



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:31 am GMT

PDB ID : 4BLO
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI6 IN COMPLEX WITH ADP
Authors : El Omari, K.; Meier, C.; Kainov, D.; Sutton, G.; Grimes, J.M.; Poranen, M.M.; Bamford, D.H.; Tuma, R.; Stuart, D.I.; Mancini, E.J.
Deposited on : 2013-05-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

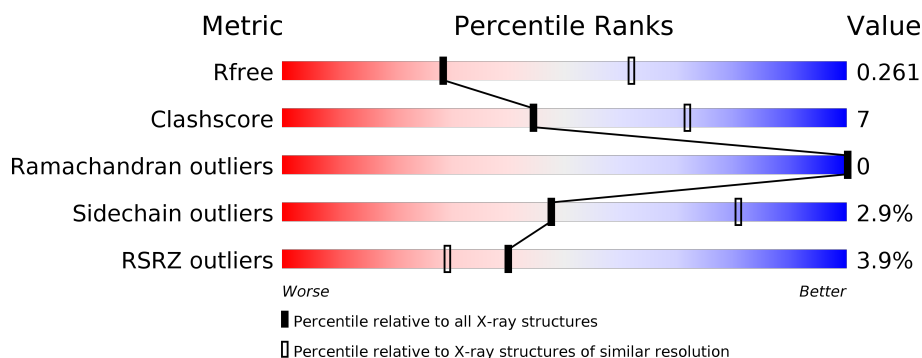
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	309	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	309	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	309	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	309	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	F	309	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	309	
1	H	309	
1	I	309	
1	J	309	
1	K	309	
1	L	309	

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
3	ADP	H	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24437 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 PACKAGING ENZYME P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2003	1276	335	382	10			
1	B	270	Total	C	N	O	S	0	0	0
			2011	1281	336	383	11			
1	C	270	Total	C	N	O	S	0	0	0
			2011	1281	336	383	11			
1	D	270	Total	C	N	O	S	0	0	0
			2011	1281	336	383	11			
1	E	269	Total	C	N	O	S	0	0	0
			2006	1278	335	382	11			
1	F	269	Total	C	N	O	S	0	0	0
			2006	1278	335	382	11			
1	G	268	Total	C	N	O	S	0	0	0
			1998	1274	333	380	11			
1	H	269	Total	C	N	O	S	0	0	0
			2003	1276	335	382	10			
1	I	269	Total	C	N	O	S	0	0	0
			2003	1276	335	382	10			
1	J	269	Total	C	N	O	S	0	0	0
			2006	1278	335	382	11			
1	K	269	Total	C	N	O	S	0	0	0
			2003	1276	335	382	10			
1	L	275	Total	C	N	O	S	0	0	0
			2040	1300	341	388	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

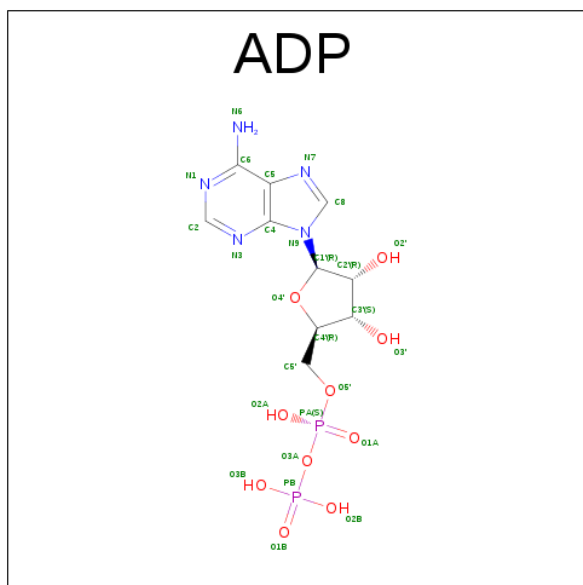
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	J	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		
2	K	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	I	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	L	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

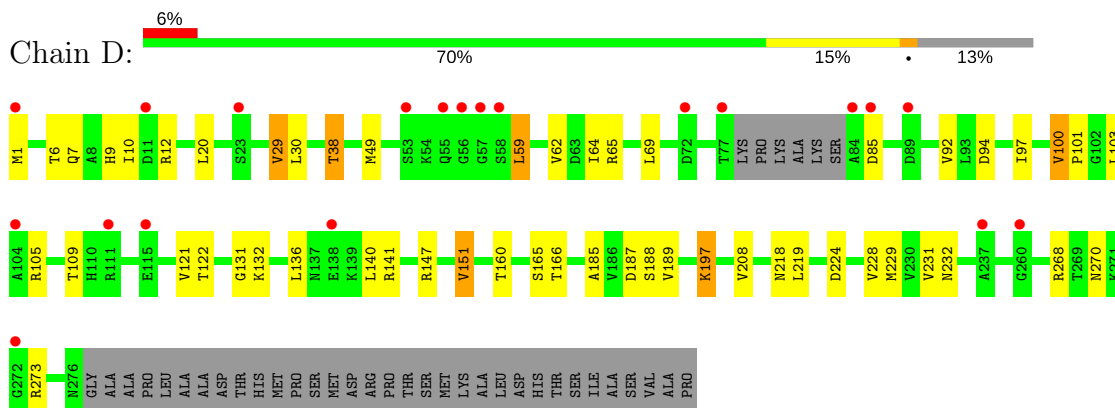
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



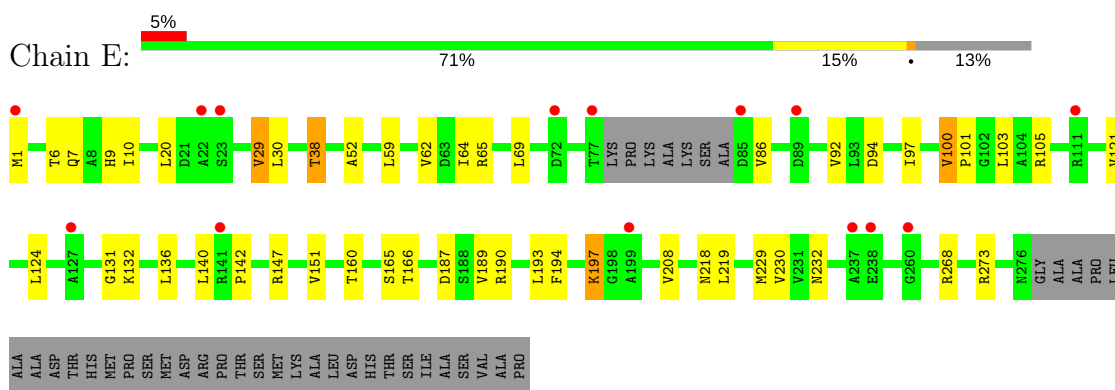
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

