



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:47 AM UTC

PDB ID : 6BBA / pdb_00006bba
Title : Crystal structure of human mitochondrial ClpP complex with acyldepsipeptide ADEP-28
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2017-10-17
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

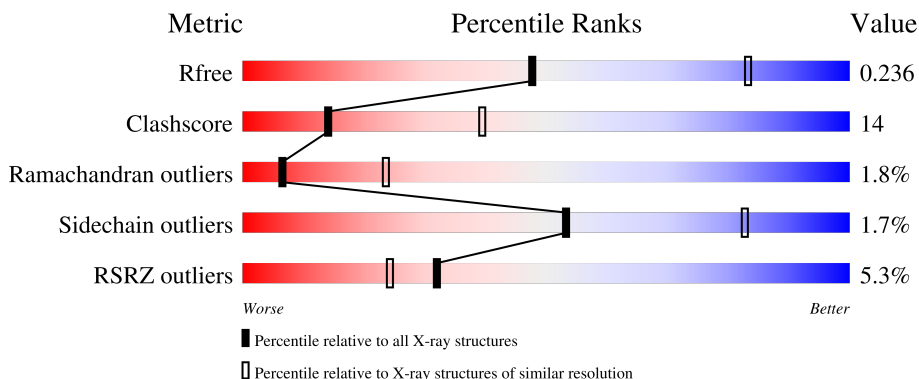
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	221	 4% 63% 20% 14%
1	B	221	 3% 64% 19% 16%
1	C	221	 6% 61% 19% 14%
1	D	221	 5% 67% 17% 14%
1	E	221	 4% 70% 14% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	221	
1	G	221	
2	H	7	
2	I	7	
2	J	7	
2	K	7	
2	L	7	
2	M	7	
2	N	7	

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
2	ALO	I	3	-	-	X	-
2	ALO	K	3	-	-	X	-
2	ALO	N	3	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10836 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 ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	189	1464	929	252	270	13	0	0	0
1	B	185	1440	914	248	265	13	0	0	0
1	C	189	1468	931	252	272	13	0	0	0
1	D	189	1468	931	252	272	13	0	0	0
1	E	188	1460	927	251	269	13	0	0	0
1	F	190	1476	936	254	272	14	0	1	0
1	G	188	1460	927	251	269	13	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	expression tag	UNP Q16740
B	57	SER	-	expression tag	UNP Q16740
C	57	SER	-	expression tag	UNP Q16740
D	57	SER	-	expression tag	UNP Q16740
E	57	SER	-	expression tag	UNP Q16740
F	57	SER	-	expression tag	UNP Q16740
G	57	SER	-	expression tag	UNP Q16740

- Molecule 2 is a protein called Acyldepsipeptide ADEP-28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
2	H	7	56	40	2	6	8	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	I	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	J	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	K	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	L	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	M	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			
2	N	7	Total	C	F	N	O	0	0	0
			56	40	2	6	8			

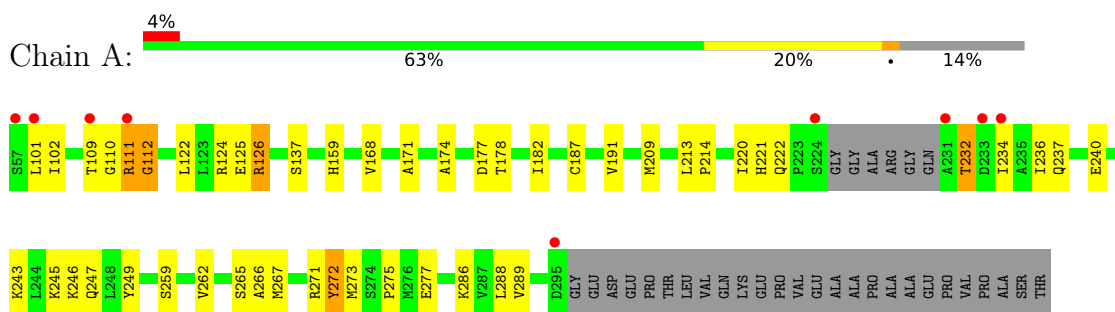
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	22	Total	O	0	0
			22	22		
3	C	22	Total	O	0	0
			22	22		
3	D	35	Total	O	0	0
			35	35		
3	E	38	Total	O	0	0
			38	38		
3	F	38	Total	O	0	0
			38	38		
3	G	30	Total	O	0	0
			30	30		
3	I	2	Total	O	0	0
			2	2		
3	M	1	Total	O	0	0
			1	1		
3	N	1	Total	O	0	0
			1	1		

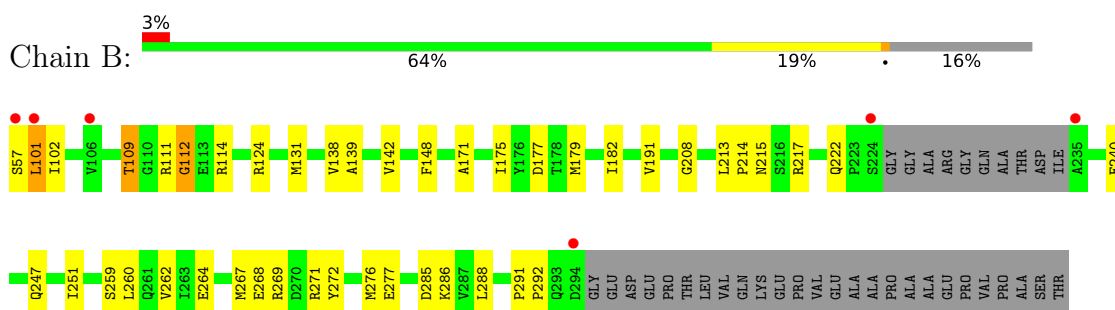
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

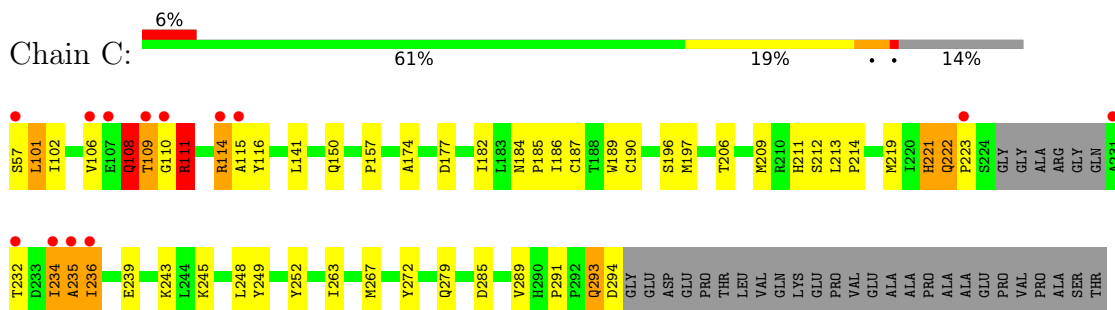
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

