



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:29 AM GMT

PDB ID : 3CMV
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 4.30 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>

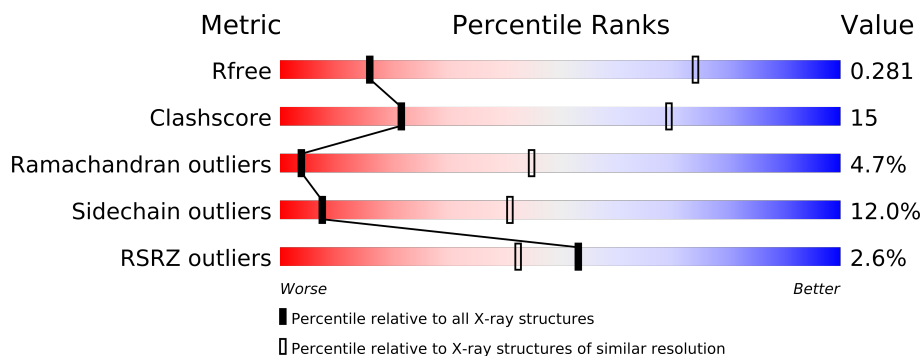
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.30 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	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
Sidechain outliers	78261	1192 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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	A	1357	
1	B	1357	
1	C	1357	
1	D	1357	
1	E	1357	
1	F	1357	
1	G	1357	
1	H	1357	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	1701	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	701	-	X
2	MG	B	1701	-	X
2	MG	B	2701	-	X
2	MG	B	701	-	X
2	MG	C	1701	-	X
2	MG	C	701	-	X
2	MG	D	1701	-	X
2	MG	D	701	-	X
2	MG	E	1701	-	X
2	MG	E	3701	-	X
2	MG	E	701	-	X
2	MG	F	1701	-	X
2	MG	F	701	-	X
2	MG	G	1701	-	X
2	MG	G	701	-	X
2	MG	H	1701	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 71761 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 protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1190	Total	C	N	O	S	0	0	0
			8970	5660	1553	1719	38			
1	B	1163	Total	C	N	O	S	0	0	0
			8769	5538	1519	1677	35			
1	C	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	D	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	E	1165	Total	C	N	O	S	0	0	0
			8787	5548	1521	1683	35			
1	F	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	G	1167	Total	C	N	O	S	0	0	0
			8799	5554	1523	1687	35			
1	H	1173	Total	C	N	O	S	0	0	0
			8844	5581	1531	1696	36			