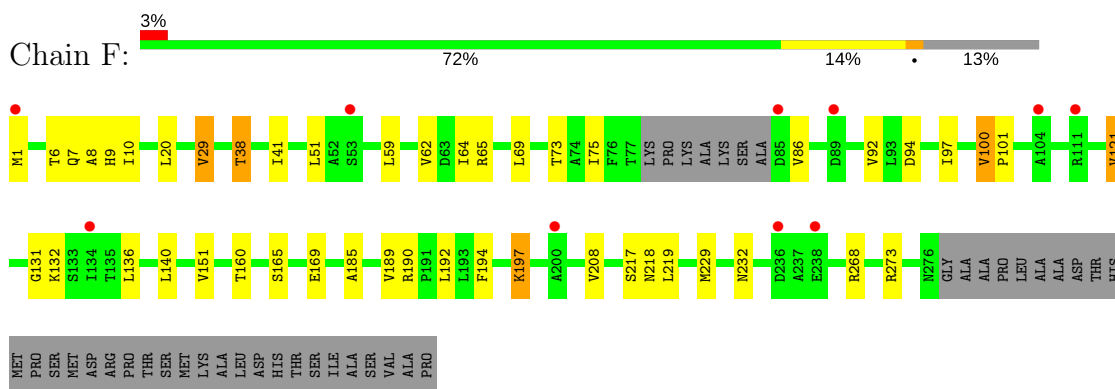
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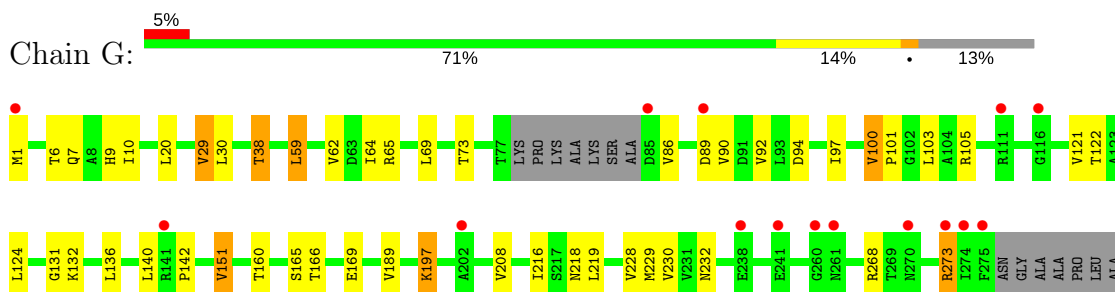
- Molecule 1: PACKAGING ENZYME P4



- Molecule 1: PACKAGING ENZYME P4

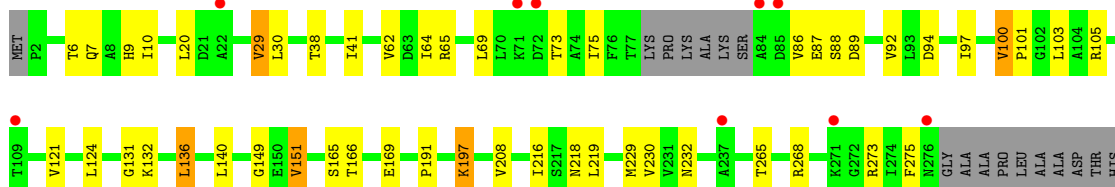


- Molecule 1: PACKAGING ENZYME P4



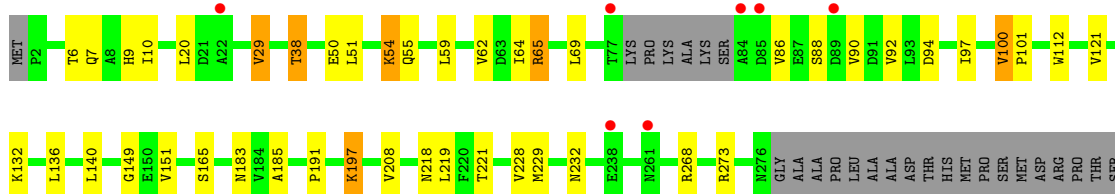
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• Molecule 1: PACKAGING ENZYME P4



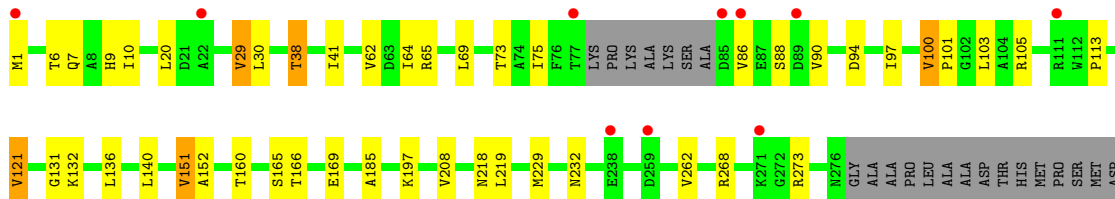
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• Molecule 1: PACKAGING ENZYME P4



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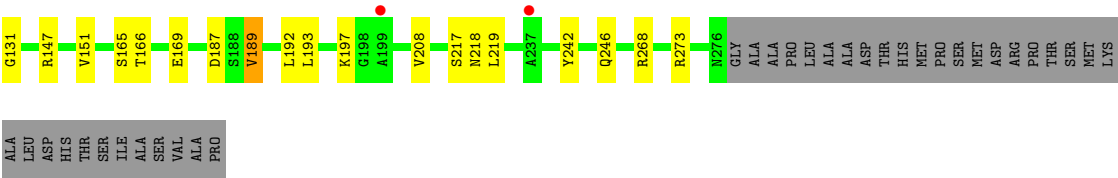
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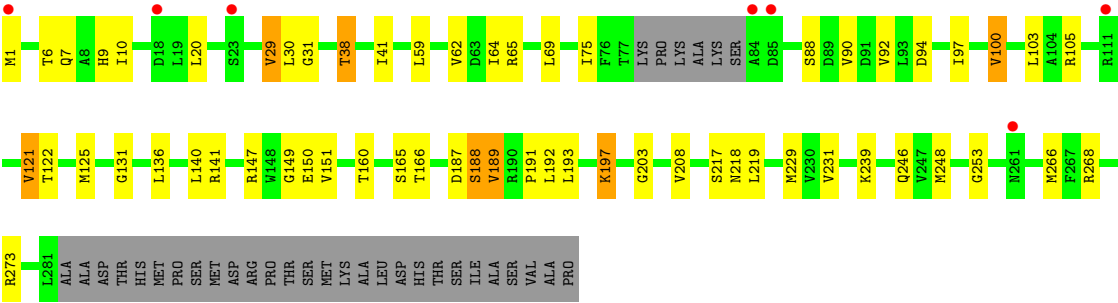
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• Molecule 1: PACKAGING ENZYME P4





● Molecule 1: PACKAGING ENZYME P4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.84Å 95.26Å 98.33Å 82.46° 86.17° 64.85°	Depositor
Resolution (Å)	19.99 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.80) 93.3 (20.00-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.79Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.217 , 0.244 0.235 , 0.261	Depositor DCC
R_{free} test set	3664 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24437	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, 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	A	0.47	0/2033	0.66	2/2767 (0.1%)
1	B	0.48	0/2041	0.67	2/2778 (0.1%)
1	C	0.44	0/2041	0.67	2/2778 (0.1%)
1	D	0.45	0/2041	0.66	2/2778 (0.1%)
1	E	0.44	0/2036	0.66	2/2771 (0.1%)
1	F	0.46	0/2036	0.66	2/2771 (0.1%)
1	G	0.46	0/2028	0.68	2/2760 (0.1%)
1	H	0.46	0/2033	0.66	2/2767 (0.1%)
1	I	0.48	0/2033	0.70	2/2767 (0.1%)
1	J	0.47	0/2036	0.68	2/2771 (0.1%)
1	K	0.46	0/2033	0.68	2/2767 (0.1%)
1	L	0.54	1/2071 (0.0%)	0.70	2/2820 (0.1%)
All	All	0.47	1/24462 (0.0%)	0.67	24/33295 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	31	GLY	C-N	10.48	1.58	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	VAL	CB-CA-C	-7.84	96.51	111.40
1	I	29	VAL	CB-CA-C	-7.83	96.53	111.40
1	J	29	VAL	CB-CA-C	-7.83	96.53	111.40
1	G	29	VAL	CB-CA-C	-7.82	96.53	111.40
1	K	29	VAL	CB-CA-C	-7.82	96.53	111.40
1	D	29	VAL	CB-CA-C	-7.82	96.54	111.40
1	L	29	VAL	CB-CA-C	-7.82	96.55	111.40
1	A	29	VAL	CB-CA-C	-7.82	96.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	29	VAL	CB-CA-C	-7.82	96.55	111.40
1	F	29	VAL	CB-CA-C	-7.81	96.55	111.40
1	E	29	VAL	CB-CA-C	-7.81	96.56	111.40
1	C	29	VAL	CB-CA-C	-7.80	96.58	111.40
1	H	29	VAL	N-CA-C	7.79	132.05	111.00
1	G	29	VAL	N-CA-C	7.79	132.03	111.00
1	E	29	VAL	N-CA-C	7.79	132.03	111.00
1	I	29	VAL	N-CA-C	7.79	132.02	111.00
1	K	29	VAL	N-CA-C	7.78	132.02	111.00
1	F	29	VAL	N-CA-C	7.78	132.01	111.00
1	D	29	VAL	N-CA-C	7.78	132.00	111.00
1	A	29	VAL	N-CA-C	7.78	132.00	111.00
1	C	29	VAL	N-CA-C	7.78	132.00	111.00
1	L	29	VAL	N-CA-C	7.78	132.00	111.00
1	J	29	VAL	N-CA-C	7.77	131.99	111.00
1	B	29	VAL	N-CA-C	7.77	131.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2003	0	2052	28	0
1	B	2011	0	2063	37	0
1	C	2011	0	2063	35	0
1	D	2011	0	2063	36	0
1	E	2006	0	2058	30	0
1	F	2006	0	2058	37	0
1	G	1998	0	2052	39	0
1	H	2003	0	2052	40	0
1	I	2003	0	2052	32	0
1	J	2006	0	2058	40	0
1	K	2003	0	2052	40	0
1	L	2040	0	2094	39	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	1	0
3	H	27	0	12	1	0
3	I	27	0	12	0	0
3	J	27	0	12	1	0
3	K	27	0	12	1	0
3	L	27	0	12	1	0
All	All	24437	0	24861	368	0

