



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 05:27 PM EST

PDB ID : 2RAM  
Title : A NOVEL DNA RECOGNITION MODE BY NF-KB P65 HOMODIMER  
Authors : Chen, Y.Q.; Ghosh, S.; Ghosh, G.  
Deposited on : 1997-11-23  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

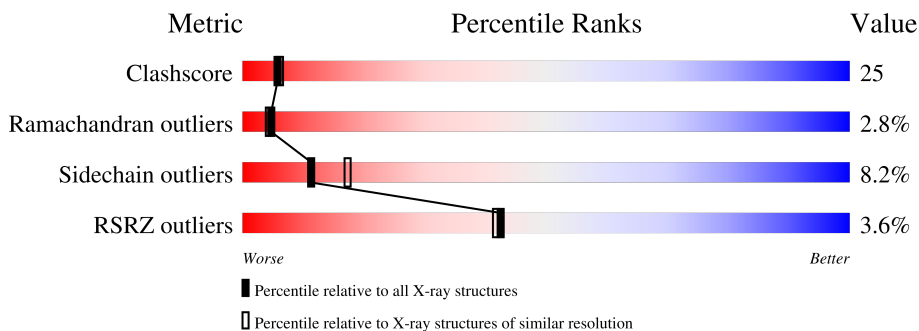
# 1 Overall quality at a glance

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)
RSRZ outliers	127900	3811 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	C	20	 5% 45% 55%
1	D	20	 5% 55% 40%
2	A	273	 3% 58% 36% 5%
2	B	273	 5% 56% 39% 2%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5314 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.

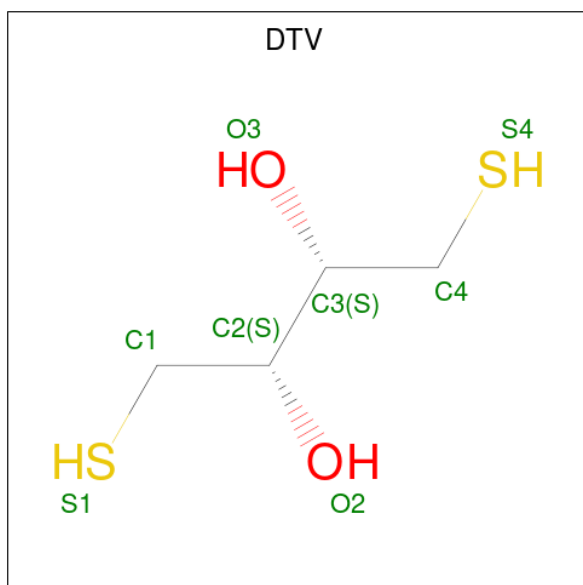
- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*GP\*AP\*AP\*AP\*TP\*(5IU)P\*(5IU)P\*CP\*CP\*AP\*GP\*CP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	I	N	O				P
1	C	20	Total 407	C 192	I 2	N 76	O 118	P 19	0	0	0
1	D	20	Total 407	C 192	I 2	N 76	O 118	P 19	0	0	0

- Molecule 2 is a protein called PROTEIN (TRANSCRIPTION FACTOR NF-KB P65).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	273	Total 2178	C 1358	N 401	O 408	S 11	0	0	0
2	B	273	Total 2178	C 1358	N 401	O 408	S 11	0	0	0

- Molecule 3 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	B	1	Total	C	O	S	0	0
			8	4	2	2		

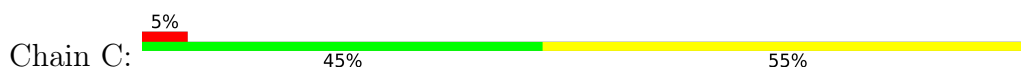
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	10	Total	O	0	0
			10	10		
4	D	15	Total	O	0	0
			15	15		
4	A	58	Total	O	0	0
			58	58		
4	B	45	Total	O	0	0
			45	45		

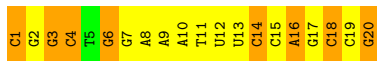
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

