



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2017 – 08:48 PM EDT

PDB ID : 3CMT
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Chen, Z.; Yang, H.; Pavletich, N.P.
Deposited on : unknown
Resolution : 3.15 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

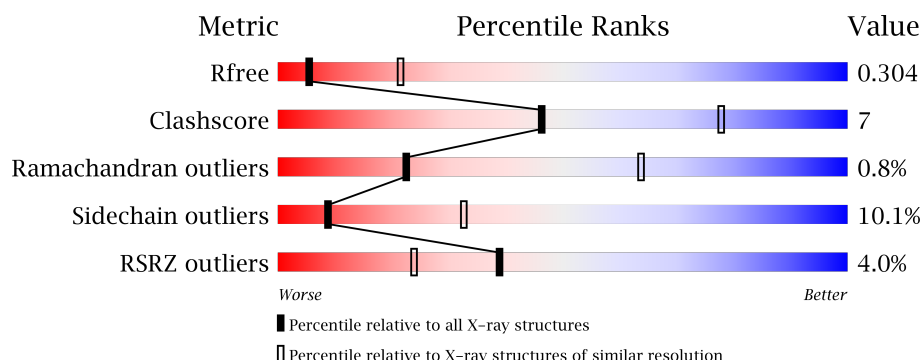
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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	
1	E	15	
2	C	6	
2	F	6	
3	A	1706	

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Mol	Chain	Length	Quality of chain
3	D	1706	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

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

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

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

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

- Molecule 3 is a protein called Protein recA.

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

There are 130 discrepancies between the modelled and reference sequences:

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

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

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

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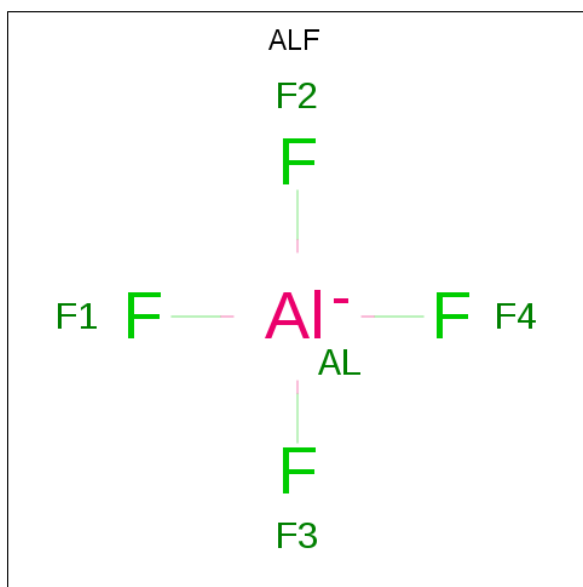
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker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

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

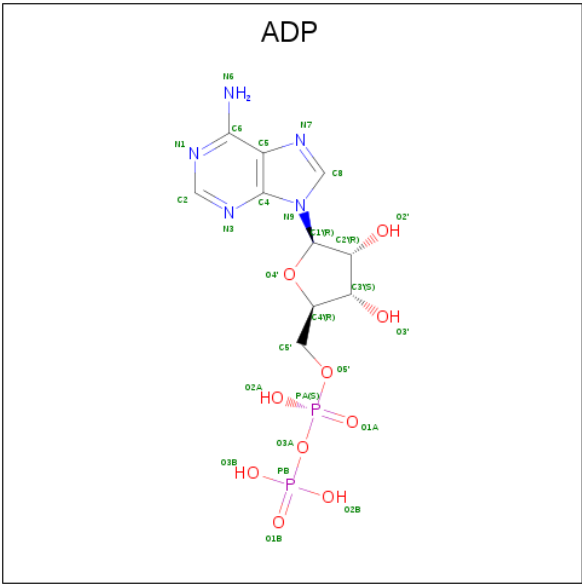
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

