Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2021 – 12:10 am BST

PDB ID	:	4WMC
Title	:	OXA-48 covalent complex with Avibactam inhibitor
Authors	:	Mangani, S.; Benvenuti, M.; Docquier, J.D.
Deposited on	:	2014-10-08
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

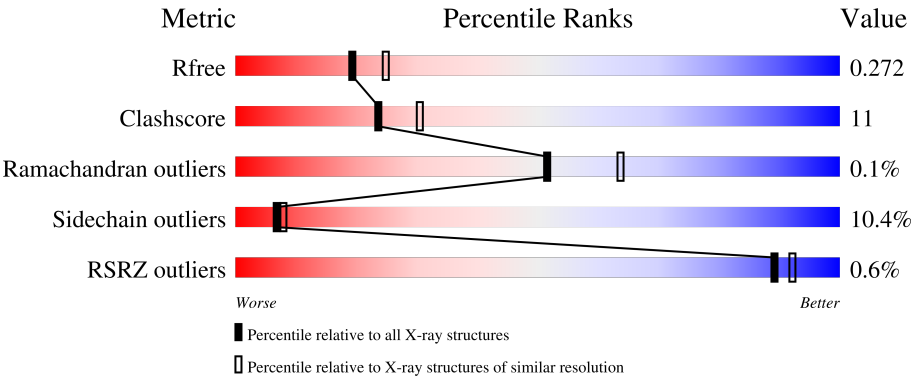
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	242	72% 23%
1	B	242	% 76% 16% 5%
1	C	242	65% 25% 5% 5%
1	F	242	% 67% 28% 5%
1	G	242	% 67% 24% 5%

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Mol	Chain	Length	Quality of chain
1	H	242	
2	D	242	
2	E	242	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15682 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.

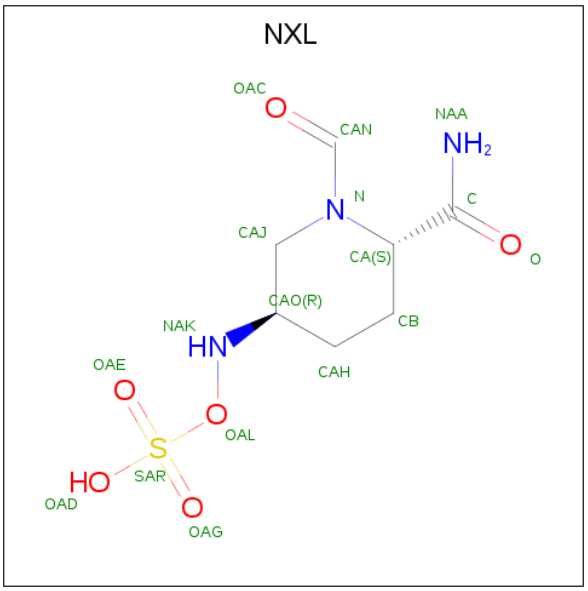
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1938	1237	341	353	7			
1	B	235	Total	C	N	O	S	0	0	0
			1922	1227	339	349	7			
1	C	230	Total	C	N	O	S	0	0	0
			1876	1199	327	343	7			
1	F	240	Total	C	N	O	S	0	0	0
			1954	1245	345	357	7			
1	G	235	Total	C	N	O	S	0	0	0
			1911	1221	334	349	7			
1	H	221	Total	C	N	O	S	0	0	0
			1794	1150	312	325	7			

- Molecule 2 is a protein called Beta-lactamase.

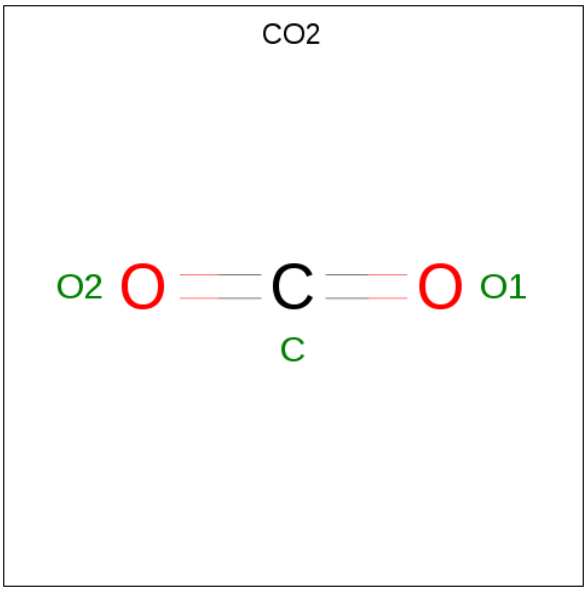
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	236	Total	C	N	O	S	0	0	0
			1935	1236	340	352	7			
2	E	239	Total	C	N	O	S	0	0	0
			1951	1242	343	359	7			

- Molecule 3 is (2S,5R)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (three-letter code: NXL) (formula: $C_7H_{13}N_3O_6S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 17 7 3 6 1	0	0
3	B	1	Total C N O S 17 7 3 6 1	0	0
3	C	1	Total C N O S 17 7 3 6 1	0	0
3	D	1	Total C N O S 17 7 3 6 1	0	0
3	E	1	Total C N O S 17 7 3 6 1	0	0
3	F	1	Total C N O S 17 7 3 6 1	0	0
3	G	1	Total C N O S 17 7 3 6 1	0	0
3	H	1	Total C N O S 17 7 3 6 1	0	0

- Molecule 4 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	F	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

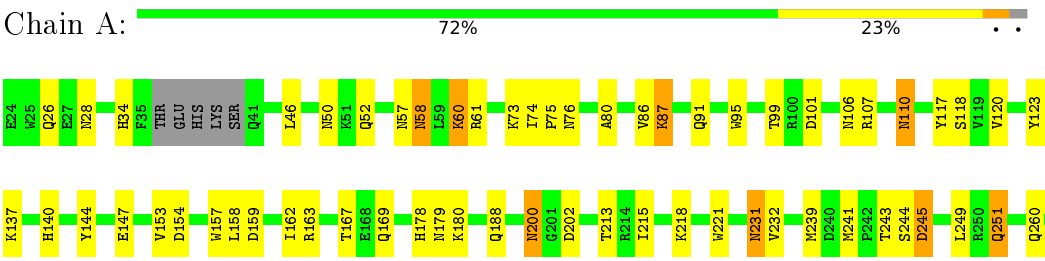
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	47	Total O 47 47	0	0
5	C	15	Total O 15 15	0	0
5	D	51	Total O 51 51	0	0
5	E	42	Total O 42 42	0	0
5	F	23	Total O 23 23	0	0
5	G	17	Total O 17 17	0	0
5	H	23	Total O 23 23	0	0

3 Residue-property plots (i)

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.

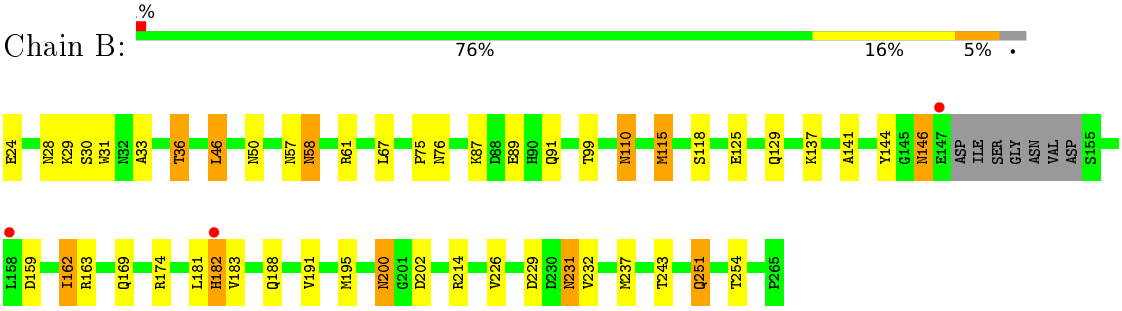
- Molecule 1: Beta-lactamase

Chain A:



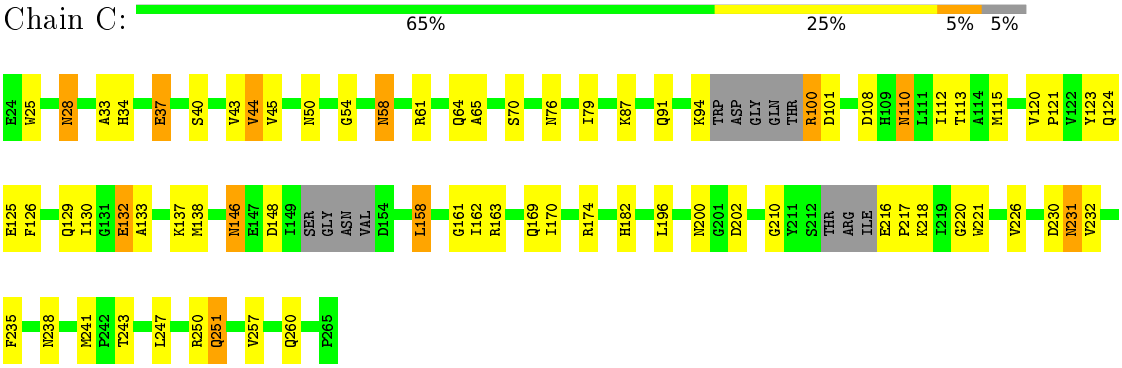
- Molecule 1: Beta-lactamase

Chain B:



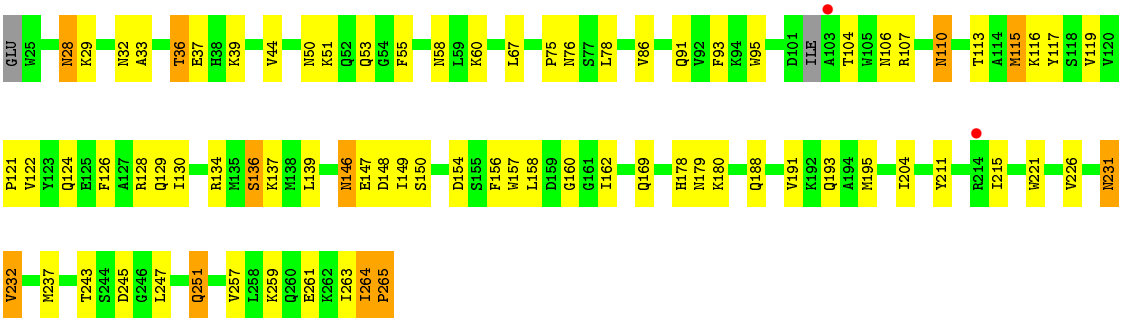
- Molecule 1: Beta-lactamase

Chain C:

