



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 1LD4
Title : Placement of the Structural Proteins in Sindbis Virus
Authors : Zhang, W.; Mukhopadhyay, S.; Pletnev, S.V.; Baker, T.S.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : 2002-04-08
Resolution : 11.40 Å (reported)
Based on PDB ID : 1SVB, 1YSA, 1I9W

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

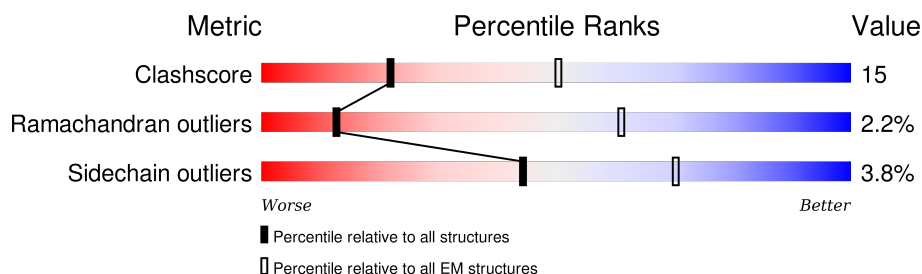
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.40 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	264	47% 9% . 43%
1	B	264	48% 8% . 43%
1	C	264	48% 8% . 43%
1	D	264	48% 8% . 43%
2	E	57	49% 51%
2	F	57	49% 51%
2	G	57	49% 51%
2	H	57	49% 51%
2	I	57	49% 51%

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Mol	Chain	Length	Quality of chain
2	J	57	<div><div></div><div>49%</div><div>51%</div></div>
2	K	57	<div><div></div><div>49%</div><div>51%</div></div>
2	L	57	<div><div></div><div>49%</div><div>51%</div></div>
3	M	439	<div><div></div><div>54%</div><div>28%</div><div>•</div><div>16%</div></div>
3	N	439	<div><div></div><div>55%</div><div>28%</div><div>•</div><div>16%</div></div>
3	O	439	<div><div></div><div>55%</div><div>28%</div><div>•</div><div>16%</div></div>
3	P	439	<div><div></div><div>55%</div><div>27%</div><div>•</div><div>16%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15680 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Coat protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	B	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	C	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		
1	D	151	Total	C	N	O	S	0	0
			1162	731	207	219	5		

- Molecule 2 is a protein called GENERAL CONTROL PROTEIN GCN4.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	E	28	Total	C	0	28
			28	28		
2	F	28	Total	C	0	28
			28	28		
2	G	28	Total	C	0	28
			28	28		
2	H	28	Total	C	0	28
			28	28		
2	I	28	Total	C	0	28
			28	28		
2	J	28	Total	C	0	28
			28	28		
2	K	28	Total	C	0	28
			28	28		
2	L	28	Total	C	0	28
			28	28		

- Molecule 3 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		
3	O	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		
3	P	369	Total	C	N	O	S	0	15
			2694	1709	446	519	20		

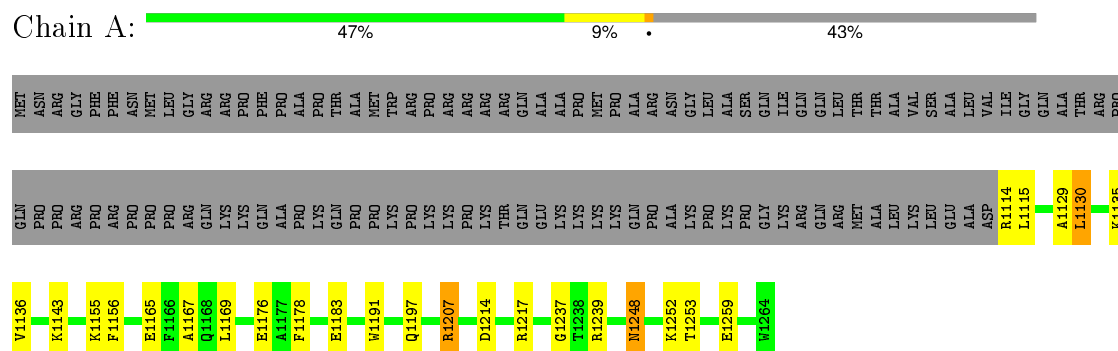
- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
4	P	6	Total	X	0
			6	6	
4	J	1	Total	X	0
			1	1	
4	H	1	Total	X	0
			1	1	
4	N	6	Total	X	0
			6	6	
4	O	8	Total	X	0
			8	8	
4	L	1	Total	X	0
			1	1	
4	F	2	Total	X	0
			2	2	
4	M	7	Total	X	0
			7	7	

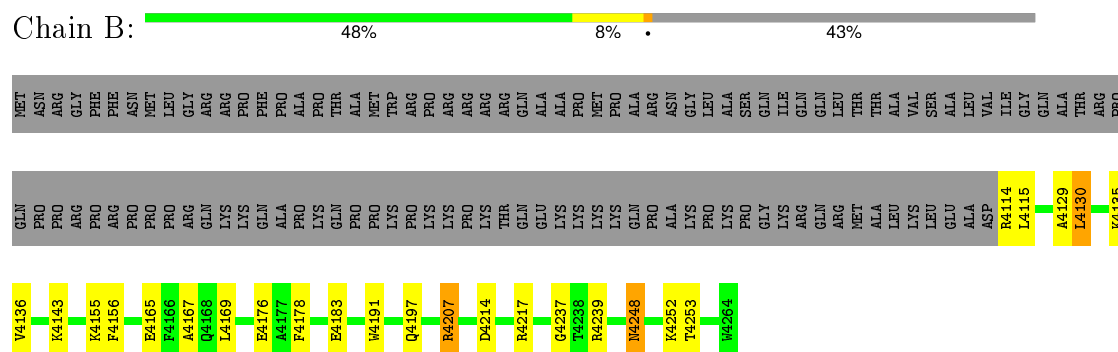
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

