



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:59 am BST

PDB ID : 1JYL
Title : Catalytic Mechanism of CTP:phosphocholine Cytidylyltransferase from *Streptococcus pneumoniae* (LicC)
Authors : Kwak, B.-Y.; Yun, M.; Park, H.-w.
Deposited on : 2001-09-12
Resolution : 2.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

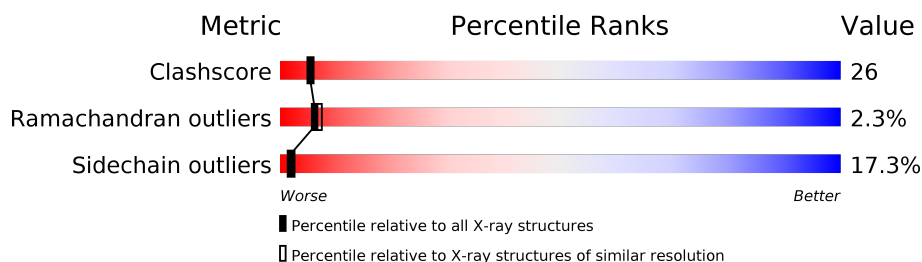
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	
1	B	254	
1	C	254	
1	D	254	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7904 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 CTP:phosphocholine Cytidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	1	0
			1905	1237	301	364	3			
1	B	228	Total	C	N	O	S	0	0	0
			1894	1231	297	363	3			
1	C	228	Total	C	N	O	S	0	1	0
			1905	1237	301	364	3			
1	D	228	Total	C	N	O	S	0	0	0
			1894	1231	297	363	3			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q97QE9
A	-18	GLY	-	EXPRESSION TAG	UNP Q97QE9
A	-17	SER	-	EXPRESSION TAG	UNP Q97QE9
A	-16	SER	-	EXPRESSION TAG	UNP Q97QE9
A	-15	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	-14	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	-13	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	-12	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	-11	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	-10	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	-9	SER	-	EXPRESSION TAG	UNP Q97QE9
A	-8	SER	-	EXPRESSION TAG	UNP Q97QE9
A	-7	GLY	-	EXPRESSION TAG	UNP Q97QE9
A	-6	LEU	-	EXPRESSION TAG	UNP Q97QE9
A	-5	VAL	-	EXPRESSION TAG	UNP Q97QE9
A	-4	PRO	-	EXPRESSION TAG	UNP Q97QE9
A	-3	ARG	-	EXPRESSION TAG	UNP Q97QE9
A	-2	GLY	-	EXPRESSION TAG	UNP Q97QE9
A	-1	SER	-	EXPRESSION TAG	UNP Q97QE9
A	0	HIS	-	EXPRESSION TAG	UNP Q97QE9
A	1	MET	-	EXPRESSION TAG	UNP Q97QE9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	-	EXPRESSION TAG	UNP Q97QE9
A	3	GLU	-	EXPRESSION TAG	UNP Q97QE9
A	4	ILE	-	EXPRESSION TAG	UNP Q97QE9
A	5	ARG	-	EXPRESSION TAG	UNP Q97QE9
A	6	VAL	-	EXPRESSION TAG	UNP Q97QE9
A	22	LEU	MET	CONFLICT	UNP Q97QE9
B	-19	MET	-	EXPRESSION TAG	UNP Q97QE9
B	-18	GLY	-	EXPRESSION TAG	UNP Q97QE9
B	-17	SER	-	EXPRESSION TAG	UNP Q97QE9
B	-16	SER	-	EXPRESSION TAG	UNP Q97QE9
B	-15	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	-14	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	-13	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	-12	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	-11	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	-10	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	-9	SER	-	EXPRESSION TAG	UNP Q97QE9
B	-8	SER	-	EXPRESSION TAG	UNP Q97QE9
B	-7	GLY	-	EXPRESSION TAG	UNP Q97QE9
B	-6	LEU	-	EXPRESSION TAG	UNP Q97QE9
B	-5	VAL	-	EXPRESSION TAG	UNP Q97QE9
B	-4	PRO	-	EXPRESSION TAG	UNP Q97QE9
B	-3	ARG	-	EXPRESSION TAG	UNP Q97QE9
B	-2	GLY	-	EXPRESSION TAG	UNP Q97QE9
B	-1	SER	-	EXPRESSION TAG	UNP Q97QE9
B	0	HIS	-	EXPRESSION TAG	UNP Q97QE9
B	1	MET	-	EXPRESSION TAG	UNP Q97QE9
B	2	LYS	-	EXPRESSION TAG	UNP Q97QE9
B	3	GLU	-	EXPRESSION TAG	UNP Q97QE9
B	4	ILE	-	EXPRESSION TAG	UNP Q97QE9
B	5	ARG	-	EXPRESSION TAG	UNP Q97QE9
B	6	VAL	-	EXPRESSION TAG	UNP Q97QE9
B	22	LEU	MET	CONFLICT	UNP Q97QE9
C	-19	MET	-	EXPRESSION TAG	UNP Q97QE9
C	-18	GLY	-	EXPRESSION TAG	UNP Q97QE9
C	-17	SER	-	EXPRESSION TAG	UNP Q97QE9
C	-16	SER	-	EXPRESSION TAG	UNP Q97QE9
C	-15	HIS	-	EXPRESSION TAG	UNP Q97QE9
C	-14	HIS	-	EXPRESSION TAG	UNP Q97QE9
C	-13	HIS	-	EXPRESSION TAG	UNP Q97QE9
C	-12	HIS	-	EXPRESSION TAG	UNP Q97QE9
C	-11	HIS	-	EXPRESSION TAG	UNP Q97QE9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	EXPRESSION TAG	UNP Q97QE9
C	-9	SER	-	EXPRESSION TAG	UNP Q97QE9
C	-8	SER	-	EXPRESSION TAG	UNP Q97QE9
C	-7	GLY	-	EXPRESSION TAG	UNP Q97QE9
C	-6	LEU	-	EXPRESSION TAG	UNP Q97QE9
C	-5	VAL	-	EXPRESSION TAG	UNP Q97QE9
C	-4	PRO	-	EXPRESSION TAG	UNP Q97QE9
C	-3	ARG	-	EXPRESSION TAG	UNP Q97QE9
C	-2	GLY	-	EXPRESSION TAG	UNP Q97QE9
C	-1	SER	-	EXPRESSION TAG	UNP Q97QE9
C	0	HIS	-	EXPRESSION TAG	UNP Q97QE9
C	1	MET	-	EXPRESSION TAG	UNP Q97QE9
C	2	LYS	-	EXPRESSION TAG	UNP Q97QE9
C	3	GLU	-	EXPRESSION TAG	UNP Q97QE9
C	4	ILE	-	EXPRESSION TAG	UNP Q97QE9
C	5	ARG	-	EXPRESSION TAG	UNP Q97QE9
C	6	VAL	-	EXPRESSION TAG	UNP Q97QE9
C	22	LEU	MET	CONFLICT	UNP Q97QE9
D	-19	MET	-	EXPRESSION TAG	UNP Q97QE9
D	-18	GLY	-	EXPRESSION TAG	UNP Q97QE9
D	-17	SER	-	EXPRESSION TAG	UNP Q97QE9
D	-16	SER	-	EXPRESSION TAG	UNP Q97QE9
D	-15	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	-14	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	-13	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	-12	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	-11	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	-10	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	-9	SER	-	EXPRESSION TAG	UNP Q97QE9
D	-8	SER	-	EXPRESSION TAG	UNP Q97QE9
D	-7	GLY	-	EXPRESSION TAG	UNP Q97QE9
D	-6	LEU	-	EXPRESSION TAG	UNP Q97QE9
D	-5	VAL	-	EXPRESSION TAG	UNP Q97QE9
D	-4	PRO	-	EXPRESSION TAG	UNP Q97QE9
D	-3	ARG	-	EXPRESSION TAG	UNP Q97QE9
D	-2	GLY	-	EXPRESSION TAG	UNP Q97QE9
D	-1	SER	-	EXPRESSION TAG	UNP Q97QE9
D	0	HIS	-	EXPRESSION TAG	UNP Q97QE9
D	1	MET	-	EXPRESSION TAG	UNP Q97QE9
D	2	LYS	-	EXPRESSION TAG	UNP Q97QE9
D	3	GLU	-	EXPRESSION TAG	UNP Q97QE9
D	4	ILE	-	EXPRESSION TAG	UNP Q97QE9

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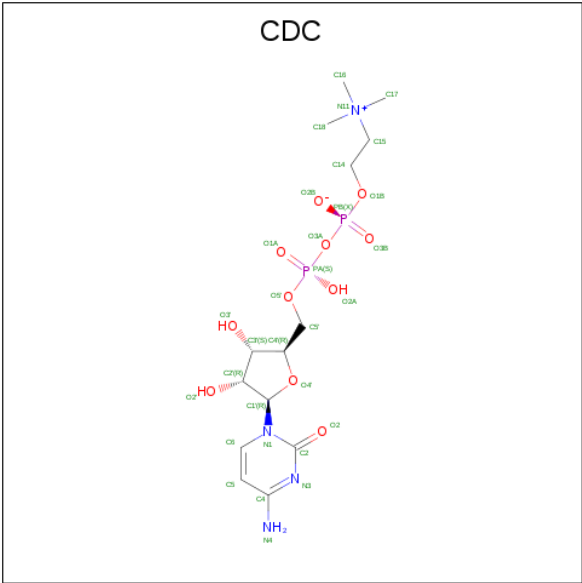
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Chain	Residue	Modelled	Actual	Comment	Reference
D	5	ARG	-	EXPRESSION TAG	UNP Q97QE9
D	6	VAL	-	EXPRESSION TAG	UNP Q97QE9
D	22	LEU	MET	CONFLICT	UNP Q97QE9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is [2-CYTIDYLATE-O'-PHOSPHONYLOXYL]-ETHYL-TRIMETHYL-AMMONIUM (three-letter code: CDC) (formula: C₁₄H₂₆N₄O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
3	B	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
3	C	1	Total	C	N	O	P	0	0
			31	14	4	11	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	14	4	11	2		

- Molecule 4 is water.