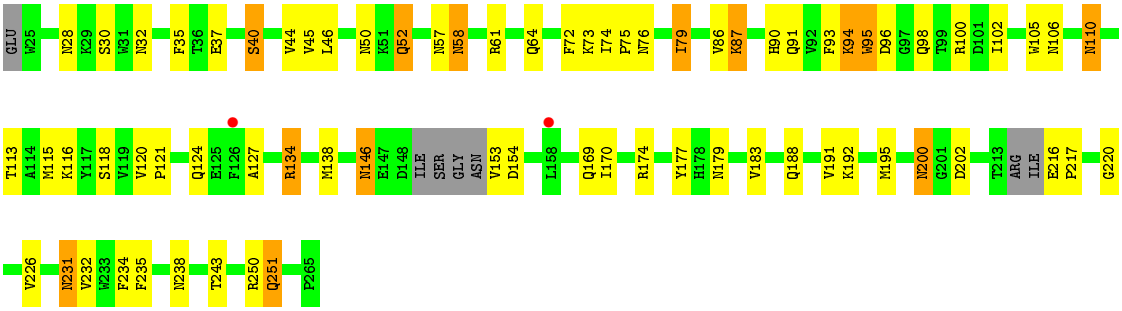


- Molecule 1: Beta-lactamase

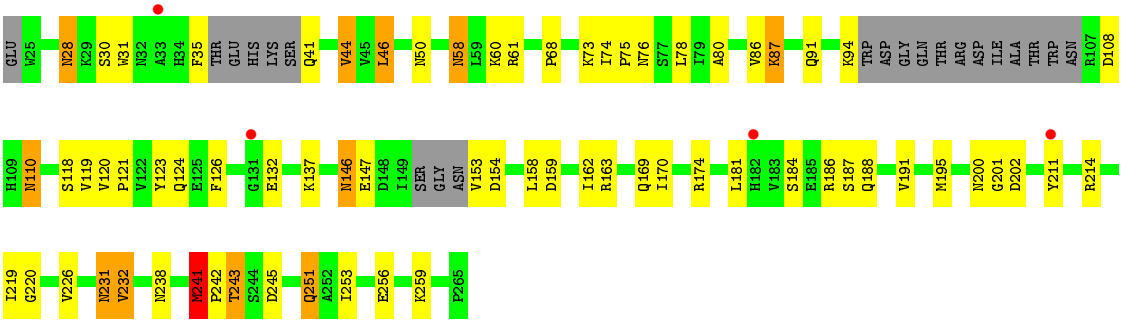
Chain F:



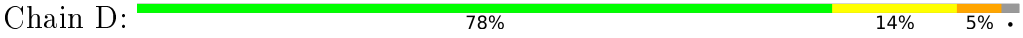
• Molecule 1: Beta-lactamase

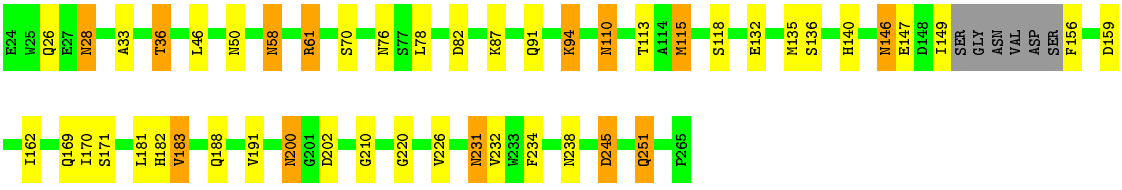


• Molecule 1: Beta-lactamase



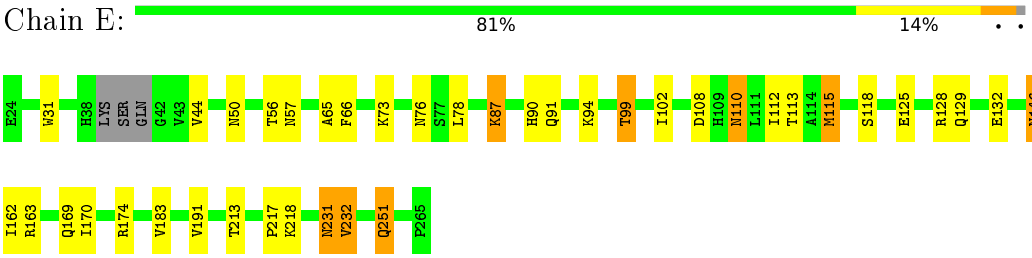
• Molecule 2: Beta-lactamase





• Molecule 2: Beta-lactamase

Chain E:


81%
14%
E24
W31
H38
LYS
SER
GLN
G42
V43
Y44
N50
T56
N57
A65
F66
K73
N76
S77
L78
K87
H90
Q91
K94
T99
I102
D108
H109
N110
L111
I112
T113
A114
M115
S118
E125
R128
Q129
E132
N146
N152
V163
I162
R163
Q169
I170
R174
V183
Y191
T213
P217
K218
N231
V232
Q251
P265

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.89Å 165.47Å 108.52Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	63.88 – 2.30 63.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (63.88-2.30) 90.7 (63.88-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.210 , 0.273 0.211 , 0.272	Depositor DCC
R_{free} test set	4546 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 11.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15682	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NXL, CO2, KCX

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	0.68	0/1985	0.81	2/2685 (0.1%)
1	B	0.75	0/1970	0.86	2/2666 (0.1%)
1	C	0.64	0/1920	0.76	1/2594 (0.0%)
1	F	0.69	0/2002	0.82	4/2708 (0.1%)
1	G	0.62	0/1958	0.77	0/2650
1	H	0.73	0/1835	0.83	1/2480 (0.0%)
2	D	0.79	0/1970	0.92	3/2665 (0.1%)
2	E	0.72	0/1986	0.85	1/2688 (0.0%)
All	All	0.71	0/15626	0.83	14/21136 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	115	MET	CG-SD-CE	-10.32	83.69	100.20
1	B	115	MET	CG-SD-CE	-7.91	87.55	100.20
2	E	115	MET	CG-SD-CE	-6.63	89.59	100.20
1	F	264	ILE	C-N-CD	6.39	141.82	128.40
1	F	265	PRO	CA-N-CD	-5.99	103.12	111.50
2	D	245	ASP	CB-CA-C	5.75	121.91	110.40
1	H	241	MET	C-N-CD	5.62	140.20	128.40
1	F	115	MET	CG-SD-CE	-5.61	91.23	100.20
2	D	61	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	C	221	TRP	CA-CB-CG	5.26	123.70	113.70
1	A	221	TRP	CA-CB-CG	5.25	123.67	113.70
1	F	221	TRP	CA-CB-CG	5.19	123.56	113.70
1	A	163	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	174	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	1938	0	1894	39	0
1	B	1922	0	1868	39	0
1	C	1876	0	1822	48	0
1	F	1954	0	1899	62	0
1	G	1911	0	1850	52	0
1	H	1794	0	1751	44	0
2	D	1935	0	1881	36	0
2	E	1951	0	1884	26	0
3	A	17	0	11	1	0
3	B	17	0	12	0	0
3	C	17	0	12	3	0
3	D	17	0	11	1	0
3	E	17	0	12	0	0
3	F	17	0	12	0	0
3	G	17	0	12	1	0
3	H	17	0	11	0	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
4	F	3	0	0	1	0
5	A	38	0	0	0	0
5	B	47	0	0	0	0
5	C	15	0	0	0	0
5	D	51	0	0	2	0
5	E	42	0	0	2	0
5	F	23	0	0	1	0
5	G	17	0	0	0	0
5	H	23	0	0	1	0
All	All	15682	0	14942	340	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 11.