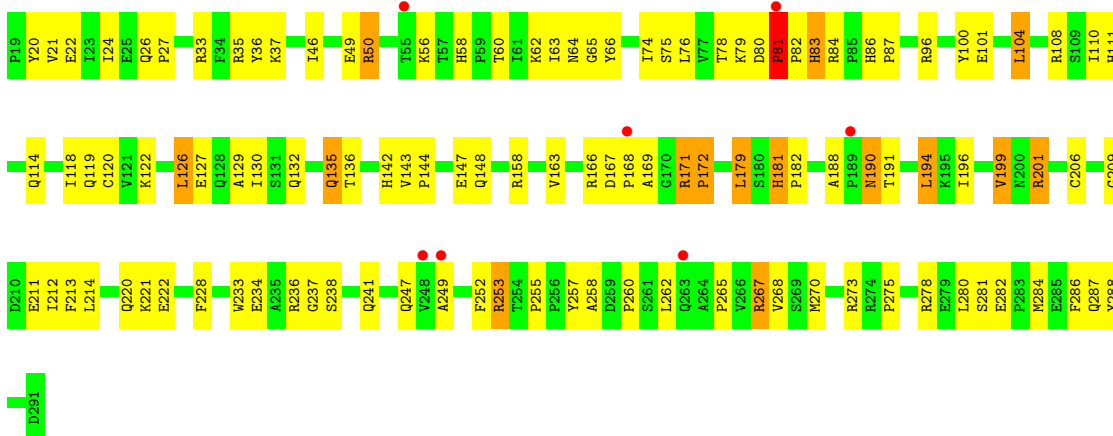
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*GP\*AP\*AP\*AP\*TP\*(5IU)P\*(5IU)P\*CP\*CP\*AP\*GP\*CP\*CP\*G)-3')



- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*GP\*AP\*AP\*AP\*TP\*(5IU)P\*(5IU)P\*CP\*CP\*AP\*GP\*CP\*CP\*G)-3')

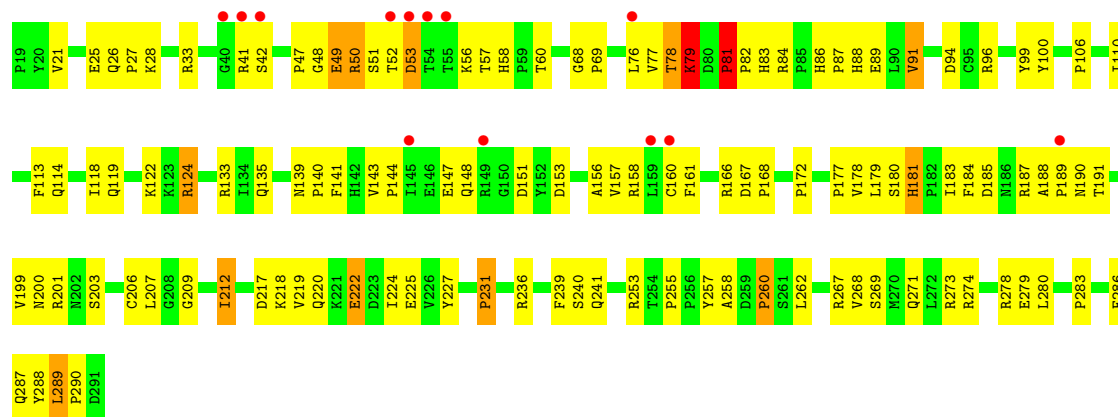


- Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)



- Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.81Å 80.62Å 167.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40 29.29 – 2.32	Depositor EDS
% Data completeness (in resolution range)	81.4 (6.00-2.40) 77.4 (29.29-2.32)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.31Å)	Xtrriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.213 , 0.308 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 92.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: DTV, 5IU

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	C	0.52	0/411	0.76	0/630
1	D	0.74	0/411	1.18	2/630 (0.3%)
2	A	0.52	1/2231 (0.0%)	0.81	0/3025
2	B	0.46	0/2231	0.77	0/3025
All	All	0.52	1/5284 (0.0%)	0.83	2/7310 (0.0%)

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	D	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	120	CYS	CB-SG	-5.41	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	DC	O4'-C4'-C3'	-5.50	102.30	104.50
1	D	6	DG	O4'-C1'-C2'	5.40	110.22	105.90

There are no chirality outliers.

All (6) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	D	14	DC	Sidechain
1	D	16	DA	Sidechain
1	D	18	DC	Sidechain
1	D	20	DG	Sidechain
1	D	3	DG	Sidechain
1	D	4	DC	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	C	407	0	220	26	0
1	D	407	0	220	52	0
2	A	2178	0	2140	93	0
2	B	2178	0	2140	94	0
3	A	8	0	10	0	0
3	B	8	0	10	1	0
4	A	58	0	0	5	0
4	B	45	0	0	2	0
4	C	10	0	0	2	0
4	D	15	0	0	0	0
All	All	5314	0	4740	246	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 25.

