Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:01 AM GMT

PDB ID	:	3GV5
Title	:	Human DNA polymerase iota in complex with T template DNA and incoming ddADP
Authors	:	Kirouac, K.N.; Ling, H.
Deposited on	:	2009-03-30
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

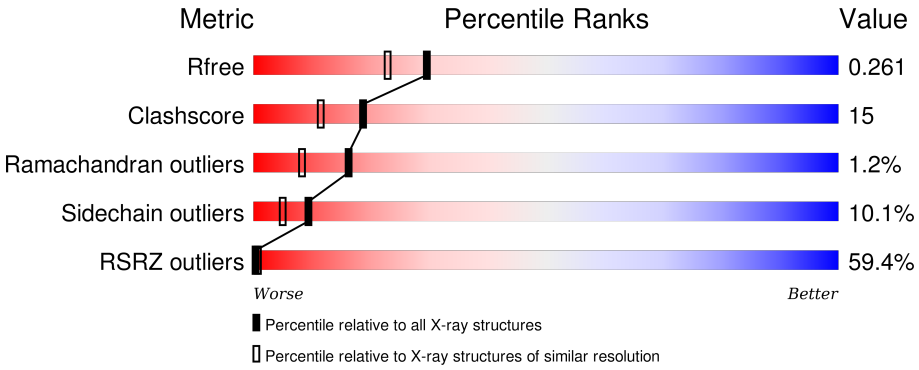
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	420	56% 62% 20% 8% 10%
1	D	420	53% 65% 20% 6% • 9%
2	E	9	22% 44% 22% 33%
2	P	9	44% 33% 44% 22%
3	F	13	8% 46% 54%

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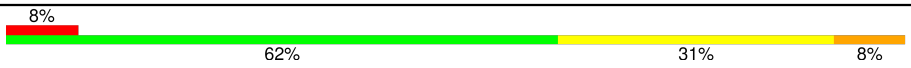
Mol	Chain	Length	Quality of chain
3	T	13	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7703 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 protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	379	Total	C	N	O	S	Se	0	0	0
			2990	1892	521	555	11	11			
1	D	383	Total	C	N	O	S	Se	0	1	0
			3020	1909	526	562	11	12			

- Molecule 2 is a DNA chain called 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	P	0	0	0
			189	90	39	52	8			
2	E	9	Total	C	N	O	P	0	0	0
			189	90	39	52	8			

- Molecule 3 is a DNA chain called 5'-D(P*CP*AP*TP*TP*CP*TP*CP*AP*TP*CP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	13	Total	C	N	O	P	0	0	0
			257	124	41	79	13			
3	F	13	Total	C	N	O	P	0	0	0
			257	124	41	79	13			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Ca	0	0
			1	1		
4	B	3	Total	Ca	0	0
			3	3		
4	D	3	Total	Ca	0	0
			3	3		

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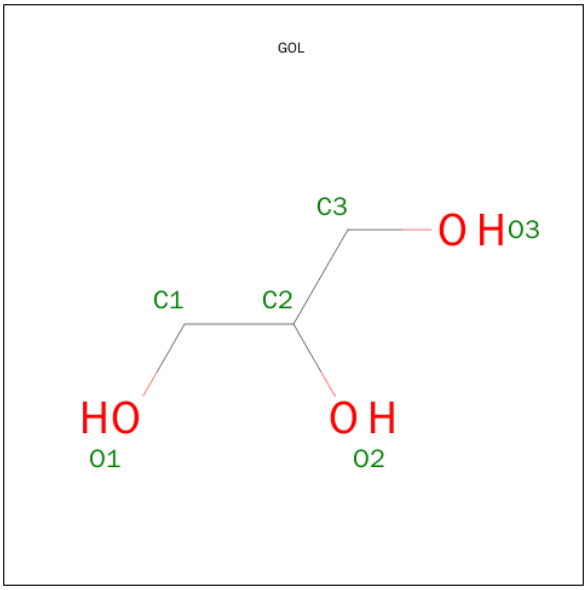
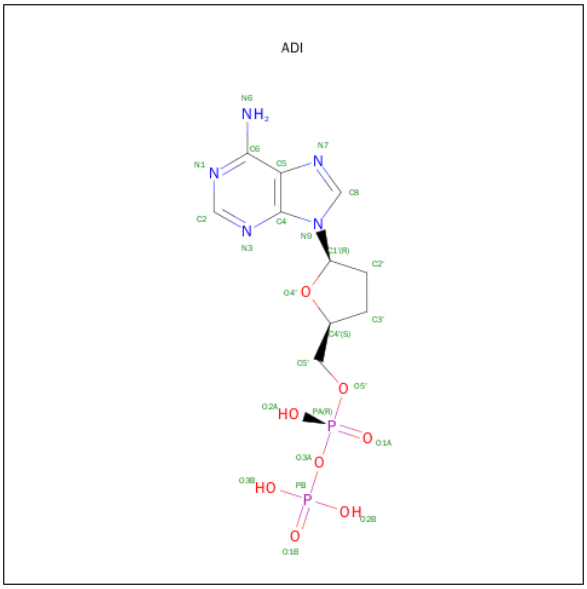
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total Ca 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-DIPHOSPHATE (three-letter code: ADI) (formula: $C_{10}H_{15}N_5O_8P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			25	10	5	8	2		
6	D	1	Total	C	N	O	P	0	0
			25	10	5	8	2		

- Molecule 7 is water.

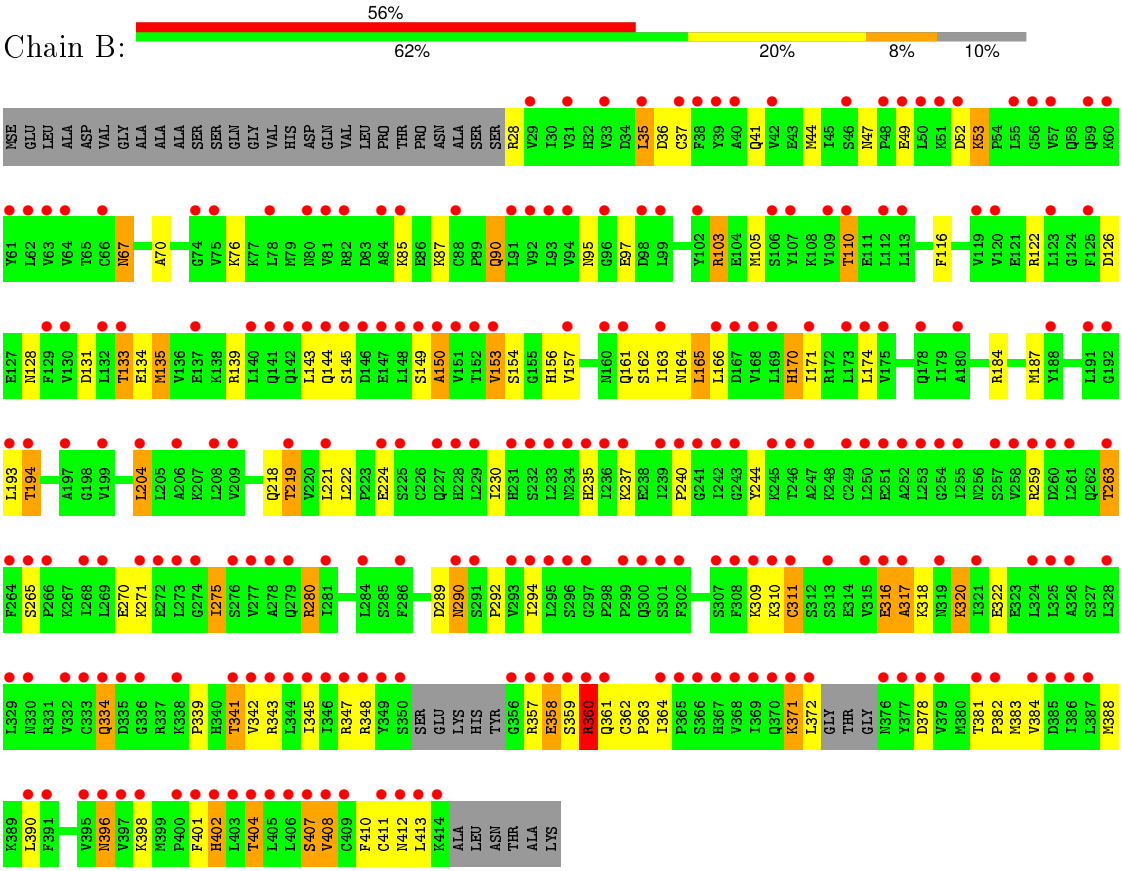
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	303	Total	O	0	0
			303	303		
7	P	32	Total	O	0	0
			32	32		
7	T	39	Total	O	0	0
			39	39		
7	D	306	Total	O	0	0
			306	306		
7	E	23	Total	O	0	0
			23	23		
7	F	34	Total	O	0	0
			34	34		

