



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:49 AM GMT

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

This is a full wwPDB 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/ValidationPDFNotes.html>

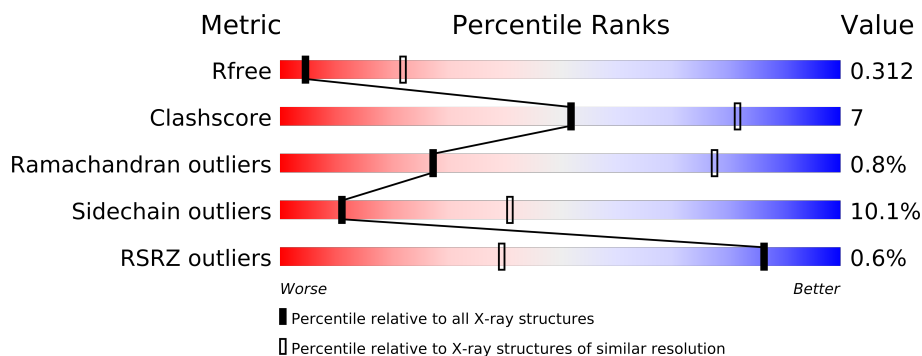
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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

Mol	Chain	Length	Quality of chain
1	B	15	
1	E	15	
2	C	6	
2	F	6	
3	A	1706	
3	D	1706	

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

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

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25312 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3').

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

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

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

- Molecule 3 is a protein called Protein recA.

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

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	3000	SER	-	linker	UNP P0A7G6
A	3986	THR	-	linker	UNP P0A7G6
A	3987	GLY	-	linker	UNP P0A7G6
A	3988	SER	-	linker	UNP P0A7G6
A	3989	THR	-	linker	UNP P0A7G6
A	3990	GLY	-	linker	UNP P0A7G6
A	3991	SER	-	linker	UNP P0A7G6
A	3992	MET	-	linker	UNP P0A7G6
A	3993	SER	-	linker	UNP P0A7G6
A	3994	GLY	-	linker	UNP P0A7G6
A	3995	ARG	-	linker	UNP P0A7G6
A	3996	THR	-	linker	UNP P0A7G6
A	3997	GLY	-	linker	UNP P0A7G6
A	3998	SER	-	linker	UNP P0A7G6
A	3999	MET	-	linker	UNP P0A7G6
A	4000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6
D	1992	MET	-	linker	UNP P0A7G6

Continued on next page...

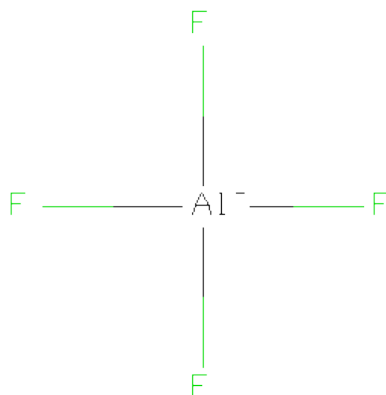
Continued from previous page...

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

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

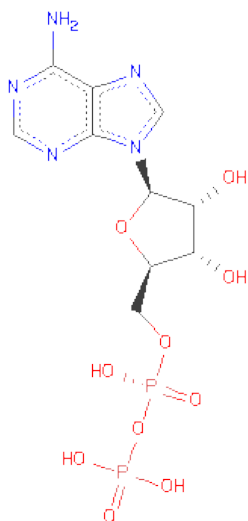
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



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

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



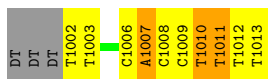
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain B: 



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

Chain E: 



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

Chain C: 



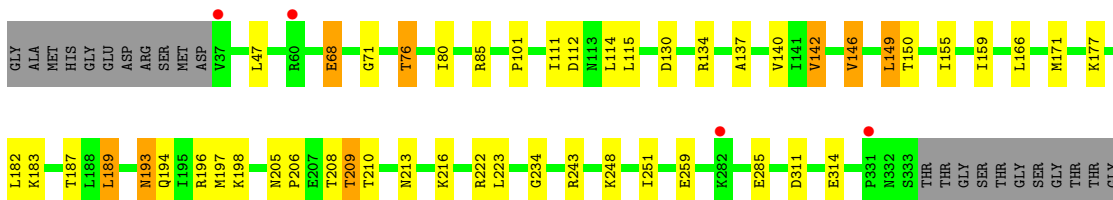
- Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

Chain F: 



- Molecule 3: Protein recA

Chain A: 



E4314	K4177	THR	I3199	F3021	R2196
L4328 SER ASN PRO ASN SER THR	L4182	GLY	M3202	G3022	R2197
	K4183	SER		K3023	K2198
	T4187	SER	N3205	R3028	I2199
	L4188	A4001	P3206	L3029	M2202
L4189	F4021	E3207	G3030	N2205	
N4193 Q4194 L4195 R4196 M4197 K4198	G4022	T3209	T3210	N2206	
	K4023	T3211	G3211	E2207	
	R4028	G3212	E3068	T2208	
	L4029	N3213	T3076	T2209	
L4047	K3216	I3080	R3085	G2211	
ILE	E4068	R3222	I3111	G2212	
GLY	S4069	L3223	L3114	N2213	
VAL	T4076	G3234	Q3124	K2216	
MET	T4076	R3243	D3130	R2222	
PHE	L4080	K3248	R3134	L2223	
GLY	R4205	I3251	E3259	G2234	
N4205	P4206	E3259	F3260	R2243	
E4207	E4086	Q3261	Q3261	K2248	
T4208	G4087	I3262	I3141	I2251	
T4209	L4114	L3263	V3142	E2259	
T4210	L4126	D4130	V3142	E2285	
G4211	D4130	R4134	N3269	N2304	
G4212	L4140	V4140	K3282	L2223	
N4213	I4141	I4141	E3285	D2311	
K4216	G4234	V4142	I3155	E2314	
	R4243	V4146	D3311		
	R4248	L4149	E3314		
	I4251	K4152	L3328		
P4254	A4153	S3329	M3171	R2332	
E4259	E4154	N3330	Q3173	S2333	
K4262	ILE	P3331	L3182	THR	
	GLU	N3332	K3183	GLY	
	GLY	S3333	T3187	ALA	
	GLU	THR	L3188	SER	
E4285	ILE	GLY	L3189	SER	
V4291	ASP	SER	L3189	GLY	
	SER	THR	THR	SER	
	HIS	GLY	N3193	THR	
	G4295	M4164	Q3194	GLY	
F4296	G4165	MET	I3195	SER	
K4297	L4166	SER	R3196	MET	
D4311	M4171	GLY	M3197	THR	
		ARG	K3198	A3001	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.15 39.75 – 2.98	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-3.15) 86.8 (39.75-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.217 , 0.243 0.275 , 0.312	Depositor DCC
R_{free} test set	1233 reflections (2.07%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -1.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 72645 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25312	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

All (2) bond length outliers are listed below:

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

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2007	DG	P-O5'-C5'	25.73	162.07	120.90
2	C	2007	DG	O5'-P-OP2	-20.43	86.18	110.70
2	C	2007	DG	O5'-P-OP1	18.46	132.85	110.70
1	E	1006	DC	O4'-C4'-C3'	-8.95	100.63	106.00
2	F	2008	DG	O4'-C1'-N9	-8.52	102.04	108.00
1	B	1006	DC	O4'-C4'-C3'	-8.51	100.89	106.00
1	E	1006	DC	C1'-O4'-C4'	-8.17	101.93	110.10
2	C	2008	DG	O4'-C1'-N9	-8.07	102.35	108.00
1	B	1006	DC	C1'-O4'-C4'	-7.84	102.26	110.10
2	F	2007	DG	O5'-P-OP2	7.55	119.76	110.70
1	E	1010	DT	O4'-C1'-N1	6.91	112.84	108.00
1	B	1010	DT	N3-C2-O2	-6.80	118.22	122.30
1	E	1002	DT	P-O3'-C3'	6.64	127.67	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1010	DT	O4'-C1'-N1	6.28	112.39	108.00
1	E	1002	DT	O4'-C1'-N1	6.28	112.39	108.00
1	E	1007	DA	O4'-C4'-C3'	-5.70	102.22	104.50
2	F	2007	DG	O4'-C1'-C2'	-5.69	101.35	105.90
2	F	2009	DT	C1'-O4'-C4'	-5.49	104.61	110.10
1	B	1007	DA	O4'-C1'-N9	5.43	111.80	108.00
1	B	1011	DT	C1'-O4'-C4'	-5.35	104.75	110.10
1	E	1004	DC	O4'-C1'-N1	-5.31	104.28	108.00
2	C	2007	DG	O4'-C1'-C2'	-5.22	101.72	105.90
1	E	1007	DA	C1'-O4'-C4'	-5.15	104.95	110.10
1	E	1007	DA	O4'-C1'-N9	5.15	111.61	108.00
1	E	1007	DA	C4'-C3'-C2'	5.14	107.72	103.10
1	E	1006	DC	O4'-C1'-N1	5.13	111.59	108.00
1	B	1008	DC	C1'-O4'-C4'	-5.11	105.00	110.10
1	E	1008	DC	C1'-O4'-C4'	-5.05	105.05	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	236	0	139	9	0
1	E	236	0	139	19	0
2	C	130	0	69	0	0
2	F	130	0	69	0	0
3	A	12125	0	12451	176	0
3	D	12125	0	12456	190	1
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	0	0
5	D	25	0	0	2	0
6	A	135	0	60	6	0
6	D	135	0	60	4	0
All	All	25312	0	25443	364	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (364) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:68:GLU:HG2	3:A:1216:LYS:HB3	1.39	1.02
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.97
3:D:160:GLY:H	3:D:1173:GLN:HE22	1.14	0.94
3:A:2068:GLU:HG2	3:A:3216:LYS:HB3	1.54	0.87
3:D:1194:GLN:HE21	3:D:1196:ARG:HH12	1.23	0.86
3:D:4194:GLN:HE21	3:D:4196:ARG:HH12	1.23	0.86
3:D:2194:GLN:HE21	3:D:2196:ARG:HH12	1.24	0.85
3:A:194:GLN:HE21	3:A:196:ARG:HH12	1.25	0.85
3:A:3194:GLN:HE21	3:A:3196:ARG:HH12	1.25	0.85
3:D:1193:ASN:HD22	3:D:1194:GLN:H	1.25	0.84
3:A:3206:PRO:HG3	3:D:3202:MET:HB3	1.58	0.84
3:D:2193:ASN:HD22	3:D:2194:GLN:H	1.26	0.84
3:D:3068:GLU:HG2	3:D:4216:LYS:HB3	1.56	0.84
3:A:4282:LYS:HG3	3:D:1282:LYS:HG3	1.59	0.83
3:A:1194:GLN:HE21	3:A:1196:ARG:HH12	1.24	0.83
3:A:3193:ASN:HD22	3:A:3194:GLN:H	1.26	0.83
3:D:1068:GLU:HG2	3:D:2216:LYS:HB3	1.61	0.82
3:A:4194:GLN:HE21	3:A:4196:ARG:HH12	1.26	0.82
3:D:194:GLN:HE21	3:D:196:ARG:HH12	1.25	0.82
3:A:2193:ASN:HD22	3:A:2194:GLN:H	1.27	0.81
3:A:2194:GLN:HE21	3:A:2196:ARG:HH12	1.24	0.81
3:D:3194:GLN:HE21	3:D:3196:ARG:HH12	1.26	0.81
3:A:193:ASN:HD22	3:A:194:GLN:H	1.28	0.80
3:A:1193:ASN:HD22	3:A:1194:GLN:H	1.28	0.80
3:D:160:GLY:H	3:D:1173:GLN:NE2	1.81	0.79
3:D:4193:ASN:HD22	3:D:4194:GLN:H	1.29	0.79
3:D:3193:ASN:HD22	3:D:3194:GLN:H	1.29	0.79
1:E:1002:DT:H2'	1:E:1003:DT:C6	2.19	0.78
3:D:2068:GLU:HG2	3:D:3216:LYS:HB3	1.66	0.77
3:D:193:ASN:HD22	3:D:194:GLN:H	1.32	0.77
3:A:1068:GLU:HG2	3:A:2216:LYS:HB3	1.66	0.77
1:E:1002:DT:P	3:D:165:GLY:HA2	2.25	0.77
3:A:71:GLY:HA2	6:A:502:ADP:H5'1	1.66	0.76
3:A:111:ILE:HG22	3:A:1030:GLY:CA	2.14	0.76
3:A:4193:ASN:HD22	3:A:4194:GLN:H	1.32	0.75
3:A:3068:GLU:HG2	3:A:4216:LYS:HB3	1.66	0.75
3:D:111:ILE:HG22	3:D:1030:GLY:CA	2.19	0.73
3:A:68:GLU:HG2	3:A:1216:LYS:CB	2.17	0.72
3:A:3146:VAL:HA	3:A:3149:LEU:HD22	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:201:VAL:HA	3:D:203:PHE:CZ	2.29	0.67
3:D:1193:ASN:HD22	3:D:1194:GLN:N	1.91	0.67
3:D:2193:ASN:HD22	3:D:2194:GLN:N	1.92	0.66
3:D:4146:VAL:HA	3:D:4149:LEU:HD22	1.77	0.66
3:D:201:VAL:HA	3:D:203:PHE:CE1	2.30	0.66
3:D:3146:VAL:HA	3:D:3149:LEU:HD22	1.78	0.66
3:A:2193:ASN:HD22	3:A:2194:GLN:N	1.94	0.65
3:D:2160:GLY:H	3:D:3173:GLN:HE22	1.41	0.65
3:D:3076:THR:HG21	3:D:3142:VAL:HG21	1.78	0.65
3:A:2068:GLU:HG2	3:A:3216:LYS:CB	2.26	0.65
3:D:146:VAL:HA	3:D:149:LEU:HD22	1.78	0.65
3:D:2160:GLY:H	3:D:3173:GLN:NE2	1.95	0.65
3:A:193:ASN:HD22	3:A:194:GLN:N	1.94	0.65
3:D:4193:ASN:HD22	3:D:4194:GLN:N	1.95	0.65
3:D:3068:GLU:HG2	3:D:4216:LYS:CB	2.27	0.65
3:A:4146:VAL:HA	3:A:4149:LEU:HD22	1.78	0.65
3:A:2329:SER:O	3:A:2330:ASN:HB2	1.94	0.65
3:A:112:ASP:O	3:A:1028:ARG:HG2	1.97	0.64
3:A:1193:ASN:HD22	3:A:1194:GLN:N	1.95	0.64
3:A:3193:ASN:HD22	3:A:3194:GLN:N	1.94	0.64
3:A:146:VAL:HA	3:A:149:LEU:HD22	1.79	0.64
3:D:3193:ASN:OD1	3:D:3209:THR:HG23	1.98	0.64
3:A:1146:VAL:HA	3:A:1149:LEU:HD22	1.78	0.64
3:D:1111:ILE:HG22	3:D:2030:GLY:CA	2.26	0.64
3:A:2146:VAL:HA	3:A:2149:LEU:HD22	1.80	0.64
