318:ASP:HB3	2.53	0.44
1:B:368:LEU:O	1:B:372:VAL:HG23	2.17	0.44
1:B:608:LYS:HG2	1:B:610:LYS:NZ	2.32	0.44
1:A:180:ASN:HB2	1:A:192:SER:HB3	2.00	0.43
1:A:635:ASN:HB3	1:A:638:THR:HG23	1.99	0.43
1:B:353:THR:CB	6:B:1395:HOH:O	2.59	0.43
1:A:58:ASN:HA	1:A:68:GLN:O	2.18	0.43
1:A:244:GLN:O	1:A:248:ARG:CG	2.64	0.43
1:B:408:LYS:HE3	1:B:408:LYS:HB2	1.89	0.43
1:B:274:PRO:CD	6:B:1060:HOH:O	2.60	0.43
1:B:640:ARG:NH2	6:B:1426:HOH:O	2.51	0.43
2:B:646:OAN:OAR	2:B:646:OAN:CAX	2.65	0.43
1:A:97:LYS:HA	6:A:759:HOH:O	2.18	0.43
1:B:240:VAL:N	6:B:1060:HOH:O	2.51	0.43
1:A:278:ASP:HA	1:A:291:LEU:CD2	2.48	0.43
1:B:100:LYS:HE2	6:B:1406:HOH:O	2.18	0.43
1:B:459:ALA:O	1:B:490:ASN:HA	2.18	0.43
1:A:170:ASN:HB3	6:A:1312:HOH:O	2.19	0.43
1:A:234:HIS:HD2	2:A:646:OAN:CAT	2.31	0.43
1:B:605:GLY:HA2	6:B:900:HOH:O	2.18	0.43
1:B:33:ILE:O	1:B:37:GLN:HG2	2.18	0.43
1:B:348:MET:N	1:B:349:PRO:HD3	2.34	0.43
1:A:181:ASN:ND2	6:A:690:HOH:O	2.45	0.43
1:A:257:LYS:NZ	6:A:1087:HOH:O	2.28	0.43
1:A:510:ILE:HD12	1:A:550:ALA:CB	2.49	0.43
1:A:355:LEU:HB2	6:A:1302:HOH:O	2.18	0.42
1:A:173:PHE:HA	1:A:219:ALA:HB3	2.01	0.42
1:A:506:GLU:OE2	6:A:1491:HOH:O	2.21	0.42
1:B:155:GLN:OE1	6:B:1328:HOH:O	2.21	0.42
1:B:338:ALA:O	1:B:343:VAL:HG22	2.19	0.42
1:A:622:LYS:NZ	6:A:823:HOH:O	2.19	0.42
1:B:110:GLN:HA	1:B:110:GLN:OE1	2.19	0.42
1:A:61:LYS:HA	1:A:76:GLU:OE1	2.19	0.42
1:A:221:LYS:HB2	1:A:222:HIS:CG	2.55	0.42
1:A:476:ILE:O	6:A:1520:HOH:O	2.21	0.42
1:B:572:GLU:HG3	6:B:1117:HOH:O	2.19	0.42
1:B:635:ASN:HA	1:B:642:LEU:HD21	2.02	0.42
1:B:636:ILE:O	1:B:636:ILE:CG1	2.68	0.42
1:A:569:ALA:CB	1:A:620:VAL:HG23	2.49	0.42
1:B:422:GLN:N	6:B:787:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HD2	6:B:950:HOH:O	2.19	0.41
1:B:635:ASN:HB2	1:B:642:LEU:CD2	2.49	0.41
1:A:409:GLU:CG	6:A:825:HOH:O	2.68	0.41