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 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.

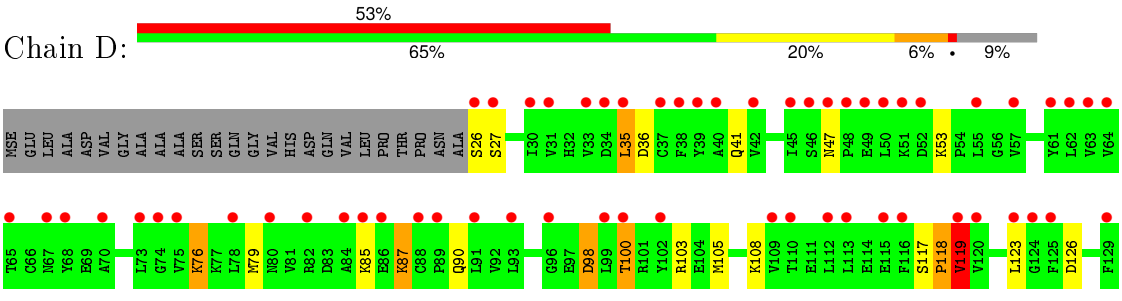
- Molecule 1: DNA polymerase iota

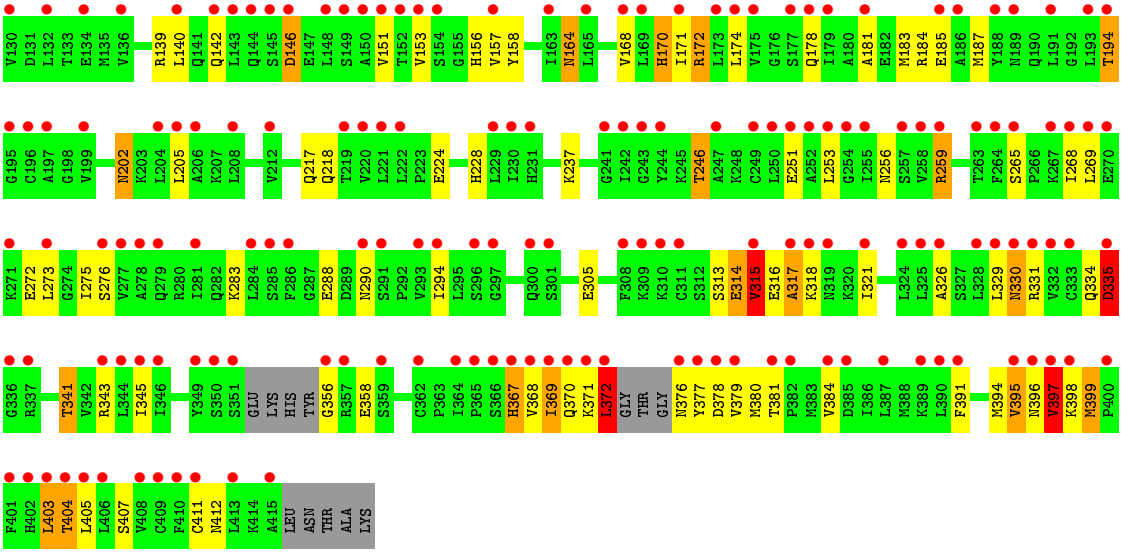
Chain B:



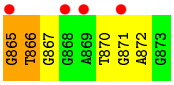
- Molecule 1: DNA polymerase iota

Chain D:

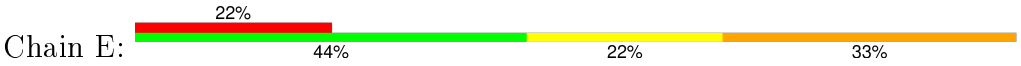


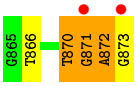


• Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'



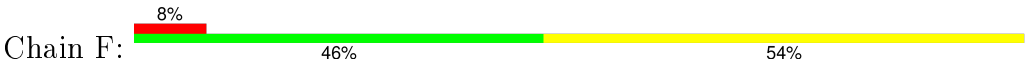
• Molecule 2: 5'-D(*GP*TP*GP*GP*AP*TP*GP*AP*G)-3'

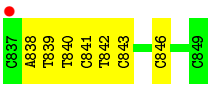




• Molecule 3: 5'-D(P*CP*AP*TP*TP*CP*TP*CP*AP*TP*CP*CP*AP*C)-3'

• Molecule 3: 5'-D(P*CP*AP*TP*TP*CP*TP*CP*AP*TP*CP*CP*AP*C)-3'





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.16Å 71.75Å 127.42Å 90.00° 112.53° 90.00°	Depositor
Resolution (Å)	51.57 – 2.00 51.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (51.57-2.00) 95.4 (51.54-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.205 , 0.253 0.216 , 0.261	Depositor DCC
R_{free} test set	1551 reflections (2.10%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 75523 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, ADI

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	0.59	1/3022 (0.0%)	0.81	7/4055 (0.2%)
1	D	0.95	8/3052 (0.3%)	0.91	16/4095 (0.4%)
2	E	1.07	0/213	1.90	8/329 (2.4%)
2	P	1.10	0/213	1.74	5/329 (1.5%)
3	F	1.11	0/285	1.84	12/435 (2.8%)
3	T	1.16	0/285	1.77	8/435 (1.8%)
All	All	0.85	9/7070 (0.1%)	1.07	56/9678 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	8
1	D	0	13
All	All	0	21