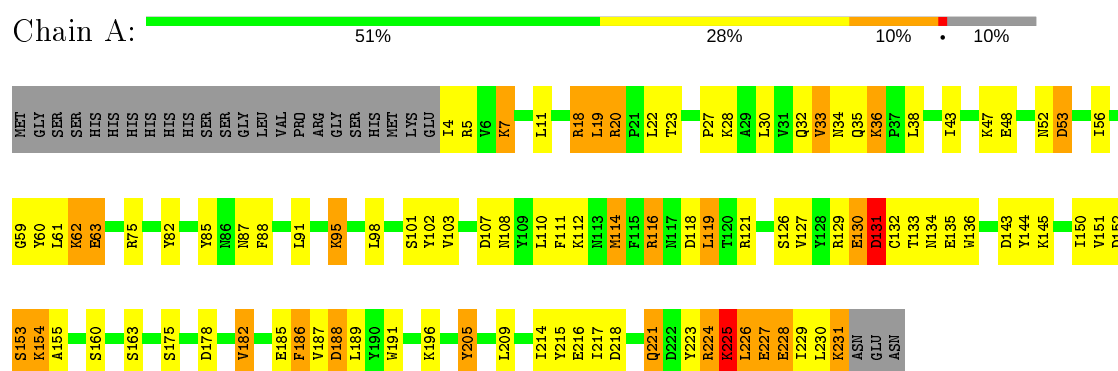
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	33	Total	O	0	0
			33	33		
4	C	50	Total	O	0	0
			50	50		
4	D	44	Total	O	0	0
			44	44		

3 Residue-property plots

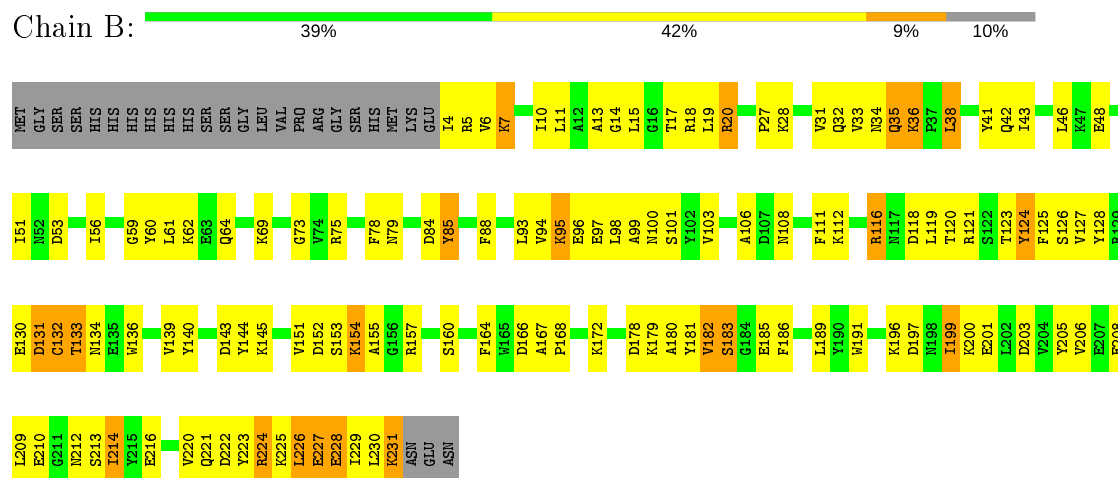
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

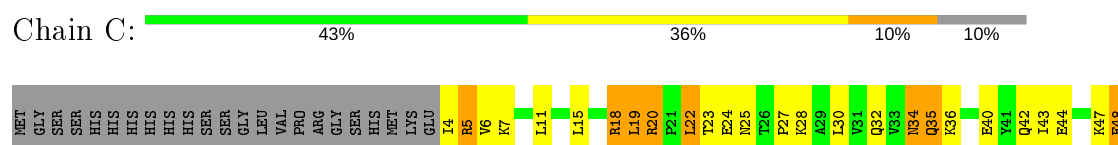
• Molecule 1: CTP:phosphocholine Cytidyltransferase

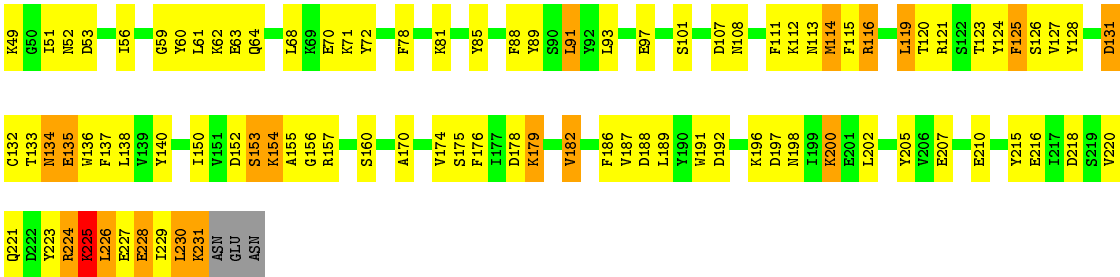


• Molecule 1: CTP:phosphocholine Cytidyltransferase

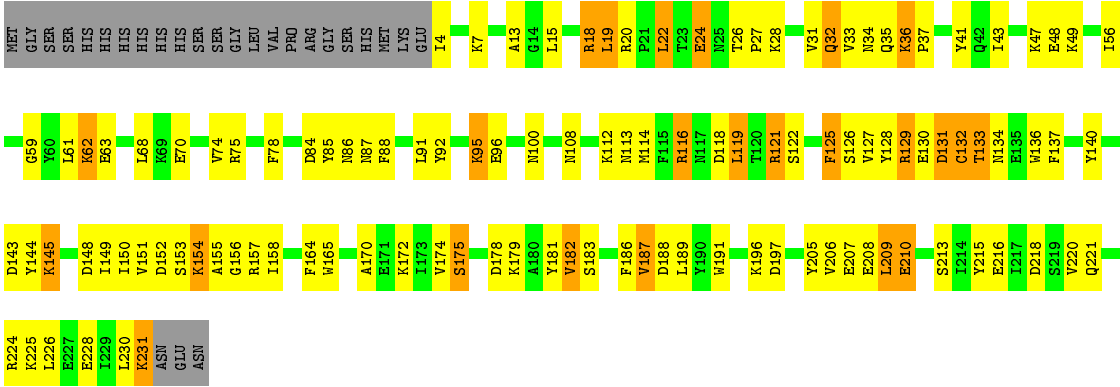


• Molecule 1: CTP:phosphocholine Cytidyltransferase





● Molecule 1: CTP:phosphocholine Cytidyltransferase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.20 Å 69.00 Å 81.60 Å 93.40° 92.80° 97.10°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	XTALVIEW	Depositor
R, R_{free}	0.208 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7904	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/1944	0.72	0/2631
1	B	0.50	0/1933	0.73	0/2616
1	C	0.48	0/1944	0.69	0/2631
1	D	0.47	0/1933	0.72	0/2616
All	All	0.49	0/7754	0.71	0/10494

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain

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	1905	0	1884	101	0
1	B	1894	0	1871	103	1
1	C	1905	0	1884	109	1
1	D	1894	0	1871	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	25	1	0
3	B	31	0	25	4	0
3	C	31	0	25	3	0
3	D	31	0	25	3	0
4	A	51	0	0	1	0
4	B	33	0	0	2	0
4	C	50	0	0	3	0
4	D	44	0	0	5	0
All	All	7904	0	7610	404	1

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 26.

