



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:49 AM GMT

PDB ID : 3CMT
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Chen, Z.; Yang, H.; Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 3.15 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

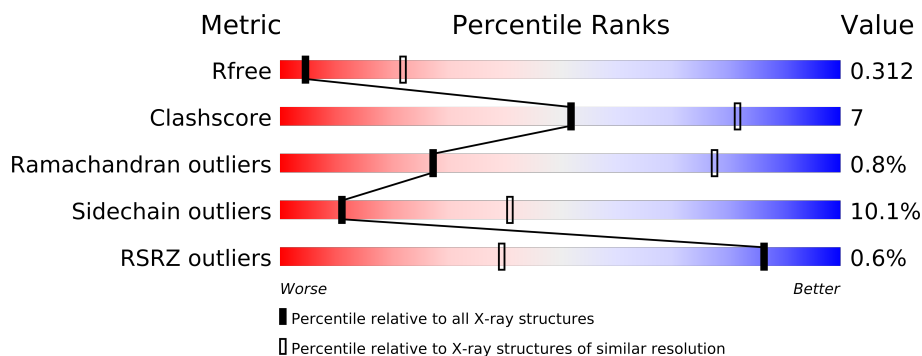
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.15 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	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. 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	6	
2	F	6	
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	1500	-	X
4	MG	A	4500	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	500	-	X
4	MG	D	1500	-	X
4	MG	D	2500	-	X
4	MG	D	500	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25312 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*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			236	115	32	77	12			
1	E	12	Total	C	N	O	P	0	0	0
			236	115	32	77	12			

- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	3	0	0
			130	60	27	37	6			
2	F	6	Total	C	N	O	P	3	0	0
			130	60	27	37	6			

- Molecule 3 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1609	Total	C	N	O	S	0	0	0
			12125	7622	2100	2347	56			
3	D	1609	Total	C	N	O	S	0	0	0
			12125	7622	2101	2345	57			

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
A	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	1992	MET	-	linker	UNP P0A7G6

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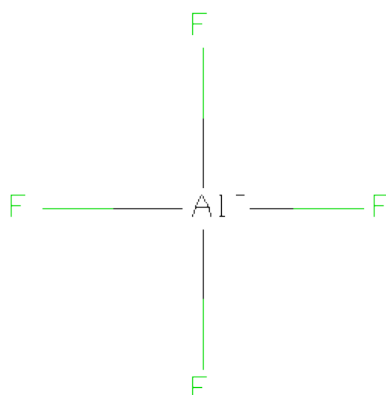
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	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).

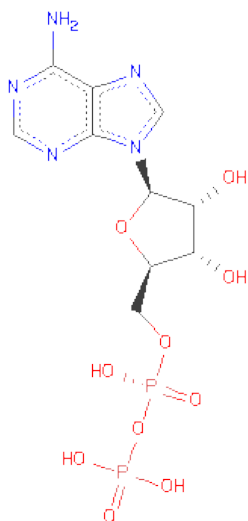
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: 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: $C_{10}H_{15}N_5O_{10}P_2$).



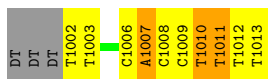
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	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*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

Chain B: 



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

Chain E: 



- Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

Chain C: 



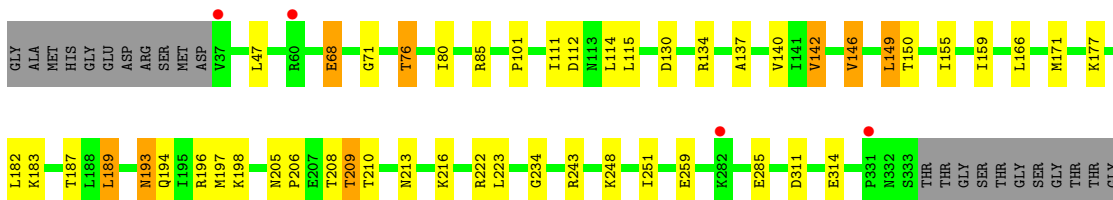
- Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