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	GLU	CG-CD	-27.52	1.10	1.51
1	D	358	GLU	CA-CB	-13.59	1.24	1.53
1	D	358	GLU	CD-OE1	12.00	1.38	1.25
1	D	358	GLU	CB-CG	11.19	1.73	1.52
1	D	358	GLU	CD-OE2	10.34	1.37	1.25
1	D	98	ASP	CB-CG	-7.46	1.36	1.51
1	D	315	VAL	N-CA	6.51	1.59	1.46
1	D	335	ASP	N-CA	5.68	1.57	1.46
1	B	334	GLN	CA-C	5.55	1.67	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	358	GLU	OE1-CD-OE2	-16.94	102.98	123.30
2	E	866	DT	O4'-C1'-N1	-10.12	100.92	108.00
1	D	318	LYS	N-CA-C	-9.64	84.97	111.00
2	P	866	DT	O4'-C1'-N1	-9.43	101.40	108.00
1	B	358	GLU	N-CA-C	8.86	134.92	111.00
1	B	311	CYS	N-CA-C	8.60	134.23	111.00
3	F	843	DC	O4'-C1'-N1	8.35	113.84	108.00
1	D	405	LEU	CA-CB-CG	8.29	134.37	115.30
3	T	839	DT	O4'-C4'-C3'	-7.97	101.22	106.00
3	T	841	DC	O4'-C1'-N1	7.30	113.11	108.00
1	D	397	VAL	N-CA-C	-7.29	91.32	111.00
3	T	839	DT	C1'-O4'-C4'	-7.17	102.93	110.10
1	D	98	ASP	CB-CG-OD1	7.01	124.61	118.30
1	D	331	ARG	N-CA-C	-7.00	92.11	111.00
3	F	842	DT	O4'-C1'-N1	6.77	112.74	108.00
1	B	103	ARG	NE-CZ-NH1	6.69	123.64	120.30
3	F	839	DT	O4'-C1'-N1	6.67	112.67	108.00
1	D	119	VAL	N-CA-C	-6.67	93.00	111.00
1	B	408	VAL	N-CA-C	6.57	128.74	111.00
1	B	103	ARG	NE-CZ-NH2	-6.55	117.02	120.30
3	F	841	DC	O4'-C1'-N1	6.50	112.55	108.00
3	F	838	DA	P-O3'-C3'	6.49	127.49	119.70
1	B	360	ARG	N-CA-C	6.37	128.19	111.00
3	F	842	DT	N3-C2-O2	-6.16	118.61	122.30
2	P	867	DG	N1-C6-O6	-6.16	116.21	119.90
3	T	839	DT	O4'-C1'-N1	6.15	112.30	108.00
1	D	404	THR	N-CA-CB	-6.11	98.70	110.30
1	D	404	THR	CB-CA-C	-6.08	95.17	111.60
2	E	872	DA	O4'-C1'-N9	6.04	112.22	108.00
1	D	98	ASP	OD1-CG-OD2	-6.02	111.86	123.30
3	F	846	DC	O4'-C1'-N1	-5.96	103.83	108.00
1	D	103	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	D	395	VAL	N-CA-C	-5.80	95.34	111.00
3	F	840	DT	C6-C5-C7	-5.76	119.44	122.90
3	T	843	DC	O4'-C1'-N1	5.75	112.03	108.00
2	P	866	DT	N1-C1'-C2'	5.74	123.50	112.60
3	F	840	DT	C4-C5-C7	5.67	122.40	119.00
1	D	372	LEU	CA-CB-CG	5.61	128.21	115.30
1	D	358	GLU	N-CA-C	-5.61	95.86	111.00
3	T	844	DA	O4'-C1'-N9	5.56	111.89	108.00
3	F	838	DA	C1'-O4'-C4'	-5.53	104.57	110.10
2	P	865	DG	O4'-C1'-N9	5.52	111.87	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	404	THR	N-CA-C	5.51	125.89	111.00
2	E	871	DG	C4'-C3'-C2'	-5.51	98.14	103.10
2	E	873	DG	C5-C6-O6	-5.51	125.29	128.60
3	F	839	DT	C1'-O4'-C4'	-5.50	104.59	110.10
2	E	870	DT	O4'-C1'-N1	5.46	111.82	108.00
3	F	843	DC	P-O3'-C3'	5.40	126.18	119.70
1	B	318	LYS	N-CA-C	5.32	125.37	111.00
3	T	842	DT	N3-C2-O2	-5.32	119.11	122.30
3	T	842	DT	O4'-C1'-N1	5.32	111.72	108.00
2	E	866	DT	N1-C1'-C2'	5.21	122.50	112.60
2	E	870	DT	C4-C5-C7	5.20	122.12	119.00
1	D	98	ASP	CB-CG-OD2	5.19	122.97	118.30
2	E	870	DT	C1'-O4'-C4'	-5.14	104.95	110.10
2	P	870	DT	O4'-C1'-N1	5.03	111.52	108.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	LYS	Peptide
1	B	316	GLU	Peptide
1	B	317	ALA	Peptide
1	B	334	GLN	Peptide
1	B	357	ARG	Peptide
1	B	359	SER	Peptide
1	B	401	PHE	Peptide
1	B	407	SER	Peptide
1	D	118	PRO	Peptide
1	D	313	SER	Peptide
1	D	314	GLU	Peptide
1	D	315	VAL	Peptide
1	D	317	ALA	Peptide
1	D	329	LEU	Peptide
1	D	330	ASN	Peptide
1	D	334	GLN	Peptide
1	D	367	HIS	Peptide
1	D	394	MSE	Peptide
1	D	396	ASN	Peptide
1	D	403	LEU	Peptide
1	D	404	THR	Peptide

