



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:56 AM GMT

PDB ID : 3CMW
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

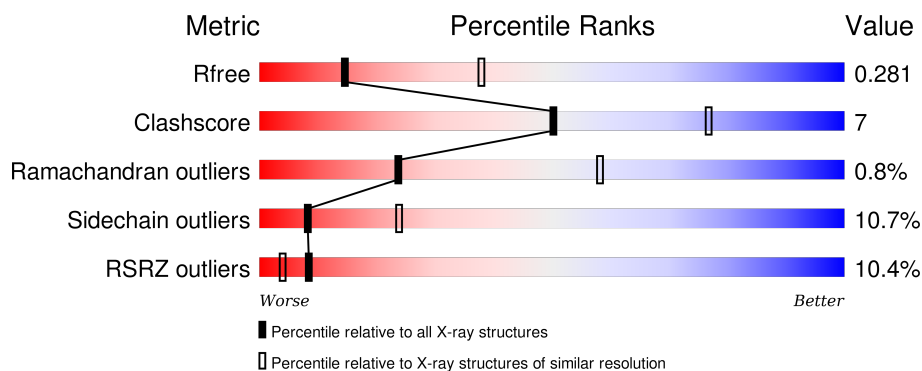
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	15	<div> <div></div> <div>20% 60% 20%</div> </div>
1	D	15	<div> <div>7%</div> <div>27% 53% 20%</div> </div>
2	A	1706	<div> <div>10%</div> <div>77% 15% • 6%</div> </div>
2	C	1706	<div> <div>9%</div> <div>77% 14% • 6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25046 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)*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			237	120	24	82	11			
1	D	12	Total	C	N	O	P	0	0	0
			237	120	24	82	11			

- Molecule 2 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1609	Total	C	N	O	S	0	0	0
			12125	7622	2100	2347	56			
2	C	1608	Total	C	N	O	S	0	0	0
			12117	7617	2100	2344	56			

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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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

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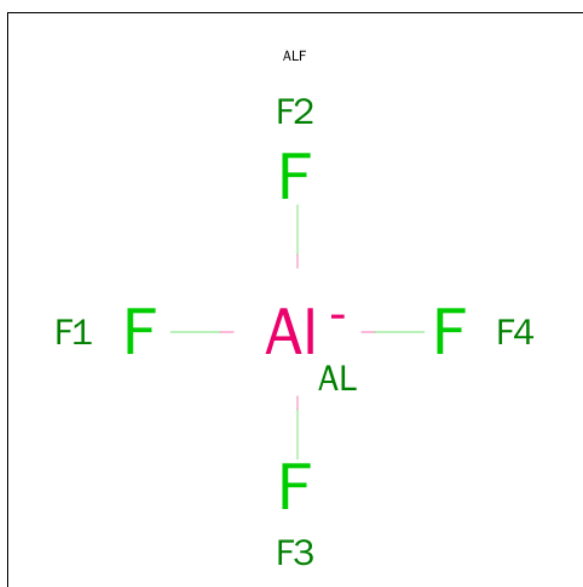
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Chain	Residue	Modelled	Actual	Comment	Reference
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	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
C	3986	THR	-	linker	UNP P0A7G6
C	3987	GLY	-	linker	UNP P0A7G6
C	3988	SER	-	linker	UNP P0A7G6
C	3989	THR	-	linker	UNP P0A7G6
C	3990	GLY	-	linker	UNP P0A7G6
C	3991	SER	-	linker	UNP P0A7G6
C	3992	MET	-	linker	UNP P0A7G6
C	3993	SER	-	linker	UNP P0A7G6
C	3994	GLY	-	linker	UNP P0A7G6
C	3995	ARG	-	linker	UNP P0A7G6
C	3996	THR	-	linker	UNP P0A7G6
C	3997	GLY	-	linker	UNP P0A7G6
C	3998	SER	-	linker	UNP P0A7G6
C	3999	MET	-	linker	UNP P0A7G6
C	4000	SER	-	linker	UNP P0A7G6

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

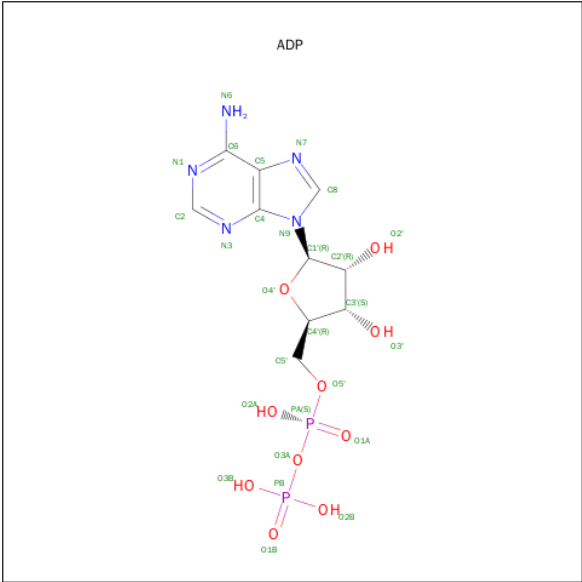
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Mg 5 5	0	0
3	C	5	Total Mg 5 5	0	0

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



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

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



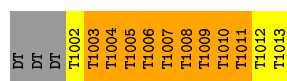
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C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

Chain B: 



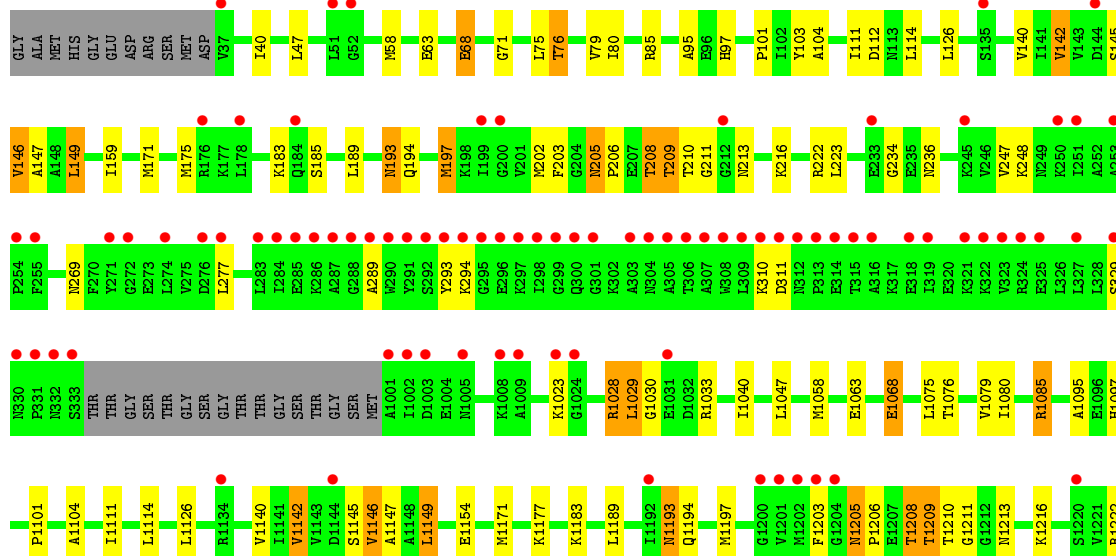
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT-3')

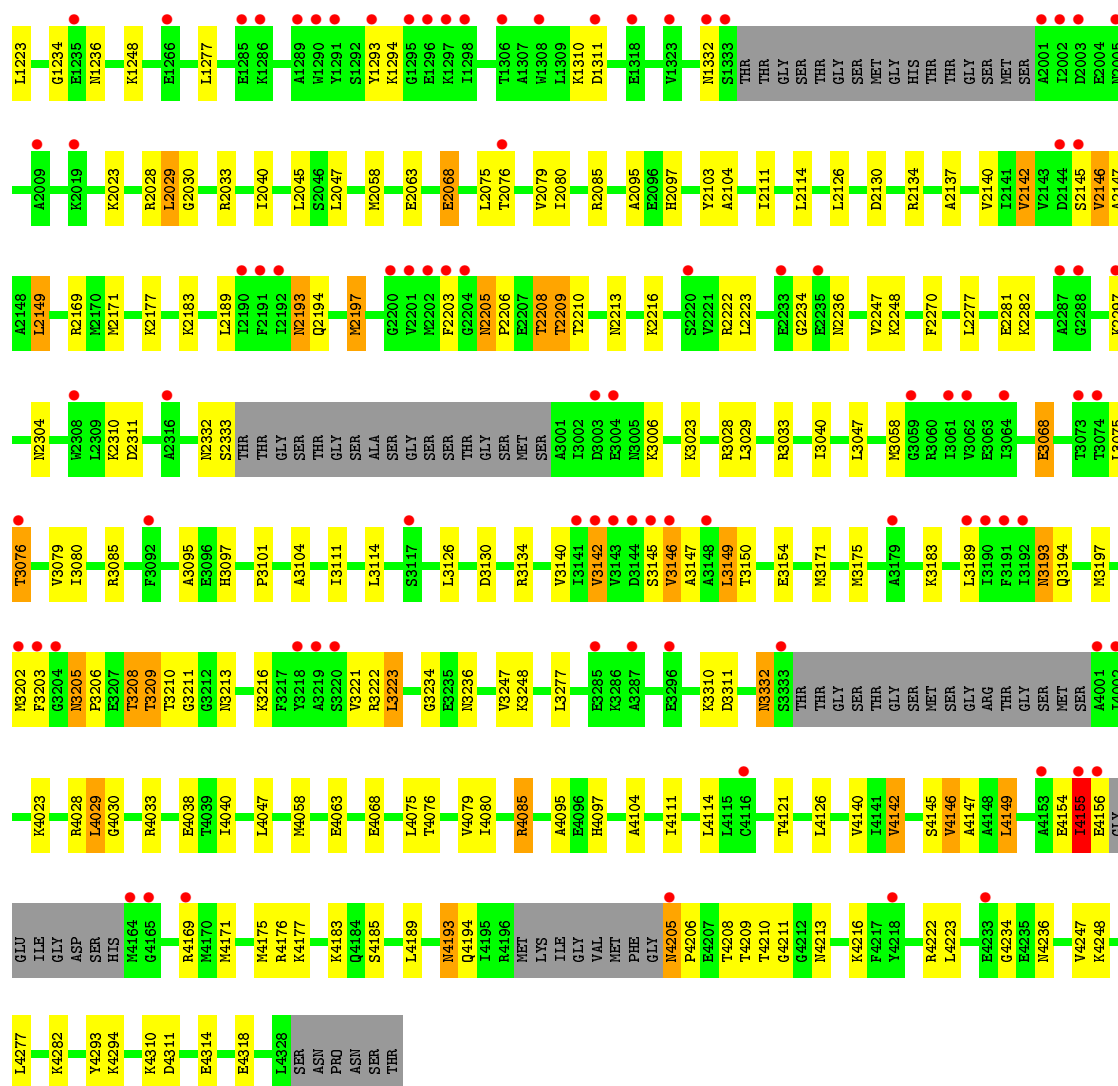
Chain D: 



