wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:34 AM GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

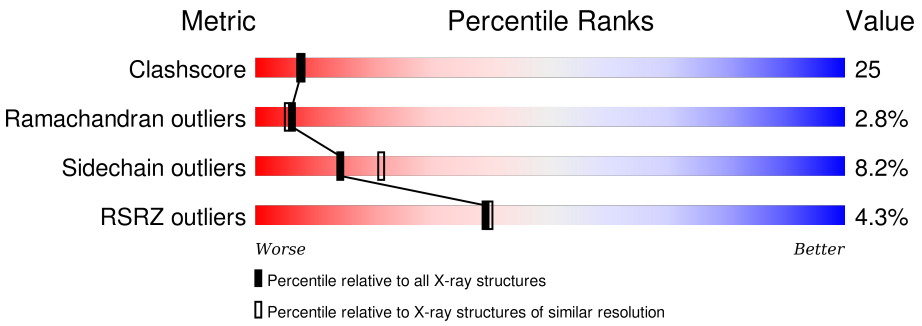
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	20	5% 45% 55%
1	D	20	5% 55% 40%
2	A	273	4% 58% 36% 5%
2	B	273	5% 56% 39% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTV	A	501	-	-	-	X
3	DTV	B	502	-	-	-	X

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.

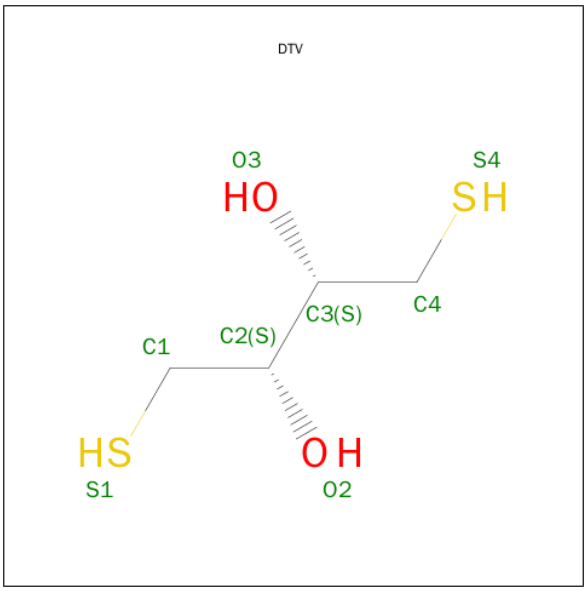
- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*TP*GP*GP*AP*AP*AP*TP*(5IU)P*(5IU)P*CP*CP*AP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	I	N	O	P			
1	C	20	407	192	2	76	118	19	0	0	0
1	D	20	407	192	2	76	118	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	2178	1358	401	408	11	0	0	0
2	B	273	2178	1358	401	408	11	0	0	0

- Molecule 3 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: $C_4H_{10}O_2S_2$).



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

- Molecule 4 is water.

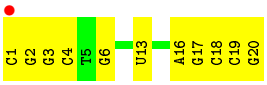
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	58	58	58	0	0
4	B	45	45	45	0	0
4	C	10	10	10	0	0
4	D	15	15	15	0	0

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.

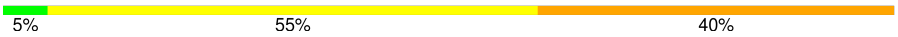
• Molecule 1: DNA (5'-D(*CP*GP*GP*CP*TP*GP*GP*AP*AP*AP*TP*(5IU)P*(5IU)P*CP*CP*AP*GP*CP*CP*G)-3')

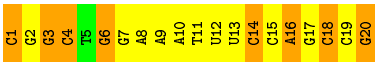
Chain C:



• 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')

