



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:29 AM GMT

PDB ID : 3CMX  
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures  
Authors : Pavletich, N.P.  
Deposited on : 2008-03-24  
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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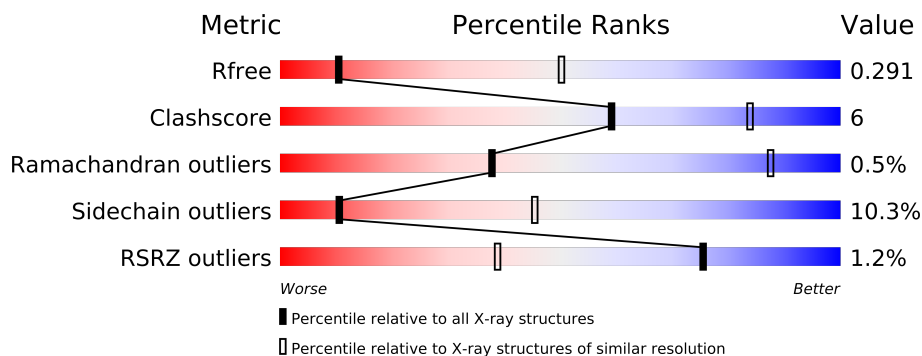
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	15	
1	E	15	
2	C	12	
2	F	12	
3	A	1706	
3	D	1706	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	2500	-	X
4	MG	A	500	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	D	1500	-	X
4	MG	D	4500	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25459 atoms, of which 0 are hydrogen and 0 are deuterium.

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\*TP\*DTP\*DTP\*DTP\*DTP\*DTP\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	13	Total	C	N	O	P	0	0	0
			260	130	26	91	13			
1	E	13	Total	C	N	O	P	0	0	0
			260	130	26	91	13			

- Molecule 2 is a DNA chain called DNA (5'-D(\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			211	100	50	51	10			
2	F	12	Total	C	N	O	P	0	0	0
			232	110	55	56	11			

- Molecule 3 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1603	Total	C	N	O	S	0	0	0
			12083	7595	2094	2339	55			
3	D	1603	Total	C	N	O	S	0	0	0
			12083	7595	2094	2339	55			

There are 130 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	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2999	MET	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
A	3986	THR	-	linker	UNP P0A7G6
A	3987	GLY	-	linker	UNP P0A7G6
A	3988	SER	-	linker	UNP P0A7G6
A	3989	THR	-	linker	UNP P0A7G6
A	3990	GLY	-	linker	UNP P0A7G6
A	3991	SER	-	linker	UNP P0A7G6
A	3992	MET	-	linker	UNP P0A7G6
A	3993	SER	-	linker	UNP P0A7G6
A	3994	GLY	-	linker	UNP P0A7G6
A	3995	ARG	-	linker	UNP P0A7G6
A	3996	THR	-	linker	UNP P0A7G6
A	3997	GLY	-	linker	UNP P0A7G6
A	3998	SER	-	linker	UNP P0A7G6
A	3999	MET	-	linker	UNP P0A7G6
A	4000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6

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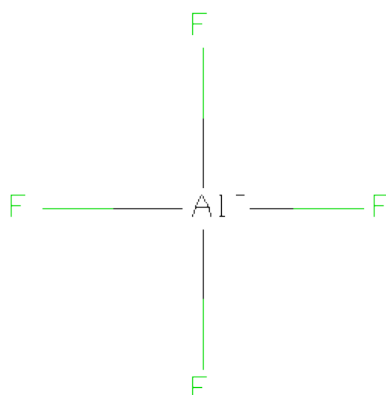
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
D	3986	THR	-	linker	UNP P0A7G6
D	3987	GLY	-	linker	UNP P0A7G6
D	3988	SER	-	linker	UNP P0A7G6
D	3989	THR	-	linker	UNP P0A7G6
D	3990	GLY	-	linker	UNP P0A7G6
D	3991	SER	-	linker	UNP P0A7G6
D	3992	MET	-	linker	UNP P0A7G6
D	3993	SER	-	linker	UNP P0A7G6
D	3994	GLY	-	linker	UNP P0A7G6
D	3995	ARG	-	linker	UNP P0A7G6
D	3996	THR	-	linker	UNP P0A7G6
D	3997	GLY	-	linker	UNP P0A7G6
D	3998	SER	-	linker	UNP P0A7G6
D	3999	MET	-	linker	UNP P0A7G6
D	4000	SER	-	linker	UNP P0A7G6

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

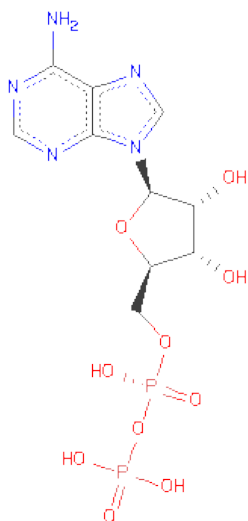
- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).



