



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:55 AM GMT

PDB ID : 3CMU
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 4.20 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 ⓘ symbol.

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

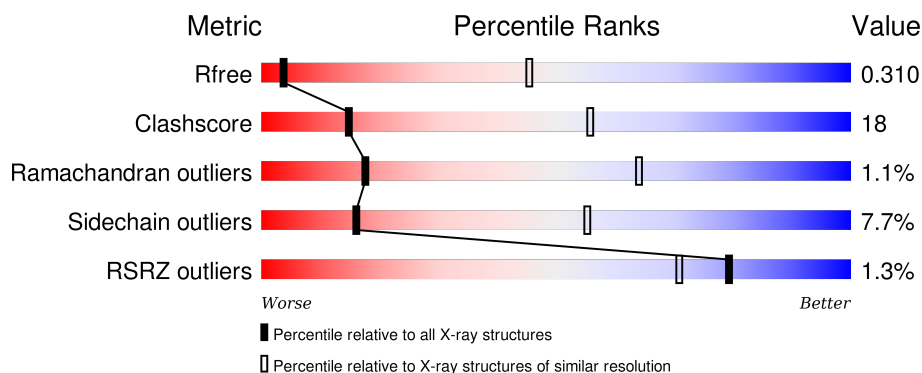
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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 $\leq 5\%$. 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	B	18	
2	A	2050	

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
4	ALF	A	3501	-	-	-	X
4	ALF	A	501	-	-	X	-
4	ALF	A	5501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15093 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(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	15	Total	C	N	O	P	0	0	0
			297	150	30	103	14			

- Molecule 2 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1937	Total	C	N	O	S	0	0	0
			14598	9178	2528	2824	68			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	LINKER	UNP P0A7G6
A	27	ALA	-	LINKER	UNP P0A7G6
A	28	HIS	-	LINKER	UNP P0A7G6
A	29	MET	-	LINKER	UNP P0A7G6
A	986	THR	-	LINKER	UNP P0A7G6
A	987	GLY	-	LINKER	UNP P0A7G6
A	988	SER	-	LINKER	UNP P0A7G6
A	989	THR	-	LINKER	UNP P0A7G6
A	990	GLY	-	LINKER	UNP P0A7G6
A	991	SER	-	LINKER	UNP P0A7G6
A	992	GLY	-	LINKER	UNP P0A7G6
A	993	THR	-	LINKER	UNP P0A7G6
A	994	THR	-	LINKER	UNP P0A7G6
A	995	GLY	-	LINKER	UNP P0A7G6
A	996	SER	-	LINKER	UNP P0A7G6
A	997	THR	-	LINKER	UNP P0A7G6
A	998	GLY	-	LINKER	UNP P0A7G6
A	999	SER	-	LINKER	UNP P0A7G6
A	1000	MET	-	LINKER	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1986	THR	-	LINKER	UNP P0A7G6
A	1987	GLY	-	LINKER	UNP P0A7G6
A	1988	SER	-	LINKER	UNP P0A7G6
A	1989	THR	-	LINKER	UNP P0A7G6
A	1990	GLY	-	LINKER	UNP P0A7G6
A	1991	SER	-	LINKER	UNP P0A7G6
A	1992	MET	-	LINKER	UNP P0A7G6
A	1993	GLY	-	LINKER	UNP P0A7G6
A	1994	HIS	-	LINKER	UNP P0A7G6
A	1995	THR	-	LINKER	UNP P0A7G6
A	1996	THR	-	LINKER	UNP P0A7G6
A	1997	GLY	-	LINKER	UNP P0A7G6
A	1998	ALA	-	LINKER	UNP P0A7G6
A	1999	MET	-	LINKER	UNP P0A7G6
A	2000	SER	-	LINKER	UNP P0A7G6
A	2986	THR	-	LINKER	UNP P0A7G6
A	2987	GLY	-	LINKER	UNP P0A7G6
A	2988	SER	-	LINKER	UNP P0A7G6
A	2989	THR	-	LINKER	UNP P0A7G6
A	2990	GLY	-	LINKER	UNP P0A7G6
A	2991	SER	-	LINKER	UNP P0A7G6
A	2992	MET	-	LINKER	UNP P0A7G6
A	2993	ALA	-	LINKER	UNP P0A7G6
A	2994	SER	-	LINKER	UNP P0A7G6
A	2995	THR	-	LINKER	UNP P0A7G6
A	2996	GLY	-	LINKER	UNP P0A7G6
A	2997	SER	-	LINKER	UNP P0A7G6
A	2998	THR	-	LINKER	UNP P0A7G6
A	2999	GLY	-	LINKER	UNP P0A7G6
A	3000	SER	-	LINKER	UNP P0A7G6
A	3989	THR	-	LINKER	UNP P0A7G6
A	3990	GLY	-	LINKER	UNP P0A7G6
A	3991	ALA	-	LINKER	UNP P0A7G6
A	3992	THR	-	LINKER	UNP P0A7G6
A	3993	GLY	-	LINKER	UNP P0A7G6
A	3994	ALA	-	LINKER	UNP P0A7G6
A	3995	MET	-	LINKER	UNP P0A7G6
A	3996	SER	-	LINKER	UNP P0A7G6
A	3997	GLY	-	LINKER	UNP P0A7G6
A	3998	ARG	-	LINKER	UNP P0A7G6
A	3999	MET	-	LINKER	UNP P0A7G6
A	4000	SER	-	LINKER	UNP P0A7G6