5.2 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	2990	0	3082	108	0
1	D	3020	0	3112	96	0
2	E	189	0	103	4	0
2	P	189	0	103	2	0
3	F	257	0	148	0	0
3	T	257	0	148	1	0
4	B	3	0	0	0	1
4	D	3	0	0	0	1
4	F	1	0	0	0	0
4	P	1	0	0	0	0
5	B	6	0	8	3	0
6	B	25	0	12	1	0
6	D	25	0	12	1	0
7	B	303	0	0	19	0
7	D	306	0	0	15	0
7	E	23	0	0	0	0
7	F	34	0	0	0	0
7	P	32	0	0	0	0
7	T	39	0	0	0	0
All	All	7703	0	6728	211	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 15.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASN:HD21	1:B:49:GLU:HG2	1.16	1.08
1:D:172:ARG:HG3	1:D:172:ARG:HH11	0.93	1.07
1:D:35:LEU:HD21	1:D:187:MSE:HE1	1.38	1.02
1:D:172:ARG:HG3	1:D:172:ARG:NH1	1.46	1.01
1:D:87:LYS:HB2	7:D:645:HOH:O	1.59	1.00
1:D:153:VAL:HG22	1:D:174:LEU:HD22	1.45	0.97
1:D:305:GLU:HB3	1:D:407:SER:HB3	1.46	0.96
1:B:47:ASN:ND2	1:B:49:GLU:HG2	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:OD2	1:B:194:THR:HG23	1.68	0.93
1:B:41:GLN:HE22	1:B:194:THR:H	1.08	0.93
1:D:172:ARG:HH11	1:D:172:ARG:CG	1.76	0.93
1:D:36:ASP:OD1	1:D:194:THR:HG22	1.68	0.93
1:B:164:ASN:H	1:B:170:HIS:HD2	1.19	0.89
1:B:342:VAL:HG21	1:B:383:MSE:HE1	1.56	0.88
1:B:184:ARG:HE	1:B:218:GLN:HE21	1.19	0.88
1:D:123:LEU:HD21	2:E:872:DA:H2"	1.53	0.88
1:D:36:ASP:OD1	1:D:194:THR:CG2	2.22	0.87
1:B:347:ARG:HE	1:B:404:THR:CG2	1.89	0.85
1:D:372:LEU:HG	1:D:377:TYR:H	1.41	0.85
1:D:35:LEU:CD2	1:D:187:MSE:HE1	2.09	0.82
1:D:140:LEU:HD11	1:D:172:ARG:HD2	1.61	0.81
1:D:275:ILE:H	1:D:275:ILE:HD12	1.43	0.81
1:B:35:LEU:HD11	1:B:187:MSE:HE1	1.62	0.81
1:B:290:ASN:HB3	7:B:480:HOH:O	1.82	0.80
1:D:398:LYS:H	1:D:399[B]:MSE:HB2	1.47	0.80
1:B:90:GLN:HE21	1:B:90:GLN:H	1.30	0.80
1:B:371:LYS:HG2	1:B:372:LEU:H	1.47	0.79
1:D:153:VAL:HG22	1:D:174:LEU:CD2	2.13	0.79
1:B:163:ILE:HG21	1:B:174:LEU:HD11	1.64	0.78
1:B:149:SER:HB2	1:B:150:ALA:HB2	1.64	0.78
6:B:425:ADI:H1'	7:B:572:HOH:O	1.83	0.77
1:D:246:THR:HG23	2:E:871:DG:OP1	1.84	0.77
1:B:131:ASP:OD2	1:B:133:THR:HG23	1.85	0.76
6:D:424:ADI:H5'1	7:D:480:HOH:O	1.86	0.75
1:D:184:ARG:HH21	1:D:218:GLN:HE21	1.34	0.75
1:B:347:ARG:HE	1:B:404:THR:HG22	1.51	0.75
1:B:131:ASP:OD2	1:B:133:THR:CG2	2.35	0.75
1:B:343:ARG:HH21	1:B:361:GLN:HE22	1.34	0.74
1:B:47:ASN:HD21	1:B:49:GLU:CG	1.98	0.74
1:D:370:GLN:HA	1:D:371:LYS:HB3	1.69	0.74
1:D:341:THR:HG23	1:D:412:ASN:HB3	1.68	0.73
1:D:164:ASN:H	1:D:170:HIS:HD2	1.37	0.72
1:B:404:THR:HG21	7:B:473:HOH:O	1.90	0.71
1:D:118:PRO:HB2	1:D:119:VAL:HG13	1.72	0.70
1:B:170:HIS:HE1	1:B:224:GLU:OE2	1.73	0.70
1:B:371:LYS:HG2	1:B:372:LEU:N	2.05	0.70
1:B:110:THR:CG2	1:B:122:ARG:HH11	2.05	0.70
1:D:259:ARG:HD2	1:D:259:ARG:H	1.57	0.70
1:B:184:ARG:HE	1:B:218:GLN:NE2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:SER:HB2	1:B:150:ALA:CB	2.22	0.70
1:B:149:SER:N	1:B:150:ALA:HB3	2.06	0.70
1:B:343:ARG:NH2	1:B:361:GLN:HE22	1.90	0.69
1:B:153:VAL:HG13	1:B:174:LEU:HD22	1.74	0.69
1:B:348:ARG:HD2	1:B:358:GLU:OE1	1.93	0.69
1:B:35:LEU:CD1	1:B:187:MSE:HE1	2.22	0.69
1:B:164:ASN:H	1:B:170:HIS:CD2	2.09	0.68
1:D:98:ASP:OD1	1:D:100:THR:HG23	1.95	0.66
1:B:28:ARG:N	7:B:603:HOH:O	2.28	0.66
1:B:110:THR:HG21	1:B:122:ARG:HH11	1.59	0.66
1:B:381:THR:HG23	1:B:382:PRO:HD3	1.77	0.66
1:D:172:ARG:NH1	1:D:172:ARG:CG	2.31	0.66
1:B:388:MSE:HE1	7:B:503:HOH:O	1.97	0.65
1:D:168:VAL:O	1:D:172:ARG:HG2	1.95	0.65
1:B:317:ALA:HB3	7:B:503:HOH:O	1.96	0.65
1:B:347:ARG:NE	1:B:404:THR:CG2	2.60	0.65
1:B:52:ASP:O	7:B:464:HOH:O	2.14	0.65
1:D:290:ASN:ND2	1:D:290:ASN:H	1.95	0.65
1:D:251:GLU:HG3	1:D:256:ASN:HD21	1.61	0.64
1:B:90:GLN:NE2	1:B:90:GLN:H	1.94	0.64
1:B:116:PHE:HB3	1:B:135:MSE:HE1	1.80	0.64
1:B:35:LEU:HD11	1:B:187:MSE:CE	2.28	0.63
1:B:110:THR:HG21	1:B:122:ARG:HG2	1.81	0.63
1:B:259:ARG:O	1:B:263:THR:HB	1.99	0.63
1:D:305:GLU:CB	1:D:407:SER:HB3	2.26	0.63
1:B:103:ARG:NH2	7:B:684:HOH:O	2.32	0.63
1:D:140:LEU:CD1	1:D:172:ARG:HD2	2.27	0.62
1:D:123:LEU:C	1:D:123:LEU:HD23	2.20	0.62
1:B:52:ASP:HB3	7:B:590:HOH:O	1.99	0.62
1:D:398:LYS:N	1:D:399[B]:MSE:HB2	2.15	0.61
1:D:202:ASN:ND2	1:D:205:LEU:H	1.98	0.61
1:B:144:GLN:HG3	1:B:145:SER:H	1.66	0.61
1:D:156:HIS:HE1	1:D:217:GLN:HE21	1.46	0.60
1:D:98:ASP:OD1	1:D:100:THR:CG2	2.49	0.60
1:D:253:LEU:HD21	1:D:272:GLU:HG2	1.82	0.60
1:B:184:ARG:NE	1:B:218:GLN:HE21	1.97	0.59
1:B:41:GLN:HA	1:B:44:MSE:HE3	1.85	0.59
1:D:305:GLU:HB3	1:D:407:SER:CB	2.29	0.58
1:B:371:LYS:HG2	1:B:372:LEU:HD12	1.85	0.58
1:D:140:LEU:HD21	1:D:171:ILE:HG13	1.86	0.58
1:D:367:HIS:HA	1:D:370:GLN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:THR:HG23	1:D:412:ASN:CB	2.34	0.57
1:B:156:HIS:HB2	1:B:219:THR:HB	1.85	0.57
1:B:41:GLN:HE22	1:B:194:THR:N	1.91	0.56
1:B:341:THR:HG23	1:B:412:ASN:CB	2.35	0.56
1:B:161:GLN:HG3	1:B:222:LEU:HD12	1.88	0.56
1:B:309:LYS:O	1:B:402:HIS:HE1	1.87	0.56
1:D:151:VAL:HG11	1:D:171:ILE:HD12	1.86	0.56
1:D:202:ASN:C	1:D:202:ASN:HD22	2.08	0.56
1:D:372:LEU:HB2	1:D:376:ASN:HA	1.87	0.56
1:D:345:ILE:HB	1:D:407:SER:OG	2.05	0.56