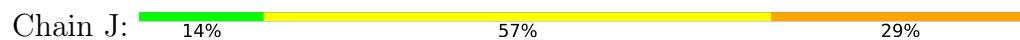


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial





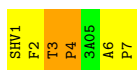
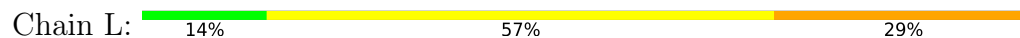
- Molecule 2: Acyldepsipeptide ADEP-28



- Molecule 2: Acyldepsipeptide ADEP-28



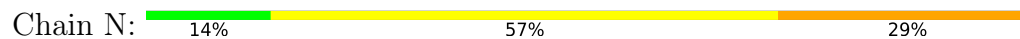
- Molecule 2: Acyldepsipeptide ADEP-28



- Molecule 2: Acyldepsipeptide ADEP-28



- Molecule 2: Acyldepsipeptide ADEP-28



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.40Å 172.40Å 135.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.73 – 2.80 46.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.73-2.80) 99.8 (46.73-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.187 , 0.235 0.192 , 0.236	Depositor DCC
R_{free} test set	2017 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtrriage
Anisotropy	0.236	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10836	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ALO, SHV, WFP, 3A0

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	0.49	0/1490	0.64	2/2016 (0.1%)
1	B	0.38	0/1466	0.56	0/1983
1	C	0.46	0/1494	0.68	0/2022
1	D	0.46	0/1494	0.69	0/2022
1	E	0.44	0/1486	0.61	0/2011
1	F	0.47	0/1505	0.63	0/2036
1	G	0.47	0/1486	0.60	1/2011 (0.0%)
2	H	6.54	7/19 (36.8%)	1.41	0/24
2	I	6.51	7/19 (36.8%)	1.65	0/24
2	J	6.51	7/19 (36.8%)	1.48	0/24
2	K	6.48	7/19 (36.8%)	1.95	0/24
2	L	6.50	7/19 (36.8%)	1.51	0/24
2	M	6.33	7/19 (36.8%)	2.00	0/24
2	N	6.43	7/19 (36.8%)	1.52	0/24
All	All	0.86	49/10554 (0.5%)	0.65	3/14269 (0.0%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	PRO	N-CA	14.72	1.69	1.47
2	K	4	PRO	N-CA	14.09	1.68	1.47
2	J	4	PRO	N-CA	14.03	1.68	1.47
2	H	4	PRO	N-CA	14.02	1.68	1.47
2	I	4	PRO	N-CA	13.74	1.67	1.47
2	N	4	PRO	N-CA	13.73	1.67	1.47
2	M	4	PRO	N-CA	13.71	1.67	1.47
2	I	4	PRO	N-CD	-11.46	1.31	1.47
2	K	4	PRO	N-CD	-10.98	1.32	1.47
2	N	4	PRO	N-CD	-10.95	1.32	1.47
2	L	4	PRO	N-CD	-10.85	1.32	1.47
2	J	4	PRO	N-CD	-10.84	1.32	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	4	PRO	N-CD	-10.71	1.32	1.47
2	H	4	PRO	N-CD	-10.71	1.32	1.47
2	H	7	PRO	N-CD	-10.51	1.33	1.47
2	J	7	PRO	N-CD	-10.37	1.33	1.47
2	N	7	PRO	N-CD	-10.35	1.33	1.47
2	I	7	PRO	N-CD	-10.24	1.33	1.47
2	K	7	PRO	N-CD	-10.22	1.33	1.47
2	J	7	PRO	N-CA	10.11	1.62	1.47
2	N	4	PRO	CA-CB	-10.04	1.33	1.53
2	M	7	PRO	N-CD	-10.02	1.33	1.47
2	L	7	PRO	N-CA	10.00	1.62	1.47
2	L	7	PRO	N-CD	-9.98	1.33	1.47
2	H	4	PRO	CA-CB	-9.90	1.33	1.53
2	H	7	PRO	N-CA	9.89	1.61	1.47
2	M	7	PRO	N-CA	9.88	1.61	1.47
2	I	4	PRO	CA-CB	-9.82	1.33	1.53
2	I	7	PRO	N-CA	9.71	1.61	1.47
2	K	7	PRO	N-CA	9.70	1.61	1.47
2	K	4	PRO	CA-CB	-9.69	1.34	1.53
2	L	4	PRO	CA-CB	-9.52	1.34	1.53
2	H	7	PRO	CA-CB	-9.49	1.34	1.53
2	M	4	PRO	CA-CB	-9.32	1.34	1.53
2	J	4	PRO	CA-CB	-9.25	1.34	1.53
2	N	7	PRO	N-CA	9.21	1.60	1.47
2	J	7	PRO	CA-CB	-9.14	1.35	1.53
2	N	7	PRO	CA-CB	-9.11	1.35	1.53
2	K	7	PRO	CA-CB	-8.96	1.35	1.53
2	I	7	PRO	CA-CB	-8.94	1.35	1.53
2	L	7	PRO	CA-CB	-8.91	1.35	1.53
2	M	7	PRO	CA-CB	-8.89	1.35	1.53
2	J	6	ALA	C-N	8.64	1.48	1.34
2	I	6	ALA	C-N	8.58	1.48	1.34
2	K	6	ALA	C-N	8.35	1.48	1.34
2	H	6	ALA	C-N	8.26	1.47	1.34
2	N	6	ALA	C-N	8.05	1.47	1.34
2	L	6	ALA	C-N	7.86	1.47	1.34
2	M	6	ALA	C-N	7.65	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	THR	N-CA-C	-6.29	100.64	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	101	LEU	N-CA-C	-5.79	98.31	108.20
1	A	126	ARG	N-CA-C	5.45	119.22	111.92

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	1464	0	1498	46	0
1	B	1440	0	1474	41	0
1	C	1468	0	1501	60	0
1	D	1468	0	1501	36	0
1	E	1460	0	1497	27	0
1	F	1476	0	1513	50	0
1	G	1460	0	1497	36	0
2	H	56	0	49	8	0
2	I	56	0	49	8	0
2	J	56	0	50	6	0
2	K	56	0	49	6	0
2	L	56	0	49	6	0
2	M	56	0	50	5	0
2	N	56	0	50	8	0
3	A	19	0	0	1	0
3	B	22	0	0	5	0
3	C	22	0	0	0	0
3	D	35	0	0	1	0
3	E	38	0	0	3	0
3	F	38	0	0	1	0
3	G	30	0	0	3	0
3	I	2	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
All	All	10836	0	10827	307	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 14.