All (404) 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:C:231:LYS:O	1:C:231:LYS:HG2	1.63	0.99
1:A:223:TYR:O	1:A:227:GLU:HG2	1.67	0.95
1:A:116:ARG:HG3	1:A:119:LEU:HD23	1.47	0.93
1:A:28:LYS:HD3	1:A:107:ASP:HB2	1.52	0.91
1:D:225:LYS:O	1:D:228:GLU:HG3	1.71	0.91
1:D:178:ASP:O	1:D:182:VAL:HG13	1.70	0.91
1:B:116:ARG:HG3	1:B:119:LEU:HD23	1.53	0.90
1:D:209:LEU:HD23	1:D:213:SER:CB	2.03	0.89
1:A:224:ARG:O	1:A:227:GLU:HB2	1.72	0.89
1:C:178:ASP:O	1:C:182:VAL:HG13	1.74	0.87
1:D:85:TYR:HD1	1:D:187:VAL:HG13	1.37	0.87
1:B:116:ARG:HG3	1:B:119:LEU:CD2	2.03	0.87
1:C:49:LYS:HD2	1:C:115:PHE:O	1.74	0.87
1:C:223:TYR:O	1:C:227:GLU:HG2	1.75	0.86
1:A:116:ARG:HB3	1:A:116:ARG:NH1	1.91	0.85
1:B:228:GLU:O	1:B:231:LYS:HB3	1.76	0.84
1:A:178:ASP:O	1:A:182:VAL:HG13	1.78	0.83
1:C:228:GLU:O	1:C:231:LYS:HB3	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:TYR:HD1	1:C:187:VAL:HG13	1.43	0.83
1:D:209:LEU:HD23	1:D:213:SER:HB2	1.58	0.83
1:A:228:GLU:O	1:A:231:LYS:HB3	1.78	0.82
1:A:85:TYR:HD1	1:A:187:VAL:HG13	1.46	0.80
1:D:157:ARG:CZ	1:D:208:GLU:HB3	2.12	0.80
1:A:28:LYS:HD3	1:A:107:ASP:CB	2.12	0.79
1:A:121:ARG:HD2	1:A:205:TYR:CD1	2.17	0.79
1:B:178:ASP:O	1:B:182:VAL:HG13	1.80	0.79
1:D:231:LYS:O	1:D:231:LYS:HG2	1.82	0.77
1:A:127:VAL:HG22	1:A:160:SER:OG	1.85	0.77
1:A:116:ARG:HG3	1:A:119:LEU:CD2	2.13	0.76
1:A:88:PHE:HB2	1:A:189:LEU:O	1.84	0.76
1:D:132:CYS:HA	1:D:154:LYS:O	1.87	0.75
1:D:24:GLU:HA	1:D:24:GLU:OE1	1.85	0.74
1:C:116:ARG:HB3	1:C:116:ARG:CZ	2.17	0.74
1:D:228:GLU:O	1:D:231:LYS:HB3	1.88	0.74
1:C:62:LYS:HD3	1:C:78:PHE:CD2	2.23	0.73
1:B:132:CYS:HA	1:B:154:LYS:O	1.89	0.73
1:C:114:MET:CE	1:C:114:MET:H	2.03	0.72
1:D:27:PRO:HG3	1:D:61:LEU:HB2	1.70	0.72
1:A:225:LYS:O	1:A:227:GLU:N	2.24	0.71
1:D:151:VAL:HG23	1:D:196:LYS:HE3	1.72	0.71
1:D:209:LEU:HD23	1:D:213:SER:OG	1.90	0.71
1:C:15:LEU:HD23	1:C:60:TYR:CD2	2.27	0.70
1:D:129:ARG:HH11	1:D:158:ILE:HD11	1.56	0.70
1:C:85:TYR:CD1	1:C:187:VAL:HG13	2.26	0.70
1:A:62:LYS:HG3	1:A:63:GLU:N	2.07	0.69
1:B:108:ASN:HD22	1:B:216:GLU:HA	1.58	0.69
1:C:34:ASN:C	1:C:35:GLN:HG2	2.13	0.69
1:B:19:LEU:HD12	1:B:28:LYS:CD	2.22	0.69
1:A:221:GLN:OE1	1:A:221:GLN:HA	1.92	0.68
1:A:108:ASN:HD21	1:A:216:GLU:HB2	1.57	0.68
1:B:231:LYS:HG2	1:B:231:LYS:O	1.94	0.68
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.59	0.67
1:C:7:LYS:HE2	1:C:97:GLU:O	1.93	0.67
1:D:209:LEU:CD2	1:D:213:SER:HB2	2.24	0.67
1:A:131:ASP:OD2	1:A:132:CYS:N	2.28	0.67
1:C:116:ARG:HG3	1:C:119:LEU:HD23	1.77	0.66
1:D:85:TYR:CD1	1:D:187:VAL:HG13	2.27	0.66
1:B:134:ASN:HA	1:B:152:ASP:O	1.96	0.65
1:A:28:LYS:HE2	1:A:217:ILE:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LEU:CD1	1:B:214:ILE:HD11	2.26	0.65
1:D:4:ILE:HG22	1:D:4:ILE:O	1.96	0.65
1:B:42:GLN:O	1:B:46:LEU:HD12	1.97	0.64
1:C:114:MET:H	1:C:114:MET:HE3	1.61	0.64
1:A:18:ARG:HG2	1:A:218:ASP:O	1.97	0.64
1:B:151:VAL:HG23	1:B:196:LYS:HE3	1.78	0.64
1:A:134:ASN:HA	1:A:153:SER:HA	1.77	0.64
1:D:128:TYR:CE2	1:D:156:GLY:HA2	2.33	0.63
1:A:231:LYS:O	1:A:231:LYS:HG2	1.98	0.63
1:B:88:PHE:HB2	1:B:189:LEU:O	1.99	0.63
1:A:110:LEU:CD2	1:A:214:ILE:HG12	2.29	0.63
1:B:10:ILE:CG2	1:B:106:ALA:HB2	2.29	0.63
1:B:209:LEU:HD11	1:B:214:ILE:HD11	1.79	0.63
1:C:121:ARG:HD2	1:C:205:TYR:CD1	2.34	0.63
1:A:53:ASP:HB2	4:A:5084:HOH:O	1.99	0.62
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.64	0.62
1:B:32:GLN:NE2	1:B:35:GLN:HA	2.15	0.62
1:C:111:PHE:HE2	1:C:215:TYR:HB2	1.64	0.62
1:D:70:GLU:HB2	4:D:5143:HOH:O	1.99	0.62
1:C:228:GLU:O	1:C:231:LYS:N	2.28	0.62
1:A:111:PHE:HE2	1:A:215:TYR:HB2	1.64	0.61
1:A:4:ILE:O	1:A:4:ILE:HG22	1.99	0.61
1:A:18:ARG:HG3	1:A:18:ARG:O	1.99	0.61
1:B:225:LYS:O	1:B:228:GLU:OE2	2.18	0.61
1:B:136:TRP:NE1	3:B:2991:CDC:H181	2.15	0.61
1:A:151:VAL:HG23	1:A:196:LYS:HE3	1.81	0.61
1:C:116:ARG:HG3	1:C:119:LEU:CD2	2.30	0.61
1:A:221:GLN:O	1:A:224:ARG:HB2	2.00	0.61
1:B:131:ASP:O	1:B:155:ALA:HB2	2.01	0.61
1:B:180:ALA:O	1:B:183:SER:HB2	2.00	0.61
1:B:32:GLN:HE21	1:B:35:GLN:HA	1.66	0.61
1:D:157:ARG:NH2	1:D:208:GLU:HB3	2.14	0.61
1:A:88:PHE:CB	1:A:189:LEU:O	2.48	0.61
1:C:18:ARG:HG2	1:C:18:ARG:HH11	1.66	0.61
1:B:62:LYS:HD3	1:B:78:PHE:CD2	2.35	0.60
1:C:127:VAL:HG22	1:C:160:SER:OG	2.00	0.60
1:C:176:PHE:HE1	1:C:202:LEU:HD21	1.67	0.60
1:D:131:ASP:CG	1:D:132:CYS:N	2.53	0.60
1:D:175:SER:O	1:D:179:LYS:HG3	2.01	0.60
1:D:92:TYR:O	1:D:95:LYS:HB3	2.00	0.60
1:A:228:GLU:OE2	1:A:229:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:ND2	1:A:216:GLU:HB2	2.16	0.60
1:C:221:GLN:NE2	1:D:84:ASP:OD1	2.34	0.60
1:D:231:LYS:CG	1:D:231:LYS:O	2.50	0.60
1:A:134:ASN:C	1:A:135:GLU:HG2	2.21	0.59
1:A:19:LEU:HB3	1:A:23:THR:HG23	1.83	0.59
1:C:11:LEU:HD21	1:C:91:LEU:HD12	1.85	0.59
1:D:126:SER:OG	1:D:157:ARG:HB3	2.03	0.59
1:A:18:ARG:NH1	1:A:18:ARG:HG2	2.18	0.59
1:C:61:LEU:HD13	1:C:64:GLN:NE2	2.18	0.59
1:C:6:VAL:HG12	1:C:51:ILE:HG12	1.85	0.59
1:C:174:VAL:HG12	1:C:174:VAL:O	2.02	0.58
1:C:25:ASN:HD22	1:D:134:ASN:HD22	1.50	0.58
1:A:95:LYS:NZ	1:A:178:ASP:OD2	2.35	0.58
1:C:207:GLU:HG3	1:C:207:GLU:O	2.03	0.58
1:C:18:ARG:HB3	1:C:218:ASP:O	2.04	0.58
1:D:34:ASN:OD1	1:D:230:LEU:HD13	2.03	0.58
1:A:116:ARG:HH11	1:A:116:ARG:HB3	1.66	0.57
1:C:136:TRP:CZ3	1:C:196:LYS:HD3	2.39	0.57
1:D:210:GLU:HG3	4:D:5150:HOH:O	2.04	0.57
1:B:19:LEU:HD12	1:B:28:LYS:HD2	1.85	0.57
1:A:85:TYR:CD1	1:A:187:VAL:HG13	2.34	0.57
1:C:224:ARG:O	1:C:227:GLU:HB2	2.05	0.57
1:B:15:LEU:HD23	1:B:60:TYR:CD2	2.40	0.57
1:B:225:LYS:O	1:B:227:GLU:N	2.38	0.56
1:C:4:ILE:O	1:C:4:ILE:HG22	2.05	0.56
1:A:131:ASP:CG	1:A:132:CYS:N	2.59	0.56
1:D:136:TRP:NE1	3:D:4991:CDC:H181	2.20	0.56
1:A:63:GLU:CD	1:A:63:GLU:H	2.09	0.56
1:A:134:ASN:O	1:A:135:GLU:HG2	2.05	0.56
1:B:196:LYS:O	1:B:196:LYS:HG3	2.03	0.56
1:B:228:GLU:OE2	1:B:229:ILE:N	2.39	0.56
1:D:18:ARG:NH1	4:D:5161:HOH:O	2.36	0.56
1:A:133:THR:O	1:A:153:SER:HA	2.06	0.56
1:A:110:LEU:HD23	1:A:214:ILE:HG12	1.87	0.56
1:D:129:ARG:HH11	1:D:158:ILE:CD1	2.17	0.56
1:D:62:LYS:HG2	1:D:63:GLU:N	2.21	0.56
1:C:108:ASN:HD22	1:C:216:GLU:HA	1.70	0.56
1:A:150:ILE:HD11	1:A:154:LYS:NZ	2.21	0.56
1:C:125:PHE:N	1:C:125:PHE:CD2	2.73	0.55
1:D:131:ASP:O	1:D:155:ALA:HB2	2.06	0.55
1:C:137:PHE:HE2	1:C:152:ASP:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD22	1:A:114:MET:HE1	1.88	0.55
1:A:151:VAL:CG2	1:A:196:LYS:HE3	2.37	0.55
1:D:26:THR:HG22	1:D:27:PRO:O	2.06	0.55
1:C:34:ASN:O	1:C:35:GLN:HG2	2.06	0.55
1:A:103:VAL:HG11	1:A:191:TRP:CZ2	2.42	0.55
1:C:49:LYS:HG3	1:C:113:ASN:HD21	1.72	0.55
1:A:116:ARG:CZ	1:A:116:ARG:HB3	2.37	0.54
1:C:126:SER:HB2	1:C:138:LEU:CD1	2.36	0.54
1:B:145:LYS:HD3	1:B:205:TYR:CZ	2.42	0.54
1:B:85:TYR:N	1:B:85:TYR:CD1	2.75	0.54
1:A:32:GLN:HB2	1:A:36:LYS:H	1.72	0.54
1:A:143:ASP:O	1:A:144:TYR:HB2	2.07	0.54
1:B:4:ILE:O	1:B:4:ILE:HG22	2.07	0.54
1:D:136:TRP:CE2	3:D:4991:CDC:H181	2.43	0.54
1:A:188:ASP:N	1:A:188:ASP:OD2	2.41	0.54
1:C:32:GLN:HE21	1:C:35:GLN:HA	1.73	0.54
1:B:116:ARG:NH1	1:B:118:ASP:OD1	2.41	0.53
1:B:225:LYS:O	1:B:226:LEU:C	2.46	0.53
1:A:231:LYS:O	1:A:231:LYS:CG	2.56	0.53
1:C:89:TYR:CE2	1:C:93:LEU:HD21	2.43	0.53
1:B:18:ARG:HG2	1:B:18:ARG:NH1	2.22	0.53
1:B:199:ILE:O	1:B:199:ILE:HD12	2.08	0.53
1:A:230:LEU:O	1:A:231:LYS:C	2.47	0.53
1:C:114:MET:HG3	1:C:125:PHE:HD1	1.74	0.53
1:C:134:ASN:C	1:C:135:GLU:HG2	2.29	0.53
1:C:32:GLN:NE2	1:C:35:GLN:HA	2.24	0.53
1:A:19:LEU:HB3	1:A:23:THR:CG2	2.39	0.53
1:B:136:TRP:CE2	3:B:2991:CDC:H181	2.44	0.53
1:B:27:PRO:HD3	1:B:64:GLN:OE1	2.09	0.53
1:B:186:PHE:HA	1:B:189:LEU:HG	1.89	0.52
1:B:88:PHE:CB	1:B:189:LEU:O	2.57	0.52
1:C:231:LYS:CG	1:C:231:LYS:O	2.48	0.52
1:A:114:MET:HG2	1:A:114:MET:O	2.08	0.52
1:A:103:VAL:HG11	1:A:191:TRP:CE2	2.45	0.52
1:B:28:LYS:HA	1:B:31:VAL:HG23	1.91	0.52
1:B:84:ASP:C	1:B:85:TYR:HD1	2.12	0.52
1:C:114:MET:HG3	1:C:125:PHE:CD1	2.44	0.52
1:B:231:LYS:O	1:B:231:LYS:CG	2.56	0.52
1:C:133:THR:HG22	1:C:134:ASN:H	1.73	0.52
1:B:225:LYS:O	1:B:228:GLU:N	2.42	0.52
1:C:27:PRO:HG2	1:C:30:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:HG22	1:A:134:ASN:H	1.75	0.52
1:B:7:LYS:HB3	1:B:53:ASP:HB3	1.91	0.52
1:C:131:ASP:OD2	1:C:132:CYS:N	2.43	0.52
1:B:181:TYR:HA	1:B:186:PHE:CD1	2.45	0.52
1:C:198:ASN:ND2	4:C:5132:HOH:O	2.39	0.52
1:B:7:LYS:CB	1:B:53:ASP:HB3	2.39	0.52
1:C:230:LEU:O	1:C:231:LYS:C	2.48	0.52
1:D:226:LEU:O	1:D:230:LEU:HG	2.10	0.52
1:A:225:LYS:O	1:A:226:LEU:C	2.49	0.51
1:C:18:ARG:HG2	1:C:18:ARG:NH1	2.26	0.51
1:D:129:ARG:HG2	1:D:131:ASP:OD2	2.11	0.51
1:A:20[B]:ARG:NH2	1:A:60:TYR:OH	2.44	0.51
1:B:224:ARG:O	1:B:227:GLU:HB2	2.10	0.51
1:B:127:VAL:HG22	1:B:160:SER:OG	2.11	0.51
1:B:7:LYS:HB2	1:B:53:ASP:O	2.11	0.50
1:D:108:ASN:OD1	1:D:216:GLU:HA	2.11	0.50
1:A:150:ILE:HD11	1:A:154:LYS:HZ3	1.76	0.50
1:B:103:VAL:HG11	1:B:191:TRP:CZ2	2.46	0.50