1:B:170:HIS:CE1	1:B:224:GLU:OE2	2.57	0.56
1:B:345:ILE:HB	1:B:407:SER:HB3	1.87	0.56
1:B:342:VAL:HG23	1:B:364:ILE:CG1	2.37	0.55
1:D:172:ARG:NH1	7:D:598:HOH:O	2.40	0.55
7:B:435:HOH:O	1:D:156:HIS:HD2	1.89	0.55
1:B:347:ARG:HE	1:B:404:THR:HG23	1.71	0.54
1:D:146:ASP:HB2	7:D:444:HOH:O	2.06	0.54
1:B:131:ASP:OD2	1:B:133:THR:HG22	2.08	0.54
5:B:422:GOL:H12	7:B:479:HOH:O	2.07	0.54
1:D:35:LEU:HD21	1:D:187:MSE:CE	2.26	0.53
1:B:348:ARG:NH2	7:B:544:HOH:O	2.41	0.53
1:B:90:GLN:HG2	7:D:604:HOH:O	2.09	0.53
1:D:290:ASN:HD22	1:D:290:ASN:H	1.55	0.53
1:B:280:ARG:NH2	1:B:289:ASP:OD1	2.41	0.53
1:B:292:PRO:HG2	1:B:294:ILE:HD11	1.89	0.53
1:B:290:ASN:H	1:B:290:ASN:HD22	1.57	0.53
1:B:341:THR:HG23	1:B:412:ASN:HB2	1.90	0.53
1:B:270:GLU:HG2	1:B:275:ILE:HA	1.91	0.53
1:D:47:ASN:HB2	7:D:541:HOH:O	2.09	0.52
1:B:204:LEU:HD23	1:B:240:PRO:HG2	1.91	0.52
1:D:181:ALA:O	1:D:185:GLU:HG3	2.08	0.52
1:D:356:GLY:N	7:D:583:HOH:O	2.43	0.52
5:B:422:GOL:H11	3:T:841:DC:H5"	1.92	0.52
1:B:110:THR:HB	1:B:128:ASN:OD1	2.09	0.52
1:B:347:ARG:HH11	1:B:404:THR:HG23	1.74	0.52
1:B:320:LYS:HG3	7:B:432:HOH:O	2.09	0.52
1:D:164:ASN:H	1:D:170:HIS:CD2	2.25	0.51
1:B:396:ASN:HD21	1:B:398:LYS:HB2	1.76	0.51
1:B:153:VAL:CG1	1:B:174:LEU:HD22	2.39	0.51
1:D:368:VAL:O	1:D:371:LYS:HB2	2.11	0.51
1:B:157:VAL:HG11	1:B:161:GLN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LYS:HE2	1:B:244:TYR:HA	1.92	0.51
1:D:371:LYS:HD3	1:D:379:VAL:HG11	1.93	0.50
1:D:369:ILE:O	1:D:369:ILE:HG22	2.10	0.50
1:D:178:GLN:NE2	7:D:481:HOH:O	2.45	0.50
1:D:251:GLU:HG3	1:D:256:ASN:ND2	2.27	0.50
1:D:151:VAL:HG11	1:D:171:ILE:CD1	2.42	0.49
1:D:384:VAL:HG22	7:D:626:HOH:O	2.13	0.49
1:D:183:MSE:O	1:D:187:MSE:HG3	2.11	0.49
1:B:378:ASP:HA	7:B:695:HOH:O	2.13	0.49
1:B:322:GLU:HG2	1:B:384:VAL:HG11	1.94	0.49
1:D:275:ILE:CD1	1:D:275:ILE:H	2.16	0.49
1:D:391:PHE:CZ	1:D:395:VAL:HG11	2.47	0.49
2:P:865:DG:H2'	2:P:866:DT:H71	1.95	0.49
1:B:360:ARG:HB3	1:B:390:LEU:HD22	1.95	0.49
1:D:53:LYS:HE2	7:D:627:HOH:O	2.12	0.49
1:B:358:GLU:HG3	1:B:358:GLU:H	1.22	0.49
1:D:36:ASP:OD1	1:D:194:THR:HG23	2.12	0.48
1:B:342:VAL:HG23	1:B:364:ILE:HG12	1.95	0.48
1:D:372:LEU:H	1:D:372:LEU:HD23	1.78	0.48
1:D:321:ILE:HG22	7:D:626:HOH:O	2.13	0.48
1:B:230:ILE:HD11	7:B:589:HOH:O	2.13	0.48
1:B:360:ARG:HD3	1:B:360:ARG:N	2.29	0.48
1:B:372:LEU:HD12	1:B:372:LEU:H	1.78	0.48
1:D:343:ARG:HD2	1:D:345:ILE:HD11	1.95	0.47
1:D:370:GLN:HA	1:D:371:LYS:CB	2.40	0.47
1:D:380:MSE:O	1:D:384:VAL:HG23	2.14	0.47
1:D:172:ARG:HG2	1:D:172:ARG:H	1.38	0.47
1:D:184:ARG:NH2	1:D:218:GLN:HE21	2.08	0.47
1:D:275:ILE:N	1:D:275:ILE:HD12	2.21	0.47
1:B:149:SER:CA	1:B:150:ALA:HB3	2.44	0.47
1:D:123:LEU:CD2	1:D:123:LEU:C	2.83	0.47
1:B:95:ASN:ND2	1:B:97:GLU:H	2.13	0.47
1:B:396:ASN:HD22	1:B:396:ASN:C	2.18	0.46
1:B:316:GLU:O	1:B:320:LYS:HD3	2.14	0.46
1:D:76:LYS:HE3	7:D:510:HOH:O	2.15	0.46
1:D:158:TYR:OH	1:D:228:HIS:HD2	1.99	0.46
1:D:76:LYS:HE2	1:D:76:LYS:HB2	1.73	0.45
1:D:391:PHE:O	1:D:395:VAL:HB	2.17	0.45
1:D:283:LYS:HG2	1:D:288:GLU:HG3	1.97	0.45
1:D:202:ASN:HD21	1:D:205:LEU:H	1.62	0.45
1:D:316:GLU:O	1:D:317:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:NH1	1:B:404:THR:HG23	2.32	0.45
1:B:149:SER:CB	1:B:150:ALA:CB	2.94	0.45
1:B:165:LEU:HD23	1:B:171:ILE:HD11	1.97	0.45
1:D:168:VAL:O	1:D:171:ILE:HG22	2.17	0.45
1:B:67:ASN:ND2	1:B:70:ALA:H	2.15	0.45
1:B:411:CYS:HB2	7:B:678:HOH:O	2.16	0.45
1:B:53:LYS:HD2	7:B:590:HOH:O	2.16	0.44
1:B:35:LEU:HB2	1:B:126:ASP:HB2	2.00	0.44
1:B:341:THR:HG23	1:B:412:ASN:HB3	1.99	0.44
1:D:26:SER:HA	1:D:27:SER:HA	1.55	0.44
1:D:156:HIS:CE1	1:D:217:GLN:HE21	2.30	0.44
1:D:153:VAL:HG21	1:D:157:VAL:CG2	2.48	0.44
1:B:342:VAL:HG21	1:B:383:MSE:CE	2.37	0.44
1:B:67:ASN:HD22	1:B:67:ASN:C	2.21	0.44
1:D:315:VAL:HG23	7:D:667:HOH:O	2.18	0.44
1:D:411:CYS:HB2	7:D:643:HOH:O	2.18	0.44
1:B:347:ARG:NE	1:B:404:THR:HG23	2.31	0.43
1:D:397:VAL:HG22	7:D:449:HOH:O	2.18	0.43
1:B:339:PRO:HB3	1:B:410:PHE:HB3	1.99	0.43
2:P:871:DG:H2'	2:P:872:DA:C8	2.53	0.43
2:E:870:DT:H2"	2:E:871:DG:H8	1.83	0.43
1:D:76:LYS:HD3	1:D:79:MSE:HE3	2.00	0.43
1:B:362:CYS:HB2	1:B:363:PRO:HD2	2.00	0.43
1:D:253:LEU:CD2	1:D:272:GLU:HG2	2.47	0.43
1:D:398:LYS:H	1:D:399[A]:MSE:HB2	1.83	0.43
1:D:326:ALA:HB2	1:D:380:MSE:HE1	2.00	0.43
1:B:105:MSE:CG	1:B:193:LEU:HD11	2.48	0.43
1:B:97:GLU:HB3	5:B:422:GOL:H11	2.01	0.42
1:B:110:THR:CG2	1:B:122:ARG:NH1	2.78	0.42
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.86	0.42
1:B:162:SER:HB3	7:B:652:HOH:O	2.19	0.42
1:D:170:HIS:HE1	1:D:224:GLU:OE2	2.04	0.41
1:D:378:ASP:OD2	1:D:381:THR:HG23	2.21	0.41
1:B:235:HIS:HD2	7:B:433:HOH:O	2.03	0.41
1:B:41:GLN:NE2	1:B:194:THR:H	1.92	0.41
1:B:396:ASN:C	1:B:396:ASN:ND2	2.75	0.41
1:D:372:LEU:N	1:D:372:LEU:HD23	2.35	0.41
1:B:139:ARG:O	1:B:143:LEU:HD13	2.21	0.41
1:D:246:THR:CG2	2:E:871:DG:OP1	2.61	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	Interatomic distance (Å)	Clash overlap (Å)
4:B:421:CA:CA	4:D:423:CA:CA[1_565]	0.43	1.77

