Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 12:59 PM EDT

PDB ID	:	6DJ8
Title	:	Structure of DNA polymerase III subunit beta from Borrelia burgdorferi in complex with a natural product
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2018-05-24
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

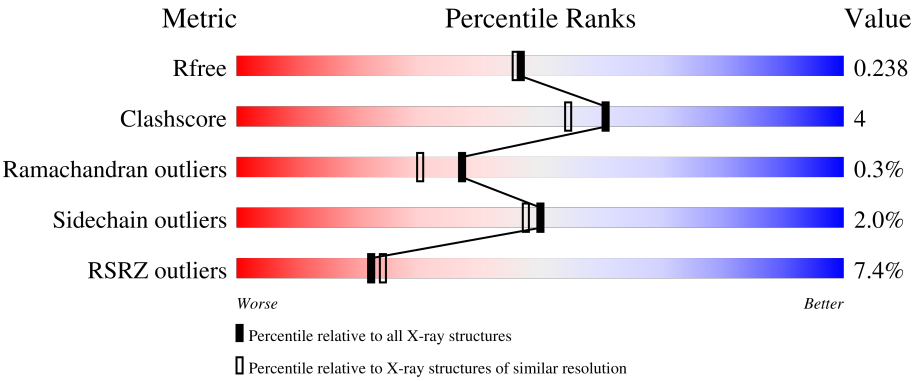
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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 >=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 <=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	393	8% 87% 10%
1	B	393	5% 87% 9%
2	C	11	18% 36% 64%
2	D	11	9% 36% 55% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6451 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	6	0
			3086	1994	497	581	14			
1	B	376	Total	C	N	O	S	0	9	0
			3000	1944	484	560	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P33761
A	-6	ALA	-	expression tag	UNP P33761
A	-5	HIS	-	expression tag	UNP P33761
A	-4	HIS	-	expression tag	UNP P33761
A	-3	HIS	-	expression tag	UNP P33761
A	-2	HIS	-	expression tag	UNP P33761
A	-1	HIS	-	expression tag	UNP P33761
A	0	HIS	-	expression tag	UNP P33761
B	-7	MET	-	initiating methionine	UNP P33761
B	-6	ALA	-	expression tag	UNP P33761
B	-5	HIS	-	expression tag	UNP P33761
B	-4	HIS	-	expression tag	UNP P33761
B	-3	HIS	-	expression tag	UNP P33761
B	-2	HIS	-	expression tag	UNP P33761
B	-1	HIS	-	expression tag	UNP P33761
B	0	HIS	-	expression tag	UNP P33761

- Molecule 2 is a protein called Natural product peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			79	57	10	12			
2	D	11	Total	C	N	O	0	0	0
			79	57	10	12			

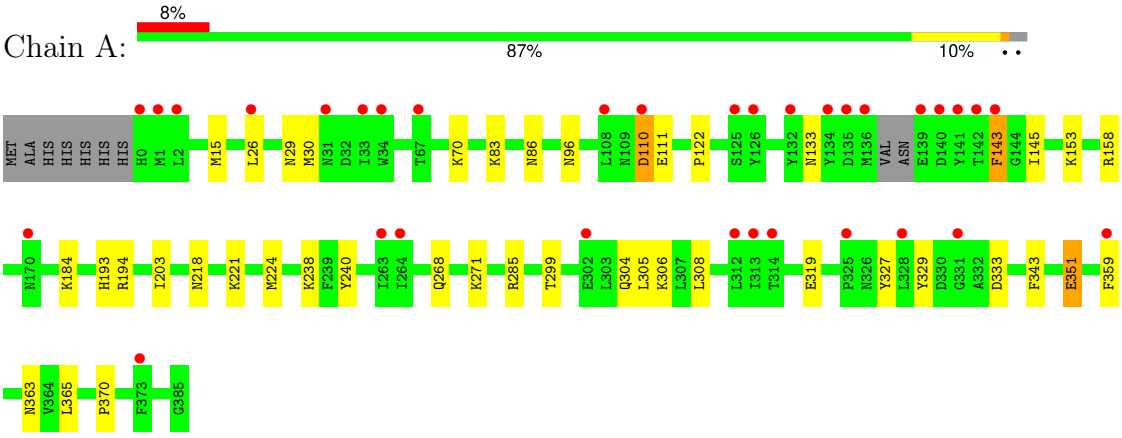
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	103	Total O 103 103	0	0
3	D	2	Total O 2 2	0	0

