



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:48 am GMT

PDB ID : 2A30  
Title : Crystal structure of human deoxycytidine kinase in complex with deoxycytidine  
Authors : Godsey, M.H.; Ort, S.; Sabini, E.; Konrad, M.; Lavie, A.  
Deposited on : 2005-06-23  
Resolution : 3.02 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

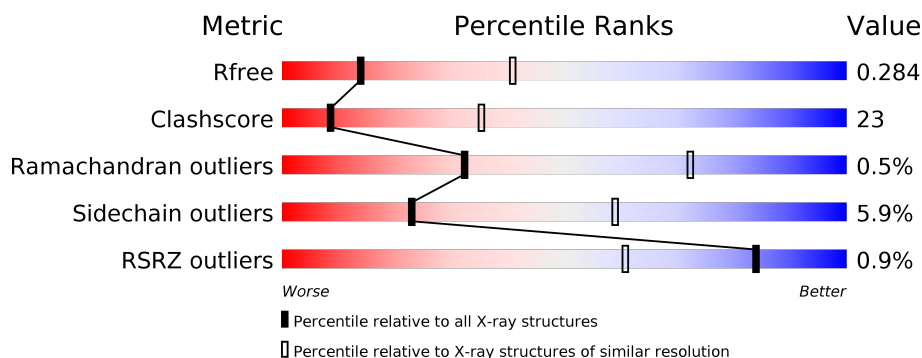
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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))
$R_{free}$	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	<div> <div>53%</div> <div>33%</div> <div>•</div> <div>11%</div> </div>
1	B	248	<div> <div>49%</div> <div>33%</div> <div>•</div> <div>15%</div> </div>
1	C	248	<div> <div>2%</div> <div>56%</div> <div>31%</div> <div>•</div> <div>11%</div> </div>
1	D	248	<div> <div>2%</div> <div>52%</div> <div>30%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6944 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1759	1130	296	325	8			
1	B	212	Total	C	N	O	S	0	0	0
			1673	1081	277	307	8			
1	C	221	Total	C	N	O	S	0	0	0
			1739	1117	293	321	8			
1	D	215	Total	C	N	O	S	0	0	0
			1681	1080	283	310	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P27707
A	-1	SER	-	CLONING ARTIFACT	UNP P27707
A	0	HIS	-	CLONING ARTIFACT	UNP P27707
A	?	-	GLN	DELETION	UNP P27707
A	?	-	ASP	DELETION	UNP P27707
A	?	-	GLU	DELETION	UNP P27707
A	?	-	PHE	DELETION	UNP P27707
A	?	-	GLU	DELETION	UNP P27707
A	?	-	GLU	DELETION	UNP P27707
A	?	-	LEU	DELETION	UNP P27707
A	?	-	THR	DELETION	UNP P27707
A	?	-	MET	DELETION	UNP P27707
A	?	-	SER	DELETION	UNP P27707
A	?	-	GLN	DELETION	UNP P27707
A	?	-	LYS	DELETION	UNP P27707
A	?	-	ASN	DELETION	UNP P27707
A	?	-	GLY	DELETION	UNP P27707
A	?	-	GLY	DELETION	UNP P27707
B	-2	GLY	-	CLONING ARTIFACT	UNP P27707
B	-1	SER	-	CLONING ARTIFACT	UNP P27707
B	0	HIS	-	CLONING ARTIFACT	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	DELETION	UNP P27707
B	?	-	ASP	DELETION	UNP P27707
B	?	-	GLU	DELETION	UNP P27707
B	?	-	PHE	DELETION	UNP P27707
B	?	-	GLU	DELETION	UNP P27707
B	?	-	GLU	DELETION	UNP P27707
B	?	-	LEU	DELETION	UNP P27707
B	?	-	THR	DELETION	UNP P27707
B	?	-	MET	DELETION	UNP P27707
B	?	-	SER	DELETION	UNP P27707
B	?	-	GLN	DELETION	UNP P27707
B	?	-	LYS	DELETION	UNP P27707
B	?	-	ASN	DELETION	UNP P27707
B	?	-	GLY	DELETION	UNP P27707
B	?	-	GLY	DELETION	UNP P27707
C	-2	GLY	-	CLONING ARTIFACT	UNP P27707
C	-1	SER	-	CLONING ARTIFACT	UNP P27707
C	0	HIS	-	CLONING ARTIFACT	UNP P27707
C	?	-	GLN	DELETION	UNP P27707
C	?	-	ASP	DELETION	UNP P27707
C	?	-	GLU	DELETION	UNP P27707
C	?	-	PHE	DELETION	UNP P27707
C	?	-	GLU	DELETION	UNP P27707
C	?	-	GLU	DELETION	UNP P27707
C	?	-	LEU	DELETION	UNP P27707
C	?	-	THR	DELETION	UNP P27707
C	?	-	MET	DELETION	UNP P27707
C	?	-	SER	DELETION	UNP P27707
C	?	-	GLN	DELETION	UNP P27707
C	?	-	LYS	DELETION	UNP P27707
C	?	-	ASN	DELETION	UNP P27707
C	?	-	GLY	DELETION	UNP P27707
C	?	-	GLY	DELETION	UNP P27707
D	-2	GLY	-	CLONING ARTIFACT	UNP P27707
D	-1	SER	-	CLONING ARTIFACT	UNP P27707
D	0	HIS	-	CLONING ARTIFACT	UNP P27707
D	?	-	GLN	DELETION	UNP P27707
D	?	-	ASP	DELETION	UNP P27707
D	?	-	GLU	DELETION	UNP P27707
D	?	-	PHE	DELETION	UNP P27707
D	?	-	GLU	DELETION	UNP P27707
D	?	-	GLU	DELETION	UNP P27707