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



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

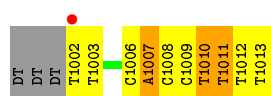
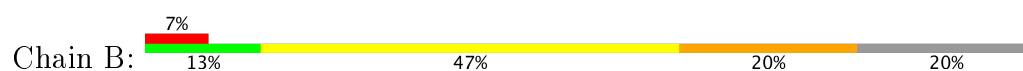


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D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

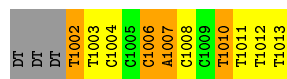
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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')



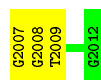
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')



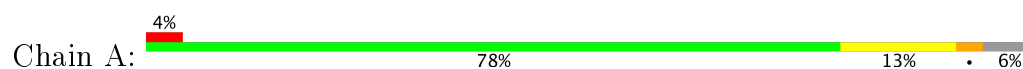
- Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')



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



- Molecule 3: Protein recA







4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	1.15	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

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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.

4.2 Too-close contacts [i](#)

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	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

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 (364) 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)
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:A:4194:GLN:HE21	3:A:4196:ARG:HH12	1.26	0.82
3:D:1068:GLU:HG2	3:D:2216:LYS:HB3	1.61	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:A:1068:GLU:HG2	3:A:2216:LYS:HB3	1.66	0.77
3:D:193:ASN:HD22	3:D:194:GLN:H	1.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:2329:SER:O	3:A:2330:ASN:HB2	1.94	0.65
3:A:4146:VAL:HA	3:A:4149:LEU:HD22	1.78	0.65
3:D:3068:GLU:HG2	3:D:4216:LYS:CB	2.27	0.65
3:D:4193:ASN:HD22	3:D:4194:GLN:N	1.95	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: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:D:3193:ASN:OD1	3:D:3209:THR:HG23	1.98	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:A:76:THR:HG21	3:A:142:VAL:HG21	1.80	0.63
3:D:193:ASN:OD1	3:D:209:THR:HG23	1.98	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:E:1013:DT:C7	3:D:3197:MET:HG3	2.29	0.63
1:B:1007:DA:H5'	3:A:2212:GLY:HA2	1.80	0.63
3:A:1076:THR:HG21	3:A:1142:VAL:HG21	1.81	0.62
1:E:1013:DT:H71	3:D:3197:MET:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1146:VAL:HA	3:D:1149:LEU:HD22	1.80	0.62
3:D:4193:ASN:OD1	3:D:4209:THR:HG23	1.99	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
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.84	0.60
1:E:1003:DT:O2	3:D:199:ILE:HG22	2.00	0.60
3:A:2193:ASN:OD1	3:A:2209:THR:HG23	2.01	0.60
3:A:3111:ILE:HG22	3:A:4030:GLY:CA	2.32	0.60
3:D:1076:THR:HG21	3:D:1142:VAL:HG21	1.82	0.60
3:A:150:THR:HB	3:A:155:ILE:HD11	1.83	0.59
3:A:4121:THR:HG22	3:A:4155:ILE:HD12	1.85	0.59
1:B:1002:DT:H2'	1:B:1003:DT:C6	2.38	0.59
3:D:193:ASN:HD22	3:D:194:GLN:N	1.98	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:3111:ILE:HG23	3:D:4029:LEU:HD13	1.86	0.58
3:D:4198:LYS:HG2	3:D:4206:PRO:O	2.03	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
3:A:2329:SER:O	3:A:2330:ASN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1013:DT:H5'	3:D:4212:GLY:HA2	1.86	0.56
3:A:198:LYS:HG2	3:A:206:PRO:O	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
