Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 04:47 AM EDT

PDB ID	:	4IQR
Title	:	Multi-Domain Organization of the HNF4alpha Nuclear Receptor Complex on DNA
Authors	:	Chandra, V.; Huang, P.; Kim, Y.; Rastinejad, F.
Deposited on	:	2013-01-13
Resolution	:	2.90 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:

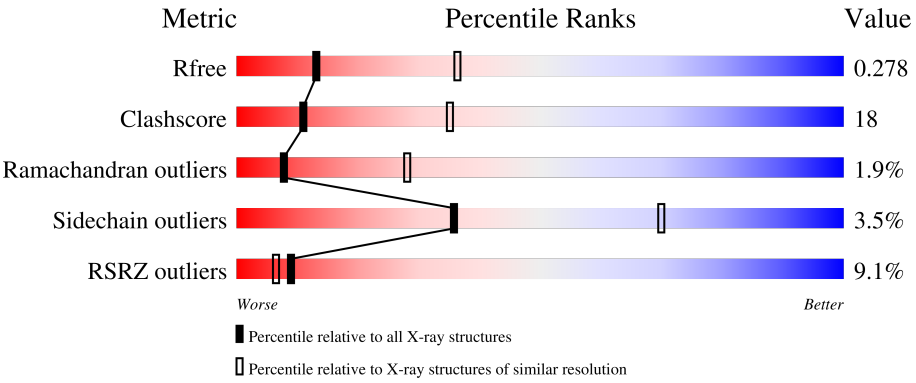
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	338	6% 58% 30% • 11%
1	B	338	7% 56% 32% • 9%
1	E	338	6% 56% 32% • 10%
1	F	338	10% 59% 30% • 7%
2	C	20	5% 40% 60%

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Mol	Chain	Length	Quality of chain
2	G	20	5% 60% 35% 5%
3	D	20	5% 35% 65%
3	H	20	40% 60%
4	I	13	62% 54% 8% 38%
4	J	13	8% 46% 31% 23%
4	K	13	62% 38% 23% 38%
4	L	13	54% 31% 31% 38%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11783 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 Hepatocyte nuclear factor 4-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2403	1521	427	435	20			
1	B	308	Total	C	N	O	S	0	0	0
			2465	1555	440	450	20			
1	E	303	Total	C	N	O	S	0	0	0
			2407	1524	428	435	20			
1	F	314	Total	C	N	O	S	0	0	0
			2506	1578	450	458	20			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP P41235
A	32	ALA	-	expression tag	UNP P41235
A	33	HIS	-	expression tag	UNP P41235
A	34	HIS	-	expression tag	UNP P41235
A	35	HIS	-	expression tag	UNP P41235
A	36	HIS	-	expression tag	UNP P41235
A	37	HIS	-	expression tag	UNP P41235
A	38	HIS	-	expression tag	UNP P41235
A	39	VAL	-	expression tag	UNP P41235
A	40	ASP	-	expression tag	UNP P41235
A	41	ASP	-	expression tag	UNP P41235
A	42	ASP	-	expression tag	UNP P41235
A	43	ASP	-	expression tag	UNP P41235
A	44	LYS	-	expression tag	UNP P41235
A	45	MET	-	expression tag	UNP P41235
B	31	MET	-	initiating methionine	UNP P41235
B	32	ALA	-	expression tag	UNP P41235
B	33	HIS	-	expression tag	UNP P41235
B	34	HIS	-	expression tag	UNP P41235
B	35	HIS	-	expression tag	UNP P41235
B	36	HIS	-	expression tag	UNP P41235

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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	HIS	-	expression tag	UNP P41235
B	38	HIS	-	expression tag	UNP P41235
B	39	VAL	-	expression tag	UNP P41235
B	40	ASP	-	expression tag	UNP P41235
B	41	ASP	-	expression tag	UNP P41235
B	42	ASP	-	expression tag	UNP P41235
B	43	ASP	-	expression tag	UNP P41235
B	44	LYS	-	expression tag	UNP P41235
B	45	MET	-	expression tag	UNP P41235
E	31	MET	-	initiating methionine	UNP P41235
E	32	ALA	-	expression tag	UNP P41235
E	33	HIS	-	expression tag	UNP P41235
E	34	HIS	-	expression tag	UNP P41235
E	35	HIS	-	expression tag	UNP P41235
E	36	HIS	-	expression tag	UNP P41235
E	37	HIS	-	expression tag	UNP P41235
E	38	HIS	-	expression tag	UNP P41235
E	39	VAL	-	expression tag	UNP P41235
E	40	ASP	-	expression tag	UNP P41235
E	41	ASP	-	expression tag	UNP P41235
E	42	ASP	-	expression tag	UNP P41235
E	43	ASP	-	expression tag	UNP P41235
E	44	LYS	-	expression tag	UNP P41235
E	45	MET	-	expression tag	UNP P41235
F	31	MET	-	initiating methionine	UNP P41235
F	32	ALA	-	expression tag	UNP P41235
F	33	HIS	-	expression tag	UNP P41235
F	34	HIS	-	expression tag	UNP P41235
F	35	HIS	-	expression tag	UNP P41235
F	36	HIS	-	expression tag	UNP P41235
F	37	HIS	-	expression tag	UNP P41235
F	38	HIS	-	expression tag	UNP P41235
F	39	VAL	-	expression tag	UNP P41235
F	40	ASP	-	expression tag	UNP P41235
F	41	ASP	-	expression tag	UNP P41235
F	42	ASP	-	expression tag	UNP P41235
F	43	ASP	-	expression tag	UNP P41235
F	44	LYS	-	expression tag	UNP P41235
F	45	MET	-	expression tag	UNP P41235

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			415	197	85	114	19			
2	G	20	Total	C	N	O	P	0	0	0
			415	197	85	114	19			

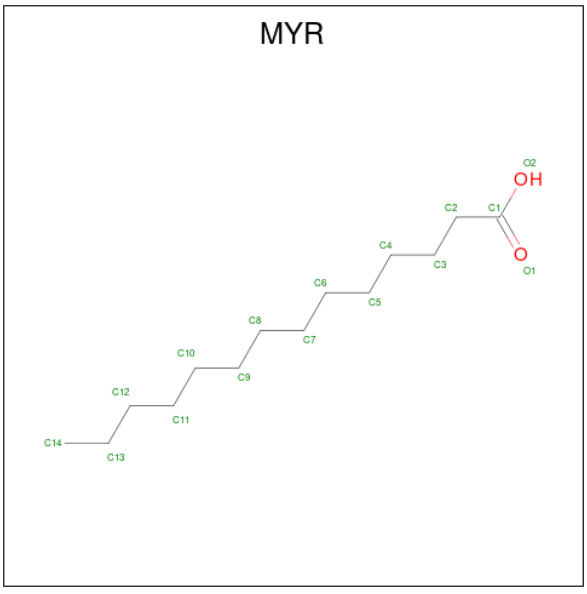
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*CP*TP*TP*TP*GP*AP*CP*CP*TP*AP*GP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			399	193	65	122	19			
3	H	20	Total	C	N	O	P	0	0	0
			399	193	65	122	19			

- Molecule 4 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	8	Total	C	N	O	0	0	0
			71	47	15	9			
4	J	10	Total	C	N	O	0	0	0
			89	57	19	13			
4	K	8	Total	C	N	O	0	0	0
			71	47	15	9			
4	L	8	Total	C	N	O	0	0	0
			71	47	15	9			

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 14 2	0	0
5	B	1	Total C O 16 14 2	0	0
5	E	1	Total C O 16 14 2	0	0
5	F	1	Total C O 16 14 2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

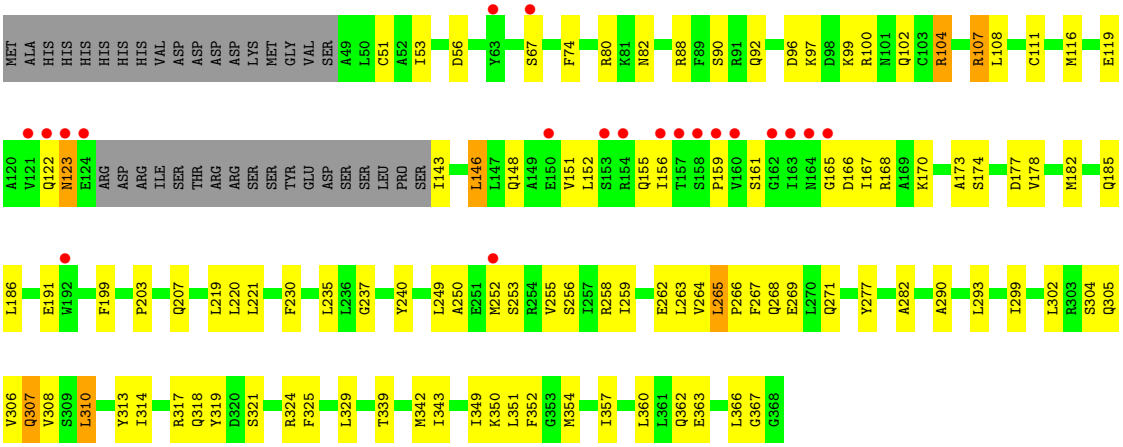
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0
6	B	2	Total Zn 2 2	0	0
6	E	2	Total Zn 2 2	0	0
6	F	2	Total Zn 2 2	0	0

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.