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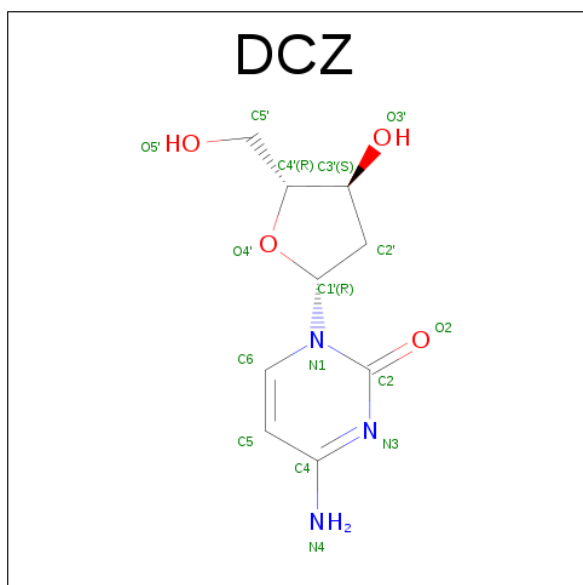
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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	UNP P27707
D	?	-	THR	DELETION	UNP P27707
D	?	-	MET	DELETION	UNP P27707
D	?	-	SER	DELETION	UNP P27707
D	?	-	GLN	DELETION	UNP P27707
D	?	-	LYS	DELETION	UNP P27707
D	?	-	ASN	DELETION	UNP P27707
D	?	-	GLY	DELETION	UNP P27707
D	?	-	GLY	DELETION	UNP P27707

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is 2'-DEOXYCYTIDINE (three-letter code: DCZ) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 16 9 3 4	0	0
3	B	1	Total C N O 16 9 3 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			16	9	3	4		
3	D	1	Total	C	N	O	0	0
			16	9	3	4		

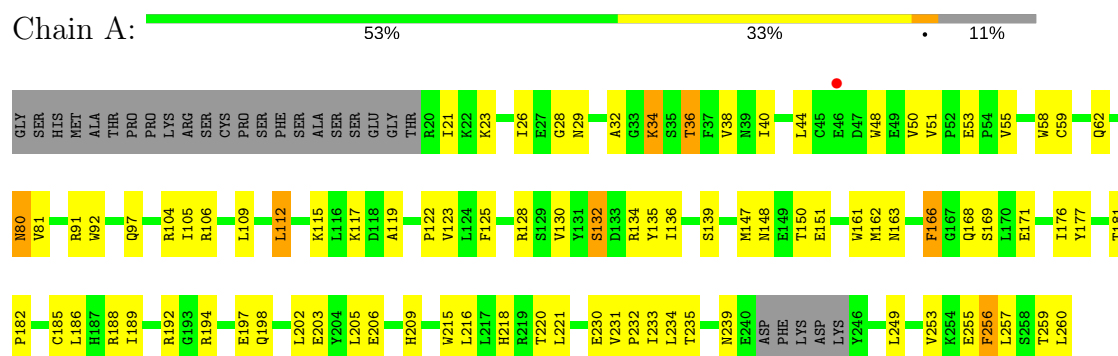
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	4	Total	O	0	0
			4	4		
4	C	12	Total	O	0	0
			12	12		
4	D	1	Total	O	0	0
			1	1		

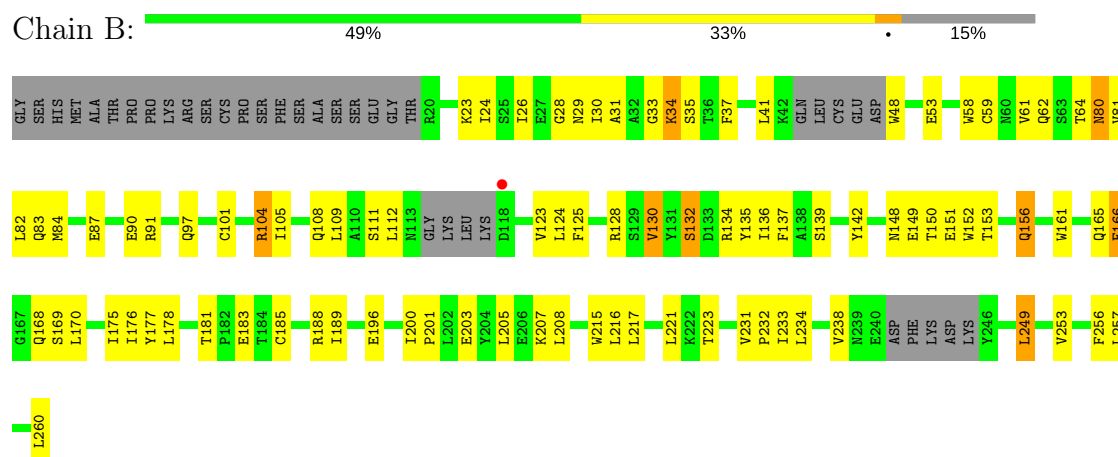
### 3 Residue-property plots

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 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.