1:B:243:GLY:CA	6:B:714:HOH:O	2.68	0.41
1:A:548:LYS:HE3	6:A:1239:HOH:O	2.19	0.41
1:A:438:LEU:HB2	1:A:577:LEU:HD23	2.01	0.41
1:B:455:ILE:CD1	1:B:484:VAL:HG21	2.50	0.41
1:B:457:ILE:HG22	1:B:465:THR:HG22	2.02	0.41
1:A:131:ARG:NH2	6:A:999:HOH:O	2.53	0.41
1:A:640:ARG:O	1:A:641:PRO:C	2.63	0.41
1:B:515:TYR:C	6:B:1360:HOH:O	2.63	0.41
1:A:55:ASP:CB	6:A:1140:HOH:O	2.49	0.41
1:A:201:SER:CB	6:A:1310:HOH:O	2.69	0.41
1:B:305:LEU:HD23	1:B:315:ILE:CD1	2.50	0.41
1:A:61:LYS:O	1:A:62:GLU:C	2.62	0.41
1:A:348:MET:CG	6:A:1140:HOH:O	2.65	0.41
1:B:370:GLU:O	1:B:374:ASN:N	2.54	0.41
1:A:152:ASN:HB3	1:A:430:LEU:HD22	2.01	0.40
1:B:422:GLN:HA	6:B:787:HOH:O	2.20	0.40
1:B:520:ASP:N	1:B:521:PRO:CD	2.85	0.40
1:A:409:GLU:CD	6:A:825:HOH:O	2.65	0.40
1:B:365:ILE:O	1:B:369:LYS:HG3	2.22	0.40
1:B:451:LYS:HB3	6:B:985:HOH:O	2.21	0.40
1:A:284:LYS:HE2	1:A:284:LYS:HB3	1.91	0.40
1:A:597:PRO:O	1:A:601:MET:HG2	2.20	0.40
1:B:56:PHE:CD2	6:B:953:HOH:O	2.74	0.40
1:B:236:GLY:O	1:B:238:PRO:HD3	2.21	0.40
1:A:143:ALA:HB1	1:A:434:ALA:CB	2.52	0.40
1:A:221:LYS:HA	1:A:222:HIS:HA	1.87	0.40
1:A:185:ASN:ND2	6:A:1338:HOH:O	2.53	0.40
1:A:202:ARG:NE	6:A:907:HOH:O	2.52	0.40
1:B:218:SER:H	1:B:264:ASP:HB2	1.87	0.40
1:B:336:VAL:HG22	1:B:368:LEU:HD23	2.03	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1227:HOH:O	6:A:1228:HOH:O[1_455]	1.92	0.28
6:A:1038:HOH:O	6:B:987:HOH:O[1_556]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HG21	6:B:1429:HOH:O[1_655]	1.48	0.12
6:A:975:HOH:O	6:B:1194:HOH:O[1_556]	2.10	0.10
6:A:985:HOH:O	6:B:741:HOH:O[1_556]	2.10	0.10
1:B:37:GLN:OE1	6:B:784:HOH:O[1_565]	2.10	0.10
6:A:1082:HOH:O	6:B:1102:HOH:O[1_556]	2.15	0.05
1:A:151:ILE:CG2	6:B:1429:HOH:O[1_655]	2.16	0.04
1:B:517:VAL:HG21	6:A:975:HOH:O[1_554]	1.56	0.04