3:D:68:GLU:HG2	3:D:1216:LYS:CB	2.26	0.64
3:A:3193:ASN:OD1	3:A:3209:THR:HG23	1.99	0.63
3:A:111:ILE:HG22	3:A:1030:GLY:N	2.13	0.63
3:A:1071:GLY:HA2	6:A:1502:ADP:H5'1	1.79	0.63
3:D:193:ASN:OD1	3:D:209:THR:HG23	1.98	0.63
3:A:76:THR:HG21	3:A:142:VAL:HG21	1.80	0.63
1:E:1013:DT:C7	3:D:3197:MET:HG3	2.29	0.63
3:A:115:LEU:HD21	3:A:1014:LEU:HD21	1.81	0.63
3:D:2146:VAL:HA	3:D:2149:LEU:HD22	1.80	0.63
1:B:1007:DA:H5'	3:A:2212:GLY:HA2	1.80	0.63
1:E:1013:DT:H71	3:D:3197:MET:HG3	1.81	0.62
3:A:1076:THR:HG21	3:A:1142:VAL:HG21	1.81	0.62
3:D:3193:ASN:HD22	3:D:3194:GLN:N	1.96	0.62
3:A:4193:ASN:HD22	3:A:4194:GLN:N	1.97	0.62
3:D:2193:ASN:OD1	3:D:2209:THR:HG23	2.00	0.62
3:A:193:ASN:OD1	3:A:209:THR:HG23	2.00	0.62
3:D:4076:THR:HG21	3:D:4142:VAL:HG21	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:4193:ASN:OD1	3:D:4209:THR:HG23	1.99	0.62
3:D:1146:VAL:HA	3:D:1149:LEU:HD22	1.80	0.62
3:A:4076:THR:HG21	3:A:4142:VAL:HG21	1.82	0.61
3:A:4193:ASN:OD1	3:A:4209:THR:HG23	2.00	0.61
3:D:2124:GLN:HG3	3:D:3021:PHE:CD1	2.36	0.61
3:A:2160:GLY:H	3:A:3173:GLN:NE2	1.98	0.61
3:A:3076:THR:HG21	3:A:3142:VAL:HG21	1.82	0.61
3:D:1193:ASN:OD1	3:D:1209:THR:HG23	2.00	0.61
3:A:2330:ASN:H	3:A:2331:PRO:HD3	1.65	0.60
3:A:1193:ASN:OD1	3:A:1209:THR:HG23	2.02	0.60
3:D:111:ILE:HG22	3:D:1030:GLY:HA2	1.83	0.60
1:E:1003:DT:O2	3:D:199:ILE:HG22	2.00	0.60
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.84	0.60
3:A:2193:ASN:OD1	3:A:2209:THR:HG23	2.01	0.60
3:D:1076:THR:HG21	3:D:1142:VAL:HG21	1.82	0.60
3:A:3111:ILE:HG22	3:A:4030:GLY:CA	2.32	0.60
3:D:193:ASN:HD22	3:D:194:GLN:N	1.98	0.59
1:B:1002:DT:H2'	1:B:1003:DT:C6	2.38	0.59
3:A:4121:THR:HG22	3:A:4155:ILE:HD12	1.85	0.59
3:A:150:THR:HB	3:A:155:ILE:HD11	1.83	0.59
3:A:2160:GLY:H	3:A:3173:GLN:HE22	1.50	0.59
1:E:1010:DT:H5'	3:D:3212:GLY:HA2	1.84	0.59
3:D:2076:THR:HG21	3:D:2142:VAL:HG21	1.84	0.59
3:A:2076:THR:HG21	3:A:2142:VAL:HG21	1.85	0.59
3:D:2111:ILE:HG22	3:D:3030:GLY:CA	2.33	0.58
3:D:3328:LEU:HB2	3:D:3331:PRO:HG3	1.84	0.58
3:D:4198:LYS:HG2	3:D:4206:PRO:O	2.03	0.58
3:D:3111:ILE:HG23	3:D:4029:LEU:HD13	1.86	0.58
1:E:1007:DA:H5'	3:D:2212:GLY:HA2	1.86	0.58
3:D:202:MET:HG2	3:D:202:MET:O	2.03	0.57
3:A:4213:ASN:OD1	3:A:4216:LYS:HE2	2.04	0.57
3:D:3243:ARG:NH1	3:D:3259:GLU:OE2	2.37	0.57
3:D:1243:ARG:NH1	3:D:1259:GLU:OE2	2.38	0.57
3:D:213:ASN:OD1	3:D:216:LYS:HE2	2.05	0.57
3:D:2243:ARG:NH1	3:D:2259:GLU:OE2	2.38	0.57
3:D:1194:GLN:NE2	3:D:1196:ARG:HH12	1.99	0.57
3:A:1243:ARG:NH1	3:A:1259:GLU:OE2	2.38	0.56
1:E:1013:DT:H5'	3:D:4212:GLY:HA2	1.86	0.56
3:A:2329:SER:O	3:A:2330:ASN:CB	2.53	0.56
3:D:3213:ASN:OD1	3:D:3216:LYS:HE2	2.05	0.56
3:A:2213:ASN:OD1	3:A:2216:LYS:HE2	2.05	0.56
3:D:1160:GLY:H	3:D:2173:GLN:NE2	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:198:LYS:HG2	3:A:206:PRO:O	2.05	0.56
3:D:2213:ASN:OD1	3:D:2216:LYS:HE2	2.05	0.56
3:D:3222:ARG:HG3	3:D:3248:LYS:HB3	1.87	0.56
3:D:1213:ASN:OD1	3:D:1216:LYS:HE2	2.05	0.56
3:A:2149:LEU:HD23	3:A:2171:MET:HE1	1.87	0.56
3:D:3076:THR:CG2	3:D:3142:VAL:HG21	2.35	0.56
3:A:4243:ARG:NH1	3:A:4259:GLU:OE2	2.39	0.56
3:D:4213:ASN:OD1	3:D:4216:LYS:HE2	2.05	0.56
3:A:2194:GLN:NE2	3:A:2196:ARG:HH12	2.01	0.55
3:A:3222:ARG:HG3	3:A:3248:LYS:HB3	1.88	0.55
3:A:2304:ASN:ND2	3:D:2304:ASN:OD1	2.27	0.55
3:A:76:THR:CG2	3:A:142:VAL:HG21	2.37	0.55
3:A:3243:ARG:NH1	3:A:3259:GLU:OE2	2.39	0.55
3:D:2222:ARG:HG3	3:D:2248:LYS:HB3	1.89	0.55
3:A:3213:ASN:OD1	3:A:3216:LYS:HE2	2.07	0.55
1:E:1013:DT:H5"	3:D:4213:ASN:ND2	2.21	0.55
3:A:3076:THR:CG2	3:A:3142:VAL:HG21	2.36	0.55
3:D:1076:THR:CG2	3:D:1142:VAL:HG21	2.37	0.55
3:A:243:ARG:NH1	3:A:259:GLU:OE2	2.40	0.54
3:A:149:LEU:HD23	3:A:171:MET:HE1	1.90	0.54
3:A:1111:ILE:HG22	3:A:2030:GLY:CA	2.37	0.54
3:D:4243:ARG:NH1	3:D:4259:GLU:OE2	2.41	0.54
3:A:4076:THR:CG2	3:A:4142:VAL:HG21	2.38	0.54
1:E:1010:DT:C2	3:D:2199:ILE:HD12	2.43	0.54
3:D:4194:GLN:NE2	3:D:4196:ARG:HH12	2.00	0.54
3:D:1160:GLY:H	3:D:2173:GLN:HE22	1.56	0.54
3:A:4261:GLN:HB2	3:A:4269:ASN:HB3	1.89	0.54
3:D:149:LEU:HD23	3:D:171:MET:HE1	1.89	0.54
3:A:1076:THR:CG2	3:A:1142:VAL:HG21	2.37	0.54
3:D:4076:THR:CG2	3:D:4142:VAL:HG21	2.38	0.54
3:A:213:ASN:OD1	3:A:216:LYS:HE2	2.08	0.54
3:D:222:ARG:HG3	3:D:248:LYS:HB3	1.91	0.53
3:D:1068:GLU:HG2	3:D:2216:LYS:CB	2.37	0.53
3:D:243:ARG:NH1	3:D:259:GLU:OE2	2.41	0.53
3:A:2243:ARG:NH1	3:A:2259:GLU:OE2	2.40	0.53
3:A:111:ILE:HG22	3:A:1030:GLY:HA2	1.89	0.53
3:D:4222:ARG:HG3	3:D:4248:LYS:HB3	1.89	0.53
3:A:4206:PRO:HG3	3:D:2202:MET:HB3	1.90	0.53
3:A:1160:GLY:H	3:A:2173:GLN:NE2	2.06	0.53
3:A:1222:ARG:HG3	3:A:1248:LYS:HB3	1.90	0.53
3:A:1213:ASN:OD1	3:A:1216:LYS:HE2	2.07	0.53
3:A:222:ARG:HG3	3:A:248:LYS:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:2076:THR:CG2	3:D:2142:VAL:HG21	2.38	0.53