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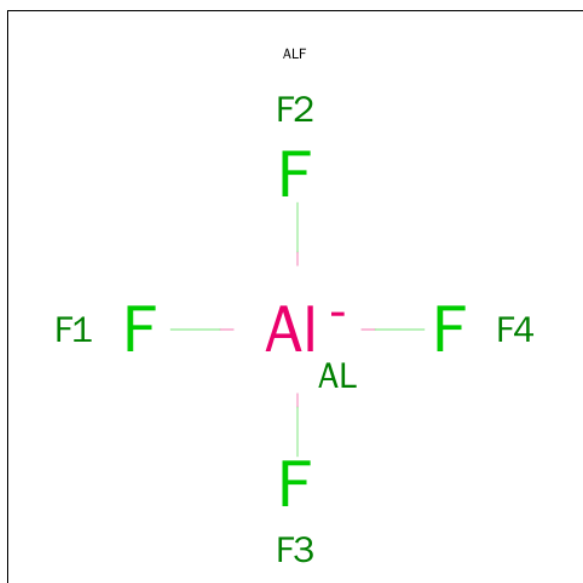
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Chain	Residue	Modelled	Actual	Comment	Reference
A	4987	THR	-	LINKER	UNP P0A7G6
A	4988	GLY	-	LINKER	UNP P0A7G6
A	4989	SER	-	LINKER	UNP P0A7G6
A	4990	THR	-	LINKER	UNP P0A7G6
A	4991	GLY	-	LINKER	UNP P0A7G6
A	4992	SER	-	LINKER	UNP P0A7G6
A	4993	GLY	-	LINKER	UNP P0A7G6
A	4994	SER	-	LINKER	UNP P0A7G6
A	4995	SER	-	LINKER	UNP P0A7G6
A	4996	THR	-	LINKER	UNP P0A7G6
A	4997	GLY	-	LINKER	UNP P0A7G6
A	4998	SER	-	LINKER	UNP P0A7G6
A	4999	MET	-	LINKER	UNP P0A7G6
A	5000	SER	-	LINKER	UNP P0A7G6

