Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:26 PM GMT

PDB ID	:	1TNV
Title	:	CRYSTAL STRUCTURAL ANALYSIS OF TOBACCO NECROSIS VIRUS (TNV) AT 5 ANGSTROMS RESOLUTION
Authors	:	Tsukihara, T.
Deposited on	:	1994-03-11
Resolution	:	5.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

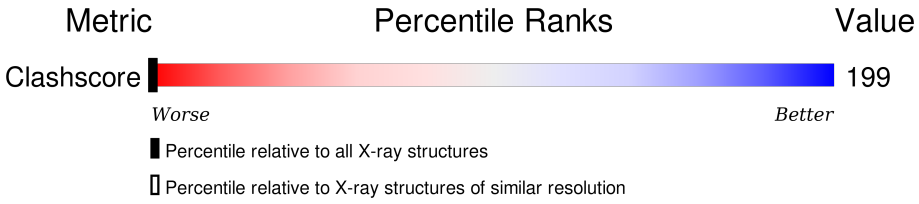
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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))
Clashscore	102246	1019 (6.22-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	186	33% 53% 13%
1	B	186	33% 55% 11%
2	C	210	39% 50% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2328 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 TOBACCO NECROSIS VIRUS (SUBUNIT VP1).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	0	0	0
			744	372	186	186			
1	B	186	Total	C	N	O	0	0	0
			744	372	186	186			

- Molecule 2 is a protein called TOBACCO NECROSIS VIRUS (SUBUNIT VP3).

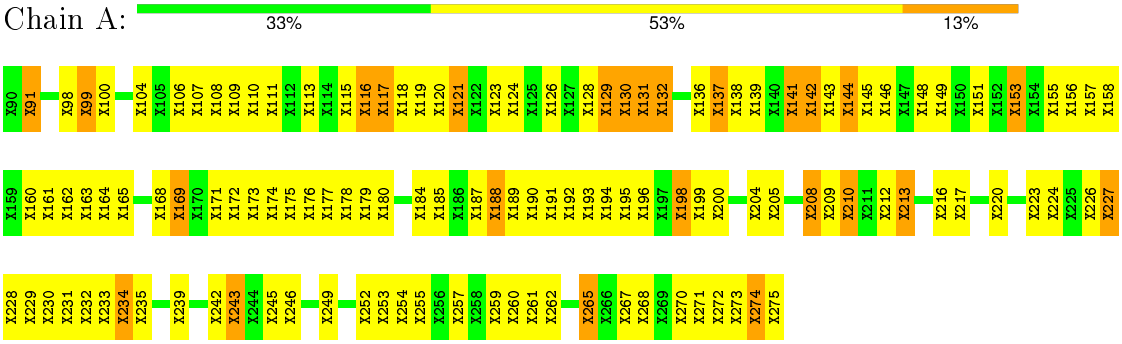
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	0	0	0
			840	420	210	210			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

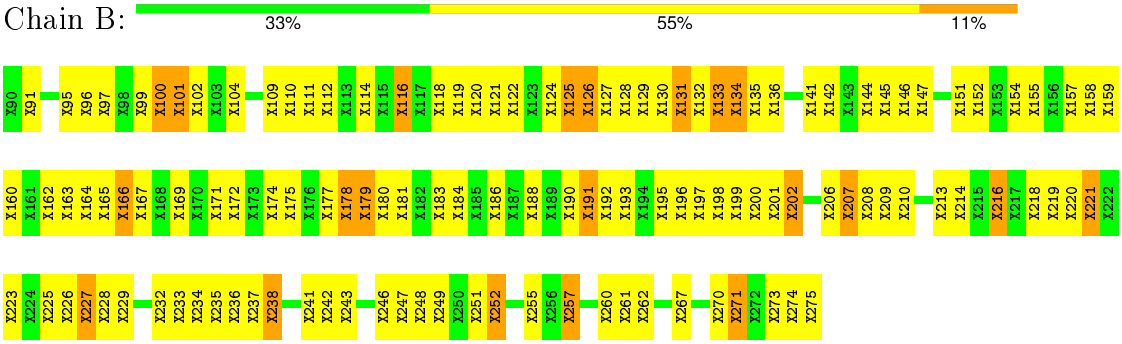
- Molecule 1: TOBACCO NECROSIS VIRUS (SUBUNIT VP1)

Chain A:



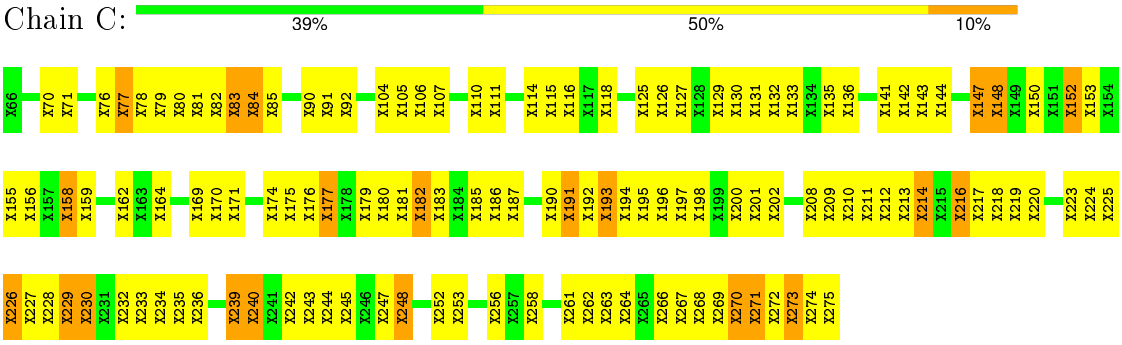
- Molecule 1: TOBACCO NECROSIS VIRUS (SUBUNIT VP1)

Chain B:



- Molecule 2: TOBACCO NECROSIS VIRUS (SUBUNIT VP3)

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α, β, γ	338.00Å 338.00Å 338.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 5.00 97.57 – 5.52	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-5.00) 42.8 (97.57-5.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.390 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Outliers	1 of 9350 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	2328	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	41
1	B	0	49
2	C	0	45
All	All	0	135