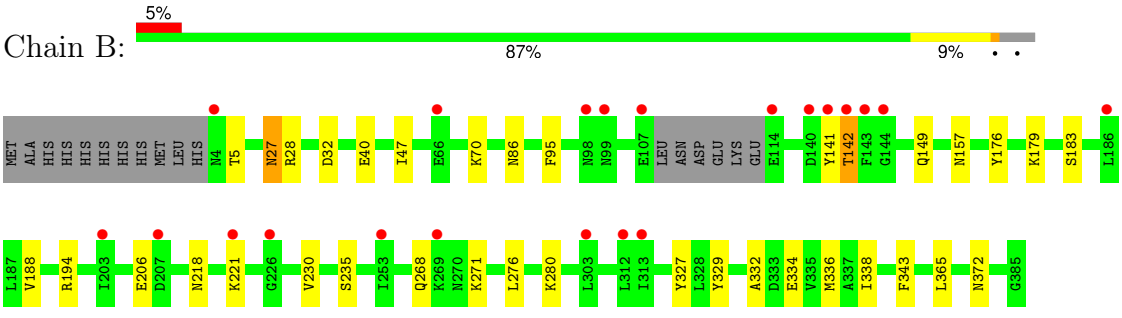
3 Residue-property plots (i)

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: Beta sliding clamp

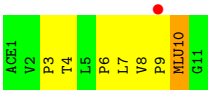


• Molecule 1: Beta sliding clamp



• Molecule 2: Natural product peptide

• Molecule 2: Natural product peptide


ACE1
V2
P3
T4
L5
P6
L7
V8
P9
MIU10
G11

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.38Å 68.29Å 86.32Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	42.00 – 2.05 42.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.00-2.05) 99.6 (42.00-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.05Å)	Xtriage
Refinement program	PHENIX DEV_3126	Depositor
R, R_{free}	0.202 , 0.235 0.204 , 0.238	Depositor DCC
R_{free} test set	54625 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6451	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MP8, NZC, MVA, ACE, MLU

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	0.42	0/3155	0.60	0/4254
1	B	0.38	0/3073	0.58	0/4151
2	C	0.29	0/24	1.19	0/26
2	D	0.30	0/24	1.21	0/26
All	All	0.40	0/6276	0.59	0/8457

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

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	3086	0	3039	22	0
1	B	3000	0	2936	24	0
2	C	79	0	96	3	0
2	D	79	0	96	4	0
3	A	102	0	0	1	0
3	B	103	0	0	1	0
3	D	2	0	0	0	0
All	All	6451	0	6167	51	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 4.