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



- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	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 ( $RSRZ > 2$ ). 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\*DT)-3')

Chain B: 



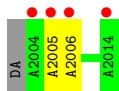
- Molecule 1: DNA (5'-D(\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DTP\*DT)-3')

Chain E: 



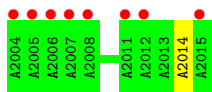
- Molecule 2: DNA (5'-D(\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*A)-3')

Chain C: 



- Molecule 2: DNA (5'-D(\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*DAP\*A)-3')

Chain F: 



- Molecule 3: Protein recA

Chain A: 





T4209	T4210	G4211	G4212	N4213	K4216	V4221	R4222	L4223	K4232	E4233	I4251	P4254	K4282	E4285	Y4291	S4292	Y4293	K4294	K4310	D4311	N4312	P4313	E4314	T4315	A4316	K4317	L4328	SER	ASN	PRO	ASN	SER	THR												
R4085	C4090	A4095	E4096	H4097	L4114	V4140	V4142	V4146	L4149	E4154	ILE	GLU	GLY	GLU	ILE	GLY	ASP	SER	HIS	MET	GLY	LEU	ALA	S4172	Q4173	R4176	K4177	K4183	Q4184	L4189	N4193	Q4194	L4195	R4196	MET	LYS	ILE	GLY	VAL	MET	PHE	GLY	N4205	T4208	
E3207	T3208	T3209	T3210	K3216	V3221	R3222	L3223	E3233	K3248	T3251	P3254	Q3261	N3269	E3285	S3333	THR	THR	GLY	SER	THR	GLY	SER	MET	SER	GLY	ARG	THR	GLY	SER	MET	SER	A4001	K4019	M4027	R4028	L4029	E4068	S4069	T4073	T4076	V4079	T4080			
G3071	K3072	T3073	T3076	V3079	I3080	R3085	C3090	A3095	E3096	H3097	I3111	L3114	V3140	I3141	V3142	V3146	L3149	T3150	I3155	G3160	M3164	G3165	S3172	Q3173	R3176	K3177	Q3184	L3189	N3193	Q3194	T3195	R3196	K3197	I3198	I3199	G3200	V3201	K3202	N3205	P3206					
E2068	S2069	T2073	T2076	V2079	I2080	R2085	C2090	A2095	E2096	H2097	D2100	P2101	I2111	L2114	V2140	I2141	V2142	V2146	L2149	T2150	E2154	I2155	G2160	H2163	M2164	G2165	S2172	Q2173	R2176	K2183	Q2184	L2189	N2193	Q2194	I2195	R2196	I2199								
M2202	N2205	P2206	E2207	T2208	T2209	T2210	K2216	V2221	R2222	L2223	E2233	I2251	P2254	E2285	N2304	M2330	P2331	N2332	S2333	THR	THR	GLY	SER	THR	GLY	SER	ALA	SER	GLY	SER	SER	THR	GLY	SER	NET	SER	A3001	K3019	K3023	M3027	R3028	L3029	E3068	S3069	S3070

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 39.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (40.00-3.40) 94.7 (39.75-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, $R_{free}$	0.238 , 0.256 0.277 , 0.291	Depositor DCC
$R_{free}$ test set	1589 reflections (3.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 52124 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	25459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.18	0/285	1.85	10/438 (2.3%)
1	E	1.19	1/285 (0.4%)	1.87	13/438 (3.0%)
2	C	0.68	0/240	1.33	1/369 (0.3%)
2	F	0.72	0/264	1.49	3/406 (0.7%)
3	A	0.43	0/12222	0.56	0/16447
3	D	0.43	0/12222	0.57	0/16447
All	All	0.47	1/25518 (0.0%)	0.66	27/34545 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1006	DT	O3'-P	-5.02	1.55	1.61