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Mg 6 6	0	0

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



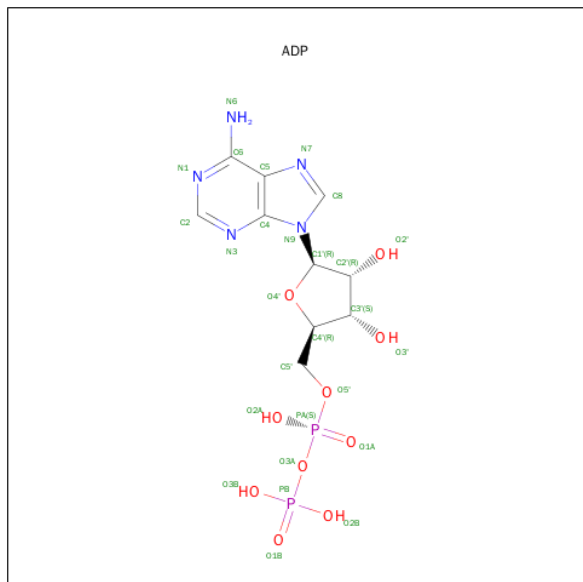
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Al F 5 1 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			5	1	4		
4	A	1	Total	Al	F	0	0
			5	1	4		
4	A	1	Total	Al	F	0	0
			5	1	4		
4	A	1	Total	Al	F	0	0
			5	1	4		
4	A	1	Total	Al	F	0	0
			5	1	4		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

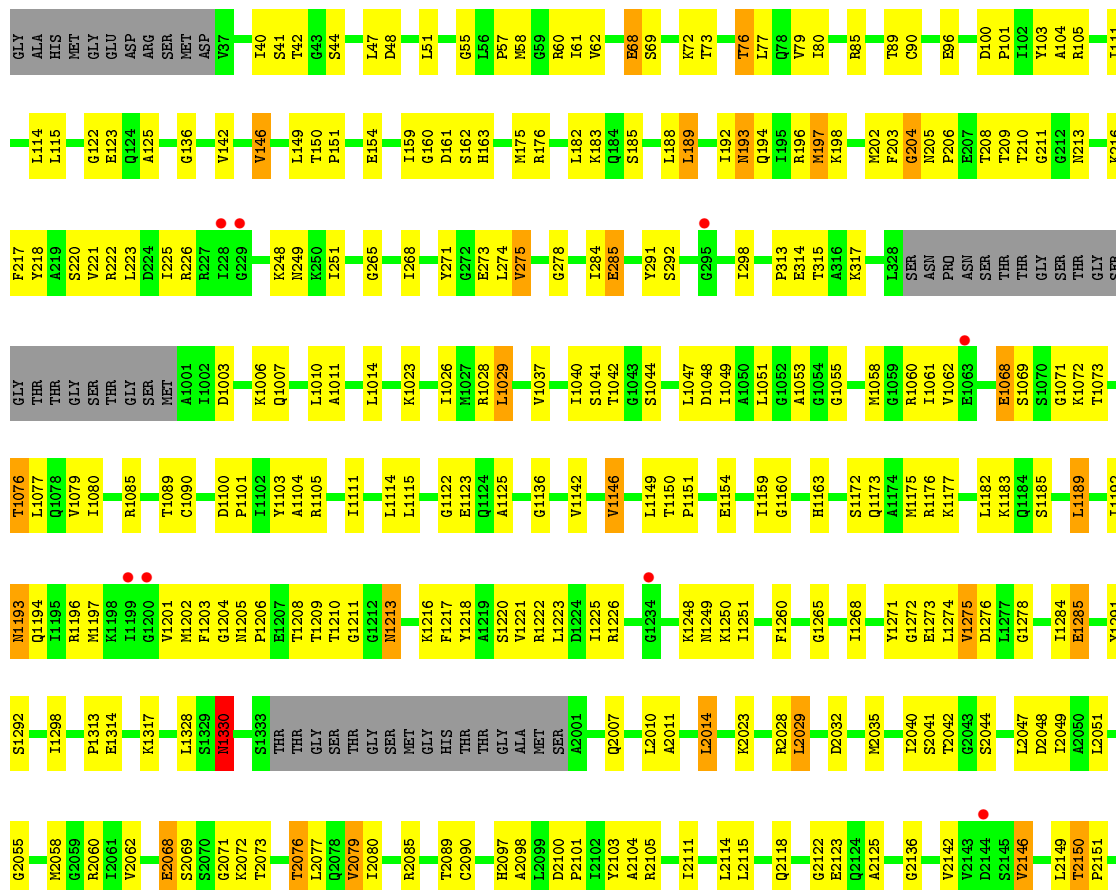
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain B: 