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 (368) 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:A:29:VAL:O	1:A:208:VAL:HG21	1.42	1.18
1:F:29:VAL:O	1:F:208:VAL:HG21	1.45	1.17
1:L:29:VAL:O	1:L:208:VAL:HG21	1.43	1.17
1:K:29:VAL:O	1:K:208:VAL:HG21	1.42	1.16
1:H:29:VAL:O	1:H:208:VAL:HG21	1.47	1.13
1:G:29:VAL:O	1:G:208:VAL:HG21	1.46	1.13
1:I:29:VAL:O	1:I:208:VAL:HG21	1.49	1.12
1:E:29:VAL:O	1:E:208:VAL:HG21	1.45	1.12
1:C:29:VAL:O	1:C:208:VAL:HG21	1.49	1.12
1:D:29:VAL:O	1:D:208:VAL:HG21	1.47	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:VAL:O	1:J:208:VAL:HG21	1.46	1.10
1:B:29:VAL:O	1:B:208:VAL:HG21	1.49	1.10
1:C:30:LEU:O	1:D:197:LYS:NZ	2.03	0.92
1:D:30:LEU:O	1:E:197:LYS:NZ	2.01	0.91
1:K:52:ALA:HA	1:K:59:LEU:HD11	1.51	0.91
1:J:88:SER:O	1:K:197:LYS:HD2	1.75	0.85
1:J:73:THR:HG21	1:J:169:GLU:CG	2.07	0.85
1:H:73:THR:HG21	1:H:169:GLU:CG	2.07	0.84
1:B:73:THR:HG21	1:B:169:GLU:CG	2.08	0.83
1:C:197:LYS:NZ	1:H:30:LEU:O	2.12	0.82
1:D:94:ASP:OD2	1:E:86:VAL:HG12	1.79	0.82
1:G:73:THR:HG21	1:G:169:GLU:CG	2.10	0.82
1:K:73:THR:HG21	1:K:169:GLU:CG	2.10	0.82
1:F:73:THR:HG21	1:F:169:GLU:CG	2.10	0.82
1:B:30:LEU:O	1:I:197:LYS:NZ	2.14	0.81
1:C:6:THR:H	1:C:9:HIS:HD2	1.31	0.78
1:K:6:THR:H	1:K:9:HIS:HD2	1.30	0.78
1:B:6:THR:H	1:B:9:HIS:HD2	1.31	0.77
1:G:6:THR:H	1:G:9:HIS:HD2	1.31	0.77
1:H:6:THR:H	1:H:9:HIS:HD2	1.33	0.76
1:L:6:THR:H	1:L:9:HIS:HD2	1.32	0.75
1:J:6:THR:H	1:J:9:HIS:HD2	1.34	0.75
1:J:90:VAL:O	1:K:197:LYS:HE3	1.87	0.75
1:G:89:ASP:OD1	1:H:88:SER:HB2	1.87	0.75
1:I:6:THR:H	1:I:9:HIS:HD2	1.33	0.74
1:D:6:THR:H	1:D:9:HIS:HD2	1.32	0.74
1:A:6:THR:H	1:A:9:HIS:HD2	1.34	0.74
1:C:86:VAL:HG12	1:H:94:ASP:OD2	1.89	0.73
1:E:52:ALA:HA	1:E:59:LEU:HD11	1.71	0.73
1:A:30:LEU:O	1:B:197:LYS:NZ	2.21	0.73
1:E:30:LEU:O	1:F:197:LYS:NZ	2.21	0.73
1:G:30:LEU:O	1:H:197:LYS:NZ	2.22	0.72
1:F:136:LEU:HA	1:F:140:LEU:HD12	1.74	0.70
1:H:73:THR:HG21	1:H:169:GLU:HG2	1.72	0.70
1:B:73:THR:HG21	1:B:169:GLU:HG3	1.74	0.70
1:C:136:LEU:HA	1:C:140:LEU:HD12	1.74	0.70
1:E:94:ASP:OD2	1:F:86:VAL:HG12	1.92	0.70
1:B:94:ASP:OD2	1:I:86:VAL:HG12	1.92	0.69
1:J:73:THR:HG21	1:J:169:GLU:HG3	1.73	0.69
1:F:94:ASP:OD2	1:G:86:VAL:HG12	1.93	0.69
1:A:136:LEU:HA	1:A:140:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:LEU:HA	1:I:140:LEU:HD12	1.75	0.69
1:E:136:LEU:HA	1:E:140:LEU:HD12	1.75	0.69
1:H:73:THR:HG21	1:H:169:GLU:HG3	1.75	0.68
1:K:73:THR:HG21	1:K:169:GLU:HG3	1.75	0.68
1:B:136:LEU:HA	1:B:140:LEU:HD12	1.76	0.68
1:G:136:LEU:HA	1:G:140:LEU:HD12	1.77	0.67
1:F:73:THR:HG21	1:F:169:GLU:HG2	1.75	0.67
1:G:73:THR:HG21	1:G:169:GLU:HG3	1.77	0.66
1:J:73:THR:HG21	1:J:169:GLU:HG2	1.78	0.66
1:E:6:THR:H	1:E:9:HIS:HD2	1.44	0.65
1:K:73:THR:HG21	1:K:169:GLU:HG2	1.79	0.65
1:D:101:PRO:HG3	1:E:165:SER:HB3	1.78	0.65
1:J:94:ASP:OD2	1:K:86:VAL:HG12	1.97	0.65
1:G:73:THR:HG21	1:G:169:GLU:HG2	1.79	0.64
1:C:101:PRO:HG3	1:D:165:SER:HB3	1.79	0.64
1:J:73:THR:CG2	1:J:169:GLU:HG3	2.28	0.63
1:A:94:ASP:OD2	1:B:86:VAL:HG12	1.98	0.63
1:J:90:VAL:O	1:K:197:LYS:CE	2.45	0.63
1:F:73:THR:HG21	1:F:169:GLU:HG3	1.79	0.63
1:H:136:LEU:HA	1:H:140:LEU:HD12	1.80	0.63
1:C:7:GLN:HA	1:C:10:ILE:HD12	1.80	0.63
1:B:73:THR:HG21	1:B:169:GLU:HG2	1.78	0.63
1:I:132:LYS:HE3	1:I:232:ASN:HB3	1.80	0.62
1:I:94:ASP:OD2	1:J:86:VAL:HG12	1.99	0.62
1:I:88:SER:O	1:J:197:LYS:HD2	2.00	0.62
1:B:73:THR:CG2	1:B:169:GLU:HG3	2.30	0.61
1:L:189:VAL:HG13	1:L:193:LEU:HD13	1.81	0.61
1:J:73:THR:CG2	1:J:169:GLU:CG	2.79	0.61
1:B:101:PRO:HG3	1:I:165:SER:HB3	1.83	0.60
1:B:89:ASP:OD1	1:I:88:SER:HB2	2.02	0.60
1:K:73:THR:CG2	1:K:169:GLU:HG3	2.32	0.59
1:C:88:SER:HB2	1:H:89:ASP:OD1	2.02	0.59
1:K:52:ALA:CA	1:K:59:LEU:HD11	2.28	0.59
1:G:94:ASP:OD2	1:H:86:VAL:HG12	2.03	0.59
1:C:94:ASP:OD2	1:D:85:ASP:HA	2.02	0.59
1:F:6:THR:H	1:F:9:HIS:HD2	1.51	0.58
1:J:7:GLN:HA	1:J:10:ILE:HD12	1.85	0.58
1:G:73:THR:CG2	1:G:169:GLU:HG3	2.32	0.58
1:L:203:GLY:HA2	1:L:239:LYS:HD2	1.85	0.58
1:B:205:ILE:HD11	1:B:210:TYR:OH	2.02	0.58
1:B:73:THR:CG2	1:B:169:GLU:CG	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:THR:CG2	1:G:169:GLU:CG	2.82	0.57
1:L:136:LEU:HA	1:L:140:LEU:HD12	1.86	0.57
1:B:7:GLN:HA	1:B:10:ILE:HD12	1.86	0.57
1:D:62:VAL:O	1:D:65:ARG:HD2	2.05	0.57
1:F:73:THR:CG2	1:F:169:GLU:CG	2.82	0.57
1:K:62:VAL:O	1:K:65:ARG:HD2	2.04	0.57