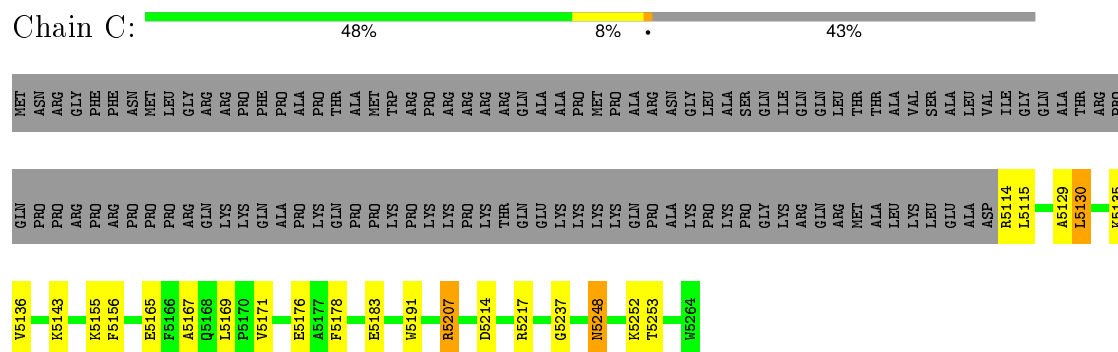
- Molecule 1: Coat protein C



- Molecule 1: Coat protein C

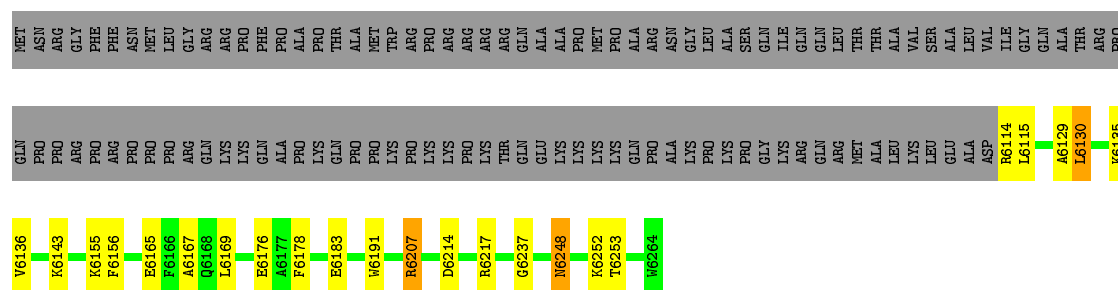


- Molecule 1: Coat protein C



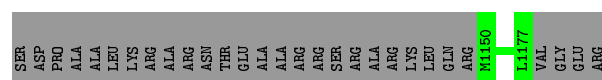
- Molecule 1: Coat protein C

Chain D:  48% 8% 43%



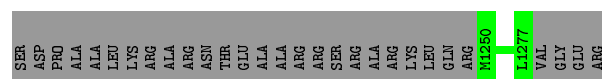
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain E:  49% 51%



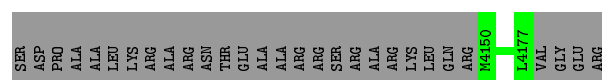
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain F:  49% 51%



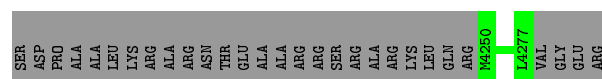
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain G:  49% 51%



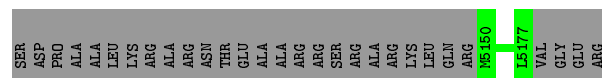
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain H:  49% 51%



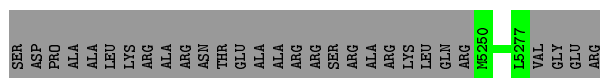
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain I:  49% 51%



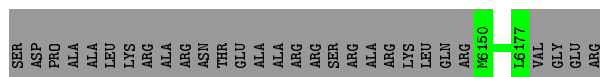
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain J:  49% 51%



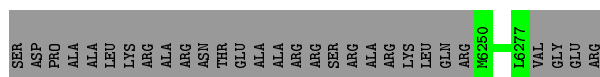
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain K: 49% 51%



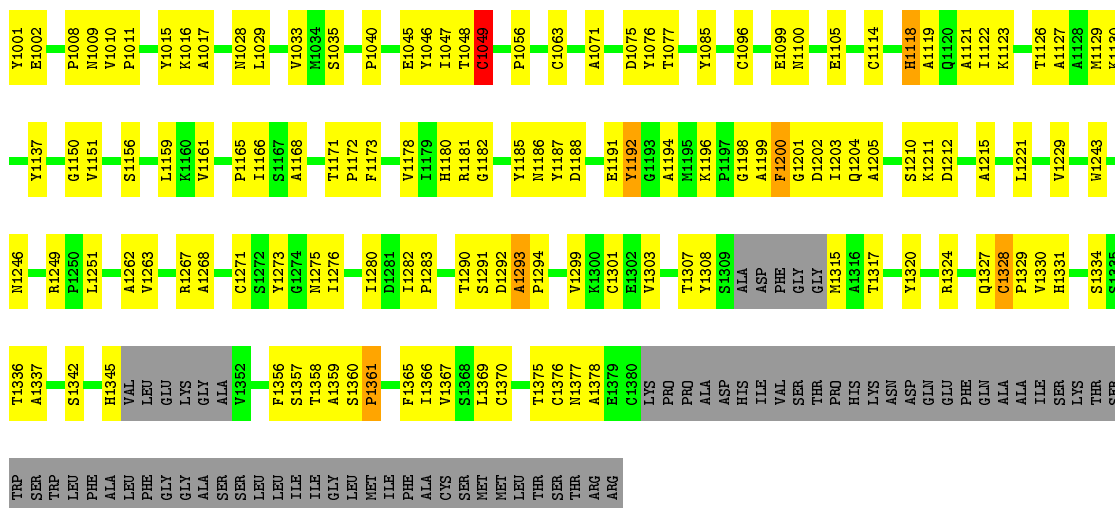
- Molecule 2: GENERAL CONTROL PROTEIN GCN4

Chain L: 49% 51%



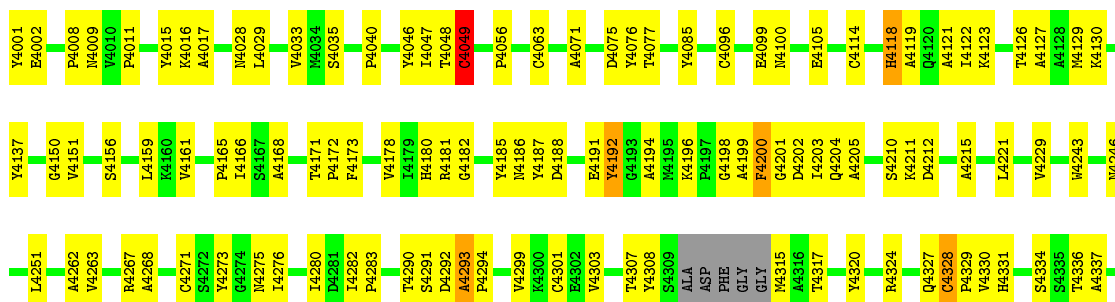
- Molecule 3: Spike glycoprotein E1

Chain M: 54% 28% 16%



- Molecule 3: Spike glycoprotein E1

Chain N: 55% 28% 16%



S4342	LEU
H4345	PHE
VAL	ALA
LEU	LEU
LEU	PHE
GLY	GLY
LYS	GLY
ALA	ALA
V4352	SER
F4356	LEU
S4357	LEU
T4358	ILE
A4359	ILE
S4360	GLY
P4361	LEU
F4365	MET
I4366	ILE
V4367	PHE
S4368	ALA
L4369	CYS
C4370	SER
T4375	SER
C4376	THR
M4377	THR
A4378	ARG
E4379	ARG
C4380	LYS
LYS	PRO
PRO	PRO
ALA	ALA
ASP	ALA
HIS	ASP
ILE	HIS
VAL	ILE
SER	VAL
THR	SER
PRO	THR
HIS	PRO
LYS	HIS
ASN	LYS
ASP	ASN
GLN	ASP
GLU	GLN
PHE	GLU
GLN	PHE
ALA	GLN
ALA	ALA
ILE	ALA
SER	ILE
LYS	SER
THR	LYS
SER	THR
TRP	SER
TRP	TRP