All (340) 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:F:264:ILE:HB	1:F:265:PRO:HA	1.40	0.99
1:G:200:ASN:HD22	1:G:202:ASP:H	1.15	0.94
1:B:200:ASN:HD22	1:B:202:ASP:H	1.09	0.93
1:A:200:ASN:HD22	1:A:202:ASP:H	1.16	0.91
1:C:87:LYS:H	1:C:91:GLN:NE2	1.70	0.90
1:A:87:LYS:H	1:A:91:GLN:NE2	1.71	0.89
2:D:87:LYS:H	2:D:91:GLN:NE2	1.68	0.89
3:D:301:NXL:NAA	5:D:401:HOH:O	2.07	0.86
1:A:251:GLN:H	1:A:251:GLN:HE21	1.25	0.84
1:C:170:ILE:O	1:C:174:ARG:HG3	1.78	0.84
1:H:200:ASN:HD22	1:H:202:ASP:H	1.24	0.84
1:B:30:SER:HA	2:D:36:THR:HG21	1.60	0.82
1:B:87:LYS:H	1:B:91:GLN:NE2	1.80	0.80
1:A:50:ASN:H	1:A:231:ASN:HD21	1.30	0.80
1:H:94:LYS:HA	1:H:108:ASP:OD1	1.81	0.80
1:B:146:ASN:HD22	1:B:146:ASN:H	1.30	0.79
1:C:251:GLN:H	1:C:251:GLN:HE21	1.30	0.78
2:D:87:LYS:H	2:D:91:GLN:HE22	1.26	0.78
1:B:200:ASN:ND2	1:B:202:ASP:H	1.82	0.77
1:B:231:ASN:HD22	1:B:232:VAL:H	1.31	0.77
1:F:149:ILE:HG22	1:F:149:ILE:O	1.82	0.77
1:C:158:LEU:HD11	3:C:301:NXL:NAA	2.00	0.76
1:C:50:ASN:H	1:C:231:ASN:HD21	1.32	0.76
1:B:251:GLN:HE21	1:B:251:GLN:H	1.32	0.75
1:G:200:ASN:ND2	1:G:202:ASP:H	1.83	0.75
1:G:72:PHE:O	1:G:75:PRO:HD2	1.86	0.74
1:G:251:GLN:HE21	1:G:251:GLN:H	1.33	0.74
2:D:200:ASN:HD22	2:D:202:ASP:H	1.36	0.73
1:H:78:LEU:HG	1:H:191:VAL:HG21	1.70	0.73
1:H:50:ASN:H	1:H:231:ASN:HD21	1.37	0.73
1:H:200:ASN:ND2	1:H:202:ASP:H	1.85	0.72
1:F:124:GLN:HG2	1:F:154:ASP:HB2	1.70	0.72
2:D:200:ASN:ND2	2:D:202:ASP:H	1.87	0.72
1:A:87:LYS:H	1:A:91:GLN:HE22	1.37	0.72
1:F:136:SER:HA	1:F:149:ILE:CD1	2.20	0.72
1:C:251:GLN:H	1:C:251:GLN:NE2	1.87	0.71
1:F:149:ILE:O	1:F:149:ILE:CG2	2.38	0.71
1:A:213:THR:O	1:A:218:LYS:HE3	1.91	0.71
2:E:125:GLU:OE2	2:E:129:GLN:NE2	2.21	0.70
1:C:87:LYS:H	1:C:91:GLN:HE22	1.40	0.70
1:G:52:GLN:HE21	1:G:52:GLN:HA	1.57	0.70
1:H:243:THR:OG1	1:H:245:ASP:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:HG23	1:A:245:ASP:HB2	1.73	0.68
1:G:28:ASN:ND2	1:G:30:SER:H	1.91	0.68
1:C:218:LYS:HB3	1:C:241:MET:O	1.92	0.68
2:E:146:ASN:HD21	2:E:162:ILE:HA	1.58	0.68
1:G:191:VAL:O	1:G:195:MET:HG3	1.95	0.67
2:D:50:ASN:H	2:D:231:ASN:HD21	1.43	0.67
2:D:251:GLN:H	2:D:251:GLN:HE21	1.40	0.66
1:G:58:ASN:ND2	1:G:61:ARG:H	1.93	0.66
1:A:140:HIS:HD2	1:A:147:GLU:OE1	1.80	0.65
2:D:110:ASN:ND2	2:D:113:THR:H	1.94	0.65
1:C:158:LEU:HD11	3:C:301:NXL:H6	1.62	0.65
2:E:132:GLU:HG3	2:E:153:VAL:HG13	1.78	0.65
1:G:134:ARG:O	1:G:138:MET:HG2	1.97	0.65
1:F:136:SER:HB2	1:F:149:ILE:HD12	1.79	0.65
1:F:50:ASN:H	1:F:231:ASN:HD21	1.43	0.64
1:H:121:PRO:HA	1:H:124:GLN:HE21	1.62	0.64
1:A:95:TRP:CZ2	1:A:106:ASN:HB3	2.33	0.64
1:F:136:SER:CB	1:F:149:ILE:HD12	2.27	0.64
1:F:251:GLN:H	1:F:251:GLN:HE21	1.44	0.64
1:F:121:PRO:HA	1:F:124:GLN:HE21	1.63	0.64
1:B:29:LYS:C	2:D:36:THR:HG21	2.18	0.64
2:E:110:ASN:C	2:E:110:ASN:HD22	2.01	0.63
1:F:119:VAL:CG1	1:F:122:VAL:HG23	2.28	0.63
1:B:181:LEU:H	1:B:188:GLN:HE22	1.47	0.63
1:H:181:LEU:H	1:H:188:GLN:HE22	1.47	0.63
2:D:28:ASN:C	2:D:28:ASN:HD22	2.02	0.63
1:A:159:ASP:HA	1:A:215:ILE:HD12	1.80	0.62
1:B:146:ASN:HD21	1:B:162:ILE:HA	1.64	0.62
1:G:50:ASN:H	1:G:231:ASN:HD21	1.47	0.62
1:A:200:ASN:ND2	1:A:202:ASP:H	1.95	0.62
1:C:216:GLU:OE2	1:C:217:PRO:HA	1.99	0.62
1:F:51:LYS:HB3	1:F:53:GLN:HE21	1.65	0.62
2:D:200:ASN:HD22	2:D:200:ASN:C	2.04	0.61
5:D:446:HOH:O	2:E:90:HIS:HE1	1.82	0.61
1:B:231:ASN:HD22	1:B:232:VAL:N	1.96	0.61
1:C:161:GLY:O	1:C:163:ARG:NH1	2.33	0.61
1:G:79:ILE:HG23	1:G:138:MET:HG3	1.82	0.61
1:C:65:ALA:HB1	1:C:163:ARG:HB3	1.81	0.61
1:F:136:SER:CA	1:F:149:ILE:CD1	2.78	0.61
1:G:116:LYS:NZ	1:H:201:GLY:O	2.27	0.61
2:E:251:GLN:H	2:E:251:GLN:HE21	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:VAL:HG12	1:F:122:VAL:HG23	1.83	0.61
1:G:216:GLU:OE2	1:G:217:PRO:HA	2.01	0.61
1:C:28:ASN:C	1:C:28:ASN:HD22	2.04	0.60
1:C:120:VAL:N	1:C:121:PRO:HD2	2.16	0.60
1:F:136:SER:HA	1:F:149:ILE:HD12	1.82	0.60
2:D:70:SER:HB2	2:D:210:GLY:HA2	1.84	0.60
1:F:44:VAL:HG21	1:F:257:VAL:HG21	1.83	0.59
1:H:170:ILE:O	1:H:174:ARG:HG3	2.02	0.59
1:C:94:LYS:HE3	1:C:108:ASP:OD2	2.03	0.59
1:G:232:VAL:HG22	1:G:234:PHE:CE1	2.36	0.59
2:E:87:LYS:H	2:E:91:GLN:NE2	1.99	0.59
2:E:94:LYS:HA	2:E:108:ASP:OD1	2.02	0.59
1:G:61:ARG:HA	1:G:64:GLN:HE21	1.66	0.59
1:F:146:ASN:HD21	1:F:162:ILE:HA	1.68	0.58
1:A:58:ASN:C	1:A:58:ASN:HD22	2.07	0.58
1:B:146:ASN:H	1:B:146:ASN:ND2	1.98	0.58
1:F:178:HIS:CB	1:F:180:LYS:HE3	2.33	0.58
1:H:74:ILE:HB	1:H:75:PRO:CD	2.34	0.58
1:H:251:GLN:H	1:H:251:GLN:HE21	1.50	0.58
1:B:67:LEU:HD23	1:B:162:ILE:O	2.04	0.57
1:F:178:HIS:HB3	1:F:180:LYS:HE3	1.84	0.57
1:B:30:SER:CA	2:D:36:THR:HG21	2.31	0.57
1:B:200:ASN:HD21	1:B:202:ASP:HB2	1.70	0.57
1:B:87:LYS:H	1:B:91:GLN:HE21	1.53	0.56
1:F:136:SER:CA	1:F:149:ILE:HD12	2.35	0.56
2:E:78:LEU:HG	2:E:191:VAL:HG21	1.85	0.56
1:F:95:TRP:HB2	1:F:107:ARG:O	2.05	0.56
1:C:58:ASN:C	1:C:58:ASN:HD22	2.07	0.56
1:H:123:TYR:CD1	1:H:126:PHE:HD2	2.23	0.56
2:D:58:ASN:ND2	2:D:61:ARG:H	2.04	0.56
1:F:251:GLN:H	1:F:251:GLN:NE2	2.04	0.56
1:G:75:PRO:O	1:G:79:ILE:HG12	2.05	0.56
1:A:239:MET:HE3	1:A:241:MET:HE2	1.87	0.56
1:A:251:GLN:HE21	1:A:251:GLN:N	2.00	0.56
1:F:110:ASN:C	1:F:110:ASN:HD22	2.09	0.56
1:A:200:ASN:HD22	1:A:202:ASP:N	1.97	0.55
1:B:191:VAL:O	1:B:195:MET:HG3	2.06	0.55
1:A:239:MET:HE3	1:A:241:MET:CE	2.36	0.55
2:E:31:TRP:HB2	2:E:57:ASN:HB3	1.88	0.55
1:H:243:THR:HG1	1:H:245:ASP:HB2	1.69	0.55
1:F:44:VAL:HG12	1:F:237:MET:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:GLN:O	1:F:134:ARG:NH1	2.40	0.55
1:B:159:ASP:HB3	1:B:214:ARG:HD2	1.89	0.55
1:C:44:VAL:HG11	1:C:257:VAL:HG21	1.88	0.55
1:A:239:MET:HE1	1:A:249:LEU:HB2	1.89	0.55
2:E:132:GLU:HG3	2:E:153:VAL:CG1	2.37	0.55
1:C:34:HIS:NE2	1:C:260:GLN:NE2	2.55	0.55
2:D:78:LEU:HD23	2:D:191:VAL:HG21	1.89	0.55
1:H:220:GLY:O	1:H:238:ASN:HA	2.07	0.55
1:C:126:PHE:O	1:C:130:ILE:HG13	2.06	0.54
1:C:100:ARG:HG2	1:C:101:ASP:H	1.71	0.54
1:F:91:GLN:OE1	1:F:93:PHE:CE1	2.61	0.54
2:D:110:ASN:C	2:D:110:ASN:HD22	2.10	0.54
1:A:110:ASN:C	1:A:110:ASN:HD22	2.10	0.54
2:E:213:THR:O	2:E:218:LYS:HE2	2.07	0.54
1:A:58:ASN:ND2	1:A:61:ARG:H	2.06	0.54
2:D:170:ILE:HD12	2:D:234:PHE:HB3	1.88	0.53
1:H:119:VAL:HG12	1:H:121:PRO:HD2	1.89	0.53
1:B:58:ASN:C	1:B:58:ASN:HD22	2.11	0.53
1:C:110:ASN:ND2	1:C:113:THR:H	2.06	0.53
1:H:211:TYR:CE1	1:H:241:MET:HG3	2.43	0.53
1:C:200:ASN:HB3	1:C:202:ASP:H	1.73	0.53
1:B:58:ASN:ND2	1:B:61:ARG:H	2.07	0.53
1:B:146:ASN:ND2	1:B:163:ARG:H	2.06	0.53
2:D:87:LYS:N	2:D:91:GLN:HE22	2.01	0.53
1:H:184:SER:OG	1:H:187:SER:HB2	2.09	0.53
1:G:110:ASN:ND2	1:G:113:THR:H	2.06	0.53
2:D:33:ALA:O	2:D:36:THR:HB	2.08	0.53
1:F:67:LEU:HD11	1:F:215:ILE:HD12	1.89	0.53
1:A:74:ILE:HB	1:A:75:PRO:HD3	1.90	0.53
1:A:157:TRP:HA	1:A:162:ILE:CG2	2.40	0.53
1:H:159:ASP:HB3	1:H:214:ARG:HB3	1.89	0.52
1:F:264:ILE:CB	1:F:265:PRO:HA	2.14	0.52
1:C:196:LEU:HD23	1:F:204:ILE:HD13	1.91	0.52
2:E:146:ASN:ND2	2:E:163:ARG:H	2.07	0.52
2:E:50:ASN:H	2:E:231:ASN:HD21	1.56	0.52
1:F:264:ILE:HB	1:F:265:PRO:CA	2.28	0.52
1:G:87:LYS:H	1:G:91:GLN:NE2	2.07	0.52
1:G:87:LYS:HG3	1:G:91:GLN:NE2	2.24	0.52
1:B:31:TRP:HB2	1:B:57:ASN:HB3	1.91	0.52
1:F:136:SER:HA	1:F:149:ILE:HD11	1.90	0.52
1:G:95:TRP:CD1	1:G:96:ASP:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:VAL:HG22	1:G:93:PHE:HZ	1.75	0.52
1:B:125:GLU:OE2	1:B:129:GLN:NE2	2.32	0.52
1:F:146:ASN:HD22	1:F:147:GLU:N	2.08	0.52
1:G:58:ASN:C	1:G:58:ASN:HD22	2.13	0.52
1:C:120:VAL:HG12	1:C:124:GLN:HE21	1.75	0.51
2:D:251:GLN:H	2:D:251:GLN:NE2	2.08	0.51
1:H:31:TRP:CZ3	1:H:44:VAL:HG22	2.45	0.51
1:C:146:ASN:HD21	1:C:162:ILE:HA	1.75	0.51
1:F:150:SER:O	1:F:160:GLY:HA3	2.11	0.51
1:H:73:LYS:HE2	5:H:420:HOH:O	2.09	0.51