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1012	DT	C4-C5-C7	8.48	124.09	119.00
1	E	1009	DT	C4-C5-C7	8.41	124.05	119.00
1	B	1006	DT	C4-C5-C7	8.17	123.90	119.00
1	B	1009	DT	C4-C5-C7	8.03	123.82	119.00
2	F	2014	DA	C1'-O4'-C4'	-7.97	102.13	110.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	260	0	157	7	0
1	E	260	0	157	13	0
2	C	211	0	111	1	0
2	F	232	0	122	0	0
3	A	12083	0	12406	158	1
3	D	12083	0	12406	162	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	1	0
5	D	25	0	0	0	0
6	A	135	0	60	7	0
6	D	135	0	60	7	0
All	All	25459	0	25479	313	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 313 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.46	0.95
3:A:4076:THR:HG21	3:A:4142:VAL:HG21	1.48	0.95
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.95
3:D:2076:THR:HG21	3:D:2142:VAL:HG21	1.49	0.94
3:A:2076:THR:HG21	3:A:2142:VAL:HG21	1.51	0.93

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	Distance(Å)	Clash(Å)
3:A:4087:GLY:O	3:A:4314:GLU:OE2[2_555]	2.07	0.13

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	
3	A	1589/1706 (93%)	1494 (94%)	87 (6%)	8 (0%)	38	87
3	D	1589/1706 (93%)	1501 (94%)	81 (5%)	7 (0%)	43	90
All	All	3178/3412 (93%)	2995 (94%)	168 (5%)	15 (0%)	38	87

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1332	ASN
3	A	4269	ASN
3	D	164	MET
3	D	1332	ASN
3	D	2332	ASN

### 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	
3	A	1263/1339 (94%)	1133 (90%)	130 (10%)	10	45
3	D	1263/1339 (94%)	1133 (90%)	130 (10%)	10	45
All	All	2526/2678 (94%)	2266 (90%)	260 (10%)	10	45

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4146	VAL
3	D	197	MET
3	D	4069	SER
3	A	4189	LEU
3	D	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:



Mol	Chain	Res	Type
3	A	4173	GLN
3	D	181	ASN
3	D	4173	GLN
3	A	4181	ASN
3	A	4300	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	$\# Z  > 2$
5	ALF	A	1501	-	4,4,4	1.85	1 (25%)	0,6,6	0.00	-
6	ADP	A	1502	4	29,29,29	1.29	4 (13%)	45,45,45	1.78	7 (15%)
5	ALF	A	2501	-	4,4,4	1.88	1 (25%)	0,6,6	0.00	-
6	ADP	A	2502	4	29,29,29	1.08	2 (6%)	45,45,45	1.78	7 (15%)
5	ALF	A	3501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	A	3502	4	29,29,29	1.19	2 (6%)	45,45,45	1.68	5 (11%)
5	ALF	A	4501	-	4,4,4	2.00	1 (25%)	0,6,6	0.00	-
6	ADP	A	4502	-	29,29,29	1.08	2 (6%)	45,45,45	1.87	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ALF	A	501	-	4,4,4	1.92	1 (25%)	0,6,6	0.00	-
6	ADP	A	502	4	29,29,29	1.09	1 (3%)	45,45,45	2.11	9 (20%)
5	ALF	D	1501	-	4,4,4	1.79	0	0,6,6	0.00	-
6	ADP	D	1502	4	29,29,29	1.18	2 (6%)	45,45,45	1.74	8 (17%)
5	ALF	D	2501	-	4,4,4	1.82	0	0,6,6	0.00	-
6	ADP	D	2502	4	29,29,29	1.24	4 (13%)	45,45,45	1.72	9 (20%)
5	ALF	D	3501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	D	3502	4	29,29,29	1.23	2 (6%)	45,45,45	1.75	10 (22%)
5	ALF	D	4501	-	4,4,4	2.07	4 (100%)	0,6,6	0.00	-
6	ADP	D	4502	4	29,29,29	1.25	3 (10%)	45,45,45	1.64	7 (15%)
5	ALF	D	501	-	4,4,4	1.92	1 (25%)	0,6,6	0.00	-
6	ADP	D	502	4	29,29,29	1.24	2 (6%)	45,45,45	1.77	6 (13%)