All (51) 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:153:LYS:HG3	1:A:224:MET:HE2	1.64	0.80
1:A:218:ASN:HA	1:A:221[A]:LYS:HE2	1.68	0.75
1:B:218:ASN:HA	1:B:221[A]:LYS:HE2	1.71	0.73
1:B:27[A]:ASN:ND2	1:B:32:ASP:OD2	2.22	0.73
1:B:336:MET:SD	1:B:365:LEU:HD11	2.33	0.68
1:B:40[A]:GLU:HG3	1:B:47:ILE:HB	1.80	0.63
1:A:333:ASP:OD1	3:A:401:HOH:O	2.16	0.62
1:A:15:MET:HE1	1:A:86:ASN:HB3	1.83	0.61
1:B:176:TYR:HB3	1:B:188[A]:VAL:HG13	1.83	0.60
1:B:268:GLN:O	1:B:271:LYS:NZ	2.38	0.57
1:A:299:THR:HB	1:A:306:LYS:HB3	1.87	0.57
1:A:110:ASP:OD1	1:A:111:GLU:N	2.37	0.56
1:A:359:PHE:HB3	1:A:365:LEU:HD12	1.89	0.55
1:A:268:GLN:O	1:A:271:LYS:NZ	2.39	0.55
1:B:28[B]:ARG:NH2	1:B:32:ASP:OD2	2.41	0.53
1:A:308:LEU:HD13	1:A:319:GLU:HG2	1.91	0.52
1:B:276:LEU:HG	1:B:280:LYS:HE3	1.92	0.52
1:A:305:LEU:HB2	1:A:327:TYR:CE1	2.46	0.51
1:B:372:ASN:HB3	3:B:489:HOH:O	2.10	0.51
1:B:142:THR:HG23	1:B:235:SER:HA	1.95	0.49
1:B:338:ILE:HD12	1:B:365:LEU:HD22	1.95	0.49
1:A:184:LYS:HD3	1:A:203:ILE:HG13	1.94	0.48
1:A:158:ARG:NH2	1:A:351:GLU:HG3	2.28	0.48
1:A:285:ARG:HH22	1:B:86:ASN:CG	2.17	0.48
1:A:193:HIS:NE2	2:C:4:NZC:HG2	2.28	0.47
2:D:10:MLU:HG	2:D:10:MLU:HCN3	1.97	0.46
1:B:176:TYR:HB3	1:B:188[A]:VAL:CG1	2.44	0.46
1:A:83:LYS:O	1:A:86:ASN:ND2	2.48	0.46
1:A:143:PHE:CE1	1:A:145:ILE:HG23	2.50	0.46
1:B:179:LYS:HG2	1:B:183:SER:HA	1.98	0.46
1:A:238:LYS:HZ2	1:A:240:TYR:HB2	1.81	0.46
1:A:70:LYS:NZ	1:A:133:ASN:HD21	2.14	0.46
1:B:327:TYR:CZ	1:B:329:TYR:HB2	2.52	0.45
2:C:7:LEU:HA	2:C:8:MVA:HN1	1.56	0.45
1:B:40[A]:GLU:HB3	1:B:70:LYS:HG2	1.99	0.44
1:B:141:TYR:HD1	1:B:235:SER:HB3	1.82	0.44
2:D:7:LEU:HA	2:D:8:MVA:HN1	1.57	0.44
1:A:143:PHE:HE1	1:A:145:ILE:HG23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:GLU:OE1	1:B:206:GLU:N	2.38	0.43
1:B:332:ALA:O	1:B:334[B]:GLU:HG2	2.19	0.43
1:B:157:ASN:HB2	1:B:221[B]:LYS:HE3	2.02	0.42
1:B:157:ASN:OD1	1:B:221[B]:LYS:NZ	2.31	0.42
1:B:27[B]:ASN:O	1:B:28[B]:ARG:HG2	2.18	0.42
1:B:149:GLN:HG2	1:B:230:VAL:HG23	2.01	0.42
1:A:30:MET:CE	1:A:122:PRO:HG2	2.50	0.41
2:D:8:MVA:HA	2:D:9:PRO:HA	1.83	0.41
2:D:3:MP8:HA	2:D:4:NZC:H40	1.57	0.41
1:A:327:TYR:CZ	1:A:329:TYR:HB2	2.56	0.41
1:B:5:THR:HG22	1:B:95:PHE:HB3	2.03	0.40
1:A:158:ARG:HH21	1:A:351:GLU:HG3	1.86	0.40
2:C:3:MP8:HA	2:C:4:NZC:H40	1.65	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	386/393 (98%)	372 (96%)	12 (3%)	2 (0%)	25 17
1	B	381/393 (97%)	366 (96%)	13 (3%)	2 (0%)	25 17
2	C	3/11 (27%)	3 (100%)	0	0	100 100
2	D	3/11 (27%)	3 (100%)	0	0	100 100
All	All	773/808 (96%)	744 (96%)	25 (3%)	4 (0%)	37 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370[A]	PRO
1	A	370[B]	PRO