There are 400 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	3000	SER	-	linker	UNP P0A7G6
B	26	GLY	-	linker	UNP P0A7G6
B	27	ALA	-	linker	UNP P0A7G6
B	28	MET	-	linker	UNP P0A7G6
B	29	HIS	-	linker	UNP P0A7G6
B	986	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	GLY	-	linker	UNP P0A7G6
B	988	SER	-	linker	UNP P0A7G6
B	989	THR	-	linker	UNP P0A7G6
B	990	GLY	-	linker	UNP P0A7G6
B	991	SER	-	linker	UNP P0A7G6
B	992	GLY	-	linker	UNP P0A7G6
B	993	THR	-	linker	UNP P0A7G6
B	994	THR	-	linker	UNP P0A7G6
B	995	GLY	-	linker	UNP P0A7G6
B	996	SER	-	linker	UNP P0A7G6
B	997	THR	-	linker	UNP P0A7G6
B	998	GLY	-	linker	UNP P0A7G6
B	999	SER	-	linker	UNP P0A7G6
B	1000	MET	-	linker	UNP P0A7G6
B	1986	THR	-	linker	UNP P0A7G6
B	1987	GLY	-	linker	UNP P0A7G6
B	1988	SER	-	linker	UNP P0A7G6
B	1989	THR	-	linker	UNP P0A7G6
B	1990	GLY	-	linker	UNP P0A7G6
B	1991	SER	-	linker	UNP P0A7G6
B	1992	MET	-	linker	UNP P0A7G6
B	1993	GLY	-	linker	UNP P0A7G6
B	1994	HIS	-	linker	UNP P0A7G6
B	1995	THR	-	linker	UNP P0A7G6
B	1996	THR	-	linker	UNP P0A7G6
B	1997	GLY	-	linker	UNP P0A7G6
B	1998	SER	-	linker	UNP P0A7G6
B	1999	MET	-	linker	UNP P0A7G6
B	2000	SER	-	linker	UNP P0A7G6
B	2985	THR	-	linker	UNP P0A7G6
B	2986	GLY	-	linker	UNP P0A7G6
B	2987	SER	-	linker	UNP P0A7G6
B	2988	THR	-	linker	UNP P0A7G6
B	2989	GLY	-	linker	UNP P0A7G6
B	2990	SER	-	linker	UNP P0A7G6
B	2991	ALA	-	linker	UNP P0A7G6
B	2992	SER	-	linker	UNP P0A7G6
B	2993	GLY	-	linker	UNP P0A7G6
B	2994	SER	-	linker	UNP P0A7G6
B	2995	SER	-	linker	UNP P0A7G6
B	2996	THR	-	linker	UNP P0A7G6
B	2997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2998	SER	-	linker	UNP P0A7G6
B	2999	MET	-	linker	UNP P0A7G6
B	3000	SER	-	linker	UNP P0A7G6
C	26	GLY	-	linker	UNP P0A7G6
C	27	ALA	-	linker	UNP P0A7G6
C	28	MET	-	linker	UNP P0A7G6
C	29	HIS	-	linker	UNP P0A7G6
C	986	THR	-	linker	UNP P0A7G6
C	987	GLY	-	linker	UNP P0A7G6
C	988	SER	-	linker	UNP P0A7G6
C	989	THR	-	linker	UNP P0A7G6
C	990	GLY	-	linker	UNP P0A7G6
C	991	SER	-	linker	UNP P0A7G6
C	992	GLY	-	linker	UNP P0A7G6
C	993	THR	-	linker	UNP P0A7G6
C	994	THR	-	linker	UNP P0A7G6
C	995	GLY	-	linker	UNP P0A7G6
C	996	SER	-	linker	UNP P0A7G6
C	997	THR	-	linker	UNP P0A7G6
C	998	GLY	-	linker	UNP P0A7G6
C	999	SER	-	linker	UNP P0A7G6
C	1000	MET	-	linker	UNP P0A7G6
C	1986	THR	-	linker	UNP P0A7G6
C	1987	GLY	-	linker	UNP P0A7G6
C	1988	SER	-	linker	UNP P0A7G6
C	1989	THR	-	linker	UNP P0A7G6
C	1990	GLY	-	linker	UNP P0A7G6
C	1991	SER	-	linker	UNP P0A7G6
C	1992	MET	-	linker	UNP P0A7G6
C	1993	GLY	-	linker	UNP P0A7G6
C	1994	HIS	-	linker	UNP P0A7G6
C	1995	THR	-	linker	UNP P0A7G6
C	1996	THR	-	linker	UNP P0A7G6
C	1997	GLY	-	linker	UNP P0A7G6
C	1998	SER	-	linker	UNP P0A7G6
C	1999	MET	-	linker	UNP P0A7G6
C	2000	SER	-	linker	UNP P0A7G6
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	GLY	-	linker	UNP P0A7G6
C	2994	SER	-	linker	UNP P0A7G6
C	2995	SER	-	linker	UNP P0A7G6
C	2996	THR	-	linker	UNP P0A7G6
C	2997	GLY	-	linker	UNP P0A7G6
C	2998	SER	-	linker	UNP P0A7G6
C	2999	MET	-	linker	UNP P0A7G6
C	3000	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	26	GLY	-	linker	UNP P0A7G6
E	27	ALA	-	linker	UNP P0A7G6
E	28	MET	-	linker	UNP P0A7G6
E	29	HIS	-	linker	UNP P0A7G6
E	986	THR	-	linker	UNP P0A7G6
E	987	GLY	-	linker	UNP P0A7G6
E	988	SER	-	linker	UNP P0A7G6
E	989	THR	-	linker	UNP P0A7G6
E	990	GLY	-	linker	UNP P0A7G6
E	991	SER	-	linker	UNP P0A7G6
E	992	GLY	-	linker	UNP P0A7G6
E	993	THR	-	linker	UNP P0A7G6
E	994	THR	-	linker	UNP P0A7G6
E	995	GLY	-	linker	UNP P0A7G6
E	996	SER	-	linker	UNP P0A7G6
E	997	THR	-	linker	UNP P0A7G6
E	998	GLY	-	linker	UNP P0A7G6
E	999	SER	-	linker	UNP P0A7G6
E	1000	MET	-	linker	UNP P0A7G6
E	1986	THR	-	linker	UNP P0A7G6
E	1987	GLY	-	linker	UNP P0A7G6
E	1988	SER	-	linker	UNP P0A7G6
E	1989	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1990	GLY	-	linker	UNP P0A7G6
E	1991	SER	-	linker	UNP P0A7G6
E	1992	MET	-	linker	UNP P0A7G6
E	1993	GLY	-	linker	UNP P0A7G6
E	1994	HIS	-	linker	UNP P0A7G6
E	1995	THR	-	linker	UNP P0A7G6
E	1996	THR	-	linker	UNP P0A7G6
E	1997	GLY	-	linker	UNP P0A7G6
E	1998	SER	-	linker	UNP P0A7G6
E	1999	MET	-	linker	UNP P0A7G6
E	2000	SER	-	linker	UNP P0A7G6
E	2985	THR	-	linker	UNP P0A7G6
E	2986	GLY	-	linker	UNP P0A7G6
E	2987	SER	-	linker	UNP P0A7G6
E	2988	THR	-	linker	UNP P0A7G6
E	2989	GLY	-	linker	UNP P0A7G6
E	2990	SER	-	linker	UNP P0A7G6
E	2991	ALA	-	linker	UNP P0A7G6
E	2992	SER	-	linker	UNP P0A7G6
E	2993	GLY	-	linker	UNP P0A7G6
E	2994	SER	-	linker	UNP P0A7G6
E	2995	SER	-	linker	UNP P0A7G6
E	2996	THR	-	linker	UNP P0A7G6
E	2997	GLY	-	linker	UNP P0A7G6