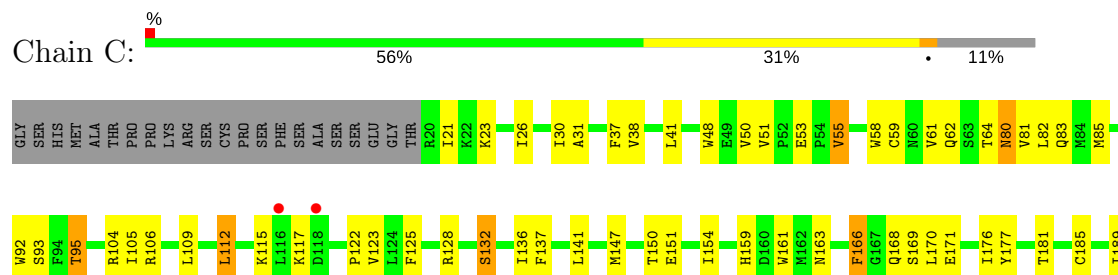
#### • Molecule 1: Deoxycytidine kinase

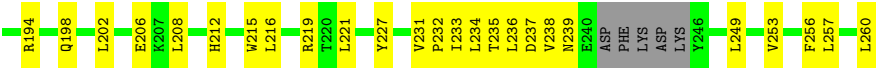


#### • Molecule 1: Deoxycytidine kinase

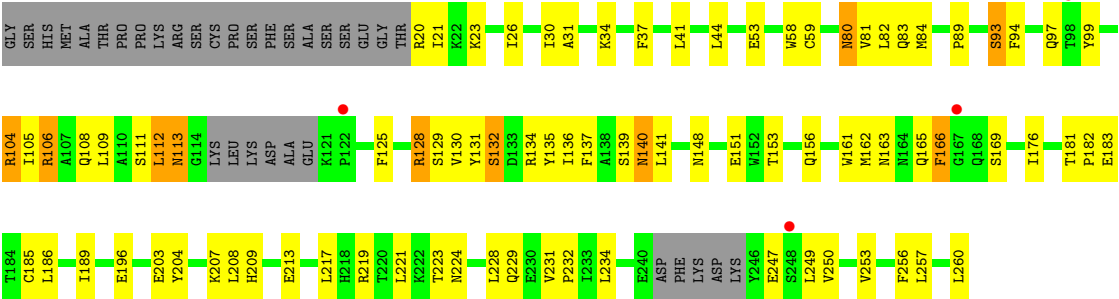


#### • Molecule 1: Deoxycytidine kinase





● Molecule 1: Deoxycytidine kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.34Å 64.94Å 108.60Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	19.90 – 3.02 19.90 – 3.02	Depositor EDS
% Data completeness (in resolution range)	91.9 (19.90-3.02) 91.9 (19.90-3.02)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.04Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.285 0.234 , 0.284	Depositor DCC
$R_{free}$ test set	2011 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.48	0/1803	0.62	0/2456
1	B	0.44	0/1714	0.60	0/2337
1	C	0.45	0/1783	0.62	0/2434
1	D	0.44	0/1722	0.62	0/2349
All	All	0.45	0/7022	0.61	0/9576

There are no bond length outliers.

There are no bond angle outliers.

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	1759	0	1635	77	0
1	B	1673	0	1552	84	0
1	C	1739	0	1594	75	0
1	D	1681	0	1543	86	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	16	0	13	1	0
3	B	16	0	13	1	0
3	C	16	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	16	0	13	1	0
4	A	9	0	0	0	0
4	B	4	0	0	0	0
4	C	12	0	0	0	0
4	D	1	0	0	0	0
All	All	6944	0	6376	305	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 23.