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (135) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	UNK	Mainchain
1	A	113	UNK	Mainchain
1	A	116	UNK	Mainchain
1	A	117	UNK	Mainchain
1	A	121	UNK	Mainchain
1	A	129	UNK	Mainchain
1	A	130	UNK	Mainchain
1	A	131	UNK	Mainchain
1	A	132	UNK	Mainchain
1	A	137	UNK	Mainchain
1	A	141	UNK	Mainchain
1	A	142	UNK	Mainchain
1	A	144	UNK	Mainchain
1	A	145	UNK	Mainchain
1	A	146	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	A	148	UNK	Mainchain
1	A	149	UNK	Mainchain
1	A	153	UNK	Mainchain
1	A	169	UNK	Mainchain
1	A	180	UNK	Mainchain
1	A	188	UNK	Mainchain
1	A	198	UNK	Mainchain
1	A	199	UNK	Mainchain
1	A	208	UNK	Mainchain
1	A	210	UNK	Mainchain
1	A	213	UNK	Mainchain
1	A	220	UNK	Mainchain
1	A	227	UNK	Mainchain
1	A	229	UNK	Mainchain
1	A	234	UNK	Mainchain
1	A	242	UNK	Mainchain
1	A	243	UNK	Mainchain
1	A	249	UNK	Mainchain
1	A	255	UNK	Mainchain
1	A	257	UNK	Mainchain
1	A	259	UNK	Mainchain
1	A	260	UNK	Mainchain
1	A	265	UNK	Mainchain
1	A	274	UNK	Mainchain
1	A	91	UNK	Mainchain
1	A	99	UNK	Mainchain
1	B	100	UNK	Mainchain
1	B	101	UNK	Mainchain
1	B	111	UNK	Peptide
1	B	112	UNK	Mainchain
1	B	114	UNK	Mainchain
1	B	116	UNK	Mainchain
1	B	121	UNK	Mainchain
1	B	122	UNK	Mainchain
1	B	125	UNK	Mainchain
1	B	126	UNK	Mainchain
1	B	131	UNK	Mainchain
1	B	133	UNK	Mainchain
1	B	134	UNK	Mainchain
1	B	141	UNK	Mainchain
1	B	142	UNK	Mainchain
1	B	145	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	B	154	UNK	Mainchain
1	B	155	UNK	Mainchain
1	B	157	UNK	Mainchain
1	B	166	UNK	Mainchain
1	B	169	UNK	Mainchain
1	B	174	UNK	Mainchain
1	B	178	UNK	Mainchain
1	B	179	UNK	Mainchain
1	B	191	UNK	Mainchain
1	B	193	UNK	Mainchain
1	B	202	UNK	Mainchain
1	B	207	UNK	Mainchain
1	B	208	UNK	Mainchain
1	B	213	UNK	Mainchain
1	B	214	UNK	Mainchain
1	B	216	UNK	Mainchain
1	B	221	UNK	Mainchain
1	B	223	UNK	Mainchain
1	B	227	UNK	Mainchain
1	B	232	UNK	Mainchain
1	B	238	UNK	Mainchain
1	B	241	UNK	Mainchain
1	B	243	UNK	Mainchain
1	B	249	UNK	Mainchain
1	B	251	UNK	Mainchain
1	B	252	UNK	Mainchain
1	B	257	UNK	Mainchain
1	B	260	UNK	Mainchain
1	B	261	UNK	Mainchain
1	B	262	UNK	Mainchain
1	B	271	UNK	Mainchain
1	B	91	UNK	Mainchain
1	B	97	UNK	Mainchain
2	C	105	UNK	Mainchain
2	C	107	UNK	Mainchain
2	C	110	UNK	Mainchain
2	C	111	UNK	Mainchain
2	C	118	UNK	Mainchain
2	C	127	UNK	Mainchain
2	C	129	UNK	Mainchain
2	C	130	UNK	Mainchain
2	C	135	UNK	Mainchain

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Mol	Chain	Res	Type	Group
2	C	136	UNK	Mainchain
2	C	141	UNK	Mainchain
2	C	147	UNK	Mainchain
2	C	148	UNK	Mainchain
2	C	152	UNK	Mainchain
2	C	156	UNK	Mainchain
2	C	158	UNK	Mainchain
2	C	171	UNK	Mainchain
2	C	177	UNK	Mainchain
2	C	182	UNK	Mainchain
2	C	183	UNK	Mainchain
2	C	185	UNK	Mainchain
2	C	190	UNK	Mainchain
2	C	191	UNK	Mainchain
2	C	193	UNK	Mainchain
2	C	194	UNK	Mainchain
2	C	197	UNK	Mainchain
2	C	208	UNK	Mainchain
2	C	209	UNK	Mainchain
2	C	214	UNK	Mainchain
2	C	216	UNK	Mainchain
2	C	220	UNK	Mainchain
2	C	226	UNK	Mainchain
2	C	229	UNK	Mainchain
2	C	230	UNK	Mainchain
2	C	239	UNK	Mainchain
2	C	240	UNK	Mainchain
2	C	248	UNK	Mainchain
2	C	253	UNK	Mainchain
2	C	256	UNK	Mainchain
2	C	270	UNK	Mainchain
2	C	271	UNK	Mainchain
2	C	273	UNK	Mainchain
2	C	77	UNK	Mainchain
2	C	83	UNK	Mainchain
2	C	84	UNK	Mainchain

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	744	0	53	172	0
1	B	744	0	33	153	0
2	C	840	0	52	167	0
All	All	2328	0	138	491	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 199.