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Mol	Chain	Res	Type
1	B	27[A]	ASN
1	B	27[B]	ASN

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	
1	A	340/365 (93%)	330 (97%)	10 (3%)	37	32
1	B	325/365 (89%)	322 (99%)	3 (1%)	75	77
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	671/736 (91%)	658 (98%)	13 (2%)	50	50

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	29	ASN
1	A	96	ASN
1	A	110	ASP
1	A	143	PHE
1	A	194	ARG
1	A	304	GLN
1	A	343	PHE
1	A	351	GLU
1	A	363	ASN
1	B	142	THR
1	B	194	ARG
1	B	343	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
2	MVA	C	8	2	6,7,8	0.24	0	6,8,10	1.00	0
2	MP8	D	3	2	6,8,9	0.78	0	3,10,12	1.22	0
2	MVA	C	2	2	6,7,8	0.25	0	6,8,10	1.02	1 (16%)
2	NZC	C	4	2	6,7,8	0.53	0	6,8,10	0.89	0
2	MVA	D	2	2	6,7,8	0.28	0	6,8,10	0.88	0
2	MP8	C	6	2	6,8,9	0.69	0	3,10,12	1.92	1 (33%)
2	MLU	D	10	2	7,8,9	0.23	0	7,9,11	0.91	1 (14%)
2	NZC	D	4	2	6,7,8	0.33	0	6,8,10	0.95	0
2	MP8	D	6	2	6,8,9	0.69	0	3,10,12	1.98	1 (33%)
2	MLU	C	10	2	7,8,9	0.24	0	7,9,11	1.60	1 (14%)
2	MP8	C	3	2	6,8,9	0.70	0	3,10,12	1.28	0
2	MVA	D	8	2	6,7,8	0.61	0	6,8,10	0.75	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
2	MVA	C	8	2	-	1/6/8/10	-
2	MP8	D	3	2	-	0/0/11/13	0/1/1/1
2	MVA	C	2	2	-	2/6/8/10	-
2	NZC	C	4	2	-	1/6/8/10	-
2	MVA	D	2	2	-	3/6/8/10	-
2	MP8	C	6	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLU	D	10	2	-	2/5/8/10	-
2	NZC	D	4	2	-	1/6/8/10	-
2	MP8	D	6	2	-	0/0/11/13	0/1/1/1
2	MLU	C	10	2	-	2/5/8/10	-
2	MP8	C	3	2	-	0/0/11/13	0/1/1/1
2	MVA	D	8	2	-	1/6/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	10	MLU	CB-CA-N	4.09	116.81	110.59
2	C	6	MP8	CG-CD-N	2.60	109.78	106.65
2	D	6	MP8	CG-CD-N	2.50	109.66	106.65
2	C	2	MVA	CB-CA-C	-2.12	110.22	112.96
2	D	10	MLU	CB-CA-N	2.12	113.81	110.59