- Molecule 2: Protein recA

Chain A: 



G5211	E5123	G4265	H4163	I4061	N3330	N3205	Y3103	L3014	E2154
G5212	Q5124	G4268	R4169	V4062	S3333	P3206	A3104	P2254	I2159
N5213	A5125	I4268	R4169	E4063	THR	T3207	R3105	F2260	G2160
K5216	G5136	I4268	Q4173	E4068	THR	T3208	I3111	K3023	A2168
F5217	L5029	Y4271	A4174	S4069	GLY	T3209	D3112	I3026	R2169
S5220	G5030	G4272	H4175	S4070	ALA	G3211	N3113	N3027	
V5221	E5031	E4273	R4176	G4071	THR	G3212	I3114	R3028	Q2173
R5222	B5032	I4274	R4177	R4072	GLY	N3213	I3115	I3029	A2174
L5223	B5035	V4275	L4182	T4073	ALA	G3214	G3030	G3030	M2175
R5224	I5040	G4278	L4182	T4076	MET	L3215	G3122	E3031	R2176
I5225	S5041	Q4183	Q4183	L4077	SER	K3216	E3123	D3032	K2177
R5226	T5042	Q4184	Q4184	Q4078	GLY	F3217	Q3124	L2274	
E5235	T5042	S4185	S4185	Q4079	ARG	Y3218	A3125	Y2275	
K5248	S5043	L4189	L4189	I4080	MET	A3219	G3136	P3036	L2182
N5249	GLY	L4192	L4192	R4085	SER	S3220	G3136	V3037	K2183
K5250	L5047	I4192	I4192	R4085	A4001	R3221	V3142	I3040	L2184
I5251	D5048	H4193	H4193	E4089	I4002	V3222	V3143	S3041	S2185
I5251	GLY	Q4194	Q4194	C4090	D4003	L3223	R3144	T3042	L2189
ASP	L5051	I4195	I4195	C4090	K4006	D3224	R3144	G3043	
HIS	ASP	R4196	R4196	H4097	Q4007	I3225	S3145	S3044	I2192
F5260	SER	I4197	I4197	H4097	Q4007	R3226	V3146	S3044	I2193
G5265	HIS	K4198	K4198	A4098	L4010	K3248	L3149	L3047	Q2194
G5265	GLY	I4199	I4199	A4098	A4011	N3249	T3150	D3048	T2195
I5268	L5165	G4200	G4200	P4101	L4014	K3250	P3151	I2298	R2196
Y5271	L5166	V4201	V4201	I4102	I4014	I3251	E3154	I3051	M2197
G5273	GLY	M4202	M4202	I4103	F4021	A3252	E3154	G3052	V2201
L5274	L5061	I4209	I4209	I4113	A4022	G3265	A3053	G3052	M2202
E5275	V5062	T4210	T4210	I4115	G4021	P3254	I3159	G3054	F2203
G5278	E5068	G4211	G4211	R4105	K4023	F3260	G3160	G3055	G2204
G5278	R5072	P4206	P4206	I4111	I4026	I3268	H3163	P3058	F2203
L5283	T5073	T4207	T4207	D4112	M4027	Y3264	R3175	G3061	G2204
I5284	L5074	G4209	G4209	I4113	R4028	G3265	R3176	I3062	T2209
E5285	K5183	T4210	T4210	I4115	L4029	I3268	R3177	V3062	T2210
L5285	Q5184	G4211	G4211	Q4118	G4030	Y3271	K3177	E3068	G2212
L5285	S5185	Q4212	Q4212	Q4118	S4034	G3272	E3068	S3069	GLY
Y5291	L5189	I4213	I4213	Q4122	M4035	E3273	G3180	S3070	N2213
S5292	L5192	K4216	K4216	E4123	I4040	L3274	G3180	G3071	A2214
I5298	N5193	F4217	F4217	Q4124	S4041	V3275	L3182	K3072	L2215
P5313	Q5194	Y4218	Y4218	A4125	T4042	G3278	K3183	T3073	K2216
E5314	L5195	S4220	S4220	Q4136	G4043	G3278	Q3184	Y3076	F2217
K5317	MET	V4221	V4221	V4142	S4044	L3283	S3185	L3077	Y2218
L5328	LYS	R4222	R4222	V4146	L4047	E3285	L3189	A2218	A2218
SER	ILE	L4223	L4223	A4146	D4048	I3284	I3192	L3077	S2220
ASN	GLY	I4225	I4225	A4146	I4049	E3285	I3192	V3079	V2221
PRO	VAL	R4226	R4226	A4146	A4050	Y3291	R3193	I3080	R2222
ASN	MET	K4248	K4248	A4146	L4051	S3292	Q3194	R3085	L2223
SER	PHE	I4249	I4249	P4151	A4052	I3298	R3195	E3086	I2224
THR	GLY	N4250	N4250	E4154	A4053	I3298	R3196	G3087	I2225
	N5205	I4251	I4251	E4154	G4054	I3298	R3197	A3001	R2226
	P5206	A5011	A5011	E4154	G4055	P3313	T3089	I3002	R2227
	E5207	L5014	L5014	I4159	M4058	E3314	C3090	Q3007	K2248
	T5208	L5114	L5114	G4160	G4059	K3317	P3101	L3010	N2249
	T5210	G5122	G5122	G4160	R4060		I3102	A3011	K2250
									I2251