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	616/642 (96%)	592 (96%)	24 (4%)	0	100	100
1	B	616/642 (96%)	584 (95%)	32 (5%)	0	100	100
All	All	1232/1284 (96%)	1176 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	520/541 (96%)	508 (98%)	12 (2%)	44	27
1	B	520/541 (96%)	508 (98%)	12 (2%)	44	27
All	All	1040/1082 (96%)	1016 (98%)	24 (2%)	44	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	181	ASN
1	A	297	SER
1	A	323	LYS
1	A	408	LYS
1	A	413	LYS
1	A	429	LYS
1	A	477	LYS
1	A	493	SER
1	A	536	SER
1	A	610	LYS
1	A	641	PRO
1	B	72	LYS
1	B	205	LEU
1	B	221	LYS
1	B	233	SER
1	B	376	ASP
1	B	428	LYS
1	B	430	LEU
1	B	497	LYS
1	B	523	VAL
1	B	608	LYS
1	B	638	THR
1	B	640	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	321	ASN
1	A	366	GLN
1	A	380	GLN
1	A	422	GLN
1	A	470	GLN
1	A	494	GLN
1	B	68	GLN
1	B	155	GLN
1	B	214	GLN
1	B	312	ASN
1	B	321	ASN
1	B	366	GLN

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Mol	Chain	Res	Type
1	B	380	GLN
1	B	473	HIS
1	B	553	HIS

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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	OAN	A	646	-	23,26,26	5.05	11 (47%)	24,35,35	1.77	4 (16%)
3	PG4	A	647	-	10,10,12	0.75	0	9,9,11	1.38	1 (11%)
2	OAN	B	646	-	23,26,26	5.09	16 (69%)	24,35,35	2.55	8 (33%)
5	ACT	B	644	-	3,3,3	0.74	0	3,3,3	1.35	0
5	ACT	B	645	-	3,3,3	0.75	0	3,3,3	1.29	0
5	ACT	A	645	-	3,3,3	0.71	0	3,3,3	1.32	0
5	ACT	A	644	-	3,3,3	0.92	0	3,3,3	0.85	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	OAN	B	646	-	-	4/12/35/35	0/2/2/2
3	PG4	A	647	-	-	4/8/8/10	-
2	OAN	A	646	-	-	8/12/35/35	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	646	OAN	CAX-CAS	9.57	1.55	1.39
2	A	646	OAN	CAX-CAS	9.38	1.55	1.39
2	A	646	OAN	CAW-CAX	8.99	1.54	1.38
2	B	646	OAN	CAU-CAT	8.92	1.54	1.38
2	B	646	OAN	CAT-CAS	8.78	1.54	1.39
2	A	646	OAN	CAU-CAT	8.78	1.53	1.38
2	A	646	OAN	CAT-CAS	8.69	1.53	1.39
2	B	646	OAN	CAW-CAX	8.44	1.53	1.38
2	B	646	OAN	CAV-CAU	7.83	1.55	1.38
2	A	646	OAN	CAV-CAU	7.79	1.55	1.38
2	B	646	OAN	CAW-CAV	7.45	1.54	1.38
2	A	646	OAN	CAW-CAV	7.41	1.54	1.38
2	B	646	OAN	CAA-NAY	7.40	1.44	1.27
2	A	646	OAN	CAA-NAY	7.04	1.43	1.27
2	A	646	OAN	OAM-CAF	-5.99	1.17	1.42
2	A	646	OAN	CAP-NAO	5.65	1.47	1.36
2	B	646	OAN	OAM-CAF	-5.43	1.19	1.42
2	B	646	OAN	CAP-NAO	5.37	1.46	1.36
2	A	646	OAN	CAG-NAI	3.63	1.46	1.34
2	B	646	OAN	OAL-CAE	-3.21	1.42	1.46
2	B	646	OAN	CAG-NAI	3.01	1.44	1.34
2	A	646	OAN	CAS-NAO	2.48	1.46	1.41
2	B	646	OAN	CAS-NAO	2.44	1.46	1.41
2	B	646	OAN	OAN-CAG	-2.36	1.18	1.23
2	B	646	OAN	CAC-CAB	-2.35	1.49	1.52
2	B	646	OAN	OAJ-CAC	-2.10	1.37	1.43
2	B	646	OAN	OAR-CAP	-2.08	1.17	1.21