All (305) 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:B:34:LYS:HD2	1:B:35:SER:H	0.98	1.15
1:A:234:LEU:HB2	1:A:256:PHE:CD2	1.97	0.99
1:D:97:GLN:HE22	3:D:602:DCZ:HN41	1.12	0.98
1:B:34:LYS:HD2	1:B:35:SER:N	1.79	0.96
1:D:106:ARG:HH11	1:D:106:ARG:CB	1.79	0.95
1:A:234:LEU:HB2	1:A:256:PHE:HD2	1.28	0.93
1:A:38:VAL:CG1	1:A:50:VAL:HG11	2.00	0.90
1:D:129:SER:HG	1:D:131:TYR:HD1	0.94	0.89
1:C:181:THR:HG23	1:C:239:ASN:HD21	1.38	0.89
1:C:38:VAL:HG13	1:C:50:VAL:HG11	1.53	0.88
1:B:101:CYS:SG	1:B:130:VAL:HG12	2.13	0.88
1:A:38:VAL:HG13	1:A:50:VAL:HG11	1.58	0.86
1:B:104:ARG:NH1	1:B:128:ARG:HB3	1.91	0.86
1:C:38:VAL:CG1	1:C:50:VAL:HG11	2.06	0.84
1:B:104:ARG:HH12	1:B:128:ARG:HB3	1.40	0.83
1:B:59:CYS:HA	1:B:80:ASN:ND2	1.94	0.83
1:B:23:LYS:HE2	1:B:169:SER:O	1.80	0.80
1:D:58:TRP:O	1:D:81:VAL:HG12	1.81	0.79
1:D:59:CYS:HA	1:D:80:ASN:ND2	1.97	0.79
1:B:134:ARG:NH2	1:B:156:GLN:HG2	1.96	0.78
1:C:26:ILE:HD12	1:C:26:ILE:N	1.98	0.78
1:D:140:ASN:HD22	1:D:140:ASN:C	1.87	0.77
1:C:21:ILE:HG23	1:C:122:PRO:HB2	1.67	0.76
1:A:59:CYS:HA	1:A:80:ASN:ND2	2.00	0.76
1:D:106:ARG:HB3	1:D:106:ARG:HH11	1.50	0.75
1:B:178:LEU:HD22	1:B:238:VAL:HG11	1.70	0.74
1:C:136:ILE:HD13	1:C:212:HIS:CE1	2.22	0.74
1:D:176:ILE:HD12	1:D:234:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:TRP:HB2	1:C:221:LEU:HD23	1.69	0.74
1:C:177:TYR:HD2	1:C:235:THR:HG23	1.53	0.73
1:B:97:GLN:HE22	3:B:402:DCZ:HN41	1.35	0.73
1:D:106:ARG:HB2	1:D:106:ARG:HH11	1.53	0.73
1:D:104:ARG:HH12	1:D:128:ARG:HB3	1.55	0.72
1:D:93:SER:OG	1:D:141:LEU:HD13	1.90	0.72
1:D:23:LYS:HE2	1:D:169:SER:O	1.90	0.71
1:A:26:ILE:N	1:A:26:ILE:HD12	2.06	0.70
1:A:38:VAL:HG11	1:A:50:VAL:HG11	1.73	0.70
1:B:249:LEU:O	1:B:253:VAL:HG23	1.93	0.69
1:A:176:ILE:HD12	1:A:234:LEU:HD23	1.75	0.69
1:D:104:ARG:NH1	1:D:128:ARG:HB3	2.07	0.69
1:B:33:GLY:H	1:B:34:LYS:HE3	1.57	0.69
1:C:185:CYS:O	1:C:189:ILE:HG12	1.94	0.68
1:B:31:ALA:O	1:B:188:ARG:HD2	1.94	0.67
1:C:95:THR:HG23	1:D:94:PHE:CE2	2.30	0.67
1:A:106:ARG:HD3	1:B:161:TRP:NE1	2.10	0.67
1:C:181:THR:HG23	1:C:239:ASN:ND2	2.08	0.66
1:D:104:ARG:O	1:D:108:GLN:HG3	1.95	0.66
1:C:147:MET:HA	1:C:151:GLU:OE1	1.96	0.66
1:D:112:LEU:HD12	1:D:113:ASN:H	1.59	0.66
1:B:111:SER:OG	1:B:124:LEU:HD21	1.96	0.65
1:A:185:CYS:O	1:A:189:ILE:HG12	1.96	0.65
1:B:185:CYS:O	1:B:189:ILE:HG12	1.96	0.65
1:C:215:TRP:CE3	1:C:216:LEU:HG	2.32	0.64
1:D:80:ASN:O	1:D:84:MET:HG3	1.98	0.64
1:D:249:LEU:O	1:D:253:VAL:HG23	1.97	0.64
1:D:106:ARG:NH1	1:D:106:ARG:CB	2.57	0.64
1:B:200:ILE:HG21	1:B:205:LEU:HD21	1.80	0.64
1:D:21:ILE:HD12	1:D:21:ILE:N	2.13	0.63
1:B:109:LEU:HD13	1:B:170:LEU:HD11	1.79	0.63
1:B:201:PRO:HB2	1:B:203:GLU:OE1	1.98	0.63
1:A:106:ARG:HD3	1:B:161:TRP:CD1	2.34	0.63
1:D:130:VAL:HG21	1:D:163:ASN:HD21	1.63	0.62
1:D:129:SER:OG	1:D:131:TYR:HD1	1.75	0.62
1:A:134:ARG:HD3	1:A:135:TYR:CE1	2.34	0.62
1:D:106:ARG:HB2	1:D:106:ARG:NH1	2.14	0.61
1:B:134:ARG:HH21	1:B:156:GLN:HG2	1.65	0.61
1:A:256:PHE:CD1	1:A:256:PHE:C	2.72	0.61
1:D:219:ARG:NH2	1:D:229:GLN:HA	2.14	0.61
1:A:256:PHE:CE1	1:A:260:LEU:HD21	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:HB2	1:A:220:THR:HG23	1.83	0.61
1:B:217:LEU:HD23	1:B:217:LEU:O	2.01	0.61
1:B:34:LYS:CD	1:B:35:SER:H	1.92	0.60
1:C:249:LEU:O	1:C:253:VAL:HG23	2.02	0.60
1:D:135:TYR:HB3	1:D:221:LEU:HD21	1.82	0.60
1:B:165:GLN:HE21	1:B:165:GLN:HA	1.66	0.60
1:D:112:LEU:HD12	1:D:113:ASN:N	2.16	0.60
1:D:228:LEU:HA	1:D:231:VAL:HG23	1.82	0.60
1:B:109:LEU:HD21	1:B:166:PHE:HB2	1.84	0.59
1:B:203:GLU:H	1:B:203:GLU:CD	2.05	0.59
1:B:83:GLN:O	1:B:87:GLU:HG3	2.02	0.59
1:A:249:LEU:O	1:A:253:VAL:HG23	2.03	0.59
1:B:80:ASN:O	1:B:84:MET:HG3	2.03	0.58
1:A:216:LEU:HD22	1:A:233:ILE:HD12	1.85	0.58
1:A:181:THR:HG23	1:A:239:ASN:HD21	1.67	0.58
1:D:37:PHE:O	1:D:41:LEU:HD13	2.04	0.58
1:B:58:TRP:O	1:B:81:VAL:HG12	2.04	0.57
1:B:80:ASN:OD1	1:B:83:GLN:HB2	2.03	0.57
1:C:171:GLU:HG3	1:C:227:TYR:CE1	2.38	0.57
1:D:134:ARG:HH12	1:D:224:ASN:HD22	1.53	0.57
1:C:234:LEU:HB2	1:C:256:PHE:CD2	2.40	0.57
1:D:140:ASN:C	1:D:140:ASN:ND2	2.57	0.57
1:D:140:ASN:O	1:D:140:ASN:ND2	2.35	0.57
1:D:185:CYS:O	1:D:189:ILE:HG12	2.03	0.57
1:A:53:GLU:C	1:A:55:VAL:H	2.08	0.56
1:C:176:ILE:HD12	1:C:234:LEU:HD23	1.86	0.56
1:C:53:GLU:C	1:C:55:VAL:H	2.08	0.56
1:A:29:ASN:O	1:A:34:LYS:HE2	2.05	0.56
1:A:147:MET:HA	1:A:151:GLU:OE1	2.06	0.56
1:A:168:GLN:O	1:A:171:GLU:HG3	2.05	0.56
1:C:235:THR:O	1:C:236:LEU:HD23	2.06	0.56
1:C:154:ILE:HG12	1:D:99:TYR:CE1	2.41	0.56
1:B:128:ARG:HG3	1:B:132:SER:OG	2.06	0.56
1:B:135:TYR:CE1	1:B:223:THR:HB	2.41	0.56
1:D:228:LEU:HA	1:D:231:VAL:CG2	2.36	0.56