1:A:46:LEU:HD12	1:A:46:LEU:N	2.25	0.51
1:C:247:LEU:HB3	1:C:250:ARG:NH1	2.26	0.51
1:G:74:ILE:HB	1:G:75:PRO:HD3	1.92	0.51
1:H:110:ASN:C	1:H:110:ASN:HD22	2.14	0.51
1:F:36:THR:O	1:F:39:LYS:N	2.34	0.51
1:H:120:VAL:HB	1:H:121:PRO:HD3	1.94	0.51
1:F:157:TRP:NE1	4:F:302:CO2:C	2.74	0.50
1:F:110:ASN:ND2	1:F:113:THR:H	2.08	0.50
1:G:220:GLY:O	1:G:238:ASN:HA	2.11	0.50
1:B:31:TRP:CH2	1:B:46:LEU:HD22	2.47	0.50
2:E:99:THR:CG2	5:E:408:HOH:O	2.59	0.50
1:G:251:GLN:HE21	1:G:251:GLN:N	2.06	0.50
1:H:58:ASN:OD1	1:H:61:ARG:HB2	2.11	0.50
1:A:178:HIS:HB2	1:A:180:LYS:HE2	1.93	0.50
1:A:80:ALA:HB1	1:A:86:VAL:HG23	1.93	0.49
1:G:179:ASN:HA	1:G:188:GLN:NE2	2.27	0.49
1:H:146:ASN:HD22	1:H:147:GLU:N	2.11	0.49
1:A:178:HIS:CB	1:A:180:LYS:HE2	2.42	0.49
1:B:237:MET:HG2	1:B:254:THR:OG1	2.12	0.49
1:G:87:LYS:H	1:G:91:GLN:HE21	1.60	0.49
1:B:200:ASN:HD22	1:B:202:ASP:N	1.93	0.49
1:B:181:LEU:H	1:B:188:GLN:NE2	2.11	0.49
1:F:191:VAL:O	1:F:195:MET:HG3	2.13	0.49
1:G:200:ASN:HD22	1:G:200:ASN:C	2.15	0.49
1:F:124:GLN:HB3	1:F:128:ARG:NH2	2.28	0.49
1:G:251:GLN:H	1:G:251:GLN:NE2	2.07	0.49
1:A:87:LYS:H	1:A:91:GLN:HE21	1.58	0.49
1:H:200:ASN:HD21	1:H:202:ASP:HB2	1.78	0.48
1:C:61:ARG:HA	1:C:64:GLN:HE21	1.79	0.48
1:H:123:TYR:O	1:H:126:PHE:HB2	2.13	0.48
1:B:33:ALA:HA	1:B:36:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:ILE:O	1:H:163:ARG:HD2	2.14	0.48
1:C:79:ILE:HA	1:C:138:MET:HE3	1.96	0.48
1:F:28:ASN:HD22	1:F:28:ASN:C	2.15	0.48
1:G:61:ARG:HA	1:G:64:GLN:NE2	2.29	0.48
1:C:146:ASN:ND2	1:C:163:ARG:H	2.11	0.48
1:A:75:PRO:HG3	1:A:144:TYR:CE2	2.49	0.47
1:B:30:SER:N	2:D:36:THR:HG21	2.29	0.47
2:E:65:ALA:HB1	2:E:163:ARG:HB3	1.97	0.47
2:E:231:ASN:HD22	2:E:232:VAL:H	1.62	0.47
1:C:110:ASN:C	1:C:110:ASN:HD22	2.18	0.47
1:C:132:GLU:HG3	1:C:133:ALA:N	2.29	0.47
1:G:105:TRP:CH2	1:G:120:VAL:HG23	2.48	0.47
1:H:31:TRP:CH2	1:H:46:LEU:HD22	2.50	0.47
2:D:181:LEU:H	2:D:188:GLN:HE22	1.61	0.47
1:F:146:ASN:ND2	1:F:148:ASP:H	2.13	0.46
1:G:232:VAL:CG2	1:G:234:PHE:CE1	2.98	0.46
1:G:127:ALA:HB1	1:G:153:VAL:O	2.16	0.46
1:C:25:TRP:CZ3	1:C:54:GLY:HA3	2.51	0.46
1:F:179:ASN:HA	1:F:188:GLN:NE2	2.30	0.46
1:A:140:HIS:CD2	1:A:147:GLU:OE1	2.66	0.46
1:A:179:ASN:HA	1:A:188:GLN:NE2	2.31	0.46
1:C:162:ILE:HG13	1:C:163:ARG:H	1.81	0.46
1:C:162:ILE:HG13	1:C:163:ARG:N	2.30	0.46
2:D:159:ASP:OD1	2:D:159:ASP:N	2.49	0.46
1:A:239:MET:CE	1:A:241:MET:HE1	2.46	0.46
1:G:86:VAL:HG22	1:G:93:PHE:CZ	2.50	0.46
1:H:242:PRO:HG2	1:H:243:THR:HG23	1.98	0.46
1:G:120:VAL:N	1:G:121:PRO:HD2	2.30	0.46
1:H:146:ASN:HD21	1:H:162:ILE:HA	1.81	0.46
1:B:141:ALA:HB1	1:B:182:HIS:CD2	2.51	0.46
1:H:28:ASN:HD22	1:H:30:SER:H	1.63	0.46
1:C:33:ALA:O	1:C:37:GLU:HB2	2.16	0.45
1:H:87:LYS:HB2	1:H:91:GLN:NE2	2.31	0.45
1:H:137:LYS:O	1:H:137:LYS:HG2	2.14	0.45
2:D:82:ASP:CG	2:D:183:VAL:HG12	2.36	0.45
2:E:66:PHE:HE1	2:E:217:PRO:HG2	1.81	0.45
1:H:80:ALA:HB1	1:H:86:VAL:HG23	1.98	0.45
1:H:146:ASN:HD22	1:H:146:ASN:C	2.20	0.45
2:D:146:ASN:HD21	2:D:162:ILE:HA	1.81	0.45
2:E:170:ILE:O	2:E:174:ARG:HG3	2.17	0.45
1:F:146:ASN:HD22	1:F:146:ASN:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:PHE:HB3	1:G:40:SER:O	2.17	0.45
1:A:120:VAL:O	1:A:124:GLN:HG3	2.16	0.45
1:C:148:ASP:O	1:C:162:ILE:HB	2.17	0.45
1:H:35:PHE:HB3	1:H:41:GLN:HA	1.99	0.45
2:D:135:MET:HB3	2:D:149:ILE:HD11	1.99	0.45
1:F:156:PHE:C	1:F:158:LEU:H	2.20	0.45
1:H:73:LYS:HE3	1:H:118:SER:OG	2.17	0.45
1:H:231:ASN:ND2	1:H:232:VAL:H	2.15	0.45
1:G:250:ARG:NH2	3:G:301:NXL:OAG	2.49	0.44
1:C:94:LYS:HA	1:C:108:ASP:OD1	2.17	0.44
2:D:110:ASN:HD21	2:D:113:THR:H	1.64	0.44
2:D:220:GLY:O	2:D:238:ASN:HA	2.17	0.44
1:G:170:ILE:O	1:G:174:ARG:HG3	2.18	0.44
1:A:58:ASN:HD22	1:A:60:LYS:H	1.66	0.44
1:B:75:PRO:HG3	1:B:144:TYR:CE2	2.53	0.44
2:D:94:LYS:HE2	2:D:94:LYS:HB3	1.67	0.44
2:E:125:GLU:OE1	2:E:128:ARG:NH2	2.48	0.44
1:F:75:PRO:HA	1:F:78:LEU:HD12	2.00	0.44
1:F:116:LYS:HD3	1:F:117:TYR:CE2	2.53	0.44
1:A:128:ARG:NH1	1:A:154:ASP:OD2	2.51	0.44
2:E:78:LEU:CG	2:E:191:VAL:HG21	2.47	0.44
1:F:86:VAL:HG22	1:F:126:PHE:CE1	2.53	0.44
1:F:259:LYS:HG2	1:F:265:PRO:HG3	1.99	0.44
1:G:188:GLN:O	1:G:192:LYS:HE2	2.18	0.44
2:D:140:HIS:HD2	2:D:147:GLU:OE1	2.01	0.43
1:G:28:ASN:ND2	1:G:28:ASN:C	2.71	0.43
1:A:157:TRP:HA	1:A:162:ILE:HG21	1.98	0.43
2:E:99:THR:HG23	5:E:408:HOH:O	2.16	0.43
1:G:73:LYS:NZ	1:G:118:SER:OG	2.36	0.43
1:C:70:SER:HB2	1:C:210:GLY:HA2	2.00	0.43
1:B:200:ASN:ND2	1:B:202:ASP:HB2	2.32	0.43
1:C:158:LEU:CD1	3:C:301:NXL:H6	2.28	0.43
1:C:125:GLU:HG3	1:C:129:GLN:HE21	1.83	0.43
1:C:58:ASN:C	1:C:58:ASN:ND2	2.72	0.43
1:F:121:PRO:HA	1:F:124:GLN:NE2	2.32	0.43
1:A:243:THR:CG2	1:A:245:ASP:HB2	2.46	0.43
1:F:55:PHE:N	1:F:55:PHE:CD1	2.87	0.43
1:H:253:ILE:O	1:H:256:GLU:HB2	2.18	0.43
1:F:150:SER:O	1:F:160:GLY:CA	2.66	0.43
1:F:261:GLU:HB2	1:F:263:ILE:HD12	2.00	0.43
1:A:34:HIS:NE2	1:A:260:GLN:NE2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ASN:ND2	1:F:146:ASN:C	2.73	0.42
1:G:87:LYS:HB2	1:G:87:LYS:HE3	1.81	0.42
1:B:251:GLN:H	1:B:251:GLN:NE2	2.07	0.42
1:C:45:VAL:O	1:C:235:PHE:HA	2.19	0.42
1:C:220:GLY:O	1:C:238:ASN:HA	2.19	0.42
2:D:58:ASN:C	2:D:58:ASN:HD22	2.23	0.42
1:F:36:THR:HG22	1:F:37:GLU:N	2.34	0.42
1:G:120:VAL:N	1:G:121:PRO:CD	2.82	0.42
1:F:158:LEU:HD12	1:F:158:LEU:HA	1.90	0.42
1:F:193:GLN:NE2	5:F:404:HOH:O	2.53	0.42
1:G:100:ARG:H	1:G:106:ASN:HD21	1.68	0.42
1:B:50:ASN:H	1:B:231:ASN:HD21	1.65	0.42
1:B:231:ASN:ND2	1:B:232:VAL:H	2.06	0.42
1:F:33:ALA:HA	1:F:36:THR:HB	2.02	0.42
1:G:90:HIS:O	1:G:91:GLN:C	2.57	0.42
1:A:239:MET:CE	1:A:249:LEU:HB2	2.49	0.42
1:B:89:GLU:O	1:B:110:ASN:HB2	2.19	0.42
1:C:146:ASN:HD21	1:C:163:ARG:H	1.67	0.41
1:G:32:ASN:OD1	1:G:57:ASN:ND2	2.45	0.41
1:H:191:VAL:O	1:H:195:MET:HG3	2.20	0.41
2:D:28:ASN:C	2:D:28:ASN:ND2	2.72	0.41
2:E:56:THR:OG1	2:E:57:ASN:N	2.53	0.41
1:G:177:TYR:CZ	1:G:232:VAL:HG11	2.55	0.41
1:C:28:ASN:C	1:C:28:ASN:ND2	2.73	0.41
2:D:200:ASN:HD21	2:D:202:ASP:HB2	1.85	0.41
1:H:74:ILE:HB	1:H:75:PRO:HD3	2.01	0.41
1:F:231:ASN:ND2	1:F:232:VAL:H	2.19	0.41
1:F:130:ILE:O	1:F:134:ARG:NE	2.46	0.41
1:H:120:VAL:O	1:H:124:GLN:HG3	2.20	0.41
1:B:29:LYS:O	2:D:36:THR:HG21	2.20	0.41
1:G:94:LYS:H	1:G:94:LYS:HG2	1.62	0.41
1:A:73:LYS:HD3	1:A:123:TYR:CE1	2.56	0.41
1:C:123:TYR:O	1:C:126:PHE:HB2	2.20	0.41
1:F:29:LYS:O	1:F:32:ASN:HB2	2.20	0.41
1:H:68:PRO:CD	1:H:162:ILE:HG23	2.51	0.41
1:G:146:ASN:C	1:G:146:ASN:HD22	2.24	0.41
3:A:301:NXL:OAL	3:A:301:NXL:H7	2.20	0.40
2:D:200:ASN:ND2	2:D:200:ASN:C	2.73	0.40
1:F:211:TYR:CG	1:F:247:LEU:HD21	2.55	0.40
1:G:183:VAL:HG23	1:G:188:GLN:HG3	2.02	0.40
2:E:110:ASN:ND2	2:E:113:THR:H	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ASN:C	1:F:107:ARG:HG2	2.42	0.40
1:F:139:LEU:HD23	1:F:139:LEU:HA	1.84	0.40
1:G:45:VAL:O	1:G:235:PHE:HA	2.21	0.40
1:A:117:TYR:OH	1:B:229:ASP:OD2	2.26	0.40
1:B:231:ASN:ND2	1:B:232:VAL:N	2.66	0.40
1:C:110:ASN:HD22	1:C:112:ILE:N	2.18	0.40
2:D:200:ASN:HD22	2:D:202:ASP:N	2.13	0.40
2:E:110:ASN:HD21	2:E:112:ILE:HB	1.87	0.40
1:G:124:GLN:HG2	1:G:154:ASP:O	2.21	0.40
1:C:43:VAL:HG12	1:C:238:ASN:OD1	2.20	0.40
2:E:31:TRP:CZ3	2:E:56:THR:HA	2.57	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	233/242 (96%)	226 (97%)	7 (3%)	0	100	100
1	B	231/242 (96%)	225 (97%)	6 (3%)	0	100	100
1	C	222/242 (92%)	206 (93%)	16 (7%)	0	100	100
1	F	236/242 (98%)	214 (91%)	21 (9%)	1 (0%)	34	42
1	G	229/242 (95%)	212 (93%)	16 (7%)	1 (0%)	34	42
1	H	213/242 (88%)	196 (92%)	17 (8%)	0	100	100
2	D	231/242 (96%)	225 (97%)	6 (3%)	0	100	100
2	E	234/242 (97%)	224 (96%)	10 (4%)	0	100	100
All	All	1829/1936 (94%)	1728 (94%)	99 (5%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	104	THR
1	G	37	GLU

