



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:58 AM GMT

PDB ID : 3KEE  
Title : HCV NS3/NS4A complexed with Non-covalent macrocyclic compound TMC435  
Authors : Lindberg, J.D.; Nystrom, S.; Cummings, M.D.  
Deposited on : 2009-10-26  
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](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 (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

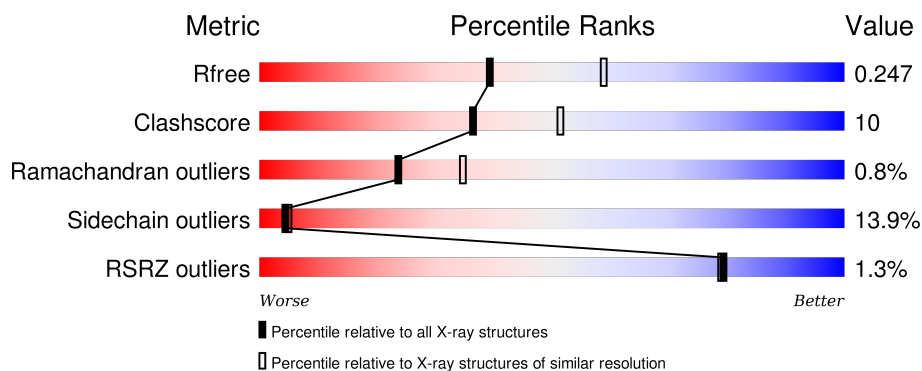
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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  $\geq 3$ , 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	190	 2% 71% 18% 5% 6%
1	B	190	 1% 66% 23% • 6%
1	C	190	 1% 67% 22% • 6%
1	D	190	 2% 71% 18% • 6%
2	E	23	 48% 48%

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Mol	Chain	Length	Quality of chain
2	F	23	<div><div></div><div>43%9%48%</div></div>
2	G	23	<div><div>4%</div><div>43%9%48%</div></div>
2	H	23	<div><div></div><div>43%. .48%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5877 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			
1	B	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			
1	C	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			
1	D	178	Total	C	N	O	S	0	0	0
			1312	815	238	249	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P90191
A	181	SER	-	EXPRESSION TAG	UNP P90191
A	182	GLY	-	EXPRESSION TAG	UNP P90191
A	183	SER	-	EXPRESSION TAG	UNP P90191
A	184	HIS	-	EXPRESSION TAG	UNP P90191
A	185	HIS	-	EXPRESSION TAG	UNP P90191
A	186	HIS	-	EXPRESSION TAG	UNP P90191
A	187	HIS	-	EXPRESSION TAG	UNP P90191
A	188	HIS	-	EXPRESSION TAG	UNP P90191
A	189	HIS	-	EXPRESSION TAG	UNP P90191
B	0	MET	-	EXPRESSION TAG	UNP P90191
B	181	SER	-	EXPRESSION TAG	UNP P90191
B	182	GLY	-	EXPRESSION TAG	UNP P90191
B	183	SER	-	EXPRESSION TAG	UNP P90191
B	184	HIS	-	EXPRESSION TAG	UNP P90191
B	185	HIS	-	EXPRESSION TAG	UNP P90191
B	186	HIS	-	EXPRESSION TAG	UNP P90191
B	187	HIS	-	EXPRESSION TAG	UNP P90191
B	188	HIS	-	EXPRESSION TAG	UNP P90191
B	189	HIS	-	EXPRESSION TAG	UNP P90191
C	0	MET	-	EXPRESSION TAG	UNP P90191

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Chain	Residue	Modelled	Actual	Comment	Reference
C	181	SER	-	EXPRESSION TAG	UNP P90191
C	182	GLY	-	EXPRESSION TAG	UNP P90191
C	183	SER	-	EXPRESSION TAG	UNP P90191
C	184	HIS	-	EXPRESSION TAG	UNP P90191
C	185	HIS	-	EXPRESSION TAG	UNP P90191
C	186	HIS	-	EXPRESSION TAG	UNP P90191
C	187	HIS	-	EXPRESSION TAG	UNP P90191
C	188	HIS	-	EXPRESSION TAG	UNP P90191
C	189	HIS	-	EXPRESSION TAG	UNP P90191
D	0	MET	-	EXPRESSION TAG	UNP P90191
D	181	SER	-	EXPRESSION TAG	UNP P90191
D	182	GLY	-	EXPRESSION TAG	UNP P90191
D	183	SER	-	EXPRESSION TAG	UNP P90191
D	184	HIS	-	EXPRESSION TAG	UNP P90191
D	185	HIS	-	EXPRESSION TAG	UNP P90191
D	186	HIS	-	EXPRESSION TAG	UNP P90191
D	187	HIS	-	EXPRESSION TAG	UNP P90191
D	188	HIS	-	EXPRESSION TAG	UNP P90191
D	189	HIS	-	EXPRESSION TAG	UNP P90191