All (307) 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:F:110:GLY:O	1:F:111:ARG:HG2	1.22	1.33
2:J:4:PRO:N	2:J:4:PRO:CA	1.68	1.32
2:L:4:PRO:N	2:L:4:PRO:CA	1.69	1.31
2:N:4:PRO:N	2:N:4:PRO:CA	1.67	1.29
2:M:4:PRO:N	2:M:4:PRO:CA	1.67	1.27
2:H:4:PRO:N	2:H:4:PRO:CA	1.68	1.24
2:I:4:PRO:N	2:I:4:PRO:CA	1.67	1.18
2:K:4:PRO:N	2:K:4:PRO:CA	1.68	1.13
1:C:235:ALA:HA	1:C:236:ILE:HG23	1.21	1.09
1:F:110:GLY:C	1:F:111:ARG:HG2	1.72	1.07
1:C:235:ALA:HB1	1:C:236:ILE:HG12	1.33	1.07
1:C:234:ILE:CG2	1:C:235:ALA:H	1.68	1.07
1:F:110:GLY:O	1:F:111:ARG:CG	2.04	1.04
1:C:235:ALA:HA	1:C:236:ILE:CG2	1.87	1.02
1:B:101:LEU:HD22	1:B:102:ILE:N	1.77	0.99
1:C:234:ILE:HG22	1:C:235:ALA:N	1.64	0.99
1:C:234:ILE:HG22	1:C:235:ALA:H	0.81	0.97
1:C:235:ALA:CB	1:C:236:ILE:HG12	1.95	0.96
1:C:108:GLN:HB3	1:C:109:THR:HA	1.44	0.95
1:C:108:GLN:HB3	1:C:109:THR:CA	1.98	0.93
1:G:185:PRO:HB2	1:G:209:MET:HE1	1.54	0.89
1:F:220:ILE:HG22	1:F:267:MET:HG2	1.54	0.89
1:F:109:THR:HG22	1:F:110:GLY:H	1.36	0.88
1:A:101:LEU:HB3	3:G:524:HOH:O	1.76	0.85
1:G:107:GLU:HG3	1:G:121:ARG:HE	1.43	0.84
1:B:101:LEU:HD13	3:B:516:HOH:O	1.78	0.82
1:C:235:ALA:CA	1:C:236:ILE:HG12	2.11	0.81
1:A:111:ARG:NH1	1:A:111:ARG:HB2	1.98	0.78
1:C:108:GLN:HB3	1:C:109:THR:CB	2.13	0.78
1:A:191:VAL:HG23	1:A:213:LEU:HD12	1.65	0.78
1:C:235:ALA:HA	1:C:236:ILE:CB	2.12	0.77
1:D:177:ASP:HB3	1:E:213:LEU:HD13	1.68	0.76
1:C:235:ALA:CA	1:C:236:ILE:HG23	2.11	0.75
1:G:109:THR:HG22	1:G:110:GLY:H	1.52	0.75
1:F:109:THR:HG22	1:F:110:GLY:N	2.02	0.74
1:C:114:ARG:HG2	1:C:116:TYR:CE2	2.24	0.73
1:D:182:ILE:HD11	1:D:186:ILE:HD11	1.71	0.72
1:F:191:VAL:HG23	1:F:213:LEU:HD12	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ILE:H	1:E:206:THR:HG23	1.55	0.71
2:K:4:PRO:N	2:K:4:PRO:C	2.49	0.71
1:E:273:MET:HE1	1:E:283:ILE:HD12	1.73	0.70
1:D:185:PRO:HB2	1:D:209:MET:HE1	1.74	0.69
1:E:233:ASP:O	1:E:234:ILE:HG12	1.92	0.69
1:B:101:LEU:CD1	3:B:516:HOH:O	2.39	0.69
1:D:179:MET:HB2	1:D:186:ILE:HD12	1.75	0.69
1:A:232:THR:CG2	1:A:234:ILE:O	2.41	0.68
2:N:3:ALO:C	2:N:4:PRO:CA	2.70	0.68
1:D:222:GLN:NE2	3:D:501:HOH:O	2.23	0.68
1:F:106:VAL:HG13	1:F:114:ARG:O	1.93	0.68
1:C:279:GLN:NE2	1:C:285:ASP:O	2.26	0.68
1:D:107:GLU:HA	1:D:107:GLU:OE1	1.91	0.68
1:E:114:ARG:HH22	1:F:113:GLU:HB3	1.59	0.67
1:F:261:GLN:O	1:F:261:GLN:NE2	2.28	0.67
1:B:276:MET:HE1	3:B:522:HOH:O	1.94	0.67
1:A:111:ARG:O	1:A:112:GLY:O	2.13	0.67
1:B:101:LEU:HD22	1:B:102:ILE:H	1.60	0.67
1:A:236:ILE:HD11	1:B:272:TYR:CE2	2.29	0.67
1:A:245:LYS:HE2	1:A:249:TYR:OH	1.96	0.66
1:E:114:ARG:HH22	1:F:113:GLU:CB	2.08	0.66
2:M:4:PRO:N	2:M:4:PRO:C	2.53	0.66
1:D:191:VAL:HG23	1:D:213:LEU:HD12	1.78	0.66
1:F:187[A]:CYS:SG	1:F:209:MET:HE2	2.36	0.66
2:H:4:PRO:N	2:H:4:PRO:C	2.52	0.65
1:F:107:GLU:HG2	1:F:121:ARG:HE	1.61	0.65
1:F:179:MET:HE3	1:F:204:ALA:HB3	1.79	0.65
1:B:101:LEU:HD22	1:B:101:LEU:C	2.22	0.65
2:N:4:PRO:N	2:N:4:PRO:C	2.51	0.65
1:G:191:VAL:HG12	1:G:213:LEU:HD12	1.79	0.64
1:G:234:ILE:O	1:G:236:ILE:HG23	1.96	0.64
2:I:3:ALO:C	2:I:4:PRO:CA	2.74	0.64
1:C:108:GLN:OE1	1:C:109:THR:HA	1.98	0.63
2:J:4:PRO:N	2:J:4:PRO:C	2.53	0.63
1:B:276:MET:CE	3:B:522:HOH:O	2.46	0.63
1:G:178:THR:HG22	2:H:2:WFP:HZ	1.80	0.63
2:K:3:ALO:C	2:K:4:PRO:CA	2.74	0.62
1:B:222:GLN:NE2	3:B:501:HOH:O	2.31	0.62
2:I:4:PRO:N	2:I:4:PRO:C	2.55	0.62
2:L:3:ALO:C	2:L:4:PRO:CA	2.75	0.62
1:A:232:THR:HG23	1:A:234:ILE:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:3:ALO:C	2:M:4:PRO:CA	2.73	0.61
1:A:286:LYS:HE3	1:A:288:LEU:HD21	1.83	0.61
2:J:3:ALO:C	2:J:4:PRO:CA	2.76	0.61
1:A:101:LEU:HD12	1:A:102:ILE:H	1.66	0.61
1:A:214:PRO:HG3	1:A:289:VAL:HG22	1.81	0.60
1:C:196:SER:OG	1:C:197:MET:N	2.34	0.60
2:K:3:ALO:HA	2:K:4:PRO:CA	2.31	0.60
2:I:3:ALO:HA	2:I:4:PRO:CA	2.32	0.60
1:D:160:MET:SD	1:D:179:MET:HE1	2.41	0.60
1:A:110:GLY:HA3	1:A:111:ARG:O	2.02	0.60
1:C:232:THR:HG22	1:C:234:ILE:H	1.67	0.60
1:E:143:ILE:HG23	1:E:178:THR:HG21	1.84	0.59
1:F:234:ILE:HD11	1:G:272:TYR:OH	2.01	0.59
1:C:108:GLN:HB3	1:C:109:THR:OG1	2.03	0.59
1:D:134:ILE:HA	1:D:138:VAL:HG21	1.84	0.58
1:E:279:GLN:NE2	3:E:501:HOH:O	2.36	0.58
1:F:107:GLU:OE2	1:F:107:GLU:HA	2.04	0.58
2:H:3:ALO:C	2:H:4:PRO:CA	2.75	0.58
2:M:1:SHV:C1	2:M:3:ALO:H	2.17	0.58
1:A:137:SER:HA	1:B:131:MET:HE2	1.86	0.57
1:C:174:ALA:HB1	1:D:191:VAL:HG22	1.87	0.57
1:C:235:ALA:HB1	1:C:236:ILE:CG1	2.21	0.57
1:D:109:THR:HG23	1:D:109:THR:O	2.04	0.57
1:A:110:GLY:HA2	1:A:111:ARG:CB	2.34	0.57
1:D:148:PHE:HA	2:L:1:SHV:H73	1.85	0.57