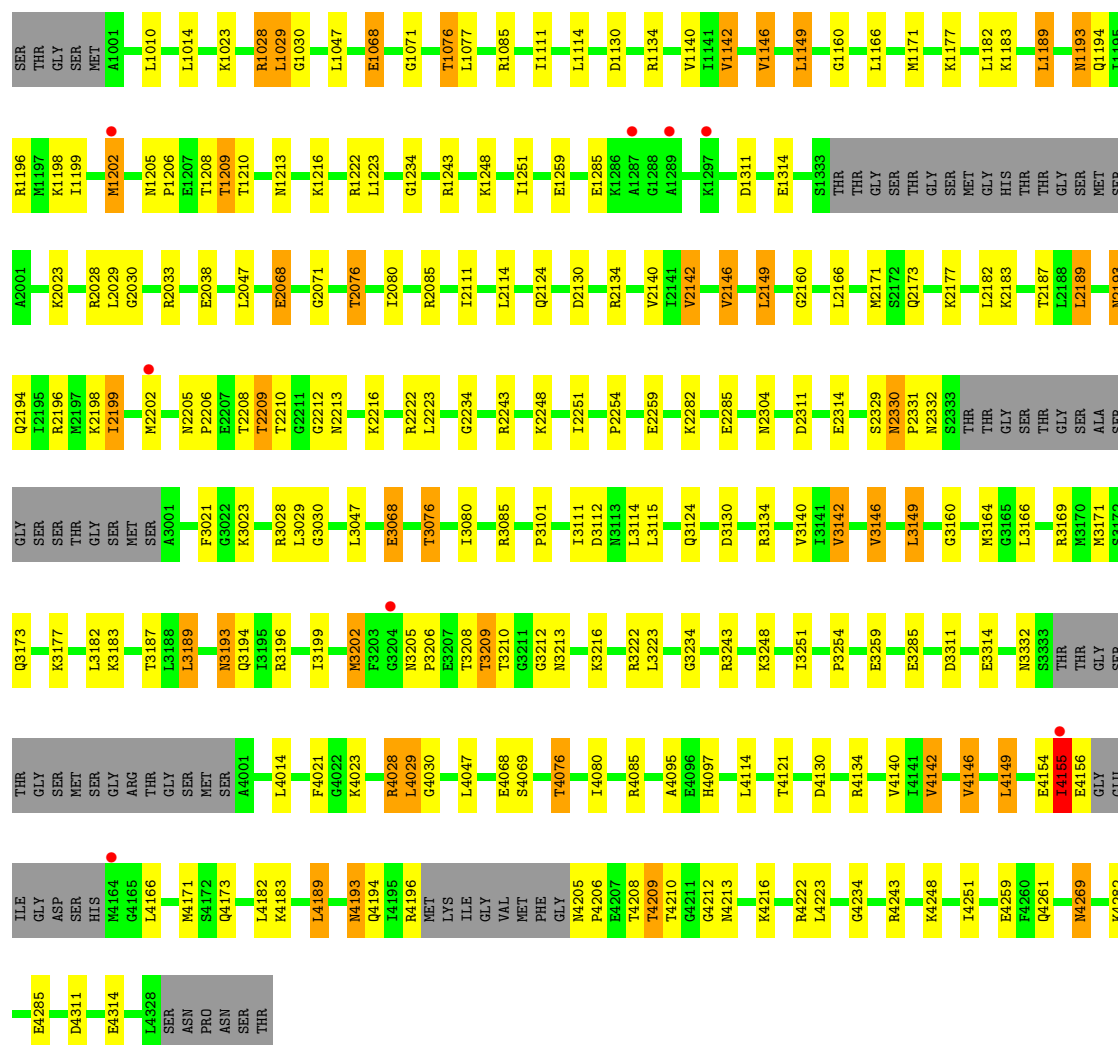
Chain F: 