- Molecule 2 is a protein called 19-mer peptide from Genome polyprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	0	0
			86	57	16	13			
2	F	12	Total	C	N	O	0	0	0
			86	57	16	13			
2	G	12	Total	C	N	O	0	0	0
			86	57	16	13			
2	H	12	Total	C	N	O	0	0	0
			86	57	16	13			

There are 16 discrepancies between the modelled and reference sequences:

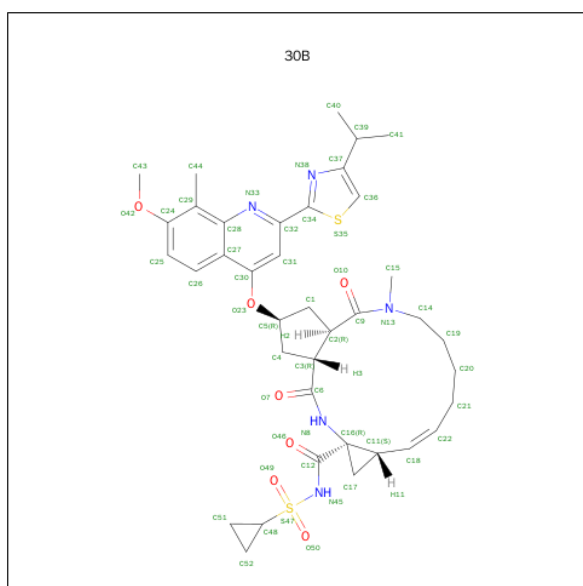
Chain	Residue	Modelled	Actual	Comment	Reference
E	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
E	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
E	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8
E	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8
F	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
F	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
F	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8
G	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	19	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	20	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	40	LYS	-	EXPRESSION TAG	UNP Q6GYR8
H	41	LYS	-	EXPRESSION TAG	UNP Q6GYR8

- Molecule 3 is (2R,3AR,10Z,11AS,12AR,14AR)-N-(CYCLOPROPYLSULFONYL)-2-({7-METHOXY-8-METHYL-2-[4-(1-METHYLETHYL)-1,3-THIAZOL-2-YL]QUINOLIN-4-YL}OXY)-5-METHYL-4,14-DIOXO-2,3,3A,4,5,6,7,8,9,11A,12,13,14,14A-TETRADECAHYDROCYCLOPENTA[C]CYCLOPROPA[G][1,6]DIAZACYCLOTETRADECINE-12A(1H)-CARBOXAMIDE (three-letter code: 30B) (formula: C<sub>38</sub>H<sub>47</sub>N<sub>5</sub>O<sub>7</sub>S<sub>2</sub>).

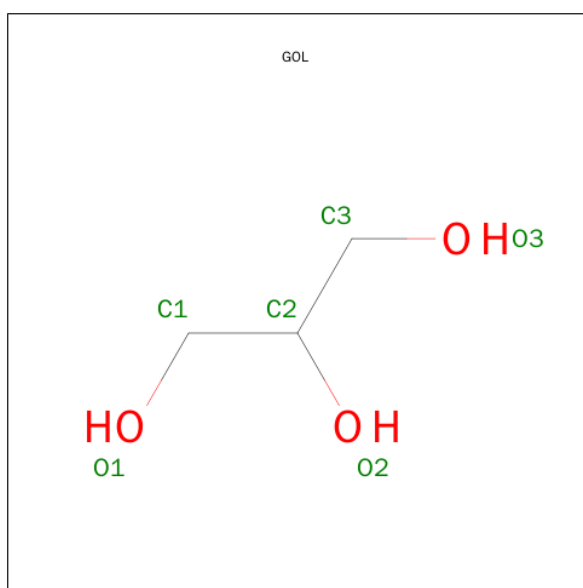


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			52	38	5	7	2		
3	B	1	Total	C	N	O	S	0	0
			52	38	5	7	2		
3	C	1	Total	C	N	O	S	0	0
			52	38	5	7	2		
3	D	1	Total	C	N	O	S	0	0
			52	38	5	7	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 12	C 6	O 6	0	1
5	D	1	Total 12	C 6	O 6	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total 11	O 11	0	0
6	E	1	Total 1	O 1	0	0
6	B	11	Total 11	O 11	0	0
6	F	1	Total 1	O 1	0	0

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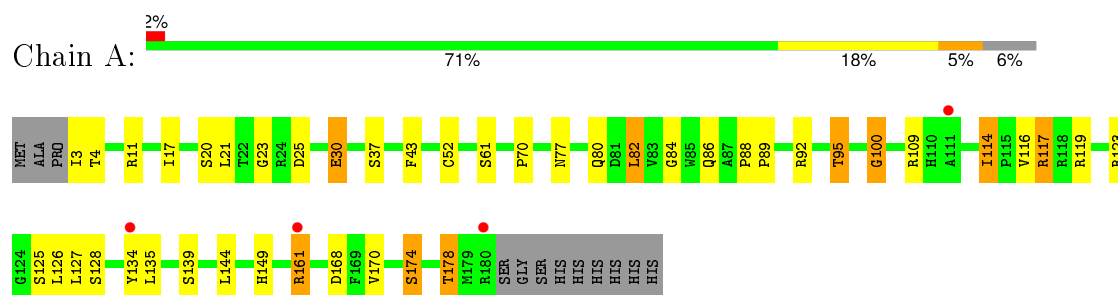
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	10	Total 10	O 10	0	0
6	D	13	Total 13	O 13	0	0
6	H	2	Total 2	O 2	0	0