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	206/211 (98%)	182 (88%)	24 (12%)	5 6
1	B	203/211 (96%)	182 (90%)	21 (10%)	7 8
1	C	199/211 (94%)	178 (89%)	21 (11%)	6 7
1	F	207/211 (98%)	190 (92%)	17 (8%)	11 14
1	G	202/211 (96%)	180 (89%)	22 (11%)	6 7
1	H	190/211 (90%)	167 (88%)	23 (12%)	5 5
2	D	203/210 (97%)	179 (88%)	24 (12%)	5 5
2	E	205/210 (98%)	189 (92%)	16 (8%)	12 16
All	All	1615/1686 (96%)	1447 (90%)	168 (10%)	7 8

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	28	ASN
1	A	52	GLN
1	A	57	ASN
1	A	58	ASN
1	A	60	LYS
1	A	76	ASN
1	A	87	LYS
1	A	99	THR
1	A	101	ASP
1	A	107	ARG
1	A	110	ASN
1	A	118	SER
1	A	137	LYS

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Mol	Chain	Res	Type
1	A	153	VAL
1	A	158	LEU
1	A	167	THR
1	A	169	GLN
1	A	200	ASN
1	A	231	ASN
1	A	232	VAL
1	A	244	SER
1	A	245	ASP
1	A	251	GLN
1	B	24	GLU
1	B	28	ASN
1	B	36	THR
1	B	46	LEU
1	B	58	ASN
1	B	76	ASN
1	B	99	THR
1	B	110	ASN
1	B	115	MET
1	B	118	SER
1	B	137	LYS
1	B	146	ASN
1	B	162	ILE
1	B	169	GLN
1	B	182	HIS
1	B	183	VAL
1	B	200	ASN
1	B	226	VAL
1	B	231	ASN
1	B	243	THR
1	B	251	GLN
1	C	28	ASN
1	C	37	GLU
1	C	40	SER
1	C	44	VAL
1	C	58	ASN
1	C	76	ASN
1	C	100	ARG
1	C	110	ASN
1	C	115	MET
1	C	132	GLU
1	C	137	LYS

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	158	LEU
1	C	169	GLN
1	C	182	HIS
1	C	226	VAL
1	C	230	ASP
1	C	231	ASN
1	C	232	VAL
1	C	243	THR
1	C	251	GLN
2	D	26	GLN
2	D	28	ASN
2	D	36	THR
2	D	46	LEU
2	D	58	ASN
2	D	76	ASN
2	D	94	LYS
2	D	110	ASN
2	D	115	MET
2	D	118	SER
2	D	132	GLU
2	D	136	SER
2	D	146	ASN
2	D	156	PHE
2	D	169	GLN
2	D	171	SER
2	D	182	HIS
2	D	183	VAL
2	D	200	ASN
2	D	226	VAL
2	D	231	ASN
2	D	232	VAL
2	D	245	ASP
2	D	251	GLN
2	E	44	VAL
2	E	76	ASN
2	E	87	LYS
2	E	99	THR
2	E	102	ILE
2	E	110	ASN
2	E	115	MET
2	E	118	SER

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Mol	Chain	Res	Type
2	E	146	ASN
2	E	152	ASN
2	E	153	VAL
2	E	169	GLN
2	E	183	VAL
2	E	231	ASN
2	E	232	VAL
2	E	251	GLN
1	F	28	ASN
1	F	36	THR
1	F	58	ASN
1	F	60	LYS
1	F	76	ASN
1	F	110	ASN
1	F	115	MET
1	F	136	SER
1	F	137	LYS
1	F	146	ASN
1	F	169	GLN
1	F	226	VAL
1	F	231	ASN
1	F	232	VAL
1	F	243	THR
1	F	245	ASP
1	F	251	GLN
1	G	40	SER
1	G	44	VAL
1	G	46	LEU
1	G	52	GLN
1	G	58	ASN
1	G	76	ASN
1	G	79	ILE
1	G	87	LYS
1	G	94	LYS
1	G	95	TRP
1	G	98	GLN
1	G	102	ILE
1	G	110	ASN
1	G	115	MET
1	G	134	ARG
1	G	146	ASN
1	G	169	GLN

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Mol	Chain	Res	Type
1	G	200	ASN
1	G	226	VAL
1	G	231	ASN
1	G	243	THR
1	G	251	GLN
1	H	28	ASN
1	H	44	VAL
1	H	46	LEU
1	H	58	ASN
1	H	60	LYS
1	H	76	ASN
1	H	87	LYS
1	H	110	ASN
1	H	132	GLU
1	H	146	ASN
1	H	153	VAL
1	H	154	ASP
1	H	158	LEU
1	H	169	GLN
1	H	186	ARG
1	H	219	ILE
1	H	226	VAL
1	H	231	ASN
1	H	232	VAL
1	H	241	MET
1	H	243	THR
1	H	251	GLN
1	H	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	52	GLN
1	A	58	ASN
1	A	63	ASN
1	A	76	ASN
1	A	91	GLN
1	A	110	ASN
1	A	124	GLN
1	A	140	HIS
1	A	169	GLN

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Mol	Chain	Res	Type
1	A	188	GLN
1	A	193	GLN
1	A	200	ASN
1	A	231	ASN
1	A	251	GLN
1	A	260	GLN
1	B	58	ASN
1	B	63	ASN
1	B	64	GLN
1	B	91	GLN
1	B	110	ASN
1	B	146	ASN
1	B	169	GLN
1	B	188	GLN
1	B	193	GLN
1	B	200	ASN
1	B	231	ASN
1	B	251	GLN
1	C	28	ASN
1	C	52	GLN
1	C	58	ASN
1	C	63	ASN
1	C	64	GLN
1	C	76	ASN
1	C	91	GLN
1	C	110	ASN
1	C	124	GLN
1	C	129	GLN
1	C	146	ASN
1	C	169	GLN
1	C	188	GLN
1	C	193	GLN
1	C	231	ASN
1	C	251	GLN
1	C	260	GLN
2	D	28	ASN
2	D	52	GLN
2	D	58	ASN
2	D	63	ASN
2	D	64	GLN
2	D	76	ASN
2	D	91	GLN

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Mol	Chain	Res	Type
2	D	110	ASN
2	D	124	GLN
2	D	140	HIS
2	D	146	ASN
2	D	169	GLN
2	D	188	GLN
2	D	200	ASN
2	D	231	ASN
2	D	251	GLN
2	E	76	ASN
2	E	90	HIS
2	E	91	GLN
2	E	110	ASN
2	E	124	GLN
2	E	146	ASN
2	E	169	GLN
2	E	188	GLN
2	E	193	GLN
2	E	231	ASN
2	E	251	GLN
2	E	260	GLN
1	F	28	ASN
1	F	38	HIS
1	F	53	GLN
1	F	58	ASN
1	F	63	ASN
1	F	76	ASN
1	F	91	GLN
1	F	110	ASN
1	F	124	GLN
1	F	140	HIS
1	F	146	ASN
1	F	169	GLN
1	F	188	GLN
1	F	193	GLN
1	F	231	ASN
1	F	251	GLN
1	F	260	GLN
1	G	26	GLN
1	G	28	ASN
1	G	52	GLN
1	G	58	ASN