1:D:89:PRO:O	1:D:93:SER:HB2	2.05	0.56
1:C:80:ASN:HD21	1:C:82:LEU:HB3	1.70	0.56
1:B:48:TRP:CD1	1:B:123:VAL:HB	2.41	0.56
1:B:26:ILE:HD11	1:B:125:PHE:HD2	1.70	0.56
1:A:194:ARG:O	1:A:198:GLN:HG2	2.06	0.55
1:C:58:TRP:O	1:C:81:VAL:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLU:O	1:D:207:LYS:HG2	2.06	0.55
1:A:192:ARG:HH21	1:A:197:GLU:CD	2.10	0.55
1:D:26:ILE:HD12	1:D:26:ILE:N	2.22	0.55
1:C:154:ILE:HG12	1:D:99:TYR:CD1	2.42	0.55
1:C:38:VAL:HG11	1:C:50:VAL:HG11	1.87	0.55
1:C:105:ILE:O	1:C:109:LEU:HB2	2.07	0.54
1:A:58:TRP:O	1:A:81:VAL:HG12	2.06	0.54
1:A:234:LEU:HB2	1:A:256:PHE:CE2	2.42	0.54
1:A:132:SER:O	1:A:136:ILE:HB	2.07	0.54
1:A:256:PHE:HE1	1:A:260:LEU:HD11	1.71	0.54
1:B:132:SER:HA	1:B:136:ILE:HD12	1.89	0.54
1:B:33:GLY:N	1:B:34:LYS:HE3	2.23	0.54
1:A:181:THR:HG23	1:A:239:ASN:ND2	2.22	0.54
1:B:203:GLU:O	1:B:207:LYS:HG2	2.09	0.53
1:B:217:LEU:C	1:B:217:LEU:HD23	2.28	0.53
1:C:112:LEU:O	1:C:112:LEU:HD12	2.07	0.53
1:A:181:THR:CG2	1:A:239:ASN:HD21	2.22	0.53
1:B:112:LEU:O	1:B:112:LEU:HD12	2.08	0.53
1:B:148:ASN:OD1	1:B:151:GLU:HG3	2.09	0.53
1:D:53:GLU:HG3	1:D:104:ARG:NH1	2.24	0.53
1:A:26:ILE:CD1	1:A:26:ILE:N	2.72	0.53
1:A:28:GLY:O	1:A:128:ARG:NH1	2.42	0.53
1:C:106:ARG:NH2	1:D:161:TRP:HB2	2.24	0.53
1:A:256:PHE:HD1	1:A:256:PHE:C	2.12	0.52
1:C:62:GLN:HG3	1:D:153:THR:OG1	2.08	0.52
1:A:104:ARG:NH1	1:A:128:ARG:HB3	2.23	0.52
1:B:26:ILE:HD11	1:B:125:PHE:CD2	2.44	0.52
1:A:181:THR:HG23	1:A:239:ASN:OD1	2.09	0.52
1:B:61:VAL:O	1:B:64:THR:OG1	2.23	0.52
1:D:219:ARG:HH21	1:D:229:GLN:HA	1.74	0.52
1:C:59:CYS:HA	1:C:80:ASN:ND2	2.25	0.51
1:D:148:ASN:OD1	1:D:151:GLU:HG3	2.10	0.51
1:C:93:SER:HB3	1:C:141:LEU:HD13	1.91	0.51
1:B:196:GLU:CD	1:B:196:GLU:H	2.14	0.51
1:D:217:LEU:C	1:D:217:LEU:HD23	2.31	0.51
1:D:59:CYS:HA	1:D:80:ASN:HD22	1.75	0.51
1:A:104:ARG:HH12	1:A:128:ARG:HB3	1.75	0.51
1:A:50:VAL:HG22	1:A:125:PHE:HB2	1.92	0.51
1:A:186:LEU:HD22	1:A:202:LEU:HD12	1.93	0.51
1:B:105:ILE:O	1:B:109:LEU:HB2	2.10	0.51
1:D:213:GLU:OE1	1:D:217:LEU:HD13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TYR:CD2	1:D:223:THR:HG22	2.45	0.51
1:C:109:LEU:HD12	1:C:170:LEU:HD21	1.92	0.51
1:B:135:TYR:HB3	1:B:221:LEU:HD21	1.91	0.50
1:A:105:ILE:O	1:A:109:LEU:HB2	2.11	0.50
1:B:137:PHE:CE2	1:B:208:LEU:HD13	2.46	0.50
1:C:50:VAL:HG22	1:C:125:PHE:HB2	1.93	0.50
1:D:134:ARG:HH12	1:D:224:ASN:ND2	2.09	0.50
1:D:137:PHE:O	1:D:141:LEU:HG	2.12	0.50
1:B:28:GLY:O	1:B:128:ARG:NH1	2.45	0.50
1:C:50:VAL:HG12	1:C:51:VAL:N	2.27	0.50
1:D:105:ILE:O	1:D:109:LEU:HB2	2.12	0.50
1:C:106:ARG:HD3	1:D:161:TRP:NE1	2.27	0.50
1:D:217:LEU:O	1:D:217:LEU:HD23	2.12	0.50
1:B:142:TYR:CE2	1:B:152:TRP:CD1	3.00	0.49
1:C:235:THR:C	1:C:236:LEU:HD23	2.33	0.49
1:A:115:LYS:C	1:A:117:LYS:H	2.15	0.49
1:D:204:TYR:CE2	1:D:208:LEU:HD11	2.46	0.49
1:C:104:ARG:NH1	1:C:128:ARG:HB3	2.28	0.49
1:C:234:LEU:CG	1:C:236:LEU:HD21	2.43	0.49
1:A:148:ASN:OD1	1:A:150:THR:HB	2.13	0.49
1:D:128:ARG:HG3	1:D:132:SER:OG	2.13	0.49
1:C:80:ASN:HB3	1:C:83:GLN:HB3	1.94	0.49
1:D:257:LEU:HA	1:D:260:LEU:HG	1.95	0.49
1:A:36:THR:O	1:A:40:ILE:HG13	2.13	0.48
1:C:136:ILE:HG22	1:C:137:PHE:N	2.28	0.48
1:A:109:LEU:HD12	1:A:112:LEU:HD21	1.96	0.48
1:A:106:ARG:HD3	1:B:161:TRP:CE2	2.49	0.48
1:D:20:ARG:C	1:D:21:ILE:HD12	2.33	0.48
1:B:175:ILE:HB	1:B:233:ILE:HD12	1.95	0.48
1:C:234:LEU:HG	1:C:236:LEU:HD21	1.95	0.48
1:C:202:LEU:HG	1:C:206:GLU:HG3	1.95	0.48
1:A:257:LEU:HA	1:A:260:LEU:HD12	1.96	0.48
1:A:91:ARG:HD2	1:B:91:ARG:HE	1.77	0.48
1:A:256:PHE:CE1	1:A:260:LEU:HD11	2.47	0.47
1:B:165:GLN:NE2	1:B:165:GLN:HA	2.29	0.47
1:A:166:PHE:CE2	1:B:166:PHE:CE2	3.02	0.47
1:C:234:LEU:HD11	1:C:236:LEU:HD21	1.96	0.47
1:C:26:ILE:CD1	1:C:26:ILE:N	2.69	0.47
1:D:134:ARG:CZ	1:D:156:GLN:HG2	2.44	0.47
1:A:218:HIS:CB	1:A:220:THR:HG23	2.44	0.47
1:B:104:ARG:O	1:B:108:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:CYS:HB2	1:A:205:LEU:HD13	1.97	0.47
1:B:59:CYS:HA	1:B:80:ASN:HD22	1.75	0.47
1:A:119:ALA:O	1:A:122:PRO:HD3	2.15	0.47
1:C:132:SER:O	1:C:136:ILE:HB	2.15	0.47
1:C:109:LEU:HD21	1:C:166:PHE:HB2	1.97	0.47
1:C:92:TRP:HH2	1:D:148:ASN:HD21	1.61	0.47
1:D:196:GLU:CD	1:D:196:GLU:H	2.18	0.47
1:D:80:ASN:OD1	1:D:83:GLN:HB2	2.15	0.46
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.78	0.46
1:A:203:GLU:HA	1:A:206:GLU:OE1	2.16	0.46
1:D:134:ARG:O	1:D:139:SER:HB2	2.15	0.46
1:B:125:PHE:HZ	1:B:257:LEU:HD11	1.80	0.46
1:A:148:ASN:OD1	1:A:150:THR:N	2.48	0.46
1:C:238:VAL:O	1:C:238:VAL:HG23	2.14	0.46
1:A:21:ILE:HG23	1:A:122:PRO:HB2	1.98	0.46
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.68	0.46
1:C:26:ILE:HD11	1:C:125:PHE:HB3	1.97	0.46