1:A:111:ARG:HB2	1:A:111:ARG:HH11	1.69	0.57
1:A:177:ASP:HB3	1:B:213:LEU:HD13	1.85	0.56
1:A:232:THR:HG21	1:A:234:ILE:O	2.05	0.56
1:C:141:LEU:HD11	1:D:103:PRO:HD2	1.88	0.56
1:D:196:SER:OG	1:D:197:MET:N	2.37	0.56
1:B:111:ARG:HG3	1:B:112:GLY:H	1.71	0.56
1:C:234:ILE:CG2	1:C:235:ALA:N	2.39	0.56
1:C:234:ILE:O	1:C:235:ALA:HB2	2.04	0.56
2:N:3:ALO:HA	2:N:4:PRO:CA	2.36	0.56
1:E:185:PRO:HA	1:E:206:THR:HG21	1.88	0.56
1:C:235:ALA:CA	1:C:236:ILE:CG1	2.85	0.55
1:D:217:ARG:HH22	1:D:274:SER:CA	2.20	0.54
1:D:242:MET:HA	1:D:242:MET:HE2	1.89	0.54
1:F:109:THR:CG2	1:F:110:GLY:H	2.14	0.54
1:A:122:LEU:HD23	2:H:1:SHV:H61	1.91	0.53
1:A:271:ARG:O	1:A:272:TYR:HB2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:PRO:HB3	2:J:4:PRO:HD2	1.88	0.53
1:B:260:LEU:O	1:B:264:GLU:HG3	2.09	0.53
1:C:114:ARG:HG2	1:C:116:TYR:CZ	2.44	0.53
1:F:139:ALA:HA	1:F:175:ILE:HD11	1.90	0.53
1:C:108:GLN:CB	1:C:109:THR:CB	2.85	0.53
1:G:202:LEU:HD21	1:G:284:LEU:HD21	1.90	0.53
1:A:111:ARG:CB	1:A:111:ARG:HH11	2.21	0.53
1:E:174:ALA:HB1	1:F:191:VAL:HG22	1.90	0.53
1:F:179:MET:CE	1:F:204:ALA:HB3	2.38	0.53
1:G:185:PRO:HA	1:G:206:THR:HG21	1.91	0.53
1:D:234:ILE:HG22	1:D:235:ALA:H	1.73	0.52
1:D:237:GLN:O	1:D:241:ILE:HG13	2.08	0.52
1:D:113:GLU:O	1:D:114:ARG:HD2	2.09	0.52
1:G:178:THR:CG2	2:H:2:WFP:HZ	2.40	0.52
1:C:185:PRO:HA	1:C:206:THR:HG21	1.91	0.52
1:C:111:ARG:HG3	1:D:113:GLU:OE1	2.10	0.51
1:C:150:GLN:HG3	1:C:184:ASN:OD1	2.11	0.51
1:F:110:GLY:O	1:F:111:ARG:CD	2.58	0.51
1:F:109:THR:CG2	1:F:110:GLY:N	2.73	0.51
1:F:148:PHE:HD1	2:N:1:SHV:H73	1.75	0.51
1:F:240:GLU:OE2	1:G:217:ARG:HD3	2.10	0.51
1:G:182:ILE:HD11	1:G:186:ILE:HD11	1.93	0.51
1:G:214:PRO:HG3	1:G:289:VAL:HG22	1.92	0.51
1:B:269:ARG:CZ	1:B:271:ARG:HD3	2.41	0.51
1:B:271:ARG:NH1	1:B:277:GLU:OE2	2.41	0.51
2:L:4:PRO:N	2:L:4:PRO:C	2.59	0.51
1:C:235:ALA:HA	1:C:236:ILE:CG1	2.40	0.51
1:F:141:LEU:HD11	1:G:103:PRO:HD2	1.93	0.51
2:N:1:SHV:C1	2:N:3:ALO:H	2.24	0.50
1:F:261:GLN:HE21	1:F:261:GLN:HA	1.77	0.50
1:D:217:ARG:NH2	1:D:274:SER:N	2.59	0.50
1:F:261:GLN:HE21	1:F:261:GLN:CA	2.24	0.50
1:B:291:PRO:HB3	2:I:4:PRO:HD2	1.94	0.50
1:D:214:PRO:HD3	1:D:288:LEU:O	2.12	0.49
1:C:219:MET:HE3	1:C:221:HIS:N	2.28	0.49
2:L:3:ALO:HA	2:L:4:PRO:CA	2.42	0.49
1:A:240:GLU:OE1	1:B:272:TYR:HB2	2.12	0.49
1:B:139:ALA:HB2	1:B:171:ALA:HB1	1.94	0.49
1:F:131:MET:HG2	1:F:132:GLY:N	2.28	0.49
1:A:109:THR:HA	1:A:110:GLY:C	2.38	0.49
1:A:110:GLY:CA	1:A:111:ARG:C	2.85	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:GLY:C	1:F:111:ARG:CG	2.58	0.49
1:G:168:VAL:HA	1:G:231:ALA:HA	1.94	0.48
1:A:125:GLU:O	1:A:126:ARG:HB2	2.13	0.48
1:A:168:VAL:HG12	1:A:171:ALA:H	1.78	0.48
1:E:124:ARG:HD3	3:E:532:HOH:O	2.14	0.48
2:K:3:ALO:HA	2:K:4:PRO:C	2.38	0.48
1:G:109:THR:HG22	1:G:110:GLY:N	2.23	0.48
1:D:217:ARG:NH2	1:D:274:SER:HA	2.29	0.48
2:N:3:ALO:CA	2:N:4:PRO:CA	2.91	0.48
1:C:101:LEU:HG	1:C:102:ILE:N	2.28	0.48
1:F:239:GLU:O	1:F:243:LYS:HG3	2.13	0.48
1:F:261:GLN:NE2	1:F:261:GLN:CA	2.77	0.48
2:I:3:ALO:HA	2:I:4:PRO:HA	1.94	0.48
1:A:246:LYS:NZ	3:A:503:HOH:O	2.44	0.48
1:E:249:TYR:CZ	1:E:264:GLU:HG2	2.49	0.48
1:G:174:ALA:O	1:G:178:THR:HG23	2.14	0.48
1:B:208:GLY:N	1:B:285:ASP:OD2	2.47	0.47
1:C:232:THR:HG22	1:C:234:ILE:N	2.28	0.47
1:D:252:TYR:CD1	1:D:267:MET:HE2	2.50	0.47
1:E:222:GLN:NE2	3:E:503:HOH:O	2.44	0.47
1:F:107:GLU:HG2	1:F:121:ARG:NE	2.28	0.47
1:F:213:LEU:HB3	1:F:214:PRO:HD2	1.96	0.47
1:F:261:GLN:NE2	1:F:261:GLN:C	2.73	0.47
1:A:220:ILE:HG13	1:A:267:MET:HG2	1.97	0.47
1:D:217:ARG:NH2	1:D:274:SER:CA	2.77	0.47
1:G:249:TYR:CZ	1:G:264:GLU:HG2	2.50	0.47
1:C:214:PRO:HG3	1:C:289:VAL:HG22	1.96	0.47
1:D:194:ALA:O	1:D:199:SER:HB3	2.14	0.47
2:K:3:ALO:CA	2:K:4:PRO:CA	2.93	0.47
1:E:110:GLY:C	1:E:112:GLY:H	2.23	0.47
1:A:221:HIS:CE1	1:A:222:GLN:O	2.68	0.47
2:H:3:ALO:HA	2:H:4:PRO:CA	2.45	0.47
1:A:272:TYR:OH	1:G:234:ILE:HD11	2.15	0.46
1:C:141:LEU:HD21	1:D:103:PRO:HD3	1.97	0.46
1:D:232:THR:HG23	1:D:234:ILE:O	2.14	0.46
2:I:4:PRO:HA	2:I:7:PRO:O	2.15	0.46
1:C:235:ALA:C	1:C:236:ILE:HG12	2.40	0.46
1:E:104:ILE:HG21	1:E:115:ALA:HB1	1.97	0.46
1:C:252:TYR:HB3	1:C:263:ILE:HD12	1.98	0.46
1:C:235:ALA:CA	1:C:236:ILE:CB	2.91	0.46
1:E:182:ILE:HD11	1:E:186:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ILE:HD11	1:F:186:ILE:HD11	1.98	0.46
1:A:110:GLY:HA2	1:A:111:ARG:HB3	1.95	0.46
2:I:3:ALO:CA	2:I:4:PRO:CA	2.94	0.46
1:A:111:ARG:NH1	1:A:111:ARG:CB	2.75	0.46