3:D:3213:ASN:OD1	3:D:3216:LYS:HE2	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:A:2149:LEU:HD23	3:A:2171:MET:HE1	1.87	0.56
3:D:1213:ASN:OD1	3:D:1216:LYS:HE2	2.05	0.56
3:A:4243:ARG:NH1	3:A:4259:GLU:OE2	2.39	0.56
3:D:3076:THR:CG2	3:D:3142:VAL:HG21	2.35	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:3076:THR:CG2	3:A:3142:VAL:HG21	2.36	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: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:A:4261:GLN:HB2	3:A:4269:ASN:HB3	1.89	0.54
3:D:1160:GLY:H	3:D:2173:GLN:HE22	1.56	0.54
3:D:4194:GLN:NE2	3:D:4196:ARG:HH12	2.00	0.54
3:A:1076:THR:CG2	3:A:1142:VAL:HG21	2.37	0.54
3:D:149:LEU:HD23	3:D:171:MET:HE1	1.89	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:A:1160:GLY:H	3:A:2173:GLN:NE2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4206:PRO:HG3	3:D:2202:MET:HB3	1.90	0.53
3:D:4222:ARG:HG3	3:D:4248:LYS:HB3	1.89	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
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:A:4069:SER:HB3	6:A:4502:ADP:H3'	1.91	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
1:E:1013:DT:H73	3:D:3198:LYS:O	2.09	0.52
3:A:2222:ARG:HG3	3:A:2248:LYS:HB3	1.90	0.52
3:D:1254:PRO:HG3	6:D:502:ADP:O2'	2.10	0.52
3:D:76:THR:CG2	3:D:142:VAL:HG21	2.39	0.52
3:A:3124:GLN:HG3	3:A:4021:PHE:CD1	2.45	0.52
3:D:2194:GLN:NE2	3:D:2196:ARG:HH12	2.00	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:2194:GLN:HE22	3:A:2196:ARG:HH22	1.59	0.50
3:A:3194:GLN:NE2	3:A:3196:ARG:HH12	2.01	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:A:101:PRO:HB3	3:A:1029:LEU:HD22	1.93	0.50
3:D:4194:GLN:HE22	3:D:4196:ARG:HH22	1.58	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:A:1194:GLN:NE2	3:A:1196:ARG:HH12	2.00	0.49
3:A:194:GLN:HE22	3:A:196:ARG:HH22	1.59	0.49
3:D:2194:GLN:HE22	3:D:2196:ARG:HH22	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1182:LEU:HD11	3:A:1189:LEU:HD12	1.95	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: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:3160:GLY:H	3:A:4173:GLN:HE22	1.61	0.47
3:A:4194:GLN:NE2	3:A:4196:ARG:HH12	2.04	0.47
3:A:1149:LEU:HD23	3:A:1171:MET:HE1	1.96	0.47
3:A:4282:LYS:HG3	3:D:1282:LYS:CG	2.40	0.47
3:D:115:LEU:HD21	3:D:1014:LEU:HD21	1.97	0.47
3:D:2194:GLN:NE2	3:D:2196:ARG:HH22	2.13	0.47
3:D:4194:GLN:NE2	3:D:4196:ARG:HH22	2.13	0.47
3:A:111:ILE:CG2	3:A:1030:GLY:HA2	2.44	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:2038:GLU:HA	3:A:2332:ASN:HD21	1.80	0.47
3:D:1149:LEU:HD23	3:D:1171:MET:HE1	1.95	0.47
3:D:2182:LEU:HD11	3:D:2189:LEU:HD12	1.96	0.47
3:A:4182:LEU:HD11	3:A:4189:LEU:HD12	1.95	0.47
3:D:2111:ILE:HG22	3:D:3030:GLY:N	2.30	0.47
3:D:3149:LEU:HD23	3:D:3171:MET:HE1	1.96	0.47
3:D:2130:ASP:OD2	3:D:2134:ARG:NH1	2.47	0.47
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:1068:GLU:HA	5:D:1501:ALF:F1	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1010:DT:C2	3:A:2199:ILE:HD12	2.51	0.45
3:A:3080:ILE:HD11	3:A:3142:VAL:CG1	2.46	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
3:A:159:ILE:HG12	3:A:1177:LYS:HD3	1.98	0.45
1:E:1013:DT:H72	3:D:3197:MET:HG3	1.99	0.45
3:D:111:ILE:CG2	3:D:1030:GLY:HA2	2.47	0.45
1:B:1013:DT:H5'	3:A:4212:GLY:HA2	1.97	0.45
3:D:3263:LEU:HG	3:D:3269:ASN:HB2	1.99	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:A:2130:ASP:OD2	3:A:2134:ARG:NH1	2.50	0.45