1:G:62:VAL:O	1:G:65:ARG:HD2	2.04	0.56
1:L:7:GLN:HA	1:L:10:ILE:HD12	1.88	0.56
1:A:7:GLN:HA	1:A:10:ILE:HD12	1.88	0.56
1:F:73:THR:CG2	1:F:169:GLU:HG3	2.34	0.56
1:G:7:GLN:HA	1:G:10:ILE:HD12	1.88	0.56
1:H:62:VAL:O	1:H:65:ARG:HD2	2.06	0.56
1:H:73:THR:CG2	1:H:169:GLU:CG	2.83	0.56
1:H:73:THR:CG2	1:H:169:GLU:HG3	2.35	0.56
1:I:7:GLN:HA	1:I:10:ILE:HD12	1.87	0.56
1:K:189:VAL:HG13	1:K:193:LEU:HD13	1.88	0.56
1:C:121:VAL:HG12	1:C:217:SER:OG	2.06	0.56
1:F:6:THR:HG22	1:F:8:ALA:H	1.71	0.56
1:A:62:VAL:O	1:A:65:ARG:HD2	2.06	0.55
1:D:12:ARG:HH22	1:D:224:ASP:HB2	1.70	0.55
1:F:62:VAL:O	1:F:65:ARG:HD2	2.06	0.55
1:J:101:PRO:HG3	1:K:165:SER:HB3	1.87	0.55
1:K:7:GLN:HA	1:K:10:ILE:HD12	1.88	0.55
1:B:62:VAL:O	1:B:65:ARG:HD2	2.06	0.55
1:I:50:GLU:O	1:I:54:LYS:HG2	2.06	0.55
1:J:62:VAL:O	1:J:65:ARG:HD2	2.07	0.55
1:K:88:SER:O	1:L:197:LYS:HD2	2.06	0.55
1:F:7:GLN:HA	1:F:10:ILE:HD12	1.88	0.55
1:D:7:GLN:HA	1:D:10:ILE:HD12	1.89	0.55
1:C:165:SER:HB3	1:H:101:PRO:HG3	1.90	0.54
1:C:62:VAL:O	1:C:65:ARG:HD2	2.07	0.54
1:E:62:VAL:O	1:E:65:ARG:HD2	2.06	0.54
1:L:62:VAL:O	1:L:65:ARG:HD2	2.07	0.54
1:C:53:SER:O	1:C:55:GLN:O	2.24	0.54
1:F:6:THR:H	1:F:9:HIS:CD2	2.26	0.54
1:I:62:VAL:O	1:I:65:ARG:HD2	2.08	0.54
1:K:59:LEU:HD23	1:K:64:ILE:CG2	2.38	0.54
1:C:39:VAL:HG11	1:J:262:VAL:O	2.08	0.54
1:K:131:GLY:HA2	3:K:401:ADP:H5'1	1.90	0.54
1:F:20:LEU:HB3	1:F:38:THR:HG23	1.90	0.53
1:A:30:LEU:HD12	1:A:197:LYS:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:GLN:HA	1:E:10:ILE:HD12	1.89	0.53
1:H:7:GLN:HA	1:H:10:ILE:HD12	1.89	0.53
1:K:73:THR:CG2	1:K:169:GLU:CG	2.82	0.53
1:J:41:ILE:HD11	1:J:75:ILE:HD11	1.90	0.53
1:E:190:ARG:HD2	1:E:194:PHE:CE2	2.44	0.53
1:A:166:THR:HA	1:L:97:ILE:O	2.09	0.53
1:G:218:ASN:HD21	1:H:151:VAL:HA	1.73	0.52
1:E:189:VAL:HG13	1:E:193:LEU:HD13	1.92	0.52
1:B:92:VAL:CG1	1:B:97:ILE:HD11	2.40	0.52
1:C:20:LEU:HB3	1:C:38:THR:HG23	1.91	0.52
1:D:121:VAL:HG21	1:D:229:MET:HE2	1.92	0.51
1:G:101:PRO:HG3	1:H:165:SER:HB3	1.92	0.51
1:A:197:LYS:HE3	1:L:90:VAL:O	2.10	0.51
1:A:121:VAL:HG21	1:A:229:MET:HE2	1.92	0.51
1:I:20:LEU:HB3	1:I:38:THR:HG23	1.92	0.51
1:K:20:LEU:HB3	1:K:38:THR:HG23	1.91	0.51
1:K:89:ASP:OD1	1:L:88:SER:HB2	2.11	0.51
1:I:268:ARG:HG2	1:I:273:ARG:HG2	1.92	0.51
1:E:20:LEU:HB3	1:E:38:THR:HG23	1.92	0.51
1:H:92:VAL:HG12	1:H:97:ILE:HD11	1.91	0.51
1:J:20:LEU:HB3	1:J:38:THR:HG23	1.93	0.51
1:C:92:VAL:HG12	1:C:97:ILE:HD11	1.91	0.51
1:B:20:LEU:HB3	1:B:38:THR:HG23	1.91	0.51
1:C:218:ASN:HD21	1:D:151:VAL:HA	1.75	0.51
1:B:268:ARG:HG2	1:B:273:ARG:HG2	1.92	0.51
1:L:121:VAL:HG21	1:L:229:MET:HE2	1.92	0.51
1:D:20:LEU:HB3	1:D:38:THR:HG23	1.91	0.51
1:K:59:LEU:HD23	1:K:64:ILE:HG21	1.93	0.50
1:E:101:PRO:HG3	1:F:165:SER:HB3	1.92	0.50
1:K:268:ARG:HG2	1:K:273:ARG:HG2	1.94	0.50
1:I:218:ASN:HD21	1:J:151:VAL:HA	1.76	0.50
1:A:197:LYS:HD2	1:L:88:SER:O	2.12	0.50
1:C:151:VAL:HA	1:H:218:ASN:HD21	1.77	0.50
1:L:189:VAL:HG11	1:L:231:VAL:HG12	1.94	0.50
1:L:20:LEU:HB3	1:L:38:THR:HG23	1.94	0.50
1:A:101:PRO:HG3	1:B:165:SER:HB3	1.94	0.49
1:D:136:LEU:HD11	1:D:185:ALA:HB1	1.93	0.49
1:J:268:ARG:HG2	1:J:273:ARG:HG2	1.94	0.49
1:G:20:LEU:HB3	1:G:38:THR:HG23	1.93	0.49
1:I:221:THR:HG21	1:J:152:ALA:HB2	1.95	0.49
1:A:20:LEU:HB3	1:A:38:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:MET:HE2	1:L:266:MET:HB2	1.95	0.49
1:H:268:ARG:HG2	1:H:273:ARG:HG2	1.94	0.49
1:H:265:THR:O	1:H:275:PHE:O	2.30	0.49
1:B:1:MET:O	1:B:160:THR:HG23	2.13	0.49
1:C:268:ARG:HG2	1:C:273:ARG:HG2	1.94	0.49
1:H:92:VAL:CG1	1:H:97:ILE:HD11	2.42	0.49
1:G:97:ILE:O	1:H:166:THR:HA	2.12	0.49
1:E:268:ARG:HG2	1:E:273:ARG:HG2	1.94	0.49
1:G:1:MET:O	1:G:160:THR:HG23	2.13	0.49
1:J:136:LEU:O	1:J:140:LEU:HB2	2.12	0.49
1:G:122:THR:HB	1:G:228:VAL:HG22	1.95	0.49
1:G:124:LEU:HB3	1:G:230:VAL:HA	1.95	0.49
1:L:92:VAL:HG12	1:L:97:ILE:HD11	1.95	0.49
1:L:147:ARG:HA	1:L:187:ASP:O	2.12	0.48
1:D:136:LEU:O	1:D:140:LEU:HB2	2.13	0.48
1:G:132:LYS:HE3	1:G:232:ASN:HB2	1.95	0.48
1:D:268:ARG:HG2	1:D:273:ARG:HG2	1.96	0.48
1:A:268:ARG:HG2	1:A:273:ARG:HG2	1.96	0.48
1:A:97:ILE:O	1:B:166:THR:HA	2.14	0.48
1:H:132:LYS:HE3	1:H:232:ASN:HB2	1.96	0.48
1:K:97:ILE:O	1:L:166:THR:HA	2.14	0.48
1:J:1:MET:O	1:J:160:THR:HG23	2.14	0.48
1:K:29:VAL:O	1:K:208:VAL:CG2	2.36	0.48
1:L:122:THR:HA	1:L:253:GLY:O	2.13	0.48
1:J:73:THR:CG2	1:J:169:GLU:HG2	2.43	0.47
1:F:1:MET:O	1:F:160:THR:HG23	2.14	0.47