1:C:71:LYS:HD3	1:C:72:TYR:CE1	2.46	0.50
1:D:36:LYS:HG2	1:D:37:PRO:HD2	1.93	0.50
1:B:196:LYS:HG2	1:B:197:ASP:OD2	2.11	0.50
1:C:132:CYS:HA	1:C:154:LYS:O	2.12	0.50
1:B:140:TYR:OH	1:B:157:ARG:HG3	2.11	0.50
1:B:166:ASP:OD1	1:B:168:PRO:HG2	2.12	0.50
1:D:134:ASN:HA	1:D:152:ASP:O	2.11	0.50
1:A:126:SER:O	1:A:209:LEU:HB2	2.12	0.50
1:C:228:GLU:OE2	1:C:229:ILE:HG13	2.11	0.50
1:A:225:LYS:O	1:A:228:GLU:N	2.45	0.50
1:A:43:ILE:HD11	1:A:56:ILE:HD11	1.93	0.50
1:C:5:ARG:NH1	1:C:5:ARG:HB2	2.26	0.50
1:C:114:MET:HE3	1:C:114:MET:N	2.25	0.49
1:B:126:SER:OG	1:B:157:ARG:HB3	2.13	0.49
1:A:4:ILE:CG2	1:A:4:ILE:O	2.61	0.49
1:C:6:VAL:CG1	1:C:51:ILE:HG12	2.43	0.49
1:D:145:LYS:HB2	1:D:205:TYR:CE2	2.47	0.49
1:D:18:ARG:HB3	1:D:218:ASP:O	2.13	0.49
1:B:103:VAL:HG11	1:B:191:TRP:CE2	2.48	0.49
1:C:128:TYR:CE1	1:C:156:GLY:HA2	2.48	0.49
1:B:154:LYS:CG	1:B:155:ALA:N	2.72	0.49
1:C:91:LEU:HD22	1:C:191:TRP:CE3	2.47	0.49
1:D:28:LYS:HA	1:D:31:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ILE:O	1:D:4:ILE:CG2	2.59	0.49
1:C:114:MET:H	1:C:114:MET:HE2	1.77	0.48
1:A:132:CYS:SG	1:A:154:LYS:HA	2.52	0.48
1:C:196:LYS:HG2	1:C:197:ASP:OD2	2.13	0.48
1:B:133:THR:O	1:B:153:SER:HA	2.14	0.48
1:B:223:TYR:O	1:B:227:GLU:HG2	2.12	0.48
1:C:125:PHE:HD2	1:C:125:PHE:N	2.10	0.48
1:B:36:LYS:HD2	1:B:41:TYR:CE1	2.48	0.48
1:C:140:TYR:OH	1:C:157:ARG:HG3	2.12	0.48
1:C:225:LYS:O	1:C:226:LEU:C	2.51	0.48
1:C:136:TRP:CG	3:C:3991:CDC:H171	2.48	0.48
1:D:230:LEU:O	1:D:231:LYS:C	2.52	0.48
1:B:167:ALA:HB3	1:B:168:PRO:HD3	1.95	0.48
1:A:27:PRO:HG2	1:A:30:LEU:HD12	1.96	0.48
1:B:27:PRO:HG3	1:B:61:LEU:HB2	1.96	0.48
1:C:154:LYS:HE3	4:C:5018:HOH:O	2.12	0.48
1:C:116:ARG:HB3	1:C:116:ARG:NH1	2.29	0.48
1:A:130:GLU:OE2	1:D:154:LYS:HD2	2.14	0.48
1:C:24:GLU:HA	1:C:24:GLU:OE1	2.13	0.47
1:B:121:ARG:HD2	1:B:205:TYR:CD1	2.49	0.47
1:B:62:LYS:HD3	1:B:78:PHE:CE2	2.48	0.47
1:C:49:LYS:HG3	1:C:113:ASN:ND2	2.29	0.47
1:A:108:ASN:HD22	1:A:216:GLU:HA	1.80	0.47
1:B:222:ASP:OD2	1:B:222:ASP:N	2.47	0.47
3:B:2991:CDC:H183	3:B:2991:CDC:H141	1.72	0.47
1:B:79:ASN:HA	1:B:93:LEU:HD11	1.96	0.47
1:A:91:LEU:HD22	1:A:191:TRP:CE3	2.49	0.47
1:A:134:ASN:HA	1:A:152:ASP:O	2.14	0.47
1:B:43:ILE:HD11	1:B:56:ILE:HD11	1.95	0.47
1:C:81:LYS:HB3	1:C:85:TYR:CD2	2.49	0.47
1:D:18:ARG:NH2	4:D:5113:HOH:O	2.46	0.47
1:C:137:PHE:HB2	1:C:150:ILE:CD1	2.45	0.47
1:C:228:GLU:C	1:C:231:LYS:H	2.17	0.47
1:D:152:ASP:OD1	1:D:153:SER:N	2.45	0.47
1:D:88:PHE:HB2	1:D:189:LEU:O	2.14	0.47
1:D:151:VAL:CG2	1:D:196:LYS:HE3	2.43	0.47
1:A:116:ARG:NH2	1:A:118:ASP:OD2	2.48	0.47
1:C:200:LYS:HB2	4:C:5134:HOH:O	2.15	0.47
1:C:170:ALA:O	1:C:174:VAL:HG23	2.15	0.47
1:C:225:LYS:O	1:C:227:GLU:N	2.48	0.47
1:A:60:TYR:HB2	1:A:82:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:HG2	1:D:197:ASP:OD1	2.16	0.46
1:A:20[B]:ARG:NH2	1:A:60:TYR:CZ	2.83	0.46
1:A:225:LYS:C	1:A:227:GLU:N	2.69	0.46
1:B:220:VAL:HG12	1:B:220:VAL:O	2.16	0.46
1:B:228:GLU:OE2	1:B:229:ILE:HG13	2.16	0.46
1:D:122:SER:HA	1:D:164:PHE:O	2.15	0.46
1:A:33:VAL:O	1:A:34:ASN:HB2	2.15	0.46
1:D:121:ARG:HD2	1:D:205:TYR:CD1	2.50	0.46
1:D:129:ARG:NH1	1:D:158:ILE:HD11	2.29	0.46
1:D:140:TYR:CD2	1:D:206:VAL:HG21	2.50	0.46
1:B:4:ILE:O	1:B:4:ILE:CG2	2.64	0.46
1:D:137:PHE:O	1:D:149:ILE:HA	2.16	0.46
1:C:19:LEU:HB3	1:C:23:THR:HG23	1.98	0.45
1:C:27:PRO:HG3	1:C:61:LEU:HB2	1.98	0.45
1:C:81:LYS:HG3	1:C:85:TYR:HE2	1.80	0.45
1:D:125:PHE:N	1:D:125:PHE:CD2	2.83	0.45
1:D:62:LYS:CD	1:D:78:PHE:CE2	2.99	0.45
1:A:20[B]:ARG:NH2	1:A:23:THR:O	2.44	0.45
1:C:131:ASP:O	1:C:155:ALA:HB2	2.16	0.45
1:C:20[B]:ARG:HD2	1:C:24:GLU:OE1	2.15	0.45
1:A:28:LYS:HD3	1:A:107:ASP:HB3	1.95	0.45
1:B:84:ASP:HB3	1:B:85:TYR:CE1	2.52	0.45
1:A:225:LYS:HE2	1:A:225:LYS:HB3	1.43	0.45
1:B:6:VAL:HG12	1:B:51:ILE:HG12	1.98	0.45
1:B:84:ASP:C	1:B:85:TYR:CD1	2.89	0.45
1:B:116:ARG:HG3	1:B:119:LEU:HD21	1.92	0.45
1:B:99:ALA:HB1	1:B:167:ALA:HA	1.98	0.45
1:C:174:VAL:CG1	1:C:174:VAL:O	2.65	0.45
1:C:179:LYS:HE2	1:C:179:LYS:HB3	1.70	0.45
1:D:131:ASP:CG	1:D:132:CYS:H	2.17	0.45
1:C:133:THR:O	1:C:153:SER:HA	2.17	0.45
1:D:91:LEU:HD22	1:D:191:TRP:CE3	2.51	0.45
1:C:28:LYS:HE3	1:C:107:ASP:HB3	1.98	0.45
1:C:4:ILE:CG2	1:C:4:ILE:O	2.64	0.45
1:D:206:VAL:HG12	1:D:207:GLU:N	2.32	0.45
1:B:182:VAL:HG11	4:B:5106:HOH:O	2.16	0.45
1:B:94:VAL:O	1:B:96:GLU:N	2.50	0.45
1:C:126:SER:OG	1:C:157:ARG:HB3	2.17	0.44
1:A:136:TRP:CG	3:A:1991:CDL:H171	2.52	0.44
1:A:32:GLN:OE1	1:A:35:GLN:HA	2.17	0.44
1:B:36:LYS:HB3	1:B:41:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LYS:CG	1:D:113:ASN:HD21	2.30	0.44
1:A:186:PHE:HA	1:A:189:LEU:HG	1.98	0.44
1:B:100:ASN:HA	1:B:164:PHE:CZ	2.53	0.44
1:D:92:TYR:CE1	1:D:95:LYS:HE2	2.52	0.44
1:A:18:ARG:CG	1:A:218:ASP:O	2.64	0.44
1:B:182:VAL:CG1	4:B:5106:HOH:O	2.64	0.44
1:B:59:GLY:O	1:B:60:TYR:C	2.56	0.44
1:A:102:TYR:HA	1:A:163:SER:O	2.18	0.44
1:C:19:LEU:HA	1:C:19:LEU:HD23	1.69	0.44
1:C:136:TRP:CE2	3:C:3991:CDC:H181	2.53	0.44
1:D:153:SER:O	1:D:154:LYS:HB3	2.18	0.44
1:D:62:LYS:HD3	1:D:78:PHE:CE2	2.53	0.44
1:D:62:LYS:HD2	1:D:78:PHE:CD2	2.53	0.44
1:C:5:ARG:CB	1:C:5:ARG:CZ	2.96	0.44
1:B:10:ILE:HG22	1:B:106:ALA:HB2	1.98	0.43
1:C:48:GLU:OE2	1:C:113:ASN:ND2	2.33	0.43
1:B:125:PHE:CD2	1:B:125:PHE:N	2.84	0.43
1:D:116:ARG:HD2	4:D:5057:HOH:O	2.17	0.43
1:D:88:PHE:CB	1:D:189:LEU:O	2.66	0.43
1:A:59:GLY:O	1:A:62:LYS:HB3	2.18	0.43
1:A:27:PRO:HD2	1:A:30:LEU:HB2	2.00	0.43
1:C:40:GLU:O	1:C:44:GLU:HG3	2.18	0.43
1:D:68:LEU:O	1:D:74:VAL:HG22	2.18	0.43
1:A:150:ILE:HD12	1:A:150:ILE:O	2.18	0.43
1:C:24:GLU:O	1:D:134:ASN:ND2	2.52	0.43
1:D:118:ASP:O	1:D:119:LEU:C	2.57	0.43
1:D:170:ALA:O	1:D:174:VAL:HG23	2.18	0.43
1:D:114:MET:HG2	1:D:125:PHE:CD1	2.54	0.43
1:B:225:LYS:C	1:B:227:GLU:N	2.73	0.42
1:C:179:LYS:O	1:C:182:VAL:HG22	2.19	0.42
1:C:62:LYS:HG3	1:C:63:GLU:N	2.34	0.42
1:D:13:ALA:HB3	3:D:4991:CDC:N3	2.34	0.42
1:B:94:VAL:C	1:B:96:GLU:H	2.23	0.42
1:D:207:GLU:HG3	1:D:207:GLU:O	2.18	0.42
1:D:62:LYS:HD3	1:D:78:PHE:HE2	1.84	0.42
1:B:123:THR:HG22	1:B:124:TYR:N	2.35	0.42
1:B:154:LYS:HG2	1:B:155:ALA:N	2.35	0.42
1:B:157:ARG:NH2	1:B:208:GLU:HB3	2.34	0.42
1:A:116:ARG:CZ	1:A:116:ARG:CB	2.97	0.42
1:C:7:LYS:O	1:C:101:SER:HA	2.19	0.42
1:D:220:VAL:O	1:D:224:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ILE:HD11	1:D:56:ILE:HD11	2.02	0.42
1:A:110:LEU:HD22	1:A:114:MET:CE	2.49	0.42
1:A:154:LYS:HG3	1:A:155:ALA:O	2.19	0.42
1:A:47:LYS:HE3	1:A:52:ASN:OD1	2.19	0.42
1:B:69:LYS:O	1:B:73:GLY:HA2	2.20	0.42
1:D:86:ASN:O	1:D:88:PHE:N	2.53	0.42
1:C:88:PHE:HB2	1:C:189:LEU:O	2.20	0.42
1:D:32:GLN:HB3	1:D:36:LYS:C	2.40	0.42
1:A:7:LYS:O	1:A:101:SER:HB2	2.20	0.42
1:A:27:PRO:HG3	1:A:61:LEU:HB2	2.02	0.41
1:B:230:LEU:O	1:B:231:LYS:C	2.57	0.41
1:C:15:LEU:O	1:C:20[B]:ARG:NH2	2.49	0.41
1:D:19:LEU:O	1:D:22:LEU:HB2	2.21	0.41
1:D:43:ILE:O	1:D:47:LYS:HG3	2.21	0.41
1:B:139:VAL:HG12	1:B:139:VAL:O	2.20	0.41
1:B:145:LYS:HD3	1:B:205:TYR:CE2	2.55	0.41
1:B:228:GLU:O	1:B:231:LYS:N	2.49	0.41
1:C:22:LEU:HD23	1:C:22:LEU:HA	1.91	0.41
1:A:114:MET:N	1:A:114:MET:SD	2.94	0.41
1:C:128:TYR:HE1	1:C:156:GLY:HA2	1.85	0.41
1:C:228:GLU:O	1:C:231:LYS:CB	2.58	0.41
1:A:215:TYR:C	1:A:215:TYR:CD2	2.94	0.41
1:A:91:LEU:HD22	1:A:191:TRP:CD2	2.56	0.41
1:B:17:THR:HA	1:B:20:ARG:HD3	2.02	0.41
1:B:140:TYR:CD2	1:B:206:VAL:HG21	2.56	0.41
1:D:100:ASN:N	1:D:165:TRP:O	2.54	0.41
1:C:68:LEU:HA	1:C:68:LEU:HD23	1.89	0.41
1:D:215:TYR:OH	1:D:225:LYS:HB2	2.21	0.41
1:D:228:GLU:O	1:D:231:LYS:N	2.46	0.41
1:D:28:LYS:O	1:D:31:VAL:HG23	2.21	0.41
1:A:98:LEU:HA	1:A:98:LEU:HD12	1.92	0.41
1:B:111:PHE:CD2	1:B:212:ASN:HB3	2.56	0.41
1:B:131:ASP:HB3	1:B:132:CYS:H	1.59	0.41
1:D:143:ASP:O	1:D:144:TYR:HB2	2.21	0.41
1:A:154:LYS:CG	1:A:155:ALA:N	2.83	0.41
1:C:123:THR:HG22	1:C:124:TYR:N	2.36	0.41
1:C:43:ILE:HD11	1:C:56:ILE:HD11	2.03	0.41
1:A:111:PHE:CE1	1:A:230:LEU:HD21	2.55	0.41
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.94	0.41
1:C:150:ILE:HD12	1:C:150:ILE:O	2.21	0.41
1:D:125:PHE:N	1:D:125:PHE:HD2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:OG1	1:D:134:ASN:N	2.54	0.41
1:A:108:ASN:ND2	1:A:216:GLU:HA	2.36	0.40
1:B:7:LYS:O	1:B:101:SER:HA	2.21	0.40
1:C:228:GLU:OE2	1:C:229:ILE:N	2.54	0.40
1:B:143:ASP:O	1:B:144:TYR:HB2	2.21	0.40
1:B:145:LYS:HE2	1:B:203:ASP:OD2	2.21	0.40
1:C:42:GLN:HG3	1:C:42:GLN:H	1.73	0.40
1:C:47:LYS:HE3	1:C:52:ASN:ND2	2.37	0.40
1:C:7:LYS:HG3	1:C:101:SER:HB2	2.03	0.40
1:D:62:LYS:HD2	1:D:78:PHE:CE2	2.56	0.40
1:B:13:ALA:HB3	3:B:2991:CDC:N3	2.37	0.40
1:D:36:LYS:HD2	1:D:41:TYR:CZ	2.56	0.40
1:A:145:LYS:HA	1:A:205:TYR:CD2	2.56	0.40
1:B:108:ASN:ND2	1:B:216:GLU:HB2	2.37	0.40
1:B:33:VAL:O	1:B:34:ASN:HB2	2.21	0.40
3:C:3991:CDC:H183	3:C:3991:CDC:H141	1.79	0.40
1:D:181:TYR:HA	1:D:186:PHE:CD1	2.57	0.40