• Molecule 3: Spike glycoprotein E1

Chain O:  55% 28% 16%

LEU	PHE	ALA	LEU	PHE	GLY	GLY	ALA	SER	SER	LEU	LEU	LEU	LEU	ILE	PHE	ALA	CYS	SER	SER	LEU	THR	SER	THR	ARG	ARG	LYS	PRO	PRO	ALA	ASP	HIS	ILE	VAL	SER	GLY	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA	ALA	ILE	SER	THR	TRP	TRP
S5342			H5345	VAL	LEU	GLY	GLY	ALA	V5352	F5356	S5357	T5358	A5359	S5360	P5361	F5365	V5367	S5368	L5369	C5370	T5375	C5376	N5377	E5379	C5380	LYS	PRO	PRO	ALA	ASP	HIS	ILE	VAL	SER	GLY	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA	ALA	ILE	SER	THR	TRP	TRP
P5250	L5251	A5262	V5263	R5267	A5268	C5271	S5272	Y5273	G5274	N5275	I5276	I5280	D5281	F5282	P5283	T5290	S5291	D5292	A5293	P5294	V5299	R5300	C5301	F5302	V5303	T5307	Y5308	S5309	ALA	ASP	PHE	GLY	M5315	A5316	T5317	Y5320	R5324	Q5327	C5328	P5329	V5330	H5331	S5334	S5335	T5336	A5337						
K5130	Y5137	G5150	S5156	L5159	V5161	P5165	L5166	S5167	A5168	T5171	P5172	F5173	V5178	I5179	H5180	R5181	G5182	Y5185	N5186	Y5187	D5188	Y5192	K5196	P5197	G5198	A5199	F5200	G5201	D5202	T5203	Q5204	A5205	S5210	K5211	D5212	A5215	L5221	V5229	W5243	N5246	A5247	R5249										
Y5001	E5002	P5008	N5009	P5010	P5011	Y5015	K5016	A5017	N5028	L5029	V5033	P5034	S5035	P5040	Y5046	I5047	T5048	C5049	P5056	C5063	A5071	H5072	H5073	A5074	D5075	Y5076	T5077	Y5085	C5096	E5099	N5100	E5105	R5210	K5211	D5212	A5215	L5221	V5229	W5243	N5246	A5247	R5249										

• Molecule 3: Spike glycoprotein E1

Chain P:  55% 27% 16%

LEU	PHE	GLY	GLY	ALA	GLY	SER	SER	LEU	ILE	ILE	PHE	ALA	ALA	CYS	MET	MET	LEU	THR	THR	SER	THR	ARG	ARG																																	
VAL	A6262	V6263	LEU	G6150	A6268	ALA	V6352	F6356	S6357	T6358	A6359	S6360	P6361	F6365	I6366	V6367	S6368	L6369	C6370	T6375	C6376	N6377	A6378	E6379	C6380	LYS	PRO	PRO	ALA	ASP	HIS	ILE	ILE	VAL	SER	THR	PRO	HIS	LYS	ASN	ASP	GLN	GLU	PHE	GLN	ALA	ALA	ILE	SER	THR	THR	TRP	TRP	LEU	PHE	ALA
Y6001	E6002	P6008	N6009	W6010	P6011	Y6015	R6016	A6017	N6028	L6029	V6033	W6034	S6035	P6040	E6045	Y6046	I6047	W6048	C6049	P6056	C6063	A6071	D6075	Y6076	T6077	Y6085	C6096	E6099	N6100	E6105	C6114	H6118	A6119	Q6120	A6121	I6122	K6123	T6126	A6127	A6128	N6129	K6130														
Y6137	G6150	S6156	L6159	R6160	V6161	P6165	L6166	S6167	A6168	T6171	P6172	F6173	V6178	I6179	H6180	R6181	G6182	Y6185	N6186	Y6187	D6188	Y6192	K6196	P6197	G6198	A6199	F6200	G6201	D6202	I6203	Q6204	A6205	S6210	K6211	D6212	A6215	L6221	V6229	W6243	N6246	A6247	L6251	H6252													
A6262	V6263	R6267	A6268	C6271	S6272	Y6273	N6274	I6275	I6276	T6280	D6281	P6283	T6290	S6291	A6293	P6294	V6299	W6300	C6301	E6302	V6303	T6307	Y6308	S6309	ALA	ASP	PHE	GLY	GLY	P6315	A6316	T6317	Y6320	R6324	Q6327	C6328	P6329	V6330	H6331	S6334	S6335	T6336	A6337	S6342	H6345											

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	each viral image was CTF corrected before reconstruction, based on the following equation: $F(\text{corr})=F(\text{obs})/[CTF +wiener]$	Depositor
Microscope	PHILLIPS CM200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1840	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2580	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.52	0/1190	0.81	1/1607 (0.1%)
1	B	0.52	0/1190	0.81	1/1607 (0.1%)
1	C	0.52	0/1190	0.81	1/1607 (0.1%)
1	D	0.52	0/1190	0.81	1/1607 (0.1%)
3	M	0.34	0/2743	0.54	0/3740
3	N	0.34	0/2743	0.54	0/3740
3	O	0.34	0/2743	0.54	0/3740
3	P	0.34	0/2743	0.54	0/3740
All	All	0.41	0/15732	0.63	4/21388 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6130	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	1130	LEU	CA-CB-CG	5.10	127.04	115.30
1	B	4130	LEU	CA-CB-CG	5.09	127.02	115.30
1	C	5130	LEU	CA-CB-CG	5.09	127.00	115.30

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	1162	0	1131	16	0
1	B	1162	0	1131	11	0
1	C	1162	0	1131	14	0
1	D	1162	0	1131	9	0
2	E	28	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	0	0
2	H	28	0	0	0	0
2	I	28	0	0	0	0
2	J	28	0	0	0	0
2	K	28	0	0	0	0
2	L	28	0	0	0	0
3	M	2694	0	2605	139	0
3	N	2694	0	2605	135	0
3	O	2694	0	2605	91	0
3	P	2694	0	2605	95	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
4	M	7	0	0	0	0
4	N	6	0	0	0	0
4	O	8	0	0	0	0
4	P	6	0	0	0	0
All	All	15680	0	14944	464	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 15.