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	373/420 (89%)	363 (97%)	7 (2%)	3 (1%)	24 15
1	D	378/420 (90%)	359 (95%)	12 (3%)	7 (2%)	10 4
All	All	751/840 (89%)	722 (96%)	19 (2%)	10 (1%)	16 7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	VAL
1	D	330	ASN
1	D	335	ASP
1	D	397	VAL
1	B	150	ALA
1	B	37	CYS
1	B	402	HIS
1	D	399[A]	MSE
1	D	399[B]	MSE
1	D	369	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	344/364 (94%)	309 (90%)	35 (10%)	9 5
1	D	348/364 (96%)	313 (90%)	35 (10%)	9 5
All	All	692/728 (95%)	622 (90%)	70 (10%)	9 5

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	LEU
1	B	53	LYS
1	B	67	ASN
1	B	76	LYS
1	B	85	LYS
1	B	87	LYS
1	B	90	GLN
1	B	110	THR
1	B	133	THR
1	B	134	GLU
1	B	135	MSE
1	B	153	VAL
1	B	154	SER
1	B	165	LEU
1	B	166	LEU
1	B	170	HIS
1	B	194	THR
1	B	204	LEU
1	B	219	THR
1	B	221	LEU
1	B	263	THR
1	B	265	SER
1	B	271	LYS
1	B	275	ILE
1	B	280	ARG
1	B	290	ASN
1	B	311	CYS
1	B	320	LYS
1	B	341	THR
1	B	360	ARG
1	B	371	LYS
1	B	396	ASN
1	B	404	THR
1	B	408	VAL
1	B	413	LEU

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Mol	Chain	Res	Type
1	D	35	LEU
1	D	41	GLN
1	D	76	LYS
1	D	85	LYS
1	D	87	LYS
1	D	90	GLN
1	D	100	THR
1	D	105	MSE
1	D	108	LYS
1	D	117	SER
1	D	119	VAL
1	D	126	ASP
1	D	139	ARG
1	D	142	GLN
1	D	146	ASP
1	D	164	ASN
1	D	170	HIS
1	D	172	ARG
1	D	194	THR
1	D	202	ASN
1	D	237	LYS
1	D	246	THR
1	D	259	ARG
1	D	265	SER
1	D	268	ILE
1	D	269	LEU
1	D	273	LEU
1	D	276	SER
1	D	294	ILE
1	D	314	GLU
1	D	335	ASP
1	D	341	THR
1	D	372	LEU
1	D	397	VAL
1	D	403	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	67	ASN
1	B	90	GLN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	217	GLN
1	B	218	GLN
1	B	227	GLN
1	B	228	HIS
1	B	290	ASN
1	B	330	ASN
1	B	361	GLN
1	B	396	ASN
1	B	402	HIS
1	D	58	GLN
1	D	142	GLN
1	D	156	HIS
1	D	161	GLN
1	D	164	ASN
1	D	170	HIS
1	D	178	GLN
1	D	202	ASN
1	D	216	ASN
1	D	218	GLN
1	D	227	GLN
1	D	228	HIS
1	D	256	ASN
1	D	290	ASN
1	D	330	ASN
1	D	412	ASN

5.3.3 RNA

There are no RNA molecules 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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	GOL	B	422	-	5,5,5	0.54	0	5,5,5	0.30	0
6	ADI	B	425	4	21,27,27	1.12	1 (4%)	24,41,41	2.47	7 (29%)
6	ADI	D	424	4	21,27,27	1.09	2 (9%)	24,41,41	2.43	6 (25%)

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	GOL	B	422	-	-	0/4/4/4	0/0/0/0
6	ADI	B	425	4	-	0/12/25/25	0/3/3/3
6	ADI	D	424	4	-	0/12/25/25	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	424	ADI	C2-N3	2.01	1.35	1.32
6	D	424	ADI	C5-C4	3.19	1.47	1.40
6	B	425	ADI	C5-C4	3.46	1.48	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	425	ADI	N3-C2-N1	-8.57	122.33	128.89
6	D	424	ADI	N3-C2-N1	-6.50	123.92	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	425	ADI	O4'-C1'-C2'	-3.50	102.88	106.67
6	B	425	ADI	C2'-C1'-N9	-3.01	106.40	112.49
6	D	424	ADI	O4'-C1'-C2'	-3.01	103.42	106.67
6	D	424	ADI	C4-C5-N7	-2.73	106.97	109.48
6	B	425	ADI	C4-C5-N7	-2.06	107.58	109.48
6	B	425	ADI	C2-N1-C6	2.19	122.68	118.77
6	D	424	ADI	O4'-C4'-C5'	2.48	113.20	109.54
6	B	425	ADI	C3'-C2'-C1'	2.71	105.74	102.71
6	D	424	ADI	C3'-C2'-C1'	3.18	106.26	102.71
6	B	425	ADI	O4'-C1'-N9	4.62	115.72	107.72
6	D	424	ADI	O4'-C1'-N9	7.06	119.94	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	422	GOL	3	0
6	B	425	ADI	1	0
6	D	424	ADI	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	368/420 (87%)	2.88	236 (64%) 0 1	45, 56, 69, 80	0
1	D	372/420 (88%)	2.50	222 (59%) 0 1	17, 54, 66, 88	0
2	E	9/9 (100%)	1.55	2 (22%) 1 1	34, 37, 40, 41	0
2	P	9/9 (100%)	1.82	4 (44%) 0 1	49, 51, 55, 57	0
3	F	13/13 (100%)	1.39	1 (7%) 16 17	31, 38, 52, 68	0
3	T	13/13 (100%)	1.72	1 (7%) 16 17	45, 54, 68, 85	0
All	All	784/884 (88%)	2.63	466 (59%) 0 1	17, 55, 68, 88	0