All (1) 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)
1:B:128:TYR:OH	1:C:128:TYR:OH[1_554]	2.12	0.08

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	227/254 (89%)	200 (88%)	21 (9%)	6 (3%)	5	5
1	B	226/254 (89%)	201 (89%)	21 (9%)	4 (2%)	8	10
1	C	227/254 (89%)	199 (88%)	22 (10%)	6 (3%)	5	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	226/254 (89%)	206 (91%)	15 (7%)	5 (2%)	6	7
All	All	906/1016 (89%)	806 (89%)	79 (9%)	21 (2%)	6	7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	LEU
1	C	131	ASP
1	A	87	ASN
1	A	131	ASP
1	A	225	LYS
1	B	131	ASP
1	B	226	LEU
1	C	186	PHE
1	D	87	ASN
1	D	131	ASP
1	B	95	LYS
1	C	226	LEU
1	D	154	LYS
1	A	154	LYS
1	A	186	PHE
1	B	14	GLY
1	C	154	LYS
1	C	225	LYS
1	C	59	GLY
1	D	187	VAL
1	D	59	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/230 (90%)	173 (83%)	35 (17%)	2	2
1	B	207/230 (90%)	170 (82%)	37 (18%)	2	2
1	C	208/230 (90%)	173 (83%)	35 (17%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	207/230 (90%)	169 (82%)	38 (18%)	1	2
All	All	830/920 (90%)	685 (82%)	145 (18%)	2	2