E	2998	SER	-	linker	UNP P0A7G6
E	2999	MET	-	linker	UNP P0A7G6
E	3000	SER	-	linker	UNP P0A7G6
F	26	GLY	-	linker	UNP P0A7G6
F	27	ALA	-	linker	UNP P0A7G6
F	28	MET	-	linker	UNP P0A7G6
F	29	HIS	-	linker	UNP P0A7G6
F	986	THR	-	linker	UNP P0A7G6
F	987	GLY	-	linker	UNP P0A7G6
F	988	SER	-	linker	UNP P0A7G6
F	989	THR	-	linker	UNP P0A7G6
F	990	GLY	-	linker	UNP P0A7G6
F	991	SER	-	linker	UNP P0A7G6
F	992	GLY	-	linker	UNP P0A7G6
F	993	THR	-	linker	UNP P0A7G6
F	994	THR	-	linker	UNP P0A7G6
F	995	GLY	-	linker	UNP P0A7G6
F	996	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	997	THR	-	linker	UNP P0A7G6
F	998	GLY	-	linker	UNP P0A7G6
F	999	SER	-	linker	UNP P0A7G6
F	1000	MET	-	linker	UNP P0A7G6
F	1986	THR	-	linker	UNP P0A7G6
F	1987	GLY	-	linker	UNP P0A7G6
F	1988	SER	-	linker	UNP P0A7G6
F	1989	THR	-	linker	UNP P0A7G6
F	1990	GLY	-	linker	UNP P0A7G6
F	1991	SER	-	linker	UNP P0A7G6
F	1992	MET	-	linker	UNP P0A7G6
F	1993	GLY	-	linker	UNP P0A7G6
F	1994	HIS	-	linker	UNP P0A7G6
F	1995	THR	-	linker	UNP P0A7G6
F	1996	THR	-	linker	UNP P0A7G6
F	1997	GLY	-	linker	UNP P0A7G6
F	1998	SER	-	linker	UNP P0A7G6
F	1999	MET	-	linker	UNP P0A7G6
F	2000	SER	-	linker	UNP P0A7G6
F	2985	THR	-	linker	UNP P0A7G6
F	2986	GLY	-	linker	UNP P0A7G6
F	2987	SER	-	linker	UNP P0A7G6
F	2988	THR	-	linker	UNP P0A7G6
F	2989	GLY	-	linker	UNP P0A7G6
F	2990	SER	-	linker	UNP P0A7G6
F	2991	ALA	-	linker	UNP P0A7G6
F	2992	SER	-	linker	UNP P0A7G6
F	2993	GLY	-	linker	UNP P0A7G6
F	2994	SER	-	linker	UNP P0A7G6
F	2995	SER	-	linker	UNP P0A7G6
F	2996	THR	-	linker	UNP P0A7G6
F	2997	GLY	-	linker	UNP P0A7G6
F	2998	SER	-	linker	UNP P0A7G6
F	2999	MET	-	linker	UNP P0A7G6
F	3000	SER	-	linker	UNP P0A7G6
G	26	GLY	-	linker	UNP P0A7G6
G	27	ALA	-	linker	UNP P0A7G6
G	28	MET	-	linker	UNP P0A7G6
G	29	HIS	-	linker	UNP P0A7G6
G	986	THR	-	linker	UNP P0A7G6
G	987	GLY	-	linker	UNP P0A7G6
G	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	989	THR	-	linker	UNP P0A7G6
G	990	GLY	-	linker	UNP P0A7G6
G	991	SER	-	linker	UNP P0A7G6
G	992	GLY	-	linker	UNP P0A7G6
G	993	THR	-	linker	UNP P0A7G6
G	994	THR	-	linker	UNP P0A7G6
G	995	GLY	-	linker	UNP P0A7G6
G	996	SER	-	linker	UNP P0A7G6
G	997	THR	-	linker	UNP P0A7G6
G	998	GLY	-	linker	UNP P0A7G6
G	999	SER	-	linker	UNP P0A7G6
G	1000	MET	-	linker	UNP P0A7G6
G	1986	THR	-	linker	UNP P0A7G6
G	1987	GLY	-	linker	UNP P0A7G6
G	1988	SER	-	linker	UNP P0A7G6
G	1989	THR	-	linker	UNP P0A7G6
G	1990	GLY	-	linker	UNP P0A7G6
G	1991	SER	-	linker	UNP P0A7G6
G	1992	MET	-	linker	UNP P0A7G6
G	1993	GLY	-	linker	UNP P0A7G6
G	1994	HIS	-	linker	UNP P0A7G6
G	1995	THR	-	linker	UNP P0A7G6
G	1996	THR	-	linker	UNP P0A7G6
G	1997	GLY	-	linker	UNP P0A7G6
G	1998	SER	-	linker	UNP P0A7G6
G	1999	MET	-	linker	UNP P0A7G6
G	2000	SER	-	linker	UNP P0A7G6
G	2985	THR	-	linker	UNP P0A7G6
G	2986	GLY	-	linker	UNP P0A7G6
G	2987	SER	-	linker	UNP P0A7G6
G	2988	THR	-	linker	UNP P0A7G6
G	2989	GLY	-	linker	UNP P0A7G6
G	2990	SER	-	linker	UNP P0A7G6
G	2991	ALA	-	linker	UNP P0A7G6
G	2992	SER	-	linker	UNP P0A7G6
G	2993	GLY	-	linker	UNP P0A7G6
G	2994	SER	-	linker	UNP P0A7G6
G	2995	SER	-	linker	UNP P0A7G6
G	2996	THR	-	linker	UNP P0A7G6
G	2997	GLY	-	linker	UNP P0A7G6
G	2998	SER	-	linker	UNP P0A7G6
G	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3000	SER	-	linker	UNP P0A7G6
H	26	GLY	-	linker	UNP P0A7G6
H	27	ALA	-	linker	UNP P0A7G6
H	28	MET	-	linker	UNP P0A7G6
H	29	HIS	-	linker	UNP P0A7G6
H	986	THR	-	linker	UNP P0A7G6
H	987	GLY	-	linker	UNP P0A7G6
H	988	SER	-	linker	UNP P0A7G6
H	989	THR	-	linker	UNP P0A7G6
H	990	GLY	-	linker	UNP P0A7G6
H	991	SER	-	linker	UNP P0A7G6
H	992	GLY	-	linker	UNP P0A7G6
H	993	THR	-	linker	UNP P0A7G6
H	994	THR	-	linker	UNP P0A7G6
H	995	GLY	-	linker	UNP P0A7G6
H	996	SER	-	linker	UNP P0A7G6
H	997	THR	-	linker	UNP P0A7G6
H	998	GLY	-	linker	UNP P0A7G6
H	999	SER	-	linker	UNP P0A7G6
H	1000	MET	-	linker	UNP P0A7G6
H	1986	THR	-	linker	UNP P0A7G6
H	1987	GLY	-	linker	UNP P0A7G6
H	1988	SER	-	linker	UNP P0A7G6
H	1989	THR	-	linker	UNP P0A7G6
H	1990	GLY	-	linker	UNP P0A7G6
H	1991	SER	-	linker	UNP P0A7G6
H	1992	MET	-	linker	UNP P0A7G6
H	1993	GLY	-	linker	UNP P0A7G6
H	1994	HIS	-	linker	UNP P0A7G6
H	1995	THR	-	linker	UNP P0A7G6
H	1996	THR	-	linker	UNP P0A7G6
H	1997	GLY	-	linker	UNP P0A7G6
H	1998	SER	-	linker	UNP P0A7G6
H	1999	MET	-	linker	UNP P0A7G6
H	2000	SER	-	linker	UNP P0A7G6
H	2985	THR	-	linker	UNP P0A7G6
H	2986	GLY	-	linker	UNP P0A7G6
H	2987	SER	-	linker	UNP P0A7G6
H	2988	THR	-	linker	UNP P0A7G6
H	2989	GLY	-	linker	UNP P0A7G6
H	2990	SER	-	linker	UNP P0A7G6
H	2991	ALA	-	linker	UNP P0A7G6