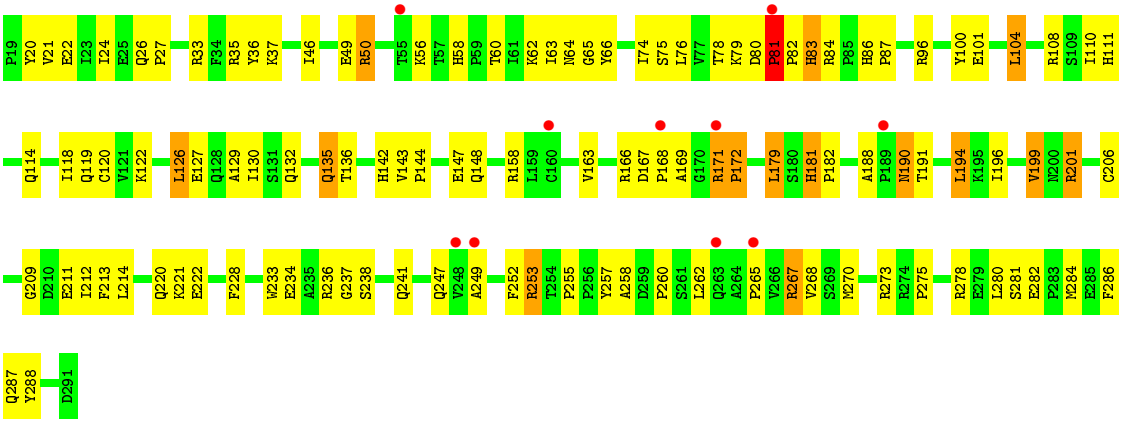
Chain D:





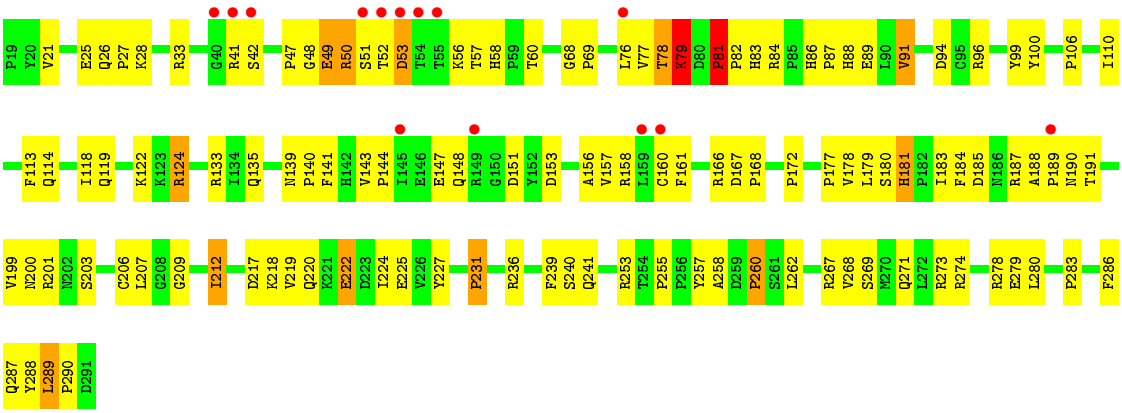
• Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)

Chain A:



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

Chain B:


P19 Y20 V21 E25 Q26 P27 K28 R33 G40 R41 S42 P47 G48 E49 R50 S51 T52 D53 T54 T55 K56 T57 H58 P59 T60 G68 P69 L76 V77 T78 K79 D80 P81 P82 H83 R84 P85 H86 P87 H88 E89 L90 V91 D94 C95 R96 Y99 Y100 P106 I110
F113 Q114 I118 Q119 K122 K123 R124 R133 I134 Q135 N139 P140 F141 H142 V143 P144 I145 E146 E147 Q148 R149 G150 D151 Y152 D153 A156 V157 R158 L159 C160 F161 R166 D167 P168 P172 P177 V178 L179 S180 H181 P182 I183 F184 D185 N186 R187 A188 P189 N190 T191
V199 N200 R201 N202 S203 C206 L207 G208 G209 I212 D217 K218 V219 Q220 K221 E222 D223 I224 E225 V226 Y227 P231 R236 F239 S240 Q241 R253 T254 P255 P256 Y257 A258 D259 P260 S261 L262 R267 V268 S269 M270 Q271 L272 R273 R274 R278 E279 L280 P283 F286
Q287 Y288 L289 P290 D291

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.39 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.213 , 0.308 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 92.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 30672 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5314	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5IU, DTV

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(^{o})	Ideal(^{o})
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.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	14	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	D	16	DA	Sidechain
1	D	18	DC	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.