1:C:132:LYS:HE3	1:C:232:ASN:HB2	1.97	0.47
1:H:41:ILE:HD11	1:H:75:ILE:HD11	1.96	0.47
1:D:92:VAL:HG12	1:D:97:ILE:HD11	1.96	0.47
1:H:216:ILE:HG21	1:H:229:MET:HE1	1.95	0.47
1:A:145:LEU:O	1:A:161:ALA:HA	2.14	0.47
1:D:109:THR:HG21	1:D:270:ASN:HD22	1.79	0.47
1:J:132:LYS:HE3	1:J:232:ASN:HB2	1.96	0.47
1:D:1:MET:O	1:D:160:THR:HG23	2.14	0.47
1:I:101:PRO:HG3	1:J:165:SER:HB3	1.97	0.47
1:G:92:VAL:HG12	1:G:97:ILE:HD11	1.97	0.47
1:D:6:THR:H	1:D:9:HIS:CD2	2.23	0.46
1:F:92:VAL:HG12	1:F:97:ILE:HD11	1.96	0.46
1:L:1:MET:O	1:L:160:THR:HG23	2.15	0.46
1:K:147:ARG:HA	1:K:187:ASP:O	2.16	0.46
1:L:100:VAL:HG11	1:L:219:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:VAL:HG21	1:E:229:MET:HE2	1.98	0.46
1:E:52:ALA:CA	1:E:59:LEU:HD11	2.44	0.46
1:C:121:VAL:HG21	1:C:229:MET:HE2	1.97	0.46
1:C:100:VAL:HG11	1:C:219:LEU:HD13	1.98	0.46
1:F:268:ARG:HG2	1:F:273:ARG:HG2	1.96	0.46
1:H:100:VAL:HG11	1:H:219:LEU:HD13	1.98	0.46
1:B:132:LYS:HE3	1:B:232:ASN:HB2	1.96	0.46
1:E:1:MET:O	1:E:160:THR:HG23	2.16	0.45
1:F:97:ILE:O	1:G:166:THR:HA	2.16	0.45
1:E:132:LYS:HE3	1:E:232:ASN:HB2	1.99	0.45
1:B:6:THR:H	1:B:9:HIS:CD2	2.22	0.45
1:I:51:LEU:HD23	1:I:59:LEU:HD22	1.99	0.45
1:D:132:LYS:HE3	1:D:232:ASN:HB2	1.98	0.45
1:C:1:MET:O	1:C:160:THR:HG23	2.17	0.45
1:A:100:VAL:HG11	1:A:219:LEU:HD13	1.99	0.45
1:F:131:GLY:HA2	3:F:401:ADP:H5'1	1.99	0.45
1:F:190:ARG:HD2	1:F:194:PHE:CE2	2.52	0.45
1:G:216:ILE:HG21	1:G:229:MET:HE1	1.99	0.45
1:G:131:GLY:HA2	3:G:401:ADP:H5'1	1.99	0.45
1:J:136:LEU:HD11	1:J:185:ALA:HB1	1.98	0.45
1:A:234:MET:HE1	1:L:246:GLN:OE1	2.16	0.45
1:G:268:ARG:HG2	1:G:273:ARG:HG3	1.99	0.45
1:A:218:ASN:HD21	1:B:151:VAL:HA	1.82	0.45
1:G:100:VAL:HG11	1:G:219:LEU:HD13	1.99	0.45
1:F:6:THR:HB	1:F:9:HIS:CD2	2.53	0.44
1:I:64:ILE:HA	1:I:69:LEU:HD11	1.99	0.44
1:J:90:VAL:H	1:K:197:LYS:HE3	1.82	0.44
1:C:136:LEU:HD11	1:C:185:ALA:HB1	1.99	0.44
1:A:88:SER:O	1:B:197:LYS:HD2	2.18	0.44
1:E:147:ARG:HA	1:E:187:ASP:O	2.17	0.44
1:B:100:VAL:HG11	1:B:219:LEU:HD13	2.00	0.44
1:I:92:VAL:CG1	1:I:97:ILE:HD11	2.48	0.44
1:L:131:GLY:HA2	3:L:401:ADP:H5'1	1.99	0.44
1:B:92:VAL:HG12	1:B:97:ILE:HD11	2.00	0.44
1:F:121:VAL:HG21	1:F:229:MET:HE2	1.98	0.44
1:L:30:LEU:HD12	1:L:197:LYS:O	2.17	0.44
1:F:64:ILE:HA	1:F:69:LEU:HD11	2.00	0.44
1:L:41:ILE:HD11	1:L:75:ILE:HD11	1.99	0.44
1:D:131:GLY:HA2	3:D:401:ADP:H5'1	2.01	0.43
1:E:100:VAL:HG11	1:E:219:LEU:HD13	2.00	0.43
1:E:92:VAL:HG12	1:E:97:ILE:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:LEU:HB3	1:H:38:THR:HB	2.00	0.43
1:I:55:GLN:OE1	1:I:59:LEU:HD23	2.18	0.43
1:D:147:ARG:HA	1:D:187:ASP:O	2.18	0.43
1:D:64:ILE:HA	1:D:69:LEU:HD11	2.00	0.43
1:H:73:THR:CG2	1:H:169:GLU:HG2	2.43	0.43
1:L:100:VAL:CG2	1:L:218:ASN:HB2	2.48	0.43
1:B:136:LEU:HD11	1:B:185:ALA:HB1	2.00	0.43
1:B:30:LEU:HD12	1:B:197:LYS:O	2.18	0.43
1:D:100:VAL:HG11	1:D:219:LEU:HD13	2.00	0.43
1:E:103:LEU:HD22	1:E:105:ARG:HG2	2.00	0.43
1:E:131:GLY:HA2	3:E:401:ADP:H5'1	2.00	0.43
1:F:73:THR:CG2	1:F:169:GLU:HG2	2.43	0.43
1:F:92:VAL:CG1	1:F:97:ILE:HD11	2.48	0.43
1:G:64:ILE:HA	1:G:69:LEU:HD11	2.01	0.43
1:I:90:VAL:O	1:J:197:LYS:HE3	2.18	0.43
1:B:64:ILE:HA	1:B:69:LEU:HD11	2.00	0.43
1:A:131:GLY:HA2	3:A:401:ADP:H5'1	2.00	0.43
1:C:6:THR:H	1:C:9:HIS:CD2	2.22	0.43
1:H:64:ILE:HA	1:H:69:LEU:HD11	2.01	0.43
1:I:100:VAL:HG11	1:I:219:LEU:HD13	2.01	0.43
1:K:64:ILE:HA	1:K:69:LEU:HD11	1.99	0.43
1:I:149:GLY:HA3	1:I:191:PRO:HG3	2.01	0.43
1:J:64:ILE:HA	1:J:69:LEU:HD11	2.00	0.43
1:K:98:TYR:HA	1:L:165:SER:O	2.19	0.43
1:C:64:ILE:HA	1:C:69:LEU:HD11	2.01	0.43
1:K:121:VAL:HG12	1:K:217:SER:HB2	2.00	0.43
1:L:149:GLY:HA3	1:L:191:PRO:HG3	2.00	0.43
1:F:101:PRO:HG3	1:G:165:SER:HB3	2.01	0.43
1:I:197:LYS:H	1:I:197:LYS:HG2	1.63	0.43
1:J:100:VAL:HG11	1:J:219:LEU:HD13	2.01	0.43
1:J:30:LEU:HD12	1:J:197:LYS:O	2.19	0.43
1:K:242:TYR:O	1:K:246:GLN:HG2	2.19	0.43
1:L:141:ARG:NH1	1:L:141:ARG:HB3	2.34	0.43
1:A:136:LEU:HD11	1:A:185:ALA:HB1	2.00	0.42
1:D:92:VAL:CG1	1:D:97:ILE:HD11	2.49	0.42
1:I:92:VAL:HG12	1:I:97:ILE:HD11	2.01	0.42
1:C:131:GLY:HA2	3:C:401:ADP:H5'1	2.01	0.42
1:H:100:VAL:CG2	1:H:218:ASN:HB2	2.49	0.42
1:K:103:LEU:HD22	1:K:105:ARG:HG2	2.01	0.42
1:B:73:THR:CG2	1:B:169:GLU:HG2	2.46	0.42
1:G:30:LEU:HD12	1:G:197:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:PRO:HG3	1:L:165:SER:HB3	1.99	0.42