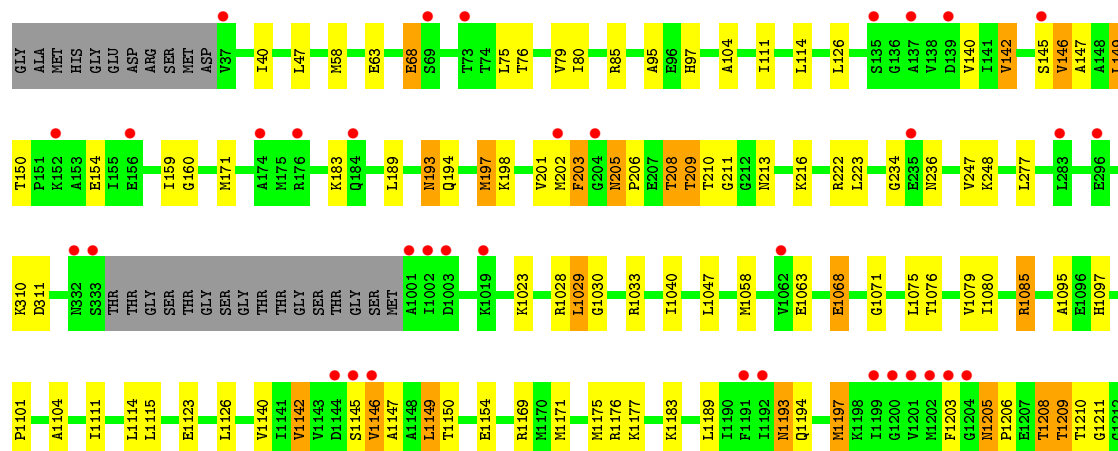
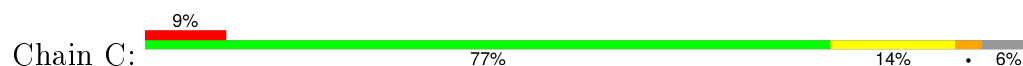
- Molecule 2: Protein recA

Chain A: 





• Molecule 2: Protein recA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.00 Å 300.50 Å 80.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 39.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.0 (20.00-2.80) 87.9 (39.41-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.214 , 0.236 0.264 , 0.281	Depositor DCC
R_{free} test set	1693 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 87028 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25046	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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	1.67	3/260 (1.2%)	2.31	18/400 (4.5%)
1	D	1.52	2/260 (0.8%)	2.15	17/400 (4.2%)
2	A	0.45	0/12264	0.59	0/16503
2	C	0.45	0/12256	0.59	0/16491
All	All	0.50	5/25040 (0.0%)	0.68	35/33794 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1010	DT	C3'-O3'	-6.92	1.34	1.44
1	B	1007	DT	C3'-O3'	-6.88	1.35	1.44
1	D	1010	DT	C3'-O3'	-6.23	1.35	1.44
1	D	1007	DT	C3'-O3'	-5.48	1.36	1.44
1	B	1009	DT	C1'-N1	5.14	1.55	1.49

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1013	DT	C1'-O4'-C4'	-12.89	97.21	110.10
1	B	1013	DT	O4'-C1'-N1	10.35	115.24	108.00
1	D	1013	DT	C1'-O4'-C4'	-9.35	100.75	110.10
1	D	1013	DT	O4'-C4'-C3'	-9.24	100.45	106.00
1	D	1007	DT	O4'-C1'-N1	8.29	113.80	108.00
1	B	1011	DT	O4'-C1'-N1	7.97	113.58	108.00
1	B	1002	DT	P-O3'-C3'	7.88	129.16	119.70
1	B	1010	DT	P-O3'-C3'	-7.86	110.27	119.70
1	D	1011	DT	O4'-C1'-N1	7.33	113.13	108.00
1	D	1013	DT	C4-C5-C7	7.32	123.39	119.00
1	D	1010	DT	O4'-C1'-N1	7.08	112.95	108.00
1	B	1010	DT	O4'-C1'-N1	7.07	112.95	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1010	DT	P-O3'-C3'	-6.46	111.95	119.70
1	D	1005	DT	O4'-C1'-N1	6.41	112.49	108.00
1	B	1003	DT	O4'-C1'-N1	6.28	112.40	108.00
1	D	1011	DT	O4'-C4'-C3'	-6.26	102.00	104.50
1	B	1007	DT	O4'-C1'-N1	6.19	112.33	108.00
1	B	1008	DT	O4'-C4'-C3'	-6.13	102.05	104.50
1	B	1013	DT	N1-C1'-C2'	6.06	124.11	112.60
1	B	1013	DT	N3-C2-O2	-5.98	118.71	122.30
1	D	1008	DT	O4'-C1'-N1	5.87	112.11	108.00
1	D	1004	DT	O4'-C1'-N1	5.80	112.06	108.00
1	B	1010	DT	C3'-C2'-C1'	-5.79	95.55	102.50
1	D	1002	DT	C4-C5-C7	5.79	122.48	119.00
1	B	1006	DT	O4'-C1'-N1	5.64	111.95	108.00
1	D	1013	DT	N3-C2-O2	-5.60	118.94	122.30
1	B	1009	DT	O4'-C1'-N1	5.30	111.71	108.00
1	B	1005	DT	O4'-C1'-N1	5.24	111.67	108.00
1	B	1009	DT	C6-C5-C7	-5.20	119.78	122.90
1	B	1004	DT	O4'-C1'-N1	5.14	111.60	108.00
1	D	1009	DT	O4'-C1'-N1	5.13	111.59	108.00
1	B	1013	DT	C2-N1-C1'	5.12	126.39	118.20
1	D	1002	DT	P-O3'-C3'	5.11	125.83	119.70
1	D	1013	DT	C6-C5-C7	-5.09	119.84	122.90
1	D	1008	DT	N3-C4-O4	5.02	122.91	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	237	0	146	11	0
1	D	237	0	146	19	0
2	A	12125	0	12452	174	2
2	C	12117	0	12447	175	1
3	A	5	0	0	0	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	25	0	0	0	0
4	C	25	0	0	0	0
5	A	135	0	60	3	0
5	C	135	0	60	1	0
All	All	25046	0	25311	351	2

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 7.