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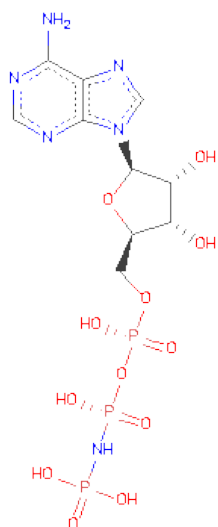
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Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker	UNP P0A7G6
H	2999	MET	-	linker	UNP P0A7G6
H	3000	SER	-	linker	UNP P0A7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0
2	E	4	Total Mg 4 4	0	0
2	H	4	Total Mg 4 4	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	A	4	Total Mg 4 4	0	0
2	F	4	Total Mg 4 4	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

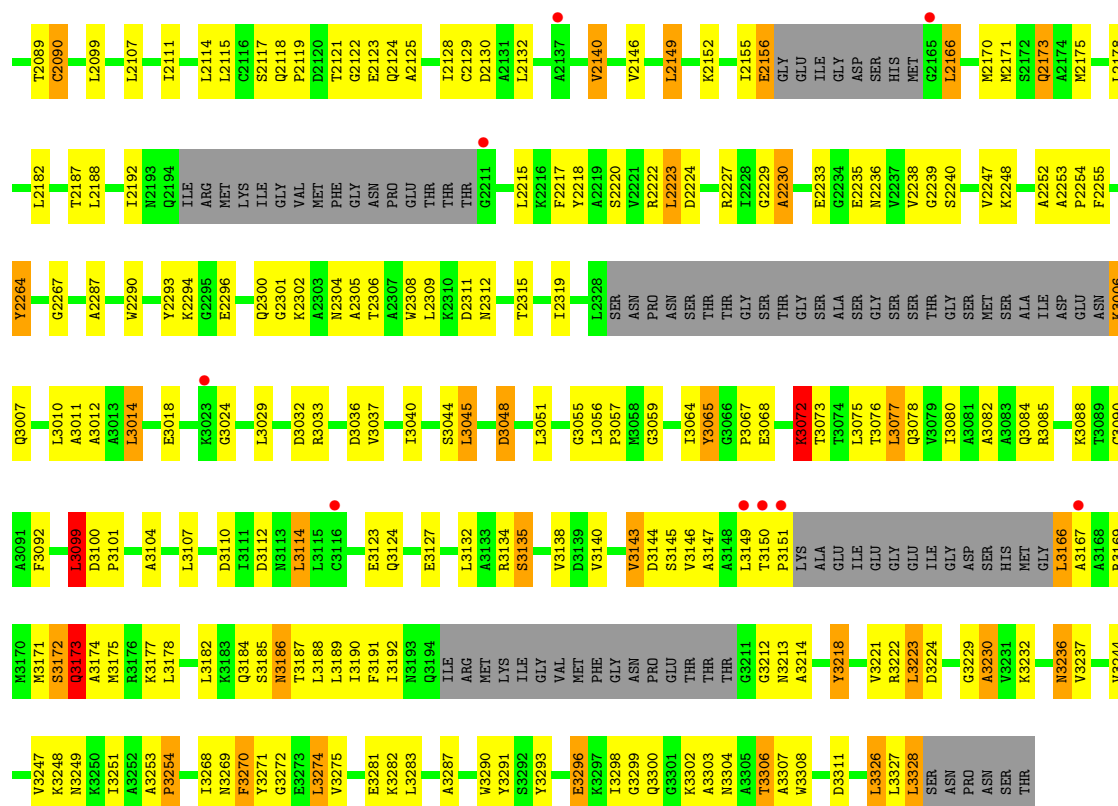
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	D	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	G	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	G	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	G	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	G	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	H	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	H	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	H	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	H	1	Total 31	C 10	N 6	O 12	P 3	0	0