1:D:131:TYR:CD2	1:D:228:LEU:HD11	2.51	0.46
1:B:29:ASN:OD1	1:B:30:ILE:N	2.45	0.46
1:D:247:GLU:HA	1:D:250:VAL:HG23	1.97	0.46
1:A:177:TYR:CD2	1:A:235:THR:HG23	2.50	0.46
1:A:62:GLN:HG3	1:B:153:THR:OG1	2.15	0.46
1:C:104:ARG:HH12	1:C:128:ARG:HB3	1.81	0.46
1:C:80:ASN:C	1:C:80:ASN:HD22	2.19	0.45
1:D:257:LEU:HA	1:D:260:LEU:CD1	2.47	0.45
1:A:48:TRP:CD1	1:A:123:VAL:HB	2.51	0.45
1:B:24:ILE:HG13	1:B:257:LEU:HD21	1.98	0.45
1:A:109:LEU:HA	1:A:112:LEU:CD2	2.47	0.45
1:A:50:VAL:HG12	1:A:51:VAL:N	2.31	0.45
1:C:23:LYS:HD2	1:C:171:GLU:O	2.17	0.45
1:C:61:VAL:O	1:C:64:THR:OG1	2.27	0.45
1:A:92:TRP:HH2	1:B:148:ASN:HD21	1.63	0.45
1:B:142:TYR:OH	1:B:149:GLU:OE2	2.29	0.45
1:C:257:LEU:HA	1:C:260:LEU:CD1	2.46	0.45
1:B:134:ARG:O	1:B:139:SER:HB2	2.17	0.44
1:B:142:TYR:CD2	1:B:152:TRP:CD1	3.04	0.44
1:C:115:LYS:C	1:C:117:LYS:H	2.19	0.44
1:A:97:GLN:HE22	3:A:302:DCZ:HN41	1.64	0.44
1:C:136:ILE:CG2	1:C:208:LEU:HD22	2.47	0.44
1:D:134:ARG:HD3	1:D:135:TYR:CE1	2.52	0.44
1:B:253:VAL:O	1:B:256:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:TYR:CD2	1:C:235:THR:HG23	2.41	0.44
1:D:204:TYR:HE2	1:D:208:LEU:HD11	1.83	0.44
1:A:34:LYS:H	1:A:34:LYS:HZ2	1.65	0.44
1:A:255:GLU:O	1:A:259:THR:HG23	2.18	0.44
1:B:231:VAL:HA	1:B:232:PRO:HD3	1.70	0.44
1:B:80:ASN:HD21	1:B:82:LEU:HB3	1.82	0.44
1:C:231:VAL:HA	1:C:232:PRO:HD3	1.70	0.44
1:D:165:GLN:NE2	1:D:165:GLN:HA	2.33	0.44
1:A:91:ARG:HD2	1:B:91:ARG:NE	2.32	0.44
1:C:257:LEU:HA	1:C:260:LEU:HG	2.00	0.43
1:D:20:ARG:CB	1:D:21:ILE:HD12	2.48	0.43
1:A:134:ARG:O	1:A:139:SER:HB2	2.19	0.43
1:A:109:LEU:HA	1:A:112:LEU:HD23	2.01	0.43
1:A:161:TRP:HE3	1:A:162:MET:HE2	1.84	0.43
1:B:37:PHE:CE1	1:B:41:LEU:HD11	2.53	0.43
1:C:48:TRP:CD1	1:C:123:VAL:HB	2.53	0.43
1:D:181:THR:HB	1:D:183:GLU:OE1	2.19	0.43
1:C:161:TRP:HH2	1:D:166:PHE:CE1	2.37	0.43
1:D:186:LEU:O	1:D:189:ILE:HB	2.19	0.43
1:D:30:ILE:O	1:D:31:ALA:HB3	2.19	0.43
1:A:182:PRO:HG3	1:A:209:HIS:HB2	2.01	0.43
1:A:21:ILE:O	1:A:23:LYS:HE2	2.19	0.43
1:A:234:LEU:CB	1:A:256:PHE:CD2	2.87	0.43
1:C:85:MET:HG3	1:C:93:SER:HA	2.01	0.42
1:D:182:PRO:HG3	1:D:209:HIS:HB2	2.01	0.42
1:B:175:ILE:HB	1:B:233:ILE:CD1	2.49	0.42
1:B:181:THR:HB	1:B:183:GLU:OE1	2.19	0.42
1:D:135:TYR:N	1:D:135:TYR:CD1	2.87	0.42
1:D:80:ASN:HD21	1:D:82:LEU:HB3	1.84	0.42
1:D:132:SER:HA	1:D:136:ILE:HD12	2.01	0.42
1:A:256:PHE:HE1	1:A:260:LEU:HD21	1.83	0.42
1:C:154:ILE:HG23	1:D:99:TYR:HD1	1.85	0.42
1:C:159:HIS:O	1:C:163:ASN:ND2	2.45	0.42
1:C:216:LEU:HB3	1:C:233:ILE:HG21	2.01	0.42
1:C:37:PHE:O	1:C:41:LEU:HD13	2.20	0.42
1:C:61:VAL:O	1:C:61:VAL:HG12	2.19	0.42
1:B:134:ARG:HD3	1:B:135:TYR:CE1	2.55	0.42
1:B:136:ILE:HD11	1:B:215:TRP:CE3	2.55	0.42
1:B:177:TYR:CD1	1:B:216:LEU:HD12	2.55	0.42
1:B:156:GLN:HE21	1:B:156:GLN:HB2	1.56	0.41
1:C:41:LEU:HD23	1:C:125:PHE:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TRP:CZ3	1:A:216:LEU:HD11	2.55	0.41
1:C:219:ARG:NH2	1:C:233:ILE:HG12	2.35	0.41
1:C:93:SER:CB	1:C:141:LEU:HD13	2.50	0.41
1:B:132:SER:CB	1:B:136:ILE:HD12	2.50	0.41
1:B:176:ILE:HD13	1:B:234:LEU:HB3	2.02	0.41
1:D:111:SER:OG	1:D:112:LEU:N	2.53	0.41
1:D:125:PHE:N	1:D:125:PHE:CD1	2.88	0.41
1:D:234:LEU:HB2	1:D:256:PHE:CD2	2.56	0.41
1:A:148:ASN:OD1	1:A:148:ASN:C	2.59	0.41
1:C:194:ARG:O	1:C:198:GLN:HG2	2.21	0.41
1:D:112:LEU:CD1	1:D:113:ASN:N	2.83	0.41
1:D:253:VAL:O	1:D:256:PHE:HB3	2.21	0.41
1:D:41:LEU:HD23	1:D:125:PHE:CD2	2.55	0.41
1:A:130:VAL:HG21	1:A:163:ASN:OD1	2.21	0.41
1:B:91:ARG:HG3	1:B:91:ARG:NH1	2.35	0.41
1:C:234:LEU:CD1	1:C:236:LEU:HD21	2.50	0.41
1:A:32:ALA:O	1:A:188:ARG:NH1	2.54	0.41
1:C:109:LEU:HD13	1:C:170:LEU:HD11	2.02	0.41
1:C:253:VAL:O	1:C:256:PHE:HB3	2.21	0.41
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.81	0.40
1:B:132:SER:CA	1:B:136:ILE:HD12	2.51	0.40
1:D:26:ILE:CD1	1:D:26:ILE:N	2.83	0.40
1:A:182:PRO:HG3	1:A:209:HIS:CB	2.52	0.40
1:B:132:SER:HA	1:B:136:ILE:CD1	2.50	0.40
1:C:237:ASP:OD2	1:C:239:ASN:HB2	2.21	0.40
1:B:26:ILE:CD1	1:B:125:PHE:HD2	2.33	0.40
1:B:257:LEU:HD23	1:B:260:LEU:HD11	2.04	0.40
1:B:37:PHE:CE1	1:B:41:LEU:CD1	3.05	0.40
1:C:30:ILE:O	1:C:31:ALA:HB3	2.22	0.40
1:D:162:MET:HA	1:D:162:MET:HE2	2.02	0.40
1:D:231:VAL:HA	1:D:232:PRO:HD3	1.73	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	217/248 (88%)	194 (89%)	22 (10%)	1 (0%)	32	72
1	B	204/248 (82%)	187 (92%)	17 (8%)	0	100	100
1	C	217/248 (88%)	191 (88%)	25 (12%)	1 (0%)	32	72
1	D	209/248 (84%)	190 (91%)	17 (8%)	2 (1%)	18	57
All	All	847/992 (85%)	762 (90%)	81 (10%)	4 (0%)	32	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	LEU
1	A	44	LEU
1	D	113	ASN
1	C	55	VAL