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	646	OAN	OAL-CAE-CAF	-7.88	98.15	106.05
2	A	646	OAN	CAS-NAO-CAP	-5.22	118.14	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	646	OAN	CAS-NAO-CAP	-4.85	118.72	126.39
2	A	646	OAN	OAL-CAE-CAF	-3.99	102.05	106.05
2	B	646	OAN	OAK-CAD-CAC	-3.62	101.84	110.38
2	A	646	OAN	OAR-CAP-NAO	-3.44	118.80	126.12
2	B	646	OAN	OAR-CAP-NAO	-3.26	119.19	126.12
2	B	646	OAN	CAF-CAE-CAD	-3.19	105.18	113.02
3	A	647	PG4	C5-O3-C4	2.86	125.78	113.26
2	B	646	OAN	CAB-NAI-CAG	-2.49	117.55	121.82
2	B	646	OAN	OAJ-CAC-CAD	-2.21	105.16	110.38
2	B	646	OAN	OAM-CAF-CAE	2.19	118.79	111.33
2	A	646	OAN	CAC-CAD-CAE	-2.06	106.50	110.23

There are no chirality outliers.

All (16) torsion outliers are listed below:

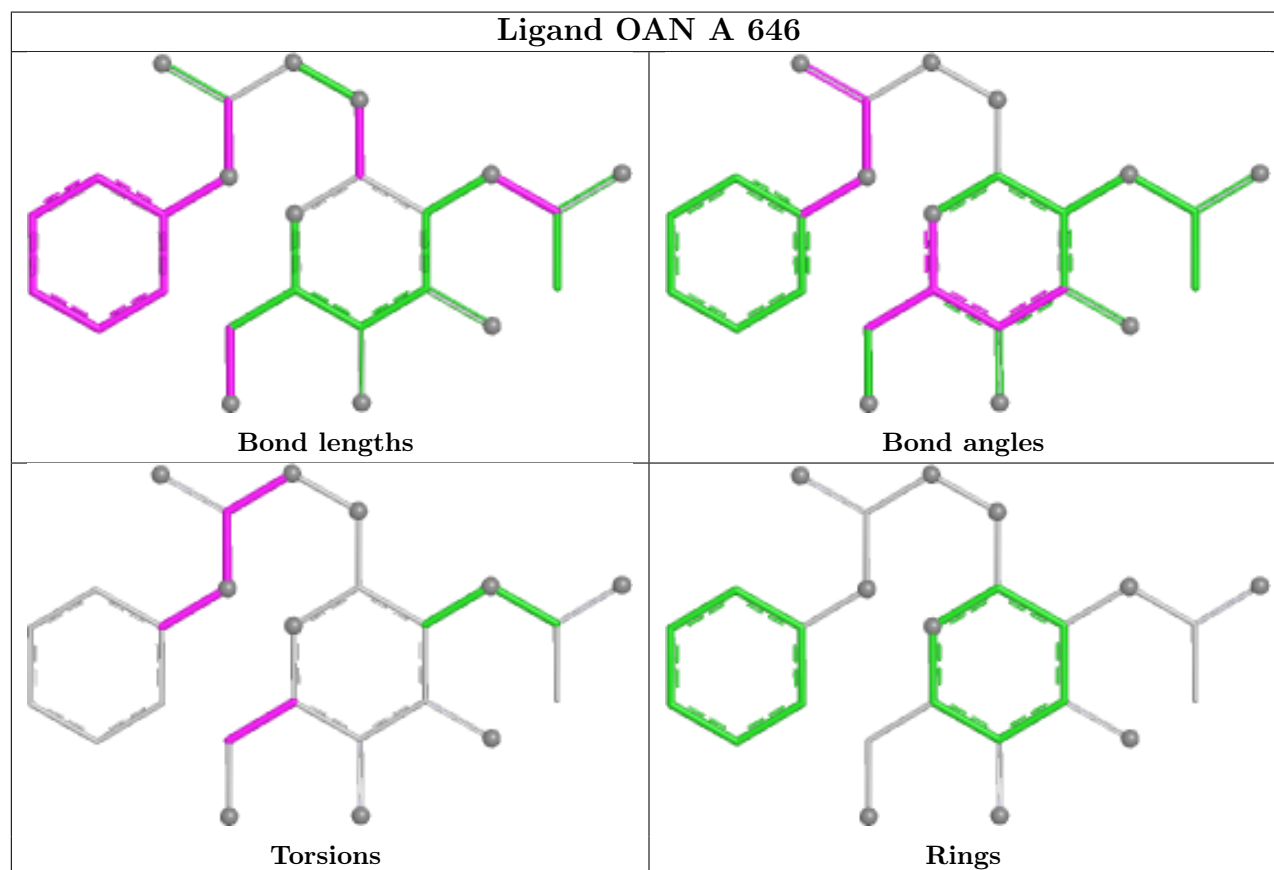
Mol	Chain	Res	Type	Atoms
2	A	646	OAN	OAR-CAP-OAQ-NAY
2	A	646	OAN	OAQ-CAP-NAO-CAS
2	A	646	OAN	OAR-CAP-NAO-CAS
2	B	646	OAN	OAR-CAP-OAQ-NAY
2	B	646	OAN	NAO-CAP-OAQ-NAY
2	B	646	OAN	OAQ-CAP-NAO-CAS
2	A	646	OAN	CAT-CAS-NAO-CAP
2	A	646	OAN	CAX-CAS-NAO-CAP
2	B	646	OAN	OAR-CAP-NAO-CAS
3	A	647	PG4	O2-C3-C4-O3
2	A	646	OAN	CAD-CAE-CAF-OAM
2	A	646	OAN	OAL-CAE-CAF-OAM
3	A	647	PG4	O3-C5-C6-O4
3	A	647	PG4	C4-C3-O2-C2
3	A	647	PG4	C8-C7-O4-C6
2	A	646	OAN	NAO-CAP-OAQ-NAY