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.00Å 156.00Å 211.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 4.20 38.35 – 4.20	Depositor EDS
% Data completeness (in resolution range)	80.7 (12.00-4.20) 81.1 (38.35-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.275 , 0.298 0.288 , 0.310	Depositor DCC
R_{free} test set	1063 reflections (6.59%)	DCC
Wilson B-factor (Å ²)	173.4	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 80.5	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21286 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15093	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, MG, ADP

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	B	2.06	5/326 (1.5%)	2.67	39/502 (7.8%)
2	A	0.59	0/14765	0.67	0/19866
All	All	0.66	5/15091 (0.0%)	0.79	39/20368 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1002	DT	N3-C4	6.64	1.44	1.38
1	B	1002	DT	C1'-N1	6.34	1.57	1.49
1	B	1012	DT	O3'-P	-6.04	1.53	1.61
1	B	1002	DT	N1-C6	5.66	1.42	1.38
1	B	1002	DT	N1-C2	5.58	1.42	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1014	DT	O4'-C1'-N1	11.00	115.70	108.00
1	B	1011	DT	O4'-C1'-N1	10.59	115.41	108.00
1	B	1005	DT	O4'-C1'-N1	9.55	114.69	108.00
1	B	1008	DT	O4'-C1'-N1	9.30	114.51	108.00
1	B	1002	DT	N3-C4-O4	9.05	125.33	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	297	0	182	25	0
2	A	14598	0	14995	523	1
3	A	6	0	0	0	0
4	A	30	0	0	8	0
5	A	162	0	72	24	0
All	All	15093	0	15249	538	1

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 18.

The worst 5 of 538 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)
2:A:4194:GLN:HE21	2:A:4196:ARG:HH12	1.10	1.00
2:A:2194:GLN:HE21	2:A:2196:ARG:HH12	1.09	0.98
2:A:194:GLN:HE21	2:A:196:ARG:HH12	1.08	0.98
2:A:5194:GLN:HE21	2:A:5196:ARG:HH12	1.11	0.95
2:A:3194:GLN:HE21	2:A:3196:ARG:HH12	1.10	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1276:ASP:OD2	2:A:5235:GLU:OE2[4_556]	2.08	0.12

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	1921/2050 (94%)	1719 (90%)	180 (9%)	22 (1%)	17 64

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	5165	GLY
2	A	1204	GLY
2	A	2204	GLY
2	A	3204	GLY
2	A	4204	GLY

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
2	A	1524/1606 (95%)	1406 (92%)	118 (8%)	16 55

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2213	ASN
2	A	3089	THR
2	A	5155	ILE
2	A	2223	LEU
2	A	2330	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2304	ASN
2	A	3181	ASN
2	A	5193	ASN
2	A	3118	GLN