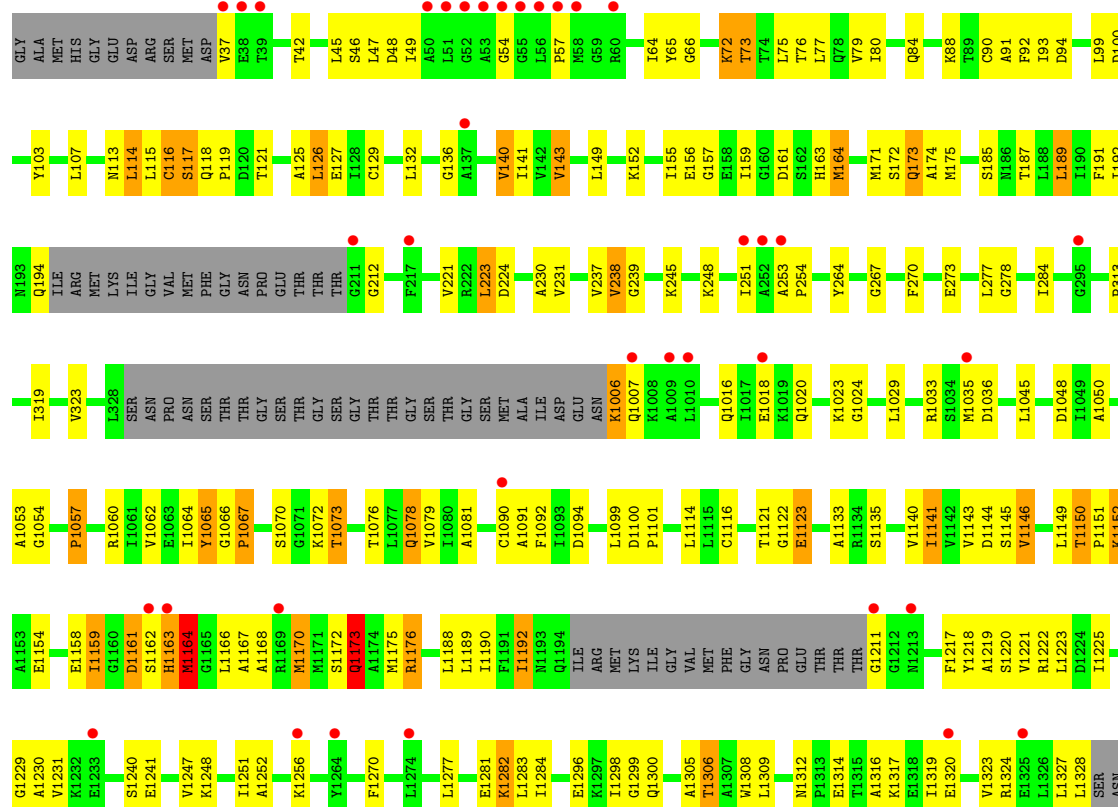




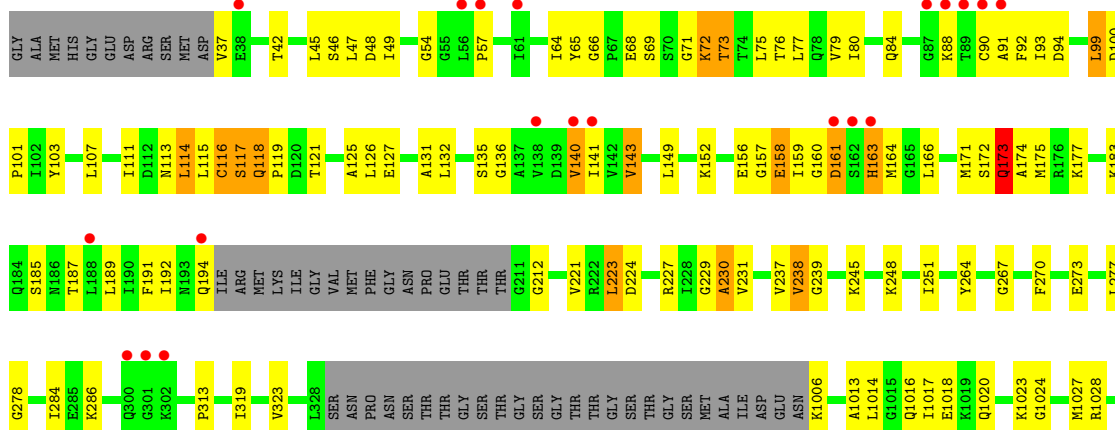


• Molecule 1: Protein recA

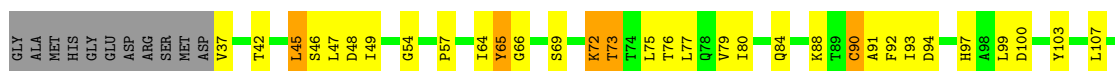
Chain D:













4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	176.60Å 189.80Å 424.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 39.93 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 92.8 (39.93-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.271 , 0.281	Depositor DCC
R_{free} test set	1823 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	170.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 119.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 96833 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	71761	wwPDB-VP
Average B, all atoms (Å ²)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MG, ANP

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	0.81	6/9068 (0.1%)	0.80	10/12192 (0.1%)
1	B	0.76	4/8861 (0.0%)	0.76	1/11910 (0.0%)
1	C	0.77	0/8951	0.77	4/12033 (0.0%)
1	D	0.74	3/8951 (0.0%)	0.75	4/12033 (0.0%)
1	E	0.72	1/8879 (0.0%)	0.75	2/11934 (0.0%)
1	F	0.77	4/8951 (0.0%)	0.77	2/12033 (0.0%)
1	G	0.77	2/8892 (0.0%)	0.76	3/11953 (0.0%)
1	H	0.72	2/8938 (0.0%)	0.75	3/12014 (0.0%)
All	All	0.76	22/71491 (0.0%)	0.77	29/96102 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	3
1	C	0	4
1	D	0	7
1	E	0	6
1	F	0	6
1	G	0	5
1	H	0	4
All	All	0	46

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	7.46	1.61	1.46
1	B	3266	GLU	CG-CD	6.68	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1164	MET	CB-CG	6.66	1.72	1.51
1	D	156	GLU	CG-CD	5.97	1.60	1.51
1	F	3270	PHE	CE1-CZ	5.74	1.48	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	MET	C-N-CA	-8.01	105.48	122.30
1	D	2166	LEU	CA-CB-CG	7.24	131.94	115.30
1	G	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	H	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	E	2166	LEU	CA-CB-CG	7.21	131.89	115.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ASP	Peptide
1	A	1163	HIS	Peptide
1	A	158	GLU	Peptide
1	A	161	ASP	Peptide
1	A	163	HIS	Peptide

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	A	8970	0	9264	308	1
1	B	8769	0	9070	275	0
1	C	8856	0	9139	294	1
1	D	8856	0	9139	268	0
1	E	8787	0	9082	304	0
1	F	8856	0	9139	314	0
1	G	8799	0	9090	269	0
1	H	8844	0	9131	304	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	124	0	52	7	0
3	B	124	0	52	2	0
3	C	124	0	52	3	0
3	D	124	0	52	2	0
3	E	124	0	52	3	0
3	F	124	0	52	9	0
3	G	124	0	52	4	0
3	H	124	0	52	4	0
All	All	71761	0	73470	2200	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 15.

The worst 5 of 2200 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1204:GLY:HA2	1:B:3115:LEU:CD2	1.50	1.42
1:A:1194:GLN:O	1:A:1195:ILE:CG2	1.73	1.37
1:A:162:SER:O	1:A:165:GLY:CA	1.71	1.35
1:A:1194:GLN:O	1:A:1195:ILE:CB	1.81	1.27
1:A:1194:GLN:O	1:A:1195:ILE:HG22	1.25	1.22

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)
1:A:1161:ASP:OD1	1:C:1314:GLU:OE2[4_456]	2.05	0.15

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	
1	A	1172/1357 (86%)	923 (79%)	191 (16%)	58 (5%)	3	43
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	4	45
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	3	43
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	4	45
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	4	45
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	4	45
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	4	46
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	3	43
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	4	45

5 of 437 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	99	LEU
1	A	238	VAL
1	A	1099	LEU
1	A	1146	VAL

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	
1	A	930/1065 (87%)	813 (87%)	117 (13%)	7	39
1	B	908/1065 (85%)	801 (88%)	107 (12%)	8	42
1	C	917/1065 (86%)	805 (88%)	112 (12%)	7	40
1	D	917/1065 (86%)	810 (88%)	107 (12%)	8	42
1	E	910/1065 (85%)	801 (88%)	109 (12%)	7	41
1	F	917/1065 (86%)	812 (88%)	105 (12%)	8	43
1	G	911/1065 (86%)	800 (88%)	111 (12%)	7	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	916/1065 (86%)	806 (88%)	110 (12%)	7	41
All	All	7326/8520 (86%)	6448 (88%)	878 (12%)	7	41