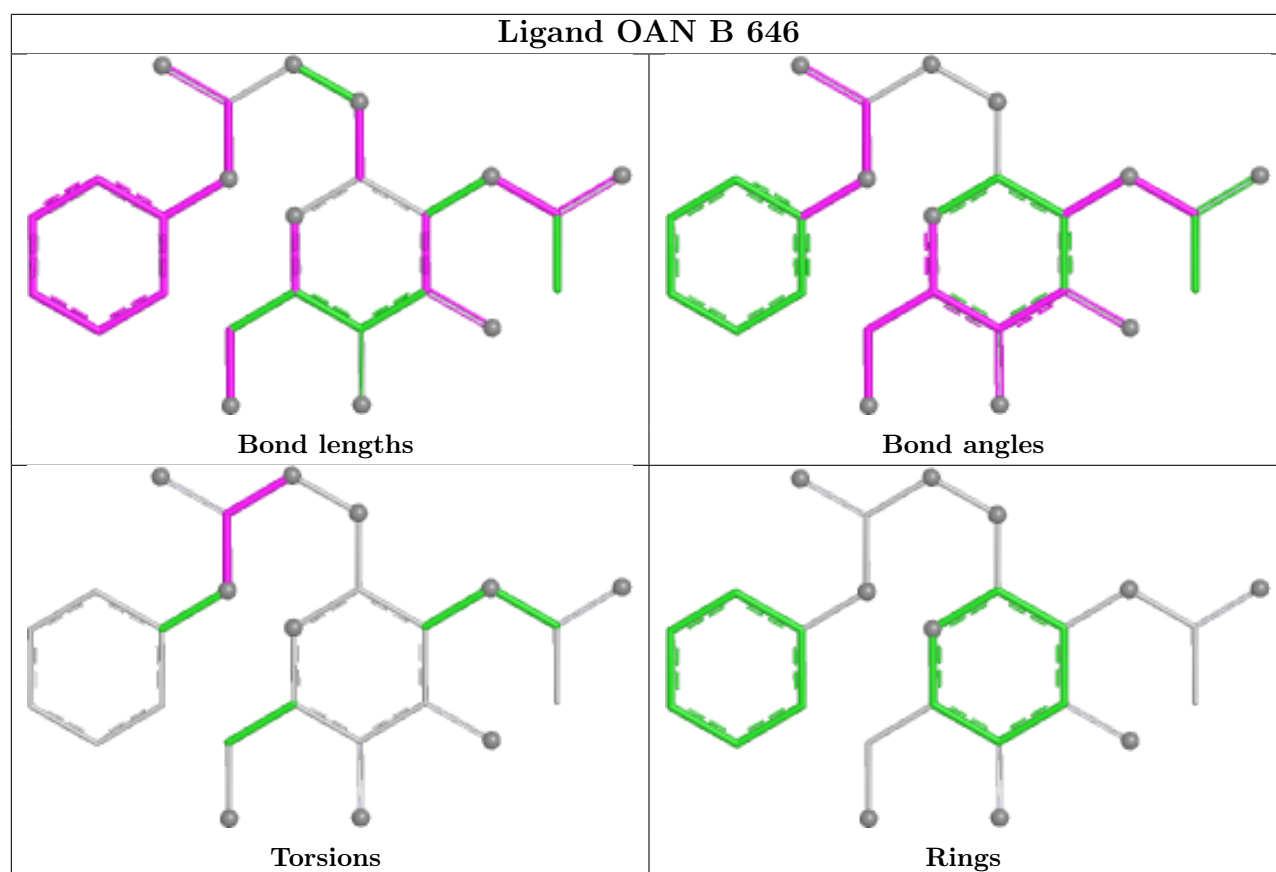
There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	646	OAN	7	0
3	A	647	PG4	5	0
2	B	646	OAN	5	0
5	A	644	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	617/642 (96%)	-1.37	0 100 100	8, 19, 44, 66	2 (0%)
1	B	617/642 (96%)	-1.34	0 100 100	8, 21, 45, 96	2 (0%)
All	All	1234/1284 (96%)	-1.36	0 100 100	8, 20, 44, 96	4 (0%)