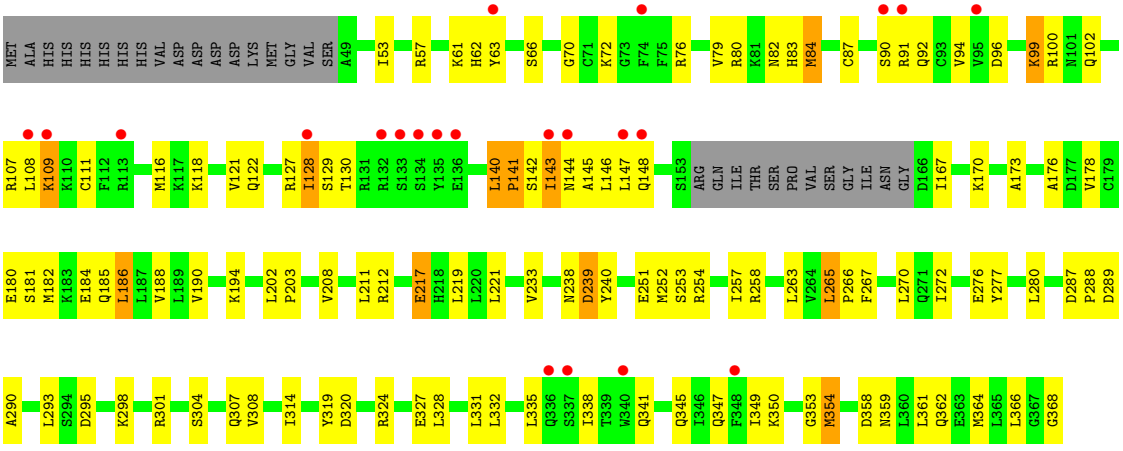
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain A:



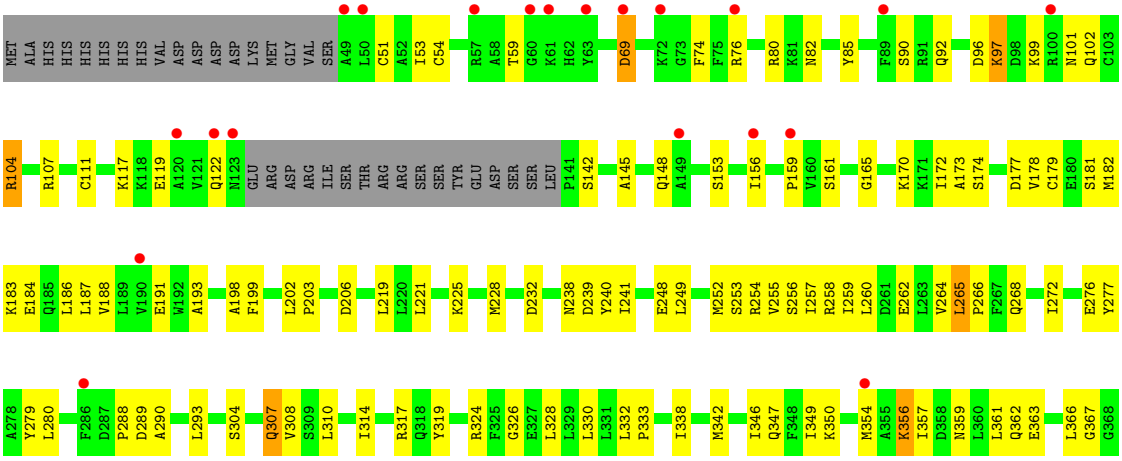
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain B:



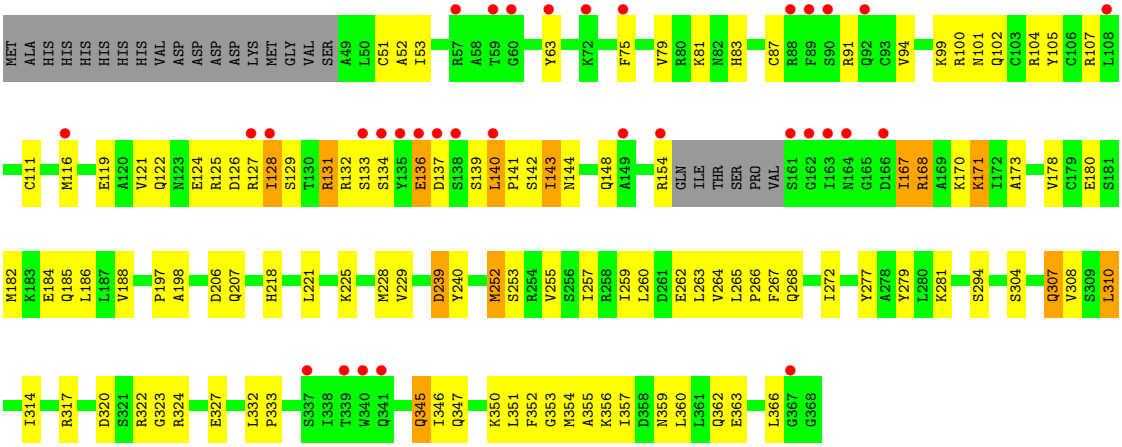
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain E:



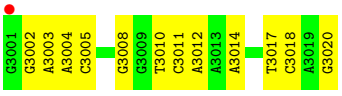
• Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain F:



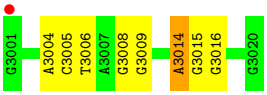
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*CP*TP*AP*GP*GP*TP*CP*AP*AP*AP*GP*GP*TP*CP*AP*G)-3')

Chain C:



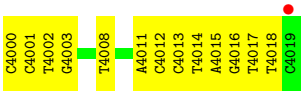
• Molecule 2: DNA (5'-D(*GP*GP*AP*AP*CP*TP*AP*GP*GP*TP*CP*AP*AP*AP*GP*GP*TP*CP*AP*G)-3')

Chain G:



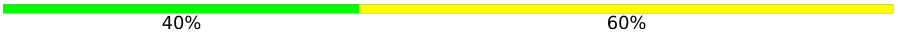
• Molecule 3: DNA (5'-D(*CP*CP*TP*GP*AP*CP*CP*TP*TP*TP*GP*AP*CP*CP*TP*AP*GP*TP*TP*C)-3')

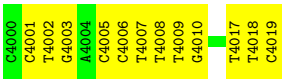
Chain D:



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

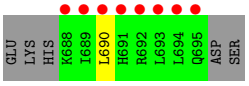
Chain H:





• Molecule 4: Nuclear receptor coactivator 2

Chain I:

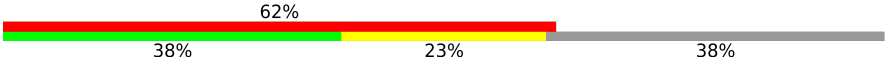


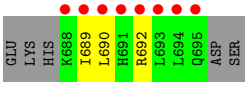
• Molecule 4: Nuclear receptor coactivator 2

Chain J:

• Molecule 4: Nuclear receptor coactivator 2

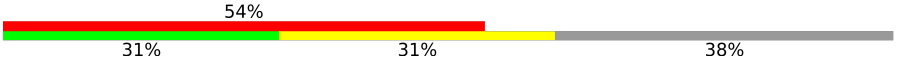
Chain K:

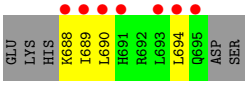




• Molecule 4: Nuclear receptor coactivator 2

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.79Å 57.60Å 166.31Å 90.00° 96.30° 90.00°	Depositor
Resolution (Å)	48.81 – 2.90 48.81 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.81-2.90) 99.1 (48.81-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.278 0.235 , 0.278	Depositor DCC
R_{free} test set	2580 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11783	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.63% 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, 0.333 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: ZN, MYR

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	0.28	0/2440	0.49	0/3276
1	B	0.28	0/2503	0.48	0/3359
1	E	0.27	0/2445	0.46	0/3283
1	F	0.26	0/2544	0.46	0/3413
2	C	0.26	0/468	0.68	0/722
2	G	0.28	0/468	0.66	0/722
3	D	0.26	0/444	0.67	0/682
3	H	0.29	0/444	0.66	0/682
4	I	0.30	0/71	0.44	0/93
4	J	0.28	0/90	0.47	0/119
4	K	0.29	0/71	0.46	0/93
4	L	0.29	0/71	0.46	0/93
All	All	0.27	0/12059	0.51	0/16537

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
2	C	0	1
2	G	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	3008	DG	Sidechain
2	G	3014	DA	Sidechain

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	A	2403	0	2451	77	0
1	B	2465	0	2504	108	0
1	E	2407	0	2458	94	0
1	F	2506	0	2546	108	0
2	C	415	0	225	10	0
2	G	415	0	225	17	0
3	D	399	0	229	13	0
3	H	399	0	229	10	0
4	I	71	0	84	1	0
4	J	89	0	95	3	0
4	K	71	0	84	7	0
4	L	71	0	84	6	0
5	A	16	0	27	3	0
5	B	16	0	27	5	0
5	E	16	0	27	2	0
5	F	16	0	27	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
All	All	11783	0	11322	417	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 18.