- Molecule 3: Protein recA

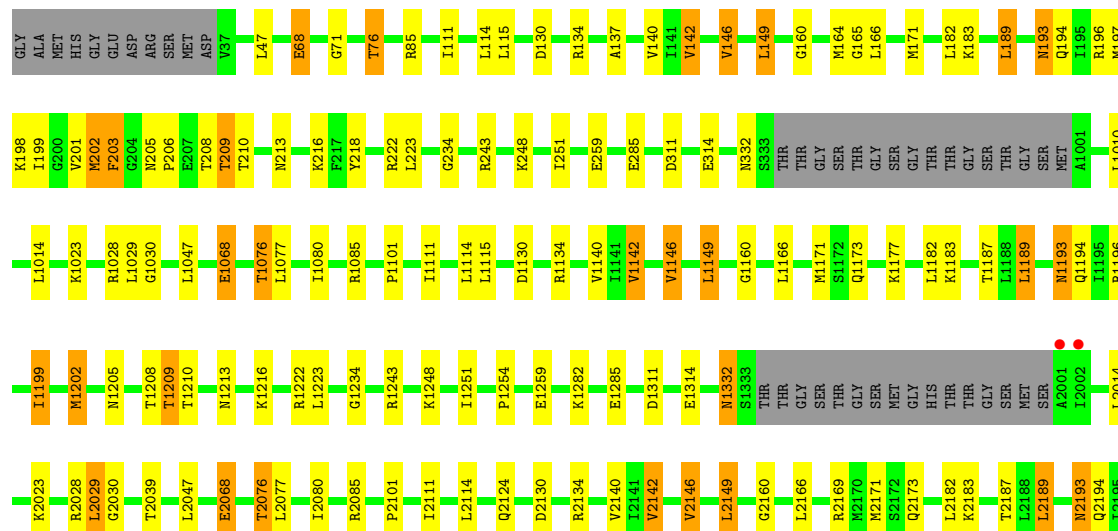
Chain A: 





• Molecule 3: Protein recA

Chain D:



E4314	K4177	THR	I3199	F3021	R2196
L4328 SER ASN PRO ASN SER THR	L4182	GLY	M3202	G3022	R2197
	K4183	SER		K3023	K2198
		MET			I2199
		SER			
	T4187	A4001	N3205	R3028	M2202
	L4188	F4021	E3207	L3029	N2205
	L4189	G4022	T3209	G3030	P2206
		K4023	T3210	L3047	E2207
	N4193		G3211		T2208
	Q4194	R4028	G3212	E3068	T2209
	L4195	L4029	N3213		T2210
	R4196			T3076	G2211
	M4197	L4047	K3216		G2212
	K4198			I3080	N2213
	ILE	E4068	R3222		K2216
	PRO	S4069	L3223	R3085	
	VAL				
	MET	T4076	G3234	I3111	R2222
	PHE				L2223
	GLY	L4080	R3243	L3114	G2234
	N4205				
	P4206	R4085	K3248	Q3124	R2243
	E4207	E4086			
	T4208	G4087	I3251	D3130	K2248
	T4209				
	T4210	L4114	E3259	R3134	
	G4211		F3260		I2251
	G4212	L4126	Q3261	V3140	
	N4213		I3262	I3141	E2259
		D4130	L3263	V3142	E2285
	K4216				
		R4134	N3269	V3146	N2304
	R4222				
	L4223	V4140	K3282	L3149	D2311
		I4141			
	G4234	V4142	E3285	I3155	E2314
	R4243	V4146	D3311	I3159	
	R4248	L4149	E3314	L3166	N2332
					S2333
	I4251	K4152	L3328	M3171	THR
		A4153	S3329	S3172	GLY
	P4254	E4154	N3330	Q3173	SER
		ILE	P3331		
	E4259	GLU	N3332	L3182	GLY
		GLY	S3333	K3183	THR
	K4262	GLU			ALA
		ILE	THR	T3187	SER
	E4265	GLY	GLY	L3188	GLY
		ASP	SER	L3189	SER
	V4291	SER	THR		SER
		HIS	GLY	N3193	THR
	G4295	M4164	SER	Q3194	GLY
	E4296	G4165	MET	I3195	SER
	K4297	L4166	SER	R3196	MET
	D4311	M4171	GLY	M3197	A3001
			ARG	K3198	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.15 39.75 – 2.98	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-3.15) 86.8 (39.75-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.217 , 0.243 0.275 , 0.312	Depositor DCC
R_{free} test set	1233 reflections (2.07%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -1.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 72645 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25312	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 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	1.15	0/260	1.79	7/397 (1.8%)
1	E	1.13	0/260	1.97	12/397 (3.0%)
2	C	3.88	1/146 (0.7%)	2.40	4/225 (1.8%)
2	F	6.25	1/146 (0.7%)	2.40	5/225 (2.2%)
3	A	0.39	0/12264	0.54	0/16503
3	D	0.39	0/12264	0.54	0/16501
All	All	0.70	2/25340 (0.0%)	0.67	28/34248 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2007	DG	P-O5'	-75.00	0.84	1.59
2	C	2007	DG	P-O5'	-45.55	1.14	1.59