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	7	LYS
1	A	11	LEU
1	A	18	ARG
1	A	19	LEU
1	A	20[A]	ARG
1	A	20[B]	ARG
1	A	22	LEU
1	A	33	VAL
1	A	36	LYS
1	A	38	LEU
1	A	48	GLU
1	A	53	ASP
1	A	62	LYS
1	A	63	GLU
1	A	75	ARG
1	A	95	LYS
1	A	112	LYS
1	A	114	MET
1	A	116	ARG
1	A	119	LEU
1	A	129	ARG
1	A	130	GLU
1	A	131	ASP
1	A	153	SER
1	A	175	SER
1	A	182	VAL
1	A	185	GLU
1	A	188	ASP
1	A	221	GLN
1	A	224	ARG
1	A	225	LYS
1	A	227	GLU
1	A	228	GLU
1	A	231	LYS
1	B	5	ARG

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Mol	Chain	Res	Type
1	B	7	LYS
1	B	11	LEU
1	B	20	ARG
1	B	35	GLN
1	B	36	LYS
1	B	38	LEU
1	B	48	GLU
1	B	75	ARG
1	B	85	TYR
1	B	95	LYS
1	B	97	GLU
1	B	98	LEU
1	B	112	LYS
1	B	116	ARG
1	B	120	THR
1	B	124	TYR
1	B	130	GLU
1	B	132	CYS
1	B	133	THR
1	B	154	LYS
1	B	172	LYS
1	B	179	LYS
1	B	182	VAL
1	B	183	SER
1	B	185	GLU
1	B	199	ILE
1	B	200	LYS
1	B	201	GLU
1	B	210	GLU
1	B	213	SER
1	B	214	ILE
1	B	221	GLN
1	B	224	ARG
1	B	227	GLU
1	B	228	GLU
1	B	231	LYS
1	C	5	ARG
1	C	18	ARG
1	C	19	LEU
1	C	20[A]	ARG
1	C	20[B]	ARG
1	C	22	LEU