All (417) 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:140:LEU:HA	1:F:144:ASN:HD22	1.29	0.96
1:B:143:ILE:HG23	1:B:144:ASN:H	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:GLU:HG2	1:F:137:ASP:H	1.33	0.93
1:A:167:ILE:HD12	1:A:170:LYS:HD2	1.56	0.88
1:B:144:ASN:HB3	1:B:148:GLN:HB2	1.55	0.87
1:B:252:MET:HB3	5:B:401:MYR:H111	1.56	0.86
1:A:146:LEU:H	1:A:146:LEU:HD23	1.42	0.85
1:B:140:LEU:H	1:B:141:PRO:HD2	1.40	0.85
1:A:152:LEU:HD23	1:A:155:GLN:HE21	1.44	0.82
1:A:156:ILE:HD11	1:A:191:GLU:HG3	1.62	0.81
1:E:122:GLN:HG2	2:G:3008:DG:OP1	1.82	0.80
1:F:125:ARG:HD3	2:G:3015:DG:H4'	1.62	0.80
1:B:173:ALA:HB2	1:B:240:TYR:HB3	1.63	0.79
1:E:173:ALA:HB2	1:E:240:TYR:HB3	1.64	0.79
2:C:3020:DG:H1	3:D:4001:DC:H42	1.29	0.78
1:F:167:ILE:HD13	1:F:167:ILE:H	1.49	0.78
1:A:252:MET:HE3	5:A:401:MYR:H142	1.66	0.78
1:B:181:SER:HB2	1:B:238:ASN:ND2	1.98	0.77
1:E:156:ILE:HD13	1:E:191:GLU:HG3	1.67	0.76
5:A:401:MYR:H112	5:A:401:MYR:H71	1.67	0.75
1:F:185:GLN:O	1:F:188:VAL:HG22	1.86	0.75
1:E:258:ARG:HD2	1:E:262:GLU:OE2	1.87	0.75
1:E:349:ILE:HG23	1:E:354:MET:HB2	1.70	0.74
1:E:253:SER:O	1:E:257:ILE:HG13	1.90	0.72
1:E:363:GLU:OE2	4:K:689:ILE:HB	1.90	0.71
1:E:265:LEU:HB3	1:E:266:PRO:HD3	1.73	0.70
1:F:221:LEU:HG	1:F:277:TYR:HE1	1.57	0.70
1:F:323:GLY:O	1:F:327:GLU:HG2	1.92	0.70
1:B:76:ARG:HD2	1:B:80:ARG:NH2	2.08	0.69
1:F:143:ILE:HD13	1:F:143:ILE:O	1.93	0.69
1:F:173:ALA:HB2	1:F:240:TYR:HB3	1.74	0.68
1:A:314:ILE:HD12	1:A:324:ARG:HD3	1.75	0.68
1:E:172:ILE:HG21	1:E:248:GLU:OE1	1.93	0.68
1:A:152:LEU:HD23	1:A:155:GLN:NE2	2.09	0.68
1:F:100:ARG:HD3	1:F:107:ARG:NH1	2.08	0.68
1:A:74:PHE:CD2	1:A:107:ARG:HD2	2.28	0.67
1:F:131:ARG:HD2	1:F:132:ARG:H	1.60	0.67
1:E:178:VAL:HG11	5:E:401:MYR:H132	1.77	0.67
1:B:270:LEU:HD23	1:B:328:LEU:HD22	1.76	0.67
1:A:74:PHE:CE2	1:A:107:ARG:HD2	2.30	0.66
1:E:304:SER:O	1:E:308:VAL:HG23	1.96	0.66
1:E:97:LYS:HB2	1:E:97:LYS:NZ	2.11	0.66
1:F:185:GLN:HA	1:F:185:GLN:NE2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:SER:O	1:E:92:GLN:HG3	1.95	0.65
1:E:363:GLU:OE1	4:K:690:LEU:HD13	1.95	0.65
1:E:314:ILE:HD12	1:E:324:ARG:HD3	1.79	0.65
1:B:280:LEU:HD11	1:B:328:LEU:HD12	1.79	0.64
1:B:61:LYS:HA	1:B:66:SER:HA	1.78	0.64
1:B:142:SER:HA	1:B:146:LEU:HD13	1.79	0.63
1:F:206:ASP:OD2	1:F:294:SER:HB3	1.97	0.63
1:B:267:PHE:HA	1:B:272:ILE:HD13	1.80	0.63
1:B:143:ILE:HG23	1:B:144:ASN:N	2.10	0.63
4:K:692:ARG:HB3	4:K:692:ARG:NH1	2.13	0.63
1:F:122:GLN:HE21	2:G:3014:DA:H4'	1.64	0.62
1:F:314:ILE:HG23	1:F:324:ARG:HD3	1.80	0.62
1:F:75:PHE:O	1:F:79:VAL:HG23	2.00	0.62
1:F:221:LEU:HG	1:F:277:TYR:CE1	2.34	0.62
1:A:156:ILE:CD1	1:A:191:GLU:HG3	2.28	0.61
1:F:252:MET:HB3	5:F:401:MYR:H101	1.81	0.61
1:A:122:GLN:O	1:A:123:ASN:HB2	2.00	0.61
1:B:184:GLU:O	1:B:188:VAL:HG23	2.00	0.61
1:F:87:CYS:HB2	1:F:105:TYR:CD2	2.36	0.61
1:B:146:LEU:N	1:B:146:LEU:HD12	2.16	0.61
2:C:3004:DA:H2"	2:C:3005:DC:H5'	1.80	0.61
1:F:167:ILE:HD13	1:F:167:ILE:N	2.14	0.61
1:B:145:ALA:HB3	1:B:146:LEU:HD12	1.83	0.61
1:B:295:ASP:OD2	1:B:298:LYS:HB2	2.01	0.61
1:F:140:LEU:HA	1:F:144:ASN:ND2	2.08	0.60
1:E:184:GLU:O	1:E:188:VAL:HG23	2.02	0.60
1:F:100:ARG:HD2	3:H:4003:DG:OP1	2.00	0.60
2:C:3020:DG:H1	3:D:4001:DC:N4	1.99	0.60
1:E:117:LYS:HB3	1:E:119:GLU:HG2	1.84	0.60
1:F:253:SER:O	1:F:257:ILE:HG13	2.01	0.60
1:A:178:VAL:HG11	5:A:401:MYR:H121	1.85	0.59
1:A:88:ARG:HD3	1:B:127:ARG:HD3	1.85	0.59
1:E:252:MET:HE2	5:E:401:MYR:H142	1.83	0.59
1:B:253:SER:O	1:B:257:ILE:HG13	2.03	0.58
1:E:179:CYS:O	1:E:183:LYS:HG2	2.02	0.58
1:F:131:ARG:CD	1:F:132:ARG:H	2.16	0.58
1:E:326:GLY:O	1:E:330:LEU:HG	2.03	0.58
1:A:178:VAL:O	1:A:182:MET:HG3	2.03	0.58
1:A:221:LEU:HG	1:A:277:TYR:HE1	1.68	0.58
1:F:178:VAL:O	1:F:182:MET:HG3	2.02	0.58
1:A:51:CYS:SG	1:A:67:SER:HA	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:NH2	1:B:368:GLY:HA2	2.19	0.57
1:E:258:ARG:HH21	1:E:338:ILE:HA	1.69	0.57
1:A:352:PHE:HB2	1:A:354:MET:CE	2.34	0.57
1:B:84:MET:CE	1:B:84:MET:H	2.17	0.57
1:B:109:LYS:HE3	1:B:109:LYS:O	2.04	0.57
1:A:56:ASP:OD1	1:A:97:LYS:HE2	2.05	0.57
1:F:104:ARG:HH22	3:H:4001:DC:H4'	1.70	0.57
1:F:140:LEU:N	1:F:141:PRO:HD2	2.19	0.57
1:A:362:GLN:HA	1:A:366:LEU:HD12	1.86	0.57
1:B:272:ILE:H	1:B:272:ILE:HD12	1.69	0.57
1:F:128:ILE:HD12	2:G:3016:DG:H4'	1.87	0.57
1:A:258:ARG:HD2	1:A:262:GLU:OE2	2.04	0.57
1:F:140:LEU:H	1:F:141:PRO:HD2	1.70	0.57
1:A:349:ILE:HG23	1:A:354:MET:HB2	1.86	0.56
3:D:4013:DC:C6	3:D:4014:DT:H72	2.39	0.56
1:F:167:ILE:H	1:F:167:ILE:CD1	2.15	0.56
1:F:63:TYR:HD2	1:F:116:MET:HE2	1.70	0.56
1:A:53:ILE:HD11	1:A:116:MET:SD	2.46	0.56
1:A:173:ALA:HB2	1:A:240:TYR:HB3	1.88	0.56
1:A:263:LEU:C	1:A:266:PRO:HD2	2.26	0.56
1:F:307:GLN:HG3	1:F:308:VAL:N	2.21	0.56
1:A:80:ARG:HG3	1:A:80:ARG:HH11	1.71	0.55
1:A:104:ARG:HG3	1:A:104:ARG:HH11	1.70	0.55
1:F:263:LEU:C	1:F:266:PRO:HD2	2.26	0.55
1:B:178:VAL:O	1:B:182:MET:HG3	2.06	0.55
1:B:298:LYS:HA	1:B:301:ARG:NH2	2.22	0.55
1:B:99:LYS:O	1:B:102:GLN:HB2	2.06	0.55
1:F:122:GLN:NE2	2:G:3014:DA:H4'	2.21	0.55
1:F:347:GLN:OE1	1:F:366:LEU:HD22	2.07	0.55
1:F:304:SER:O	1:F:308:VAL:HG23	2.05	0.55
1:F:264:VAL:O	1:F:268:GLN:HG3	2.07	0.54
1:B:141:PRO:HG2	1:B:142:SER:H	1.71	0.54
1:A:220:LEU:HD11	1:A:342:MET:SD	2.48	0.54
1:A:350:LYS:HB2	1:A:357:ILE:HG13	1.88	0.54
1:F:182:MET:O	1:F:186:LEU:HB2	2.08	0.54
1:A:199:PHE:CZ	1:A:207:GLN:HB3	2.42	0.54
1:E:254:ARG:HB2	1:E:254:ARG:NH1	2.23	0.54
1:B:217:GLU:HG3	1:B:335:LEU:HG	1.89	0.54
1:E:317:ARG:HA	1:E:317:ARG:CZ	2.38	0.54
1:A:264:VAL:O	1:A:268:GLN:HG3	2.07	0.53
1:E:362:GLN:HA	1:E:366:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HD13	3:D:4008:DT:C5'	2.38	0.53
1:A:90:SER:O	1:A:92:GLN:HG3	2.08	0.53
1:B:94:VAL:HG13	1:B:99:LYS:HD2	1.90	0.53
1:B:122:GLN:OE1	2:C:3014:DA:H4'	2.07	0.53
1:F:362:GLN:HA	1:F:366:LEU:HB2	1.91	0.53
1:B:307:GLN:HG3	1:B:308:VAL:N	2.23	0.53
1:B:63:TYR:CE2	1:B:72:LYS:HG3	2.43	0.53
2:G:3004:DA:H1'	2:G:3005:DC:H5"	1.90	0.53
1:A:186:LEU:HD13	1:A:219:LEU:HD11	1.90	0.53
1:B:170:LYS:HD2	1:B:239:ASP:O	2.09	0.53
1:E:181:SER:HB2	1:E:238:ASN:ND2	2.24	0.53
1:F:136:GLU:HG2	1:F:137:ASP:N	2.15	0.53
1:B:76:ARG:HD2	1:B:80:ARG:HH21	1.71	0.52
1:E:279:TYR:HB3	1:E:310:LEU:HD12	1.91	0.52
1:B:272:ILE:HD12	1:B:272:ILE:N	2.23	0.52
1:E:186:LEU:HD13	1:E:219:LEU:HD11	1.90	0.52