5 of 878 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2089	THR
1	E	1282	LYS
1	H	1221	VAL
1	D	2264	TYR
1	E	65	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2300	GLN
1	E	2236	ASN
1	H	2020	GLN
1	D	3181	ASN
1	E	173	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 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 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	$\# Z > 2$
3	ANP	A	1400	-	33,33,33	3.39	6 (18%)	51,52,52	2.33	11 (21%)
3	ANP	A	2400	-	33,33,33	3.76	6 (18%)	51,52,52	2.33	12 (23%)
3	ANP	A	3400	-	33,33,33	3.28	6 (18%)	51,52,52	2.50	13 (25%)
3	ANP	A	400	-	33,33,33	3.73	7 (21%)	51,52,52	2.17	11 (21%)
3	ANP	B	1400	-	33,33,33	3.70	5 (15%)	51,52,52	2.34	11 (21%)
3	ANP	B	2400	-	33,33,33	3.71	6 (18%)	51,52,52	2.31	11 (21%)
3	ANP	B	3400	-	33,33,33	3.63	5 (15%)	51,52,52	2.55	13 (25%)
3	ANP	B	400	-	33,33,33	3.55	6 (18%)	51,52,52	2.17	11 (21%)
3	ANP	C	1400	-	33,33,33	3.85	6 (18%)	51,52,52	2.34	12 (23%)
3	ANP	C	2400	-	33,33,33	3.58	5 (15%)	51,52,52	2.30	11 (21%)
3	ANP	C	3400	-	33,33,33	4.21	6 (18%)	51,52,52	2.44	13 (25%)
3	ANP	C	400	-	33,33,33	3.25	5 (15%)	51,52,52	2.21	11 (21%)
3	ANP	D	1400	-	33,33,33	3.60	6 (18%)	51,52,52	2.34	11 (21%)
3	ANP	D	2400	-	33,33,33	3.71	6 (18%)	51,52,52	2.30	12 (23%)
3	ANP	D	3400	-	33,33,33	3.54	6 (18%)	51,52,52	2.52	13 (25%)
3	ANP	D	400	-	33,33,33	3.78	6 (18%)	51,52,52	2.13	11 (21%)
3	ANP	E	1400	-	33,33,33	3.67	7 (21%)	51,52,52	2.35	11 (21%)
3	ANP	E	2400	-	33,33,33	3.78	6 (18%)	51,52,52	2.30	11 (21%)
3	ANP	E	3400	2	33,33,33	3.29	7 (21%)	51,52,52	2.52	14 (27%)
3	ANP	E	400	-	33,33,33	3.68	6 (18%)	51,52,52	2.20	10 (19%)
3	ANP	F	1400	-	33,33,33	3.75	7 (21%)	51,52,52	2.32	11 (21%)
3	ANP	F	2400	-	33,33,33	3.45	5 (15%)	51,52,52	2.32	12 (23%)
3	ANP	F	3400	-	33,33,33	3.54	7 (21%)	51,52,52	2.47	13 (25%)
3	ANP	F	400	-	33,33,33	3.46	6 (18%)	51,52,52	2.13	11 (21%)
3	ANP	G	1400	-	33,33,33	3.55	7 (21%)	51,52,52	2.33	12 (23%)
3	ANP	G	2400	-	33,33,33	3.78	6 (18%)	51,52,52	2.29	11 (21%)
3	ANP	G	3400	-	33,33,33	4.04	6 (18%)	51,52,52	2.47	13 (25%)
3	ANP	G	400	-	33,33,33	3.67	5 (15%)	51,52,52	2.16	11 (21%)
3	ANP	H	1400	-	33,33,33	3.85	6 (18%)	51,52,52	2.27	11 (21%)
3	ANP	H	2400	-	33,33,33	3.67	5 (15%)	51,52,52	2.30	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	H	3400	-	33,33,33	4.00	6 (18%)	51,52,52	2.60	13 (25%)
3	ANP	H	400	-	33,33,33	3.55	6 (18%)	51,52,52	2.18	10 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	A	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	A	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	A	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	B	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	B	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	B	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	B	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	C	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	C	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	C	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	C	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	D	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	D	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	D	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	D	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	E	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	E	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	E	3400	2	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	E	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	F	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	F	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	F	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	F	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	G	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	G	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	G	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	G	400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	H	1400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	H	2400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	H	3400	-	1/1/7/8	0/18/38/38	0/1/3/3
3	ANP	H	400	-	1/1/7/8	0/18/38/38	0/1/3/3

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3400	ANP	PG-N3B	16.61	1.78	1.64
3	H	3400	ANP	PG-N3B	15.51	1.77	1.64
3	G	3400	ANP	PG-N3B	15.36	1.77	1.64
3	C	3400	ANP	PB-N3B	15.24	1.77	1.64
3	G	3400	ANP	PB-N3B	14.89	1.77	1.64

The worst 5 of 372 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3400	ANP	O1G-PG-N3B	-7.68	100.23	111.83
3	F	3400	ANP	O1G-PG-N3B	-7.30	100.81	111.83
3	G	1400	ANP	PB-N3B-PG	-7.25	117.87	130.07
3	A	1400	ANP	PB-N3B-PG	-7.21	117.94	130.07
3	D	1400	ANP	PB-N3B-PG	-7.18	118.00	130.07

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3400	ANP	C4'
3	D	3400	ANP	C4'
3	E	400	ANP	C4'
3	F	3400	ANP	C4'
3	E	2400	ANP	C4'

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(Å ²)	Q<0.9
1	A	1190/1357 (87%)	0.20	20 (1%) 67 54	181, 217, 253, 285	0
1	B	1163/1357 (85%)	0.12	28 (2%) 56 44	175, 217, 254, 286	0
1	C	1175/1357 (86%)	0.14	26 (2%) 59 46	187, 216, 253, 284	0
1	D	1175/1357 (86%)	0.26	45 (3%) 38 33	181, 218, 256, 286	0
1	E	1165/1357 (85%)	0.21	36 (3%) 47 38	186, 218, 255, 288	0
1	F	1175/1357 (86%)	0.19	31 (2%) 53 42	185, 217, 255, 285	0
1	G	1167/1357 (85%)	0.15	34 (2%) 49 40	185, 216, 254, 291	0
1	H	1173/1357 (86%)	0.13	23 (1%) 62 48	186, 218, 255, 288	0
All	All	9383/10856 (86%)	0.18	243 (2%) 53 42	175, 217, 255, 291	0