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.

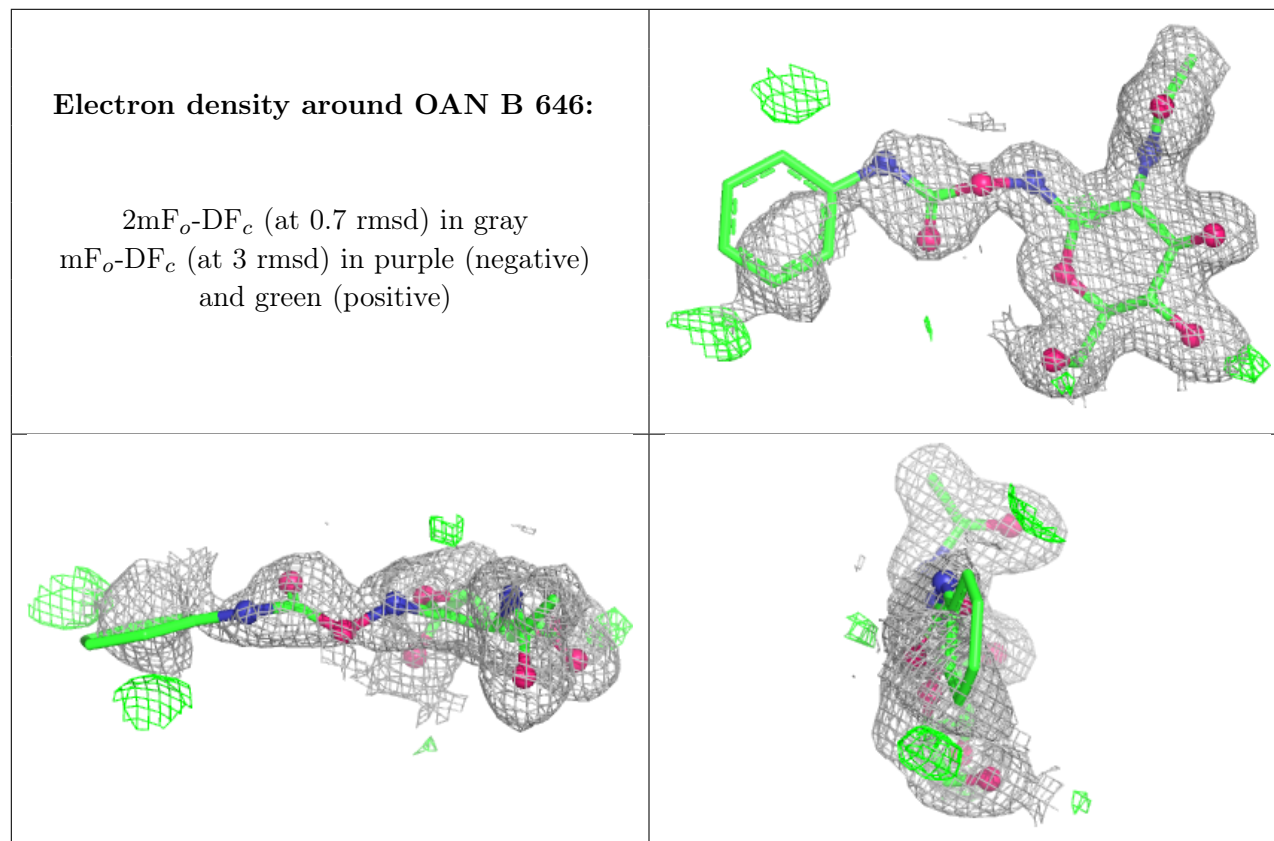
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	B	644	4/4	0.98	0.05	35,37,44,44	0
2	OAN	B	646	25/25	0.99	0.05	5,13,59,62	0
3	PG4	A	647	11/13	0.99	0.05	20,34,59,61	0
4	NA	B	643	1/1	0.99	0.02	19,19,19,19	0
5	ACT	A	644	4/4	0.99	0.03	19,30,36,39	0
5	ACT	A	645	4/4	0.99	0.05	33,37,41,46	0
2	OAN	A	646	25/25	0.99	0.06	6,14,64,68	0