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2007	DG	P-O5'-C5'	25.73	162.07	120.90
2	C	2007	DG	O5'-P-OP2	-20.43	86.18	110.70
2	C	2007	DG	O5'-P-OP1	18.46	132.85	110.70
1	E	1006	DC	O4'-C4'-C3'	-8.95	100.63	106.00
2	F	2008	DG	O4'-C1'-N9	-8.52	102.04	108.00

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	236	0	139	9	0
1	E	236	0	139	19	0
2	C	130	0	69	0	0
2	F	130	0	69	0	0
3	A	12125	0	12451	176	0
3	D	12125	0	12456	190	1
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	0	0
5	D	25	0	0	2	0
6	A	135	0	60	6	0
6	D	135	0	60	4	0
All	All	25312	0	25443	364	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 7.

The worst 5 of 364 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:68:GLU:HG2	3:A:1216:LYS:HB3	1.39	1.02
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.97
3:D:160:GLY:H	3:D:1173:GLN:HE22	1.14	0.94
3:A:2068:GLU:HG2	3:A:3216:LYS:HB3	1.54	0.87
3:D:1194:GLN:HE21	3:D:1196:ARG:HH12	1.23	0.86

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:D:218:TYR:OH	3:D:4087:GLY:O[4_456]	2.19	0.01

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	1595/1706 (94%)	1549 (97%)	33 (2%)	13 (1%)	27	77
3	D	1595/1706 (94%)	1539 (96%)	43 (3%)	13 (1%)	27	77
All	All	3190/3412 (94%)	3088 (97%)	76 (2%)	26 (1%)	27	77

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1023	LYS
3	A	2023	LYS
3	A	2330	ASN
3	A	3023	LYS
3	A	4023	LYS

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	1267/1339 (95%)	1142 (90%)	125 (10%)	11	42
3	D	1267/1339 (95%)	1136 (90%)	131 (10%)	10	40
All	All	2534/2678 (95%)	2278 (90%)	256 (10%)	11	41

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4193	ASN
3	D	209	THR
3	D	4085	ARG
3	A	4210	THR

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Mol	Chain	Res	Type
3	D	140	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	4205	ASN
3	D	304	ASN
3	D	4181	ASN
3	A	4300	GLN
3	D	193	ASN

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	1.81	0	0,6,6	0.00	-
6	ADP	A	1502	4	29,29,29	1.14	2 (6%)	45,45,45	2.00	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ALF	A	2501	-	4,4,4	1.85	0	0,6,6	0.00	-
6	ADP	A	2502	4	29,29,29	1.13	2 (6%)	45,45,45	1.78	11 (24%)
5	ALF	A	3501	-	4,4,4	1.83	0	0,6,6	0.00	-
6	ADP	A	3502	4	29,29,29	1.28	4 (13%)	45,45,45	1.81	9 (20%)
5	ALF	A	4501	-	4,4,4	1.90	0	0,6,6	0.00	-
6	ADP	A	4502	4	29,29,29	1.25	3 (10%)	45,45,45	1.75	8 (17%)
5	ALF	A	501	-	4,4,4	1.90	0	0,6,6	0.00	-
6	ADP	A	502	4	29,29,29	1.09	2 (6%)	45,45,45	1.87	9 (20%)
5	ALF	D	1501	-	4,4,4	1.82	0	0,6,6	0.00	-
6	ADP	D	1502	4	29,29,29	1.12	2 (6%)	45,45,45	1.92	11 (24%)
5	ALF	D	2501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	D	2502	4	29,29,29	1.20	3 (10%)	45,45,45	1.76	8 (17%)
5	ALF	D	3501	-	4,4,4	1.77	0	0,6,6	0.00	-
6	ADP	D	3502	4	29,29,29	1.19	2 (6%)	45,45,45	1.82	7 (15%)
5	ALF	D	4501	-	4,4,4	1.91	1 (25%)	0,6,6	0.00	-
6	ADP	D	4502	4	29,29,29	1.20	3 (10%)	45,45,45	1.79	11 (24%)
5	ALF	D	501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	D	502	4	29,29,29	1.13	2 (6%)	45,45,45	1.75	10 (22%)