All (246) 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:D:17:DG:H2'	1:D:18:DC:C6	2.09	0.88
1:D:17:DG:H2'	1:D:18:DC:H6	1.39	0.87
1:D:8:DA:H2''	1:D:9:DA:O5'	1.77	0.85
1:D:2:DG:H2''	1:D:3:DG:O5'	1.78	0.84
1:D:9:DA:H2''	1:D:10:DA:O5'	1.77	0.84
2:B:139:ASN:HD21	2:B:143:VAL:N	1.75	0.84
1:D:17:DG:H2''	1:D:18:DC:O4'	1.76	0.84
2:B:28:LYS:HB2	2:B:47:PRO:HG2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLY:O	2:B:106:PRO:HA	1.83	0.79
2:A:81:PRO:HB2	2:A:82:PRO:HD3	1.63	0.77
1:C:20:DG:OP2	1:C:20:DG:H2'	1.85	0.77
1:C:3:DG:H8	1:C:3:DG:OP2	1.66	0.77
2:A:167:ASP:HB2	2:A:168:PRO:HD2	1.65	0.76
2:B:81:PRO:HB2	2:B:82:PRO:HD3	1.66	0.76
2:A:196:ILE:HG23	2:A:214:LEU:HD21	1.68	0.76
2:B:161:PHE:HB2	2:B:178:VAL:HG13	1.67	0.76
1:C:2:DG:H2''	1:C:3:DG:OP2	1.86	0.74
2:A:104:LEU:HD21	2:A:163:VAL:HG13	1.70	0.74
1:D:1:DC:H4'	1:D:2:DG:OP1	1.88	0.73
2:A:27:PRO:O	2:A:181:HIS:HE1	1.70	0.73
1:D:3:DG:H2'	1:D:4:DC:O4'	1.88	0.73
1:C:18:DC:H1'	1:C:19:DC:H5'	1.70	0.73
2:B:189:PRO:HB2	2:B:220:GLN:HE21	1.53	0.72
2:B:200:ASN:OD1	2:B:201:ARG:HG2	1.92	0.70
2:B:139:ASN:HD21	2:B:143:VAL:H	1.38	0.69
1:C:16:DA:N6	1:D:4:DC:N4	2.39	0.69
2:A:190:ASN:HA	2:A:220:GLN:NE2	2.07	0.69
1:C:19:DC:H42	1:D:2:DG:H1	1.40	0.69
2:A:233:TRP:CD1	2:A:258:ALA:HB2	2.27	0.68
2:A:132:GLN:O	2:A:136:THR:HG22	1.94	0.67
2:B:189:PRO:HB2	2:B:220:GLN:NE2	2.09	0.67
1:D:12:5IU:H2''	1:D:13:5IU:O5'	1.95	0.66
2:B:94:ASP:HB2	2:B:100:TYR:CE2	2.29	0.66
2:B:84:ARG:HG2	2:B:143:VAL:HG11	1.77	0.66
2:A:166:ARG:HG2	2:A:166:ARG:HH11	1.60	0.66
2:A:237:GLY:HA2	2:A:255:PRO:HD3	1.79	0.64
1:C:1:DC:H1'	1:C:2:DG:C5	2.33	0.64
2:B:224:ILE:HG13	2:B:225:GLU:H	1.63	0.64
1:C:19:DC:N3	1:D:2:DG:N2	2.38	0.64
2:A:221:LYS:NZ	2:A:241:GLN:HE21	1.95	0.63
1:D:11:DT:H2''	1:D:12:5IU:O5'	1.99	0.62
2:A:46:ILE:HD11	2:A:118:ILE:HG13	1.82	0.62
1:C:4:DC:H42	1:D:17:DG:H1	1.45	0.62
2:A:221:LYS:HZ3	2:A:241:GLN:HE21	1.46	0.62
2:B:158:ARG:HD2	2:B:180:SER:O	1.99	0.61
2:B:224:ILE:HG13	2:B:225:GLU:N	2.14	0.61
1:D:14:DC:H2''	1:D:15:DC:O5'	2.00	0.61
1:D:17:DG:H2''	1:D:18:DC:O5'	1.99	0.61
2:A:158:ARG:CZ	2:A:182:PRO:HD3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ARG:HA	2:B:185:ASP:OD1	2.00	0.61
1:D:17:DG:C2'	1:D:18:DC:C6	2.84	0.61
2:A:211:GLU:HB2	2:A:253:ARG:NH1	2.16	0.60
2:B:139:ASN:ND2	2:B:143:VAL:H	1.99	0.60
2:A:49:GLU:HG3	2:A:50:ARG:HD3	1.81	0.60
2:A:206:CYS:HB3	2:A:262:LEU:HD12	1.82	0.60
2:B:190:ASN:HB3	2:B:220:GLN:OE1	2.02	0.60
2:A:171:ARG:HE	2:A:171:ARG:HA	1.67	0.60
2:A:24:ILE:HG13	2:A:62:LYS:HB2	1.82	0.60
1:C:17:DG:H2''	1:C:18:DC:OP2	2.01	0.60
1:C:17:DG:H1	1:D:4:DC:N4	2.00	0.59
2:A:56:LYS:NZ	2:A:56:LYS:HB3	2.16	0.59
1:C:17:DG:H1	1:D:4:DC:H42	1.51	0.59
2:B:48:GLY:HA3	2:B:57:THR:HG22	1.85	0.59