1:E:170:LYS:HD2	1:E:239:ASP:O	2.09	0.52
1:E:304:SER:O	1:E:307:GLN:HG3	2.10	0.52
1:A:313:TYR:O	1:A:317:ARG:NH1	2.43	0.52
1:E:104:ARG:HH21	3:H:4008:DT:H5"	1.74	0.52
1:B:63:TYR:O	1:B:116:MET:HA	2.09	0.52
1:B:128:ILE:HD13	3:D:4008:DT:H5'	1.92	0.52
1:E:99:LYS:HG2	1:E:102:GLN:HE22	1.74	0.52
3:H:4009:DT:H2"	3:H:4010:DG:C8	2.45	0.52
1:E:347:GLN:OE1	1:E:366:LEU:HD22	2.10	0.52
1:A:325:PHE:CZ	1:A:329:LEU:HD11	2.45	0.52
1:F:363:GLU:CD	4:L:688:LYS:HB2	2.30	0.52
1:A:317:ARG:HB3	1:A:319:TYR:CE1	2.45	0.52
1:B:176:ALA:O	1:B:180:GLU:HB2	2.10	0.52
1:E:182:MET:O	1:E:186:LEU:HB2	2.10	0.52
1:F:94:VAL:CG1	1:F:99:LYS:HE2	2.39	0.52
2:G:3005:DC:H2'	2:G:3006:DT:H72	1.91	0.52
1:B:108:LEU:O	1:B:111:CYS:HB2	2.10	0.52
2:C:3004:DA:H2"	2:C:3005:DC:C5'	2.40	0.52
2:C:3010:DT:H2"	2:C:3011:DC:C6	2.45	0.52
1:E:193:ALA:HB1	1:E:199:PHE:CD2	2.44	0.52
1:F:225:LYS:O	1:F:228:MET:HG2	2.09	0.52
3:H:4005:DC:H2"	3:H:4006:DC:O5'	2.10	0.52
1:E:53:ILE:HD13	1:E:111:CYS:SG	2.50	0.51
1:E:350:LYS:HE2	1:E:362:GLN:OE1	2.11	0.51
1:E:288:PRO:O	1:E:293:LEU:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3008:DG:H1'	2:G:3009:DG:H5'	1.92	0.51
1:B:358:ASP:HB3	1:B:361:LEU:HD13	1.91	0.51
1:B:79:VAL:HG13	1:B:118:LYS:HG3	1.92	0.51
1:B:221:LEU:HG	1:B:277:TYR:HE1	1.75	0.51
1:B:178:VAL:HG11	5:B:401:MYR:H131	1.92	0.51
2:C:3004:DA:H1'	2:C:3005:DC:H5"	1.91	0.51
1:A:185:GLN:NE2	1:A:237:GLY:HA3	2.26	0.51
1:E:317:ARG:HA	1:E:317:ARG:NE	2.25	0.51
1:E:350:LYS:HB2	1:E:357:ILE:HG13	1.92	0.51
4:J:688:LYS:O	4:J:692:ARG:HG3	2.11	0.51
1:A:304:SER:O	1:A:307:GLN:HG3	2.10	0.50
1:A:318:GLN:HE21	1:A:318:GLN:HA	1.76	0.50
1:B:267:PHE:HE1	1:B:331:LEU:HD13	1.76	0.50
1:E:153:SER:O	1:E:188:VAL:HG13	2.11	0.50
1:E:363:GLU:CD	4:K:690:LEU:HD13	2.31	0.50
1:A:53:ILE:HD13	1:A:111:CYS:SG	2.51	0.50
1:E:99:LYS:HG2	1:E:102:GLN:NE2	2.26	0.50
1:E:156:ILE:HG21	1:E:191:GLU:HG3	1.92	0.50
1:F:255:VAL:O	1:F:259:ILE:HG13	2.11	0.50
1:A:290:ALA:HB3	1:A:293:LEU:HG	1.93	0.50
1:F:132:ARG:HG2	1:F:133:SER:N	2.26	0.50
1:A:318:GLN:HA	1:A:318:GLN:NE2	2.27	0.50
1:B:147:LEU:C	1:B:147:LEU:HD23	2.32	0.50
1:F:185:GLN:HA	1:F:185:GLN:HE21	1.75	0.50
1:B:272:ILE:HG23	1:B:276:GLU:HB2	1.94	0.50
1:A:314:ILE:HG23	1:A:324:ARG:HD3	1.93	0.49
1:E:342:MET:O	1:E:346:ILE:HG13	2.12	0.49
1:E:238:ASN:OD1	1:E:240:TYR:HD2	1.95	0.49
1:F:125:ARG:CD	2:G:3015:DG:H4'	2.40	0.49
1:B:53:ILE:HD13	1:B:111:CYS:SG	2.52	0.49
1:B:185:GLN:OE1	1:B:185:GLN:HA	2.12	0.49
1:B:350:LYS:HE2	1:B:362:GLN:OE1	2.12	0.49
1:E:119:GLU:H	1:E:119:GLU:CD	2.14	0.49
1:A:108:LEU:HD21	1:B:319:TYR:CE1	2.48	0.49
1:E:96:ASP:OD2	1:E:99:LYS:HE2	2.13	0.49
1:E:264:VAL:O	1:E:268:GLN:HG3	2.13	0.49
1:F:127:ARG:HG2	1:F:129:SER:H	1.77	0.49
1:F:267:PHE:CD2	1:F:272:ILE:HD12	2.48	0.49
1:F:279:TYR:HB3	1:F:310:LEU:HG	1.94	0.49
1:B:252:MET:HE3	5:B:401:MYR:H121	1.94	0.49
3:D:4001:DC:H2"	3:D:4002:DT:O5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PRO:O	1:A:207:GLN:HG3	2.12	0.49
1:E:265:LEU:CB	1:E:266:PRO:HD3	2.42	0.49
1:F:143:ILE:HD13	1:F:143:ILE:C	2.33	0.49
1:B:62:HIS:CD2	1:B:72:LYS:HD2	2.48	0.49
1:B:76:ARG:O	1:B:80:ARG:HB2	2.11	0.49
1:E:290:ALA:HB3	1:E:293:LEU:CD1	2.43	0.49
1:F:363:GLU:OE1	4:L:690:LEU:HD13	2.13	0.49
1:F:119:GLU:CD	1:F:119:GLU:H	2.15	0.48
1:F:363:GLU:CD	4:L:690:LEU:HD13	2.34	0.48
1:E:289:ASP:HB3	1:F:262:GLU:OE2	2.12	0.48
4:K:692:ARG:HB3	4:K:692:ARG:HH11	1.75	0.48
1:B:307:GLN:HG3	1:B:308:VAL:H	1.78	0.48
1:B:170:LYS:HE3	1:B:239:ASP:CG	2.34	0.48
1:F:345:GLN:HA	1:F:345:GLN:HE21	1.78	0.48
1:B:100:ARG:HB2	1:B:107:ARG:HD3	1.96	0.48
1:B:252:MET:CE	5:B:401:MYR:H121	2.43	0.48
1:B:304:SER:O	1:B:308:VAL:HG23	2.14	0.48
1:B:290:ALA:HB3	1:B:293:LEU:HD11	1.95	0.48
1:F:322:ARG:HG2	1:F:322:ARG:HH11	1.78	0.48
1:B:211:LEU:HD12	4:J:694:LEU:HD11	1.97	0.47
1:B:280:LEU:HD22	1:B:332:LEU:HD11	1.95	0.47
1:B:127:ARG:C	1:B:128:ILE:HG13	2.34	0.47
1:F:124:GLU:H	1:F:124:GLU:CD	2.18	0.47
1:F:252:MET:HG3	5:F:401:MYR:H121	1.96	0.47
1:E:170:LYS:HB3	1:E:241:ILE:HG23	1.97	0.47
1:F:260:LEU:HD23	1:F:264:VAL:HG21	1.96	0.47
1:F:350:LYS:HB2	1:F:357:ILE:HG13	1.96	0.47
1:E:80:ARG:HG3	1:E:80:ARG:HH11	1.79	0.47
1:A:104:ARG:HG3	1:A:104:ARG:NH1	2.29	0.47
1:B:70:GLY:HA2	3:D:4003:DG:H2'	1.96	0.47
1:E:97:LYS:HB2	1:E:97:LYS:HZ2	1.78	0.47
1:E:161:SER:HB3	1:E:165:GLY:HA3	1.96	0.47
1:F:170:LYS:O	1:F:171:LYS:HG2	2.14	0.47
3:H:4018:DT:H2'	3:H:4019:DC:C6	2.50	0.47
1:A:182:MET:O	1:A:186:LEU:HB2	2.15	0.47
1:A:255:VAL:O	1:A:259:ILE:HG13	2.15	0.47
1:B:314:ILE:HG23	1:B:324:ARG:HD3	1.97	0.47
1:E:76:ARG:NH2	2:G:3009:DG:N7	2.62	0.47
1:F:197:PRO:HG2	1:F:198:ALA:H	1.79	0.47
1:B:170:LYS:HE3	1:B:239:ASP:OD2	2.15	0.47
1:E:249:LEU:HB3	1:E:252:MET:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:LEU:HD23	1:F:140:LEU:C	2.35	0.47
1:F:207:GLN:HB3	4:L:694:LEU:HD21	1.97	0.47
1:B:63:TYR:CE1	1:B:121:VAL:HG22	2.50	0.46
1:B:167:ILE:HA	1:B:170:LYS:HG2	1.97	0.46
3:D:4000:DC:H2"	3:D:4001:DC:O5'	2.15	0.46
1:A:166:ASP:OD2	1:A:168:ARG:HB2	2.16	0.46
1:F:144:ASN:O	1:F:148:GLN:HB2	2.15	0.46
1:F:359:ASN:HB2	4:L:689:ILE:HD11	1.96	0.46
1:B:144:ASN:HB2	1:E:159:PRO:HD3	1.97	0.46
1:F:128:ILE:HG22	1:F:128:ILE:O	2.16	0.46
1:F:346:ILE:HG22	1:F:366:LEU:HD11	1.96	0.46
1:B:167:ILE:HD11	1:B:233:VAL:HG11	1.97	0.46
1:B:185:GLN:HB3	1:B:219:LEU:CD2	2.45	0.46
1:E:74:PHE:CD2	1:E:107:ARG:HD3	2.51	0.46
1:A:339:THR:O	1:A:343:ILE:HG13	2.15	0.46
1:E:221:LEU:HG	1:E:277:TYR:HE1	1.81	0.46
1:E:359:ASN:HB3	4:K:689:ILE:HD11	1.97	0.46
1:A:174:SER:O	1:A:177:ASP:N	2.48	0.45
1:A:265:LEU:HD22	1:A:269:GLU:OE1	2.16	0.45
1:B:349:ILE:HG23	1:B:354:MET:HB3	1.97	0.45
1:A:230:PHE:CE2	1:A:235:LEU:HD22	2.50	0.45
1:E:85:TYR:CE1	1:E:104:ARG:NH1	2.84	0.45
1:A:182:MET:HE3	1:A:342:MET:SD	2.56	0.45
1:A:314:ILE:HG22	1:A:321:SER:HB2	1.99	0.45
1:B:63:TYR:HE2	1:B:72:LYS:HG3	1.81	0.45
1:F:136:GLU:O	1:F:137:ASP:HB2	2.15	0.45
1:A:253:SER:HA	1:A:256:SER:OG	2.16	0.45
1:E:59:THR:HG21	1:E:69:ASP:OD1	2.17	0.45
1:F:94:VAL:HG13	1:F:99:LYS:HE2	1.98	0.45
1:F:229:VAL:HG12	1:F:229:VAL:O	2.16	0.45
1:B:129:SER:O	1:B:130:THR:HG22	2.17	0.45
1:B:359:ASN:O	1:B:362:GLN:HB3	2.16	0.45
1:E:254:ARG:NH1	1:E:254:ARG:CB	2.80	0.45
1:F:139:SER:O	1:F:140:LEU:HB2	2.16	0.45
1:F:171:LYS:HB3	1:F:240:TYR:CD1	2.52	0.45
2:G:3004:DA:C2'	2:G:3005:DC:H5"	2.47	0.45
1:A:305:GLN:O	1:A:308:VAL:HG12	2.16	0.45