All (464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1194:ALA:CB	3:N:4151:VAL:HG12	1.36	1.54
3:M:1151:VAL:HG12	3:N:4194:ALA:CB	1.36	1.48
3:M:1151:VAL:CG1	3:N:4194:ALA:CB	2.05	1.34
3:M:1194:ALA:CB	3:N:4151:VAL:CG1	2.05	1.31
3:O:5330:VAL:HG22	3:O:5369:LEU:CA	1.62	1.29
3:P:6330:VAL:HG22	3:P:6369:LEU:CA	1.62	1.29
3:M:1330:VAL:HG22	3:M:1369:LEU:CA	1.62	1.29
3:N:4330:VAL:HG22	3:N:4369:LEU:CA	1.62	1.28
3:M:1151:VAL:CG1	3:N:4194:ALA:HB3	1.64	1.27
3:M:1194:ALA:HB3	3:N:4151:VAL:CG1	1.64	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:1151:VAL:HG21	3:N:4191:GLU:CD	1.55	1.25
3:M:1191:GLU:CD	3:N:4151:VAL:HG21	1.55	1.24
3:M:1191:GLU:CB	3:N:4151:VAL:HG11	1.75	1.15
3:M:1151:VAL:HG11	3:N:4191:GLU:CB	1.75	1.14
1:A:1259:GLU:OE1	1:C:5171:VAL:CG2	1.99	1.10
3:N:4001:TYR:CA	3:N:4282:ILE:O	2.02	1.08
3:O:5001:TYR:CA	3:O:5282:ILE:O	2.02	1.07
3:M:1001:TYR:CA	3:M:1282:ILE:O	2.02	1.07
3:P:6330:VAL:CG2	3:P:6369:LEU:CA	2.33	1.07
3:O:5330:VAL:CG2	3:O:5369:LEU:CA	2.33	1.06
3:N:4330:VAL:CG2	3:N:4369:LEU:CA	2.33	1.06
3:M:1330:VAL:CG2	3:M:1369:LEU:CA	2.33	1.05
3:P:6001:TYR:CA	3:P:6282:ILE:O	2.02	1.05
3:P:6303:VAL:HG23	3:P:6377:ASN:CA	1.88	1.04
3:M:1191:GLU:HB2	3:N:4151:VAL:CG1	1.87	1.04
3:M:1151:VAL:HG12	3:N:4194:ALA:HB2	1.08	1.04
3:M:1303:VAL:HG23	3:M:1377:ASN:CA	1.88	1.04
3:N:4303:VAL:HG23	3:N:4377:ASN:CA	1.88	1.03
3:M:1194:ALA:HB2	3:N:4151:VAL:HG12	1.08	1.03
3:M:1151:VAL:HG11	3:N:4191:GLU:HB2	1.03	1.03
3:O:5303:VAL:HG23	3:O:5377:ASN:CA	1.88	1.03
3:M:1151:VAL:CG1	3:N:4191:GLU:HB2	1.87	1.03
3:M:1191:GLU:HB2	3:N:4151:VAL:HG11	1.04	1.01
3:O:5301:CYS:CB	3:O:5376:CYS:CA	2.45	0.94
3:N:4301:CYS:CB	3:N:4376:CYS:CA	2.45	0.94
3:P:6301:CYS:CB	3:P:6376:CYS:CA	2.45	0.93
3:M:1301:CYS:CB	3:M:1376:CYS:CA	2.45	0.93
3:O:5301:CYS:HB3	3:O:5376:CYS:CA	2.00	0.92
3:N:4301:CYS:HB3	3:N:4376:CYS:CA	2.00	0.91
3:P:6301:CYS:HB3	3:P:6376:CYS:CA	2.00	0.91
3:M:1301:CYS:HB3	3:M:1376:CYS:CA	1.99	0.91
3:O:5366:ILE:HA	3:O:5375:THR:CA	2.01	0.91
3:N:4366:ILE:HA	3:N:4375:THR:CA	2.01	0.90
3:M:1366:ILE:HA	3:M:1375:THR:CA	2.01	0.90
1:A:1259:GLU:OE1	1:C:5171:VAL:HG21	1.68	0.90
3:M:1151:VAL:CG2	3:N:4191:GLU:CD	2.39	0.90
3:M:1191:GLU:CD	3:N:4151:VAL:CG2	2.39	0.90
3:P:6366:ILE:HA	3:P:6375:THR:CA	2.01	0.88
3:M:1151:VAL:HG21	3:N:4191:GLU:CG	2.06	0.86
3:M:1151:VAL:HG13	3:N:4194:ALA:CB	2.07	0.85
3:M:1194:ALA:CB	3:N:4151:VAL:HG13	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6301:CYS:HB2	3:P:6376:CYS:CA	2.07	0.84
3:M:1191:GLU:CG	3:N:4151:VAL:HG21	2.06	0.84
3:O:5301:CYS:HB2	3:O:5376:CYS:CA	2.07	0.84
3:M:1301:CYS:HB2	3:M:1376:CYS:CA	2.07	0.83
3:N:4301:CYS:HB2	3:N:4376:CYS:CA	2.07	0.82
3:P:6002:GLU:CA	3:P:6002:GLU:CG	2.58	0.82
3:M:1002:GLU:CG	3:M:1002:GLU:CA	2.58	0.82
3:N:4002:GLU:CA	3:N:4002:GLU:CG	2.58	0.82
3:O:5002:GLU:CG	3:O:5002:GLU:CA	2.58	0.81
3:M:1049:CYS:SG	3:M:1118:HIS:HA	2.24	0.78
3:O:5049:CYS:SG	3:O:5118:HIS:HA	2.24	0.78
3:P:6049:CYS:SG	3:P:6118:HIS:HA	2.24	0.78
3:N:4049:CYS:SG	3:N:4118:HIS:HA	2.24	0.78
3:M:1191:GLU:OE2	3:N:4151:VAL:HG21	1.84	0.78
3:M:1151:VAL:HG12	3:N:4194:ALA:HB3	1.32	0.77
1:A:1259:GLU:OE1	1:C:5171:VAL:HG22	1.84	0.77
3:M:1151:VAL:HG21	3:N:4191:GLU:OE2	1.84	0.76
3:M:1194:ALA:HB3	3:N:4151:VAL:HG13	1.65	0.76
3:M:1151:VAL:HG13	3:N:4194:ALA:HB3	1.65	0.75
3:O:5358:THR:HG22	3:O:5359:ALA:H	1.55	0.72
3:M:1358:THR:HG22	3:M:1359:ALA:H	1.55	0.72
3:P:6049:CYS:HB3	3:P:6114:CYS:SG	2.30	0.71
3:N:4049:CYS:HB3	3:N:4114:CYS:SG	2.30	0.71
3:P:6009:ASN:HD21	3:P:6166:ILE:HD13	1.56	0.71
3:P:6358:THR:HG22	3:P:6359:ALA:H	1.55	0.71
3:O:5049:CYS:HB3	3:O:5114:CYS:SG	2.30	0.71
3:M:1049:CYS:HB3	3:M:1114:CYS:SG	2.30	0.71
3:O:5200:PHE:H	3:O:5243:TRP:HE1	1.39	0.71
3:P:6016:LYS:HD3	3:P:6331:HIS:HE1	1.55	0.70
3:M:1009:ASN:HD21	3:M:1166:ILE:HD13	1.56	0.70
3:O:5016:LYS:HD3	3:O:5331:HIS:HE1	1.55	0.70
3:N:4009:ASN:HD21	3:N:4166:ILE:HD13	1.55	0.70
3:N:4358:THR:HG22	3:N:4359:ALA:H	1.55	0.70
3:M:1016:LYS:HD3	3:M:1331:HIS:HE1	1.55	0.70
3:N:4016:LYS:HD3	3:N:4331:HIS:HE1	1.55	0.70
3:O:5009:ASN:HD21	3:O:5166:ILE:HD13	1.56	0.70
3:P:6180:HIS:HB2	3:P:6185:TYR:HE1	1.57	0.69