All (491) 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)
2:C:175:UNK:CA	2:C:175:UNK:C	1.76	1.62
2:C:266:UNK:C	2:C:266:UNK:CA	1.76	1.62
1:A:131:UNK:C	1:A:131:UNK:CA	1.76	1.62
1:A:272:UNK:CA	1:A:272:UNK:C	1.76	1.62
1:B:270:UNK:C	1:B:270:UNK:CA	1.76	1.62
1:A:275:UNK:C	1:A:275:UNK:CA	1.76	1.61
1:B:235:UNK:CA	1:B:235:UNK:C	1.76	1.61
1:A:178:UNK:CA	1:A:178:UNK:C	1.76	1.61
1:A:191:UNK:CA	1:A:191:UNK:C	1.76	1.61
2:C:201:UNK:C	2:C:201:UNK:CA	1.76	1.60
1:B:146:UNK:CA	1:B:146:UNK:C	1.76	1.58
1:A:267:UNK:CA	1:A:267:UNK:C	1.76	1.58
1:B:133:UNK:CA	1:B:133:UNK:C	1.76	1.58
2:C:79:UNK:CA	2:C:79:UNK:C	1.76	1.58
2:C:217:UNK:CA	2:C:217:UNK:C	1.76	1.58
2:C:229:UNK:C	2:C:229:UNK:CA	1.76	1.58
1:B:246:UNK:C	1:B:246:UNK:CA	1.76	1.58
2:C:261:UNK:C	2:C:261:UNK:CA	1.76	1.58
1:A:253:UNK:CA	1:A:253:UNK:C	1.76	1.57
2:C:174:UNK:CA	2:C:174:UNK:C	1.82	1.57
1:B:201:UNK:C	1:B:201:UNK:CA	1.82	1.57
1:A:274:UNK:CA	1:A:274:UNK:C	1.82	1.56
2:C:180:UNK:C	2:C:180:UNK:CA	1.82	1.56
2:C:264:UNK:CA	2:C:264:UNK:C	1.82	1.56
1:A:129:UNK:C	1:A:129:UNK:CA	1.76	1.56
2:C:235:UNK:CA	2:C:235:UNK:C	1.76	1.55
2:C:219:UNK:CA	2:C:219:UNK:N	1.69	1.55
1:A:245:UNK:CA	1:A:245:UNK:C	1.82	1.55
2:C:143:UNK:C	2:C:143:UNK:CA	1.82	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:UNK:N	2:C:78:UNK:CA	1.69	1.55
1:B:99:UNK:CA	1:B:99:UNK:C	1.76	1.55
2:C:233:UNK:CA	2:C:233:UNK:C	1.82	1.54
1:B:95:UNK:CA	1:B:95:UNK:C	1.82	1.54
1:B:238:UNK:N	1:B:238:UNK:CA	1.69	1.54
1:A:232:UNK:C	1:A:232:UNK:CA	1.85	1.54
1:B:206:UNK:C	1:B:206:UNK:CA	1.82	1.54
1:B:210:UNK:N	1:B:210:UNK:CA	1.69	1.54
1:A:174:UNK:N	1:A:174:UNK:CA	1.69	1.54
2:C:170:UNK:CA	2:C:170:UNK:N	1.69	1.54
2:C:187:UNK:CA	2:C:187:UNK:N	1.69	1.54
2:C:225:UNK:N	2:C:225:UNK:CA	1.69	1.53
2:C:132:UNK:CA	2:C:132:UNK:C	1.82	1.53
2:C:90:UNK:C	2:C:90:UNK:CA	1.85	1.53
1:B:110:UNK:CA	1:B:110:UNK:N	1.72	1.53
1:B:101:UNK:C	1:B:101:UNK:CA	1.82	1.52
1:B:274:UNK:N	1:B:274:UNK:CA	1.69	1.52
2:C:77:UNK:N	2:C:77:UNK:CA	1.69	1.52
1:A:227:UNK:N	1:A:227:UNK:CA	1.69	1.52
1:A:213:UNK:CA	1:A:213:UNK:N	1.69	1.52
2:C:126:UNK:N	2:C:126:UNK:CA	1.69	1.52
1:B:191:UNK:CA	1:B:191:UNK:N	1.72	1.52
2:C:131:UNK:C	2:C:131:UNK:CA	1.82	1.52
1:B:160:UNK:CA	1:B:160:UNK:N	1.69	1.52
1:A:231:UNK:CA	1:A:231:UNK:N	1.69	1.52
1:A:155:UNK:CA	1:A:155:UNK:C	1.82	1.52
1:A:157:UNK:CA	1:A:157:UNK:C	1.82	1.52
1:B:179:UNK:CA	1:B:179:UNK:N	1.69	1.52
2:C:210:UNK:C	2:C:210:UNK:CA	1.82	1.51
1:A:196:UNK:CA	1:A:196:UNK:N	1.69	1.51
1:A:99:UNK:N	1:A:99:UNK:CA	1.72	1.51
1:B:172:UNK:N	1:B:172:UNK:CA	1.72	1.51
1:B:178:UNK:CA	1:B:178:UNK:N	1.72	1.51
1:B:228:UNK:C	1:B:228:UNK:CA	1.85	1.51
1:B:135:UNK:CA	1:B:135:UNK:C	1.85	1.51
2:C:82:UNK:CA	2:C:82:UNK:N	1.72	1.51
1:A:162:UNK:N	1:A:162:UNK:CA	1.72	1.51
1:A:233:UNK:N	1:A:233:UNK:CA	1.72	1.51
1:A:209:UNK:CA	1:A:209:UNK:N	1.72	1.51
1:A:205:UNK:CA	1:A:205:UNK:N	1.69	1.51
1:A:143:UNK:CA	1:A:143:UNK:N	1.72	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:UNK:N	1:A:169:UNK:CA	1.72	1.50
2:C:71:UNK:N	2:C:71:UNK:CA	1.72	1.50
1:A:194:UNK:N	1:A:194:UNK:CA	1.69	1.50
2:C:235:UNK:N	2:C:235:UNK:CA	1.72	1.49
1:B:167:UNK:CA	1:B:167:UNK:N	1.72	1.49
1:B:181:UNK:N	1:B:181:UNK:CA	1.72	1.49
2:C:245:UNK:CA	2:C:245:UNK:N	1.76	1.49
2:C:153:UNK:N	2:C:153:UNK:CA	1.72	1.49
1:A:108:UNK:CA	1:A:108:UNK:N	1.72	1.49
2:C:84:UNK:CA	2:C:84:UNK:N	1.76	1.49