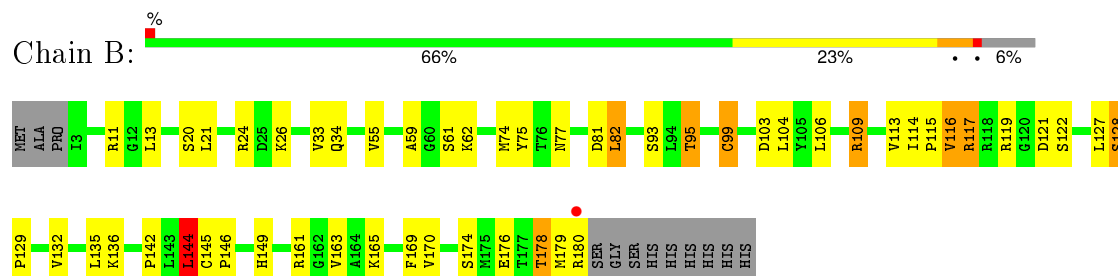
### 3 Residue-property plots [i](#)

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.

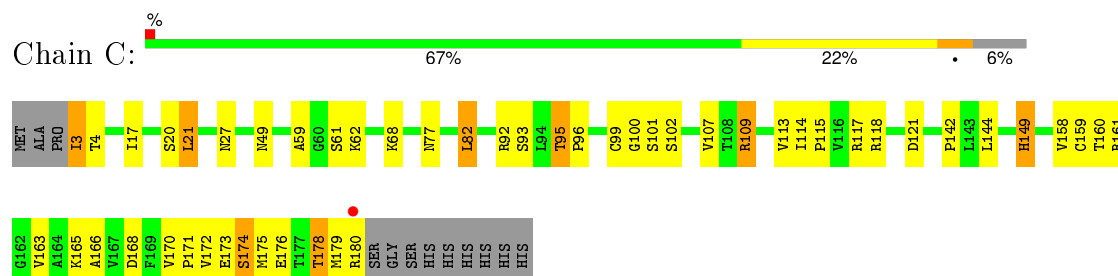
- Molecule 1: Genome polyprotein



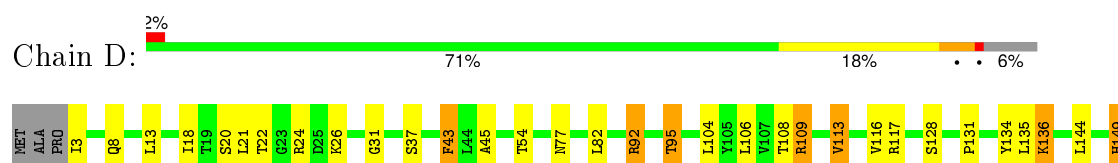
- Molecule 1: Genome polyprotein

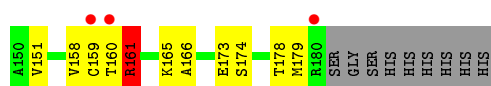


- Molecule 1: Genome polyprotein

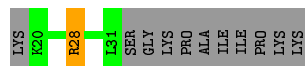


- Molecule 1: Genome polyprotein





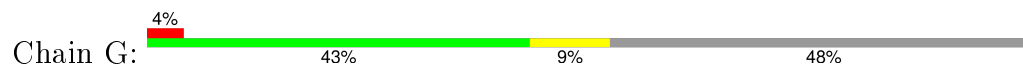
- Molecule 2: 19-mer peptide from Genome polyprotein



- Molecule 2: 19-mer peptide from Genome polyprotein



- Molecule 2: 19-mer peptide from Genome polyprotein



- Molecule 2: 19-mer peptide from Genome polyprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.03Å 54.45Å 85.50Å 92.44° 93.16° 116.04°	Depositor
Resolution (Å)	48.80 – 2.40 48.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.80-2.40) 93.6 (48.79-2.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.246 0.198 , 0.247	Depositor DCC
$R_{free}$ test set	1461 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29045 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, 30B