3:D:4149:LEU:HD23	3:D:4171:MET:HE1	1.99	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
3:A:1194:GLN:NE2	3:A:1196:ARG:HH22	2.14	0.44
3:A:4154:GLU:C	3:A:4156:GLU:H	2.19	0.44
3:A:4194:GLN:NE2	3:A:4196:ARG:HH22	2.14	0.44
1:E:1013:DT:H71	3:D:3197:MET:CG	2.45	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:1130:ASP:OD2	3:D:1134:ARG:NH1	2.51	0.43
3:D:1080:ILE:HD11	3:D:1142:VAL:CG1	2.48	0.43
3:D:194:GLN:HE21	3:D:196:ARG:NH1	2.05	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:A:130:ASP:OD2	3:A:134:ARG:NH1	2.51	0.43
3:A:2177:LYS:HB3	3:A:2177:LYS:HE2	1.83	0.43
3:A:3101:PRO:HB3	3:A:4029:LEU:HD22	1.99	0.43
3:D:3130:ASP:OD2	3:D:3134:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3202:MET:HG2	3:D:3202:MET:H	1.66	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:1149:LEU:HD23	3:D:1171:MET:CE	2.48	0.43
3:D:3080:ILE:HD11	3:D:3142:VAL:CG1	2.48	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
3:A:1149:LEU:HD23	3:A:1171:MET:CE	2.48	0.43
3:A:3194:GLN:NE2	3:A:3196:ARG:HH22	2.15	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: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:D:4194:GLN:HE21	3:D:4196:ARG:NH1	2.03	0.43
3:A:4080:ILE:HD11	3:A:4142:VAL:CG1	2.49	0.43
3:A:137:ALA:HB1	3:A:1010:LEU:HB2	2.00	0.42
3:D:2243:ARG:HG3	3:D:2259:GLU:HG2	2.01	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:1076:THR:HG22	3:D:1077:LEU:N	2.34	0.42
3:D:3198:LYS:HG2	3:D:3206:PRO:O	2.20	0.42
3:A:3202:MET:H	3:A:3202:MET:HG2	1.65	0.42
3:D:3159:ILE:HD13	3:D:4126:LEU:HB3	2.02	0.42
3:A:2071:GLY:HA2	6:A:2502:ADP:H5'1	2.02	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:CG1	2.48	0.42
1:E:1013:DT:C7	3:D:3198:LYS:O	2.67	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:A:1243:ARG:HG3	3:A:1259:GLU:HG2	2.02	0.42
3:D:1243:ARG:HG3	3:D:1259:GLU:HG2	2.01	0.42
3:A:2182:LEU:HD23	3:A:2187:THR:HB	2.02	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:D:3194:GLN:HE21	3:D:3196:ARG:NH1	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1202:MET:H	3:A:1202:MET:HG2	1.64	0.41
3:A:243:ARG:HG3	3:A:259:GLU:HG2	2.02	0.41
3:D:2182:LEU:HD23	3:D:2187:THR:HB	2.01	0.41
3:D:4243:ARG:HG3	3:D:4259:GLU:HG2	2.03	0.41
3:A:177:LYS:HB3	3:A:177:LYS:HE2	1.85	0.41
3:D:3080:ILE:HD11	3:D:3142:VAL:HG13	2.02	0.41
3:D:1080:ILE:HD11	3:D:1142:VAL:HG13	2.02	0.41
3:D:1202:MET:HG2	3:D:1202:MET:H	1.65	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:A:2080:ILE:HD11	3:A:2142:VAL:CG1	2.50	0.41
3:D:1177:LYS:HB3	3:D:1177:LYS:HE2	1.84	0.41
3:D:4080:ILE:HD11	3:D:4142:VAL:CG1	2.50	0.41
3:A:2254:PRO:HG3	6:A:1502:ADP:O2'	2.21	0.41
3:A:2330:ASN:N	3:A:2331:PRO:HD3	2.35	0.41
3:D:1182:LEU:HD23	3:D:1187:THR:HB	2.03	0.41
3:D:2076:THR:HG22	3:D:2077:LEU:N	2.36	0.41
3:D:3068:GLU:HA	5:D:3501:ALF:F1	2.11	0.41
3:D:3155:ILE:HA	3:D:4177:LYS:HE3	2.03	0.41
3:A:3243:ARG:HG3	3:A:3259:GLU:HG2	2.04	0.40
3:A:4080:ILE:HD11	3:A:4142:VAL:HG13	2.03	0.40
3:A:1076:THR:HG22	3:A:1077:LEU:N	2.36	0.40
3:A:3115:LEU:HD21	3:A:4014:LEU:HD21	2.02	0.40
3:D:4182:LEU:HD23	3:D:4187:THR:HB	2.03	0.40
3:A:2033:ARG:NE	3:A:2033:ARG:HA	2.37	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:2282:LYS:HG3	3:D:3282:LYS:HG3	2.01	0.40
3:A:2199:ILE:HD11	3:A:3164:MET:HE3	2.03	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: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 sym-