All (351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1013:DT:O4	2:A:3202:MET:HG2	1.49	1.10
2:A:2068:GLU:HG2	2:A:3216:LYS:HB3	1.33	1.08
2:A:68:GLU:HG2	2:A:1216:LYS:HB3	1.24	1.07
2:C:68:GLU:HG2	2:C:1216:LYS:HB3	1.42	0.99
2:A:3068:GLU:HG2	2:A:4216:LYS:HB3	1.48	0.95
2:C:2068:GLU:HG2	2:C:3216:LYS:HB3	1.48	0.95
2:C:1068:GLU:HG2	2:C:2216:LYS:HB3	1.51	0.91
2:A:289:ALA:HB2	2:C:4235:GLU:HG3	1.52	0.90
2:C:3068:GLU:HG2	2:C:4216:LYS:HB3	1.53	0.87
2:A:1068:GLU:HG2	2:A:2216:LYS:HB3	1.58	0.85
2:A:2304:ASN:OD1	2:C:2304:ASN:ND2	2.11	0.84
2:A:3193:ASN:HD22	2:A:3194:GLN:H	1.26	0.84
2:C:4076:THR:HG21	2:C:4142:VAL:HG21	1.61	0.82
2:A:3146:VAL:HA	2:A:3149:LEU:HD22	1.61	0.82
2:A:146:VAL:HA	2:A:149:LEU:HD22	1.62	0.82
2:C:1076:THR:HG21	2:C:1142:VAL:HG21	1.62	0.82
2:C:4146:VAL:HA	2:C:4149:LEU:HD22	1.62	0.81
2:A:4076:THR:HG21	2:A:4142:VAL:HG21	1.63	0.81
2:A:1146:VAL:HA	2:A:1149:LEU:HD22	1.61	0.81
2:C:3146:VAL:HA	2:C:3149:LEU:HD22	1.62	0.81
2:A:3076:THR:HG21	2:A:3142:VAL:HG21	1.61	0.81
2:A:76:THR:HG21	2:A:142:VAL:HG21	1.63	0.81
2:C:2193:ASN:HD22	2:C:2194:GLN:H	1.28	0.81
2:C:2146:VAL:HA	2:C:2149:LEU:HD22	1.62	0.80
2:C:3076:THR:HG21	2:C:3142:VAL:HG21	1.61	0.80
2:C:3193:ASN:HD22	2:C:3194:GLN:H	1.29	0.80
2:A:1076:THR:HG21	2:A:1142:VAL:HG21	1.62	0.80
2:A:4282:LYS:HG3	2:C:1282:LYS:HG3	1.64	0.80
2:A:2076:THR:HG21	2:A:2142:VAL:HG21	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:VAL:HA	2:C:149:LEU:HD22	1.61	0.79
2:A:4146:VAL:HA	2:A:4149:LEU:HD22	1.65	0.79
2:C:2076:THR:HG21	2:C:2142:VAL:HG21	1.63	0.79
2:A:2146:VAL:HA	2:A:2149:LEU:HD22	1.65	0.79
2:A:2193:ASN:HD22	2:A:2194:GLN:H	1.28	0.78
2:A:193:ASN:HD22	2:A:194:GLN:H	1.29	0.78
2:C:4193:ASN:HD22	2:C:4194:GLN:H	1.33	0.77
2:C:76:THR:HG21	2:C:142:VAL:HG21	1.65	0.77
1:D:1013:DT:O4	2:A:3202:MET:CG	2.31	0.76
2:C:1193:ASN:HD22	2:C:1194:GLN:H	1.30	0.76
2:A:4193:ASN:HD22	2:A:4194:GLN:H	1.33	0.76
2:C:193:ASN:HD22	2:C:194:GLN:H	1.34	0.76
1:D:1013:DT:H71	2:A:3202:MET:SD	2.26	0.76
2:C:1146:VAL:HA	2:C:1149:LEU:HD22	1.66	0.75
2:A:1193:ASN:HD22	2:A:1194:GLN:H	1.32	0.74
2:A:289:ALA:CB	2:C:4235:GLU:HG3	2.18	0.72
2:A:2281:GLU:OE1	2:C:3282:LYS:NZ	2.25	0.70
2:C:3193:ASN:HD21	2:C:3210:THR:HB	1.59	0.68
2:A:2193:ASN:HD21	2:A:2210:THR:HB	1.59	0.67
2:C:1193:ASN:HD21	2:C:1210:THR:HB	1.59	0.67
2:C:111:ILE:HG22	2:C:1030:GLY:CA	2.24	0.67
2:A:3076:THR:CG2	2:A:3142:VAL:HG21	2.25	0.67
1:B:1011:DT:O2	2:A:4169:ARG:NH1	2.27	0.67
2:C:2193:ASN:HD21	2:C:2210:THR:HB	1.60	0.66
2:A:4193:ASN:HD21	2:A:4210:THR:HB	1.61	0.66
2:A:1193:ASN:HD21	2:A:1210:THR:HB	1.61	0.66
2:C:3154:GLU:O	2:C:4177:LYS:HE2	1.96	0.65
2:A:3193:ASN:HD21	2:A:3210:THR:HB	1.61	0.65
2:C:111:ILE:HG22	2:C:1030:GLY:HA2	1.78	0.65
2:C:2150:THR:OG1	2:C:3176:ARG:HG2	1.97	0.64
2:C:193:ASN:HD21	2:C:210:THR:HB	1.61	0.64
2:A:1154:GLU:O	2:A:2177:LYS:HE2	1.97	0.64
2:A:193:ASN:HD21	2:A:210:THR:HB	1.61	0.64
2:C:3076:THR:CG2	2:C:3142:VAL:HG21	2.27	0.64
2:A:4121:THR:HG22	2:A:4155:ILE:HD12	1.78	0.64
2:C:2076:THR:CG2	2:C:2142:VAL:HG21	2.28	0.64
2:A:2076:THR:CG2	2:A:2142:VAL:HG21	2.28	0.64
2:C:4193:ASN:HD21	2:C:4210:THR:HB	1.62	0.63
2:C:1076:THR:CG2	2:C:1142:VAL:HG21	2.28	0.63
2:A:111:ILE:HD12	2:A:1029:LEU:HD13	1.81	0.63
2:A:3111:ILE:HG22	2:A:4030:GLY:CA	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1076:THR:CG2	2:A:1142:VAL:HG21	2.28	0.62
2:C:198:LYS:HG3	2:C:201:VAL:HG21	1.81	0.62
2:A:76:THR:CG2	2:A:142:VAL:HG21	2.29	0.62
2:C:76:THR:CG2	2:C:142:VAL:HG21	2.30	0.61
2:C:4076:THR:CG2	2:C:4142:VAL:HG21	2.29	0.61
2:A:111:ILE:HG22	2:A:1030:GLY:CA	2.30	0.61
2:A:4076:THR:CG2	2:A:4142:VAL:HG21	2.29	0.61
2:C:111:ILE:CG2	2:C:1030:GLY:HA2	2.31	0.61
2:C:2193:ASN:HD22	2:C:2194:GLN:N	1.97	0.60
2:A:3193:ASN:HD22	2:A:3194:GLN:N	1.96	0.60
2:A:193:ASN:HD22	2:A:194:GLN:N	1.99	0.60
2:A:3206:PRO:HD3	2:C:3202:MET:O	2.01	0.60
2:A:1205:ASN:HD22	2:A:1206:PRO:HD2	1.66	0.60
2:C:2205:ASN:HD22	2:C:2206:PRO:HD2	1.67	0.60
2:C:205:ASN:HD22	2:C:206:PRO:HD2	1.67	0.59
2:A:3205:ASN:HD22	2:A:3206:PRO:HD2	1.67	0.59
2:C:4193:ASN:HD22	2:C:4194:GLN:N	2.01	0.59
2:A:4193:ASN:HD22	2:A:4194:GLN:N	2.01	0.59
2:C:3193:ASN:HD22	2:C:3194:GLN:N	2.00	0.59
2:C:2154:GLU:CD	2:C:3176:ARG:HH21	2.05	0.59
2:A:2193:ASN:HD22	2:A:2194:GLN:N	1.98	0.58
2:A:4104:ALA:HB3	2:A:4111:ILE:HD11	1.85	0.58
2:A:2147:ALA:HA	2:A:2210:THR:HG21	1.86	0.58
1:B:1004:DT:C7	2:A:197:MET:HG3	2.34	0.58
2:A:2205:ASN:HD22	2:A:2206:PRO:HD2	1.67	0.58
2:A:1193:ASN:HD22	2:A:1194:GLN:N	2.00	0.58
2:A:2149:LEU:HD23	2:A:2171:MET:HE1	1.86	0.57
2:A:111:ILE:HD12	2:A:1029:LEU:CD1	2.33	0.57
2:A:205:ASN:HD22	2:A:206:PRO:HD2	1.68	0.57
2:C:4205:ASN:HD22	2:C:4206:PRO:HD2	1.69	0.57
2:C:1193:ASN:HD22	2:C:1194:GLN:N	2.00	0.57
2:A:4205:ASN:HD22	2:A:4206:PRO:HD2	1.68	0.57
2:A:1147:ALA:HA	2:A:1210:THR:HG21	1.86	0.57
2:C:3104:ALA:HB3	2:C:3111:ILE:HD11	1.85	0.57
2:C:3205:ASN:HD22	2:C:3206:PRO:HD2	1.69	0.57
2:C:1205:ASN:HD22	2:C:1206:PRO:HD2	1.69	0.57
2:C:4147:ALA:HA	2:C:4210:THR:HG21	1.88	0.56
2:C:3147:ALA:HA	2:C:3210:THR:HG21	1.87	0.56
2:A:4147:ALA:HA	2:A:4210:THR:HG21	1.88	0.56
2:C:154:GLU:CD	2:C:1176:ARG:HH21	2.09	0.56
2:A:2126:LEU:HD11	2:A:2171:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3147:ALA:HA	2:A:3210:THR:HG21	1.88	0.56
2:C:1147:ALA:HA	2:C:1210:THR:HG21	1.86	0.56
2:A:104:ALA:HB3	2:A:111:ILE:HD11	1.87	0.56
2:A:4206:PRO:HG3	2:C:2202:MET:O	2.06	0.56
2:C:4104:ALA:HB3	2:C:4111:ILE:HD11	1.88	0.56
2:C:4213:ASN:OD1	2:C:4216:LYS:HE2	2.06	0.56
2:A:4213:ASN:OD1	2:A:4216:LYS:HE2	2.06	0.55
2:C:3111:ILE:HD12	2:C:4029:LEU:HD13	1.88	0.55
2:C:3261:GLN:OE1	2:C:3269:ASN:ND2	2.39	0.55
2:C:1104:ALA:HB3	2:C:1111:ILE:HD11	1.87	0.55
2:C:150:THR:OG1	2:C:1176:ARG:HG2	2.07	0.55
2:A:101:PRO:HB3	2:A:1029:LEU:HD22	1.89	0.55
2:C:2104:ALA:HB3	2:C:2111:ILE:HD11	1.87	0.55
2:C:104:ALA:HB3	2:C:111:ILE:HD11	1.88	0.54
2:A:1111:ILE:HG22	2:A:2030:GLY:CA	2.37	0.54
2:A:3104:ALA:HB3	2:A:3111:ILE:HD11	1.90	0.54
2:A:147:ALA:HA	2:A:210:THR:HG21	1.89	0.54
2:C:2147:ALA:HA	2:C:2210:THR:HG21	1.88	0.54
2:A:1104:ALA:HB3	2:A:1111:ILE:HD11	1.89	0.54
2:A:3154:GLU:O	2:A:4177:LYS:HE2	2.08	0.54
2:C:159:ILE:HG12	2:C:1177:LYS:HD3	1.90	0.53
1:B:1004:DT:H2''	1:B:1005:DT:C6	2.43	0.53
2:A:2104:ALA:HB3	2:A:2111:ILE:HD11	1.91	0.53
2:C:147:ALA:HA	2:C:210:THR:HG21	1.90	0.53
2:A:111:ILE:HG22	2:A:1030:GLY:HA2	1.89	0.53
2:C:2111:ILE:HG22	2:C:3030:GLY:CA	2.39	0.53
2:C:1213:ASN:OD1	2:C:1216:LYS:HE2	2.07	0.53
2:C:193:ASN:HD22	2:C:194:GLN:N	2.04	0.53
2:C:1111:ILE:HG22	2:C:2030:GLY:CA	2.38	0.53
2:A:3111:ILE:HG22	2:A:4030:GLY:HA2	1.89	0.53
1:D:1008:DT:H2'	1:D:1009:DT:C6	2.43	0.53
2:A:112:ASP:O	2:A:1028:ARG:HG2	2.09	0.53
2:A:1076:THR:HG23	2:A:1142:VAL:HG11	1.91	0.52
2:C:2101:PRO:HB3	2:C:3029:LEU:HD22	1.91	0.52
2:C:3330:ASN:HB3	2:C:3332:ASN:H	1.74	0.52
2:A:76:THR:HG23	2:A:142:VAL:HG11	1.91	0.52
2:A:2076:THR:HG23	2:A:2142:VAL:HG11	1.91	0.52
2:C:2076:THR:HG23	2:C:2142:VAL:HG11	1.91	0.52
1:B:1010:DT:H2''	1:B:1011:DT:C6	2.44	0.52
2:C:3076:THR:HG23	2:C:3142:VAL:HG11	1.91	0.52
2:C:76:THR:HG23	2:C:142:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1010:DT:H2''	1:D:1011:DT:C6	2.45	0.52
2:A:4095:ALA:O	2:A:4097:HIS:HD2	1.93	0.52
2:C:213:ASN:OD1	2:C:216:LYS:HE2	2.10	0.52
2:A:3213:ASN:OD1	2:A:3216:LYS:HE2	2.10	0.52
2:A:4149:LEU:HD23	2:A:4171:MET:HE1	1.91	0.51
2:A:3095:ALA:O	2:A:3097:HIS:HD2	1.92	0.51
1:D:1013:DT:C4	2:A:3202:MET:HG2	2.36	0.51
2:A:3111:ILE:CG2	2:A:4030:GLY:HA2	2.40	0.51
1:D:1004:DT:H2''	1:D:1005:DT:C6	2.45	0.51
2:C:2213:ASN:OD1	2:C:2216:LYS:HE2	2.11	0.51
2:C:1076:THR:HG23	2:C:1142:VAL:HG11	1.93	0.51
2:C:3263:LEU:HG	2:C:3269:ASN:HB2	1.92	0.51
2:A:3076:THR:HG23	2:A:3142:VAL:HG11	1.91	0.51
2:C:95:ALA:O	2:C:97:HIS:HD2	1.94	0.51
1:D:1013:DT:C4	2:A:3202:MET:HE2	2.46	0.51
2:C:3213:ASN:OD1	2:C:3216:LYS:HE2	2.12	0.50
2:A:2033:ARG:NE	2:A:2033:ARG:HA	2.26	0.50
2:C:4095:ALA:O	2:C:4097:HIS:HD2	1.94	0.50
2:A:1213:ASN:OD1	2:A:1216:LYS:HE2	2.11	0.50
1:B:1008:DT:H2'	1:B:1009:DT:C6	2.47	0.50
2:A:3111:ILE:HD12	2:A:4029:LEU:HD13	1.94	0.50
2:C:4033:ARG:HA	2:C:4033:ARG:NE	2.27	0.50