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	4	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2502	ADP	C5-C4	3.63	1.48	1.40
6	D	4502	ADP	C5-C4	3.63	1.48	1.40
6	A	3502	ADP	C4-N9	-3.51	1.32	1.37
6	A	502	ADP	C5-C4	3.41	1.48	1.40
6	A	2502	ADP	C4-N9	-3.34	1.32	1.37

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	ADP	N3-C2-N1	-7.63	122.33	128.71
6	D	2502	ADP	N3-C2-N1	-7.09	122.78	128.71
6	A	3502	ADP	N3-C2-N1	-6.96	122.89	128.71
6	D	4502	ADP	N3-C2-N1	-6.55	123.24	128.71
6	A	4502	ADP	N3-C2-N1	-6.51	123.26	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, 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(Å²)	Q<0.9	
1	B	12/15 (80%)	-0.08	0	100	100	37, 42, 48, 48	0
1	E	12/15 (80%)	-0.08	0	100	100	38, 47, 53, 62	0
2	C	6/6 (100%)	0.19	0	100	100	46, 48, 63, 66	1 (16%)
2	F	6/6 (100%)	0.12	0	100	100	48, 50, 55, 56	1 (16%)
3	A	1609/1706 (94%)	0.08	12 (0%)	84	35	39, 49, 64, 96	0
3	D	1609/1706 (94%)	-0.00	9 (0%)	86	39	39, 49, 65, 96	0
All	All	3254/3454 (94%)	0.04	21 (0%)	86	39	37, 49, 64, 96	2 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	4164	MET	3.3
3	A	2202	MET	2.7
3	D	4295	GLY	2.7
3	A	1287	ALA	2.7
3	D	2001	ALA	2.7

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	1500	1/1	0.46	12.95	38,38,38,38	0
4	MG	D	1500	1/1	0.41	4.99	28,28,28,28	0
4	MG	D	2500	1/1	0.56	3.07	32,32,32,32	0
4	MG	A	500	1/1	0.43	2.85	44,44,44,44	0
4	MG	D	500	1/1	0.38	2.72	34,34,34,34	0
4	MG	A	4500	1/1	0.23	2.64	32,32,32,32	0
4	MG	A	2500	1/1	0.42	1.96	25,25,25,25	0
4	MG	A	3500	1/1	0.41	1.78	27,27,27,27	0
4	MG	D	3500	1/1	0.35	1.26	31,31,31,31	0
5	ALF	A	1501	5/5	0.31	1.06	35,35,38,41	0
5	ALF	D	3501	5/5	0.27	0.43	27,29,33,33	0
5	ALF	A	501	5/5	0.29	0.33	38,39,44,46	0
5	ALF	D	2501	5/5	0.35	0.27	24,26,29,30	0
6	ADP	A	502	27/27	0.27	0.25	42,44,48,49	0
4	MG	D	4500	1/1	0.22	0.21	39,39,39,39	0
5	ALF	D	1501	5/5	0.29	-0.08	23,24,26,26	0
5	ALF	A	3501	5/5	0.28	-0.23	28,28,31,32	0
5	ALF	D	501	5/5	0.29	-0.27	30,30,32,35	0
6	ADP	A	3502	27/27	0.21	-0.46	16,20,24,26	0
5	ALF	D	4501	5/5	0.18	-0.48	41,41,43,43	0
6	ADP	A	1502	27/27	0.21	-0.50	27,30,35,35	0
6	ADP	D	3502	27/27	0.20	-0.59	28,34,36,37	0
5	ALF	A	4501	5/5	0.17	-0.76	49,49,51,51	0
6	ADP	D	502	27/27	0.21	-0.79	16,23,29,30	0
5	ALF	A	2501	5/5	0.27	-0.85	24,25,27,28	0
6	ADP	D	4502	27/27	0.15	-0.89	41,43,45,46	0
6	ADP	A	2502	27/27	0.17	-1.07	15,20,27,27	0
6	ADP	D	2502	27/27	0.18	-1.18	25,27,29,30	0
6	ADP	D	1502	27/27	0.19	-1.28	15,19,23,24	0
6	ADP	A	4502	27/27	0.13	-1.29	31,42,44,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.