2:C:159:UNK:N	2:C:159:UNK:CA	1.76	1.49
1:B:237:UNK:N	1:B:237:UNK:CA	1.72	1.49
1:B:163:UNK:N	1:B:163:UNK:CA	1.72	1.49
1:A:110:UNK:CA	1:A:110:UNK:N	1.72	1.48
1:A:271:UNK:N	1:A:271:UNK:CA	1.72	1.48
2:C:263:UNK:CA	2:C:263:UNK:N	1.72	1.48
1:B:229:UNK:N	1:B:229:UNK:CA	1.72	1.48
1:B:129:UNK:CA	1:B:129:UNK:N	1.76	1.48
1:B:152:UNK:CA	1:B:152:UNK:N	1.72	1.48
1:B:199:UNK:N	1:B:199:UNK:CA	1.72	1.48
2:C:273:UNK:N	2:C:273:UNK:CA	1.72	1.48
1:B:125:UNK:N	1:B:125:UNK:CA	1.72	1.47
1:B:198:UNK:CA	1:B:198:UNK:N	1.72	1.47
1:B:120:UNK:N	1:B:120:UNK:CA	1.72	1.47
1:B:196:UNK:N	1:B:196:UNK:CA	1.76	1.47
1:A:217:UNK:CA	1:A:217:UNK:N	1.72	1.47
2:C:214:UNK:N	2:C:214:UNK:CA	1.72	1.47
2:C:240:UNK:CA	2:C:240:UNK:N	1.76	1.47
2:C:116:UNK:CA	2:C:116:UNK:N	1.76	1.47
1:A:189:UNK:N	1:A:189:UNK:CA	1.76	1.46
1:B:184:UNK:N	1:B:184:UNK:CA	1.72	1.46
1:A:161:UNK:CA	1:A:161:UNK:N	1.72	1.46
1:A:163:UNK:CA	1:A:163:UNK:N	1.76	1.44
2:C:91:UNK:CA	2:C:91:UNK:N	1.82	1.42
1:A:164:UNK:CA	1:A:164:UNK:N	1.82	1.41
1:B:131:UNK:CA	1:B:131:UNK:N	1.82	1.40
1:A:142:UNK:CA	1:A:142:UNK:N	1.82	1.40
2:C:198:UNK:O	2:C:200:UNK:N	1.66	1.28
1:B:134:UNK:N	1:B:219:UNK:O	1.76	1.19
1:B:183:UNK:C	1:B:184:UNK:CA	2.27	1.13
1:A:137:UNK:N	1:A:262:UNK:O	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:UNK:C	1:A:157:UNK:O	0.83	1.13
1:B:270:UNK:O	1:B:273:UNK:N	1.82	1.12
2:C:242:UNK:O	2:C:242:UNK:C	0.83	1.12
1:A:188:UNK:O	1:A:190:UNK:N	1.82	1.11
1:B:128:UNK:C	1:B:129:UNK:CA	2.29	1.09
1:A:109:UNK:C	1:A:110:UNK:CA	2.34	1.04
2:C:191:UNK:C	2:C:193:UNK:H2	1.68	1.02
1:A:226:UNK:C	1:A:227:UNK:CA	2.39	1.01
2:C:76:UNK:C	2:C:77:UNK:CA	2.39	1.01
1:A:216:UNK:C	1:A:217:UNK:CA	2.39	1.00
2:C:175:UNK:CA	2:C:176:UNK:N	2.24	1.00
1:A:195:UNK:C	1:A:196:UNK:CA	2.39	1.00
2:C:153:UNK:CA	2:C:247:UNK:CA	2.39	0.99
1:B:246:UNK:CA	1:B:247:UNK:N	2.27	0.98
1:B:177:UNK:C	1:B:178:UNK:CA	2.41	0.98
1:A:198:UNK:O	1:A:200:UNK:N	1.97	0.97
1:B:101:UNK:CA	1:B:102:UNK:N	2.27	0.97
2:C:77:UNK:C	2:C:78:UNK:CA	2.41	0.97
1:B:178:UNK:C	1:B:179:UNK:CA	2.41	0.97
2:C:90:UNK:CA	2:C:91:UNK:N	2.29	0.95
2:C:218:UNK:C	2:C:219:UNK:CA	2.44	0.95
2:C:271:UNK:C	2:C:273:UNK:N	2.29	0.95
1:A:129:UNK:CA	1:A:130:UNK:N	2.29	0.95
2:C:273:UNK:O	2:C:275:UNK:N	2.00	0.94
2:C:261:UNK:CA	2:C:262:UNK:N	2.29	0.94
1:B:120:UNK:N	1:B:120:UNK:C	2.29	0.94
1:A:120:UNK:O	1:A:121:UNK:O	1.85	0.94
2:C:242:UNK:O	2:C:243:UNK:N	2.00	0.94
1:A:253:UNK:C	1:A:253:UNK:N	2.29	0.93
1:A:141:UNK:C	1:A:142:UNK:CA	2.46	0.93
2:C:152:UNK:C	2:C:153:UNK:CA	2.46	0.93
2:C:272:UNK:C	2:C:273:UNK:CA	2.46	0.93
2:C:213:UNK:C	2:C:214:UNK:CA	2.46	0.92
1:B:228:UNK:C	1:B:229:UNK:CA	2.48	0.91
1:B:236:UNK:C	1:B:237:UNK:CA	2.48	0.91
1:A:232:UNK:C	1:A:233:UNK:CA	2.48	0.91
1:B:238:UNK:N	1:B:238:UNK:C	2.34	0.91
1:A:157:UNK:O	1:A:158:UNK:N	2.03	0.90
1:A:160:UNK:C	1:A:161:UNK:CA	2.48	0.90
1:A:161:UNK:C	1:A:162:UNK:CA	2.48	0.90
2:C:224:UNK:C	2:C:225:UNK:CA	2.48	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:UNK:O	1:B:200:UNK:N	2.06	0.89
2:C:271:UNK:O	2:C:273:UNK:N	2.06	0.89
2:C:131:UNK:CA	2:C:132:UNK:N	2.37	0.88
2:C:214:UNK:N	2:C:214:UNK:C	2.37	0.88
1:A:275:UNK:C	1:A:275:UNK:N	2.37	0.88
1:B:152:UNK:N	1:B:152:UNK:C	2.37	0.87
1:A:107:UNK:C	1:A:108:UNK:CA	2.53	0.86
1:A:270:UNK:C	1:A:271:UNK:CA	2.53	0.86
1:A:267:UNK:CA	1:A:268:UNK:N	2.39	0.86
1:B:119:UNK:C	1:B:120:UNK:CA	2.53	0.86