### 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	180/228 (79%)	170 (94%)	10 (6%)	25	61
1	B	171/228 (75%)	158 (92%)	13 (8%)	15	47
1	C	175/228 (77%)	167 (95%)	8 (5%)	31	69
1	D	169/228 (74%)	159 (94%)	10 (6%)	23	59
All	All	695/912 (76%)	654 (94%)	41 (6%)	23	59

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	36	THR
1	A	80	ASN
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	132	SER
1	A	166	PHE
1	A	169	SER
1	A	221	LEU
1	A	230	GLU
1	A	256	PHE
1	B	34	LYS
1	B	53	GLU
1	B	62	GLN
1	B	80	ASN
1	B	90	GLU
1	B	104	ARG
1	B	130	VAL
1	B	132	SER
1	B	150	THR
1	B	156	GLN
1	B	166	PHE
1	B	168	GLN
1	B	249	LEU
1	C	80	ASN
1	C	95	THR
1	C	112	LEU
1	C	132	SER
1	C	150	THR
1	C	166	PHE
1	C	168	GLN
1	C	169	SER
1	D	34	LYS
1	D	80	ASN
1	D	93	SER
1	D	104	ARG
1	D	106	ARG
1	D	112	LEU
1	D	128	ARG
1	D	132	SER
1	D	140	ASN
1	D	166	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	97	GLN
1	A	165	GLN
1	A	179	GLN
1	B	80	ASN
1	B	97	GLN
1	B	108	GLN
1	B	156	GLN
1	B	163	ASN
1	B	165	GLN
1	B	198	GLN
1	B	209	HIS
1	B	212	HIS
1	C	80	ASN
1	C	97	GLN
1	C	165	GLN
1	D	80	ASN
1	D	97	GLN
1	D	140	ASN
1	D	163	ASN
1	D	165	GLN
1	D	209	HIS
1	D	224	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 6 ligands modelled in this entry, 2 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	DCZ	A	302	-	14,17,17	1.57	3 (21%)	17,24,24	1.27	3 (17%)
3	DCZ	B	402	-	14,17,17	1.27	2 (14%)	17,24,24	1.27	2 (11%)
3	DCZ	C	502	-	14,17,17	1.50	3 (21%)	17,24,24	1.34	3 (17%)
3	DCZ	D	602	-	14,17,17	1.38	3 (21%)	17,24,24	1.19	2 (11%)