2:C:4222:ARG:HG3	2:C:4248:LYS:HB3	1.93	0.50
2:A:4033:ARG:NE	2:A:4033:ARG:HA	2.27	0.50
2:A:103:TYR:CD1	5:A:502:ADP:C6	3.00	0.50
2:C:4076:THR:HG23	2:C:4142:VAL:HG11	1.92	0.50
2:A:3101:PRO:HB3	2:A:4029:LEU:HD22	1.94	0.50
2:C:1095:ALA:O	2:C:1097:HIS:HD2	1.95	0.50
2:A:3222:ARG:HG3	2:A:3248:LYS:HB3	1.92	0.50
1:D:1013:DT:C5	2:A:3202:MET:CE	2.95	0.49
2:A:3080:ILE:HD11	2:A:3142:VAL:CG1	2.42	0.49
2:A:1111:ILE:HG22	2:A:2030:GLY:HA2	1.92	0.49
2:A:2149:LEU:HD23	2:A:2171:MET:CE	2.43	0.49
2:C:2111:ILE:HG22	2:C:3030:GLY:HA2	1.95	0.49
2:A:95:ALA:O	2:A:97:HIS:HD2	1.96	0.49
2:A:4149:LEU:HD23	2:A:4171:MET:CE	2.42	0.49
2:A:3126:LEU:HD11	2:A:3171:MET:HE2	1.94	0.49
2:C:126:LEU:HD11	2:C:171:MET:HE2	1.95	0.49
2:C:2095:ALA:O	2:C:2097:HIS:HD2	1.95	0.49
2:C:2033:ARG:HA	2:C:2033:ARG:NE	2.28	0.49
2:A:2213:ASN:OD1	2:A:2216:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1149:LEU:HD23	2:C:1171:MET:CE	2.43	0.49
2:A:3033:ARG:HA	2:A:3033:ARG:NE	2.27	0.49
2:C:3111:ILE:HG22	2:C:4030:GLY:HA2	1.95	0.49
2:A:213:ASN:OD1	2:A:216:LYS:HE2	2.12	0.49
2:A:2304:ASN:ND2	2:C:2304:ASN:OD1	2.45	0.48
2:C:40:ILE:HG12	2:C:58:MET:SD	2.53	0.48
1:B:1003:DT:H2'	2:A:197:MET:O	2.12	0.48
2:A:1095:ALA:O	2:A:1097:HIS:HD2	1.97	0.48
2:A:126:LEU:HD11	2:A:171:MET:HE2	1.94	0.48
2:C:2111:ILE:HD12	2:C:3029:LEU:HD13	1.93	0.48
2:A:4076:THR:HG23	2:A:4142:VAL:HG11	1.94	0.48
2:C:1033:ARG:HA	2:C:1033:ARG:NE	2.28	0.48
2:A:1111:ILE:CG2	2:A:2030:GLY:HA2	2.44	0.48
2:C:3126:LEU:HD11	2:C:3171:MET:HE2	1.94	0.48
2:A:149:LEU:HD23	2:A:171:MET:CE	2.44	0.48
2:A:1126:LEU:HD11	2:A:1171:MET:HE2	1.96	0.48
2:C:1149:LEU:HD23	2:C:1171:MET:HE3	1.95	0.48
2:C:154:GLU:OE1	2:C:1176:ARG:NH2	2.45	0.48
2:C:3222:ARG:HG3	2:C:3248:LYS:HB3	1.94	0.48
2:A:1222:ARG:HG3	2:A:1248:LYS:HB3	1.95	0.48
2:A:68:GLU:HG2	2:A:1216:LYS:CB	2.17	0.47
2:C:1080:ILE:HD11	2:C:1142:VAL:CG1	2.44	0.47
2:C:1154:GLU:CD	2:C:2176:ARG:HH21	2.16	0.47
2:C:149:LEU:HD23	2:C:171:MET:CE	2.44	0.47
1:D:1006:DT:H5'	2:C:2169:ARG:HA	1.96	0.47
2:A:3149:LEU:HD23	2:A:3171:MET:HE1	1.96	0.47
1:B:1007:DT:H2''	1:B:1008:DT:C6	2.49	0.47
2:C:222:ARG:HG3	2:C:248:LYS:HB3	1.96	0.47
2:C:4149:LEU:HD23	2:C:4171:MET:CE	2.44	0.47
2:C:4040:ILE:HG12	2:C:4058:MET:SD	2.55	0.47
2:A:2040:ILE:HG12	2:A:2058:MET:SD	2.55	0.47
2:A:2080:ILE:HD11	2:A:2142:VAL:CG1	2.45	0.47
2:A:4126:LEU:HD11	2:A:4171:MET:HE2	1.95	0.47
2:A:159:ILE:HG13	2:A:1177:LYS:HD3	1.96	0.47
1:B:1004:DT:H73	2:A:197:MET:HG3	1.96	0.47
2:A:2222:ARG:HG3	2:A:2248:LYS:HB3	1.97	0.47
2:A:3210:THR:HG22	2:A:3211:GLY:N	2.29	0.47
2:C:1111:ILE:CG2	2:C:2030:GLY:HA2	2.45	0.47
2:A:4222:ARG:HG3	2:A:4248:LYS:HB3	1.97	0.47
1:D:1007:DT:H2''	1:D:1008:DT:C6	2.50	0.46
2:A:1033:ARG:NE	2:A:1033:ARG:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2095:ALA:O	2:A:2097:HIS:HD2	1.98	0.46
2:C:3033:ARG:NE	2:C:3033:ARG:HA	2.30	0.46
2:A:1080:ILE:HD11	2:A:1142:VAL:CG1	2.46	0.46
2:A:1040:ILE:HG12	2:A:1058:MET:SD	2.54	0.46
2:C:80:ILE:HD11	2:C:142:VAL:CG1	2.45	0.46
1:D:1007:DT:H73	2:C:1197:MET:HG3	1.96	0.46
2:A:2282:LYS:HG3	2:C:3282:LYS:HG3	1.97	0.46
2:A:111:ILE:CG2	2:A:1030:GLY:HA2	2.45	0.46
2:C:3095:ALA:O	2:C:3097:HIS:HD2	1.98	0.46
2:C:1126:LEU:HD11	2:C:1171:MET:HE2	1.98	0.46
2:C:3111:ILE:HG22	2:C:4030:GLY:CA	2.45	0.46
2:A:3040:ILE:HG12	2:A:3058:MET:SD	2.56	0.46
2:C:1101:PRO:HB3	2:C:2029:LEU:HD22	1.96	0.46
2:A:222:ARG:HG3	2:A:248:LYS:HB3	1.97	0.46
2:C:3149:LEU:HD23	2:C:3171:MET:CE	2.45	0.46
1:D:1005:DT:H2'	1:D:1006:DT:C6	2.51	0.46
2:A:2137:ALA:HA	2:A:3006:LYS:HE3	1.97	0.46
2:A:3149:LEU:HD23	2:A:3171:MET:CE	2.46	0.46
2:C:3040:ILE:HG12	2:C:3058:MET:SD	2.55	0.46
2:C:2222:ARG:HG3	2:C:2248:LYS:HB3	1.98	0.46
2:A:2332:ASN:CG	2:A:2333:SER:H	2.20	0.45
2:C:2126:LEU:HD11	2:C:2171:MET:HE2	1.98	0.45
1:D:1011:DT:H2'	1:D:1012:DT:C6	2.51	0.45
2:C:2040:ILE:HG12	2:C:2058:MET:SD	2.56	0.45
2:A:80:ILE:HD11	2:A:142:VAL:CG1	2.46	0.45
2:A:3208:THR:HG22	2:A:3209:THR:H	1.80	0.45
2:C:4080:ILE:HD11	2:C:4142:VAL:CG1	2.47	0.45
2:C:4126:LEU:HD11	2:C:4171:MET:HE2	1.97	0.45
2:A:4080:ILE:HD11	2:A:4142:VAL:CG1	2.45	0.45
2:A:1149:LEU:HD23	2:A:1171:MET:CE	2.47	0.45
2:C:3149:LEU:HD23	2:C:3171:MET:HE1	1.99	0.45
2:C:2080:ILE:HD11	2:C:2142:VAL:CG1	2.46	0.45
2:A:3150:THR:OG1	2:A:4176:ARG:HG2	2.17	0.45
2:C:1222:ARG:HG3	2:C:1248:LYS:HB3	1.97	0.45
2:C:3080:ILE:HD11	2:C:3142:VAL:CG1	2.46	0.45
2:A:1210:THR:HG22	2:A:1211:GLY:N	2.32	0.45
2:C:1040:ILE:HG12	2:C:1058:MET:SD	2.57	0.45
2:C:111:ILE:HD12	2:C:1029:LEU:HD13	1.99	0.44
2:C:1115:LEU:HD11	2:C:2010:LEU:HD11	1.99	0.44
2:A:171:MET:O	2:A:175:MET:HG2	2.18	0.44
2:C:3111:ILE:HD12	2:C:4029:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2171:MET:O	2:C:2175:MET:HG2	2.17	0.44
2:A:4040:ILE:HG12	2:A:4058:MET:SD	2.58	0.44
2:C:2149:LEU:HD23	2:C:2171:MET:CE	2.48	0.44
2:C:4210:THR:HG22	2:C:4211:GLY:N	2.32	0.44
2:C:2154:GLU:OE1	2:C:3176:ARG:NH2	2.50	0.44
2:C:1208:THR:HG22	2:C:1209:THR:H	1.83	0.44
2:C:2208:THR:HG22	2:C:2209:THR:H	1.83	0.43
2:C:3210:THR:HG22	2:C:3211:GLY:N	2.34	0.43
2:C:1150:THR:OG1	2:C:2176:ARG:HG2	2.18	0.43
1:B:1011:DT:H2'	1:B:1012:DT:C6	2.53	0.43
2:A:2103:TYR:CD1	5:A:2502:ADP:C6	3.06	0.43
2:C:208:THR:HG22	2:C:209:THR:H	1.83	0.43
2:A:4063:GLU:OE1	2:A:4222:ARG:HD2	2.18	0.43
2:A:1208:THR:HG22	2:A:1209:THR:H	1.83	0.43
2:A:149:LEU:HD23	2:A:171:MET:HE1	2.00	0.43
2:A:4210:THR:HG22	2:A:4211:GLY:N	2.34	0.43
1:B:1010:DT:H73	2:A:2197:MET:HG3	2.00	0.43
2:C:3171:MET:O	2:C:3175:MET:HG2	2.19	0.43
2:A:208:THR:HG22	2:A:209:THR:H	1.84	0.43
2:C:1210:THR:HG22	2:C:1211:GLY:N	2.34	0.43
2:C:210:THR:HG22	2:C:211:GLY:N	2.34	0.43
2:C:1111:ILE:HG22	2:C:2030:GLY:HA2	2.00	0.43
2:C:1063:GLU:OE1	2:C:1222:ARG:HD2	2.19	0.42
2:A:210:THR:HG22	2:A:211:GLY:N	2.34	0.42
2:C:2111:ILE:CG2	2:C:3030:GLY:HA2	2.47	0.42
2:A:71:GLY:HA2	5:A:502:ADP:H5'1	2.01	0.42
2:C:201:VAL:HA	2:C:203:PHE:CE1	2.54	0.42
2:C:160:GLY:HA3	2:C:1123:GLU:HG2	2.02	0.42
2:C:3208:THR:HG22	2:C:3209:THR:H	1.85	0.42
2:C:3130:ASP:OD2	2:C:3134:ARG:NH1	2.52	0.42
1:D:1012:DT:H2'	2:C:3197:MET:O	2.20	0.42
2:A:40:ILE:HG12	2:A:58:MET:SD	2.60	0.42
2:C:4208:THR:HG22	2:C:4209:THR:H	1.84	0.42
1:D:1007:DT:C7	2:C:1197:MET:HG3	2.50	0.42
2:A:2130:ASP:OD2	2:A:2134:ARG:NH1	2.53	0.41
1:B:1006:DT:H5'	2:A:2169:ARG:HA	2.02	0.41
2:C:2130:ASP:OD2	2:C:2134:ARG:NH1	2.53	0.41
2:C:2154:GLU:O	2:C:3177:LYS:HE2	2.20	0.41
2:C:1171:MET:O	2:C:1175:MET:HG2	2.20	0.41
2:A:1063:GLU:OE1	2:A:1222:ARG:HD2	2.20	0.41
2:A:63:GLU:OE1	2:A:222:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1205:ASN:ND2	2:A:1206:PRO:HD2	2.35	0.41
2:C:63:GLU:OE1	2:C:222:ARG:HD2	2.20	0.41
2:A:1101:PRO:HB3	2:A:2029:LEU:HD22	2.03	0.41
2:A:2208:THR:HG22	2:A:2209:THR:H	1.86	0.41
1:D:1003:DT:H5'	2:C:1169:ARG:HA	2.02	0.41
2:A:3221:VAL:HG12	2:A:3223:LEU:HD13	2.03	0.41
1:D:1013:DT:C7	2:A:3202:MET:HE1	2.50	0.41
2:A:4171:MET:O	2:A:4175:MET:HG2	2.21	0.41
2:C:198:LYS:HG2	2:C:206:PRO:O	2.21	0.41
2:C:3040:ILE:HD11	2:C:3088:LYS:HE2	2.03	0.41
2:C:3085:ARG:HG2	2:C:3085:ARG:HH11	1.85	0.41
2:C:2221:VAL:HG12	2:C:2223:LEU:HD13	2.03	0.41
2:A:3130:ASP:OD2	2:A:3134:ARG:NH1	2.54	0.41
2:C:1126:LEU:HD11	2:C:1171:MET:CE	2.51	0.41
2:A:2063:GLU:OE1	2:A:2222:ARG:HD2	2.21	0.41
2:C:1085:ARG:HH11	2:C:1085:ARG:HG2	1.86	0.41
2:A:2045:LEU:HB2	2:A:2270:PHE:CE1	2.56	0.41
2:C:2040:ILE:HD11	2:C:2088:LYS:HE2	2.03	0.40
2:C:4149:LEU:HD23	2:C:4171:MET:HE1	2.03	0.40
2:A:3205:ASN:ND2	2:A:3206:PRO:HD2	2.34	0.40
1:D:1004:DT:H73	2:C:197:MET:HG3	2.03	0.40
2:A:4293:TYR:CE2	2:A:4294:LYS:HE2	2.57	0.40
2:A:1085:ARG:HG2	2:A:1085:ARG:HH11	1.87	0.40
2:C:4063:GLU:OE1	2:C:4222:ARG:HD2	2.21	0.40
2:A:1293:TYR:CE2	2:A:1294:LYS:HE2	2.56	0.40
2:A:293:TYR:CE2	2:A:294:LYS:HE2	2.57	0.40
2:C:3221:VAL:HG12	2:C:3223:LEU:HD13	2.04	0.40
2:A:3171:MET:O	2:A:3175:MET:HG2	2.20	0.40
2:C:126:LEU:HD11	2:C:171:MET:CE	2.51	0.40
2:A:2205:ASN:ND2	2:A:2206:PRO:HD2	2.35	0.40
2:C:2293:TYR:CE2	2:C:2294:LYS:HE2	2.56	0.40
2:C:3150:THR:HB	2:C:3155:ILE:CD1	2.52	0.40
2:C:1071:GLY:HA2	5:C:1502:ADP:H5'1	2.04	0.40
2:A:4085:ARG:HG2	2:A:4085:ARG:HH11	1.87	0.40
2:A:4154:GLU:C	2:A:4156:GLU:H	2.25	0.40