3:M:1290:THR:O	3:M:1294:PRO:HD2	1.92	0.69
3:N:4200:PHE:H	3:N:4243:TRP:HE1	1.39	0.69
3:M:1151:VAL:CG1	3:N:4194:ALA:HB1	2.21	0.69
3:P:6200:PHE:H	3:P:6243:TRP:HE1	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4290:THR:O	3:N:4294:PRO:HD2	1.92	0.69
3:O:5290:THR:O	3:O:5294:PRO:HD2	1.92	0.69
3:P:6290:THR:O	3:P:6294:PRO:HD2	1.92	0.69
3:M:1180:HIS:HB2	3:M:1185:TYR:HE1	1.57	0.68
3:N:4040:PRO:HA	3:N:4127:ALA:HA	1.76	0.68
3:O:5040:PRO:HA	3:O:5127:ALA:HA	1.76	0.68
3:M:1366:ILE:O	3:M:1367:VAL:CA	2.42	0.68
3:M:1200:PHE:H	3:M:1243:TRP:HE1	1.39	0.68
3:M:1040:PRO:HA	3:M:1127:ALA:HA	1.76	0.68
3:O:5366:ILE:O	3:O:5367:VAL:CA	2.42	0.68
3:O:5180:HIS:HB2	3:O:5185:TYR:HE1	1.57	0.68
3:N:4366:ILE:O	3:N:4367:VAL:CA	2.42	0.68
3:N:4180:HIS:HB2	3:N:4185:TYR:HE1	1.57	0.67
1:B:4156:PHE:HB3	1:B:4165:GLU:HG2	1.76	0.67
1:D:6156:PHE:HB3	1:D:6165:GLU:HG2	1.76	0.67
1:A:1156:PHE:HB3	1:A:1165:GLU:HG2	1.76	0.67
3:P:6040:PRO:HA	3:P:6127:ALA:HA	1.76	0.67
3:M:1191:GLU:OE2	3:N:4151:VAL:CG2	2.43	0.66
1:C:5156:PHE:HB3	1:C:5165:GLU:HG2	1.76	0.66
3:P:6366:ILE:O	3:P:6367:VAL:CA	2.42	0.66
3:O:5017:ALA:HB3	3:O:5029:LEU:HD12	1.77	0.66
3:N:4017:ALA:HB3	3:N:4029:LEU:HD12	1.77	0.66
3:P:6017:ALA:HB3	3:P:6029:LEU:HD12	1.77	0.65
3:M:1017:ALA:HB3	3:M:1029:LEU:HD12	1.77	0.65
3:M:1194:ALA:HB1	3:N:4151:VAL:CG1	2.21	0.65
3:M:1151:VAL:CG2	3:N:4191:GLU:OE2	2.43	0.65
3:M:1194:ALA:HB3	3:N:4151:VAL:HG12	1.32	0.63
3:P:6129:MET:SD	3:P:6166:ILE:HD12	2.39	0.63
3:O:5330:VAL:HG21	3:O:5369:LEU:CA	2.29	0.63
3:O:5129:MET:SD	3:O:5166:ILE:HD12	2.39	0.63
3:M:1129:MET:SD	3:M:1166:ILE:HD12	2.39	0.62
3:P:6365:PHE:O	3:P:6375:THR:CA	2.48	0.62
3:O:5365:PHE:O	3:O:5375:THR:CA	2.48	0.62
3:M:1365:PHE:O	3:M:1375:THR:CA	2.48	0.62
3:N:4365:PHE:O	3:N:4375:THR:CA	2.48	0.62
3:N:4129:MET:SD	3:N:4166:ILE:HD12	2.39	0.61
3:N:4330:VAL:HG21	3:N:4369:LEU:CA	2.29	0.61
3:O:5171:THR:HG22	3:O:5173:PHE:H	1.66	0.60
3:O:5342:SER:O	3:O:5356:PHE:HZ	1.84	0.60
3:P:6342:SER:O	3:P:6356:PHE:HZ	1.84	0.60
3:M:1171:THR:HG22	3:M:1173:PHE:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6330:VAL:HG21	3:P:6369:LEU:CA	2.29	0.60
3:N:4200:PHE:N	3:N:4243:TRP:HE1	2.00	0.60
3:M:1151:VAL:HG11	3:N:4191:GLU:HB3	1.81	0.60
3:N:4171:THR:HG22	3:N:4173:PHE:H	1.66	0.59
3:P:6171:THR:HG22	3:P:6173:PHE:H	1.66	0.59
3:O:5303:VAL:CG2	3:O:5377:ASN:CA	2.75	0.59
3:P:6200:PHE:N	3:P:6243:TRP:HE1	2.00	0.59
3:M:1342:SER:O	3:M:1356:PHE:HZ	1.84	0.59
3:O:5200:PHE:N	3:O:5243:TRP:HE1	2.00	0.59
3:N:4342:SER:O	3:N:4356:PHE:HZ	1.84	0.59
3:P:6180:HIS:NE2	3:P:6187:TYR:HE1	2.02	0.58
3:M:1180:HIS:NE2	3:M:1187:TYR:HE1	2.02	0.58
3:M:1200:PHE:N	3:M:1243:TRP:HE1	2.00	0.58
3:P:6159:LEU:CD2	3:P:6283:PRO:HD2	2.34	0.58
3:P:6360:SER:HB2	3:P:6361:PRO:HD2	1.86	0.57
3:N:4159:LEU:CD2	3:N:4283:PRO:HD2	2.34	0.57
3:M:1330:VAL:HG21	3:M:1369:LEU:CA	2.29	0.57
3:O:5159:LEU:CD2	3:O:5283:PRO:HD2	2.34	0.57
3:O:5180:HIS:NE2	3:O:5187:TYR:HE1	2.02	0.57
3:O:5121:ALA:HA	3:O:5178:VAL:HG22	1.87	0.57
3:M:1159:LEU:CD2	3:M:1283:PRO:HD2	2.34	0.57
3:N:4180:HIS:NE2	3:N:4187:TYR:HE1	2.02	0.57
3:M:1360:SER:HB2	3:M:1361:PRO:HD2	1.86	0.56
1:D:6207:ARG:HH21	1:D:6237:GLY:HA2	1.71	0.56
1:B:4207:ARG:HH21	1:B:4237:GLY:HA2	1.71	0.56
3:N:4121:ALA:HA	3:N:4178:VAL:HG22	1.86	0.56
3:O:5360:SER:HB2	3:O:5361:PRO:HD2	1.86	0.56
3:N:4360:SER:HB2	3:N:4361:PRO:HD2	1.86	0.56
3:O:5315:MET:HG2	3:O:5317:THR:H	1.71	0.56
3:P:6121:ALA:HA	3:P:6178:VAL:HG22	1.87	0.56
1:C:5207:ARG:HH21	1:C:5237:GLY:HA2	1.71	0.56
3:N:4192:TYR:HD1	3:N:4192:TYR:H	1.54	0.56
3:M:1121:ALA:HA	3:M:1178:VAL:HG22	1.87	0.56
1:A:1207:ARG:HH21	1:A:1237:GLY:HA2	1.71	0.55
3:P:6315:MET:HG2	3:P:6317:THR:H	1.71	0.55
3:P:6303:VAL:CG2	3:P:6377:ASN:CA	2.75	0.55
3:M:1192:TYR:HD1	3:M:1192:TYR:H	1.54	0.55
3:P:6161:VAL:HA	3:P:6280:ILE:HG12	1.89	0.55
3:O:5008:PRO:HA	3:O:5275:ASN:HA	1.88	0.55
3:P:6192:TYR:H	3:P:6192:TYR:HD1	1.54	0.55
3:M:1161:VAL:HA	3:M:1280:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4016:LYS:HD3	3:N:4331:HIS:CE1	2.39	0.54
3:N:4315:MET:HG2	3:N:4317:THR:H	1.71	0.54
3:O:5016:LYS:HD3	3:O:5331:HIS:CE1	2.39	0.54
3:N:4008:PRO:HA	3:N:4275:ASN:HA	1.89	0.54