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	0.73	0/1337	0.82	1/1820 (0.1%)
1	B	0.68	0/1337	0.88	2/1820 (0.1%)
1	C	0.71	0/1337	0.83	0/1820
1	D	0.70	1/1337 (0.1%)	0.84	2/1820 (0.1%)
2	E	0.83	0/85	0.77	0/113
2	F	0.82	0/85	0.76	0/113
2	G	0.72	0/85	0.79	0/113
2	H	0.73	0/85	0.78	0/113
All	All	0.71	1/5688 (0.0%)	0.84	5/7732 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	CYS	CB-SG	5.22	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	99	CYS	CA-C-N	6.50	129.21	116.20
1	D	109	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	92	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	144	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1312	0	1318	34	0
1	B	1312	0	1318	32	0
1	C	1312	0	1318	37	0
1	D	1312	0	1318	26	0
2	E	86	0	105	1	0
2	F	86	0	105	1	0
2	G	86	0	105	1	0
2	H	86	0	105	3	0
3	A	52	0	47	2	0
3	B	52	0	47	0	0
3	C	52	0	47	1	0
3	D	52	0	47	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	C	12	0	16	1	0
5	D	12	0	16	2	0
6	A	11	0	0	3	0
6	B	11	0	0	1	0
6	C	10	0	0	0	0
6	D	13	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	H	2	0	0	0	0
All	All	5877	0	5912	112	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 10.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:CG2	1:C:95:THR:HG22	1.61	1.31
1:A:114:ILE:HG21	6:A:196:HOH:O	1.46	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG23	1:C:95:THR:HG22	1.28	1.10
1:A:114:ILE:HD11	1:A:126:LEU:HD22	1.21	1.08
1:B:95:THR:HG22	1:D:95:THR:CG2	1.86	1.05
1:B:95:THR:HG22	1:D:95:THR:HG23	1.33	1.04
1:D:160:THR:O	1:D:161:ARG:HB2	1.56	1.02
1:C:179:MET:O	1:C:180:ARG:HB2	1.57	1.02
1:A:174:SER:O	1:A:178:THR:HG23	1.67	0.93
1:A:95:THR:HG23	1:C:95:THR:CG2	2.02	0.89
1:A:95:THR:HG21	1:C:95:THR:HG22	1.56	0.87
1:D:174:SER:O	1:D:178:THR:HG23	1.75	0.86
1:A:95:THR:CG2	1:C:95:THR:CG2	2.52	0.86
1:C:142:PRO:HB2	1:C:144:LEU:HD13	1.65	0.76
1:A:95:THR:HB	1:C:93:SER:O	1.87	0.75
1:C:179:MET:O	1:C:180:ARG:CB	2.35	0.74
1:A:161:ARG:HB3	1:A:161:ARG:HH11	1.50	0.74
1:B:82:LEU:HG	1:B:170:VAL:HG11	1.69	0.73
1:D:158:VAL:HB	1:D:166:ALA:HB3	1.70	0.72
1:B:99:CYS:SG	1:B:99:CYS:O	2.47	0.71
1:A:161:ARG:HB3	1:A:161:ARG:NH1	2.06	0.70
1:B:149:HIS:CE1	1:D:149:HIS:HE1	2.11	0.68
1:B:109:ARG:NH1	5:D:3968[A]:GOL:H11	2.09	0.67
1:C:174:SER:O	1:C:178:THR:HG22	1.95	0.67
1:B:95:THR:HG22	1:D:95:THR:HG21	1.74	0.66
1:C:62:LYS:HB2	2:G:23:VAL:HG23	1.77	0.66
1:B:142:PRO:HB2	1:B:144:LEU:HD13	1.79	0.65
1:C:107:VAL:HB	1:C:142:PRO:HG2	1.78	0.65
1:C:142:PRO:HB2	1:C:144:LEU:CD1	2.26	0.64
1:A:86:GLN:OE1	1:C:68:LYS:HE3	1.97	0.64
1:A:114:ILE:HD11	1:A:126:LEU:CD2	2.14	0.62
1:C:59:ALA:O	1:C:62:LYS:HG2	2.00	0.60
1:A:123:ARG:NH1	1:A:168:ASP:OD1	2.35	0.60
1:B:24:ARG:HE	1:B:26:LYS:HE3	1.67	0.59
1:D:160:THR:O	1:D:161:ARG:CB	2.41	0.58
1:C:158:VAL:HB	1:C:166:ALA:HB3	1.86	0.58
1:B:74:MET:HB2	1:B:75:TYR:CD2	2.39	0.57
1:C:49:ASN:HD21	1:C:96:PRO:CG	2.17	0.57
1:B:149:HIS:CE1	1:D:149:HIS:CE1	2.93	0.57
1:B:122:SER:HB2	1:B:169:PHE:O	2.06	0.56
1:D:108:THR:O	2:H:29:ILE:CD1	2.54	0.55
1:C:102:SER:HA	1:C:118:ARG:HB3	1.88	0.55
1:A:86:GLN:OE1	1:C:68:LYS:CE	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HB	2:F:29:ILE:HB	1.89	0.54
1:B:115:PRO:HB2	1:B:127:LEU:HG	1.90	0.52
1:A:30:GLU:HG3	2:E:28:ARG:CZ	2.40	0.52
1:A:95:THR:HG21	1:C:95:THR:CG2	2.31	0.51