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	MVA	CB-CA-N-CN
2	D	2	MVA	CB-CA-N-CN
2	D	2	MVA	N-CA-CB-CG1
2	C	10	MLU	CA-CB-CG-CD2
2	D	10	MLU	CA-CB-CG-CD1
2	D	10	MLU	CA-CB-CG-CD2
2	C	10	MLU	CA-CB-CG-CD1
2	C	2	MVA	N-CA-CB-CG1
2	C	4	NZC	CB-CA-N-C40
2	D	4	NZC	CB-CA-N-C40
2	C	8	MVA	CB-CA-N-CN
2	D	8	MVA	CB-CA-N-CN
2	D	2	MVA	N-CA-CB-CG2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	8	MVA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	MP8	1	0
2	C	4	NZC	2	0
2	D	10	MLU	1	0
2	D	4	NZC	1	0
2	C	3	MP8	1	0
2	D	8	MVA	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} 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	A	384/393 (97%)	0.53	33 (8%)	18	19	26, 46, 75, 100	6 (1%)
1	B	376/393 (95%)	0.49	21 (5%)	31	33	24, 49, 75, 121	9 (2%)
2	C	4/11 (36%)	1.95	2 (50%)	0	0	65, 82, 83, 107	0
2	D	4/11 (36%)	1.63	1 (25%)	2	1	45, 56, 59, 86	0
All	All	768/808 (95%)	0.52	57 (7%)	22	24	24, 47, 76, 121	15 (1%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	LEU	4.6
1	A	126	TYR	3.9
1	A	313	ILE	3.8
2	D	9	PRO	3.5
1	B	313	ILE	3.5
1	A	139	GLU	3.3
1	B	107	GLU	3.3
1	B	207	ASP	3.3
1	B	98	ASN	3.2
2	C	9	PRO	3.2
1	B	140	ASP	3.0
1	A	26	LEU	3.0
1	A	1	MET	3.0
1	B	143	PHE	3.0
1	A	0	HIS	2.9
1	B	221[A]	LYS	2.9
1	A	132	TYR	2.9
1	A	142	THR	2.9
1	A	312	LEU	2.8
1	A	34	TRP	2.6
1	A	141	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	314	THR	2.5
1	A	263	ILE	2.5
1	B	4	ASN	2.5
1	B	99	ASN	2.5
1	B	144	GLY	2.4
1	A	373	PHE	2.4
1	B	203	ILE	2.4
1	B	186	LEU	2.4
1	B	269	LYS	2.4
1	A	125	SER	2.4
1	B	141	TYR	2.4
1	A	33	ILE	2.3
1	A	2	LEU	2.3
1	B	142	THR	2.3
1	B	226	GLY	2.3
1	A	328	LEU	2.3
1	A	67	THR	2.2
1	A	31	ASN	2.2
1	A	359	PHE	2.2
1	A	143	PHE	2.2
1	A	264	ILE	2.2
1	B	66	GLU	2.2
1	A	135	ASP	2.2
1	A	325	PRO	2.1
1	A	108	LEU	2.1
1	B	253	ILE	2.1
1	A	134	TYR	2.1
1	A	331	GLY	2.1
1	A	110	ASP	2.1
1	A	170	ASN	2.0
1	A	302	GLU	2.0
1	B	114	GLU	2.0
1	A	140	ASP	2.0
1	A	136	MET	2.0
1	B	303	LEU	2.0
2	C	7	LEU	2.0

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^{th} 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^2)	Q<0.9
2	MLU	C	10	9/10	0.63	0.20	94,104,107,108	0
2	MVA	C	8	8/9	0.67	0.21	84,101,104,105	0
2	MVA	D	8	8/9	0.72	0.18	66,76,81,81	0
2	MP8	C	3	8/9	0.76	0.18	74,79,82,86	0
2	MVA	C	2	8/9	0.82	0.16	80,88,90,96	0
2	MLU	D	10	9/10	0.82	0.17	73,75,86,91	0
2	MP8	C	6	8/9	0.85	0.14	76,79,83,90	0
2	NZC	C	4	8/9	0.86	0.12	66,72,78,80	0
2	MP8	D	6	8/9	0.92	0.12	52,58,62,68	0
2	MP8	D	3	8/9	0.94	0.09	40,44,49,51	0
2	MVA	D	2	8/9	0.94	0.09	44,46,48,49	0
2	NZC	D	4	8/9	0.95	0.09	42,44,48,48	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.