3:P:6008:PRO:HA	3:P:6275:ASN:HA	1.89	0.54
3:M:1315:MET:HG2	3:M:1317:THR:H	1.71	0.54
3:M:1191:GLU:HB3	3:N:4151:VAL:HG11	1.81	0.54
3:M:1290:THR:HG22	3:M:1291:SER:H	1.73	0.54
3:N:4161:VAL:HA	3:N:4280:ILE:HG12	1.89	0.54
3:N:4290:THR:HG22	3:N:4291:SER:H	1.73	0.54
3:M:1008:PRO:HA	3:M:1275:ASN:HA	1.89	0.54
3:O:5161:VAL:HA	3:O:5280:ILE:HG12	1.89	0.54
3:O:5192:TYR:HD1	3:O:5192:TYR:H	1.54	0.54
3:M:1016:LYS:HD3	3:M:1331:HIS:CE1	2.39	0.54
3:O:5290:THR:HG22	3:O:5291:SER:H	1.73	0.53
3:P:6016:LYS:HD3	3:P:6331:HIS:CE1	2.39	0.53
3:P:6290:THR:HG22	3:P:6291:SER:H	1.73	0.53
3:N:4303:VAL:CG2	3:N:4377:ASN:CA	2.75	0.53
1:A:1248:ASN:ND2	1:A:1252:LYS:H	2.07	0.53
3:M:1303:VAL:CG2	3:M:1377:ASN:CA	2.75	0.52
3:N:4063:CYS:HA	3:N:4099:GLU:O	2.10	0.52
3:M:1011:PRO:HA	3:M:1033:VAL:HB	1.92	0.52
3:N:4192:TYR:N	3:N:4192:TYR:CD1	2.78	0.52
3:O:5192:TYR:CD1	3:O:5192:TYR:N	2.78	0.52
3:P:6262:ALA:HB3	3:P:6267:ARG:H	1.75	0.52
1:D:6248:ASN:ND2	1:D:6252:LYS:H	2.07	0.52
1:B:4248:ASN:ND2	1:B:4252:LYS:H	2.07	0.52
3:M:1063:CYS:HA	3:M:1099:GLU:O	2.10	0.52
3:M:1151:VAL:O	3:N:4194:ALA:CB	2.58	0.52
3:N:4243:TRP:HA	3:N:4243:TRP:CE3	2.45	0.52
3:P:6336:THR:HG22	3:P:6337:ALA:N	2.25	0.52
3:N:4011:PRO:HA	3:N:4033:VAL:HB	1.91	0.52
3:M:1194:ALA:CB	3:N:4151:VAL:O	2.58	0.51
3:O:5336:THR:HG22	3:O:5337:ALA:N	2.25	0.51
1:C:5248:ASN:ND2	1:C:5252:LYS:H	2.07	0.51
3:O:5063:CYS:HA	3:O:5099:GLU:O	2.10	0.51
3:P:6011:PRO:HA	3:P:6033:VAL:HB	1.91	0.51
3:P:6063:CYS:HA	3:P:6099:GLU:O	2.10	0.51
3:O:5262:ALA:HB3	3:O:5267:ARG:H	1.75	0.51
3:N:4262:ALA:HB3	3:N:4267:ARG:H	1.75	0.51
3:P:6243:TRP:CE3	3:P:6243:TRP:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:5028:ASN:HD22	3:O:5342:SER:HB2	1.76	0.51
3:M:1262:ALA:HB3	3:M:1267:ARG:H	1.75	0.51
3:O:5011:PRO:HA	3:O:5033:VAL:HB	1.91	0.51
3:O:5243:TRP:CE3	3:O:5243:TRP:HA	2.45	0.51
3:M:1243:TRP:CE3	3:M:1243:TRP:HA	2.45	0.51
3:N:4049:CYS:CB	3:N:4114:CYS:SG	2.99	0.50
3:M:1192:TYR:N	3:M:1192:TYR:CD1	2.78	0.50
3:N:4336:THR:HG22	3:N:4337:ALA:N	2.25	0.50
3:O:5049:CYS:CB	3:O:5114:CYS:SG	2.99	0.50
3:P:6192:TYR:CD1	3:P:6192:TYR:N	2.78	0.50
3:M:1194:ALA:HB1	3:N:4151:VAL:O	2.12	0.50
3:M:1336:THR:HG22	3:M:1337:ALA:N	2.25	0.50
3:M:1028:ASN:HD22	3:M:1342:SER:HB2	1.76	0.50
3:P:6009:ASN:OD1	3:P:6276:ILE:HG13	2.11	0.50
3:N:4028:ASN:HD22	3:N:4342:SER:HB2	1.76	0.50
3:N:4009:ASN:OD1	3:N:4276:ILE:HG13	2.11	0.49
3:O:5009:ASN:OD1	3:O:5276:ILE:HG13	2.11	0.49
3:M:1009:ASN:OD1	3:M:1276:ILE:HG13	2.11	0.49
3:M:1210:SER:O	3:M:1211:LYS:HG3	2.12	0.49
3:P:6358:THR:HG22	3:P:6359:ALA:N	2.27	0.49
3:P:6028:ASN:HD22	3:P:6342:SER:HB2	1.76	0.49
3:M:1049:CYS:CB	3:M:1114:CYS:SG	2.99	0.49
1:A:1214:ASP:O	1:A:1217:ARG:HG3	2.13	0.49
3:M:1151:VAL:O	3:N:4194:ALA:HB1	2.12	0.49
3:O:5210:SER:O	3:O:5211:LYS:HG3	2.12	0.49
1:C:5214:ASP:O	1:C:5217:ARG:HG3	2.13	0.49
1:B:4214:ASP:O	1:B:4217:ARG:HG3	2.13	0.49
3:P:6210:SER:O	3:P:6211:LYS:HG3	2.12	0.48
1:D:6214:ASP:O	1:D:6217:ARG:HG3	2.13	0.48
3:N:4210:SER:O	3:N:4211:LYS:HG3	2.12	0.48
1:A:1259:GLU:CD	1:C:5171:VAL:HG21	2.31	0.48
3:P:6049:CYS:CB	3:P:6114:CYS:SG	2.99	0.48
3:M:1186:ASN:ND2	3:M:1251:LEU:HD21	2.29	0.48
3:M:1194:ALA:HB1	3:N:4151:VAL:HG13	1.89	0.48
3:O:5172:PRO:HD3	3:O:5273:TYR:OH	2.14	0.48
3:M:1358:THR:HG22	3:M:1359:ALA:N	2.27	0.47
3:N:4172:PRO:HD3	3:N:4273:TYR:OH	2.14	0.47
3:M:1337:ALA:HB2	3:M:1360:SER:HB3	1.96	0.47
3:O:5186:ASN:ND2	3:O:5251:LEU:HD21	2.29	0.47
3:M:1172:PRO:HD3	3:M:1273:TYR:OH	2.14	0.47
3:N:4337:ALA:HB2	3:N:4360:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4192:TYR:N	3:N:4192:TYR:HD1	2.12	0.47
3:M:1192:TYR:HD1	3:M:1192:TYR:N	2.12	0.47
3:O:5192:TYR:N	3:O:5192:TYR:HD1	2.12	0.47
3:P:6172:PRO:HD3	3:P:6273:TYR:OH	2.14	0.47
3:P:6186:ASN:ND2	3:P:6251:LEU:HD21	2.29	0.47
3:O:5337:ALA:HB2	3:O:5360:SER:HB3	1.96	0.47
3:N:4186:ASN:ND2	3:N:4251:LEU:HD21	2.29	0.47
1:B:4136:VAL:HG22	1:B:4169:LEU:HD23	1.97	0.47
3:N:4290:THR:HG22	3:N:4291:SER:N	2.30	0.46
3:O:5122:ILE:HG22	3:O:5123:LYS:N	2.30	0.46
1:D:6136:VAL:HG22	1:D:6169:LEU:HD23	1.97	0.46
3:O:5166:ILE:HG22	3:O:5168:ALA:H	1.81	0.46