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Mol	Chain	Res	Type
1	G	63	ASN
1	G	64	GLN
1	G	76	ASN
1	G	91	GLN
1	G	106	ASN
1	G	110	ASN
1	G	124	GLN
1	G	146	ASN
1	G	169	GLN
1	G	188	GLN
1	G	193	GLN
1	G	200	ASN
1	G	231	ASN
1	G	251	GLN
1	H	28	ASN
1	H	53	GLN
1	H	58	ASN
1	H	63	ASN
1	H	64	GLN
1	H	76	ASN
1	H	91	GLN
1	H	110	ASN
1	H	124	GLN
1	H	146	ASN
1	H	169	GLN
1	H	188	GLN
1	H	200	ASN
1	H	231	ASN
1	H	251	GLN
1	H	260	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KCX	E	73	2	7,11,12	0.74	0	4,12,14	1.32	1 (25%)
2	KCX	D	73	2	7,11,12	0.63	0	4,12,14	0.94	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	KCX	E	73	2	-	0/7/10/12	-
2	KCX	D	73	2	-	1/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	73	KCX	CD-CE-NZ	2.03	116.94	111.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	73	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NXL	F	301	1	14,17,17	0.61	0	17,24,24	1.60	3 (17%)
3	NXL	E	301	2	14,17,17	0.69	0	17,24,24	1.45	2 (11%)
3	NXL	H	301	1	14,17,17	1.00	1 (7%)	17,24,24	1.76	4 (23%)
3	NXL	A	301	1	14,17,17	1.09	1 (7%)	17,24,24	1.66	3 (17%)
3	NXL	D	301	2	14,17,17	1.40	2 (14%)	17,24,24	2.02	7 (41%)
3	NXL	B	301	1	14,17,17	0.83	0	17,24,24	1.61	4 (23%)
4	CO2	C	302	-	2,2,2	0.18	0	1,1,1	0.40	0
4	CO2	A	302	-	2,2,2	0.17	0	1,1,1	0.48	0
4	CO2	F	302	-	2,2,2	0.26	0	1,1,1	0.36	0
3	NXL	C	301	1	14,17,17	0.61	0	17,24,24	1.63	4 (23%)
3	NXL	G	301	1	14,17,17	0.69	0	17,24,24	1.45	6 (35%)

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	NXL	F	301	1	-	1/5/25/25	0/1/1/1
3	NXL	E	301	2	-	2/5/25/25	0/1/1/1
3	NXL	H	301	1	-	4/5/25/25	0/1/1/1
3	NXL	A	301	1	-	2/5/25/25	0/1/1/1
3	NXL	D	301	2	-	1/5/25/25	0/1/1/1
3	NXL	B	301	1	-	3/5/25/25	0/1/1/1
3	NXL	C	301	1	-	2/5/25/25	0/1/1/1
3	NXL	G	301	1	-	4/5/25/25	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NXL	OAG-SAR	3.46	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	NXL	OAG-SAR	3.27	1.59	1.45
3	D	301	NXL	OAG-SAR	2.98	1.58	1.45
3	D	301	NXL	CA-C	-2.48	1.48	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	301	NXL	CAO-CAJ-N	-4.06	104.40	110.11
3	A	301	NXL	CB-CA-N	-3.97	104.58	110.31
3	B	301	NXL	OAL-SAR-OAE	3.77	115.27	103.29
3	C	301	NXL	CAO-CAJ-N	-3.73	104.86	110.11
3	D	301	NXL	OAL-SAR-OAG	3.67	114.95	103.29
3	H	301	NXL	CB-CAH-CAO	3.66	115.53	111.48
3	D	301	NXL	CB-CAH-CAO	-3.50	107.61	111.48
3	B	301	NXL	CB-CAH-CAO	3.43	115.28	111.48
3	F	301	NXL	CAO-CAJ-N	-3.19	105.62	110.11
3	E	301	NXL	CAH-CB-CA	3.14	116.89	110.30
3	G	301	NXL	OAL-SAR-OAG	2.81	112.22	103.29
3	C	301	NXL	CAH-CB-CA	2.79	116.16	110.30
3	H	301	NXL	CAH-CB-CA	2.75	116.07	110.30
3	D	301	NXL	C-CA-N	-2.62	104.99	111.27
3	D	301	NXL	OAD-SAR-OAE	-2.55	99.63	108.49
3	F	301	NXL	CB-CA-N	-2.45	106.77	110.31
3	G	301	NXL	OAG-SAR-OAE	-2.44	102.44	112.22
3	B	301	NXL	CAH-CB-CA	2.44	115.41	110.30
3	C	301	NXL	OAL-SAR-OAG	2.34	110.73	103.29
3	C	301	NXL	CB-CA-C	-2.31	107.98	112.12
3	D	301	NXL	CAH-CAO-CAJ	-2.30	106.72	109.71
3	F	301	NXL	CB-CA-C	2.22	116.11	112.12
3	B	301	NXL	CAO-CAJ-N	-2.22	106.99	110.11
3	A	301	NXL	OAC-CAN-N	-2.16	119.48	125.59
3	G	301	NXL	OAD-SAR-OAE	2.16	115.98	108.49
3	D	301	NXL	CB-CA-C	-2.14	108.28	112.12
3	D	301	NXL	CAJ-CAO-NAK	2.14	117.13	109.02
3	G	301	NXL	OAL-SAR-OAE	2.07	109.88	103.29
3	H	301	NXL	OAL-SAR-OAG	2.07	109.85	103.29
3	E	301	NXL	C-CA-N	2.02	116.12	111.27
3	G	301	NXL	CAO-CAJ-N	-2.01	107.28	110.11
3	G	301	NXL	CAH-CB-CA	2.01	114.52	110.30
3	A	301	NXL	CAO-CAJ-N	-2.01	107.29	110.11

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	NXL	OAC-CAN-N-CAJ
3	C	301	NXL	OAC-CAN-N-CA
3	D	301	NXL	OAC-CAN-N-CAJ
3	E	301	NXL	OAC-CAN-N-CAJ
3	E	301	NXL	OAC-CAN-N-CA
3	F	301	NXL	OAC-CAN-N-CAJ
3	G	301	NXL	OAC-CAN-N-CAJ
3	G	301	NXL	OAC-CAN-N-CA
3	G	301	NXL	O-C-CA-CB
3	G	301	NXL	NAA-C-CA-CB
3	H	301	NXL	OAC-CAN-N-CAJ
3	H	301	NXL	OAC-CAN-N-CA
3	H	301	NXL	O-C-CA-CB
3	H	301	NXL	NAA-C-CA-CB
3	A	301	NXL	NAA-C-CA-CB
3	A	301	NXL	O-C-CA-CB
3	B	301	NXL	NAA-C-CA-CB
3	B	301	NXL	OAC-CAN-N-CA
3	B	301	NXL	O-C-CA-CB

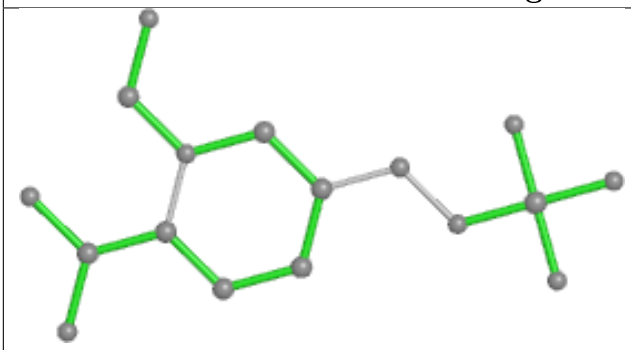
There are no ring outliers.

5 monomers are involved in 7 short contacts:

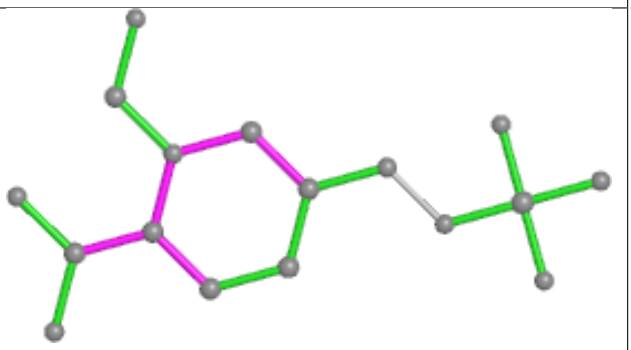
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NXL	1	0
3	D	301	NXL	1	0
4	F	302	CO2	1	0
3	C	301	NXL	3	0
3	G	301	NXL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

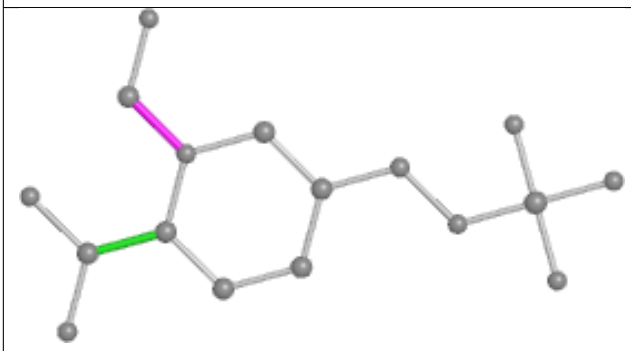
Ligand NXL F 301



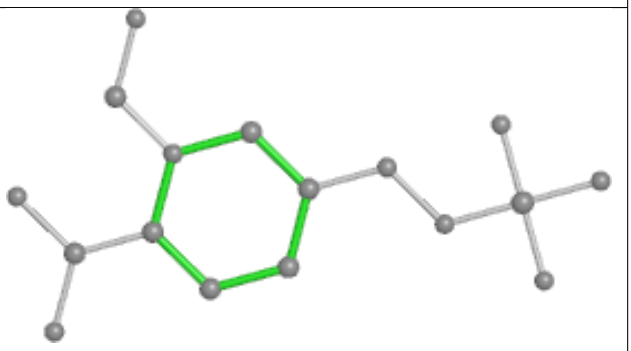
Bond lengths



Bond angles

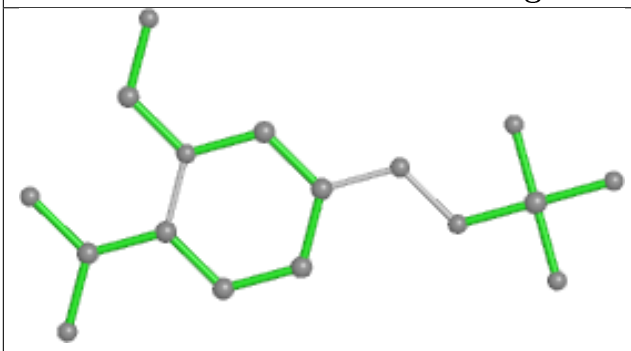


Torsions



Rings

Ligand NXL E 301



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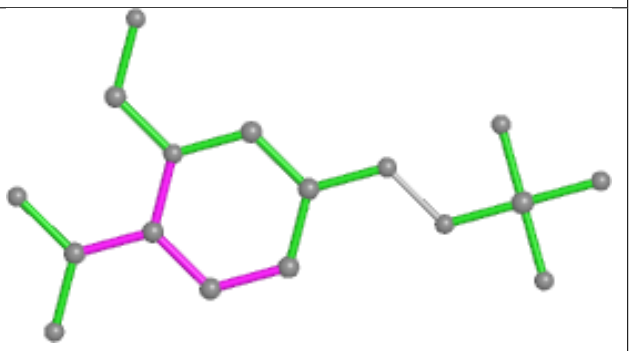