1:K:100:VAL:HG11	1:K:219:LEU:HD13	2.00	0.42
1:B:114:SER:O	1:B:117:ILE:HG22	2.19	0.42
1:B:131:GLY:HA2	3:B:401:ADP:H5'1	2.01	0.42
1:F:41:ILE:HD11	1:F:75:ILE:HD11	2.01	0.42
1:L:268:ARG:HG2	1:L:273:ARG:HG2	2.02	0.42
1:E:100:VAL:CG2	1:E:218:ASN:HB2	2.50	0.42
1:A:197:LYS:CD	1:L:88:SER:O	2.68	0.42
1:A:64:ILE:HA	1:A:69:LEU:HD11	2.01	0.42
1:D:103:LEU:HD22	1:D:105:ARG:HG2	2.01	0.42
1:D:189:VAL:HG11	1:D:231:VAL:HG12	2.01	0.42
1:E:64:ILE:HA	1:E:69:LEU:HD11	2.01	0.42
1:F:100:VAL:CG2	1:F:218:ASN:HB2	2.50	0.42
1:F:136:LEU:HD11	1:F:185:ALA:HB1	2.01	0.42
1:F:100:VAL:HG11	1:F:219:LEU:HD13	2.01	0.42
1:H:103:LEU:HD22	1:H:105:ARG:HG2	2.02	0.42
1:A:100:VAL:CG2	1:A:218:ASN:HB2	2.50	0.42
1:F:132:LYS:HE3	1:F:232:ASN:HB2	2.01	0.42
1:H:131:GLY:HA2	3:H:401:ADP:H5'1	2.01	0.42
1:L:103:LEU:HD22	1:L:105:ARG:HG2	2.02	0.42
1:A:121:VAL:HG12	1:A:217:SER:HB2	2.02	0.42
1:C:166:THR:HA	1:H:97:ILE:O	2.19	0.42
1:J:131:GLY:HA2	3:J:401:ADP:H5'1	2.02	0.42
1:K:100:VAL:CG2	1:K:218:ASN:HB2	2.50	0.41
1:C:100:VAL:CG2	1:C:218:ASN:HB2	2.50	0.41
1:C:97:ILE:O	1:D:166:THR:HA	2.20	0.41
1:D:10:ILE:HG12	1:D:49:MET:HE1	2.02	0.41
1:G:73:THR:CG2	1:G:169:GLU:HG2	2.45	0.41
1:I:136:LEU:HD11	1:I:185:ALA:HB1	2.02	0.41
1:L:64:ILE:HA	1:L:69:LEU:HD11	2.01	0.41
1:F:218:ASN:HD21	1:G:151:VAL:HA	1.85	0.41
1:J:97:ILE:O	1:K:166:THR:HA	2.19	0.41
1:K:73:THR:CG2	1:K:169:GLU:HG2	2.45	0.41
1:G:103:LEU:HD22	1:G:105:ARG:HG2	2.01	0.41
1:H:149:GLY:HA3	1:H:191:PRO:HG3	2.02	0.41
1:J:103:LEU:HD22	1:J:105:ARG:HG2	2.02	0.41
1:G:92:VAL:CG1	1:G:97:ILE:HD11	2.50	0.41
1:L:121:VAL:HG12	1:L:217:SER:HB2	2.02	0.41
1:D:122:THR:HB	1:D:228:VAL:HG22	2.02	0.41
1:F:121:VAL:HG12	1:F:217:SER:HB2	2.01	0.41
1:G:6:THR:H	1:G:9:HIS:CD2	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:VAL:HG21	1:J:229:MET:HE2	2.02	0.41
1:D:97:ILE:O	1:E:166:THR:HA	2.21	0.41
1:G:92:VAL:HG22	1:H:197:LYS:HE3	2.01	0.41
1:I:140:LEU:HD13	1:I:228:VAL:HG11	2.03	0.41
1:C:187:ASP:HA	1:C:188:SER:HA	1.84	0.41
1:C:30:LEU:HD12	1:C:197:LYS:O	2.21	0.41
1:D:59:LEU:HA	1:D:59:LEU:HD12	1.94	0.41
1:I:121:VAL:HG21	1:I:229:MET:HE2	2.03	0.41
1:I:97:ILE:O	1:J:166:THR:HA	2.20	0.41
1:K:6:THR:H	1:K:9:HIS:CD2	2.21	0.41
1:C:92:VAL:CG1	1:C:97:ILE:HD11	2.51	0.41
1:D:100:VAL:HA	1:D:101:PRO:HD3	1.98	0.41
1:G:59:LEU:HA	1:G:59:LEU:HD12	1.92	0.41
1:D:100:VAL:CG2	1:D:218:ASN:HB2	2.51	0.41
1:I:112:TRP:CE3	1:I:183:ASN:HB3	2.56	0.41
1:J:100:VAL:CG2	1:J:218:ASN:HB2	2.50	0.41
1:L:248:MET:CE	1:L:266:MET:HB2	2.51	0.41
1:G:90:VAL:HA	1:H:87:GLU:HA	2.03	0.40
1:K:100:VAL:HA	1:K:101:PRO:HD3	1.98	0.40
1:L:150:GLU:OE2	1:L:188:SER:HB2	2.21	0.40
1:A:216:ILE:HG21	1:A:229:MET:HE2	2.03	0.40
1:F:51:LEU:HD23	1:F:59:LEU:HD22	2.02	0.40
1:H:124:LEU:HB3	1:H:230:VAL:HA	2.03	0.40
1:B:197:LYS:H	1:B:197:LYS:HG2	1.61	0.40
1:C:1:MET:O	1:C:159:ASP:HB2	2.21	0.40
1:L:92:VAL:CG1	1:L:97:ILE:HD11	2.51	0.40
1:B:135:THR:HA	1:B:139:LYS:HE3	2.04	0.40
1:E:100:VAL:HG22	1:E:218:ASN:HB2	2.04	0.40
1:E:124:LEU:HB3	1:E:230:VAL:HA	2.04	0.40
1:J:113:PRO:HB3	1:J:140:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/309 (86%)	260 (98%)	5 (2%)	0	100	100
1	B	266/309 (86%)	261 (98%)	5 (2%)	0	100	100
1	C	266/309 (86%)	258 (97%)	8 (3%)	0	100	100
1	D	266/309 (86%)	257 (97%)	9 (3%)	0	100	100
1	E	265/309 (86%)	260 (98%)	5 (2%)	0	100	100
1	F	265/309 (86%)	259 (98%)	6 (2%)	0	100	100
1	G	264/309 (85%)	257 (97%)	7 (3%)	0	100	100
1	H	265/309 (86%)	259 (98%)	6 (2%)	0	100	100
1	I	265/309 (86%)	261 (98%)	4 (2%)	0	100	100
1	J	265/309 (86%)	260 (98%)	5 (2%)	0	100	100
1	K	265/309 (86%)	256 (97%)	9 (3%)	0	100	100
1	L	271/309 (88%)	266 (98%)	5 (2%)	0	100	100
All	All	3188/3708 (86%)	3114 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/250 (88%)	213 (97%)	6 (3%)	50	83
1	B	220/250 (88%)	216 (98%)	4 (2%)	64	90
1	C	220/250 (88%)	215 (98%)	5 (2%)	56	86
1	D	220/250 (88%)	213 (97%)	7 (3%)	44	78
1	E	220/250 (88%)	215 (98%)	5 (2%)	56	86
1	F	220/250 (88%)	213 (97%)	7 (3%)	44	78
1	G	219/250 (88%)	210 (96%)	9 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	219/250 (88%)	214 (98%)	5 (2%)	56	86
1	I	219/250 (88%)	213 (97%)	6 (3%)	50	83
1	J	220/250 (88%)	216 (98%)	4 (2%)	64	90
1	K	219/250 (88%)	212 (97%)	7 (3%)	44	78
1	L	222/250 (89%)	211 (95%)	11 (5%)	28	62
All	All	2637/3000 (88%)	2561 (97%)	76 (3%)	48	81