1:B:87:CYS:SG	1:B:91:ARG:HA	2.57	0.45
1:E:356:LYS:NZ	1:E:356:LYS:HB3	2.31	0.45
1:F:267:PHE:CG	1:F:272:ILE:HD12	2.52	0.45
3:H:4006:DC:H2'	3:H:4007:DT:C7	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:H	1:B:141:PRO:CD	2.20	0.45
1:B:186:LEU:HG	1:B:364:MET:SD	2.57	0.45
3:D:4002:DT:H2'	3:D:4003:DG:C8	2.50	0.45
1:E:221:LEU:HG	1:E:277:TYR:CE1	2.52	0.45
1:F:186:LEU:HD23	1:F:360:LEU:HG	1.99	0.45
1:B:347:GLN:OE1	1:B:366:LEU:HD22	2.17	0.45
1:E:156:ILE:HD13	1:E:191:GLU:CG	2.43	0.45
1:F:304:SER:O	1:F:307:GLN:HG3	2.17	0.45
1:E:332:LEU:HB2	1:E:333:PRO:HD3	1.98	0.45
1:F:63:TYR:CE1	1:F:121:VAL:HG22	2.52	0.45
3:D:4013:DC:H2'	3:D:4014:DT:H72	1.98	0.45
1:E:142:SER:O	1:E:145:ALA:HB3	2.17	0.45
1:A:96:ASP:O	1:A:100:ARG:HB3	2.17	0.44
1:B:208:VAL:HG13	4:J:690:LEU:HD23	1.98	0.44
1:A:282:ALA:HB3	1:A:306:VAL:HG11	1.99	0.44
1:F:53:ILE:HD13	1:F:111:CYS:SG	2.58	0.44
1:F:100:ARG:HG3	1:F:101:ASN:N	2.31	0.44
1:B:186:LEU:HD13	1:B:219:LEU:HD11	1.98	0.44
1:F:154:ARG:NH1	1:F:154:ARG:HG3	2.32	0.44
1:B:90:SER:O	1:B:92:GLN:HG3	2.17	0.44
1:E:256:SER:O	1:E:260:LEU:HG	2.17	0.44
1:F:168:ARG:H	1:F:168:ARG:HD2	1.81	0.44
1:A:161:SER:HB3	1:A:165:GLY:HA3	2.00	0.44
3:H:4017:DT:H2"	3:H:4018:DT:O5'	2.17	0.44
1:A:80:ARG:HG3	1:A:80:ARG:NH1	2.31	0.44
1:F:104:ARG:NH2	3:H:4001:DC:H4'	2.31	0.44
1:F:184:GLU:O	1:F:188:VAL:HG13	2.18	0.44
1:A:249:LEU:HB3	1:A:252:MET:HB2	1.99	0.44
1:A:267:PHE:O	1:A:271:GLN:N	2.49	0.44
1:E:319:TYR:H	1:E:319:TYR:HD1	1.65	0.44
1:A:351:LEU:HD23	1:A:352:PHE:HE1	1.82	0.44
1:B:94:VAL:HG22	1:B:96:ASP:OD1	2.18	0.44
1:B:212:ARG:HH22	1:B:368:GLY:HA2	1.81	0.44
1:F:132:ARG:CZ	1:F:134:SER:OG	2.66	0.44
1:B:84:MET:H	1:B:84:MET:HE2	1.83	0.44
1:E:254:ARG:CB	1:E:254:ARG:HH11	2.30	0.44
1:F:327:GLU:OE2	1:F:327:GLU:HA	2.18	0.44
1:E:174:SER:O	1:E:177:ASP:N	2.51	0.43
1:E:198:ALA:O	1:E:202:LEU:HG	2.18	0.43
1:A:221:LEU:HG	1:A:277:TYR:CE1	2.50	0.43
1:B:272:ILE:H	1:B:272:ILE:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4011:DA:H2"	3:D:4012:DC:O5'	2.18	0.43
1:E:225:LYS:O	1:E:228:MET:HG2	2.17	0.43
2:G:3004:DA:H2"	2:G:3005:DC:H5"	1.99	0.43
2:G:3004:DA:H2"	2:G:3005:DC:C5'	2.48	0.43
1:B:141:PRO:O	1:B:145:ALA:HB3	2.19	0.43
1:B:221:LEU:HG	1:B:277:TYR:CE1	2.53	0.43
1:A:167:ILE:HA	1:A:170:LYS:HE2	2.00	0.43
1:F:185:GLN:HE21	1:F:185:GLN:CA	2.31	0.43
1:B:143:ILE:CG2	1:B:144:ASN:H	2.12	0.43
1:B:270:LEU:HD23	1:B:328:LEU:CD2	2.45	0.43
1:F:168:ARG:HG3	1:F:168:ARG:HH11	1.83	0.43
2:G:3014:DA:H2"	2:G:3015:DG:OP2	2.17	0.43
1:A:191:GLU:OE2	1:A:191:GLU:HA	2.19	0.43
1:B:304:SER:O	1:B:307:GLN:HG3	2.18	0.43
1:E:280:LEU:HD11	1:E:328:LEU:HD22	2.00	0.43
1:A:146:LEU:HD13	1:A:282:ALA:HB2	2.01	0.43
2:C:3011:DC:H2"	2:C:3012:DA:N7	2.34	0.43
1:E:80:ARG:HH22	2:G:3008:DG:H3'	1.84	0.43
1:F:252:MET:CG	5:F:401:MYR:H121	2.49	0.43
1:F:350:LYS:HE2	1:F:362:GLN:OE1	2.19	0.43
1:F:351:LEU:HD23	1:F:352:PHE:CE1	2.54	0.43
1:E:101:ASN:HB3	1:F:125:ARG:HG2	2.01	0.43
1:F:307:GLN:HG3	1:F:308:VAL:H	1.83	0.43
1:E:265:LEU:HB3	1:E:266:PRO:CD	2.45	0.42
4:K:692:ARG:HH11	4:K:692:ARG:CB	2.31	0.42
1:B:109:LYS:HE3	1:B:109:LYS:HA	2.00	0.42
1:F:81:LYS:C	1:F:83:HIS:H	2.22	0.42
1:E:254:ARG:HA	1:E:257:ILE:HD12	2.02	0.42
1:E:290:ALA:HB3	1:E:293:LEU:HD11	2.01	0.42
1:F:356:LYS:HD3	1:F:356:LYS:C	2.40	0.42
3:H:4001:DC:C6	3:H:4002:DT:H72	2.54	0.42
1:A:262:GLU:HG2	1:B:289:ASP:CG	2.40	0.42
1:E:148:GLN:HA	1:E:148:GLN:OE1	2.19	0.42
1:E:272:ILE:HG23	1:E:276:GLU:HB2	2.01	0.42
1:E:310:LEU:O	1:E:310:LEU:HD23	2.19	0.42
1:A:99:LYS:HB2	1:A:102:GLN:CD	2.38	0.42
1:B:144:ASN:HB2	1:E:159:PRO:CD	2.49	0.42
1:E:203:PRO:HD2	1:E:206:ASP:OD2	2.19	0.42
1:E:290:ALA:HB3	1:E:293:LEU:HG	2.02	0.42
1:F:180:GLU:O	1:F:184:GLU:HG2	2.18	0.42
1:A:314:ILE:CG2	1:A:321:SER:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:CYS:C	1:E:53:ILE:H	2.23	0.42
2:C:3002:DG:H2"	2:C:3003:DA:C8	2.54	0.42
1:A:263:LEU:O	1:A:266:PRO:HD2	2.20	0.42
1:B:258:ARG:HH21	1:B:338:ILE:HA	1.85	0.42
1:B:265:LEU:HB3	1:B:266:PRO:HD3	2.01	0.42
1:B:263:LEU:C	1:B:266:PRO:HD2	2.40	0.42
3:D:4017:DT:H2'	3:D:4018:DT:H72	2.02	0.42
1:E:97:LYS:NZ	1:E:97:LYS:CB	2.82	0.41
1:F:332:LEU:HB2	1:F:333:PRO:HD3	2.02	0.41
1:A:310:LEU:HD13	1:A:325:PHE:CE1	2.56	0.41
1:B:109:LYS:HE3	1:B:109:LYS:CA	2.51	0.41
1:F:51:CYS:C	1:F:53:ILE:H	2.23	0.41
1:A:148:GLN:HG2	1:A:152:LEU:HD12	2.03	0.41
1:B:144:ASN:HA	1:B:147:LEU:HB3	2.01	0.41
1:F:154:ARG:HG3	1:F:154:ARG:HH11	1.85	0.41
2:G:3015:DG:H2"	2:G:3016:DG:O5'	2.20	0.41
1:F:91:ARG:HG3	1:F:91:ARG:HH11	1.86	0.41
1:F:354:MET:SD	1:F:354:MET:N	2.93	0.41
1:F:363:GLU:OE2	4:L:688:LYS:HB2	2.19	0.41
1:F:353:GLY:C	1:F:355:ALA:H	2.24	0.41
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.95	0.41
1:A:363:GLU:OE1	4:I:690:LEU:HG	2.21	0.41
1:B:181:SER:HB2	1:B:238:ASN:CG	2.39	0.41
1:B:190:VAL:O	1:B:194:LYS:HG3	2.21	0.41
1:B:251:GLU:O	1:B:254:ARG:HB2	2.21	0.41
1:B:287:ASP:HA	1:B:288:PRO:HD2	1.94	0.41
1:B:341:GLN:O	1:B:345:GLN:HG3	2.21	0.41
5:B:401:MYR:H92	5:B:401:MYR:H61	1.79	0.41
1:F:218:HIS:ND1	1:F:281:LYS:HE3	2.36	0.41
1:B:202:LEU:HA	1:B:203:PRO:HD3	1.90	0.41
1:E:319:TYR:CD1	1:E:319:TYR:N	2.89	0.41
1:F:128:ILE:HD12	2:G:3016:DG:C4'	2.49	0.41
1:E:54:CYS:O	1:E:96:ASP:HA	2.21	0.40
1:E:80:ARG:HG3	1:E:80:ARG:NH1	2.36	0.40
1:E:255:VAL:O	1:E:259:ILE:HG13	2.21	0.40
1:F:168:ARG:HG3	1:F:168:ARG:NH1	2.36	0.40
1:B:83:HIS:O	1:B:83:HIS:ND1	2.53	0.40
1:B:327:GLU:OE2	1:B:327:GLU:HA	2.22	0.40
2:C:3017:DT:H2"	2:C:3018:DC:O4'	2.21	0.40
3:D:4015:DA:H2"	3:D:4016:DG:C8	2.56	0.40
1:F:314:ILE:CG2	1:F:324:ARG:HD3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:O	1:A:146:LEU:HD21	2.20	0.40
1:A:293:LEU:HD13	1:A:299:ILE:HG13	2.04	0.40
1:B:145:ALA:CB	1:B:146:LEU:HD12	2.50	0.40
1:E:361:LEU:HD12	1:E:361:LEU:N	2.36	0.40
1:F:91:ARG:HG3	1:F:91:ARG:NH1	2.36	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	298/338 (88%)	273 (92%)	20 (7%)	5 (2%)	9 31
1	B	304/338 (90%)	266 (88%)	30 (10%)	8 (3%)	5 20
1	E	299/338 (88%)	271 (91%)	27 (9%)	1 (0%)	41 71
1	F	310/338 (92%)	265 (86%)	36 (12%)	9 (3%)	4 18
4	I	6/13 (46%)	5 (83%)	1 (17%)	0	100 100
4	J	8/13 (62%)	7 (88%)	1 (12%)	0	100 100
4	K	6/13 (46%)	5 (83%)	1 (17%)	0	100 100
4	L	6/13 (46%)	5 (83%)	1 (17%)	0	100 100
All	All	1237/1404 (88%)	1097 (89%)	117 (10%)	23 (2%)	8 28