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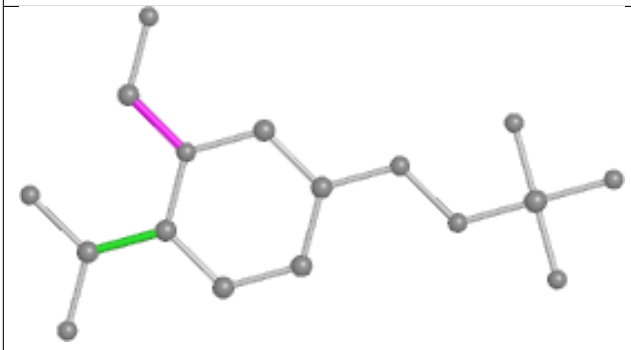

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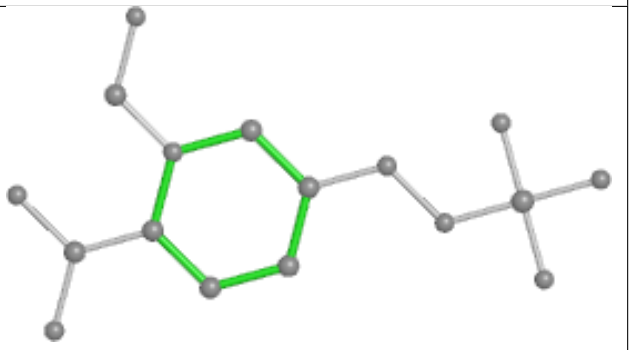
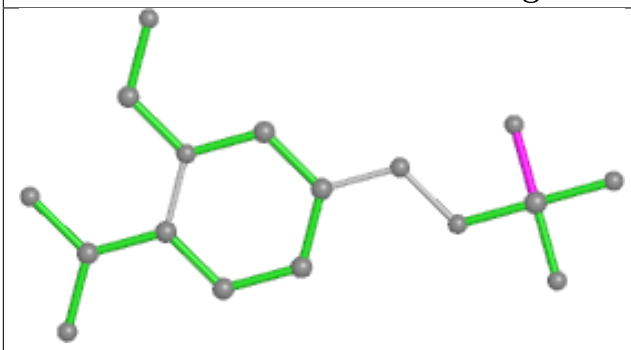


Rings

Ligand NXL H 301



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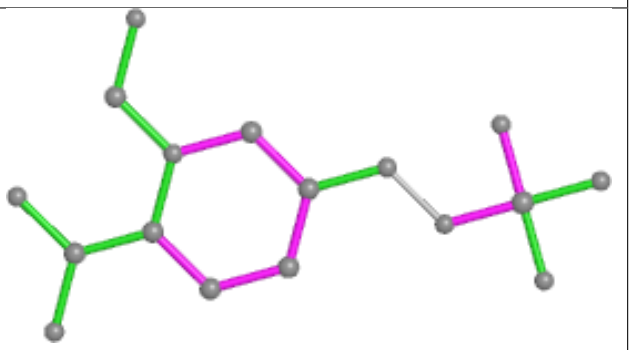

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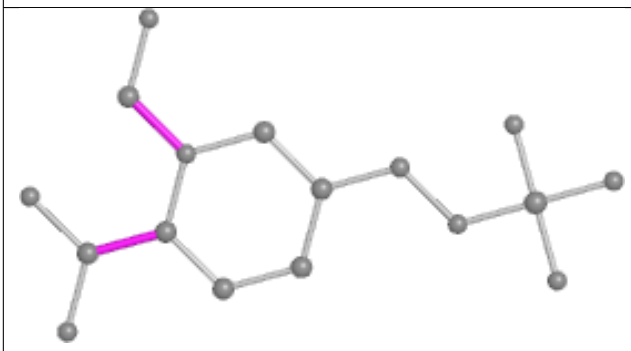
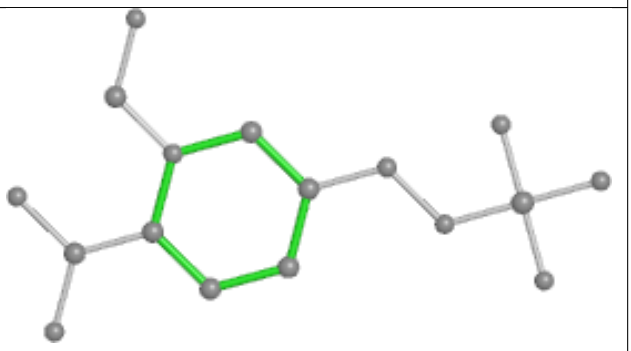
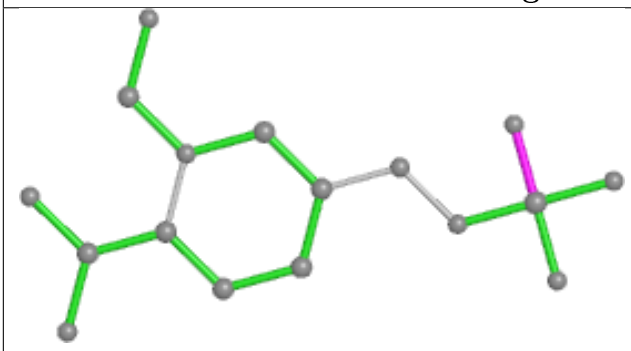


Torsions



Rings

Ligand NXL A 301



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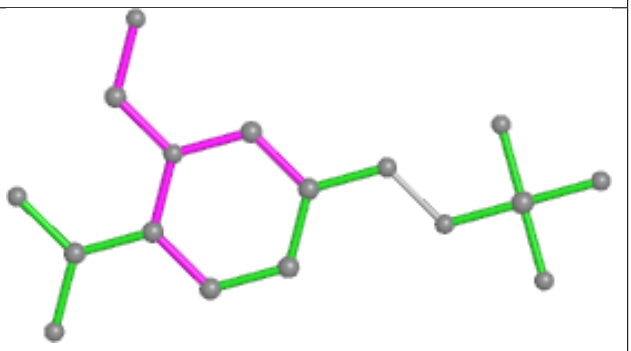

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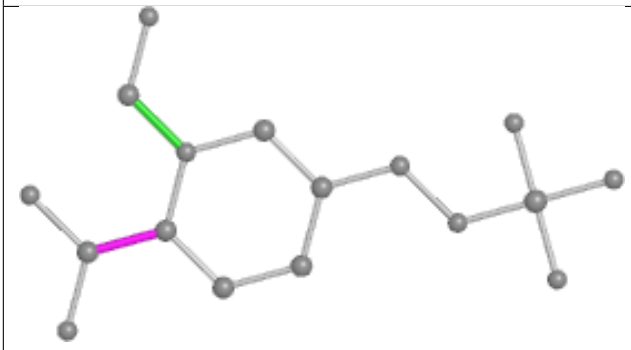
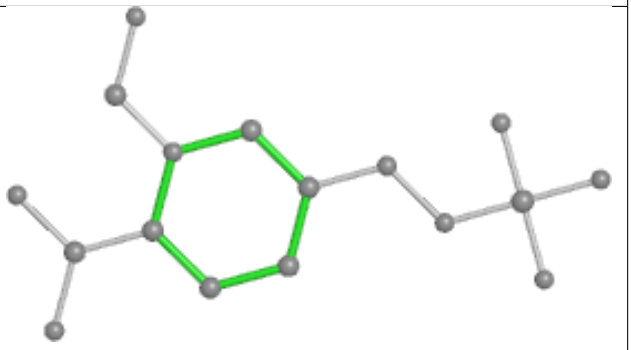
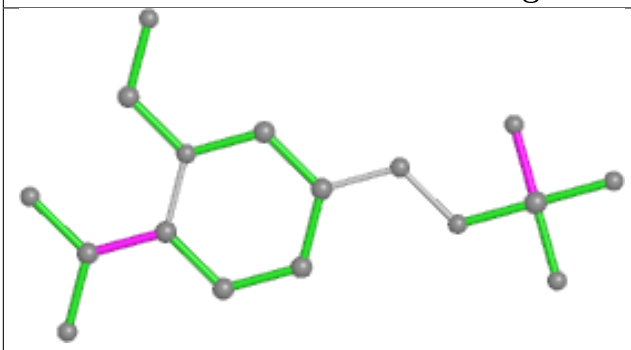


Torsions



Rings

Ligand NXL D 301



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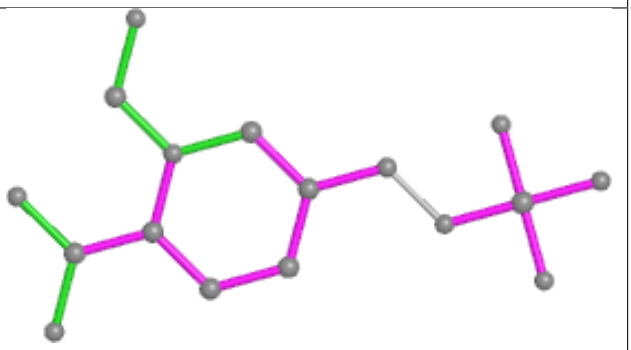

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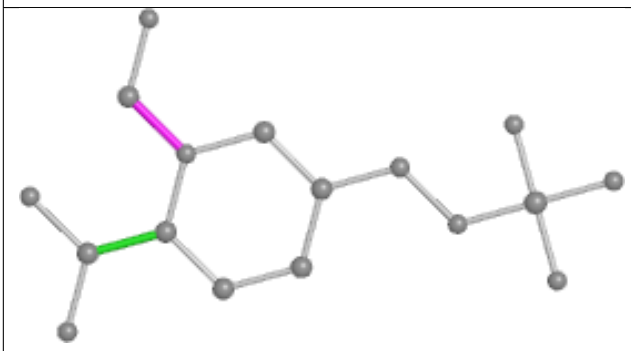

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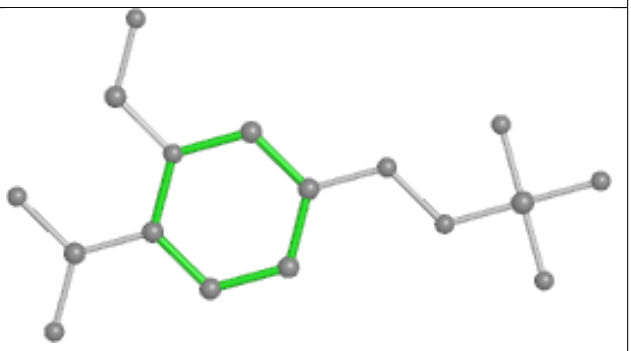