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	59	LEU
1	A	100	VAL
1	A	121	VAL
1	A	151	VAL
1	A	189	VAL
1	B	38	THR
1	B	100	VAL
1	B	151	VAL
1	B	197	LYS
1	C	38	THR
1	C	59	LEU
1	C	100	VAL
1	C	151	VAL
1	C	197	LYS
1	D	38	THR
1	D	59	LEU
1	D	100	VAL
1	D	141	ARG
1	D	151	VAL
1	D	188	SER
1	D	197	LYS
1	E	38	THR
1	E	100	VAL
1	E	142	PRO
1	E	151	VAL
1	E	197	LYS
1	F	38	THR
1	F	100	VAL
1	F	121	VAL

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Mol	Chain	Res	Type
1	F	151	VAL
1	F	189	VAL
1	F	192	LEU
1	F	197	LYS
1	G	38	THR
1	G	59	LEU
1	G	100	VAL
1	G	121	VAL
1	G	142	PRO
1	G	151	VAL
1	G	189	VAL
1	G	197	LYS
1	G	273	ARG
1	H	100	VAL
1	H	121	VAL
1	H	136	LEU
1	H	151	VAL
1	H	197	LYS
1	I	38	THR
1	I	54	LYS
1	I	65	ARG
1	I	100	VAL
1	I	151	VAL
1	I	197	LYS
1	J	38	THR
1	J	100	VAL
1	J	121	VAL
1	J	151	VAL
1	K	38	THR
1	K	92	VAL
1	K	94	ASP
1	K	100	VAL
1	K	151	VAL
1	K	189	VAL
1	K	192	LEU
1	L	38	THR
1	L	59	LEU
1	L	94	ASP
1	L	100	VAL
1	L	121	VAL
1	L	125	MET
1	L	151	VAL