1:A:17:ILE:O	1:A:20:SER:HB3	2.11	0.51
1:B:93:SER:O	1:D:95:THR:CG2	2.60	0.50
1:C:82:LEU:HG	1:C:170:VAL:HG11	1.93	0.50
1:D:18:ILE:O	1:D:22:THR:HG23	2.12	0.50
1:A:3:ILE:N	1:A:3:ILE:HD12	2.27	0.50
1:C:160:THR:O	1:C:163:VAL:HG22	2.11	0.49
1:B:59:ALA:O	1:B:62:LYS:HG3	2.13	0.49
1:D:43:PHE:CD1	1:D:43:PHE:N	2.79	0.49
1:C:99:CYS:O	1:C:101:SER:N	2.46	0.49
1:A:11:ARG:HH12	1:A:25:ASP:CG	2.16	0.48
1:A:134:TYR:HE2	6:A:196:HOH:O	1.97	0.48
1:C:109:ARG:HD3	5:C:3968[B]:GOL:O2	2.12	0.48
1:D:31:GLY:H	1:D:92:ARG:HD3	1.78	0.48
1:B:178:THR:C	1:B:180:ARG:H	2.17	0.47
1:B:34:GLN:NE2	6:B:194:HOH:O	2.46	0.47
1:A:119:ARG:HD3	1:A:125:SER:HB3	1.96	0.47
1:D:160:THR:O	1:D:160:THR:HG22	2.15	0.47
1:C:171:PRO:HB2	1:C:173:GLU:HG2	1.96	0.47
1:C:17:ILE:O	1:C:21:LEU:HD22	2.15	0.47
1:C:174:SER:O	1:C:178:THR:CG2	2.62	0.47
1:A:117:ARG:HH22	1:B:119:ARG:HB3	1.80	0.47
1:B:104:LEU:HB2	1:B:116:VAL:HG22	1.96	0.46
1:B:109:ARG:HH11	5:D:3968[A]:GOL:H11	1.80	0.46
1:D:131:PRO:O	1:D:134:TYR:HB3	2.16	0.46
1:C:107:VAL:HB	1:C:142:PRO:CG	2.46	0.46
1:B:149:HIS:HE1	1:D:149:HIS:CE1	2.33	0.46
1:C:176:GLU:HA	1:C:179:MET:CE	2.46	0.46
1:A:149:HIS:HE1	1:C:149:HIS:CE1	2.34	0.46
1:B:115:PRO:O	1:B:116:VAL:HG12	2.16	0.45
1:A:77:ASN:OD1	1:A:80:GLN:HB2	2.17	0.45
1:D:173:GLU:H	1:D:173:GLU:CD	2.20	0.45
1:D:8:GLN:OE1	2:H:28:ARG:HD3	2.16	0.45
1:D:24:ARG:HE	1:D:26:LYS:HE2	1.83	0.44
1:A:139:SER:HB3	3:A:500:30B:C12	2.48	0.44
1:C:159:CYS:HA	1:C:163:VAL:O	2.18	0.44
1:A:82:LEU:HG	1:A:170:VAL:HG11	1.99	0.44
1:B:104:LEU:HA	1:B:144:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ILE:HA	1:C:115:PRO:HD3	1.79	0.43
1:D:108:THR:O	2:H:29:ILE:HD11	2.18	0.43
1:B:55:VAL:HA	1:B:81:ASP:O	2.17	0.43
1:C:3:ILE:HG21	1:C:144:LEU:HD23	1.99	0.43
3:D:500:30B:H11	3:D:500:30B:H21	1.78	0.43
1:A:100:GLY:O	1:B:117:ARG:NH1	2.42	0.43
1:A:114:ILE:HD13	6:A:196:HOH:O	2.19	0.43
1:A:43:PHE:CD1	1:A:43:PHE:N	2.87	0.42
1:A:23:GLY:HA3	1:A:70:PRO:HG3	2.01	0.42
1:C:49:ASN:HD21	1:C:96:PRO:HG3	1.83	0.42
3:A:500:30B:H2	3:A:500:30B:H15B	1.98	0.42
1:B:106:LEU:HD23	1:B:114:ILE:HD11	2.02	0.42
1:C:59:ALA:O	1:C:62:LYS:CG	2.65	0.42
3:C:500:30B:H21	3:C:500:30B:H11	1.99	0.42
1:B:145:CYS:HB2	1:B:146:PRO:CD	2.50	0.42
1:D:104:LEU:HD22	1:D:151:VAL:HG21	2.02	0.42
1:B:128:SER:HA	1:B:129:PRO:HD2	1.75	0.41
1:C:17:ILE:O	1:C:20:SER:HB3	2.20	0.41
1:C:175:MET:O	1:C:179:MET:HG3	2.21	0.41
1:D:136:LYS:HD2	3:D:500:30B:O49	2.19	0.41
1:A:117:ARG:HH12	1:B:119:ARG:HD2	1.85	0.41
1:D:92:ARG:HG2	1:D:92:ARG:NH1	2.35	0.41
1:B:24:ARG:HH21	1:B:26:LYS:NZ	2.19	0.41
1:D:45:ALA:HB2	1:D:54:THR:HB	2.03	0.41
1:D:106:LEU:O	1:D:113:VAL:HA	2.21	0.41
1:A:88:PRO:HA	1:A:89:PRO:HD3	1.98	0.40
1:B:174:SER:O	1:B:178:THR:CG2	2.69	0.40
1:A:52:CYS:O	1:A:84:GLY:HA2	2.21	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	176/190 (93%)	170 (97%)	5 (3%)	1 (1%)	30	43
1	B	176/190 (93%)	170 (97%)	5 (3%)	1 (1%)	30	43
1	C	176/190 (93%)	168 (96%)	6 (3%)	2 (1%)	17	25
1	D	176/190 (93%)	170 (97%)	4 (2%)	2 (1%)	17	25
2	E	10/23 (44%)	10 (100%)	0	0	100	100
2	F	10/23 (44%)	10 (100%)	0	0	100	100
2	G	10/23 (44%)	10 (100%)	0	0	100	100
2	H	10/23 (44%)	10 (100%)	0	0	100	100
All	All	744/852 (87%)	718 (96%)	20 (3%)	6 (1%)	24	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	GLY
1	D	161	ARG
1	A	100	GLY
1	C	27	ASN
1	B	179	MET
1	D	179	MET