2:B:33:ARG:CG	2:B:187:ARG:HB2	2.34	0.58
2:A:26:GLN:HB3	2:A:181:HIS:CE1	2.38	0.58
1:D:4:DC:H2'	1:D:4:DC:O2	2.02	0.58
2:B:257:TYR:CG	2:B:258:ALA:N	2.71	0.58
2:B:258:ALA:O	2:B:260:PRO:HD3	2.03	0.58
2:B:139:ASN:ND2	2:B:143:VAL:N	2.48	0.58
2:A:58:HIS:CD2	2:A:114:GLN:HB3	2.39	0.57
1:D:14:DC:H2'	1:D:15:DC:H6	1.69	0.57
2:A:26:GLN:HB3	2:A:181:HIS:NE2	2.19	0.57
2:A:199:VAL:HG13	2:A:201:ARG:H	1.68	0.57
2:B:60:THR:HG21	2:B:110:ILE:HG23	1.86	0.57
2:B:153:ASP:HB2	3:B:502:DTV:S4	2.44	0.57
1:D:17:DG:C2'	1:D:18:DC:O4'	2.49	0.56
2:B:52:THR:H	2:B:56:LYS:HA	1.70	0.56
1:D:16:DA:H2''	1:D:17:DG:C5'	2.36	0.56
1:D:16:DA:H2''	1:D:17:DG:O5'	2.06	0.56
1:D:17:DG:C2'	1:D:18:DC:H6	2.15	0.56
2:A:49:GLU:CG	2:A:50:ARG:HD3	2.36	0.56
2:A:206:CYS:HB3	2:A:262:LEU:CD1	2.36	0.56
2:B:267:ARG:HG3	2:B:287:GLN:HE22	1.70	0.56
2:A:24:ILE:CG1	2:A:62:LYS:HB2	2.36	0.56
2:B:48:GLY:C	2:B:50:ARG:H	2.10	0.55
2:B:82:PRO:O	2:B:84:ARG:HG3	2.06	0.55
1:C:19:DC:N4	1:D:2:DG:H1	2.04	0.55
2:B:206:CYS:SG	2:B:207:LEU:HD22	2.46	0.55
2:A:24:ILE:CD1	2:A:62:LYS:HB2	2.36	0.55
2:B:25:GLU:HB3	2:B:60:THR:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:PRO:HD2	2:B:147:GLU:HB3	1.89	0.54
2:A:24:ILE:HD11	2:A:62:LYS:HB2	1.89	0.54
1:C:13:5IU:I5	2:A:36:TYR:CD1	3.31	0.53
2:A:236:ARG:HG3	2:A:236:ARG:HH11	1.72	0.53
2:B:267:ARG:HG2	2:B:287:GLN:OE1	2.08	0.53
2:B:273:ARG:HG3	2:B:280:LEU:CD2	2.37	0.53
2:B:21:VAL:CG1	2:B:178:VAL:HG11	2.39	0.53
2:A:190:ASN:HA	2:A:220:GLN:HE22	1.73	0.53
2:A:221:LYS:NZ	2:A:241:GLN:NE2	2.57	0.53
2:A:80:ASP:HB3	2:A:81:PRO:HD2	1.89	0.53
1:D:1:DC:H2''	1:D:2:DG:O5'	2.10	0.52
1:D:8:DA:C2'	1:D:9:DA:O5'	2.55	0.52
2:A:214:LEU:O	2:A:249:ALA:HA	2.09	0.52
2:B:41:ARG:HB3	4:B:429:HOH:O	2.10	0.52
1:D:15:DC:H2'	1:D:16:DA:C8	2.45	0.52
2:B:58:HIS:HB3	2:B:113:PHE:O	2.10	0.52
2:A:100:TYR:CD1	2:A:101:GLU:N	2.78	0.52
2:A:267:ARG:HD2	2:A:287:GLN:HE21	1.75	0.52
2:A:37:LYS:HB2	2:A:37:LYS:NZ	2.24	0.52
1:D:16:DA:C2'	1:D:17:DG:O5'	2.58	0.51
1:D:6:DG:C2'	1:D:7:DG:OP2	2.58	0.51
2:A:213:PHE:CZ	2:B:200:ASN:HA	2.46	0.51
2:A:273:ARG:O	2:A:275:PRO:HD3	2.09	0.51
2:A:83:HIS:CD2	2:A:179:LEU:HD21	2.45	0.51
1:D:11:DT:H71	2:B:187:ARG:HH11	1.74	0.51
2:B:209:GLY:O	2:B:253:ARG:HD3	2.10	0.51
2:A:196:ILE:HG23	2:A:214:LEU:CD2	2.40	0.51
2:A:24:ILE:HD12	2:A:110:ILE:HG13	1.93	0.51
2:A:282:GLU:HG2	4:A:319:HOH:O	2.10	0.51
2:B:51:SER:HB2	2:B:57:THR:O	2.11	0.51
2:A:126:LEU:O	2:A:129:ALA:HB3	2.11	0.51
2:A:104:LEU:HD21	2:A:163:VAL:CG1	2.40	0.50
2:B:60:THR:CG2	2:B:110:ILE:HG23	2.42	0.50
1:D:20:DG:C8	1:D:20:DG:O5'	2.64	0.50
1:D:7:DG:H2''	1:D:8:DA:H5'	1.93	0.50
4:C:306:HOH:O	2:A:247:GLN:HG2	2.12	0.49
1:D:9:DA:H2'	1:D:10:DA:C8	2.47	0.49
1:C:19:DC:H2''	1:C:20:DG:C8	2.46	0.49