metry operator and encoded unit-cell translations to be applied.

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

4.3 Torsion angles [i](#)

4.3.1 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	
3	A	1595/1706 (94%)	1549 (97%)	33 (2%)	13 (1%)	22	64
3	D	1595/1706 (94%)	1539 (96%)	43 (3%)	13 (1%)	22	64
All	All	3190/3412 (94%)	3088 (97%)	76 (2%)	26 (1%)	22	64

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

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Mol	Chain	Res	Type
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

4.3.2 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%)	9	34
3	D	1267/1339 (95%)	1136 (90%)	131 (10%)	8	32
All	All	2534/2678 (95%)	2278 (90%)	256 (10%)	9	32

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 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	$\# Z > 2$
5	ALF	A	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	1502	4	25,29,29	1.02	1 (4%)	24,45,45	1.92	3 (12%)
5	ALF	A	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	2502	4	25,29,29	0.98	1 (4%)	24,45,45	1.50	3 (12%)
5	ALF	A	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	3502	4	25,29,29	1.11	2 (8%)	24,45,45	1.71	2 (8%)
5	ALF	A	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	4502	4	25,29,29	1.16	2 (8%)	24,45,45	1.70	5 (20%)
5	ALF	A	501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	502	4	25,29,29	1.08	2 (8%)	24,45,45	1.62	1 (4%)
5	ALF	D	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	D	1502	4	25,29,29	0.94	2 (8%)	24,45,45	1.66	4 (16%)
5	ALF	D	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	D	2502	4	25,29,29	1.09	1 (4%)	24,45,45	1.81	2 (8%)
5	ALF	D	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	D	3502	4	25,29,29	1.05	1 (4%)	24,45,45	1.47	2 (8%)
5	ALF	D	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	D	4502	4	25,29,29	1.09	1 (4%)	24,45,45	1.77	3 (12%)
5	ALF	D	501	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	D	502	4	25,29,29	0.99	1 (4%)	24,45,45	1.45	2 (8%)