All (2) 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:4038:GLU:OE1	2:A:4318:GLU:OE2[2_555]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2297:LYS:NZ	2:C:4097:HIS:O[1_554]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1595/1706 (94%)	1545 (97%)	37 (2%)	13 (1%)	24	58
2	C	1594/1706 (93%)	1550 (97%)	33 (2%)	11 (1%)	26	62
All	All	3189/3412 (94%)	3095 (97%)	70 (2%)	24 (1%)	24	58

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1023	LYS
2	A	2023	LYS
2	A	3023	LYS
2	A	3332	ASN
2	A	4023	LYS
2	C	1023	LYS
2	C	1332	ASN
2	C	2023	LYS
2	C	3023	LYS
2	C	3269	ASN
2	C	4023	LYS
2	A	269	ASN
2	A	1332	ASN
2	A	3234	GLY
2	A	234	GLY
2	A	1234	GLY
2	C	234	GLY
2	C	1234	GLY
2	C	2234	GLY

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Mol	Chain	Res	Type
2	C	3234	GLY
2	C	4234	GLY
2	A	4234	GLY
2	A	2234	GLY
2	A	4155	ILE

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	1267/1339 (95%)	1128 (89%)	139 (11%)	8	23
2	C	1266/1339 (94%)	1134 (90%)	132 (10%)	9	25
All	All	2533/2678 (95%)	2262 (89%)	271 (11%)	8	24

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	47	LEU
2	A	68	GLU
2	A	75	LEU
2	A	76	THR
2	A	79	VAL
2	A	85	ARG
2	A	114	LEU
2	A	140	VAL
2	A	142	VAL
2	A	145	SER
2	A	146	VAL
2	A	149	LEU
2	A	183	LYS
2	A	185	SER
2	A	189	LEU
2	A	193	ASN
2	A	197	MET
2	A	202	MET