2:B:99:TYR:CD1	2:B:99:TYR:C	2.86	0.49
2:A:268:VAL:HG22	2:A:286:PHE:O	2.13	0.49
1:D:14:DC:H2'	1:D:15:DC:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:VAL:HG21	2:B:288:TYR:CE2	2.48	0.49
2:B:26:GLN:O	2:B:49:GLU:HB2	2.13	0.48
2:B:122:LYS:NZ	2:B:124:ARG:HD3	2.28	0.48
2:B:91:VAL:HG21	2:B:119:GLN:HB2	1.95	0.48
1:C:6:DG:N2	1:D:15:DC:N3	2.57	0.48
2:A:22:GLU:OE2	2:A:62:LYS:HD3	2.14	0.48
2:A:60:THR:CG2	2:A:110:ILE:HG23	2.43	0.48
2:B:161:PHE:HB2	2:B:178:VAL:CG1	2.41	0.48
1:C:3:DG:OP2	1:C:3:DG:C8	2.56	0.48
2:B:156:ALA:HB2	2:B:184:PHE:CD1	2.49	0.48
1:C:2:DG:N2	1:D:19:DC:N3	2.58	0.48
2:B:51:SER:OG	2:B:56:LYS:HB3	2.14	0.48
1:D:11:DT:H71	2:B:187:ARG:NH1	2.29	0.47
2:B:47:PRO:HB2	2:B:51:SER:HB3	1.96	0.47
2:A:199:VAL:HG22	2:A:212:ILE:CG2	2.45	0.47
2:B:156:ALA:HA	2:B:183:ILE:O	2.15	0.47
2:A:236:ARG:HG3	2:A:236:ARG:NH1	2.29	0.47
2:B:28:LYS:HE3	2:B:47:PRO:HB2	1.97	0.47
1:C:16:DA:N6	1:D:4:DC:H41	2.13	0.47
1:D:2:DG:C2'	1:D:3:DG:O5'	2.58	0.47
2:A:273:ARG:HH12	2:A:278:ARG:HG2	1.80	0.47
2:B:160:CYS:SG	2:B:177:PRO:HB3	2.56	0.46
2:B:217:ASP:O	2:B:219:VAL:HG13	2.15	0.46
2:A:27:PRO:O	2:A:181:HIS:CE1	2.60	0.46
2:A:35:ARG:O	2:A:119:GLN:HA	2.16	0.46
2:A:257:TYR:CG	2:A:258:ALA:N	2.83	0.46
2:B:58:HIS:CG	2:B:114:GLN:HG2	2.50	0.46
2:A:21:VAL:HG22	2:A:63:ILE:CD1	2.45	0.46
2:B:268:VAL:HG23	2:B:286:PHE:HB3	1.97	0.46
2:A:119:GLN:HG3	4:A:331:HOH:O	2.16	0.46
2:A:221:LYS:HZ2	2:A:241:GLN:NE2	2.14	0.46
2:A:260:PRO:HB3	4:A:303:HOH:O	2.16	0.46
2:A:24:ILE:HD11	2:A:62:LYS:HD2	1.97	0.46
2:A:78:THR:HG23	2:A:84:ARG:O	2.16	0.46
2:A:144:PRO:HB2	2:A:147:GLU:HB2	1.97	0.46
1:D:8:DA:H2'	1:D:9:DA:C8	2.51	0.46
2:B:27:PRO:O	2:B:181:HIS:HE1	1.99	0.46
2:B:271:GLN:HB3	2:B:283:PRO:HA	1.97	0.46
2:A:143:VAL:HA	2:A:144:PRO:HD3	1.76	0.45
2:B:167:ASP:HB2	2:B:168:PRO:CD	2.46	0.45
1:D:14:DC:C2'	1:D:15:DC:O5'	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:DG:C6	1:D:18:DC:N4	2.84	0.45
2:B:33:ARG:HG2	2:B:187:ARG:HB2	1.98	0.45
2:A:78:THR:HG22	2:A:86:HIS:HD2	1.82	0.45
2:A:108:ARG:HD2	2:A:110:ILE:O	2.17	0.45
2:A:126:LEU:CD1	2:A:130:ILE:HD11	2.46	0.45
2:B:26:GLN:HB3	2:B:181:HIS:NE2	2.32	0.45
2:A:79:LYS:HG3	2:A:182:PRO:HB3	1.97	0.45
2:B:262:LEU:O	2:B:290:PRO:HB3	2.17	0.45
1:C:4:DC:N3	1:D:17:DG:N2	2.49	0.44
1:C:13:5IU:O2	1:D:9:DA:C2	2.70	0.44
2:B:69:PRO:HB2	2:B:166:ARG:CZ	2.47	0.44
2:B:140:PRO:HG2	2:B:141:PHE:CD2	2.52	0.44
2:B:255:PRO:HG2	2:B:288:TYR:OH	2.17	0.44
1:C:19:DC:H2''	1:C:20:DG:OP2	2.17	0.44
4:C:353:HOH:O	2:A:122:LYS:HB3	2.17	0.44
2:A:211:GLU:N	2:A:253:ARG:NH1	2.65	0.44
2:B:268:VAL:HG22	2:B:286:PHE:O	2.18	0.44
2:A:78:THR:OG1	2:A:83:HIS:HA	2.18	0.44
2:B:279:GLU:O	2:B:280:LEU:HD23	2.17	0.44
2:B:273:ARG:HG3	2:B:280:LEU:HD23	1.98	0.44