### 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	145/155 (94%)	127 (88%)	18 (12%)	6	7
1	B	145/155 (94%)	121 (83%)	24 (17%)	3	3
1	C	145/155 (94%)	126 (87%)	19 (13%)	5	6
1	D	145/155 (94%)	124 (86%)	21 (14%)	4	4
2	E	10/19 (53%)	9 (90%)	1 (10%)	9	14
2	F	10/19 (53%)	9 (90%)	1 (10%)	9	14
2	G	10/19 (53%)	9 (90%)	1 (10%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	10/19 (53%)	9 (90%)	1 (10%)	9	14
All	All	620/696 (89%)	534 (86%)	86 (14%)	4	5

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	21	LEU
1	A	30	GLU
1	A	37	SER
1	A	61	SER
1	A	82	LEU
1	A	95	THR
1	A	109	ARG
1	A	114	ILE
1	A	116	VAL
1	A	117	ARG
1	A	127	LEU
1	A	128	SER
1	A	135	LEU
1	A	144	LEU
1	A	161	ARG
1	A	174	SER
1	A	178	THR
2	E	28	ARG
1	B	11	ARG
1	B	13	LEU
1	B	20	SER
1	B	21	LEU
1	B	61	SER
1	B	77	ASN
1	B	82	LEU
1	B	95	THR
1	B	103	ASP
1	B	109	ARG
1	B	113	VAL
1	B	116	VAL
1	B	117	ARG
1	B	121	ASP
1	B	128	SER
1	B	132	VAL
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	136	LYS
1	B	144	LEU
1	B	161	ARG
1	B	163	VAL
1	B	165	LYS
1	B	176	GLU
1	B	178	THR
2	F	28	ARG
1	C	3	ILE
1	C	4	THR
1	C	21	LEU
1	C	61	SER
1	C	77	ASN
1	C	82	LEU
1	C	92	ARG
1	C	95	THR
1	C	109	ARG
1	C	113	VAL
1	C	117	ARG
1	C	121	ASP
1	C	149	HIS
1	C	161	ARG
1	C	165	LYS
1	C	168	ASP
1	C	172	VAL
1	C	174	SER
1	C	178	THR
2	G	28	ARG
1	D	3	ILE
1	D	13	LEU
1	D	20	SER
1	D	21	LEU
1	D	37	SER
1	D	43	PHE
1	D	77	ASN
1	D	82	LEU
1	D	92	ARG
1	D	95	THR
1	D	109	ARG
1	D	113	VAL
1	D	116	VAL
1	D	117	ARG

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Mol	Chain	Res	Type
1	D	128	SER
1	D	135	LEU
1	D	136	LYS
1	D	144	LEU
1	D	149	HIS
1	D	161	ARG
1	D	165	LYS
2	H	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	34	GLN
1	A	149	HIS
1	B	27	ASN
1	B	34	GLN
1	B	77	ASN
1	B	149	HIS
1	C	9	GLN
1	C	27	ASN
1	C	49	ASN
1	C	77	ASN
1	D	9	GLN
1	D	27	ASN
1	D	49	ASN
1	D	149	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	30B	A	500	-	51,58,58	1.42	9 (17%)	61,88,88	2.85	14 (22%)
3	30B	B	500	-	51,58,58	1.41	5 (9%)	61,88,88	2.86	19 (31%)
5	GOL	C	3968[A]	-	5,5,5	0.24	0	5,5,5	0.42	0
5	GOL	C	3968[B]	-	5,5,5	0.30	0	5,5,5	0.31	0
3	30B	C	500	-	51,58,58	1.41	5 (9%)	61,88,88	2.72	14 (22%)
5	GOL	D	3968[A]	-	5,5,5	0.37	0	5,5,5	0.38	0
5	GOL	D	3968[B]	-	5,5,5	0.37	0	5,5,5	0.38	0
3	30B	D	500	-	51,58,58	1.52	6 (11%)	61,88,88	2.65	17 (27%)