1:B:198:UNK:C	1:B:198:UNK:N	2.39	0.86
2:C:180:UNK:C	2:C:180:UNK:N	2.39	0.85
1:B:246:UNK:C	1:B:246:UNK:N	2.39	0.85
1:A:232:UNK:N	1:A:233:UNK:N	2.24	0.85
2:C:239:UNK:C	2:C:240:UNK:CA	2.53	0.85
2:C:115:UNK:C	2:C:116:UNK:CA	2.53	0.85
2:C:229:UNK:C	2:C:229:UNK:N	2.39	0.85
1:B:160:UNK:C	1:B:160:UNK:N	2.39	0.85
1:A:232:UNK:C	1:A:232:UNK:N	2.39	0.85
1:A:157:UNK:N	1:A:157:UNK:C	2.39	0.85
1:B:146:UNK:C	1:B:146:UNK:N	2.39	0.84
1:B:270:UNK:CA	1:B:271:UNK:N	2.39	0.84
1:A:232:UNK:CA	1:A:233:UNK:N	2.39	0.84
2:C:82:UNK:C	2:C:82:UNK:N	2.39	0.84
1:A:188:UNK:C	1:A:189:UNK:CA	2.55	0.83
1:A:209:UNK:C	1:A:209:UNK:N	2.41	0.83
1:A:230:UNK:C	1:A:231:UNK:CA	2.48	0.83
1:B:159:UNK:C	1:B:160:UNK:CA	2.55	0.83
2:C:235:UNK:CA	2:C:236:UNK:N	2.41	0.83
2:C:169:UNK:C	2:C:170:UNK:CA	2.53	0.83
1:A:174:UNK:N	1:A:174:UNK:C	2.39	0.83
1:A:188:UNK:C	1:A:190:UNK:N	2.41	0.83
1:B:228:UNK:CA	1:B:229:UNK:N	2.39	0.83
2:C:201:UNK:C	2:C:201:UNK:N	2.41	0.82
1:B:95:UNK:CA	1:B:96:UNK:N	2.41	0.82
1:A:193:UNK:C	1:A:194:UNK:CA	2.57	0.82
1:A:208:UNK:C	1:A:209:UNK:CA	2.57	0.82
1:B:237:UNK:C	1:B:238:UNK:CA	2.57	0.81
2:C:233:UNK:CA	2:C:234:UNK:N	2.41	0.81
1:B:195:UNK:C	1:B:196:UNK:CA	2.53	0.81
1:B:216:UNK:C	1:B:218:UNK:H	1.91	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:UNK:CA	2:C:267:UNK:N	2.41	0.81
1:B:99:UNK:CA	1:B:100:UNK:N	2.37	0.81
1:B:99:UNK:N	1:B:99:UNK:C	2.44	0.81
1:B:152:UNK:O	1:B:248:UNK:N	2.14	0.81
2:C:242:UNK:O	2:C:242:UNK:CA	2.29	0.81
1:A:168:UNK:C	1:A:169:UNK:CA	2.60	0.80
1:B:274:UNK:O	1:B:275:UNK:C	2.27	0.80
1:B:184:UNK:N	1:B:184:UNK:C	2.46	0.79
2:C:219:UNK:N	2:C:219:UNK:C	2.46	0.79
1:A:226:UNK:C	1:A:227:UNK:C	2.60	0.79
2:C:158:UNK:C	2:C:159:UNK:CA	2.60	0.79
2:C:104:UNK:O	2:C:252:UNK:O	2.00	0.79
1:B:198:UNK:C	1:B:199:UNK:CA	2.60	0.78
2:C:79:UNK:CA	2:C:80:UNK:N	2.46	0.78
2:C:143:UNK:CA	2:C:144:UNK:N	2.46	0.78
1:A:173:UNK:C	1:A:174:UNK:CA	2.60	0.78
2:C:273:UNK:C	2:C:273:UNK:N	2.46	0.78
2:C:210:UNK:O	2:C:213:UNK:N	2.16	0.77
1:B:273:UNK:C	1:B:274:UNK:CA	2.60	0.77
2:C:131:UNK:C	2:C:131:UNK:N	2.48	0.77
1:B:274:UNK:C	1:B:274:UNK:N	2.48	0.76
2:C:217:UNK:CA	2:C:218:UNK:N	2.46	0.76
1:A:272:UNK:CA	1:A:273:UNK:N	2.46	0.76
1:A:204:UNK:C	1:A:205:UNK:CA	2.60	0.76
1:B:163:UNK:C	1:B:163:UNK:N	2.48	0.76
2:C:191:UNK:C	2:C:193:UNK:N	2.46	0.76
2:C:79:UNK:O	2:C:79:UNK:CA	2.29	0.76
2:C:174:UNK:CA	2:C:175:UNK:N	2.39	0.76
1:A:245:UNK:CA	1:A:246:UNK:N	2.48	0.76
2:C:143:UNK:N	2:C:143:UNK:C	2.48	0.76
1:A:169:UNK:C	1:A:169:UNK:N	2.48	0.76
1:B:167:UNK:N	1:B:167:UNK:C	2.46	0.76
1:A:189:UNK:N	1:A:189:UNK:C	2.48	0.75
1:A:232:UNK:C	1:A:234:UNK:N	2.48	0.75
2:C:90:UNK:C	2:C:90:UNK:N	2.48	0.75
1:A:171:UNK:O	1:A:175:UNK:N	2.19	0.75
1:B:95:UNK:N	1:B:95:UNK:C	2.48	0.75
1:B:133:UNK:CA	1:B:220:UNK:CA	2.64	0.75
2:C:186:UNK:C	2:C:187:UNK:CA	2.64	0.74
2:C:217:UNK:N	2:C:217:UNK:C	2.48	0.74
2:C:210:UNK:CA	2:C:211:UNK:N	2.48	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:UNK:C	2:C:84:UNK:CA	2.64	0.74
1:A:178:UNK:CA	1:A:179:UNK:N	2.48	0.74
1:A:227:UNK:N	1:A:227:UNK:C	2.48	0.74
1:A:188:UNK:C	1:A:189:UNK:C	2.66	0.74
1:A:162:UNK:O	1:A:165:UNK:N	2.22	0.73
2:C:90:UNK:C	2:C:91:UNK:CA	2.64	0.73
1:B:151:UNK:C	1:B:152:UNK:CA	2.60	0.73
1:A:91:UNK:O	1:A:265:UNK:N	2.22	0.73
1:B:119:UNK:C	1:B:120:UNK:C	2.66	0.73
1:B:135:UNK:N	1:B:135:UNK:C	2.48	0.72
1:A:142:UNK:C	1:A:143:UNK:CA	2.64	0.72