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	B	143	ILE
1	F	128	ILE
1	F	140	LEU
1	F	320	ASP

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Mol	Chain	Res	Type
1	B	128	ILE
1	B	353	GLY
1	E	367	GLY
1	A	367	GLY
1	B	99	LYS
1	F	171	LYS
1	A	159	PRO
1	A	250	ALA
1	B	57	ARG
1	B	140	LEU
1	B	141	PRO
1	F	136	GLU
1	B	320	ASP
1	F	52	ALA
1	F	142	SER
1	F	239	ASP
1	F	126	ASP
1	A	151	VAL

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	262/296 (88%)	252 (96%)	10 (4%)	33	67
1	B	270/296 (91%)	262 (97%)	8 (3%)	41	75
1	E	263/296 (89%)	254 (97%)	9 (3%)	37	71
1	F	274/296 (93%)	262 (96%)	12 (4%)	28	61
4	I	8/13 (62%)	8 (100%)	0	100	100
4	J	10/13 (77%)	10 (100%)	0	100	100
4	K	8/13 (62%)	8 (100%)	0	100	100
4	L	8/13 (62%)	8 (100%)	0	100	100
All	All	1103/1236 (89%)	1064 (96%)	39 (4%)	36	70

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	104	ARG
1	A	107	ARG
1	A	119	GLU
1	A	146	LEU
1	A	265	LEU
1	A	302	LEU
1	A	307	GLN
1	A	310	LEU
1	A	360	LEU
1	B	82	ASN
1	B	84	MET
1	B	109	LYS
1	B	186	LEU
1	B	217	GLU
1	B	239	ASP
1	B	265	LEU
1	B	354	MET
1	E	69	ASP
1	E	82	ASN
1	E	97	LYS
1	E	104	ARG
1	E	187	LEU
1	E	232	ASP
1	E	265	LEU
1	E	307	GLN
1	E	356	LYS
1	F	102	GLN
1	F	131	ARG
1	F	143	ILE
1	F	167	ILE
1	F	168	ARG
1	F	239	ASP
1	F	252	MET
1	F	265	LEU
1	F	307	GLN
1	F	310	LEU
1	F	317	ARG
1	F	345	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	101	ASN
1	A	102	GLN
1	A	155	GLN
1	A	164	ASN
1	A	318	GLN
1	A	336	GLN
1	A	345	GLN
1	B	82	ASN
1	B	101	ASN
1	B	122	GLN
1	B	144	ASN
1	B	148	GLN
1	B	305	GLN
1	B	315	ASN
1	B	318	GLN
1	B	336	GLN
1	E	92	GLN
1	E	102	GLN
1	E	164	ASN
1	E	336	GLN
1	E	345	GLN
1	F	122	GLN
1	F	144	ASN
1	F	148	GLN
1	F	185	GLN
1	F	315	ASN
1	F	336	GLN
1	F	341	GLN
1	F	345	GLN
4	L	695	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	MYR	B	401	-	15,15,15	0.57	0	15,15,15	0.98	0
5	MYR	E	401	-	15,15,15	0.53	0	15,15,15	0.96	1 (6%)
5	MYR	A	401	-	15,15,15	0.57	0	15,15,15	0.97	2 (13%)
5	MYR	F	401	-	15,15,15	0.51	0	15,15,15	1.21	3 (20%)