All (466) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	ALA	15.2
1	B	145	SER	14.0
1	D	372	LEU	13.9
1	B	148	LEU	12.9
1	D	376	ASN	12.5
1	B	143	LEU	11.2
1	B	149	SER	10.4
1	B	372	LEU	9.6
1	B	144	GLN	9.5
1	B	376	ASN	9.4
1	B	377	TYR	9.1
1	B	333	CYS	8.6
1	B	379	VAL	8.4
1	B	146	ASP	7.9
1	D	333	CYS	7.8
1	B	381	THR	7.5
1	B	168	VAL	7.3
1	D	370	GLN	7.2
1	D	381	THR	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	378	ASP	7.0
1	B	268	ILE	6.7
1	D	52	ASP	6.6
1	B	234	ASN	6.5
1	B	254	GLY	6.4
1	B	141	GLN	6.3
1	D	367	HIS	6.3
1	B	356	GLY	6.1
1	D	315	VAL	6.1
1	B	370	GLN	6.0
1	B	147	GLU	5.9
1	B	349	TYR	5.8
1	D	26	SER	5.8
1	B	366	SER	5.8
1	B	368	VAL	5.7
1	B	384	VAL	5.7
1	B	367	HIS	5.5
1	D	350	SER	5.4
1	B	403	LEU	5.3
1	B	153	VAL	5.3
1	B	232	SER	5.3
1	B	231	HIS	5.3
1	B	52	ASP	5.3
1	B	228	HIS	5.3
1	B	46	SER	5.3
1	B	62	LEU	5.3
1	D	415	ALA	5.2
1	D	268	ILE	5.2
1	D	140	LEU	5.1
1	B	413	LEU	5.1
1	D	346	ILE	5.1
1	B	273	LEU	5.1
1	D	35	LEU	5.1
1	D	368	VAL	4.9
1	B	61	TYR	4.9
1	B	93	LEU	4.8
1	D	152	THR	4.8
1	D	377	TYR	4.7
1	B	37	CYS	4.7
1	B	249	CYS	4.7
1	B	405	LEU	4.7
1	D	151	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	265	SER	4.6
1	B	317	ALA	4.6
1	D	273	LEU	4.6
1	D	403	LEU	4.6
1	B	336	GLY	4.5
1	B	295	LEU	4.4
1	D	99	LEU	4.4
1	B	120	VAL	4.4
1	B	151	VAL	4.4
1	B	311	CYS	4.4
1	B	346	ILE	4.3
1	B	142	GLN	4.3
1	B	309	LYS	4.3
1	B	140	LEU	4.3
1	D	88	CYS	4.3
1	B	409	CYS	4.2
1	D	252	ALA	4.2
1	B	308	PHE	4.2
1	D	324	LEU	4.2
1	B	369	ILE	4.2
1	D	385	ASP	4.2
1	D	308	PHE	4.2
1	D	378	ASP	4.2
1	D	384	VAL	4.1
1	D	328	LEU	4.1
1	B	241	GLY	4.1
1	B	167	ASP	4.1
1	B	250	LEU	4.1
1	B	350	SER	4.0
1	B	359	SER	4.0
1	B	284	LEU	4.0
1	B	345	ILE	4.0
1	D	157	VAL	4.0
1	D	197	ALA	4.0
1	D	47	ASN	4.0
1	D	356	GLY	4.0
1	D	259	ARG	3.9
1	B	334	GLN	3.9
1	B	57	VAL	3.9
1	B	357	ARG	3.9
1	D	357	ARG	3.9
1	D	398	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	330	ASN	3.9
1	D	62	LEU	3.9
1	D	317	ALA	3.8
1	D	387	LEU	3.8
1	D	390	LEU	3.8
1	D	249	CYS	3.8
1	B	137	GLU	3.8
1	B	326	ALA	3.8
1	B	229	LEU	3.8
1	D	33	VAL	3.8
1	D	321	ILE	3.8
1	D	336	GLY	3.8
1	D	406	LEU	3.8
1	D	397	VAL	3.7
1	B	225	SER	3.7
1	D	119	VAL	3.7
1	D	30	ILE	3.7
1	B	269	LEU	3.7
1	B	371	LYS	3.7
1	B	265	SER	3.7
1	D	366	SER	3.7
1	B	119	VAL	3.7
1	D	277	VAL	3.7
1	B	242	ILE	3.7
1	D	78	LEU	3.7
1	D	401	PHE	3.7
1	B	48	PRO	3.7
1	D	46	SER	3.7
1	B	123	LEU	3.7
1	B	335	ASP	3.7
1	D	411	CYS	3.7
1	B	63	VAL	3.6
1	B	206	ALA	3.6
1	B	401	PHE	3.6
1	B	78	LEU	3.6
1	B	264	PHE	3.6
1	B	171	ILE	3.6
1	D	255	ILE	3.6
1	D	290	ASN	3.6
1	B	259	ARG	3.6
1	D	391	PHE	3.6
1	D	369	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	241	GLY	3.5
1	D	196	CYS	3.5
1	D	395	VAL	3.5
1	D	148	LEU	3.5
1	D	326	ALA	3.5
1	D	120	VAL	3.5
1	D	250	LEU	3.5
1	B	81	VAL	3.5
1	B	342	VAL	3.5
1	B	99	LEU	3.5
1	B	188	TYR	3.5
1	D	271	LYS	3.5
1	B	365	PRO	3.5
1	D	123	LEU	3.5
1	D	150	ALA	3.5
1	D	278	ALA	3.5
1	B	125	PHE	3.5
1	D	109	VAL	3.4
1	B	175	VAL	3.4
1	B	348	ARG	3.4
1	D	332	VAL	3.4
1	D	113	LEU	3.4
1	B	84	ALA	3.4
1	B	180	ALA	3.4
1	B	382	PRO	3.4
1	D	319	ASN	3.4
1	B	347	ARG	3.4
1	B	91	LEU	3.4
1	B	406	LEU	3.4
1	D	48	PRO	3.4
1	B	42	VAL	3.3
1	B	247	ALA	3.3
1	D	229	LEU	3.3
1	D	37	CYS	3.3
1	D	163	ILE	3.3
1	B	107	TYR	3.3
1	B	94	VAL	3.3
1	D	220	VAL	3.3
1	D	169	LEU	3.3
1	B	290	ASN	3.3
1	B	64	VAL	3.3
1	B	82	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	3.3
1	D	191	LEU	3.3
1	B	386	ILE	3.3
1	D	195	GLY	3.3
1	B	293	VAL	3.3
1	D	136	VAL	3.3
1	D	143	LEU	3.3
1	D	362	CYS	3.3
1	D	45	ILE	3.2
3	F	837	DC	3.2
1	B	260	ASP	3.2
1	B	110	THR	3.2
1	B	236	ILE	3.2
1	B	411	CYS	3.2
1	D	181	ALA	3.2
1	B	277	VAL	3.2
1	D	194	THR	3.2
1	D	199	VAL	3.2
1	B	319	ASN	3.2
1	B	152	THR	3.2
1	B	33	VAL	3.2
1	B	239	ILE	3.2
1	B	255	ILE	3.2
1	B	400	PRO	3.2
1	D	74	GLY	3.2
1	B	258	VAL	3.2
1	B	395	VAL	3.2
1	D	153	VAL	3.2
1	D	173	LEU	3.2
1	D	405	LEU	3.2
1	D	85	LYS	3.1
1	B	35	LEU	3.1
1	B	328	LEU	3.1
1	B	385	ASP	3.1
1	D	64	VAL	3.1
1	B	88	CYS	3.1
1	B	271	LYS	3.1
1	B	364	ILE	3.1
1	B	163	ILE	3.1
1	D	206	ALA	3.0
1	B	109	VAL	3.0
1	B	261	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	310	LYS	3.0
1	B	315	VAL	3.0
1	D	165	LEU	3.0
1	B	402	HIS	3.0
1	D	311	CYS	3.0
1	D	364	ILE	3.0
1	B	301	SER	3.0
1	B	113	LEU	3.0
1	B	235	HIS	3.0
1	D	371	LYS	3.0
1	D	351	SER	3.0
1	D	325	LEU	3.0
1	D	344	LEU	3.0
1	B	266	PRO	3.0
1	B	85	LYS	3.0
1	B	233	LEU	3.0
1	D	129	PHE	3.0
1	D	331	ARG	2.9