1:A:163:UNK:C	1:A:164:UNK:CA	2.66	0.72
1:A:162:UNK:C	1:A:163:UNK:CA	2.66	0.72
1:A:98:UNK:C	1:A:99:UNK:CA	2.66	0.72
1:B:166:UNK:C	1:B:167:UNK:CA	2.66	0.72
2:C:244:UNK:C	2:C:245:UNK:CA	2.64	0.72
1:B:270:UNK:O	1:B:273:UNK:CA	2.37	0.72
1:A:155:UNK:N	1:A:155:UNK:C	2.48	0.72
2:C:174:UNK:C	2:C:174:UNK:N	2.48	0.71
1:A:213:UNK:N	1:A:213:UNK:C	2.53	0.71
1:A:155:UNK:CA	1:A:156:UNK:N	2.48	0.71
1:A:99:UNK:C	1:A:99:UNK:N	2.53	0.71
2:C:187:UNK:N	2:C:187:UNK:C	2.48	0.71
1:A:267:UNK:C	1:A:267:UNK:N	2.53	0.71
1:A:99:UNK:O	1:A:100:UNK:O	2.08	0.71
1:B:181:UNK:N	1:B:181:UNK:C	2.53	0.70
1:B:233:UNK:O	1:B:236:UNK:N	2.24	0.70
2:C:125:UNK:C	2:C:126:UNK:CA	2.64	0.70
1:A:131:UNK:O	1:A:131:UNK:CA	2.37	0.70
1:A:172:UNK:O	1:A:173:UNK:C	2.39	0.70
2:C:84:UNK:N	2:C:84:UNK:C	2.53	0.70
1:A:119:UNK:O	1:A:120:UNK:C	2.39	0.70
1:A:129:UNK:C	1:A:129:UNK:N	2.53	0.70
1:B:133:UNK:N	1:B:133:UNK:C	2.53	0.70
1:B:190:UNK:C	1:B:191:UNK:CA	2.57	0.70
1:A:142:UNK:C	1:A:142:UNK:N	2.55	0.69
1:A:217:UNK:N	1:A:217:UNK:C	2.53	0.69
1:B:191:UNK:C	1:B:191:UNK:N	2.55	0.69
1:B:144:UNK:O	1:B:255:UNK:CA	2.39	0.69
1:B:206:UNK:CA	1:B:207:UNK:N	2.55	0.69
2:C:201:UNK:CA	2:C:202:UNK:N	2.48	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:UNK:CA	1:A:254:UNK:N	2.55	0.68
1:A:123:UNK:O	1:A:126:UNK:N	2.27	0.68
2:C:228:UNK:O	2:C:229:UNK:C	2.41	0.68
1:A:139:UNK:O	1:A:209:UNK:N	2.27	0.68
1:B:196:UNK:N	1:B:196:UNK:C	2.55	0.68
1:A:115:UNK:N	1:A:239:UNK:O	2.27	0.68
1:B:124:UNK:C	1:B:125:UNK:CA	2.66	0.68
1:B:134:UNK:O	1:B:219:UNK:N	2.27	0.68
1:A:232:UNK:O	1:A:234:UNK:N	2.27	0.68
1:A:274:UNK:C	1:A:274:UNK:N	2.53	0.68
1:B:235:UNK:CA	1:B:236:UNK:N	2.48	0.68
2:C:177:UNK:O	2:C:179:UNK:N	2.27	0.68
1:A:132:UNK:N	1:A:267:UNK:O	2.27	0.68
1:A:153:UNK:O	1:A:185:UNK:N	2.27	0.67
1:B:146:UNK:CA	1:B:147:UNK:N	2.48	0.67
1:A:195:UNK:C	1:A:196:UNK:C	2.73	0.67
2:C:233:UNK:C	2:C:235:UNK:N	2.55	0.66
2:C:78:UNK:C	2:C:78:UNK:N	2.55	0.66
1:B:180:UNK:C	1:B:181:UNK:CA	2.64	0.66
1:B:225:UNK:O	1:B:226:UNK:C	2.41	0.66
2:C:132:UNK:CA	2:C:133:UNK:N	2.57	0.65
2:C:228:UNK:C	2:C:229:UNK:C	2.75	0.65
1:B:130:UNK:C	1:B:131:UNK:CA	2.75	0.65
1:A:110:UNK:N	1:A:110:UNK:C	2.55	0.65
2:C:155:UNK:O	2:C:182:UNK:CA	2.44	0.65
1:B:171:UNK:O	1:B:175:UNK:N	2.29	0.65
1:B:132:UNK:O	1:B:221:UNK:N	2.29	0.65
1:B:237:UNK:N	1:B:237:UNK:C	2.60	0.65
1:A:194:UNK:C	1:A:194:UNK:N	2.60	0.65
2:C:262:UNK:C	2:C:263:UNK:CA	2.75	0.65
2:C:213:UNK:C	2:C:214:UNK:C	2.75	0.65
1:A:99:UNK:C	1:A:100:UNK:O	2.39	0.65
1:A:143:UNK:N	1:A:143:UNK:C	2.55	0.64
2:C:79:UNK:N	2:C:79:UNK:C	2.60	0.64
1:A:274:UNK:O	1:A:275:UNK:C	2.46	0.64
1:A:129:UNK:N	1:A:130:UNK:N	2.46	0.64
1:A:191:UNK:O	1:A:192:UNK:O	2.16	0.64
2:C:198:UNK:C	2:C:200:UNK:N	2.60	0.64
1:B:172:UNK:N	1:B:172:UNK:C	2.60	0.63
2:C:193:UNK:O	2:C:198:UNK:O	2.16	0.63
1:A:91:UNK:N	1:A:265:UNK:O	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:UNK:CA	1:A:132:UNK:N	2.46	0.63
2:C:106:UNK:CA	2:C:248:UNK:CA	2.77	0.63
1:B:183:UNK:C	1:B:184:UNK:C	2.75	0.63
2:C:91:UNK:C	2:C:91:UNK:N	2.60	0.62
1:B:128:UNK:C	1:B:129:UNK:C	2.77	0.62
2:C:263:UNK:C	2:C:263:UNK:N	2.60	0.62
2:C:264:UNK:O	2:C:264:UNK:CA	2.41	0.62
2:C:217:UNK:N	2:C:218:UNK:N	2.48	0.61
1:B:146:UNK:N	1:B:147:UNK:N	2.46	0.61
2:C:266:UNK:O	2:C:266:UNK:CA	2.37	0.61
1:B:201:UNK:O	1:B:201:UNK:CA	2.39	0.61
2:C:232:UNK:O	2:C:235:UNK:N	2.34	0.61
1:A:162:UNK:C	1:A:164:UNK:N	2.64	0.61