1:C:221:HIS:O	1:C:222:GLN:HB3	2.16	0.46
1:A:187:CYS:HA	1:A:209:MET:O	2.16	0.46
1:G:273:MET:HB3	1:G:277:GLU:HB2	1.97	0.45
1:B:259:SER:OG	1:B:262:VAL:HG12	2.17	0.45
1:C:249:TYR:HD1	1:C:267:MET:HE3	1.81	0.45
1:C:219:MET:HE3	1:C:222:GLN:H	1.82	0.45
1:D:263:ILE:CG2	1:D:267:MET:HE3	2.47	0.45
1:B:179:MET:O	1:B:182:ILE:HG22	2.16	0.45
1:E:111:ARG:HA	1:E:111:ARG:NE	2.30	0.45
1:E:249:TYR:CE2	1:E:264:GLU:HG2	2.51	0.45
1:E:186:ILE:H	1:E:206:THR:CG2	2.28	0.45
1:E:196:SER:OG	1:E:197:MET:N	2.49	0.45
1:F:177:ASP:CG	1:G:214:PRO:HD2	2.42	0.45
1:F:249:TYR:CE2	1:F:264:GLU:HG2	2.52	0.45
1:F:261:GLN:C	1:F:261:GLN:CD	2.85	0.45
2:M:3:ALO:HA	2:M:4:PRO:CA	2.47	0.45
1:A:174:ALA:HB1	1:B:191:VAL:CG1	2.46	0.45
1:F:177:ASP:HB3	1:G:213:LEU:HD13	1.98	0.45
1:D:179:MET:HB3	1:D:179:MET:HE2	1.40	0.44
1:B:111:ARG:HG3	1:B:112:GLY:N	2.32	0.44
1:B:191:VAL:HG22	1:B:213:LEU:HD12	1.98	0.44
1:C:187:CYS:SG	1:C:209:MET:HE2	2.58	0.44
1:A:259:SER:OG	1:A:262:VAL:HG23	2.18	0.44
1:A:265:SER:O	1:A:266:ALA:HB3	2.18	0.44
1:B:109:THR:HG21	1:B:114:ARG:HD3	1.98	0.44
1:B:247:GLN:O	1:B:251:ILE:HG13	2.18	0.44
1:G:274:SER:OG	1:G:277:GLU:HG3	2.17	0.44
1:C:157:PRO:HA	1:C:185:PRO:HG2	1.99	0.44
1:E:104:ILE:CG2	1:E:115:ALA:HB1	2.48	0.44
1:G:249:TYR:CE2	1:G:264:GLU:HG2	2.53	0.44
1:B:124:ARG:HH21	1:C:106:VAL:HG21	1.83	0.44
1:B:267:MET:HE2	1:B:267:MET:HB3	1.78	0.44
1:F:245:LYS:HE2	1:F:249:TYR:OH	2.18	0.44
1:A:111:ARG:HB2	1:A:111:ARG:CZ	2.49	0.43
1:B:139:ALA:HA	1:B:175:ILE:HD11	2.01	0.43
1:C:108:GLN:CB	1:C:109:THR:CA	2.83	0.43
1:B:240:GLU:OE1	1:C:272:TYR:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ILE:HD11	1:C:186:ILE:HD11	2.00	0.43
1:C:189:TRP:CE3	1:C:211:HIS:HB2	2.54	0.43
1:E:279:GLN:NE2	1:E:285:ASP:O	2.51	0.43
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.83	0.43
1:F:111:ARG:HE	1:F:111:ARG:HB3	1.72	0.43
1:F:274:SER:OG	1:F:277:GLU:HG3	2.18	0.43
1:A:174:ALA:HB1	1:B:191:VAL:HG13	2.00	0.43
1:A:273:MET:HB3	1:A:277:GLU:HB2	2.00	0.43
1:C:222:GLN:HA	1:C:223:PRO:HD2	1.90	0.43
1:F:220:ILE:HD12	1:F:252:TYR:CE2	2.53	0.43
1:G:196:SER:HB2	3:G:518:HOH:O	2.18	0.43
1:B:286:LYS:HB2	1:B:288:LEU:HD11	2.00	0.42
1:G:239:GLU:O	1:G:243:LYS:HG3	2.18	0.42
1:A:101:LEU:HD12	1:A:102:ILE:N	2.33	0.42
1:F:273:MET:HB3	1:F:277:GLU:HB2	2.00	0.42
1:B:213:LEU:HB3	1:B:214:PRO:HD2	2.01	0.42
1:B:269:ARG:CZ	1:B:271:ARG:CD	2.98	0.42
1:C:219:MET:HB3	1:C:219:MET:HE2	1.81	0.42
1:G:125:GLU:HG3	2:N:1:SHV:H62	2.01	0.42
1:G:195:ALA:HB1	1:G:219:MET:HE2	2.00	0.42
1:E:177:ASP:OD2	1:F:215:ASN:HB2	2.20	0.42
1:G:203:ALA:HB2	1:G:283:ILE:HG23	2.02	0.42
2:L:3:ALO:CA	2:L:4:PRO:CA	2.97	0.42
1:B:177:ASP:HB3	1:C:213:LEU:HD13	2.01	0.42
1:C:190:CYS:HB3	1:C:212:SER:HB2	2.02	0.42
1:E:187:CYS:SG	1:E:209:MET:HB3	2.60	0.42
1:C:239:GLU:O	1:C:243:LYS:HG3	2.20	0.42
1:B:138:VAL:O	1:B:142:VAL:HG23	2.20	0.42
1:D:216:SER:C	1:D:217:ARG:HG2	2.45	0.42
1:A:243:LYS:O	1:A:247:GLN:HG2	2.19	0.42
1:A:247:GLN:OE1	1:B:215:ASN:ND2	2.46	0.42
1:C:249:TYR:CD1	1:C:267:MET:HE3	2.55	0.42
1:A:214:PRO:O	1:A:275:PRO:HG2	2.19	0.41
1:F:107:GLU:OE2	1:F:107:GLU:CA	2.68	0.41
1:F:286:LYS:NZ	3:F:502:HOH:O	2.37	0.41
1:G:205:GLY:O	1:G:210:ARG:HD3	2.19	0.41
1:C:293:GLN:HB3	1:C:294:ASP:H	1.63	0.41
1:F:109:THR:C	1:F:111:ARG:H	2.27	0.41
1:A:159:HIS:CE1	2:H:6:ALA:HA	2.56	0.41
1:G:232:THR:HG23	1:G:234:ILE:O	2.20	0.41
2:J:1:SHV:C1	2:J:3:ALO:H	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:HA3	1:A:111:ARG:C	2.46	0.41
1:D:113:GLU:C	1:D:114:ARG:HD2	2.45	0.41
1:E:213:LEU:HB3	1:E:214:PRO:HD2	2.01	0.41
1:E:259:SER:OG	1:E:262:VAL:HG23	2.20	0.41
1:B:148:PHE:HD1	2:J:1:SHV:H73	1.85	0.41
1:C:219:MET:CE	1:C:222:GLN:H	2.33	0.41
1:C:245:LYS:O	1:C:248:LEU:N	2.52	0.41
1:D:134:ILE:HA	1:D:138:VAL:CG2	2.51	0.41
1:F:121:ARG:HH12	1:F:125:GLU:HG2	1.86	0.41
1:G:277:GLU:OE1	3:G:501:HOH:O	2.22	0.41
1:A:191:VAL:HG23	1:A:213:LEU:CD1	2.43	0.41
1:B:217:ARG:HB3	1:B:272:TYR:CD1	2.56	0.41
1:D:109:THR:HA	1:D:110:GLY:HA3	1.75	0.40
1:G:143:ILE:HG12	1:G:178:THR:HG21	2.04	0.40
1:G:147:LEU:HD23	1:G:147:LEU:HA	1.83	0.40
1:E:150:GLN:HG3	1:E:184:ASN:OD1	2.21	0.40
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.82	0.40
1:F:196:SER:OG	1:F:197:MET:N	2.53	0.40
1:A:178:THR:O	1:A:182:ILE:HG23	2.20	0.40
1:B:291:PRO:HA	1:B:292:PRO:HD3	1.95	0.40
1:C:177:ASP:HB3	1:D:213:LEU:HD13	2.03	0.40
1:G:148:PHE:O	1:G:151:SER:HB3	2.22	0.40
1:G:139:ALA:HA	1:G:175:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