1	D	42	VAL	2.9
1	D	254	GLY	2.9
1	D	174	LEU	2.9
1	D	330	ASN	2.9
1	D	188	TYR	2.9
1	D	132	LEU	2.9
1	B	391	PHE	2.9
1	D	276	SER	2.9
1	B	253	LEU	2.9
1	B	31	VAL	2.9
1	D	168	VAL	2.9
1	D	293	VAL	2.9
1	B	245	LYS	2.9
1	D	50	LEU	2.9
1	D	205	LEU	2.9
1	D	221	LEU	2.9
1	B	75	VAL	2.9
1	B	252	ALA	2.9
1	D	365	PRO	2.9
1	D	335	ASP	2.9
1	B	281	ILE	2.8
1	D	73	LEU	2.8
1	D	89	PRO	2.8
1	B	240	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	294	ILE	2.8
1	B	50	LEU	2.8
1	B	390	LEU	2.8
1	D	57	VAL	2.8
1	D	408	VAL	2.8
1	B	39	TYR	2.8
1	D	39	TYR	2.8
1	D	61	TYR	2.8
1	B	129	PHE	2.8
1	D	409	CYS	2.8
1	D	231	HIS	2.8
1	B	55	LEU	2.8
1	B	324	LEU	2.8
1	D	31	VAL	2.8
1	B	178	GLN	2.8
1	D	359	SER	2.8
1	B	325	LEU	2.8
1	B	209	VAL	2.8
1	B	102	TYR	2.8
1	D	345	ILE	2.8
1	D	379	VAL	2.8
1	D	382	PRO	2.7
1	B	227	GLN	2.7
1	D	144	GLN	2.7
1	D	49	GLU	2.7
1	B	321	ILE	2.7
1	D	154	SER	2.7
1	B	278	ALA	2.7
1	B	174	LEU	2.7
1	D	413	LEU	2.7
1	B	313	SER	2.7
1	B	130	VAL	2.7
1	B	133	THR	2.7
1	B	316	GLU	2.7
1	D	115	GLU	2.7
1	B	80	ASN	2.6
1	B	263	THR	2.6
1	D	84	ALA	2.6
1	B	302	PHE	2.6
1	D	38	PHE	2.6
1	D	34	ASP	2.6
1	B	160	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	329	LEU	2.6
1	D	402	HIS	2.6
1	B	307	SER	2.6
1	B	407	SER	2.6
1	D	247	ALA	2.6
1	B	344	LEU	2.6
1	D	204	LEU	2.6
1	D	222	LEU	2.6
1	D	253	LEU	2.6
1	B	246	THR	2.6
1	D	257	SER	2.6
1	D	70	ALA	2.6
1	D	124	GLY	2.6
1	D	281	ILE	2.6
1	B	166	LEU	2.6
1	B	193	LEU	2.6
1	D	112	LEU	2.6
1	D	329	LEU	2.6
1	D	267	LYS	2.6
1	B	49	GLU	2.6
1	B	29	VAL	2.6
1	D	63	VAL	2.6
1	D	258	VAL	2.6
1	D	244	TYR	2.5
1	B	297	GLY	2.5
1	D	243	GLY	2.5
1	D	55	LEU	2.5
1	D	175	VAL	2.5
1	D	396	ASN	2.5
1	D	178	GLN	2.5
1	B	224	GLU	2.5
1	D	212	VAL	2.5
1	B	338	LYS	2.5
1	B	296	SER	2.5
1	D	177	SER	2.5
1	D	294	ILE	2.5
1	B	396	ASN	2.5
1	D	27	SER	2.5
1	D	310	LYS	2.5
1	B	251	GLU	2.5
1	B	332	VAL	2.5
1	B	194	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	414	LYS	2.5
1	D	68	TYR	2.5
1	D	286	PHE	2.5
1	B	358	GLU	2.4
1	B	398	LYS	2.5
1	D	82	ARG	2.5
1	B	56	GLY	2.4
1	B	38	PHE	2.4
1	B	387	LEU	2.4
1	D	263	THR	2.4
1	D	134	GLU	2.4
1	B	204	LEU	2.4
1	D	116	PHE	2.4
1	D	193	LEU	2.4
1	D	146	ASP	2.4
1	B	237	LYS	2.4
1	B	276	SER	2.4
3	T	837	DC	2.4
1	D	96	GLY	2.4
1	D	142	GLN	2.4
1	D	279	GLN	2.4
1	D	300	GLN	2.4
1	D	125	PHE	2.4
1	B	60	LYS	2.4
1	D	219	THR	2.4
1	B	92	VAL	2.4
1	D	75	VAL	2.4
1	B	169	LEU	2.4
1	D	284	LEU	2.4
1	B	404	THR	2.4
1	D	100	THR	2.4
1	B	219	THR	2.4
1	B	291	SER	2.4
1	B	106	SER	2.3
1	D	208	LEU	2.3
1	D	186	ALA	2.3
1	B	360	ARG	2.3
1	D	102	TYR	2.3
1	D	264	PHE	2.3
1	D	349	TYR	2.3
1	D	110	THR	2.3
1	D	269	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	40	ALA	2.3
1	D	86	GLU	2.3
1	B	300	GLN	2.3
1	B	74	GLY	2.3
1	D	285	SER	2.3
1	D	301	SER	2.3
1	B	157	VAL	2.3
1	D	404	THR	2.3
1	D	270	GLU	2.3
2	P	871	DG	2.3
1	D	296	SER	2.2
1	D	297	GLY	2.2
1	B	98	ASP	2.2
2	E	871	DG	2.2
1	D	145	SER	2.2
1	D	400	PRO	2.2
1	B	208	LEU	2.2
1	B	221	LEU	2.2
1	D	91	LEU	2.2
1	D	242	ILE	2.2
1	B	343	ARG	2.2
1	B	197	ALA	2.2
1	D	337	ARG	2.1
1	B	192	GLY	2.1
1	D	185	GLU	2.1
1	D	40	ALA	2.1
1	D	130	VAL	2.1
2	P	868	DG	2.1
1	D	318	LYS	2.1
1	D	389	LYS	2.1
1	D	93	LEU	2.1
1	D	67	ASN	2.1
1	B	161	GLN	2.1
1	D	343	ARG	2.1
1	D	410	PHE	2.1
1	B	272	GLU	2.1
1	D	251	GLU	2.1
1	B	199	VAL	2.1
1	B	397	VAL	2.1
1	D	149	SER	2.1
1	D	171	ILE	2.1
1	D	179	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	2.1
1	B	96	GLY	2.1
1	B	59	GLN	2.1
1	B	51	LYS	2.1
1	B	299	PRO	2.1
1	B	66	CYS	2.1
1	B	274	GLY	2.1
1	B	412	ASN	2.1
1	D	291	SER	2.1
1	B	341	THR	2.1
1	D	65	THR	2.1
1	B	173	LEU	2.1
1	B	279	GLN	2.1
1	D	189	ASN	2.1
1	D	309	LYS	2.1
1	B	257	SER	2.1
1	D	51	LYS	2.0
1	B	112	LEU	2.0
1	B	286	PHE	2.0
2	E	873	DG	2.0
2	P	869	DA	2.0
1	B	243	GLY	2.0
1	D	230	ILE	2.0
1	B	361	GLN	2.0
1	D	80	ASN	2.0
2	P	865	DG	2.0
1	B	408	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CA	B	421	1/1	1.00	0.30	0.80	35,35,35,35	0
5	GOL	B	422	6/6	0.83	0.27	0.26	32,34,34,35	0
6	ADI	D	424	25/25	0.85	0.23	-0.43	19,24,29,30	0
4	CA	D	423	1/1	0.99	0.25	-0.72	36,36,36,36	0
6	ADI	B	425	25/25	0.86	0.22	-0.75	15,21,24,26	0
4	CA	D	421	1/1	0.99	0.13	-2.29	14,14,14,14	0
4	CA	F	1	1/1	0.98	0.10	-3.21	19,19,19,19	0
4	CA	B	423	1/1	0.99	0.13	-3.48	28,28,28,28	0
4	CA	B	424	1/1	0.99	0.11	-3.94	13,13,13,13	0
4	CA	D	422	1/1	0.92	0.26	-	43,43,43,43	0
4	CA	P	1	1/1	0.99	0.09	-	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.