1:A:274:UNK:C	1:A:275:UNK:C	2.79	0.61
1:B:178:UNK:C	1:B:178:UNK:N	2.64	0.60
1:B:233:UNK:O	1:B:234:UNK:C	2.48	0.60
1:B:151:UNK:C	1:B:152:UNK:C	2.79	0.60
2:C:70:UNK:C	2:C:71:UNK:CA	2.75	0.60
1:B:104:UNK:O	1:B:252:UNK:CA	2.48	0.60
1:B:135:UNK:CA	1:B:136:UNK:N	2.64	0.60
2:C:170:UNK:N	2:C:170:UNK:C	2.55	0.60
1:A:108:UNK:C	1:A:108:UNK:N	2.60	0.60
1:A:144:UNK:O	1:A:187:UNK:O	2.19	0.59
1:A:232:UNK:C	1:A:233:UNK:C	2.81	0.59
1:A:157:UNK:CA	1:A:158:UNK:N	2.60	0.59
2:C:174:UNK:C	2:C:176:UNK:N	2.66	0.59
2:C:216:UNK:C	2:C:218:UNK:N	2.66	0.58
1:A:119:UNK:O	1:A:121:UNK:N	2.37	0.58
2:C:133:UNK:O	2:C:266:UNK:N	2.37	0.58
1:A:162:UNK:N	1:A:162:UNK:C	2.66	0.58
1:A:198:UNK:C	1:A:200:UNK:N	2.64	0.58
2:C:198:UNK:O	2:C:200:UNK:CA	2.48	0.58
1:B:116:UNK:C	1:B:118:UNK:N	2.66	0.58
1:A:151:UNK:O	1:A:153:UNK:N	2.37	0.58
2:C:261:UNK:O	2:C:261:UNK:CA	2.46	0.57
1:B:216:UNK:C	1:B:218:UNK:N	2.64	0.57
2:C:261:UNK:C	2:C:261:UNK:N	2.66	0.57
1:A:136:UNK:C	1:A:262:UNK:O	2.48	0.57
1:B:195:UNK:C	1:B:196:UNK:C	2.83	0.57
1:A:120:UNK:C	1:A:121:UNK:O	2.46	0.56
1:A:223:UNK:O	1:A:224:UNK:C	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:UNK:O	1:A:235:UNK:N	2.39	0.56
2:C:85:UNK:O	2:C:92:UNK:N	2.39	0.56
1:A:267:UNK:O	1:A:267:UNK:CA	2.41	0.56
1:B:99:UNK:N	1:B:257:UNK:O	2.39	0.56
1:B:158:UNK:N	1:B:242:UNK:O	2.39	0.56
2:C:271:UNK:O	2:C:274:UNK:N	2.39	0.56
1:B:124:UNK:O	1:B:128:UNK:N	2.39	0.56
2:C:245:UNK:N	2:C:245:UNK:C	2.64	0.55
1:B:197:UNK:C	1:B:198:UNK:CA	2.77	0.55
2:C:226:UNK:O	2:C:227:UNK:C	2.53	0.55
1:A:195:UNK:O	1:A:196:UNK:C	2.55	0.55
1:B:95:UNK:O	1:B:95:UNK:N	2.39	0.55
1:A:153:UNK:O	1:A:185:UNK:CA	2.55	0.55
2:C:175:UNK:N	2:C:176:UNK:N	2.55	0.54
2:C:234:UNK:C	2:C:235:UNK:CA	2.79	0.54
2:C:133:UNK:O	2:C:266:UNK:CA	2.55	0.54
2:C:229:UNK:CA	2:C:230:UNK:N	2.66	0.54
2:C:235:UNK:CA	2:C:235:UNK:O	2.37	0.54
2:C:148:UNK:C	2:C:150:UNK:N	2.64	0.54
1:A:245:UNK:N	1:A:245:UNK:C	2.64	0.54
1:B:177:UNK:CA	2:C:268:UNK:O	2.55	0.54
2:C:270:UNK:O	2:C:271:UNK:C	2.55	0.54
1:A:171:UNK:O	1:A:172:UNK:C	2.55	0.54
1:B:99:UNK:CA	1:B:257:UNK:O	2.55	0.54
1:A:226:UNK:O	1:A:227:UNK:C	2.55	0.54
1:B:110:UNK:N	1:B:110:UNK:C	2.60	0.53
1:A:190:UNK:O	1:A:191:UNK:O	2.27	0.53
1:B:190:UNK:O	1:B:191:UNK:O	2.27	0.53
1:A:193:UNK:O	1:A:198:UNK:N	2.41	0.53
1:A:111:UNK:N	1:A:243:UNK:O	2.41	0.53
1:B:132:UNK:N	1:B:267:UNK:O	2.41	0.53
2:C:201:UNK:O	2:C:201:UNK:CA	2.48	0.53
2:C:223:UNK:O	2:C:224:UNK:O	2.27	0.53
2:C:81:UNK:C	2:C:82:UNK:CA	2.79	0.53
1:B:270:UNK:O	1:B:271:UNK:C	2.55	0.52
2:C:192:UNK:O	2:C:196:UNK:N	2.41	0.52
1:B:201:UNK:CA	1:B:202:UNK:N	2.57	0.52
1:A:177:UNK:O	1:A:178:UNK:C	2.57	0.52
1:B:198:UNK:C	1:B:200:UNK:N	2.73	0.52
1:A:231:UNK:N	1:A:231:UNK:C	2.70	0.52
2:C:210:UNK:C	2:C:210:UNK:N	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:UNK:C	1:B:210:UNK:CA	2.77	0.51
2:C:235:UNK:N	2:C:235:UNK:C	2.73	0.51
1:B:162:UNK:C	1:B:163:UNK:CA	2.66	0.51
2:C:273:UNK:C	2:C:275:UNK:H2	2.13	0.51
2:C:142:UNK:O	2:C:258:UNK:N	2.44	0.51
2:C:213:UNK:O	2:C:214:UNK:O	2.29	0.50
1:A:116:UNK:O	1:A:117:UNK:C	2.60	0.50
2:C:233:UNK:C	2:C:233:UNK:N	2.60	0.50
2:C:232:UNK:C	2:C:234:UNK:N	2.75	0.50
1:B:206:UNK:C	1:B:206:UNK:N	2.64	0.50
2:C:175:UNK:O	2:C:175:UNK:CA	2.41	0.50
2:C:213:UNK:O	2:C:214:UNK:C	2.60	0.50
1:A:128:UNK:C	1:A:130:UNK:N	2.75	0.50
2:C:131:UNK:O	2:C:131:UNK:CA	2.48	0.49