3:A:194:GLN:NE2	3:A:196:ARG:HH12	2.01	0.53
3:A:4222:ARG:HG3	3:A:4248:LYS:HB3	1.90	0.52
3:D:1222:ARG:HG3	3:D:1248:LYS:HB3	1.91	0.52
3:A:3206:PRO:HG3	3:D:3202:MET:CB	2.34	0.52
3:D:194:GLN:NE2	3:D:196:ARG:HH12	2.03	0.52
3:D:2149:LEU:HD23	3:D:2171:MET:HE1	1.90	0.52
3:A:4069:SER:HB3	6:A:4502:ADP:H3'	1.91	0.52
1:E:1013:DT:H73	3:D:3198:LYS:O	2.09	0.52
3:D:76:THR:CG2	3:D:142:VAL:HG21	2.39	0.52
3:D:1254:PRO:HG3	6:D:502:ADP:O2'	2.10	0.52
3:A:2222:ARG:HG3	3:A:2248:LYS:HB3	1.90	0.52
3:D:2194:GLN:NE2	3:D:2196:ARG:HH12	2.00	0.52
3:A:3124:GLN:HG3	3:A:4021:PHE:CD1	2.45	0.52
3:D:198:LYS:HG2	3:D:206:PRO:O	2.09	0.51
3:D:1194:GLN:HE22	3:D:1196:ARG:HH22	1.56	0.51
1:E:1007:DA:C6	3:D:1199:ILE:HG13	2.45	0.51
3:A:2076:THR:CG2	3:A:2142:VAL:HG21	2.39	0.51
3:A:3194:GLN:NE2	3:A:3196:ARG:HH12	2.01	0.50
3:A:2194:GLN:HE22	3:A:2196:ARG:HH22	1.59	0.50
1:E:1003:DT:H2'	3:D:197:MET:O	2.11	0.50
3:D:111:ILE:HG22	3:D:1030:GLY:N	2.27	0.50
3:D:4194:GLN:HE22	3:D:4196:ARG:HH22	1.58	0.50
3:A:101:PRO:HB3	3:A:1029:LEU:HD22	1.93	0.50
3:D:4069:SER:HA	6:D:4502:ADP:O3A	2.12	0.50
1:B:1009:DC:O2	3:A:3169:ARG:NH1	2.44	0.50
3:D:201:VAL:HG23	3:D:203:PHE:CD1	2.46	0.50
3:A:3194:GLN:HE22	3:A:3196:ARG:HH22	1.60	0.49
3:A:3160:GLY:H	3:A:4173:GLN:NE2	2.10	0.49
3:D:194:GLN:HE22	3:D:196:ARG:HH22	1.58	0.49
3:D:2068:GLU:HG2	3:D:3216:LYS:CB	2.40	0.49
3:D:2194:GLN:HE22	3:D:2196:ARG:HH22	1.58	0.49
3:A:194:GLN:HE22	3:A:196:ARG:HH22	1.59	0.49
3:A:1194:GLN:NE2	3:A:1196:ARG:HH12	2.00	0.49
1:B:1010:DT:H2'	1:B:1011:DT:C6	2.47	0.49
3:D:1182:LEU:HD11	3:D:1189:LEU:HD12	1.95	0.49
3:D:1194:GLN:HE21	3:D:1196:ARG:NH1	2.03	0.49
3:A:3111:ILE:HG22	3:A:4030:GLY:N	2.27	0.49
3:D:2101:PRO:HB3	3:D:3029:LEU:HD22	1.95	0.49
3:A:2124:GLN:HG3	3:A:3021:PHE:CD1	2.48	0.49
3:D:3261:GLN:HB2	3:D:3269:ASN:HB3	1.95	0.48
3:D:3194:GLN:HE22	3:D:3196:ARG:HH22	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1194:GLN:HE22	3:A:1196:ARG:HH22	1.59	0.48
3:A:1160:GLY:H	3:A:2173:GLN:HE22	1.62	0.48
3:A:182:LEU:HD11	3:A:189:LEU:HD12	1.96	0.48
3:A:3254:PRO:HG3	6:A:2502:ADP:O2'	2.13	0.48
3:D:1194:GLN:NE2	3:D:1196:ARG:HH22	2.12	0.48
3:D:1115:LEU:HD21	3:D:2014:LEU:HD21	1.95	0.48
3:A:1182:LEU:HD11	3:A:1189:LEU:HD12	1.95	0.48
3:D:137:ALA:HB1	3:D:1010:LEU:HB2	1.95	0.48
3:D:182:LEU:HD11	3:D:189:LEU:HD12	1.96	0.47
3:A:4194:GLN:NE2	3:A:4196:ARG:HH12	2.04	0.47
3:A:3160:GLY:H	3:A:4173:GLN:HE22	1.61	0.47
3:A:4282:LYS:HG3	3:D:1282:LYS:CG	2.40	0.47
3:A:1149:LEU:HD23	3:A:1171:MET:HE1	1.96	0.47
3:D:2194:GLN:NE2	3:D:2196:ARG:HH22	2.13	0.47
3:D:115:LEU:HD21	3:D:1014:LEU:HD21	1.97	0.47
3:D:4194:GLN:NE2	3:D:4196:ARG:HH22	2.13	0.47
3:A:4194:GLN:HE22	3:A:4196:ARG:HH22	1.61	0.47
3:D:194:GLN:NE2	3:D:196:ARG:HH22	2.11	0.47
3:A:111:ILE:CG2	3:A:1030:GLY:HA2	2.44	0.47
3:D:1149:LEU:HD23	3:D:1171:MET:HE1	1.95	0.47
3:A:2038:GLU:HA	3:A:2332:ASN:HD21	1.80	0.47
3:D:2182:LEU:HD11	3:D:2189:LEU:HD12	1.96	0.47
3:D:3149:LEU:HD23	3:D:3171:MET:HE1	1.96	0.47
3:D:2111:ILE:HG22	3:D:3030:GLY:N	2.30	0.47
3:A:4182:LEU:HD11	3:A:4189:LEU:HD12	1.95	0.47
3:D:2130:ASP:OD2	3:D:2134:ARG:NH1	2.47	0.47
3:D:1068:GLU:HA	5:D:1501:ALF:F1	2.05	0.46
3:A:3068:GLU:HG2	3:A:4216:LYS:CB	2.40	0.46
1:B:1011:DT:H2'	1:B:1012:DT:C6	2.50	0.46
3:D:3182:LEU:HD11	3:D:3189:LEU:HD12	1.97	0.46
3:A:3149:LEU:HD23	3:A:3171:MET:HE1	1.96	0.46
1:E:1011:DT:H2'	1:E:1012:DT:C6	2.50	0.46
3:A:2194:GLN:HE21	3:A:2196:ARG:NH1	2.04	0.46
3:D:3194:GLN:NE2	3:D:3196:ARG:HH12	2.02	0.46
3:D:4182:LEU:HD11	3:D:4189:LEU:HD12	1.97	0.46
3:A:3112:ASP:O	3:A:4028:ARG:HG2	2.16	0.46
3:A:3111:ILE:HG23	3:A:4029:LEU:HD13	1.98	0.46
3:A:3111:ILE:HG22	3:A:4030:GLY:HA2	1.98	0.46
1:E:1006:DC:H5'	3:D:2169:ARG:HA	1.97	0.46
3:A:194:GLN:NE2	3:A:196:ARG:HH22	2.13	0.45
3:A:2194:GLN:NE2	3:A:2196:ARG:HH22	2.14	0.45
3:A:3080:ILE:HD11	3:A:3142:VAL:CG1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1010:DT:C2	3:A:2199:ILE:HD12	2.51	0.45
3:D:1111:ILE:HG22	3:D:2030:GLY:HA2	1.96	0.45
3:A:111:ILE:HG23	3:A:1029:LEU:HB3	1.98	0.45
3:D:1111:ILE:HG22	3:D:2030:GLY:N	2.31	0.45
1:E:1013:DT:H72	3:D:3197:MET:HG3	1.99	0.45
3:A:159:ILE:HG12	3:A:1177:LYS:HD3	1.98	0.45
3:D:111:ILE:CG2	3:D:1030:GLY:HA2	2.47	0.45
3:D:3263:LEU:HG	3:D:3269:ASN:HB2	1.99	0.45
1:B:1013:DT:H5'	3:A:4212:GLY:HA2	1.97	0.45
3:A:2182:LEU:HD11	3:A:2189:LEU:HD12	1.99	0.45
3:A:2111:ILE:HG22	3:A:3030:GLY:CA	2.46	0.45
3:D:4149:LEU:HD23	3:D:4171:MET:HE1	1.99	0.45
3:A:2130:ASP:OD2	3:A:2134:ARG:NH1	2.50	0.45
3:D:4177:LYS:HB3	3:D:4177:LYS:HE2	1.82	0.45
3:D:149:LEU:HD23	3:D:171:MET:CE	2.47	0.45
1:E:1013:DT:H71	3:D:3197:MET:CG	2.45	0.44
3:A:1194:GLN:NE2	3:A:1196:ARG:HH22	2.14	0.44
3:A:4194:GLN:NE2	3:A:4196:ARG:HH22	2.14	0.44
3:A:4154:GLU:C	3:A:4156:GLU:H	2.19	0.44
3:A:2149:LEU:HD23	3:A:2171:MET:CE	2.47	0.44