3:P:6182:GLY:HA2	3:P:6263:VAL:HG13	1.97	0.46
3:M:1001:TYR:CA	3:M:1282:ILE:C	2.82	0.46
3:P:6122:ILE:HG22	3:P:6123:LYS:N	2.30	0.46
3:P:6290:THR:HG22	3:P:6291:SER:N	2.30	0.46
3:M:1182:GLY:HA2	3:M:1263:VAL:HG13	1.96	0.46
3:O:5182:GLY:HA2	3:O:5263:VAL:HG13	1.96	0.46
3:N:4182:GLY:HA2	3:N:4263:VAL:HG13	1.96	0.46
3:O:5358:THR:HG22	3:O:5359:ALA:N	2.27	0.46
3:P:6337:ALA:HB2	3:P:6360:SER:HB3	1.96	0.46
3:P:6192:TYR:HD1	3:P:6192:TYR:N	2.12	0.46
3:M:1166:ILE:HG22	3:M:1168:ALA:H	1.81	0.46
3:N:4358:THR:HG22	3:N:4359:ALA:N	2.27	0.46
1:A:1136:VAL:HG22	1:A:1169:LEU:HD23	1.97	0.46
3:M:1290:THR:HG22	3:M:1291:SER:N	2.30	0.46
3:M:1356:PHE:HB3	3:M:1357:SER:H	1.63	0.46
3:M:1327:GLN:H	3:M:1345:HIS:CE1	2.34	0.46
3:P:6327:GLN:H	3:P:6345:HIS:CE1	2.34	0.46
1:A:1135:LYS:HB2	1:A:1167:ALA:O	2.16	0.46
3:N:4166:ILE:HG22	3:N:4168:ALA:H	1.81	0.46
3:O:5008:PRO:HG2	3:O:5015:TYR:CE2	2.51	0.46
1:C:5135:LYS:HB2	1:C:5167:ALA:O	2.16	0.46
1:C:5130:LEU:HD11	1:C:5178:PHE:CD2	2.52	0.45
3:N:4122:ILE:HG22	3:N:4123:LYS:N	2.30	0.45
3:N:4303:VAL:HG21	3:N:4378:ALA:CA	2.47	0.45
3:P:6356:PHE:HB3	3:P:6357:SER:H	1.63	0.45
3:M:1008:PRO:HG2	3:M:1015:TYR:CE2	2.51	0.45
1:B:4135:LYS:HB2	1:B:4167:ALA:O	2.16	0.45
1:C:5114:ARG:HH21	1:C:5176:GLU:HB2	1.82	0.45
3:M:1151:VAL:HG13	3:N:4194:ALA:HB1	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6166:ILE:HG22	3:P:6168:ALA:H	1.81	0.45
3:O:5327:GLN:H	3:O:5345:HIS:CE1	2.34	0.45
1:B:4130:LEU:HD11	1:B:4178:PHE:CD2	2.51	0.45
3:P:6303:VAL:HG21	3:P:6378:ALA:CA	2.47	0.45
1:D:6114:ARG:HH21	1:D:6176:GLU:HB2	1.82	0.45
3:M:1329:PRO:O	3:M:1370:CYS:CA	2.65	0.45
1:A:1114:ARG:HH21	1:A:1176:GLU:HB2	1.82	0.45
3:M:1122:ILE:HG22	3:M:1123:LYS:N	2.30	0.45
1:D:6130:LEU:HD11	1:D:6178:PHE:CD2	2.52	0.45
3:O:5290:THR:HG22	3:O:5291:SER:N	2.30	0.45
1:B:4114:ARG:HH21	1:B:4176:GLU:HB2	1.82	0.45
3:M:1096:CYS:HB2	3:M:1100:ASN:HD21	1.82	0.45
1:A:1130:LEU:HD11	1:A:1178:PHE:CD2	2.51	0.45
3:M:1268:ALA:HB1	3:M:1271:CYS:SG	2.57	0.45
1:D:6135:LYS:HB2	1:D:6167:ALA:O	2.16	0.45
1:C:5136:VAL:HG22	1:C:5169:LEU:HD23	1.97	0.45
3:M:1303:VAL:HG21	3:M:1378:ALA:CA	2.47	0.45
3:N:4008:PRO:HG2	3:N:4015:TYR:CE2	2.51	0.45
3:P:6329:PRO:O	3:P:6370:CYS:CA	2.65	0.45
3:O:5329:PRO:O	3:O:5370:CYS:CA	2.65	0.45
3:N:4268:ALA:HB1	3:N:4271:CYS:SG	2.57	0.45
3:O:5303:VAL:HG21	3:O:5378:ALA:CA	2.47	0.44
3:N:4047:ILE:HG23	3:N:4119:ALA:O	2.18	0.44
3:N:4327:GLN:H	3:N:4345:HIS:CE1	2.34	0.44
3:P:6268:ALA:HB1	3:P:6271:CYS:SG	2.57	0.44
3:O:5268:ALA:HB1	3:O:5271:CYS:SG	2.57	0.44
3:O:5001:TYR:CA	3:O:5282:ILE:C	2.82	0.44
3:P:6008:PRO:HG2	3:P:6015:TYR:CE2	2.51	0.44
3:N:4096:CYS:HB2	3:N:4100:ASN:HD21	1.82	0.44
3:N:4329:PRO:O	3:N:4370:CYS:CA	2.65	0.44
3:O:5307:THR:HG22	3:O:5308:TYR:N	2.32	0.44
3:N:4307:THR:HG22	3:N:4308:TYR:N	2.32	0.44
3:M:1085:TYR:OH	3:M:1229:VAL:HA	2.18	0.44
3:P:6096:CYS:HB2	3:P:6100:ASN:HD21	1.82	0.44
3:P:6327:GLN:H	3:P:6345:HIS:HE1	1.66	0.44
3:P:6085:TYR:OH	3:P:6229:VAL:HA	2.18	0.44
3:P:6307:THR:HG22	3:P:6308:TYR:N	2.32	0.44
3:M:1200:PHE:HA	3:M:1200:PHE:HD2	1.61	0.43
3:O:5096:CYS:HB2	3:O:5100:ASN:HD21	1.82	0.43
3:O:5047:ILE:HG23	3:O:5119:ALA:O	2.18	0.43
3:P:6047:ILE:HG23	3:P:6119:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4356:PHE:HB3	3:N:4357:SER:H	1.63	0.43
3:M:1327:GLN:H	3:M:1345:HIS:HE1	1.66	0.43
3:P:6203:ILE:HA	3:P:6215:ALA:HB2	2.00	0.43
3:M:1249:ARG:H	3:M:1249:ARG:HG3	1.67	0.43
3:P:6077:THR:HG22	3:P:6221:LEU:HG	2.01	0.43
3:M:1199:ALA:HB1	3:M:1243:TRP:NE1	2.33	0.43
3:M:1047:ILE:HG23	3:M:1119:ALA:O	2.18	0.43
3:O:5077:THR:HG22	3:O:5221:LEU:HG	2.01	0.43
3:M:1307:THR:HG22	3:M:1308:TYR:N	2.32	0.43
3:M:1077:THR:HG22	3:M:1221:LEU:HG	2.01	0.43
3:N:4085:TYR:OH	3:N:4229:VAL:HA	2.18	0.43
3:M:1071:ALA:HB3	3:M:1076:TYR:OH	2.19	0.43
3:O:5071:ALA:HB3	3:O:5076:TYR:OH	2.19	0.43
3:P:6056:PRO:HD2	3:P:6105:GLU:O	2.19	0.43
3:O:5249:ARG:H	3:O:5249:ARG:HG3	1.67	0.43
1:C:5115:LEU:HD12	1:C:5129:ALA:O	2.19	0.43
3:P:6320:TYR:CE1	3:P:6369:LEU:CA	3.02	0.43
3:M:1320:TYR:CE1	3:M:1369:LEU:CA	3.02	0.43
3:N:4001:TYR:CA	3:N:4282:ILE:C	2.82	0.43
3:P:6199:ALA:HB1	3:P:6243:TRP:NE1	2.34	0.43