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Mol	Chain	Res	Type
2	A	203	PHE
2	A	205	ASN
2	A	208	THR
2	A	209	THR
2	A	223	LEU
2	A	236	ASN
2	A	247	VAL
2	A	277	LEU
2	A	310	LYS
2	A	311	ASP
2	A	329	SER
2	A	1028	ARG
2	A	1029	LEU
2	A	1047	LEU
2	A	1068	GLU
2	A	1075	LEU
2	A	1079	VAL
2	A	1085	ARG
2	A	1114	LEU
2	A	1140	VAL
2	A	1142	VAL
2	A	1145	SER
2	A	1146	VAL
2	A	1149	LEU
2	A	1183	LYS
2	A	1189	LEU
2	A	1193	ASN
2	A	1197	MET
2	A	1203	PHE
2	A	1205	ASN
2	A	1208	THR
2	A	1209	THR
2	A	1223	LEU
2	A	1236	ASN
2	A	1277	LEU
2	A	1310	LYS
2	A	1311	ASP
2	A	2028	ARG
2	A	2029	LEU
2	A	2047	LEU
2	A	2068	GLU
2	A	2075	LEU

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Mol	Chain	Res	Type
2	A	2079	VAL
2	A	2085	ARG
2	A	2114	LEU
2	A	2140	VAL
2	A	2142	VAL
2	A	2145	SER
2	A	2146	VAL
2	A	2149	LEU
2	A	2183	LYS
2	A	2189	LEU
2	A	2193	ASN
2	A	2197	MET
2	A	2203	PHE
2	A	2205	ASN
2	A	2208	THR
2	A	2209	THR
2	A	2223	LEU
2	A	2236	ASN
2	A	2247	VAL
2	A	2277	LEU
2	A	2310	LYS
2	A	2311	ASP
2	A	3028	ARG
2	A	3029	LEU
2	A	3047	LEU
2	A	3068	GLU
2	A	3075	LEU
2	A	3076	THR
2	A	3079	VAL
2	A	3085	ARG
2	A	3114	LEU
2	A	3140	VAL
2	A	3142	VAL
2	A	3145	SER
2	A	3146	VAL
2	A	3149	LEU
2	A	3183	LYS
2	A	3189	LEU
2	A	3193	ASN
2	A	3197	MET
2	A	3203	PHE
2	A	3205	ASN

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Mol	Chain	Res	Type
2	A	3208	THR
2	A	3209	THR
2	A	3223	LEU
2	A	3236	ASN
2	A	3247	VAL
2	A	3277	LEU
2	A	3310	LYS
2	A	3311	ASP
2	A	3332	ASN
2	A	4028	ARG
2	A	4029	LEU
2	A	4047	LEU
2	A	4068	GLU
2	A	4075	LEU
2	A	4079	VAL
2	A	4085	ARG
2	A	4114	LEU
2	A	4140	VAL
2	A	4142	VAL
2	A	4145	SER
2	A	4146	VAL
2	A	4149	LEU
2	A	4155	ILE
2	A	4183	LYS
2	A	4185	SER
2	A	4189	LEU
2	A	4193	ASN
2	A	4205	ASN
2	A	4208	THR
2	A	4209	THR
2	A	4223	LEU
2	A	4236	ASN
2	A	4247	VAL
2	A	4277	LEU
2	A	4310	LYS
2	A	4311	ASP
2	A	4314	GLU
2	C	47	LEU
2	C	68	GLU
2	C	75	LEU
2	C	79	VAL
2	C	85	ARG

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Mol	Chain	Res	Type
2	C	114	LEU
2	C	140	VAL
2	C	142	VAL
2	C	145	SER
2	C	146	VAL
2	C	149	LEU
2	C	183	LYS
2	C	189	LEU
2	C	193	ASN
2	C	197	MET
2	C	202	MET
2	C	203	PHE
2	C	205	ASN
2	C	208	THR
2	C	209	THR
2	C	223	LEU
2	C	236	ASN
2	C	247	VAL
2	C	277	LEU
2	C	310	LYS
2	C	311	ASP
2	C	1028	ARG
2	C	1029	LEU
2	C	1047	LEU
2	C	1068	GLU
2	C	1075	LEU
2	C	1079	VAL
2	C	1085	ARG
2	C	1114	LEU
2	C	1140	VAL
2	C	1142	VAL
2	C	1145	SER
2	C	1146	VAL
2	C	1149	LEU
2	C	1183	LYS
2	C	1189	LEU
2	C	1193	ASN
2	C	1197	MET
2	C	1203	PHE
2	C	1205	ASN
2	C	1208	THR
2	C	1209	THR

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Mol	Chain	Res	Type
2	C	1223	LEU
2	C	1236	ASN
2	C	1277	LEU
2	C	1310	LYS
2	C	1311	ASP
2	C	2028	ARG
2	C	2029	LEU
2	C	2047	LEU
2	C	2068	GLU
2	C	2075	LEU
2	C	2079	VAL
2	C	2085	ARG
2	C	2114	LEU
2	C	2140	VAL
2	C	2142	VAL
2	C	2145	SER
2	C	2146	VAL
2	C	2149	LEU
2	C	2183	LYS
2	C	2189	LEU
2	C	2193	ASN
2	C	2197	MET
2	C	2203	PHE
2	C	2205	ASN
2	C	2208	THR
2	C	2209	THR
2	C	2223	LEU
2	C	2236	ASN
2	C	2247	VAL
2	C	2277	LEU
2	C	2310	LYS
2	C	2311	ASP
2	C	3028	ARG
2	C	3029	LEU
2	C	3047	LEU
2	C	3068	GLU
2	C	3075	LEU
2	C	3079	VAL
2	C	3085	ARG
2	C	3114	LEU
2	C	3140	VAL
2	C	3142	VAL

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Mol	Chain	Res	Type
2	C	3145	SER
2	C	3146	VAL
2	C	3149	LEU
2	C	3183	LYS
2	C	3189	LEU
2	C	3193	ASN
2	C	3197	MET
2	C	3203	PHE
2	C	3205	ASN
2	C	3208	THR
2	C	3209	THR
2	C	3223	LEU
2	C	3236	ASN
2	C	3247	VAL
2	C	3277	LEU
2	C	3310	LYS
2	C	3311	ASP
2	C	4028	ARG
2	C	4029	LEU
2	C	4047	LEU
2	C	4068	GLU
2	C	4075	LEU
2	C	4079	VAL
2	C	4085	ARG
2	C	4114	LEU
2	C	4140	VAL
2	C	4142	VAL
2	C	4145	SER
2	C	4146	VAL
2	C	4149	LEU
2	C	4183	LYS
2	C	4185	SER
2	C	4189	LEU
2	C	4193	ASN
2	C	4205	ASN
2	C	4208	THR
2	C	4209	THR
2	C	4223	LEU
2	C	4236	ASN
2	C	4247	VAL
2	C	4277	LEU
2	C	4310	LYS

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Mol	Chain	Res	Type
2	C	4311	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	97	HIS
2	A	181	ASN
2	A	193	ASN
2	A	205	ASN
2	A	304	ASN
2	A	1097	HIS
2	A	1181	ASN
2	A	1184	GLN
2	A	1193	ASN
2	A	1205	ASN
2	A	1304	ASN
2	A	1332	ASN
2	A	2097	HIS
2	A	2181	ASN
2	A	2184	GLN
2	A	2193	ASN
2	A	2205	ASN
2	A	2330	ASN
2	A	3097	HIS
2	A	3181	ASN
2	A	3193	ASN
2	A	3205	ASN
2	A	3304	ASN
2	A	4097	HIS
2	A	4181	ASN
2	A	4184	GLN
2	A	4193	ASN
2	A	4205	ASN
2	A	4304	ASN
2	C	97	HIS
2	C	181	ASN
2	C	193	ASN
2	C	205	ASN
2	C	304	ASN
2	C	330	ASN
2	C	1097	HIS
2	C	1181	ASN

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Mol	Chain	Res	Type
2	C	1193	ASN
2	C	1205	ASN
2	C	1304	ASN
2	C	2097	HIS
2	C	2181	ASN
2	C	2193	ASN
2	C	2205	ASN
2	C	2332	ASN
2	C	3097	HIS
2	C	3118	GLN
2	C	3181	ASN
2	C	3193	ASN
2	C	3205	ASN
2	C	3304	ASN
2	C	4097	HIS
2	C	4181	ASN
2	C	4184	GLN
2	C	4193	ASN
2	C	4205	ASN
2	C	4304	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 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	$\# Z > 2$
4	ALF	A	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	1502	3	22,29,29	0.83	1 (4%)	27,45,45	2.42	7 (25%)
4	ALF	A	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	2502	3	22,29,29	0.97	1 (4%)	27,45,45	2.07	5 (18%)
4	ALF	A	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	3502	3	22,29,29	1.00	2 (9%)	27,45,45	2.34	6 (22%)
4	ALF	A	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	4502	3	22,29,29	1.24	2 (9%)	27,45,45	1.91	6 (22%)
4	ALF	A	501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	502	3	22,29,29	1.07	1 (4%)	27,45,45	2.09	4 (14%)
4	ALF	C	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	1502	3	22,29,29	0.89	1 (4%)	27,45,45	1.86	5 (18%)
4	ALF	C	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	2502	3	22,29,29	0.98	1 (4%)	27,45,45	2.28	7 (25%)
4	ALF	C	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	3502	3	22,29,29	0.90	1 (4%)	27,45,45	2.25	6 (22%)
4	ALF	C	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	4502	3	22,29,29	1.06	1 (4%)	27,45,45	2.12	7 (25%)
4	ALF	C	501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	502	3	22,29,29	0.90	1 (4%)	27,45,45	2.06	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ALF	C	1501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	1502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	2501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	2502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	3501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	3502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	4501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	4502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	502	3	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4502	ADP	O4'-C1'	2.35	1.44	1.41
5	A	3502	ADP	C5-C4	2.42	1.46	1.40
5	A	3502	ADP	O4'-C1'	2.45	1.44	1.41
5	C	1502	ADP	C5-C4	2.45	1.46	1.40
5	A	1502	ADP	C5-C4	2.57	1.46	1.40
5	C	502	ADP	C5-C4	2.68	1.46	1.40
5	C	2502	ADP	C5-C4	3.00	1.47	1.40
5	A	2502	ADP	C5-C4	3.01	1.47	1.40
5	C	3502	ADP	C5-C4	3.12	1.47	1.40
5	A	502	ADP	C5-C4	3.17	1.47	1.40
5	C	4502	ADP	C5-C4	3.53	1.48	1.40
5	A	4502	ADP	C5-C4	3.78	1.49	1.40