1:B:274:UNK:N	1:B:275:UNK:N	2.60	0.49
1:B:131:UNK:N	1:B:131:UNK:C	2.73	0.49
1:B:226:UNK:O	1:B:227:UNK:C	2.60	0.49
2:C:126:UNK:N	2:C:126:UNK:C	2.66	0.49
1:A:123:UNK:O	1:A:124:UNK:C	2.60	0.49
1:A:273:UNK:C	1:A:274:UNK:C	2.91	0.49
2:C:106:UNK:N	2:C:248:UNK:CA	2.75	0.49
1:B:270:UNK:O	1:B:270:UNK:CA	2.46	0.49
1:B:177:UNK:C	1:B:178:UNK:C	2.91	0.49
1:B:128:UNK:O	1:B:131:UNK:N	2.46	0.49
1:A:171:UNK:O	1:A:174:UNK:N	2.46	0.49
2:C:224:UNK:C	2:C:225:UNK:C	2.91	0.49
1:A:227:UNK:O	1:A:228:UNK:C	2.60	0.49
2:C:132:UNK:N	2:C:267:UNK:O	2.46	0.49
1:B:162:UNK:C	1:B:163:UNK:C	2.91	0.49
1:B:125:UNK:N	1:B:125:UNK:C	2.64	0.49
1:B:186:UNK:O	1:B:188:UNK:N	2.46	0.49
2:C:232:UNK:C	2:C:233:UNK:C	2.91	0.48
2:C:233:UNK:O	2:C:236:UNK:N	2.46	0.48
1:A:271:UNK:C	1:A:271:UNK:N	2.64	0.48
1:A:191:UNK:O	1:A:192:UNK:C	2.48	0.48
2:C:162:UNK:C	2:C:164:UNK:N	2.77	0.48
2:C:180:UNK:CA	2:C:181:UNK:N	2.66	0.48
1:B:210:UNK:N	1:B:210:UNK:C	2.53	0.48
2:C:76:UNK:C	2:C:77:UNK:C	2.91	0.48
1:B:109:UNK:C	1:B:110:UNK:CA	2.75	0.47
1:A:162:UNK:C	1:A:163:UNK:C	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:UNK:C	1:B:167:UNK:C	2.93	0.47
1:A:270:UNK:C	1:A:271:UNK:C	2.93	0.47
1:A:245:UNK:O	1:A:245:UNK:CA	2.48	0.47
1:B:190:UNK:C	1:B:191:UNK:C	2.93	0.46
1:A:162:UNK:O	1:A:164:UNK:N	2.48	0.46
2:C:224:UNK:C	2:C:226:UNK:N	2.79	0.46
1:A:104:UNK:CA	1:A:252:UNK:CA	2.93	0.46
1:B:127:UNK:O	1:B:128:UNK:C	2.64	0.46
1:A:271:UNK:O	1:A:274:UNK:CA	2.64	0.46
1:B:233:UNK:C	1:B:235:UNK:N	2.66	0.45
1:A:118:UNK:O	1:A:119:UNK:C	2.64	0.45
2:C:233:UNK:N	2:C:234:UNK:N	2.64	0.45
2:C:192:UNK:O	2:C:193:UNK:C	2.64	0.45
2:C:273:UNK:N	2:C:274:UNK:N	2.64	0.45
1:A:129:UNK:O	1:A:271:UNK:CA	2.64	0.45
1:B:125:UNK:O	1:B:126:UNK:C	2.64	0.45
1:A:274:UNK:CA	1:A:275:UNK:N	2.66	0.45
1:A:162:UNK:O	1:A:163:UNK:C	2.64	0.45
1:A:138:UNK:O	1:A:261:UNK:CA	2.64	0.45
1:B:101:UNK:CA	1:B:102:UNK:H	2.27	0.44
1:A:216:UNK:C	1:A:217:UNK:C	2.91	0.44
1:A:212:UNK:C	1:A:213:UNK:CA	2.73	0.44
2:C:210:UNK:O	2:C:213:UNK:CA	2.66	0.44
1:B:129:UNK:C	1:B:131:UNK:N	2.73	0.44
2:C:269:UNK:O	2:C:270:UNK:C	2.66	0.44
2:C:195:UNK:O	2:C:196:UNK:C	2.66	0.44
1:A:174:UNK:C	1:A:176:UNK:N	2.81	0.43
1:A:184:UNK:C	1:A:185:UNK:O	2.64	0.43
1:B:195:UNK:O	1:B:196:UNK:C	2.66	0.43
2:C:77:UNK:C	2:C:77:UNK:N	2.64	0.43
1:B:163:UNK:N	1:B:164:UNK:N	2.66	0.43
1:A:191:UNK:CA	1:A:192:UNK:N	2.66	0.42
1:B:201:UNK:C	1:B:201:UNK:N	2.66	0.42
1:A:210:UNK:C	1:A:212:UNK:H	2.32	0.42
1:A:157:UNK:C	1:A:157:UNK:H	2.25	0.42
1:A:131:UNK:C	1:A:131:UNK:N	2.66	0.42
1:B:179:UNK:C	1:B:179:UNK:N	2.64	0.42
2:C:212:UNK:C	2:C:214:UNK:N	2.79	0.42
2:C:77:UNK:C	2:C:78:UNK:C	2.97	0.42
1:B:162:UNK:O	1:B:165:UNK:N	2.53	0.42
1:B:151:UNK:O	1:B:152:UNK:C	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:UNK:O	2:C:148:UNK:C	2.66	0.42
1:A:273:UNK:O	1:A:275:UNK:N	2.53	0.42
1:B:133:UNK:CA	1:B:134:UNK:N	2.66	0.42
1:B:164:UNK:O	1:B:165:UNK:C	2.66	0.42
2:C:114:UNK:O	2:C:116:UNK:N	2.53	0.42
1:A:173:UNK:C	1:A:174:UNK:C	2.91	0.41
1:A:194:UNK:N	1:A:195:UNK:N	2.66	0.41
1:B:192:UNK:O	1:B:195:UNK:N	2.53	0.41
1:A:210:UNK:C	1:A:212:UNK:N	2.83	0.41
1:A:157:UNK:N	1:A:157:UNK:O	2.53	0.40
1:B:229:UNK:C	1:B:229:UNK:N	2.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	0/186	-	-	-	-
1	B	0/186	-	-	-	-
2	C	0/210	-	-	-	-
All	All	0/582	-	-	-	-

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.