2:B:28:LYS:CB	2:B:47:PRO:HG2	2.38	0.44
2:B:86:HIS:ND1	2:B:87:PRO:HD2	2.33	0.43
1:D:4:DC:O2	1:D:4:DC:C2'	2.62	0.43
2:A:166:ARG:HD2	4:A:357:HOH:O	2.19	0.43
2:B:79:LYS:HA	2:B:158:ARG:HG3	2.00	0.43
2:A:126:LEU:O	2:A:130:ILE:HG12	2.18	0.43
2:A:65:GLY:O	2:A:66:TYR:HB2	2.19	0.43
1:C:6:DG:H1	1:D:15:DC:N4	2.17	0.43
2:B:21:VAL:HG11	2:B:178:VAL:HG11	2.00	0.43
2:B:89:GLU:HG2	2:B:133:ARG:NH2	2.33	0.43
2:B:267:ARG:CG	2:B:287:GLN:HE22	2.31	0.43
1:C:3:DG:H2''	1:C:4:DC:C6	2.54	0.43
2:B:69:PRO:HG2	2:B:166:ARG:NH2	2.33	0.43
2:B:188:ALA:HB3	2:B:191:THR:OG1	2.19	0.43
2:B:227:TYR:CD1	2:B:236:ARG:NH1	2.87	0.43
2:B:48:GLY:N	2:B:57:THR:O	2.48	0.42
1:D:16:DA:H2''	1:D:17:DG:H5'	2.00	0.42
1:D:17:DG:C2'	1:D:18:DC:O5'	2.65	0.42
2:A:228:PHE:O	2:A:234:GLU:HA	2.19	0.42
2:B:77:VAL:O	2:B:78:THR:O	2.37	0.42
2:B:144:PRO:O	2:B:148:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:74:ILE:HB	2:A:100:TYR:HB3	2.01	0.42
2:A:273:ARG:HB2	2:A:280:LEU:HD23	2.01	0.42
2:A:20:TYR:CE1	2:A:64:ASN:OD1	2.72	0.42
2:A:270:MET:CE	2:A:284:MET:SD	3.07	0.42
2:A:144:PRO:O	2:A:148:GLN:N	2.52	0.42
2:B:58:HIS:ND1	2:B:114:GLN:HG2	2.35	0.42
1:C:16:DA:H61	1:D:4:DC:N4	2.14	0.42
2:B:289:LEU:HB3	2:B:290:PRO:HD2	2.01	0.42
2:B:206:CYS:SG	2:B:260:PRO:C	2.98	0.42
2:B:271:GLN:NE2	4:B:412:HOH:O	2.47	0.42
2:A:132:GLN:HA	2:A:135:GLN:CG	2.50	0.42
2:A:188:ALA:HB1	2:A:190:ASN:HD22	1.84	0.42
2:B:274:ARG:O	2:B:278:ARG:N	2.51	0.42
2:B:218:LYS:HB2	2:B:218:LYS:HE3	1.84	0.42
2:A:127:GLU:HA	2:A:130:ILE:HG12	2.02	0.41
2:A:86:HIS:HA	2:A:87:PRO:HD3	1.96	0.41
2:B:222:GLU:HA	2:B:241:GLN:OE1	2.20	0.41
2:B:239:PHE:HD2	2:B:240:SER:O	2.04	0.41
2:A:267:ARG:H	2:A:267:ARG:HG2	1.40	0.41
2:A:194:LEU:HB3	2:A:281:SER:HB3	2.03	0.41
2:B:124:ARG:NH1	2:B:124:ARG:HB2	2.36	0.41
1:D:11:DT:H2''	1:D:12:5IU:C5'	2.51	0.41
2:A:167:ASP:OD1	2:A:169:ALA:HB3	2.20	0.41
2:B:118:ILE:HD13	2:B:157:VAL:HG21	2.02	0.41
2:B:201:ARG:CG	2:B:212:ILE:HD13	2.51	0.41
2:A:171:ARG:NE	2:A:172:PRO:HD2	2.36	0.41
2:B:188:ALA:HB3	2:B:191:THR:CG2	2.51	0.41
2:B:78:THR:O	2:B:79:LYS:HB3	2.21	0.41
2:A:111:HIS:HD2	4:A:387:HOH:O	2.03	0.40
2:A:166:ARG:HG2	2:A:166:ARG:NH1	2.32	0.40
2:A:214:LEU:HB2	2:A:252:PHE:HE1	1.86	0.40
2:A:265:PRO:HA	2:A:288:TYR:O	2.21	0.40
2:A:209:GLY:O	2:A:253:ARG:NH1	2.54	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	
2	A	271/273 (99%)	239 (88%)	27 (10%)	5 (2%)	8	10
2	B	271/273 (99%)	228 (84%)	33 (12%)	10 (4%)	3	2
All	All	542/546 (99%)	467 (86%)	60 (11%)	15 (3%)	5	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	81	PRO
2	B	50	ARG
2	B	53	ASP
2	B	78	THR
2	B	81	PRO
2	A	142	HIS
2	B	42	SER
2	B	79	LYS
2	B	83	HIS
2	A	83	HIS
2	B	88	HIS
2	A	96	ARG
2	B	49	GLU
2	A	191	THR
2	B	231	PRO