3:D:130:ASP:OD2	3:D:134:ARG:NH1	2.50	0.44
3:A:1130:ASP:OD2	3:A:1134:ARG:NH1	2.51	0.44
3:A:3182:LEU:HD11	3:A:3189:LEU:HD12	1.99	0.44
1:E:1007:DA:C5'	3:D:2212:GLY:HA2	2.47	0.44
3:D:2149:LEU:HD23	3:D:2171:MET:CE	2.48	0.44
3:D:194:GLN:HE21	3:D:196:ARG:NH1	2.05	0.43
3:D:1080:ILE:HD11	3:D:1142:VAL:CG1	2.48	0.43
3:D:1130:ASP:OD2	3:D:1134:ARG:NH1	2.51	0.43
3:A:1111:ILE:HG22	3:A:2030:GLY:HA2	2.01	0.43
3:D:4254:PRO:HG3	6:D:3502:ADP:O2'	2.18	0.43
3:D:3202:MET:HG2	3:D:3202:MET:H	1.66	0.43
3:A:3101:PRO:HB3	3:A:4029:LEU:HD22	1.99	0.43
3:A:2177:LYS:HB3	3:A:2177:LYS:HE2	1.83	0.43
3:A:130:ASP:OD2	3:A:134:ARG:NH1	2.51	0.43
3:D:3130:ASP:OD2	3:D:3134:ARG:NH1	2.51	0.43
3:D:3080:ILE:HD11	3:D:3142:VAL:CG1	2.48	0.43
3:D:1149:LEU:HD23	3:D:1171:MET:CE	2.48	0.43
3:A:2243:ARG:HG3	3:A:2259:GLU:HG2	2.00	0.43
3:A:3130:ASP:OD2	3:A:3134:ARG:NH1	2.51	0.43
3:D:2194:GLN:HE21	3:D:2196:ARG:NH1	2.04	0.43
3:D:3194:GLN:NE2	3:D:3196:ARG:HH22	2.16	0.43
3:D:4149:LEU:HD23	3:D:4171:MET:CE	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:3194:GLN:NE2	3:A:3196:ARG:HH22	2.15	0.43
3:A:1149:LEU:HD23	3:A:1171:MET:CE	2.48	0.43
3:A:4149:LEU:HD23	3:A:4171:MET:CE	2.49	0.43
3:A:3182:LEU:HD23	3:A:3187:THR:HB	2.00	0.43
3:D:4194:GLN:HE21	3:D:4196:ARG:NH1	2.03	0.43
3:D:2111:ILE:HG22	3:D:3030:GLY:HA2	2.01	0.43
3:D:2039:THR:HG23	3:D:2332:ASN:HD21	1.84	0.43
3:A:4080:ILE:HD11	3:A:4142:VAL:CG1	2.49	0.43
3:D:2243:ARG:HG3	3:D:2259:GLU:HG2	2.01	0.42
3:A:137:ALA:HB1	3:A:1010:LEU:HB2	2.00	0.42
3:A:1198:LYS:HG2	3:A:1206:PRO:O	2.19	0.42
3:D:3124:GLN:HG3	3:D:4021:PHE:CD1	2.54	0.42
3:D:3198:LYS:HG2	3:D:3206:PRO:O	2.20	0.42
3:D:1076:THR:HG22	3:D:1077:LEU:N	2.34	0.42
3:D:3159:ILE:HD13	3:D:4126:LEU:HB3	2.02	0.42
3:A:3202:MET:H	3:A:3202:MET:HG2	1.65	0.42
1:E:1013:DT:C7	3:D:3198:LYS:O	2.67	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:CG1	2.48	0.42
3:A:2071:GLY:HA2	6:A:2502:ADP:H5'1	2.02	0.42
3:D:4130:ASP:OD2	3:D:4134:ARG:NH1	2.52	0.42
3:A:4095:ALA:O	3:A:4097:HIS:HD2	2.03	0.42
3:A:4130:ASP:OD2	3:A:4134:ARG:NH1	2.53	0.42
3:D:1243:ARG:HG3	3:D:1259:GLU:HG2	2.01	0.42
3:A:1243:ARG:HG3	3:A:1259:GLU:HG2	2.02	0.42
3:A:2182:LEU:HD23	3:A:2187:THR:HB	2.02	0.42
3:D:3194:GLN:HE21	3:D:3196:ARG:NH1	2.06	0.42
3:A:1068:GLU:HG2	3:A:2216:LYS:CB	2.43	0.42
3:A:149:LEU:HD23	3:A:171:MET:CE	2.48	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:HG13	2.02	0.42
3:A:2198:LYS:HG2	3:A:2206:PRO:O	2.20	0.41
3:A:3177:LYS:HB3	3:A:3177:LYS:HE2	1.82	0.41
3:A:80:ILE:HD11	3:A:142:VAL:CG1	2.50	0.41
3:D:4023:LYS:H	3:D:4023:LYS:HG2	1.74	0.41
3:A:3149:LEU:HD23	3:A:3171:MET:CE	2.50	0.41
3:D:3149:LEU:HD23	3:D:3171:MET:CE	2.50	0.41
3:D:71:GLY:HA2	6:D:502:ADP:H5'1	2.03	0.41
3:A:3080:ILE:HD11	3:A:3142:VAL:HG13	2.02	0.41
1:B:1003:DT:H2'	3:A:197:MET:O	2.20	0.41
3:A:243:ARG:HG3	3:A:259:GLU:HG2	2.02	0.41
3:D:4243:ARG:HG3	3:D:4259:GLU:HG2	2.03	0.41
3:D:2182:LEU:HD23	3:D:2187:THR:HB	2.01	0.41
3:A:1202:MET:H	3:A:1202:MET:HG2	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:3080:ILE:HD11	3:D:3142:VAL:HG13	2.02	0.41
3:A:177:LYS:HB3	3:A:177:LYS:HE2	1.85	0.41
3:D:4080:ILE:HD11	3:D:4142:VAL:CG1	2.50	0.41
3:D:1080:ILE:HD11	3:D:1142:VAL:HG13	2.02	0.41
3:A:2080:ILE:HD11	3:A:2142:VAL:CG1	2.50	0.41
3:D:3243:ARG:HG3	3:D:3259:GLU:HG2	2.02	0.41
3:A:182:LEU:HD23	3:A:187:THR:HB	2.03	0.41
3:D:1202:MET:HG2	3:D:1202:MET:H	1.65	0.41
3:D:1177:LYS:HB3	3:D:1177:LYS:HE2	1.84	0.41
3:D:3068:GLU:HA	5:D:3501:ALF:F1	2.11	0.41
3:A:2330:ASN:N	3:A:2331:PRO:HD3	2.35	0.41
3:A:2254:PRO:HG3	6:A:1502:ADP:O2'	2.21	0.41
3:D:2076:THR:HG22	3:D:2077:LEU:N	2.36	0.41
3:D:1182:LEU:HD23	3:D:1187:THR:HB	2.03	0.41
3:D:3155:ILE:HA	3:D:4177:LYS:HE3	2.03	0.41
3:A:4080:ILE:HD11	3:A:4142:VAL:HG13	2.03	0.40
3:A:3243:ARG:HG3	3:A:3259:GLU:HG2	2.04	0.40
3:A:1076:THR:HG22	3:A:1077:LEU:N	2.36	0.40
3:D:4182:LEU:HD23	3:D:4187:THR:HB	2.03	0.40
3:A:3115:LEU:HD21	3:A:4014:LEU:HD21	2.02	0.40
3:D:201:VAL:HG23	3:D:203:PHE:CE1	2.57	0.40
3:D:2146:VAL:O	3:D:2149:LEU:HB2	2.22	0.40
3:D:3182:LEU:HD23	3:D:3187:THR:HB	2.03	0.40
3:A:2033:ARG:NE	3:A:2033:ARG:HA	2.37	0.40
3:A:2282:LYS:HG3	3:D:3282:LYS:HG3	2.01	0.40
3:A:4149:LEU:HD23	3:A:4171:MET:HE1	2.01	0.40
3:A:4243:ARG:HG3	3:A:4259:GLU:HG2	2.02	0.40
3:A:2199:ILE:HD11	3:A:3164:MET:HE3	2.03	0.40
3:D:1101:PRO:HB3	3:D:2029:LEU:HD22	2.04	0.40
1:B:1010:DT:H5'	3:A:3212:GLY:HA2	2.04	0.40
3:D:2198:LYS:HG2	3:D:2206:PRO:O	2.22	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:218:TYR:OH	3:D:4087:GLY:O[4_456]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1595/1706 (94%)	1549 (97%)	33 (2%)	13 (1%)	27	77
3	D	1595/1706 (94%)	1539 (96%)	43 (3%)	13 (1%)	27	77
All	All	3190/3412 (94%)	3088 (97%)	76 (2%)	26 (1%)	27	77