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	A	185/221 (84%)	171 (92%)	12 (6%)	2 (1%)	11 36
1	B	181/221 (82%)	166 (92%)	12 (7%)	3 (2%)	7 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	185/221 (84%)	168 (91%)	8 (4%)	9 (5%)	1	6
1	D	185/221 (84%)	175 (95%)	6 (3%)	4 (2%)	5	19
1	E	184/221 (83%)	174 (95%)	6 (3%)	4 (2%)	5	19
1	F	187/221 (85%)	181 (97%)	5 (3%)	1 (0%)	24	55
1	G	184/221 (83%)	177 (96%)	7 (4%)	0	100	100
2	H	2/7 (29%)	2 (100%)	0	0	100	100
2	I	2/7 (29%)	2 (100%)	0	0	100	100
2	J	2/7 (29%)	2 (100%)	0	0	100	100
2	K	2/7 (29%)	2 (100%)	0	0	100	100
2	L	2/7 (29%)	2 (100%)	0	0	100	100
2	M	2/7 (29%)	2 (100%)	0	0	100	100
2	N	2/7 (29%)	2 (100%)	0	0	100	100
All	All	1305/1596 (82%)	1226 (94%)	56 (4%)	23 (2%)	6	23

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	C	236	ILE
1	C	293	GLN
1	D	113	GLU
1	D	236	ILE
1	E	114	ARG
1	E	234	ILE
1	F	111	ARG
1	C	110	GLY
1	C	111	ARG
1	C	235	ALA
1	B	109	THR
1	C	108	GLN
1	D	110	GLY
1	D	112	GLY
1	E	112	GLY
1	B	112	GLY
1	C	115	ALA
1	C	222	GLN
1	B	268	GLU
1	E	110	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	TYR
1	C	234	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	A	162/185 (88%)	159 (98%)	3 (2%)	50	81
1	B	160/185 (86%)	158 (99%)	2 (1%)	61	86
1	C	163/185 (88%)	156 (96%)	7 (4%)	26	60
1	D	163/185 (88%)	162 (99%)	1 (1%)	78	92
1	E	162/185 (88%)	162 (100%)	0	100	100
1	F	164/185 (89%)	160 (98%)	4 (2%)	43	77
1	G	162/185 (88%)	160 (99%)	2 (1%)	63	87
2	H	2/2 (100%)	2 (100%)	0	100	100
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
2	M	2/2 (100%)	2 (100%)	0	100	100
2	N	2/2 (100%)	2 (100%)	0	100	100
All	All	1150/1309 (88%)	1131 (98%)	19 (2%)	53	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	124	ARG
1	A	237	GLN
1	B	57	SER
1	B	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	57	SER
1	C	101	LEU
1	C	108	GLN
1	C	109	THR
1	C	111	ARG
1	C	114	ARG
1	C	221	HIS
1	D	101	LEU
1	F	107	GLU
1	F	111	ARG
1	F	237	GLN
1	F	261	GLN
1	G	57	SER
1	G	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	221	HIS
1	A	237	GLN
1	B	221	HIS
1	B	222	GLN
1	C	180	GLN
1	C	193	GLN
1	C	279	GLN
1	D	159	HIS
1	D	221	HIS
1	D	279	GLN
1	E	108	GLN
1	E	221	HIS
1	E	237	GLN
1	F	159	HIS
1	F	180	GLN
1	F	222	GLN
1	F	237	GLN
1	F	247	GLN
1	F	261	GLN
1	G	108	GLN
1	G	154	ASN
1	G	159	HIS
1	G	193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	215	ASN
1	G	221	HIS
1	G	279	GLN
1	G	290	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	ALO	I	3	2	5,6,7	0.42	0	5,7,9	0.50	0
2	WFP	M	2	2	12,13,14	1.02	1 (8%)	12,17,19	1.48	3 (25%)
2	ALO	L	3	2	5,6,7	0.61	0	5,7,9	1.20	1 (20%)
2	WFP	K	2	2	12,13,14	1.13	2 (16%)	12,17,19	1.49	4 (33%)
2	WFP	N	2	2	12,13,14	1.06	1 (8%)	12,17,19	1.77	3 (25%)
2	ALO	J	3	2	5,6,7	0.45	0	5,7,9	1.67	1 (20%)
2	ALO	N	3	2	5,6,7	0.43	0	5,7,9	1.52	1 (20%)
2	WFP	L	2	2	12,13,14	1.00	1 (8%)	12,17,19	2.15	6 (50%)
2	ALO	M	3	2	5,6,7	0.40	0	5,7,9	1.08	0
2	ALO	H	3	2	5,6,7	0.47	0	5,7,9	0.80	0
2	ALO	K	3	2	5,6,7	0.54	0	5,7,9	1.13	0
2	WFP	H	2	2	12,13,14	1.01	1 (8%)	12,17,19	1.76	2 (16%)
2	WFP	J	2	2	12,13,14	1.01	1 (8%)	12,17,19	1.40	2 (16%)
2	WFP	I	2	2	12,13,14	1.15	1 (8%)	12,17,19	1.92	5 (41%)