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3502	ADP	N3-C2-N1	-9.03	121.98	128.89
5	A	1502	ADP	N3-C2-N1	-8.11	122.69	128.89
5	C	3502	ADP	N3-C2-N1	-8.00	122.77	128.89
5	C	2502	ADP	N3-C2-N1	-7.54	123.12	128.89
5	C	4502	ADP	N3-C2-N1	-7.37	123.25	128.89
5	A	502	ADP	N3-C2-N1	-7.36	123.26	128.89
5	A	4502	ADP	N3-C2-N1	-7.36	123.26	128.89
5	C	502	ADP	N3-C2-N1	-6.60	123.84	128.89
5	A	2502	ADP	N3-C2-N1	-6.57	123.86	128.89
5	A	1502	ADP	C2'-C1'-N9	-6.43	104.47	114.29
5	C	2502	ADP	C2'-C1'-N9	-6.09	104.99	114.29
5	C	1502	ADP	N3-C2-N1	-5.90	124.38	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3502	ADP	C2'-C1'-N9	-5.72	105.55	114.29
5	A	2502	ADP	C2'-C1'-N9	-5.49	105.90	114.29
5	C	502	ADP	C2'-C1'-N9	-5.29	106.21	114.29
5	A	502	ADP	C2'-C1'-N9	-4.88	106.83	114.29
5	A	3502	ADP	C2'-C1'-N9	-4.79	106.97	114.29
5	C	1502	ADP	C2'-C1'-N9	-4.71	107.10	114.29
5	C	4502	ADP	C2'-C1'-N9	-4.62	107.23	114.29
5	A	502	ADP	PA-O3A-PB	-3.27	121.70	132.67
5	C	2502	ADP	C4-C5-N7	-3.07	106.66	109.48
5	A	4502	ADP	C2'-C1'-N9	-3.07	109.61	114.29
5	A	2502	ADP	PA-O3A-PB	-3.06	122.41	132.67
5	A	1502	ADP	C1'-N9-C4	-3.02	122.39	126.94
5	C	1502	ADP	C4-C5-N7	-2.81	106.90	109.48
5	C	502	ADP	C4-C5-N7	-2.79	106.91	109.48
5	A	3502	ADP	PA-O3A-PB	-2.57	124.06	132.67
5	A	2502	ADP	C4-C5-N7	-2.52	107.16	109.48
5	A	3502	ADP	C1'-N9-C4	-2.46	123.22	126.94
5	C	4502	ADP	PA-O3A-PB	-2.42	124.56	132.67
5	A	4502	ADP	PA-O3A-PB	-2.40	124.63	132.67
5	C	2502	ADP	C1'-N9-C4	-2.39	123.33	126.94
5	A	1502	ADP	PA-O3A-PB	-2.36	124.75	132.67
5	C	2502	ADP	PA-O3A-PB	-2.23	125.18	132.67
5	C	3502	ADP	PA-O3A-PB	-2.22	125.22	132.67
5	C	502	ADP	PA-O3A-PB	-2.19	125.31	132.67
5	A	4502	ADP	C1'-N9-C4	-2.08	123.81	126.94
5	C	1502	ADP	N6-C6-N1	2.02	123.53	119.20
5	C	3502	ADP	O3B-PB-O2B	2.03	115.09	107.38
5	C	4502	ADP	O2B-PB-O1B	2.03	117.13	110.58
5	A	502	ADP	N6-C6-N1	2.12	123.76	119.20
5	C	3502	ADP	O4'-C1'-N9	2.21	112.73	108.10
5	C	4502	ADP	C2-N1-C6	2.23	122.75	118.77
5	A	3502	ADP	C2-N1-C6	2.25	122.79	118.77
5	A	1502	ADP	O4'-C1'-N9	2.28	112.87	108.10
5	A	4502	ADP	C2-N1-C6	2.30	122.88	118.77
5	C	3502	ADP	C2-N1-C6	2.30	122.88	118.77
5	A	2502	ADP	O4'-C1'-N9	2.30	112.92	108.10
5	C	502	ADP	O4'-C1'-N9	2.31	112.94	108.10
5	C	2502	ADP	O4'-C1'-N9	2.33	112.97	108.10
5	A	4502	ADP	O2B-PB-O1B	2.35	118.14	110.58
5	A	3502	ADP	O4'-C1'-N9	2.36	113.04	108.10
5	A	1502	ADP	C2-N1-C6	2.41	123.07	118.77
5	C	2502	ADP	C2-N1-C6	2.57	123.35	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	C	4502	ADP	O3B-PB-O2B	2.58	117.21	107.38
5	C	1502	ADP	O4'-C1'-N9	2.59	113.51	108.10
5	C	4502	ADP	N6-C6-N1	2.63	124.85	119.20
5	A	1502	ADP	O3B-PB-O2B	2.68	117.60	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2502	ADP	1	0
5	A	502	ADP	2	0
5	C	1502	ADP	1	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 ⓘ