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Mol	Chain	Res	Type
1	C	34	ASN
1	C	35	GLN
1	C	36	LYS
1	C	48	GLU
1	C	53	ASP
1	C	70	GLU
1	C	91	LEU
1	C	112	LYS
1	C	114	MET
1	C	116	ARG
1	C	119	LEU
1	C	120	THR
1	C	125	PHE
1	C	134	ASN
1	C	135	GLU
1	C	153	SER
1	C	175	SER
1	C	179	LYS
1	C	182	VAL
1	C	188	ASP
1	C	192	ASP
1	C	200	LYS
1	C	210	GLU
1	C	220	VAL
1	C	224	ARG
1	C	225	LYS
1	C	228	GLU
1	C	230	LEU
1	C	231	LYS
1	D	7	LYS
1	D	15	LEU
1	D	18	ARG
1	D	19	LEU
1	D	20	ARG
1	D	22	LEU
1	D	24	GLU
1	D	32	GLN
1	D	33	VAL
1	D	35	GLN
1	D	36	LYS
1	D	48	GLU
1	D	62	LYS

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Mol	Chain	Res	Type
1	D	75	ARG
1	D	95	LYS
1	D	96	GLU
1	D	112	LYS
1	D	116	ARG
1	D	119	LEU
1	D	121	ARG
1	D	125	PHE
1	D	127	VAL
1	D	129	ARG
1	D	130	GLU
1	D	132	CYS
1	D	133	THR
1	D	145	LYS
1	D	148	ASP
1	D	150	ILE
1	D	172	LYS
1	D	175	SER
1	D	182	VAL
1	D	183	SER
1	D	188	ASP
1	D	209	LEU
1	D	210	GLU
1	D	221	GLN
1	D	231	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	100	ASN
1	A	108	ASN
1	B	32	GLN
1	B	108	ASN
1	B	212	ASN
1	C	25	ASN
1	C	32	GLN
1	C	64	GLN
1	C	108	ASN
1	C	212	ASN
1	C	221	GLN
1	D	64	GLN

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Mol	Chain	Res	Type
1	D	134	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	CDC	C	3991	2	27,32,32	1.18	3 (11%)	34,49,49	1.53	6 (17%)
3	CDC	D	4991	2	27,32,32	1.12	0	34,49,49	1.71	7 (20%)
3	CDC	A	1991	2	27,32,32	1.17	3 (11%)	34,49,49	1.61	7 (20%)
3	CDC	B	2991	2	27,32,32	1.17	1 (3%)	34,49,49	1.69	8 (23%)

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	CDC	C	3991	2	-	11/22/40/40	0/2/2/2
3	CDC	D	4991	2	-	12/22/40/40	0/2/2/2
3	CDC	A	1991	2	-	11/22/40/40	0/2/2/2
3	CDC	B	2991	2	-	12/22/40/40	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3991	CDC	C2-N3	-2.71	1.32	1.38
3	C	3991	CDC	C2'-C1'	-2.66	1.49	1.53
3	A	1991	CDC	C2'-C1'	-2.50	1.50	1.53
3	B	2991	CDC	C6-N1	2.27	1.38	1.35
3	A	1991	CDC	C6-N1	2.21	1.38	1.35
3	C	3991	CDC	C6-N1	2.07	1.38	1.35
3	A	1991	CDC	C2-N3	-2.03	1.34	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2991	CDC	C5'-C4'-C3'	-4.63	97.83	115.18
3	C	3991	CDC	C2-N3-C4	4.45	120.86	116.34
3	D	4991	CDC	C2-N3-C4	4.43	120.83	116.34
3	A	1991	CDC	C2-N3-C4	4.20	120.60	116.34
3	B	2991	CDC	C2-N3-C4	4.20	120.59	116.34
3	D	4991	CDC	C5'-C4'-C3'	-4.18	99.53	115.18
3	A	1991	CDC	PB-O3A-PA	-3.72	120.05	132.83
3	A	1991	CDC	C5'-C4'-C3'	-3.59	101.72	115.18
3	B	2991	CDC	C6-N1-C2	-3.38	115.83	121.20
3	D	4991	CDC	C6-N1-C2	-3.31	115.94	121.20
3	D	4991	CDC	O4'-C1'-C2'	-3.28	102.14	106.93
3	C	3991	CDC	PB-O3A-PA	-3.21	121.82	132.83
3	D	4991	CDC	PB-O3A-PA	-3.12	122.12	132.83
3	C	3991	CDC	C6-N1-C2	-2.91	116.57	121.20
3	C	3991	CDC	C5'-C4'-C3'	-2.88	104.39	115.18
3	A	1991	CDC	C6-N1-C2	-2.84	116.69	121.20
3	A	1991	CDC	O4'-C1'-C2'	-2.62	103.09	106.93
3	B	2991	CDC	O4'-C1'-C2'	-2.60	103.12	106.93
3	B	2991	CDC	PB-O3A-PA	-2.56	124.05	132.83
3	B	2991	CDC	O4'-C4'-C5'	2.42	117.34	109.37
3	D	4991	CDC	O4'-C4'-C5'	2.39	117.23	109.37
3	C	3991	CDC	O3'-C3'-C4'	-2.31	104.36	111.05
3	A	1991	CDC	PB-O1B-C14	-2.26	110.46	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2991	CDC	O5'-C5'-C4'	2.11	116.25	108.99
3	D	4991	CDC	PB-O1B-C14	-2.09	111.28	121.59
3	B	2991	CDC	O3'-C3'-C4'	-2.09	105.00	111.05
3	C	3991	CDC	PB-O1B-C14	-2.04	111.54	121.59
3	A	1991	CDC	O3'-C3'-C4'	-2.02	105.21	111.05

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3991	CDC	C3'-C4'-C5'-O5'
3	C	3991	CDC	O4'-C4'-C5'-O5'
3	C	3991	CDC	C5'-O5'-PA-O2A
3	C	3991	CDC	O1B-C14-C15-N11
3	A	1991	CDC	O4'-C4'-C5'-O5'
3	A	1991	CDC	C5'-O5'-PA-O2A
3	A	1991	CDC	C5'-O5'-PA-O3A
3	A	1991	CDC	O1B-C14-C15-N11
3	D	4991	CDC	C2'-C1'-N1-C6
3	D	4991	CDC	O4'-C1'-N1-C6
3	D	4991	CDC	O4'-C4'-C5'-O5'
3	D	4991	CDC	C5'-O5'-PA-O2A
3	D	4991	CDC	C5'-O5'-PA-O3A
3	D	4991	CDC	PB-O3A-PA-O5'
3	D	4991	CDC	O1B-C14-C15-N11
3	B	2991	CDC	C2'-C1'-N1-C6
3	B	2991	CDC	O4'-C1'-N1-C6
3	B	2991	CDC	O4'-C4'-C5'-O5'
3	B	2991	CDC	C5'-O5'-PA-O2A
3	B	2991	CDC	O1B-C14-C15-N11
3	A	1991	CDC	C3'-C4'-C5'-O5'
3	D	4991	CDC	C3'-C4'-C5'-O5'
3	B	2991	CDC	C3'-C4'-C5'-O5'
3	A	1991	CDC	C14-C15-N11-C18
3	C	3991	CDC	C14-C15-N11-C18
3	A	1991	CDC	C14-C15-N11-C17
3	B	2991	CDC	C14-C15-N11-C18
3	C	3991	CDC	C14-C15-N11-C17
3	A	1991	CDC	C14-C15-N11-C16
3	C	3991	CDC	C14-C15-N11-C16
3	B	2991	CDC	C14-C15-N11-C16
3	C	3991	CDC	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
3	A	1991	CDC	PB-O3A-PA-O5'
3	B	2991	CDC	PB-O3A-PA-O5'
3	B	2991	CDC	C5'-O5'-PA-O3A
3	C	3991	CDC	C5'-O5'-PA-O1A
3	A	1991	CDC	C5'-O5'-PA-O1A
3	D	4991	CDC	C5'-O5'-PA-O1A
3	B	2991	CDC	C5'-O5'-PA-O1A
3	B	2991	CDC	C14-C15-N11-C17
3	D	4991	CDC	C4'-C5'-O5'-PA
3	D	4991	CDC	C14-C15-N11-C18
3	C	3991	CDC	C5'-O5'-PA-O3A
3	C	3991	CDC	C4'-C5'-O5'-PA
3	A	1991	CDC	C4'-C5'-O5'-PA
3	D	4991	CDC	C14-C15-N11-C16