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
2	ALO	I	3	2	-	1/5/6/8	-
2	WFP	M	2	2	-	2/5/6/8	0/1/1/1
2	ALO	L	3	2	-	1/5/6/8	-
2	WFP	K	2	2	-	1/5/6/8	0/1/1/1
2	WFP	N	2	2	-	2/5/6/8	0/1/1/1
2	ALO	J	3	2	-	1/5/6/8	-
2	ALO	N	3	2	-	1/5/6/8	-
2	WFP	L	2	2	-	0/5/6/8	0/1/1/1
2	ALO	M	3	2	-	1/5/6/8	-
2	ALO	H	3	2	-	1/5/6/8	-
2	ALO	K	3	2	-	1/5/6/8	-
2	WFP	H	2	2	-	0/5/6/8	0/1/1/1
2	WFP	J	2	2	-	1/5/6/8	0/1/1/1
2	WFP	I	2	2	-	1/5/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	WFP	CB-CG	2.53	1.57	1.51
2	M	2	WFP	CB-CG	2.53	1.57	1.51
2	J	2	WFP	CB-CG	2.46	1.57	1.51
2	L	2	WFP	CB-CG	2.38	1.56	1.51
2	N	2	WFP	CB-CG	2.34	1.56	1.51
2	K	2	WFP	CB-CG	2.31	1.56	1.51
2	H	2	WFP	CB-CG	2.17	1.56	1.51
2	K	2	WFP	CD1-CE1	2.09	1.41	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	WFP	CD2-CE2-CZ	-3.73	118.97	123.50
2	L	2	WFP	CD2-CE2-CZ	-3.65	119.06	123.50
2	L	2	WFP	CE2-CZ-CE1	3.64	121.39	116.08
2	H	2	WFP	CD1-CE1-CZ	-3.61	119.11	123.50
2	N	2	WFP	CD2-CE2-CZ	-3.35	119.43	123.50
2	J	3	ALO	OG1-CB-CA	3.24	115.86	109.01
2	H	2	WFP	CE2-CZ-CE1	3.07	120.55	116.08
2	N	2	WFP	CE2-CZ-CE1	2.98	120.42	116.08
2	I	2	WFP	CE2-CZ-CE1	2.93	120.34	116.08
2	L	2	WFP	CD1-CE1-CZ	-2.83	120.07	123.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	WFP	F2-CE2-CD2	2.79	122.25	118.28
2	L	2	WFP	F1-CE1-CD1	2.73	122.17	118.28
2	J	2	WFP	CD2-CE2-CZ	-2.71	120.21	123.50
2	N	2	WFP	CD1-CE1-CZ	-2.62	120.32	123.50
2	I	2	WFP	F2-CE2-CD2	2.52	121.86	118.28
2	M	2	WFP	CD1-CE1-CZ	-2.50	120.47	123.50
2	M	2	WFP	CD2-CE2-CZ	-2.43	120.55	123.50
2	K	2	WFP	CD1-CE1-CZ	-2.39	120.60	123.50
2	J	2	WFP	CE2-CZ-CE1	2.37	119.54	116.08
2	I	2	WFP	CG-CD2-CE2	2.31	120.77	118.75
2	K	2	WFP	CE2-CZ-CE1	2.29	119.42	116.08
2	L	3	ALO	CG2-CB-CA	-2.27	107.00	112.16
2	K	2	WFP	CD2-CE2-CZ	-2.23	120.80	123.50
2	N	3	ALO	OG1-CB-CA	2.22	113.71	109.01
2	I	2	WFP	CD1-CE1-CZ	-2.22	120.80	123.50
2	M	2	WFP	CE2-CZ-CE1	2.18	119.26	116.08
2	K	2	WFP	F1-CE1-CD1	2.12	121.29	118.28
2	L	2	WFP	CG-CD2-CE2	2.03	120.52	118.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	3	ALO	O-C-CA-CB
2	L	3	ALO	O-C-CA-CB
2	M	3	ALO	O-C-CA-CB
2	K	2	WFP	N-CA-CB-CG
2	N	2	WFP	N-CA-CB-CG
2	I	2	WFP	N-CA-CB-CG
2	J	2	WFP	N-CA-CB-CG
2	M	2	WFP	N-CA-CB-CG
2	H	3	ALO	O-C-CA-CB
2	I	3	ALO	O-C-CA-CB
2	N	3	ALO	O-C-CA-CB
2	M	2	WFP	C-CA-CB-CG
2	N	2	WFP	C-CA-CB-CG
2	J	3	ALO	N-CA-CB-CG2