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	B	12/15 (80%)	0.52	0 100 100	29, 56, 64, 65	0
1	D	12/15 (80%)	0.63	1 (8%) 14 7	22, 52, 61, 61	0
2	A	1609/1706 (94%)	0.71	176 (10%) 7 3	52, 62, 78, 107	0
2	C	1608/1706 (94%)	0.65	159 (9%) 9 4	50, 62, 79, 108	0
All	All	3241/3442 (94%)	0.68	336 (10%) 8 4	22, 62, 79, 108	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1001	ALA	12.4
2	A	4164	MET	7.8
2	C	3330	ASN	7.7
2	C	4291	TYR	7.7
2	C	3202	MET	7.6
2	C	3331	PRO	7.5
2	A	331	PRO	7.3
2	C	2001	ALA	7.0
2	C	3329	SER	7.0
2	A	1333	SER	6.9
2	C	4296	GLU	6.7
2	A	2001	ALA	6.7
2	C	4290	TRP	6.5
2	A	1202	MET	6.3
2	C	3332	ASN	6.3
2	A	315	THR	6.0
2	C	4297	LYS	5.5
2	A	1002	ILE	5.5
2	C	1202	MET	5.4
2	C	4314	GLU	5.4
2	A	2202	MET	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	4295	GLY	5.2
2	A	1298	ILE	5.2
2	C	37	VAL	5.2
2	A	330	ASN	5.2
2	A	316	ALA	5.0
2	A	1024	GLY	5.0
2	A	300	GLN	5.0
2	C	4002	ILE	4.9
2	A	2203	PHE	4.9
2	C	3203	PHE	4.9
2	C	2002	ILE	4.8
2	A	3287	ALA	4.8
2	A	3203	PHE	4.8
2	A	4001	ALA	4.8
2	A	1308	TRP	4.6
2	A	329	SER	4.6
2	C	4306	THR	4.6
2	C	4198	LYS	4.6
2	A	4002	ILE	4.6
2	C	2333	SER	4.6
2	A	309	LEU	4.6
2	A	323	VAL	4.5
2	A	289	ALA	4.4
2	A	3202	MET	4.4
2	C	4285	GLU	4.4
2	C	1333	SER	4.4
2	C	2008	LYS	4.4
2	C	176	ARG	4.3
2	C	4293	TYR	4.3
2	A	3003	ASP	4.3
2	C	3001	ALA	4.3
2	A	3204	GLY	4.3
2	A	298	ILE	4.3
2	C	283	LEU	4.2
2	A	287	ALA	4.2
2	C	4278	GLY	4.2
2	A	1332	ASN	4.2
2	C	4315	THR	4.2
2	C	202	MET	4.2
2	A	296	GLU	4.1
2	C	4005	ASN	4.1
2	A	2200	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	C	1201	VAL	4.0
2	C	4300	GLN	4.0
2	C	4286	LYS	4.0
2	A	297	LYS	3.9
2	C	3333	SER	3.9
2	C	2202	MET	3.9
2	A	314	GLU	3.9
2	A	1201	VAL	3.9
2	A	3145	SER	3.8
2	C	4309	LEU	3.8
2	A	1203	PHE	3.8
2	A	307	ALA	3.8
2	C	4294	LYS	3.8
2	A	3296	GLU	3.7
2	A	135	SER	3.7
2	C	2003	ASP	3.7
2	A	1297	LYS	3.7
2	A	1204	GLY	3.7
2	C	3296	GLU	3.7
2	C	1200	GLY	3.7
2	A	311	ASP	3.7
2	C	2006	LYS	3.7
2	A	306	THR	3.6
2	A	308	TRP	3.6
2	A	271	TYR	3.6
2	C	296	GLU	3.6
2	C	4298	ILE	3.6
2	C	2145	SER	3.6
2	C	1235	GLU	3.5
2	C	69	SER	3.5
2	C	1002	ILE	3.5
2	C	1203	PHE	3.5
2	C	2005	ASN	3.4
2	C	4310	LYS	3.4
2	A	293	TYR	3.4
2	C	2204	GLY	3.4
2	C	3002	ILE	3.4
2	A	303	ALA	3.4
2	A	274	LEU	3.4
2	A	288	GLY	3.4
2	A	276	ASP	3.4
2	A	299	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	291	TYR	3.3
2	A	2297	LYS	3.3
2	A	3144	ASP	3.3
2	A	1200	GLY	3.3
2	A	313	PRO	3.3
2	A	2019	LYS	3.3
2	C	4284	ILE	3.2
2	A	3062	VAL	3.2
2	C	3233	GLU	3.2
2	A	2145	SER	3.2
2	C	4282	LYS	3.2
2	A	144	ASP	3.2
2	A	1311	ASP	3.2
2	C	4205	ASN	3.2
2	C	4313	PRO	3.2
2	C	333	SER	3.2
2	A	200	GLY	3.1
2	A	4233	GLU	3.1
2	A	1295	GLY	3.1
2	C	3005	ASN	3.1
2	A	3189	LEU	3.1
2	A	295	GLY	3.1
2	C	2200	GLY	3.1
2	C	3237	VAL	3.1
2	A	2287	ALA	3.1
2	C	4206	PRO	3.1
2	C	3204	GLY	3.1
2	A	3190	ILE	3.1
2	C	73	THR	3.1
2	A	4155	ILE	3.1
2	C	1204	GLY	3.1
2	A	2201	VAL	3.1
2	A	2233	GLU	3.1
2	C	4008	LYS	3.1
2	A	1291	TYR	3.0
2	A	272	GLY	3.0
2	C	4003	ASP	3.0
2	A	2204	GLY	3.0
2	C	4301	GLY	3.0
2	C	135	SER	3.0
2	A	1293	TYR	3.0
2	A	1285	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	3314	GLU	3.0
2	A	322	LYS	2.9
2	C	4234	GLY	2.9
2	C	3004	GLU	2.9
2	C	4009	ALA	2.9
2	A	3073	THR	2.9
2	A	305	ALA	2.9
2	C	4292	SER	2.9
2	C	332	ASN	2.9
2	A	1023	LYS	2.9
2	A	332	ASN	2.9
2	C	4287	ALA	2.9
2	C	4279	VAL	2.8
2	C	4318	GLU	2.8
2	A	290	TRP	2.8
2	C	3145	SER	2.8
2	A	37	VAL	2.8
2	C	4235	GLU	2.8
2	C	3287	ALA	2.8
2	A	2003	ASP	2.8
2	A	251	ILE	2.8
2	A	284	ILE	2.8
1	D	1013	DT	2.8
2	C	4001	ALA	2.8
2	C	137	ALA	2.7
2	C	4311	ASP	2.7
2	A	1009	ALA	2.7
2	A	3191	PHE	2.7
2	A	325	GLU	2.7
2	C	3236	ASN	2.7
2	A	3061	ILE	2.7
2	A	184	GLN	2.7
2	A	1005	ASN	2.7
2	A	1235	GLU	2.7
2	A	1323	VAL	2.7
2	C	4238	VAL	2.7
2	C	4312	ASN	2.7
2	A	318	GLU	2.7
2	C	4006	LYS	2.7
2	A	1003	ASP	2.7
2	A	52	GLY	2.7
2	A	3143	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	1318	GLU	2.6
2	C	3003	ASP	2.6
2	A	304	ASN	2.6
2	C	139	ASP	2.6
2	A	1266	GLU	2.6
2	C	4152	LYS	2.6
2	A	1031	GLU	2.6
2	A	3192	ILE	2.6
2	A	1134	ARG	2.6
2	A	2005	ASN	2.6
2	C	1001	ALA	2.6
2	A	3218	TYR	2.5
2	A	4169	ARG	2.5
2	A	301	GLY	2.5
2	A	3064	ILE	2.5
2	A	4153	ALA	2.5
2	A	1286	LYS	2.5
2	A	253	ALA	2.5
2	A	4165	GLY	2.5
2	A	286	LYS	2.5
2	A	3148	ALA	2.5
2	A	3285	GLU	2.5
2	C	3062	VAL	2.5
2	A	250	LYS	2.5
2	C	3328	LEU	2.5
2	A	2002	ILE	2.5
2	A	292	SER	2.5
2	C	4120	ASP	2.5
2	A	3142	VAL	2.5
2	C	2192	ILE	2.5
2	C	3295	GLY	2.5
2	A	3076	THR	2.4
2	C	1220	SER	2.4
2	A	1296	GLU	2.4
2	C	3219	ALA	2.4
2	C	235	GLU	2.4
2	A	4156	GLU	2.4
2	C	2004	GLU	2.4
2	C	184	GLN	2.4
2	A	3333	SER	2.4
2	C	2147	ALA	2.4
2	A	255	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	1003	ASP	2.4
2	A	321	LYS	2.4
2	A	2220	SER	2.4
2	A	4205	ASN	2.4
2	A	254	PRO	2.4
2	C	1241	GLU	2.4
2	C	3006	LYS	2.4
2	A	324	ARG	2.3
2	A	294	LYS	2.3
2	A	3179	ALA	2.3
2	A	310	LYS	2.3
2	A	1289	ALA	2.3
2	A	3219	ALA	2.3
2	C	4232	LYS	2.3
2	C	2203	PHE	2.3
2	A	3220	SER	2.3
2	A	319	ILE	2.3
2	A	2192	ILE	2.3
2	C	2023	LYS	2.3
2	C	4283	LEU	2.3
2	C	4197	MET	2.3
2	C	156	GLU	2.3
2	A	4116	CYS	2.3
2	C	4137	ALA	2.3
2	C	1062	VAL	2.3
2	A	176	ARG	2.3
2	A	2144	ASP	2.3
2	C	4016	GLN	2.3
2	C	4020	GLN	2.3
2	A	1220	SER	2.3
2	C	2064	ILE	2.3
2	C	3306	THR	2.3
2	C	4281	GLU	2.3
2	A	283	LEU	2.3
2	A	1192	ILE	2.2
2	C	3191	PHE	2.2
2	A	3074	THR	2.2
2	A	2009	ALA	2.2
2	C	174	ALA	2.2
2	A	233	GLU	2.2
2	C	3220	SER	2.2
2	C	3293	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	3323	VAL	2.2
2	C	3294	LYS	2.2
2	C	4271	TYR	2.2
2	A	2191	PHE	2.2
2	A	199	ILE	2.2
2	C	3298	ILE	2.2
2	A	212	GLY	2.2
2	C	3218	TYR	2.2
2	C	3169	ARG	2.2
2	C	3209	THR	2.2
2	C	2271	TYR	2.2
2	C	4007	GLN	2.2
2	A	245	LYS	2.2
2	A	2235	GLU	2.2
2	C	4136	GLY	2.2
2	C	2146	VAL	2.2
2	C	4019	LYS	2.2
2	A	3141	ILE	2.2
2	C	4154	GLU	2.2
2	C	1223	LEU	2.2
2	C	1145	SER	2.1
2	C	3008	LYS	2.1
2	A	312	ASN	2.1
2	A	3004	GLU	2.1
2	C	152	LYS	2.1
2	A	1144	ASP	2.1
2	A	1290	TRP	2.1
2	C	1290	TRP	2.1
2	C	1192	ILE	2.1
2	C	2301	GLY	2.1
2	C	1146	VAL	2.1
2	C	3174	ALA	2.1
2	A	4218	TYR	2.1
2	C	4299	GLY	2.1
2	A	3146	VAL	2.1
2	C	3146	VAL	2.1
2	A	2316	ALA	2.1
2	C	204	GLY	2.1
2	A	333	SER	2.1
2	A	1306	THR	2.1
2	C	2193	ASN	2.1
2	A	2288	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	3190	ILE	2.1
2	C	1019	LYS	2.1
2	A	178	LEU	2.1
2	A	2076	THR	2.1
2	C	1144	ASP	2.0
2	A	2308	TRP	2.0
2	A	3092	PHE	2.0
2	C	3192	ILE	2.0
2	A	51	LEU	2.0
2	A	1008	LYS	2.0
2	A	3117	SER	2.0
2	C	145	SER	2.0
2	A	3059	GLY	2.0
2	A	2190	ILE	2.0
2	A	327	LEU	2.0
2	C	1191	PHE	2.0
2	C	3235	GLU	2.0
2	C	1199	ILE	2.0
2	A	277	LEU	2.0
2	A	285	GLU	2.0
2	C	2069	SER	2.0

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(Å ²)	Q<0.9
4	ALF	A	501	5/5	0.95	0.32	0.58	60,60,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ALF	C	2501	5/5	0.95	0.33	0.53	45,47,50,50	0
4	ALF	C	3501	5/5	0.94	0.28	0.50	47,49,52,53	0
4	ALF	C	501	5/5	0.97	0.34	0.15	44,49,49,52	0
4	ALF	A	1501	5/5	0.94	0.28	0.13	45,47,50,53	0
4	ALF	C	1501	5/5	0.97	0.28	-0.02	40,42,46,47	0
4	ALF	A	3501	5/5	0.96	0.28	-0.17	42,46,49,51	0
4	ALF	A	2501	5/5	0.97	0.29	-0.19	40,44,45,47	0
5	ADP	A	502	27/27	0.93	0.22	-0.34	50,53,57,60	0
5	ADP	C	502	27/27	0.97	0.23	-0.64	37,40,43,47	0
5	ADP	C	4502	27/27	0.94	0.15	-0.89	54,56,61,63	0
5	ADP	A	1502	27/27	0.96	0.19	-0.95	33,40,44,46	0
5	ADP	A	4502	27/27	0.94	0.15	-0.97	47,62,63,68	0
5	ADP	C	3502	27/27	0.94	0.18	-1.03	40,50,52,53	0
5	ADP	C	2502	27/27	0.96	0.18	-1.03	41,46,49,49	0
5	ADP	C	1502	27/27	0.97	0.19	-1.10	32,36,39,41	0
5	ADP	A	2502	27/27	0.96	0.18	-1.13	37,42,45,47	0
4	ALF	A	4501	5/5	0.80	0.16	-1.14	78,79,81,82	0
4	ALF	C	4501	5/5	0.88	0.14	-1.15	67,71,73,75	0
5	ADP	A	3502	27/27	0.97	0.19	-1.16	28,35,39,40	0
3	MG	A	1500	1/1	0.88	0.39	-	47,47,47,47	0
3	MG	C	500	1/1	0.86	0.49	-	50,50,50,50	0
3	MG	C	2500	1/1	0.94	0.51	-	48,48,48,48	0
3	MG	A	4500	1/1	0.95	0.29	-	60,60,60,60	0
3	MG	C	3500	1/1	0.88	0.43	-	45,45,45,45	0
3	MG	C	4500	1/1	0.89	0.31	-	56,56,56,56	0
3	MG	A	500	1/1	0.95	0.55	-	57,57,57,57	0
3	MG	A	2500	1/1	0.82	0.42	-	42,42,42,42	0
3	MG	A	3500	1/1	0.90	0.50	-	46,46,46,46	0
3	MG	C	1500	1/1	0.95	0.46	-	45,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.