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	-	0/12/32/32	0/3/3/3
5	ALF	A	2501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	2502	4	-	0/12/32/32	0/3/3/3
5	ALF	A	3501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	3502	4	-	0/12/32/32	0/3/3/3
5	ALF	A	4501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	4502	4	-	0/12/32/32	0/3/3/3
5	ALF	A	501	-	-	0/0/0/0	0/0/0/0
6	ADP	A	502	4	-	0/12/32/32	0/3/3/3
5	ALF	D	1501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	1502	4	-	0/12/32/32	0/3/3/3
5	ALF	D	2501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	2502	4	-	0/12/32/32	0/3/3/3
5	ALF	D	3501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	3502	4	-	0/12/32/32	0/3/3/3
5	ALF	D	4501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	4502	4	-	0/12/32/32	0/3/3/3
5	ALF	D	501	-	-	0/0/0/0	0/0/0/0
6	ADP	D	502	4	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1502	ADP	PB-O3A	2.05	1.63	1.60
6	A	502	ADP	C2-N3	2.10	1.35	1.32
6	A	4502	ADP	O4'-C1'	2.17	1.44	1.41
6	D	1502	ADP	C5-C4	2.66	1.46	1.40
6	A	1502	ADP	C5-C4	2.95	1.47	1.40
6	A	3502	ADP	PB-O3A	2.95	1.64	1.60
6	A	3502	ADP	C5-C4	2.98	1.47	1.40
6	D	502	ADP	C5-C4	3.07	1.47	1.40
6	A	2502	ADP	C5-C4	3.11	1.47	1.40
6	D	3502	ADP	C5-C4	3.18	1.47	1.40
6	A	4502	ADP	C5-C4	3.32	1.48	1.40
6	A	502	ADP	C5-C4	3.41	1.48	1.40
6	D	4502	ADP	C5-C4	3.63	1.48	1.40
6	D	2502	ADP	C5-C4	3.63	1.48	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	ADP	N3-C2-N1	-7.50	122.33	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2502	ADP	N3-C2-N1	-6.98	122.78	128.86
6	A	3502	ADP	N3-C2-N1	-6.85	122.89	128.86
6	D	4502	ADP	N3-C2-N1	-6.46	123.24	128.86
6	A	4502	ADP	N3-C2-N1	-6.43	123.26	128.86
6	D	1502	ADP	N3-C2-N1	-6.07	123.57	128.86
6	A	502	ADP	N3-C2-N1	-5.98	123.65	128.86
6	D	3502	ADP	N3-C2-N1	-5.52	124.05	128.86
6	A	2502	ADP	N3-C2-N1	-5.41	124.15	128.86
6	D	502	ADP	N3-C2-N1	-4.63	124.83	128.86
6	D	502	ADP	C4-C5-N7	-2.57	106.92	109.41
6	A	4502	ADP	C4-C5-N7	-2.27	107.21	109.41
6	D	1502	ADP	C4-C5-N7	-2.16	107.32	109.41
6	D	3502	ADP	N6-C6-N1	2.01	122.75	118.77
6	A	2502	ADP	O2B-PB-O1B	2.04	118.47	110.50
6	A	1502	ADP	C2-N1-C6	2.08	122.42	118.77
6	A	4502	ADP	C2-N1-C6	2.14	122.52	118.77
6	A	2502	ADP	N6-C6-N1	2.17	123.07	118.77
6	D	1502	ADP	O2B-PB-O1B	2.20	119.09	110.50
6	A	4502	ADP	O2B-PB-O1B	2.20	119.11	110.50
6	A	4502	ADP	N6-C6-N1	2.22	123.17	118.77
6	D	4502	ADP	O3B-PB-O2B	2.26	116.73	107.61
6	D	1502	ADP	N6-C6-N1	2.41	123.54	118.77
6	A	3502	ADP	C2-N1-C6	2.42	123.00	118.77
6	D	4502	ADP	C2-N1-C6	2.64	123.39	118.77
6	A	1502	ADP	N6-C6-N1	2.75	124.22	118.77
6	D	2502	ADP	C2-N1-C6	3.00	124.01	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1502	ADP	2	0
6	A	2502	ADP	2	0
6	A	4502	ADP	1	0
6	A	502	ADP	1	0
5	D	1501	ALF	1	0
5	D	3501	ALF	1	0
6	D	3502	ADP	1	0
6	D	4502	ADP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	502	ADP	2	0