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
5	ALF	A	1501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	1502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	2501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	2502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	3501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	3502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	4501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	4502	-	-	0/16/32/32	0/1/3/3
5	ALF	A	501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	1501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	1502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	2501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	2502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	3501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	3502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	4501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	4502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	502	4	-	0/16/32/32	0/1/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3502	ADP	C5-C4	3.75	1.49	1.40
6	D	2502	ADP	C5-C4	3.75	1.48	1.40
6	D	4502	ADP	C5-C4	3.61	1.48	1.40
6	D	502	ADP	C4-N9	-3.61	1.32	1.37
6	D	502	ADP	C5-C4	3.61	1.48	1.40

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	502	ADP	N3-C2-N1	-8.11	121.93	128.71
6	A	2502	ADP	N3-C2-N1	-6.60	123.19	128.71
6	A	4502	ADP	N3-C2-N1	-6.48	123.29	128.71
6	A	1502	ADP	N3-C2-N1	-6.37	123.38	128.71
6	A	3502	ADP	N3-C2-N1	-6.22	123.51	128.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	B	13/15 (86%)	0.17	0 100 100	14, 20, 22, 24	0
1	E	13/15 (86%)	-0.00	0 100 100	11, 19, 23, 28	0
2	C	11/12 (91%)	1.65	4 (36%) 1 1	46, 49, 51, 56	0
2	F	12/12 (100%)	2.63	8 (66%) 0 0	47, 49, 51, 51	0
3	A	1603/1706 (93%)	0.10	13 (0%) 83 49	19, 30, 45, 76	0
3	D	1603/1706 (93%)	0.06	14 (0%) 81 47	18, 30, 45, 75	0
All	All	3255/3466 (93%)	0.10	39 (1%) 75 39	11, 30, 48, 76	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2012	DA	5.3
2	C	2014	DA	4.4
2	F	2004	DA	4.2
3	D	4316	ALA	3.6
3	D	4291	TYR	3.6

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	D	4500	1/1	0.27	4.66	17,17,17,17	0
4	MG	A	500	1/1	0.55	3.22	24,24,24,24	0
4	MG	A	2500	1/1	0.39	2.63	2,2,2,2	0
4	MG	D	1500	1/1	0.41	2.14	2,2,2,2	0
4	MG	A	3500	1/1	0.39	1.98	2,2,2,2	0
5	ALF	D	4501	5/5	0.23	0.85	26,30,32,32	0
4	MG	D	2500	1/1	0.38	0.75	2,2,2,2	0
5	ALF	A	501	5/5	0.35	0.36	17,21,22,23	0
5	ALF	A	2501	5/5	0.30	0.24	2,2,2,2	0
6	ADP	A	502	27/27	0.28	0.21	18,21,27,29	0
5	ALF	A	1501	5/5	0.30	0.19	2,2,4,5	0
5	ALF	D	2501	5/5	0.34	0.17	2,2,2,2	0
5	ALF	D	1501	5/5	0.30	0.12	2,2,2,2	0
4	MG	D	3500	1/1	0.29	0.08	6,6,6,6	0
5	ALF	D	501	5/5	0.28	-0.05	2,2,2,2	0
4	MG	A	1500	1/1	0.32	-0.08	3,3,3,3	0
5	ALF	A	3501	5/5	0.28	-0.15	2,2,2,2	0
6	ADP	A	1502	27/27	0.24	-0.21	2,2,3,5	0
4	MG	D	500	1/1	0.26	-0.29	5,5,5,5	0
6	ADP	D	1502	27/27	0.23	-0.41	2,2,3,5	0
6	ADP	A	3502	27/27	0.20	-0.68	2,2,2,2	0
6	ADP	A	2502	27/27	0.20	-0.73	2,2,2,5	0
6	ADP	D	2502	27/27	0.20	-0.83	2,5,6,7	0
6	ADP	D	502	27/27	0.20	-0.88	2,2,4,5	0
5	ALF	D	3501	5/5	0.23	-0.90	2,2,3,6	0
6	ADP	D	3502	27/27	0.18	-1.07	2,4,9,9	0
5	ALF	A	4501	5/5	0.14	-1.17	36,38,40,40	0
6	ADP	D	4502	27/27	0.14	-1.25	17,19,21,24	0
6	ADP	A	4502	27/27	0.13	-1.34	11,19,23,23	0
4	MG	A	4500	1/1	0.14	-1.41	2,2,2,2	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.