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	ALO	4	0
2	L	3	ALO	3	0
2	J	3	ALO	2	0
2	N	3	ALO	4	0
2	M	3	ALO	3	0
2	H	3	ALO	2	0
2	K	3	ALO	4	0
2	H	2	WFP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	189/221 (85%)	0.08	9 (4%) 35 28	51, 64, 101, 137	0
1	B	185/221 (83%)	0.10	6 (3%) 50 40	51, 67, 99, 132	0
1	C	189/221 (85%)	0.15	13 (6%) 23 16	47, 64, 100, 145	0
1	D	189/221 (85%)	-0.17	11 (5%) 29 22	42, 53, 94, 152	0
1	E	188/221 (85%)	-0.29	9 (4%) 35 28	42, 51, 86, 134	0
1	F	190/221 (85%)	-0.22	12 (6%) 26 19	32, 49, 85, 145	1 (0%)
1	G	188/221 (85%)	-0.11	11 (5%) 28 21	43, 56, 88, 143	0
2	H	3/7 (42%)	-0.28	0 100 100	72, 72, 72, 75	0
2	I	3/7 (42%)	0.26	0 100 100	73, 73, 75, 77	0
2	J	3/7 (42%)	-0.23	0 100 100	65, 65, 71, 73	0
2	K	3/7 (42%)	-0.02	0 100 100	62, 62, 64, 68	0
2	L	3/7 (42%)	-0.26	0 100 100	55, 55, 55, 57	0
2	M	3/7 (42%)	-0.32	0 100 100	54, 54, 55, 57	0
2	N	3/7 (42%)	-0.25	0 100 100	52, 52, 55, 56	0
All	All	1339/1596 (83%)	-0.07	71 (5%) 32 24	32, 58, 100, 152	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	236	ILE	6.8
1	F	293	GLN	5.9
1	C	231	ALA	5.2
1	C	235	ALA	5.0
1	B	106	VAL	4.2
1	F	110	GLY	4.2
1	F	109	THR	4.1
1	B	235	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	234	ILE	3.8
1	A	234	ILE	3.8
1	B	57	SER	3.8
1	G	109	THR	3.7
1	A	101	LEU	3.7
1	A	295	ASP	3.7
1	D	231	ALA	3.6
1	F	57	SER	3.6
1	G	107	GLU	3.5
1	A	231	ALA	3.4
1	A	109	THR	3.4
1	G	232	THR	3.4
1	G	234	ILE	3.3
1	A	57	SER	3.3
1	C	110	GLY	3.2
1	F	229	GLY	3.1
1	F	107	GLU	3.1
1	D	232	THR	3.1
1	C	223	PRO	3.0
1	G	235	ALA	3.0
1	C	109	THR	3.0
1	D	109	THR	2.9
1	G	57	SER	2.9
1	A	233	ASP	2.9
1	F	233	ASP	2.8
1	E	231	ALA	2.8
1	C	234	ILE	2.8
1	G	110	GLY	2.7
1	E	293	GLN	2.7
1	F	261	GLN	2.7
1	B	101	LEU	2.7
1	G	231	ALA	2.6
1	D	57	SER	2.6
1	F	112	GLY	2.6
1	C	232	THR	2.5
1	E	232	THR	2.5
1	D	234	ILE	2.5
1	D	116	TYR	2.5
1	E	57	SER	2.4
1	E	233	ASP	2.4
1	C	114	ARG	2.4
1	C	57	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	107	GLU	2.4
1	D	106	VAL	2.4
1	F	235	ALA	2.4
1	D	107	GLU	2.3
1	G	224	SER	2.3
1	E	108	GLN	2.3
1	G	101	LEU	2.3
1	A	224	SER	2.3
1	B	294	ASP	2.3
1	B	224	SER	2.3
1	D	233	ASP	2.2
1	C	106	VAL	2.2
1	C	115	ALA	2.2
1	D	108	GLN	2.2
1	E	101	LEU	2.2
1	G	233	ASP	2.1
1	F	108	GLN	2.1
1	A	111	ARG	2.0
1	E	115	ALA	2.0
1	D	235	ALA	2.0
1	E	234	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
2	ALO	H	3	7/8	0.91	0.10	64,66,70,72	0
2	ALO	K	3	7/8	0.91	0.12	58,62,69,70	0
2	ALO	I	3	7/8	0.93	0.10	62,69,73,75	0
2	ALO	N	3	7/8	0.93	0.10	44,52,59,61	0
2	ALO	M	3	7/8	0.94	0.08	51,53,56,57	0
2	ALO	J	3	7/8	0.94	0.10	61,67,72,75	0
2	WFP	H	2	13/14	0.95	0.08	53,60,69,69	0
2	ALO	L	3	7/8	0.95	0.08	50,54,56,63	0
2	WFP	I	2	13/14	0.95	0.09	63,67,71,71	0
2	WFP	K	2	13/14	0.95	0.08	54,58,63,65	0
2	WFP	M	2	13/14	0.96	0.07	45,48,54,55	0
2	WFP	N	2	13/14	0.96	0.10	46,50,54,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	WFP	J	2	13/14	0.96	0.09	55,66,70,70	0
2	WFP	L	2	13/14	0.97	0.07	44,49,54,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.