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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%)	0.07	1 (8%) 12 6	37, 42, 48, 48	0
1	E	12/15 (80%)	0.04	0 100 100	38, 47, 53, 62	0
2	C	6/6 (100%)	0.31	0 100 100	46, 48, 63, 66	1 (16%)
2	F	6/6 (100%)	0.22	0 100 100	48, 50, 55, 56	1 (16%)
3	A	1609/1706 (94%)	0.24	69 (4%) 36 21	39, 49, 64, 96	0
3	D	1609/1706 (94%)	0.12	59 (3%) 42 26	39, 49, 65, 96	0
All	All	3254/3454 (94%)	0.18	129 (3%) 39 24	37, 49, 64, 96	2 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	4295	GLY	5.1
3	A	37	VAL	5.1
3	A	4164	MET	4.9
3	D	2001	ALA	4.3
3	A	1333	SER	4.3
3	A	1287	ALA	4.3
3	D	4297	LYS	4.2
3	A	3203	PHE	4.2
3	D	333	SER	4.1
3	A	288	GLY	4.0
3	A	3204	GLY	3.8
3	A	205	ASN	3.7
3	A	1202	MET	3.7
3	A	2202	MET	3.7
3	A	4155	ILE	3.7
3	D	4291	TYR	3.6
3	D	3204	GLY	3.6
3	A	276	ASP	3.6
3	D	3202	MET	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	1289	ALA	3.6
3	D	3203	PHE	3.6
3	A	3202	MET	3.5
3	A	299	GLY	3.5
3	A	251	ILE	3.5
3	A	60	ARG	3.4
3	D	2002	ILE	3.4
3	D	4290	TRP	3.4
3	A	314	GLU	3.3
3	D	4001	ALA	3.3
3	D	3001	ALA	3.2
3	A	1204	GLY	3.2
3	D	4318	GLU	3.2
3	D	3330	ASN	3.2
3	D	4317	LYS	3.1
3	A	315	THR	3.0
3	A	282	LYS	3.0
3	A	331	PRO	3.0
3	D	4282	LYS	3.0
3	D	3023	LYS	3.0
3	D	4275	VAL	2.9
3	A	204	GLY	2.9
3	A	4001	ALA	2.9
3	A	55	GLY	2.9
3	D	3296	GLU	2.8
3	A	253	ALA	2.8
3	A	326	LEU	2.8
3	D	4313	PRO	2.8
3	D	3295	GLY	2.8
3	D	3287	ALA	2.8
3	A	1298	ILE	2.7
3	A	332	ASN	2.7
3	A	2287	ALA	2.7
3	D	4314	GLU	2.6
3	D	4164	MET	2.6
3	A	168	ALA	2.6
3	D	4311	ASP	2.6
3	A	2200	GLY	2.6
3	D	176	ARG	2.6
3	A	333	SER	2.6
3	A	1286	LYS	2.6
3	A	1300	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	1299	GLY	2.6
3	A	274	LEU	2.6
3	D	4315	THR	2.6
3	D	2023	LYS	2.5
3	A	3003	ASP	2.5
3	A	4208	THR	2.5
3	D	4278	GLY	2.5
3	D	4321	LYS	2.5
3	A	197	MET	2.5
3	A	1297	LYS	2.5
3	A	4002	ILE	2.5
3	A	4023	LYS	2.4
3	D	4277	LEU	2.4
3	D	332	ASN	2.4
3	D	4294	LYS	2.4
3	D	4316	ALA	2.4
3	A	1321	LYS	2.4
3	D	4152	LYS	2.4
3	D	4312	ASN	2.3
3	D	1202	MET	2.3
3	A	53	ALA	2.3
3	D	4235	GLU	2.3
3	D	3329	SER	2.3
3	D	1333	SER	2.3
3	D	2333	SER	2.3
3	D	2145	SER	2.3
3	A	2201	VAL	2.3
3	A	1332	ASN	2.3
3	A	3220	SER	2.2
3	A	287	ALA	2.2
3	A	289	ALA	2.2
3	D	1200	GLY	2.2
3	D	4296	GLU	2.2