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3151	PRO	7.7
1	H	3151	PRO	7.0
1	E	3151	PRO	7.0
1	B	3151	PRO	6.2
1	C	3151	PRO	6.1

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
2	MG	D	1701	1/1	1.45	14.47	212,212,212,212	0
2	MG	D	701	1/1	1.44	13.02	261,261,261,261	0
2	MG	B	701	1/1	1.17	11.87	184,184,184,184	0
2	MG	H	1701	1/1	1.07	11.00	188,188,188,188	0
2	MG	E	701	1/1	0.88	8.25	204,204,204,204	0
2	MG	F	701	1/1	0.96	8.08	189,189,189,189	0
2	MG	G	1701	1/1	0.67	7.07	191,191,191,191	0
2	MG	G	701	1/1	0.69	6.39	215,215,215,215	0
2	MG	A	701	1/1	0.82	5.28	143,143,143,143	0
2	MG	F	1701	1/1	0.64	5.07	175,175,175,175	0
2	MG	B	1701	1/1	0.54	4.75	214,214,214,214	0
2	MG	B	2701	1/1	0.88	4.58	238,238,238,238	0
2	MG	A	1701	1/1	0.51	3.19	181,181,181,181	0
2	MG	C	701	1/1	0.77	3.17	177,177,177,177	0
2	MG	E	1701	1/1	0.56	3.10	190,190,190,190	0
2	MG	C	1701	1/1	0.43	2.38	132,132,132,132	0
2	MG	E	3701	1/1	0.34	2.21	131,131,131,131	0
2	MG	E	2701	1/1	0.41	1.51	228,228,228,228	0
3	ANP	G	2400	31/31	0.36	1.46	303,308,315,315	0
2	MG	D	3701	1/1	0.24	1.42	108,108,108,108	0
3	ANP	F	2400	31/31	0.34	0.98	286,303,310,310	0
3	ANP	D	1400	31/31	0.41	0.83	287,290,294,294	0
3	ANP	H	2400	31/31	0.33	0.80	298,312,316,316	0
3	ANP	A	2400	31/31	0.29	0.79	308,311,315,315	0
3	ANP	A	1400	31/31	0.30	0.74	267,280,283,283	0
3	ANP	D	2400	31/31	0.34	0.71	305,310,315,315	0
2	MG	D	2701	1/1	0.36	0.71	237,237,237,237	0
3	ANP	D	400	31/31	0.31	0.69	263,273,274,274	0
3	ANP	E	1400	31/31	0.24	0.68	287,293,296,296	0
3	ANP	H	1400	31/31	0.25	0.64	296,299,304,304	0
3	ANP	B	2400	31/31	0.31	0.63	306,312,314,314	0
3	ANP	G	400	31/31	0.23	0.60	253,262,264,265	0
3	ANP	A	400	31/31	0.35	0.52	246,250,255,256	0
3	ANP	B	400	31/31	0.40	0.50	242,255,259,260	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	F	2701	1/1	0.35	0.46	232,232,232,232	0
2	MG	B	3701	1/1	0.18	0.39	69,69,69,69	0
3	ANP	F	1400	31/31	0.23	0.24	271,280,286,286	0
3	ANP	H	400	31/31	0.22	0.21	254,263,265,265	0
2	MG	H	2701	1/1	0.35	0.18	271,271,271,271	0
2	MG	G	3701	1/1	0.27	0.13	100,100,100,100	0
3	ANP	C	1400	31/31	0.22	0.13	288,291,293,294	0
3	ANP	C	2400	31/31	0.23	0.07	296,309,314,315	0
3	ANP	G	1400	31/31	0.23	-0.01	279,285,289,290	0
3	ANP	E	3400	31/31	0.19	-0.09	163,180,187,187	0
3	ANP	G	3400	31/31	0.24	-0.13	153,176,191,192	0
3	ANP	B	1400	31/31	0.18	-0.13	275,286,290,290	0
3	ANP	D	3400	31/31	0.21	-0.14	149,170,188,189	0
3	ANP	E	2400	31/31	0.22	-0.20	307,317,320,320	0
3	ANP	C	3400	31/31	0.17	-0.20	176,190,200,200	0
3	ANP	E	400	31/31	0.24	-0.26	256,261,264,265	0
2	MG	H	701	1/1	0.16	-0.28	200,200,200,200	0
3	ANP	H	3400	31/31	0.17	-0.32	180,187,196,197	0
3	ANP	C	400	31/31	0.29	-0.33	226,245,250,250	0
2	MG	H	3701	1/1	0.21	-0.39	121,121,121,121	0
3	ANP	F	400	31/31	0.25	-0.39	243,257,263,263	0
3	ANP	B	3400	31/31	0.17	-0.40	143,159,176,178	0
3	ANP	F	3400	31/31	0.15	-0.94	148,171,183,183	0
2	MG	C	3701	1/1	0.14	-0.95	140,140,140,140	0
2	MG	G	2701	1/1	0.19	-0.96	192,192,192,192	0
3	ANP	A	3400	31/31	0.17	-1.20	152,165,180,181	0
2	MG	A	2701	1/1	0.15	-1.47	247,247,247,247	0
2	MG	C	2701	1/1	0.22	-1.67	211,211,211,211	0
2	MG	A	3701	1/1	0.08	-1.69	116,116,116,116	0
2	MG	F	3701	1/1	0.10	-3.09	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.