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	243/243 (100%)	223 (92%)	20 (8%)	11	17
2	B	243/243 (100%)	223 (92%)	20 (8%)	11	17
All	All	486/486 (100%)	446 (92%)	40 (8%)	11	17

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	33	ARG
2	A	50	ARG
2	A	75	SER
2	A	76	LEU
2	A	81	PRO
2	A	104	LEU
2	A	126	LEU
2	A	135	GLN
2	A	171	ARG
2	A	172	PRO
2	A	179	LEU
2	A	181	HIS
2	A	190	ASN
2	A	194	LEU
2	A	199	VAL
2	A	201	ARG
2	A	222	GLU
2	A	238	SER
2	A	253	ARG
2	A	267	ARG
2	B	53	ASP
2	B	76	LEU
2	B	79	LYS
2	B	81	PRO
2	B	91	VAL
2	B	96	ARG
2	B	124	ARG
2	B	135	GLN
2	B	151	ASP
2	B	172	PRO
2	B	179	LEU
2	B	181	HIS
2	B	199	VAL
2	B	203	SER
2	B	212	ILE

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Mol	Chain	Res	Type
2	B	222	GLU
2	B	231	PRO
2	B	260	PRO
2	B	269	SER
2	B	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	58	HIS
2	A	115	ASN
2	A	132	GLN
2	A	137	ASN
2	A	162	GLN
2	A	181	HIS
2	A	190	ASN
2	A	220	GLN
2	A	241	GLN
2	A	287	GLN
2	B	64	ASN
2	B	114	GLN
2	B	139	ASN
2	B	190	ASN
2	B	220	GLN
2	B	271	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5IU	C	13	1	18,21,22	0.58	0	26,30,33	0.63	0
1	5IU	D	13	1	18,21,22	0.72	0	26,30,33	0.74	0
1	5IU	D	12	1	18,21,22	0.56	0	26,30,33	0.78	0
1	5IU	C	12	1	18,21,22	0.62	0	26,30,33	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5IU	C	13	1	-	1/7/21/22	0/2/2/2
1	5IU	D	13	1	-	2/7/21/22	0/2/2/2
1	5IU	D	12	1	-	0/7/21/22	0/2/2/2
1	5IU	C	12	1	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	13	5IU	C3'-C4'-C5'-O5'
1	D	13	5IU	O4'-C4'-C5'-O5'
1	C	13	5IU	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	13	5IU	2	0
1	D	13	5IU	1	0
1	D	12	5IU	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DTV	A	501	-	7,7,7	0.76	0	4,8,8	0.30	0
3	DTV	B	502	-	7,7,7	0.86	0	4,8,8	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTV	A	501	-	-	0/8/8/8	-
3	DTV	B	502	-	-	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	DTV	C1-C2-C3-O3
3	B	502	DTV	C1-C2-C3-C4
3	B	502	DTV	O2-C2-C3-O3
3	B	502	DTV	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	DTV	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