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Mol	Chain	Res	Type
1	L	188	SER
1	L	189	VAL
1	L	192	LEU
1	L	197	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	37	ASN
1	A	183	ASN
1	A	218	ASN
1	B	9	HIS
1	B	37	ASN
1	B	183	ASN
1	B	218	ASN
1	C	9	HIS
1	C	37	ASN
1	C	183	ASN
1	C	218	ASN
1	D	9	HIS
1	D	37	ASN
1	D	183	ASN
1	D	218	ASN
1	E	9	HIS
1	E	37	ASN
1	E	183	ASN
1	E	218	ASN
1	F	9	HIS
1	F	37	ASN
1	F	183	ASN
1	F	218	ASN
1	G	9	HIS
1	G	37	ASN
1	G	183	ASN
1	G	218	ASN
1	H	9	HIS
1	H	37	ASN
1	H	183	ASN
1	H	218	ASN
1	I	9	HIS
1	I	37	ASN

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Mol	Chain	Res	Type
1	I	218	ASN
1	J	9	HIS
1	J	37	ASN
1	J	183	ASN
1	J	218	ASN
1	K	9	HIS
1	K	37	ASN
1	K	183	ASN
1	K	218	ASN
1	L	9	HIS
1	L	37	ASN
1	L	183	ASN
1	L	218	ASN
1	L	232	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	401	2	25,29,29	0.70	0	24,45,45	0.53	0
3	ADP	B	401	2	25,29,29	0.66	0	24,45,45	0.54	0
3	ADP	C	401	2	25,29,29	0.63	0	24,45,45	0.58	0
3	ADP	D	401	2	25,29,29	0.61	0	24,45,45	0.54	0
3	ADP	E	401	2	25,29,29	0.67	0	24,45,45	0.52	0
3	ADP	F	401	2	25,29,29	0.63	0	24,45,45	0.54	0
3	ADP	G	401	2	25,29,29	0.64	0	24,45,45	0.56	0
3	ADP	H	401	2	25,29,29	0.63	0	24,45,45	0.62	0
3	ADP	I	401	2	25,29,29	0.59	0	24,45,45	0.55	0
3	ADP	J	401	2	25,29,29	0.64	0	24,45,45	0.54	0
3	ADP	K	401	2	25,29,29	0.65	0	24,45,45	0.49	0
3	ADP	L	401	2	25,29,29	0.66	0	24,45,45	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	401	2	-	0/12/32/32	0/3/3/3
3	ADP	B	401	2	-	0/12/32/32	0/3/3/3
3	ADP	C	401	2	-	0/12/32/32	0/3/3/3
3	ADP	D	401	2	-	0/12/32/32	0/3/3/3
3	ADP	E	401	2	-	0/12/32/32	0/3/3/3
3	ADP	F	401	2	-	0/12/32/32	0/3/3/3
3	ADP	G	401	2	-	0/12/32/32	0/3/3/3
3	ADP	H	401	2	-	0/12/32/32	0/3/3/3
3	ADP	I	401	2	-	0/12/32/32	0/3/3/3
3	ADP	J	401	2	-	0/12/32/32	0/3/3/3
3	ADP	K	401	2	-	0/12/32/32	0/3/3/3
3	ADP	L	401	2	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	1	0
3	B	401	ADP	1	0
3	C	401	ADP	1	0
3	D	401	ADP	1	0
3	E	401	ADP	1	0
3	F	401	ADP	1	0
3	G	401	ADP	1	0
3	H	401	ADP	1	0
3	J	401	ADP	1	0
3	K	401	ADP	1	0
3	L	401	ADP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/309 (87%)	-0.19	6 (2%) 62 52	22, 44, 77, 113	0
1	B	270/309 (87%)	-0.19	8 (2%) 51 39	23, 41, 73, 100	0
1	C	270/309 (87%)	0.24	13 (4%) 31 21	26, 64, 107, 130	0
1	D	270/309 (87%)	0.30	20 (7%) 15 8	26, 73, 112, 158	0
1	E	269/309 (87%)	0.16	14 (5%) 28 19	26, 63, 98, 115	0
1	F	269/309 (87%)	0.05	10 (3%) 42 31	26, 54, 87, 120	0
1	G	268/309 (86%)	0.06	15 (5%) 25 16	26, 52, 93, 137	0
1	H	269/309 (87%)	0.05	9 (3%) 47 36	26, 55, 92, 123	0
1	I	269/309 (87%)	-0.20	7 (2%) 56 45	25, 41, 73, 95	0
1	J	269/309 (87%)	-0.14	10 (3%) 42 31	26, 44, 80, 107	0
1	K	269/309 (87%)	-0.15	6 (2%) 62 52	26, 45, 81, 106	0
1	L	275/309 (88%)	-0.15	7 (2%) 58 47	26, 48, 82, 101	0
All	All	3236/3708 (87%)	-0.01	125 (3%) 40 29	22, 52, 93, 158	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	GLY	7.5
1	J	1	MET	6.1
1	F	1	MET	6.1
1	I	84	ALA	6.0
1	C	1	MET	6.0
1	D	57	GLY	5.7
1	E	1	MET	5.3
1	F	238	GLU	4.8
1	K	85	ASP	4.6
1	C	104	ALA	4.6
1	E	85	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.4
1	G	1	MET	4.4
1	K	84	ALA	4.1
1	C	84	ALA	4.1
1	G	275	PHE	3.9
1	C	261	ASN	3.9
1	H	85	ASP	3.8
1	B	238	GLU	3.6
1	L	23	SER	3.5
1	E	22	ALA	3.5
1	H	84	ALA	3.5
1	G	85	ASP	3.5
1	G	261	ASN	3.5
1	F	85	ASP	3.4
1	I	85	ASP	3.4
1	D	237	ALA	3.4
1	C	238	GLU	3.4
1	J	238	GLU	3.3
1	L	85	ASP	3.3
1	B	89	ASP	3.3
1	B	84	ALA	3.2
1	D	89	ASP	3.2
1	E	199	ALA	3.1
1	B	77	THR	3.1
1	C	199	ALA	3.0
1	C	237	ALA	3.0
1	D	77	THR	2.9
1	L	111	ARG	2.9
1	D	260	GLY	2.9
1	L	1	MET	2.9
1	D	272	GLY	2.9
1	E	77	THR	2.9
1	G	260	GLY	2.9
1	A	54	LYS	2.9
1	I	89	ASP	2.9
1	H	237	ALA	2.8
1	H	271	LYS	2.8
1	L	261	ASN	2.8
1	D	1	MET	2.8
1	D	85	ASP	2.8
1	A	84	ALA	2.8
1	C	111	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	23	SER	2.7
1	D	84	ALA	2.7
1	I	22	ALA	2.7
1	H	71	LYS	2.7
1	I	261	ASN	2.7
1	E	89	ASP	2.7
1	J	85	ASP	2.7
1	G	111	ARG	2.7
1	A	85	ASP	2.7
1	F	104	ALA	2.7
1	D	53	SER	2.7
1	K	89	ASP	2.7
1	G	238	GLU	2.7
1	K	199	ALA	2.6
1	L	18	ASP	2.6
1	C	239	LYS	2.6
1	C	259	ASP	2.6
1	C	141	ARG	2.6
1	A	261	ASN	2.6
1	G	202	ALA	2.6
1	E	260	GLY	2.6
1	G	274	ILE	2.5
1	I	77	THR	2.5
1	D	72	ASP	2.5
1	F	89	ASP	2.5
1	E	238	GLU	2.5
1	I	238	GLU	2.5
1	G	89	ASP	2.4
1	J	22	ALA	2.4
1	F	111	ARG	2.4
1	D	11	ASP	2.4
1	G	270	ASN	2.4
1	D	104	ALA	2.4
1	D	115	GLU	2.4
1	J	86	VAL	2.4
1	F	53	SER	2.4
1	F	236	ASP	2.4
1	G	273	ARG	2.4
1	J	271	LYS	2.4
1	D	58	SER	2.4
1	E	141	ARG	2.4
1	L	84	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	55	GLN	2.3
1	B	85	ASP	2.3
1	H	22	ALA	2.3
1	H	72	ASP	2.3
1	C	23	SER	2.2
1	A	89	ASP	2.2
1	B	237	ALA	2.2
1	J	77	THR	2.2
1	H	276	ASN	2.2
1	G	141	ARG	2.2
1	J	111	ARG	2.1
1	E	111	ARG	2.1
1	A	53	SER	2.1
1	J	89	ASP	2.1
1	C	115	GLU	2.1
1	K	71	LYS	2.1
1	E	23	SER	2.1
1	G	241	GLU	2.1
1	J	259	ASP	2.1
1	H	109	THR	2.1
1	K	237	ALA	2.0
1	B	55	GLN	2.0
1	D	111	ARG	2.0
1	D	138	GLU	2.0
1	E	127	ALA	2.0
1	F	200	ALA	2.0
1	E	72	ASP	2.0
1	F	134	ILE	2.0
1	E	237	ALA	2.0
1	G	116	GLY	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ADP	H	401	27/27	0.81	0.41	1.48	77,127,140,143	0
3	ADP	K	401	27/27	0.90	0.27	1.18	49,73,79,80	0
3	ADP	L	401	27/27	0.90	0.23	0.75	39,71,76,77	0
3	ADP	J	401	27/27	0.89	0.23	0.54	48,59,67,70	0
3	ADP	B	401	27/27	0.91	0.21	0.53	24,57,64,65	0
3	ADP	E	401	27/27	0.87	0.27	0.48	62,87,96,98	0
3	ADP	F	401	27/27	0.84	0.25	0.44	62,91,106,108	0
3	ADP	I	401	27/27	0.92	0.24	0.39	33,63,77,79	0
3	ADP	G	401	27/27	0.89	0.25	0.33	63,88,99,102	0
3	ADP	C	401	27/27	0.83	0.28	0.30	70,100,119,121	0
3	ADP	D	401	27/27	0.83	0.27	0.25	82,120,135,138	0
3	ADP	A	401	27/27	0.93	0.19	0.03	33,57,62,63	0
2	CA	B	400	1/1	0.92	0.19	-	55,55,55,55	0
2	CA	K	400	1/1	0.97	0.24	-	61,61,61,61	0
2	CA	D	400	1/1	0.95	0.17	-	70,70,70,70	0
2	CA	C	400	1/1	0.94	0.12	-	68,68,68,68	0
2	CA	E	400	1/1	0.95	0.14	-	76,76,76,76	0
2	CA	I	400	1/1	0.93	0.13	-	49,49,49,49	0
2	CA	G	400	1/1	0.96	0.16	-	80,80,80,80	0
2	CA	A	400	1/1	0.94	0.26	-	65,65,65,65	0
2	CA	J	400	1/1	0.93	0.18	-	48,48,48,48	0
2	CA	L	400	1/1	0.98	0.15	-	50,50,50,50	0
2	CA	F	400	1/1	0.87	0.25	-	70,70,70,70	0
2	CA	H	400	1/1	0.94	0.15	-	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.