3	A	298	ILE	2.2
3	D	1298	ILE	2.2
3	A	311	ASP	2.2
3	A	327	LEU	2.2
3	A	49	ILE	2.2
3	D	1289	ALA	2.2
3	D	2203	PHE	2.2
3	A	1325	GLU	2.2
3	D	4328	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	1308	TRP	2.2
3	D	3317	LYS	2.2
3	A	296	GLU	2.2
3	D	1201	VAL	2.2
3	A	280	LYS	2.2
3	A	254	PRO	2.1
3	A	3144	ASP	2.1
3	D	2144	ASP	2.1
3	A	330	ASN	2.1
3	D	1204	GLY	2.1
1	B	1002	DT	2.1
3	D	4005	ASN	2.1
3	D	202	MET	2.1
3	D	4002	ILE	2.1
3	A	300	GLN	2.1
3	D	204	GLY	2.1
3	D	1332	ASN	2.1
3	A	4156	GLU	2.1
3	A	206	PRO	2.1
3	A	1203	PHE	2.0
3	A	1291	TYR	2.0
3	A	199	ILE	2.0
3	D	203	PHE	2.0
3	D	3200	GLY	2.0
3	A	216	LYS	2.0
3	A	1031	GLU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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(\AA^2)	Q<0.9
4	MG	A	500	1/1	0.90	0.43	2.82	44,44,44,44	0
5	ALF	A	1501	5/5	0.93	0.30	1.47	35,35,38,41	0
5	ALF	D	3501	5/5	0.93	0.29	0.57	27,29,33,33	0
5	ALF	D	2501	5/5	0.96	0.36	0.37	24,26,29,30	0
5	ALF	A	501	5/5	0.92	0.30	0.32	38,39,44,46	0
6	ADP	A	502	27/27	0.91	0.26	0.06	42,44,48,49	0
5	ALF	D	501	5/5	0.97	0.31	0.05	30,30,32,35	0
5	ALF	D	1501	5/5	0.97	0.28	-0.10	23,24,26,26	0
5	ALF	A	3501	5/5	0.94	0.28	-0.33	28,28,31,32	0
6	ADP	A	3502	27/27	0.94	0.21	-0.57	16,20,24,26	0
5	ALF	D	4501	5/5	0.90	0.17	-0.58	41,41,43,43	0
6	ADP	D	3502	27/27	0.93	0.20	-0.58	28,34,36,37	0
6	ADP	A	1502	27/27	0.96	0.20	-0.65	27,30,35,35	0
5	ALF	A	4501	5/5	0.90	0.17	-0.74	49,49,51,51	0
6	ADP	D	502	27/27	0.96	0.21	-0.77	16,23,29,30	0
5	ALF	A	2501	5/5	0.96	0.26	-0.94	24,25,27,28	0
6	ADP	D	4502	27/27	0.93	0.14	-1.07	41,43,45,46	0
6	ADP	A	4502	27/27	0.93	0.14	-1.24	31,42,44,45	0
6	ADP	A	2502	27/27	0.96	0.17	-1.25	15,20,27,27	0
6	ADP	D	2502	27/27	0.95	0.19	-1.31	25,27,29,30	0
6	ADP	D	1502	27/27	0.96	0.19	-1.38	15,19,23,24	0
4	MG	A	3500	1/1	0.95	0.42	-	27,27,27,27	0
4	MG	A	4500	1/1	0.95	0.24	-	32,32,32,32	0
4	MG	A	1500	1/1	0.92	0.43	-	38,38,38,38	0
4	MG	D	500	1/1	0.92	0.39	-	34,34,34,34	0
4	MG	D	1500	1/1	0.96	0.41	-	28,28,28,28	0
4	MG	D	3500	1/1	0.87	0.36	-	31,31,31,31	0
4	MG	A	2500	1/1	0.94	0.42	-	25,25,25,25	0
4	MG	D	2500	1/1	0.94	0.55	-	32,32,32,32	0
4	MG	D	4500	1/1	0.80	0.19	-	39,39,39,39	0

5.5 Other polymers ⓘ

There are no such residues in this entry.