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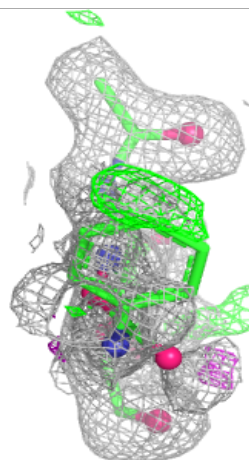
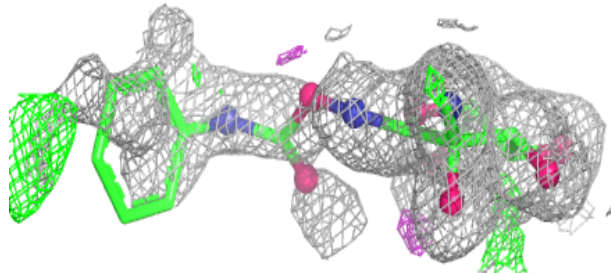
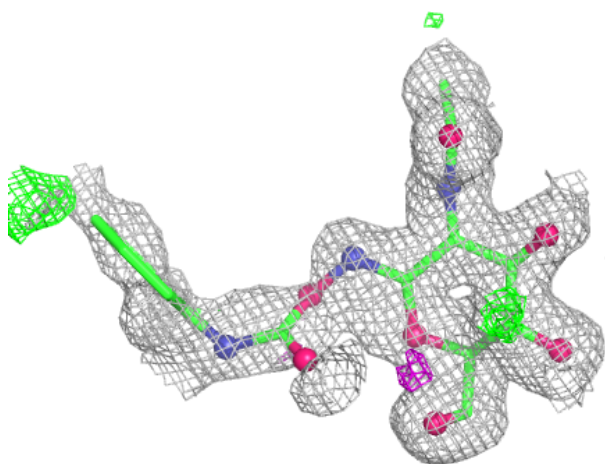
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	B	645	4/4	0.99	0.04	34,38,46,46	0
4	NA	A	643	1/1	1.00	0.01	20,20,20,20	0

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 OAN A 646:

$2mF_o-DF_c$ (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.