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	MYR	B	401	-	-	5/13/13/13	-
5	MYR	E	401	-	-	4/13/13/13	-
5	MYR	A	401	-	-	3/13/13/13	-
5	MYR	F	401	-	-	1/13/13/13	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	401	MYR	O2-C1-C2	2.49	122.03	114.03
5	F	401	MYR	C3-C2-C1	-2.46	108.28	114.47
5	E	401	MYR	O2-C1-C2	2.21	121.14	114.03
5	A	401	MYR	O2-C1-O1	-2.10	118.06	123.30
5	A	401	MYR	O2-C1-C2	2.09	120.74	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	401	MYR	O2-C1-O1	-2.05	118.20	123.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	MYR	C4-C5-C6-C7
5	B	401	MYR	C3-C4-C5-C6
5	F	401	MYR	C3-C4-C5-C6
5	A	401	MYR	C7-C8-C9-C10
5	B	401	MYR	C6-C7-C8-C9
5	A	401	MYR	O2-C1-C2-C3
5	B	401	MYR	O2-C1-C2-C3
5	E	401	MYR	O2-C1-C2-C3
5	A	401	MYR	O1-C1-C2-C3
5	E	401	MYR	O1-C1-C2-C3
5	E	401	MYR	C5-C6-C7-C8
5	B	401	MYR	O1-C1-C2-C3
5	E	401	MYR	C7-C8-C9-C10

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	MYR	5	0
5	E	401	MYR	2	0
5	A	401	MYR	3	0
5	F	401	MYR	3	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	A	302/338 (89%)	0.59	20 (6%) 18 14	47, 72, 126, 169	0
1	B	308/338 (91%)	0.62	22 (7%) 16 12	45, 77, 129, 163	0
1	E	303/338 (89%)	0.50	20 (6%) 18 14	53, 86, 116, 133	0
1	F	314/338 (92%)	0.75	33 (10%) 6 5	56, 90, 158, 208	0
2	C	20/20 (100%)	0.32	1 (5%) 28 25	69, 86, 111, 120	0
2	G	20/20 (100%)	0.37	1 (5%) 28 25	65, 78, 100, 110	0
3	D	20/20 (100%)	0.47	1 (5%) 28 25	58, 96, 139, 144	0
3	H	20/20 (100%)	0.38	0 100 100	56, 85, 107, 109	0
4	I	8/13 (61%)	4.09	8 (100%) 0 0	135, 145, 155, 158	0
4	J	10/13 (76%)	0.75	1 (10%) 7 5	107, 114, 121, 129	0
4	K	8/13 (61%)	6.58	8 (100%) 0 0	168, 171, 172, 176	0
4	L	8/13 (61%)	4.19	7 (87%) 0 0	153, 156, 161, 165	0
All	All	1341/1484 (90%)	0.68	122 (9%) 9 6	45, 82, 144, 208	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	SER	11.0
1	B	135	TYR	10.7
4	K	693	LEU	9.0
4	K	694	LEU	8.6
1	F	135	TYR	8.4
4	I	691	HIS	8.3
1	A	158	SER	8.3
1	F	161	SER	8.2
4	L	693	LEU	7.7
1	A	157	THR	7.6
4	K	689	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
4	K	690	LEU	6.6
4	K	691	HIS	6.6
4	K	688	LYS	6.5
1	B	136	GLU	6.5
1	B	133	SER	6.3
1	F	166	ASP	6.3
4	L	694	LEU	5.9
4	K	695	GLN	5.9
1	A	160	VAL	5.9
1	A	156	ILE	5.4
4	I	690	LEU	5.4
1	E	49	ALA	5.2
4	I	694	LEU	5.0
4	L	690	LEU	5.0
4	L	691	HIS	4.5
1	A	159	PRO	4.3
4	I	693	LEU	4.3
1	F	136	GLU	4.1
2	G	3001	DG	4.0
1	A	124	GLU	3.8
1	F	154	ARG	3.8
1	F	163	ILE	3.8
1	B	108	LEU	3.7
1	B	91	ARG	3.6
1	B	143	ILE	3.5
1	F	75	PHE	3.5
1	A	163	ILE	3.5
1	E	122	GLN	3.5
1	E	159	PRO	3.5
1	F	134	SER	3.4
1	E	50	LEU	3.4
1	A	162	GLY	3.4
1	F	138	SER	3.2
1	F	133	SER	3.2
1	E	286	PHE	3.2
1	A	122	GLN	3.2
1	F	63	TYR	3.1
1	B	144	ASN	3.1
1	A	153	SER	3.1
1	A	123	ASN	3.1
1	E	120	ALA	3.1
1	F	137	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
4	L	689	ILE	3.0
1	E	63	TYR	3.0
1	F	127	ARG	3.0
1	B	109	LYS	3.0
1	B	128	ILE	2.9
1	B	337	SER	2.9
1	E	190	VAL	2.9
4	I	695	GLN	2.9
4	L	695	GLN	2.9
1	F	162	GLY	2.9
1	F	340	TRP	2.8
1	F	339	THR	2.8
1	A	165	GLY	2.8
1	B	74	PHE	2.7
1	E	69	ASP	2.7
1	E	57	ARG	2.7
1	F	57	ARG	2.7
1	F	164	ASN	2.7
1	A	121	VAL	2.6
1	B	348	PHE	2.6
1	F	88	ARG	2.6
1	A	63	TYR	2.6
1	F	337	SER	2.6
4	L	688	LYS	2.5
1	B	113	ARG	2.5
4	I	689	ILE	2.5
1	E	354	MET	2.5
1	A	67	SER	2.5
4	K	692	ARG	2.5
1	A	164	ASN	2.5
1	A	154	ARG	2.4
1	B	63	TYR	2.4
1	B	132	ARG	2.4
1	A	192	TRP	2.4
1	F	116	MET	2.3
1	E	100	ARG	2.3
1	B	340	TRP	2.3
1	E	149	ALA	2.3
1	E	61	LYS	2.2
1	F	341	GLN	2.2
1	E	76	ARG	2.2
4	J	695	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	59	THR	2.2
1	F	60	GLY	2.2
1	B	147	LEU	2.2
2	C	3001	DG	2.2
1	F	89	PHE	2.2
1	E	60	GLY	2.2
1	E	89	PHE	2.2
1	F	140	LEU	2.2
1	F	92	GLN	2.2
1	F	90	SER	2.2
4	I	692	ARG	2.2
1	F	128	ILE	2.1
4	I	688	LYS	2.1
1	A	150	GLU	2.1
3	D	4019	DC	2.1
1	B	90	SER	2.1
1	A	252	MET	2.1
1	E	72	LYS	2.1
1	E	156	ILE	2.1
1	F	108	LEU	2.1
1	B	148	GLN	2.1
1	F	367	GLY	2.1
1	F	149	ALA	2.0
1	F	72	LYS	2.0
1	B	95	VAL	2.0
1	E	123	ASN	2.0
1	B	336	GLN	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
5	MYR	E	401	16/16	0.90	0.57	69,81,96,96	0
5	MYR	A	401	16/16	0.91	0.51	63,74,89,90	0
5	MYR	F	401	16/16	0.93	0.42	68,80,95,95	0
6	ZN	F	403	1/1	0.93	0.09	100,100,100,100	0
5	MYR	B	401	16/16	0.94	0.35	58,69,84,84	0
6	ZN	A	403	1/1	0.95	0.18	77,77,77,77	0
6	ZN	B	402	1/1	0.96	0.14	98,98,98,98	0
6	ZN	B	403	1/1	0.97	0.07	98,98,98,98	0
6	ZN	A	402	1/1	0.98	0.14	74,74,74,74	0
6	ZN	F	402	1/1	0.99	0.16	103,103,103,103	0
6	ZN	E	402	1/1	1.00	0.13	88,88,88,88	0
6	ZN	E	403	1/1	1.00	0.15	95,95,95,95	0

6.5 Other polymers (i)

There are no such residues in this entry.