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1023	LYS
3	A	2023	LYS
3	A	2330	ASN
3	A	3023	LYS
3	A	4023	LYS
3	D	1023	LYS
3	D	2023	LYS
3	D	3023	LYS
3	D	4023	LYS
3	D	1332	ASN
3	D	3269	ASN
3	D	332	ASN
3	D	2332	ASN
3	A	234	GLY
3	A	1234	GLY
3	A	2234	GLY
3	A	3234	GLY
3	A	3332	ASN
3	A	4234	GLY
3	A	4269	ASN
3	D	234	GLY
3	D	1234	GLY
3	D	2234	GLY
3	D	3234	GLY
3	D	4234	GLY
3	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	
3	A	1267/1339 (95%)	1142 (90%)	125 (10%)	11	42
3	D	1267/1339 (95%)	1136 (90%)	131 (10%)	10	40
All	All	2534/2678 (95%)	2278 (90%)	256 (10%)	11	41

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	47	LEU
3	A	68	GLU
3	A	76	THR
3	A	85	ARG
3	A	114	LEU
3	A	140	VAL
3	A	142	VAL
3	A	146	VAL
3	A	149	LEU
3	A	166	LEU
3	A	183	LYS
3	A	189	LEU
3	A	193	ASN
3	A	205	ASN
3	A	208	THR
3	A	209	THR
3	A	210	THR
3	A	223	LEU
3	A	251	ILE
3	A	285	GLU
3	A	311	ASP
3	A	314	GLU
3	A	1028	ARG
3	A	1029	LEU
3	A	1047	LEU
3	A	1068	GLU
3	A	1076	THR
3	A	1085	ARG
3	A	1114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1140	VAL
3	A	1142	VAL
3	A	1146	VAL
3	A	1149	LEU
3	A	1166	LEU
3	A	1183	LYS
3	A	1189	LEU
3	A	1193	ASN
3	A	1199	ILE
3	A	1202	MET
3	A	1205	ASN
3	A	1208	THR
3	A	1209	THR
3	A	1210	THR
3	A	1223	LEU
3	A	1251	ILE
3	A	1285	GLU
3	A	1311	ASP
3	A	1314	GLU
3	A	2028	ARG
3	A	2029	LEU
3	A	2047	LEU
3	A	2068	GLU
3	A	2076	THR
3	A	2085	ARG
3	A	2114	LEU
3	A	2140	VAL
3	A	2142	VAL
3	A	2146	VAL
3	A	2149	LEU
3	A	2166	LEU
3	A	2183	LYS
3	A	2189	LEU
3	A	2193	ASN
3	A	2199	ILE
3	A	2202	MET
3	A	2205	ASN
3	A	2208	THR
3	A	2209	THR
3	A	2210	THR
3	A	2223	LEU
3	A	2251	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2285	GLU
3	A	2311	ASP
3	A	2314	GLU
3	A	3028	ARG
3	A	3029	LEU
3	A	3047	LEU
3	A	3068	GLU
3	A	3076	THR
3	A	3085	ARG
3	A	3114	LEU
3	A	3140	VAL
3	A	3142	VAL
3	A	3146	VAL
3	A	3149	LEU
3	A	3166	LEU
3	A	3183	LYS
3	A	3189	LEU
3	A	3193	ASN
3	A	3199	ILE
3	A	3202	MET
3	A	3205	ASN
3	A	3208	THR
3	A	3209	THR
3	A	3210	THR
3	A	3223	LEU
3	A	3251	ILE
3	A	3285	GLU
3	A	3311	ASP
3	A	3314	GLU
3	A	4028	ARG
3	A	4029	LEU
3	A	4047	LEU
3	A	4068	GLU
3	A	4076	THR
3	A	4085	ARG
3	A	4114	LEU
3	A	4140	VAL
3	A	4142	VAL
3	A	4146	VAL
3	A	4149	LEU
3	A	4155	ILE
3	A	4166	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	4183	LYS
3	A	4189	LEU
3	A	4193	ASN
3	A	4205	ASN
3	A	4208	THR
3	A	4209	THR
3	A	4210	THR
3	A	4223	LEU
3	A	4251	ILE
3	A	4285	GLU
3	A	4311	ASP
3	A	4314	GLU
3	D	47	LEU
3	D	68	GLU
3	D	76	THR
3	D	85	ARG
3	D	114	LEU
3	D	140	VAL
3	D	142	VAL
3	D	146	VAL
3	D	149	LEU
3	D	164	MET
3	D	166	LEU
3	D	183	LYS
3	D	189	LEU
3	D	193	ASN
3	D	202	MET
3	D	203	PHE
3	D	205	ASN
3	D	208	THR
3	D	209	THR
3	D	210	THR
3	D	223	LEU
3	D	251	ILE
3	D	285	GLU
3	D	311	ASP
3	D	314	GLU
3	D	1028	ARG
3	D	1029	LEU
3	D	1047	LEU
3	D	1068	GLU
3	D	1076	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1085	ARG
3	D	1114	LEU
3	D	1140	VAL
3	D	1142	VAL
3	D	1146	VAL
3	D	1149	LEU
3	D	1166	LEU
3	D	1183	LYS
3	D	1189	LEU
3	D	1193	ASN
3	D	1199	ILE
3	D	1202	MET
3	D	1205	ASN
3	D	1208	THR
3	D	1209	THR
3	D	1210	THR
3	D	1223	LEU
3	D	1251	ILE
3	D	1285	GLU
3	D	1311	ASP
3	D	1314	GLU
3	D	1332	ASN
3	D	2028	ARG
3	D	2029	LEU
3	D	2047	LEU
3	D	2068	GLU
3	D	2076	THR
3	D	2085	ARG
3	D	2114	LEU
3	D	2140	VAL
3	D	2142	VAL
3	D	2146	VAL
3	D	2149	LEU
3	D	2166	LEU
3	D	2183	LYS
3	D	2189	LEU
3	D	2193	ASN
3	D	2199	ILE
3	D	2202	MET
3	D	2205	ASN
3	D	2208	THR
3	D	2209	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	2210	THR
3	D	2223	LEU
3	D	2251	ILE
3	D	2285	GLU
3	D	2311	ASP
3	D	2314	GLU
3	D	2332	ASN
3	D	3028	ARG
3	D	3029	LEU
3	D	3047	LEU
3	D	3068	GLU
3	D	3076	THR
3	D	3085	ARG
3	D	3114	LEU
3	D	3140	VAL
3	D	3142	VAL
3	D	3146	VAL
3	D	3149	LEU
3	D	3166	LEU
3	D	3183	LYS
3	D	3189	LEU
3	D	3193	ASN
3	D	3199	ILE
3	D	3202	MET
3	D	3205	ASN
3	D	3208	THR
3	D	3209	THR
3	D	3210	THR
3	D	3223	LEU
3	D	3251	ILE
3	D	3285	GLU
3	D	3311	ASP
3	D	3314	GLU
3	D	3329	SER
3	D	4028	ARG
3	D	4029	LEU
3	D	4047	LEU
3	D	4068	GLU
3	D	4076	THR
3	D	4085	ARG
3	D	4114	LEU
3	D	4140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	4142	VAL
3	D	4146	VAL
3	D	4149	LEU
3	D	4164	MET
3	D	4166	LEU
3	D	4183	LYS
3	D	4189	LEU
3	D	4193	ASN
3	D	4205	ASN
3	D	4208	THR
3	D	4209	THR
3	D	4210	THR
3	D	4223	LEU
3	D	4251	ILE
3	D	4285	GLU
3	D	4311	ASP
3	D	4314	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	97	HIS
3	A	181	ASN
3	A	193	ASN
3	A	194	GLN