### 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	C	18/20 (90%)	0.26	1 (5%) 24 23	27, 58, 78, 81	0
1	D	18/20 (90%)	0.11	0 100 100	25, 58, 81, 83	0
2	A	273/273 (100%)	-0.06	7 (2%) 56 54	19, 38, 62, 71	0
2	B	273/273 (100%)	0.10	13 (4%) 30 29	21, 45, 74, 89	0
All	All	582/586 (99%)	0.03	21 (3%) 42 42	19, 42, 72, 89	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	42	SER	8.9
2	B	54	THR	3.7
2	B	52	THR	3.5
2	B	149	ARG	3.4
2	B	41	ARG	3.2
2	B	40	GLY	3.1
2	A	55	THR	2.8
2	A	189	PRO	2.8
2	B	55	THR	2.8
2	A	248	VAL	2.7
1	C	1	DC	2.6
2	B	160	CYS	2.6
2	A	168	PRO	2.5
2	B	76	LEU	2.4
2	B	53	ASP	2.3
2	A	263	GLN	2.2
2	B	159	LEU	2.2
2	B	145	ILE	2.2
2	B	189	PRO	2.2
2	A	81	PRO	2.2
2	A	249	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
1	5IU	D	13	20/21	0.97	0.11	31,40,54,59	0
1	5IU	C	13	20/21	0.99	0.11	16,29,41,47	0
1	5IU	D	12	20/21	0.99	0.14	26,33,41,43	0
1	5IU	C	12	20/21	0.99	0.14	17,30,38,39	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
3	DTV	B	502	8/8	0.68	0.37	51,65,72,85	0
3	DTV	A	501	8/8	0.81	0.26	47,59,65,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.