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Mol	Chain	Res	Type
2	A	3193	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\# Z > 2$
4	ALF	A	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	1502	3	22,29,29	1.17	2 (9%)	27,45,45	2.08	4 (14%)
4	ALF	A	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	2502	3	22,29,29	1.05	1 (4%)	27,45,45	1.98	4 (14%)
4	ALF	A	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	3502	3	22,29,29	1.07	1 (4%)	27,45,45	2.13	6 (22%)
4	ALF	A	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	4502	3	22,29,29	1.04	1 (4%)	27,45,45	2.18	5 (18%)
4	ALF	A	501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	502	3	22,29,29	1.08	1 (4%)	27,45,45	2.10	6 (22%)
4	ALF	A	5501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	5502	3	22,29,29	1.07	2 (9%)	27,45,45	2.09	5 (18%)

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
4	ALF	A	1501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	1502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	2501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	2502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	3501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	3502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	4501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	4502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	5501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	5502	3	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5502	ADP	C2-N3	2.11	1.35	1.32
5	A	1502	ADP	C2-N3	2.13	1.36	1.32
5	A	502	ADP	C5-C4	3.10	1.47	1.40
5	A	2502	ADP	C5-C4	3.12	1.47	1.40
5	A	4502	ADP	C5-C4	3.13	1.47	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	ADP	N3-C2-N1	-8.28	122.56	128.89
5	A	1502	ADP	N3-C2-N1	-8.17	122.64	128.89
5	A	4502	ADP	N3-C2-N1	-8.00	122.77	128.89
5	A	3502	ADP	N3-C2-N1	-7.92	122.83	128.89
5	A	2502	ADP	N3-C2-N1	-7.23	123.36	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	ALF	1	0
5	A	1502	ADP	5	0
4	A	2501	ALF	1	0
5	A	2502	ADP	7	0
5	A	3502	ADP	5	0
4	A	4501	ALF	1	0
5	A	4502	ADP	4	0
4	A	501	ALF	3	0
4	A	5501	ALF	2	0
5	A	5502	ADP	3	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	B	15/18 (83%)	0.46	0 100 100	118, 147, 162, 174	0
2	A	1937/2050 (94%)	-0.23	25 (1%) 79 71	147, 196, 220, 220	0
All	All	1952/2068 (94%)	-0.23	25 (1%) 79 71	118, 195, 220, 220	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1200	GLY	3.1
2	A	5001	ALA	3.1
2	A	5205	ASN	2.9
2	A	295	GLY	2.7
2	A	3283	LEU	2.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
4	ALF	A	3501	5/5	0.98	0.52	0.89	181,181,182,183	0
5	ADP	A	502	27/27	0.93	0.37	0.62	169,190,193,193	0
4	ALF	A	1501	5/5	0.95	0.33	0.37	190,194,195,196	0
4	ALF	A	501	5/5	0.97	0.39	0.18	165,168,169,169	0
5	ADP	A	1502	27/27	0.92	0.25	-0.12	191,198,201,202	0
5	ADP	A	3502	27/27	0.91	0.29	-0.21	182,190,197,197	0
4	ALF	A	4501	5/5	0.99	0.26	-0.33	159,160,161,162	0
5	ADP	A	2502	27/27	0.93	0.20	-0.57	176,188,192,193	0
5	ADP	A	4502	27/27	0.97	0.18	-0.76	157,178,183,183	0
4	ALF	A	5501	5/5	0.95	0.17	-0.95	167,172,172,172	0
4	ALF	A	2501	5/5	0.94	0.23	-0.96	177,177,179,180	0
5	ADP	A	5502	27/27	0.96	0.13	-1.26	173,185,193,193	0
3	MG	A	4500	1/1	0.99	0.35	-	162,162,162,162	0
3	MG	A	1500	1/1	0.99	0.47	-	186,186,186,186	0
3	MG	A	3500	1/1	0.99	0.60	-	180,180,180,180	0
3	MG	A	500	1/1	0.98	0.55	-	162,162,162,162	0
3	MG	A	2500	1/1	0.97	0.32	-	177,177,177,177	0
3	MG	A	5500	1/1	0.98	0.10	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.