The worst 5 of 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

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%)	11	13
2	B	271/273 (99%)	228 (84%)	33 (12%)	10 (4%)	4	3
All	All	542/546 (99%)	467 (86%)	60 (11%)	15 (3%)	6	5

5 of 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

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%)	14	21
2	B	243/243 (100%)	223 (92%)	20 (8%)	14	21
All	All	486/486 (100%)	446 (92%)	40 (8%)	14	21

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	253	ARG

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Mol	Chain	Res	Type
2	B	79	LYS
2	B	231	PRO
2	B	53	ASP
2	B	81	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	220	GLN
2	A	241	GLN
2	B	139	ASN
2	A	190	ASN
2	B	190	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)

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	12	1	12,21,22	1.09	1 (8%)	14,30,33	3.87	1 (7%)
1	5IU	C	13	1	12,21,22	1.23	2 (16%)	14,30,33	3.66	1 (7%)
1	5IU	D	12	1	12,21,22	1.11	2 (16%)	14,30,33	3.73	1 (7%)
1	5IU	D	13	1	12,21,22	1.16	2 (16%)	14,30,33	3.75	1 (7%)

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	12	1	-	0/3/21/22	0/2/2/2
1	5IU	C	13	1	-	0/3/21/22	0/2/2/2
1	5IU	D	12	1	-	0/3/21/22	0/2/2/2
1	5IU	D	13	1	-	0/3/21/22	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	5IU	C6-C5	-2.25	1.33	1.38
1	D	12	5IU	C6-C5	-2.16	1.33	1.38
1	C	13	5IU	C6-C5	-2.03	1.33	1.38
1	D	13	5IU	C4-N3	2.21	1.37	1.33
1	D	12	5IU	C4-N3	2.26	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	12	5IU	C4-N3-C2	13.58	126.99	115.25
1	C	13	5IU	C4-N3-C2	13.61	127.01	115.25
1	D	13	5IU	C4-N3-C2	13.63	127.03	115.25
1	C	12	5IU	C4-N3-C2	14.27	127.58	115.25

There are no chirality outliers.

There are no torsion outliers.

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	12	5IU	3	0
1	D	13	5IU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	0.79	0	4,8,8	0.65	0
3	DTV	B	502	-	7,7,7	0.91	0	4,8,8	1.31	1 (25%)

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	0/0/0/0
3	DTV	B	502	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	DTV	C3-C4-S4	2.56	118.15	113.91

There are no chirality outliers.

There are no torsion outliers.

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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	18/20 (90%)	0.32	1 (5%) 28 28	27, 58, 78, 81	0
1	D	18/20 (90%)	0.16	0 100 100	25, 58, 81, 83	0
2	A	273/273 (100%)	-0.01	10 (3%) 45 46	19, 38, 62, 71	0
2	B	273/273 (100%)	0.16	14 (5%) 32 32	21, 45, 74, 89	0
All	All	582/586 (99%)	0.09	25 (4%) 39 40	19, 42, 72, 89	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	42	SER	9.2
2	B	54	THR	3.8
2	B	52	THR	3.6
2	B	149	ARG	3.5
2	B	40	GLY	3.3

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. 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, 95th 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^2)	Q<0.9
1	5IU	C	12	20/21	0.99	0.13	-	17,30,38,39	0
1	5IU	C	13	20/21	0.99	0.11	-	16,29,41,47	0
1	5IU	D	13	20/21	0.97	0.11	-	31,40,54,59	0
1	5IU	D	12	20/21	0.99	0.14	-	26,33,41,43	0

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, 95th 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^2)	Q<0.9
3	DTV	B	502	8/8	0.68	0.37	7.95	51,65,72,85	0
3	DTV	A	501	8/8	0.81	0.26	3.11	47,59,65,76	0

6.5 Other polymers (i)

There are no such residues in this entry.