3	A	205	ASN
3	A	300	GLN
3	A	304	ASN
3	A	1097	HIS
3	A	1173	GLN
3	A	1181	ASN
3	A	1193	ASN
3	A	1194	GLN
3	A	1205	ASN
3	A	1300	GLN
3	A	1304	ASN
3	A	2097	HIS
3	A	2173	GLN
3	A	2181	ASN
3	A	2193	ASN
3	A	2194	GLN
3	A	2300	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2304	ASN
3	A	2332	ASN
3	A	3097	HIS
3	A	3173	GLN
3	A	3181	ASN
3	A	3193	ASN
3	A	3194	GLN
3	A	3205	ASN
3	A	3300	GLN
3	A	3304	ASN
3	A	4097	HIS
3	A	4173	GLN
3	A	4181	ASN
3	A	4193	ASN
3	A	4194	GLN
3	A	4205	ASN
3	A	4300	GLN
3	A	4304	ASN
3	D	97	HIS
3	D	181	ASN
3	D	193	ASN
3	D	194	GLN
3	D	205	ASN
3	D	300	GLN
3	D	304	ASN
3	D	332	ASN
3	D	1097	HIS
3	D	1173	GLN
3	D	1181	ASN
3	D	1193	ASN
3	D	1194	GLN
3	D	1205	ASN
3	D	1300	GLN
3	D	1304	ASN
3	D	1332	ASN
3	D	2097	HIS
3	D	2173	GLN
3	D	2181	ASN
3	D	2193	ASN
3	D	2194	GLN
3	D	2205	ASN
3	D	2300	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	2304	ASN
3	D	3097	HIS
3	D	3173	GLN
3	D	3181	ASN
3	D	3193	ASN
3	D	3194	GLN
3	D	3205	ASN
3	D	3300	GLN
3	D	3304	ASN
3	D	4097	HIS
3	D	4173	GLN
3	D	4181	ASN
3	D	4184	GLN
3	D	4193	ASN
3	D	4194	GLN
3	D	4205	ASN
3	D	4300	GLN
3	D	4304	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ALF	A	1501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	A	1502	4	29,29,29	1.14	2 (6%)	45,45,45	2.00	12 (26%)
5	ALF	A	2501	-	4,4,4	1.85	0	0,6,6	0.00	-
6	ADP	A	2502	4	29,29,29	1.13	2 (6%)	45,45,45	1.78	11 (24%)
5	ALF	A	3501	-	4,4,4	1.83	0	0,6,6	0.00	-
6	ADP	A	3502	4	29,29,29	1.28	4 (13%)	45,45,45	1.81	9 (20%)
5	ALF	A	4501	-	4,4,4	1.90	0	0,6,6	0.00	-
6	ADP	A	4502	4	29,29,29	1.25	3 (10%)	45,45,45	1.75	8 (17%)
5	ALF	A	501	-	4,4,4	1.90	0	0,6,6	0.00	-
6	ADP	A	502	4	29,29,29	1.09	2 (6%)	45,45,45	1.87	9 (20%)
5	ALF	D	1501	-	4,4,4	1.82	0	0,6,6	0.00	-
6	ADP	D	1502	4	29,29,29	1.12	2 (6%)	45,45,45	1.92	11 (24%)
5	ALF	D	2501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	D	2502	4	29,29,29	1.20	3 (10%)	45,45,45	1.76	8 (17%)
5	ALF	D	3501	-	4,4,4	1.77	0	0,6,6	0.00	-
6	ADP	D	3502	4	29,29,29	1.19	2 (6%)	45,45,45	1.82	7 (15%)
5	ALF	D	4501	-	4,4,4	1.91	1 (25%)	0,6,6	0.00	-
6	ADP	D	4502	4	29,29,29	1.20	3 (10%)	45,45,45	1.79	11 (24%)
5	ALF	D	501	-	4,4,4	1.81	0	0,6,6	0.00	-
6	ADP	D	502	4	29,29,29	1.13	2 (6%)	45,45,45	1.75	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ALF	A	1501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	1502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	2501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	2502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	3501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	3502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	4501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	4502	4	-	0/16/32/32	0/1/3/3
5	ALF	A	501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	502	4	-	0/16/32/32	0/1/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ALF	D	1501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	1502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	2501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	2502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	3501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	3502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	4501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	4502	4	-	0/16/32/32	0/1/3/3
5	ALF	D	501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	502	4	-	0/16/32/32	0/1/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2502	ADP	C5-C4	3.63	1.48	1.40
6	D	4502	ADP	C5-C4	3.63	1.48	1.40
6	A	3502	ADP	C4-N9	-3.51	1.32	1.37
6	A	502	ADP	C5-C4	3.41	1.48	1.40
6	A	2502	ADP	C4-N9	-3.34	1.32	1.37
6	A	4502	ADP	C5-C4	3.32	1.48	1.40
6	D	3502	ADP	C4-N9	-3.32	1.32	1.37
6	A	1502	ADP	C4-N9	-3.29	1.33	1.37
6	D	502	ADP	C4-N9	-3.20	1.33	1.37
6	D	3502	ADP	C5-C4	3.18	1.47	1.40
6	A	2502	ADP	C5-C4	3.11	1.47	1.40
6	D	502	ADP	C5-C4	3.07	1.47	1.40
6	D	1502	ADP	C4-N9	-3.01	1.33	1.37
6	D	2502	ADP	C4-N9	-2.99	1.33	1.37
6	A	3502	ADP	C5-C4	2.98	1.47	1.40
6	A	1502	ADP	C5-C4	2.95	1.47	1.40
6	D	4502	ADP	C4-N9	-2.92	1.33	1.37
6	A	4502	ADP	C4-N9	-2.86	1.33	1.37
6	A	3502	ADP	PB-O3A	2.67	1.64	1.60
6	D	1502	ADP	C5-C4	2.66	1.46	1.40
6	A	502	ADP	C4-N9	-2.61	1.33	1.37
6	A	3502	ADP	PA-O3A	2.48	1.64	1.59
6	A	4502	ADP	PA-O3A	2.18	1.63	1.59
6	D	4502	ADP	PA-O3A	2.15	1.63	1.59
6	D	2502	ADP	PA-O3A	2.09	1.63	1.59
5	D	4501	ALF	F4-AL	2.05	1.80	1.58