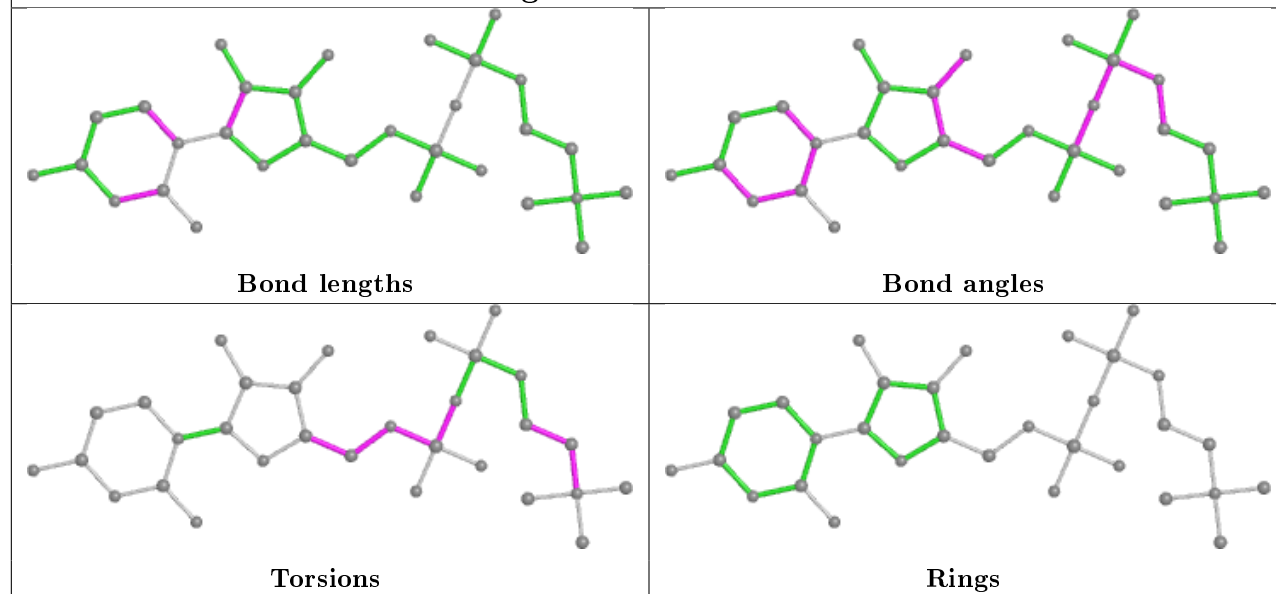
There are no ring outliers.

4 monomers are involved in 11 short contacts:

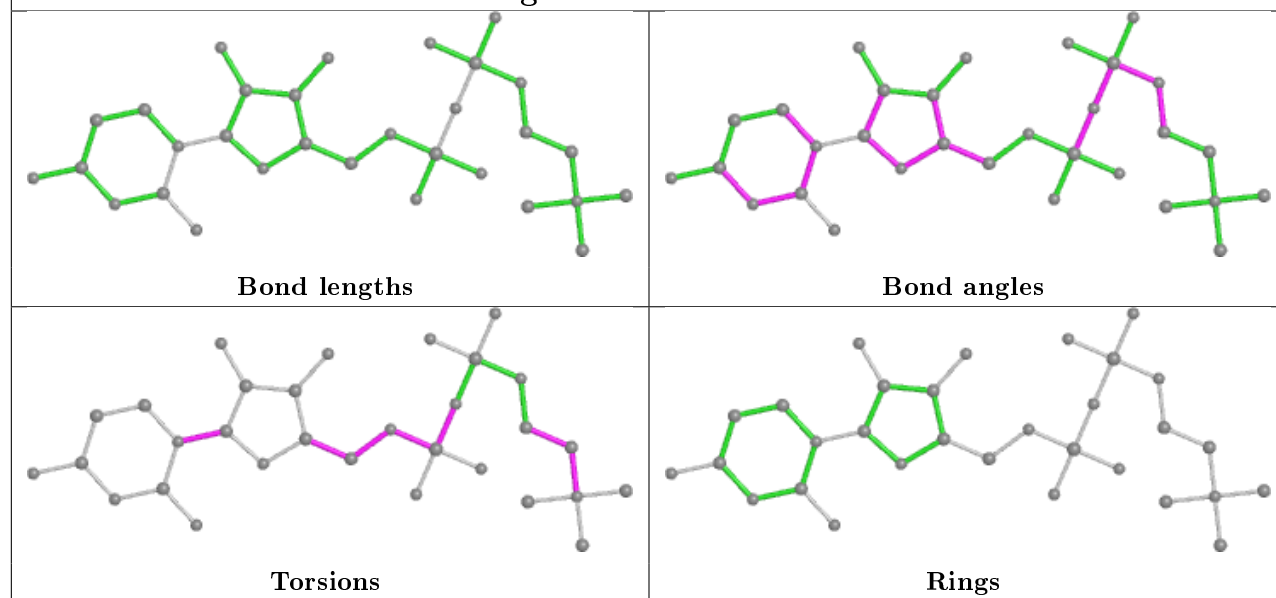
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3991	CDC	3	0
3	D	4991	CDC	3	0
3	A	1991	CDC	1	0
3	B	2991	CDC	4	0

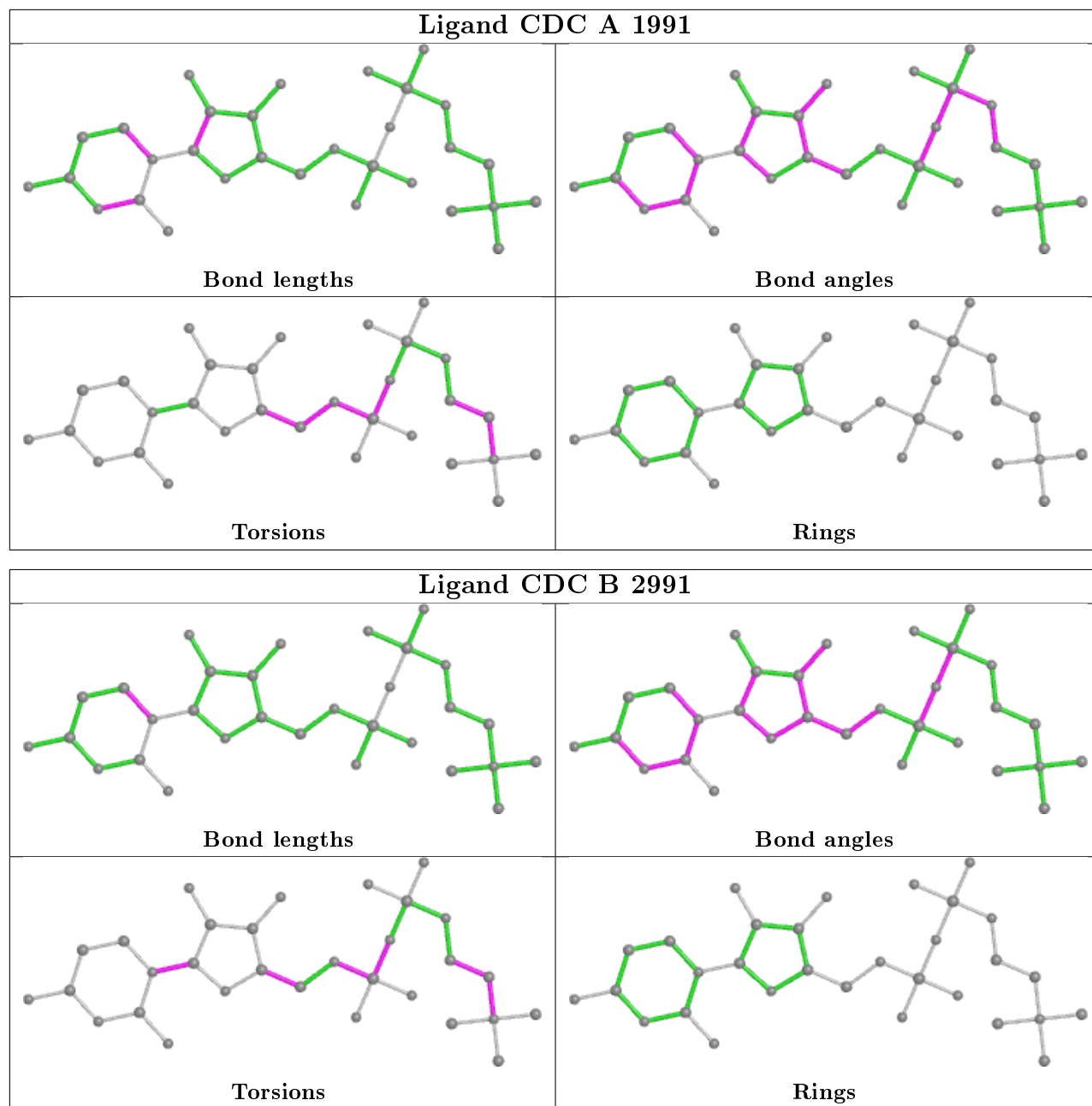
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand CDC C 3991



Ligand CDC D 4991





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.