Rings

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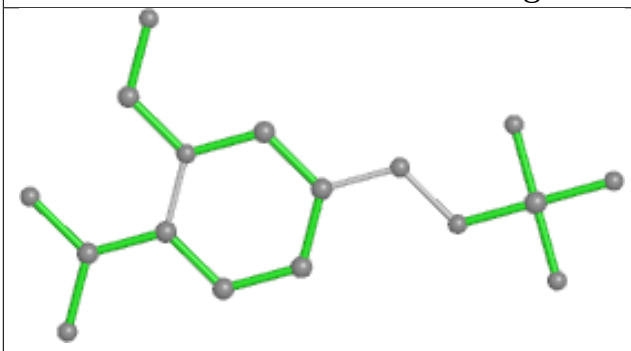

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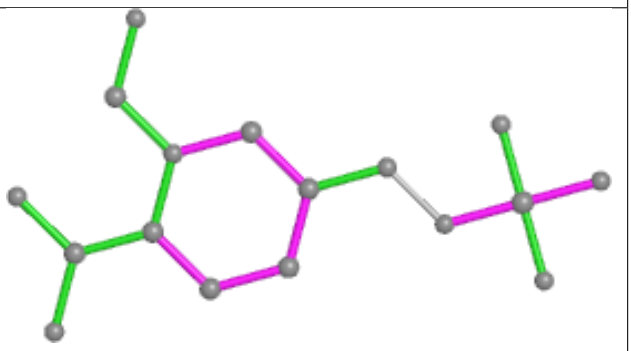

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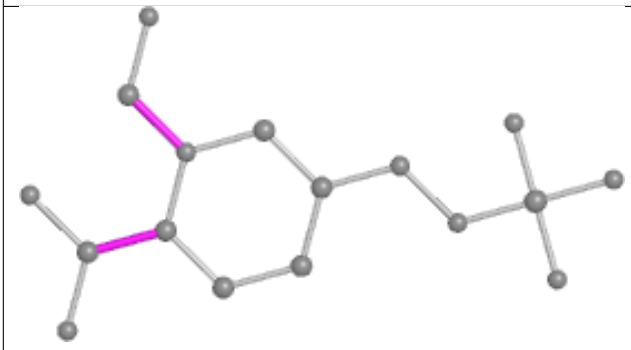

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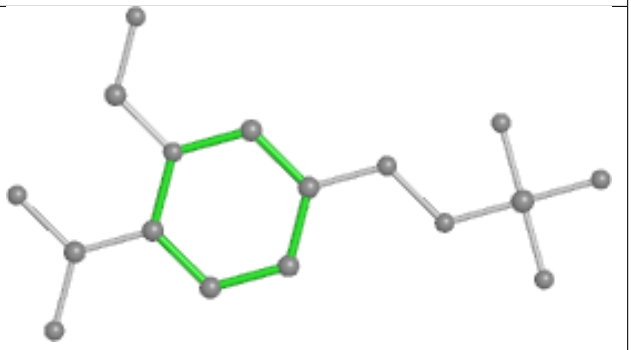

Rings

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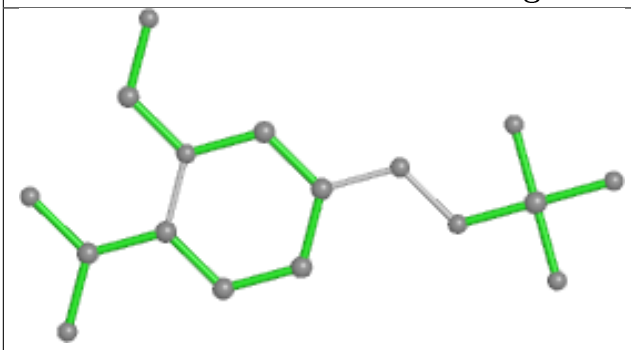

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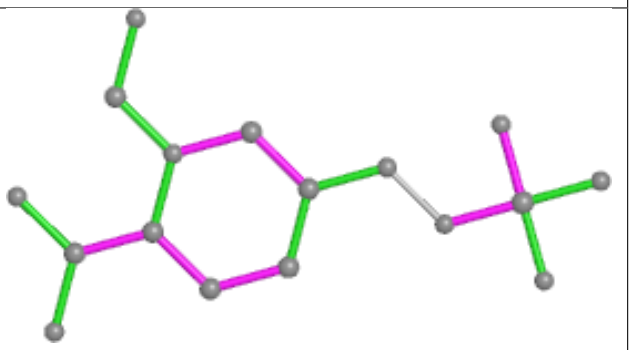

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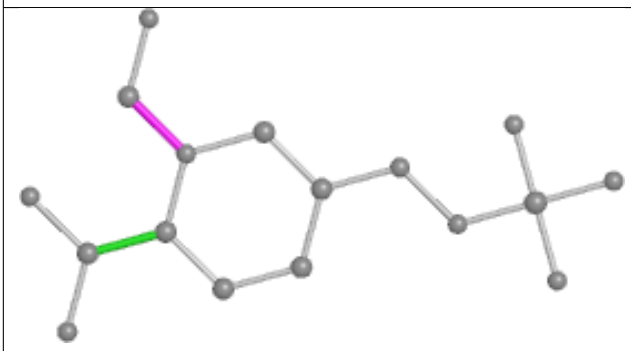

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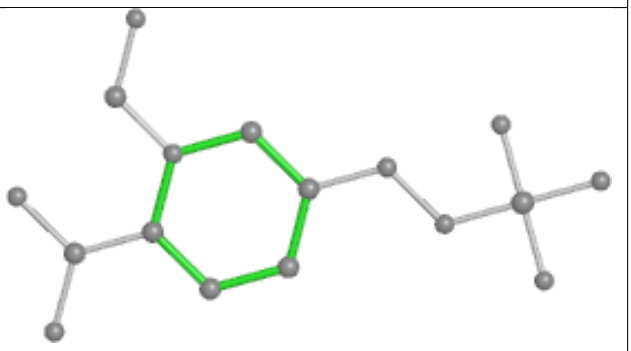
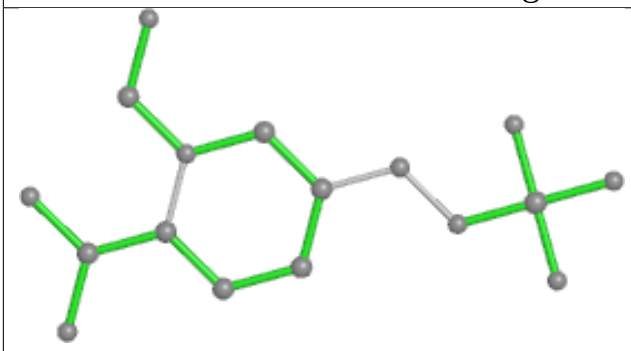


Rings

Ligand NXL G 301



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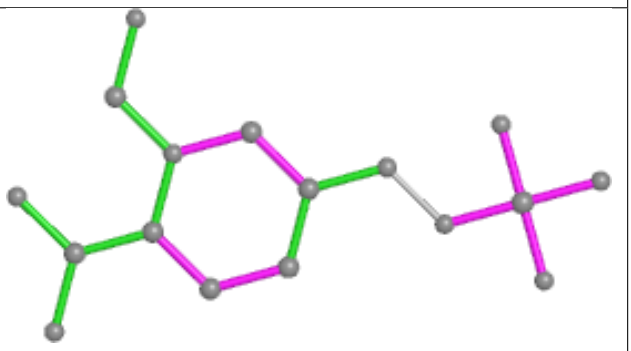
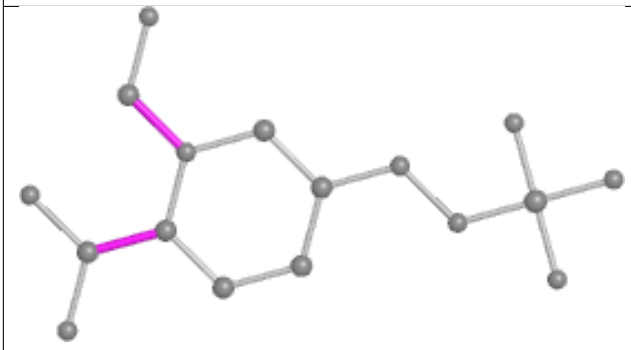
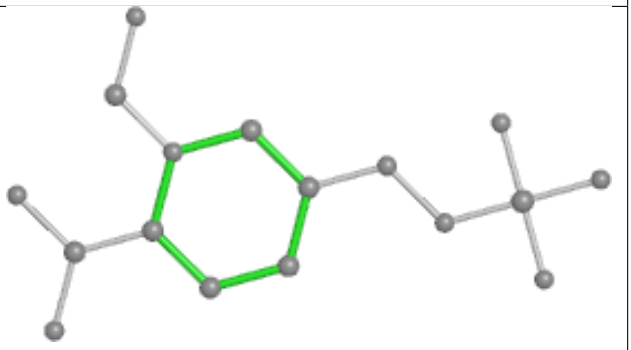


Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	237/242 (97%)	-0.40	0 100 100	12, 27, 46, 57	0
1	B	235/242 (97%)	-0.50	3 (1%) 77 81	8, 18, 41, 82	0
1	C	230/242 (95%)	-0.20	0 100 100	16, 34, 57, 73	0
1	F	240/242 (99%)	-0.24	2 (0%) 86 89	11, 31, 59, 74	0
1	G	235/242 (97%)	-0.16	2 (0%) 84 88	14, 35, 60, 75	0
1	H	221/242 (91%)	-0.21	4 (1%) 68 74	11, 30, 55, 76	0
2	D	235/242 (97%)	-0.54	0 100 100	7, 17, 37, 63	0
2	E	238/242 (98%)	-0.47	0 100 100	11, 24, 42, 56	0
All	All	1871/1936 (96%)	-0.34	11 (0%) 89 92	7, 27, 53, 82	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	158	LEU	3.6
1	G	126	PHE	3.1
1	H	211	TYR	2.9
1	F	214	ARG	2.8
1	G	158	LEU	2.5
1	H	131	GLY	2.4
1	H	182	HIS	2.4
1	H	33	ALA	2.3
1	B	147	GLU	2.2
1	B	182	HIS	2.1
1	F	103	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KCX	D	73	12/13	0.92	0.13	12,17,37,42	0
2	KCX	E	73	12/13	0.97	0.10	14,17,28,29	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CO2	A	302	3/3	0.81	0.15	38,38,39,46	0
4	CO2	C	302	3/3	0.88	0.17	41,41,43,45	0
3	NXL	G	301	17/17	0.92	0.16	46,49,55,59	0
4	CO2	F	302	3/3	0.92	0.16	42,42,43,47	0
3	NXL	H	301	17/17	0.93	0.12	40,46,62,62	0
3	NXL	F	301	17/17	0.94	0.12	32,37,48,49	0
3	NXL	D	301	17/17	0.95	0.13	16,21,31,33	0
3	NXL	C	301	17/17	0.96	0.13	38,48,57,59	0
3	NXL	A	301	17/17	0.97	0.12	22,28,40,42	0
3	NXL	E	301	17/17	0.97	0.10	17,21,30,32	0
3	NXL	B	301	17/17	0.98	0.10	19,24,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.