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	ADP	N3-C2-N1	-7.63	122.33	128.71
6	D	2502	ADP	N3-C2-N1	-7.09	122.78	128.71
6	A	3502	ADP	N3-C2-N1	-6.96	122.89	128.71
6	D	4502	ADP	N3-C2-N1	-6.55	123.24	128.71
6	A	4502	ADP	N3-C2-N1	-6.51	123.26	128.71
6	D	1502	ADP	N3-C2-N1	-6.15	123.57	128.71
6	A	502	ADP	N3-C2-N1	-6.05	123.65	128.71
6	D	1502	ADP	N3-C4-N9	5.65	135.63	125.43
6	D	3502	ADP	N3-C2-N1	-5.57	124.05	128.71
6	A	2502	ADP	N3-C2-N1	-5.46	124.15	128.71
6	D	3502	ADP	O4'-C1'-N9	5.43	113.49	108.44
6	A	1502	ADP	N3-C4-N9	5.41	135.20	125.43
6	A	502	ADP	N3-C4-N9	5.39	135.16	125.43
6	A	4502	ADP	N3-C4-N9	5.36	135.12	125.43
6	D	3502	ADP	N3-C4-N9	5.28	134.96	125.43
6	A	3502	ADP	N3-C4-N9	5.10	134.64	125.43
6	A	2502	ADP	N3-C4-N9	5.07	134.59	125.43
6	D	502	ADP	N3-C4-N9	5.00	134.46	125.43
6	D	4502	ADP	N3-C4-N9	4.95	134.37	125.43
6	D	2502	ADP	N3-C4-N9	4.74	133.98	125.43
6	D	502	ADP	N3-C2-N1	-4.64	124.83	128.71
6	D	502	ADP	O4'-C1'-N9	4.43	112.56	108.44
6	A	3502	ADP	O4'-C1'-N9	4.09	112.24	108.44
6	D	1502	ADP	O4'-C1'-N9	4.04	112.20	108.44
6	A	502	ADP	PA-O3A-PB	-4.04	119.84	131.68
6	A	2502	ADP	O4'-C1'-N9	3.51	111.70	108.44
6	D	1502	ADP	C5-C4-N3	-3.27	118.57	125.70
6	A	2502	ADP	PA-O3A-PB	-3.21	122.26	131.68
6	A	1502	ADP	C8-N9-C4	3.17	109.32	106.90
6	D	3502	ADP	C2'-C1'-N9	-3.11	105.27	113.27
6	D	502	ADP	C5-C4-N3	-3.08	119.00	125.70
6	D	502	ADP	C4-C5-N7	-3.03	106.92	109.52
6	A	4502	ADP	C5-C4-N3	-2.96	119.26	125.70
6	D	3502	ADP	C5-C4-N3	-2.92	119.34	125.70
6	A	502	ADP	C8-N9-C4	2.92	109.12	106.90
6	D	2502	ADP	C2-N1-C6	2.90	124.01	118.77
6	A	502	ADP	C5-C4-N3	-2.88	119.44	125.70
6	A	502	ADP	O4'-C1'-N9	2.82	111.06	108.44
6	A	2502	ADP	C5-C4-N3	-2.80	119.61	125.70
6	D	1502	ADP	C2'-C1'-N9	-2.79	106.10	113.27
6	A	1502	ADP	C5-C4-N3	-2.74	119.73	125.70
6	A	1502	ADP	PA-O3A-PB	-2.73	123.67	131.68
6	A	4502	ADP	C4-C5-N7	-2.69	107.21	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	4502	ADP	C8-N9-C4	2.66	108.93	106.90
6	A	4502	ADP	O2B-PB-O1B	2.65	119.11	110.44
6	D	1502	ADP	O2B-PB-O1B	2.65	119.09	110.44
6	A	1502	ADP	O4'-C1'-N9	2.64	110.89	108.44
6	A	3502	ADP	C5-C4-N3	-2.62	120.00	125.70
6	A	2502	ADP	C3'-C2'-C1'	2.59	104.96	100.91
6	D	1502	ADP	C8-N9-C4	2.58	108.87	106.90
6	A	4502	ADP	C8-N9-C4	2.57	108.86	106.90
6	D	1502	ADP	C4-C5-N7	-2.57	107.32	109.52
6	D	4502	ADP	C2-N1-C6	2.56	123.39	118.77
6	A	2502	ADP	C2'-C1'-N9	-2.55	106.72	113.27
6	D	2502	ADP	C8-N9-C4	2.55	108.84	106.90
6	D	4502	ADP	C5-C4-N3	-2.50	120.27	125.70
6	A	1502	ADP	C2'-C1'-N9	-2.49	106.87	113.27
6	A	502	ADP	C3'-C2'-C1'	2.48	104.79	100.91
6	A	1502	ADP	N6-C6-N1	2.48	124.22	119.36
6	A	1502	ADP	C2-N3-C4	2.47	121.04	114.01
6	D	4502	ADP	C3'-C2'-C1'	2.46	104.75	100.91
6	A	3502	ADP	C8-N9-C4	2.46	108.78	106.90
6	A	2502	ADP	O2B-PB-O1B	2.45	118.47	110.44
6	D	1502	ADP	C2-N3-C4	2.40	120.84	114.01
6	D	2502	ADP	C2'-C1'-N9	-2.36	107.21	113.27
6	D	4502	ADP	O3B-PB-O2B	2.34	116.73	107.61
6	A	3502	ADP	C2-N1-C6	2.34	123.00	118.77
6	D	502	ADP	C3'-C2'-C1'	2.33	104.56	100.91
6	D	502	ADP	C2'-C1'-N9	-2.28	107.40	113.27
6	D	2502	ADP	C5-C4-N3	-2.27	120.75	125.70
6	A	502	ADP	C4-C5-N7	-2.27	107.58	109.52
6	A	2502	ADP	C4-C5-N7	-2.26	107.59	109.52
6	A	502	ADP	C2-N3-C4	2.26	120.43	114.01
6	D	502	ADP	O2B-PB-O1B	2.22	117.68	110.44
6	D	1502	ADP	C3'-C2'-C1'	2.21	104.37	100.91
6	D	502	ADP	PA-O3A-PB	-2.20	125.22	131.68
6	A	2502	ADP	C8-N9-C4	2.20	108.58	106.90
6	A	1502	ADP	C3'-C2'-C1'	2.18	104.31	100.91
6	A	3502	ADP	O2B-PB-O1B	2.17	117.53	110.44
6	D	4502	ADP	O4'-C1'-N9	2.15	110.44	108.44
6	A	4502	ADP	C2-N3-C4	2.15	120.12	114.01
6	D	4502	ADP	PA-O3A-PB	-2.13	125.44	131.68
6	D	1502	ADP	N6-C6-N1	2.13	123.54	119.36
6	D	2502	ADP	PA-O3A-PB	-2.10	125.52	131.68
6	D	2502	ADP	O4'-C1'-N9	2.10	110.39	108.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3502	ADP	PA-O3A-PB	-2.08	125.59	131.68
6	A	4502	ADP	C2-N1-C6	2.07	122.52	118.77
6	A	3502	ADP	C2'-C1'-N9	-2.07	107.94	113.27
6	A	1502	ADP	O3B-PB-O2B	2.07	115.68	107.61
6	D	4502	ADP	C2'-C1'-N9	-2.07	107.96	113.27
6	A	3502	ADP	C2-N3-C4	2.06	119.87	114.01
6	A	2502	ADP	C2-N3-C4	2.03	119.79	114.01
6	D	4502	ADP	C4-C5-N7	-2.03	107.78	109.52
6	A	1502	ADP	C2-N1-C6	2.02	122.42	118.77
6	D	3502	ADP	C2-N3-C4	2.01	119.73	114.01
6	D	502	ADP	C2-N3-C4	2.01	119.72	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	B	12/15 (80%)	-0.08	0	100	100	37, 42, 48, 48	0
1	E	12/15 (80%)	-0.08	0	100	100	38, 47, 53, 62	0
2	C	6/6 (100%)	0.19	0	100	100	46, 48, 63, 66	1 (16%)
2	F	6/6 (100%)	0.12	0	100	100	48, 50, 55, 56	1 (16%)
3	A	1609/1706 (94%)	0.08	12 (0%)	84	35	39, 49, 64, 96	0
3	D	1609/1706 (94%)	-0.00	9 (0%)	86	39	39, 49, 65, 96	0
All	All	3254/3454 (94%)	0.04	21 (0%)	86	39	37, 49, 64, 96	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	4164	MET	3.3
3	A	2202	MET	2.7
3	D	4295	GLY	2.7
3	A	1287	ALA	2.7
3	D	2001	ALA	2.7
3	A	1289	ALA	2.6
3	A	37	VAL	2.5
3	A	1202	MET	2.5
3	A	282	LYS	2.4
3	A	60	ARG	2.3
3	D	4291	TYR	2.3
3	D	4297	LYS	2.3
3	A	1297	LYS	2.3
3	D	4001	ALA	2.3
3	A	4155	ILE	2.2
3	D	3202	MET	2.2
3	A	331	PRO	2.1
3	D	2002	ILE	2.1
3	D	4282	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	4152	LYS	2.0
3	A	3204	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	1500	1/1	0.46	12.95	38,38,38,38	0
4	MG	D	1500	1/1	0.41	4.99	28,28,28,28	0
4	MG	D	2500	1/1	0.56	3.07	32,32,32,32	0
4	MG	A	500	1/1	0.43	2.85	44,44,44,44	0
4	MG	D	500	1/1	0.38	2.72	34,34,34,34	0
4	MG	A	4500	1/1	0.23	2.64	32,32,32,32	0
4	MG	A	2500	1/1	0.42	1.96	25,25,25,25	0
4	MG	A	3500	1/1	0.41	1.78	27,27,27,27	0
4	MG	D	3500	1/1	0.35	1.26	31,31,31,31	0
5	ALF	A	1501	5/5	0.31	1.06	35,35,38,41	0
5	ALF	D	3501	5/5	0.27	0.43	27,29,33,33	0
5	ALF	A	501	5/5	0.29	0.33	38,39,44,46	0
5	ALF	D	2501	5/5	0.35	0.27	24,26,29,30	0
6	ADP	A	502	27/27	0.27	0.25	42,44,48,49	0
4	MG	D	4500	1/1	0.22	0.21	39,39,39,39	0
5	ALF	D	1501	5/5	0.29	-0.08	23,24,26,26	0
5	ALF	A	3501	5/5	0.28	-0.23	28,28,31,32	0
5	ALF	D	501	5/5	0.29	-0.27	30,30,32,35	0
6	ADP	A	3502	27/27	0.21	-0.46	16,20,24,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ALF	D	4501	5/5	0.18	-0.48	41,41,43,43	0
6	ADP	A	1502	27/27	0.21	-0.50	27,30,35,35	0
6	ADP	D	3502	27/27	0.20	-0.59	28,34,36,37	0
5	ALF	A	4501	5/5	0.17	-0.76	49,49,51,51	0
6	ADP	D	502	27/27	0.21	-0.79	16,23,29,30	0
5	ALF	A	2501	5/5	0.27	-0.85	24,25,27,28	0
6	ADP	D	4502	27/27	0.15	-0.89	41,43,45,46	0
6	ADP	A	2502	27/27	0.17	-1.07	15,20,27,27	0
6	ADP	D	2502	27/27	0.18	-1.18	25,27,29,30	0
6	ADP	D	1502	27/27	0.19	-1.28	15,19,23,24	0
6	ADP	A	4502	27/27	0.13	-1.29	31,42,44,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.