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	30B	A	500	-	-	0/51/79/79	0/4/7/7
3	30B	B	500	-	-	0/51/79/79	0/4/7/7
5	GOL	C	3968[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3968[B]	-	-	0/4/4/4	0/0/0/0
3	30B	C	500	-	-	0/51/79/79	0/4/7/7
5	GOL	D	3968[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3968[B]	-	-	0/4/4/4	0/0/0/0
3	30B	D	500	-	-	0/51/79/79	0/4/7/7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	30B	S47-N45	-3.54	1.53	1.62
3	A	500	30B	S47-N45	-3.39	1.53	1.62
3	B	500	30B	S47-N45	-3.25	1.54	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	30B	C12-N45	-2.78	1.32	1.37
3	D	500	30B	S47-N45	-2.44	1.56	1.62
3	B	500	30B	C28-N33	-2.34	1.32	1.37
3	C	500	30B	O49-S47	-2.01	1.41	1.43
3	A	500	30B	C2-C9	2.00	1.56	1.51
3	A	500	30B	C26-C25	2.05	1.40	1.36
3	D	500	30B	C17-C16	2.14	1.53	1.51
3	A	500	30B	C17-C16	2.21	1.53	1.51
3	A	500	30B	C3-C6	2.25	1.55	1.52
3	D	500	30B	C34-S35	2.80	1.77	1.73
3	A	500	30B	C34-S35	3.04	1.77	1.73
3	D	500	30B	C11-C18	3.35	1.53	1.50
3	B	500	30B	O42-C24	3.46	1.42	1.37
3	D	500	30B	O42-C24	3.48	1.42	1.37
3	B	500	30B	C11-C18	3.62	1.53	1.50
3	A	500	30B	C11-C18	3.66	1.54	1.50
3	C	500	30B	C11-C18	3.74	1.54	1.50
3	C	500	30B	O42-C24	3.82	1.43	1.37
3	A	500	30B	C36-S35	3.97	1.76	1.70
3	C	500	30B	C36-S35	5.28	1.78	1.70
3	B	500	30B	C36-S35	5.63	1.79	1.70
3	D	500	30B	C36-S35	6.55	1.80	1.70

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	30B	C36-C37-C39	-13.91	108.64	129.21
3	C	500	30B	C36-C37-C39	-10.38	113.86	129.21
3	B	500	30B	C36-C37-C39	-9.59	115.03	129.21
3	B	500	30B	C11-C16-N8	-9.47	98.55	117.66
3	D	500	30B	O50-S47-O49	-8.02	106.16	119.34
3	D	500	30B	C11-C16-N8	-8.01	101.50	117.66
3	C	500	30B	O50-S47-O49	-7.97	106.24	119.34
3	C	500	30B	C11-C16-N8	-7.94	101.63	117.66
3	A	500	30B	C11-C16-N8	-7.90	101.71	117.66
3	D	500	30B	C36-C37-C39	-7.30	118.41	129.21
3	B	500	30B	O50-S47-O49	-5.34	110.58	119.34
3	B	500	30B	O42-C24-C25	-4.43	116.89	124.35
3	A	500	30B	O50-S47-O49	-4.38	112.15	119.34
3	D	500	30B	O42-C24-C25	-4.24	117.21	124.35
3	D	500	30B	C31-C32-C34	-3.68	115.82	120.18
3	A	500	30B	O42-C24-C25	-3.20	118.97	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	30B	C25-C26-C27	-3.11	117.04	121.13
3	C	500	30B	O42-C24-C25	-3.07	119.19	124.35
3	A	500	30B	C41-C39-C37	-2.78	105.36	112.01
3	D	500	30B	C3-C6-N8	-2.75	112.66	116.30
3	C	500	30B	C3-C6-N8	-2.74	112.67	116.30
3	A	500	30B	C17-C11-C18	-2.63	113.57	119.32
3	B	500	30B	C19-C14-N13	-2.54	103.17	112.53
3	B	500	30B	C3-C6-N8	-2.47	113.03	116.30
3	B	500	30B	C40-C39-C37	-2.38	106.31	112.01
3	D	500	30B	C40-C39-C37	-2.30	106.51	112.01
3	A	500	30B	C26-C25-C24	-2.09	116.35	119.80
3	B	500	30B	C12-N45-S47	-2.08	120.07	123.88
3	D	500	30B	C1-C2-C9	2.04	117.05	112.63
3	B	500	30B	C11-C16-C12	2.05	120.95	117.09
3	D	500	30B	O7-C6-C3	2.05	123.92	121.56
3	C	500	30B	C1-C2-C9	2.06	117.10	112.63
3	A	500	30B	O23-C5-C4	2.14	114.48	108.70
3	C	500	30B	C32-N33-C28	2.20	119.69	118.33
3	C	500	30B	C17-C16-N8	2.21	120.91	117.84
3	B	500	30B	C44-C29-C24	2.29	124.17	120.80
3	B	500	30B	O7-C6-C3	2.32	124.22	121.56
3	B	500	30B	C1-C2-C9	2.36	117.75	112.63
3	B	500	30B	C4-C5-C1	2.47	108.44	104.63
3	D	500	30B	C43-O42-C24	2.51	121.35	117.54
3	D	500	30B	C32-N33-C28	2.65	119.96	118.33
3	A	500	30B	C29-C28-N33	2.83	120.66	117.59
3	D	500	30B	C29-C28-N33	2.86	120.69	117.59
3	C	500	30B	C4-C5-C1	2.87	109.06	104.63
3	C	500	30B	O23-C30-C27	2.96	118.68	114.36
3	D	500	30B	C39-C37-N38	3.06	125.61	120.26
3	B	500	30B	C32-N33-C28	3.24	120.33	118.33
3	A	500	30B	C16-N8-C6	3.29	128.62	121.51
3	D	500	30B	O23-C30-C27	3.53	119.51	114.36
3	A	500	30B	O23-C30-C27	3.62	119.63	114.36
3	A	500	30B	O42-C24-C29	3.65	118.08	115.04
3	B	500	30B	C39-C37-N38	3.70	126.72	120.26
3	B	500	30B	O23-C30-C27	3.85	119.97	114.36
3	D	500	30B	C16-N8-C6	3.99	130.13	121.51
3	C	500	30B	C16-N8-C6	4.40	131.02	121.51
3	C	500	30B	C39-C37-N38	4.65	128.38	120.26
3	C	500	30B	O42-C24-C29	5.30	119.45	115.04
3	D	500	30B	C12-C16-N8	6.26	123.55	116.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	30B	C39-C37-N38	6.57	131.75	120.26
3	D	500	30B	O42-C24-C29	7.09	120.95	115.04
3	A	500	30B	C12-C16-N8	7.47	124.98	116.09
3	C	500	30B	C12-C16-N8	7.53	125.06	116.09
3	B	500	30B	C12-C16-N8	7.87	125.46	116.09
3	B	500	30B	O42-C24-C29	8.72	122.31	115.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	30B	2	0
5	C	3968[B]	GOL	1	0
3	C	500	30B	1	0
5	D	3968[A]	GOL	2	0
3	D	500	30B	2	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 ⓘ