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	DCZ	A	302	-	-	0/2/18/18	0/2/2/2
3	DCZ	B	402	-	-	0/2/18/18	0/2/2/2
3	DCZ	C	502	-	-	0/2/18/18	0/2/2/2
3	DCZ	D	602	-	-	0/2/18/18	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	DCZ	C5-C4	-3.53	1.32	1.41
3	C	502	DCZ	C5-C4	-3.50	1.32	1.41
3	D	602	DCZ	C5-C4	-2.95	1.33	1.41
3	B	402	DCZ	C5-C4	-2.82	1.34	1.41
3	A	302	DCZ	C6-C5	-2.74	1.32	1.38
3	C	502	DCZ	C6-C5	-2.52	1.32	1.38
3	D	602	DCZ	C6-C5	-2.47	1.32	1.38
3	B	402	DCZ	C6-C5	-2.33	1.33	1.38
3	D	602	DCZ	O4'-C1'	2.16	1.47	1.42
3	C	502	DCZ	O4'-C1'	2.24	1.47	1.42
3	A	302	DCZ	O4'-C1'	2.42	1.47	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	DCZ	C6-N1-C2	-3.12	116.22	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	DCZ	C6-N1-C2	-2.78	116.78	121.28
3	B	402	DCZ	C6-N1-C2	-2.75	116.82	121.28
3	A	302	DCZ	C6-N1-C2	-2.51	117.21	121.28
3	A	302	DCZ	C2'-C3'-C4'	2.19	107.39	102.73
3	C	502	DCZ	C2'-C3'-C4'	2.20	107.41	102.73
3	D	602	DCZ	C2'-C1'-N1	2.23	119.51	114.23
3	B	402	DCZ	C2'-C1'-N1	2.60	120.38	114.23
3	A	302	DCZ	C2'-C1'-N1	2.71	120.64	114.23
3	C	502	DCZ	C2'-C1'-N1	2.87	121.01	114.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	DCZ	1	0
3	B	402	DCZ	1	0
3	D	602	DCZ	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	221/248 (89%)	-0.57	1 (0%) 90 73	40, 66, 100, 109	0
1	B	212/248 (85%)	-0.49	1 (0%) 90 73	48, 71, 96, 108	0
1	C	221/248 (89%)	-0.54	2 (0%) 84 61	38, 66, 101, 108	0
1	D	215/248 (86%)	-0.40	4 (1%) 67 37	47, 73, 101, 108	0
All	All	869/992 (87%)	-0.50	8 (0%) 84 61	38, 70, 101, 109	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	PRO	3.3
1	A	46	GLU	2.9
1	D	167	GLY	2.7
1	C	116	LEU	2.7
1	C	118	ASP	2.7
1	D	248	SER	2.6
1	D	98	THR	2.1
1	B	118	ASP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DCZ	D	602	16/16	0.95	0.22	0.77	63,70,71,71	0
3	DCZ	A	302	16/16	0.97	0.19	0.23	36,41,46,46	0
3	DCZ	C	502	16/16	0.96	0.18	-0.10	40,42,47,49	0
3	DCZ	B	402	16/16	0.97	0.17	-0.25	45,51,54,55	0
2	CA	A	261	1/1	0.91	0.11	-1.94	75,75,75,75	0
2	CA	C	261	1/1	0.93	0.09	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.