### 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<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	178/190 (93%)	-0.19	4 (2%) 65 64	11, 22, 36, 51	1 (0%)
1	B	178/190 (93%)	-0.26	1 (0%) 90 90	13, 24, 38, 46	1 (0%)
1	C	178/190 (93%)	-0.31	1 (0%) 90 90	11, 24, 39, 48	1 (0%)
1	D	178/190 (93%)	-0.23	3 (1%) 73 72	12, 24, 39, 49	1 (0%)
2	E	12/23 (52%)	-0.30	0 100 100	19, 24, 31, 35	0
2	F	12/23 (52%)	-0.36	0 100 100	19, 23, 28, 37	0
2	G	12/23 (52%)	-0.32	1 (8%) 14 14	19, 22, 29, 39	0
2	H	12/23 (52%)	-0.49	0 100 100	19, 24, 32, 37	0
All	All	760/852 (89%)	-0.25	10 (1%) 79 79	11, 24, 38, 51	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ARG	5.6
1	A	161	ARG	4.6
1	C	180	ARG	4.6
1	B	180	ARG	4.1
1	D	180	ARG	3.9
1	D	160	THR	2.7
1	A	134	TYR	2.7
1	A	111	ALA	2.4
1	D	159	CYS	2.3
2	G	20	LYS	2.1

### 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 [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
4	ZN	C	2000	1/1	0.99	0.11	-0.35	31,31,31,31	0
3	30B	C	500	52/52	0.97	0.12	-0.41	9,14,17,18	0
4	ZN	D	2000	1/1	1.00	0.10	-0.51	27,27,27,27	0
3	30B	B	500	52/52	0.97	0.12	-0.54	5,13,17,19	0
3	30B	A	500	52/52	0.97	0.12	-0.68	4,10,17,17	0
3	30B	D	500	52/52	0.97	0.12	-0.79	6,15,19,23	0
4	ZN	B	2000	1/1	0.98	0.11	-1.26	32,32,32,32	0
4	ZN	A	2000	1/1	0.99	0.10	-1.73	24,24,24,24	0
5	GOL	D	3968[A]	6/6	0.95	0.20	-	33,34,34,34	6
5	GOL	D	3968[B]	6/6	0.95	0.20	-	25,27,27,28	6
5	GOL	C	3968[B]	6/6	0.91	0.20	-	28,29,30,31	6
5	GOL	C	3968[A]	6/6	0.91	0.20	-	34,35,35,35	6

### 6.5 Other polymers [i](#)

There are no such residues in this entry.