1:D:6115:LEU:HD12	1:D:6129:ALA:O	2.19	0.43
3:O:5056:PRO:HD2	3:O:5105:GLU:O	2.19	0.43
3:M:1029:LEU:HD22	3:M:1137:TYR:CE2	2.54	0.43
3:O:5085:TYR:OH	3:O:5229:VAL:HA	2.18	0.43
3:N:4203:ILE:HA	3:N:4215:ALA:HB2	2.00	0.43
3:N:4029:LEU:HD22	3:N:4137:TYR:CE2	2.54	0.43
3:O:5327:GLN:H	3:O:5345:HIS:HE1	1.66	0.43
3:N:4327:GLN:H	3:N:4345:HIS:HE1	1.66	0.43
3:N:4056:PRO:HD2	3:N:4105:GLU:O	2.19	0.43
3:P:6071:ALA:HB3	3:P:6076:TYR:OH	2.19	0.43
3:N:4199:ALA:HB1	3:N:4243:TRP:NE1	2.33	0.42
3:P:6001:TYR:CA	3:P:6282:ILE:C	2.82	0.42
3:O:5203:ILE:HA	3:O:5215:ALA:HB2	2.01	0.42
3:M:1203:ILE:HA	3:M:1215:ALA:HB2	2.01	0.42
3:O:5199:ALA:HB1	3:O:5243:TRP:NE1	2.33	0.42
3:P:6029:LEU:HD22	3:P:6137:TYR:CE2	2.54	0.42
3:O:5130:LYS:HD2	3:O:5267:ARG:NH2	2.35	0.42
3:N:4320:TYR:CE1	3:N:4369:LEU:CA	3.02	0.42
3:N:4077:THR:HG22	3:N:4221:LEU:HG	2.01	0.42
1:B:4115:LEU:HD12	1:B:4129:ALA:O	2.19	0.42
3:O:5320:TYR:CE1	3:O:5369:LEU:CA	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6130:LYS:HD2	3:P:6267:ARG:NH2	2.35	0.42
3:N:4071:ALA:HB3	3:N:4076:TYR:OH	2.19	0.42
1:A:1115:LEU:HD12	1:A:1129:ALA:O	2.19	0.42
3:O:5063:CYS:N	3:O:5096:CYS:SG	2.93	0.42
3:M:1056:PRO:HD2	3:M:1105:GLU:O	2.19	0.42
3:P:6048:THR:CG2	3:P:6204:GLN:HG2	2.50	0.42
3:P:6299:VAL:HG13	3:P:6320:TYR:HE2	1.85	0.42
3:O:5009:ASN:ND2	3:O:5166:ILE:HD13	2.31	0.42
3:O:5029:LEU:HD22	3:O:5137:TYR:CE2	2.54	0.42
3:P:6327:GLN:O	3:P:6328:CYS:HB3	2.20	0.42
3:N:4327:GLN:O	3:N:4328:CYS:HB3	2.20	0.42
3:P:6048:THR:HG23	3:P:6204:GLN:HG2	2.02	0.42
3:M:1320:TYR:OH	3:M:1369:LEU:CA	2.68	0.42
3:P:6203:ILE:HG12	3:P:6215:ALA:CB	2.50	0.42
3:O:5046:TYR:HA	3:O:5205:ALA:O	2.20	0.42
3:M:1299:VAL:HG13	3:M:1320:TYR:HE2	1.85	0.42
3:N:4203:ILE:HG12	3:N:4215:ALA:CB	2.50	0.42
3:N:4048:THR:CG2	3:N:4204:GLN:HG2	2.50	0.42
3:O:5048:THR:CG2	3:O:5204:GLN:HG2	2.50	0.42
3:O:5150:GLY:N	3:O:5165:PRO:HD3	2.35	0.42
3:N:4063:CYS:N	3:N:4096:CYS:SG	2.93	0.41
3:M:1063:CYS:N	3:M:1096:CYS:SG	2.93	0.41
3:M:1151:VAL:HG21	3:N:4191:GLU:CB	2.50	0.41
3:N:4299:VAL:HG13	3:N:4320:TYR:HE2	1.85	0.41
3:N:4200:PHE:HD2	3:N:4200:PHE:HA	1.61	0.41
3:O:5029:LEU:HD22	3:O:5137:TYR:HE2	1.85	0.41
3:M:1327:GLN:O	3:M:1328:CYS:HB3	2.20	0.41
3:M:1150:GLY:N	3:M:1165:PRO:HD3	2.35	0.41
3:O:5299:VAL:HG13	3:O:5320:TYR:HE2	1.85	0.41
3:N:4029:LEU:HD22	3:N:4137:TYR:HE2	1.85	0.41
3:P:6342:SER:O	3:P:6356:PHE:CZ	2.71	0.41
3:M:1130:LYS:HD2	3:M:1267:ARG:NH2	2.35	0.41
3:O:5327:GLN:O	3:O:5328:CYS:HB3	2.20	0.41
3:P:6320:TYR:OH	3:P:6369:LEU:CA	2.68	0.41
3:P:6009:ASN:ND2	3:P:6166:ILE:HD13	2.31	0.41
3:P:6029:LEU:HD22	3:P:6137:TYR:HE2	1.85	0.41
3:N:4130:LYS:HD2	3:N:4267:ARG:NH2	2.35	0.41
3:M:1048:THR:HG23	3:M:1204:GLN:HG2	2.02	0.41
3:M:1191:GLU:CB	3:N:4151:VAL:HG21	2.50	0.41
3:N:4317:THR:O	3:N:4317:THR:HG22	2.20	0.41
3:P:6063:CYS:N	3:P:6096:CYS:SG	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:4196:LYS:C	3:N:4198:GLY:H	2.24	0.41
3:P:6046:TYR:HA	3:P:6205:ALA:O	2.20	0.41
3:M:1293:ALA:HB3	3:M:1294:PRO:CD	2.51	0.41
3:N:4293:ALA:HB3	3:N:4294:PRO:CD	2.51	0.41
3:M:1317:THR:HG22	3:M:1317:THR:O	2.20	0.41
3:M:1010:VAL:HA	3:M:1011:PRO:HD2	1.92	0.41
1:B:4248:ASN:C	1:B:4248:ASN:HD22	2.24	0.41
1:B:4197:GLN:NE2	1:B:4239:ARG:HH12	2.19	0.41
1:A:1197:GLN:NE2	1:A:1239:ARG:HH12	2.19	0.41
3:P:6150:GLY:N	3:P:6165:PRO:HD3	2.35	0.41
3:O:5320:TYR:OH	3:O:5369:LEU:CA	2.68	0.41
3:O:5243:TRP:HZ3	3:O:5246:ASN:HB3	1.86	0.41
3:P:6336:THR:O	3:P:6337:ALA:HB3	2.21	0.41
3:M:1336:THR:O	3:M:1337:ALA:HB3	2.21	0.41
3:O:5336:THR:O	3:O:5337:ALA:HB3	2.21	0.41
3:M:1203:ILE:HG12	3:M:1215:ALA:CB	2.50	0.41
3:N:4320:TYR:OH	3:N:4369:LEU:CA	2.68	0.41
3:N:4243:TRP:HZ3	3:N:4246:ASN:HB3	1.86	0.41
3:M:1243:TRP:HZ3	3:M:1246:ASN:HB3	1.86	0.41
3:N:4336:THR:O	3:N:4337:ALA:HB3	2.21	0.41
1:A:1248:ASN:C	1:A:1248:ASN:HD22	2.24	0.41
3:M:1196:LYS:C	3:M:1198:GLY:H	2.24	0.41
3:M:1049:CYS:HG	3:M:1118:HIS:HA	1.86	0.41
3:P:6293:ALA:HB3	3:P:6294:PRO:CD	2.51	0.41
3:O:5317:THR:HG22	3:O:5317:THR:O	2.20	0.41
3:P:6317:THR:O	3:P:6317:THR:HG22	2.20	0.41
3:O:5073:HIS:H	3:O:5076:TYR:HE1	1.69	0.41
3:M:1046:TYR:HA	3:M:1205:ALA:O	2.20	0.41
3:N:4150:GLY:N	3:N:4165:PRO:HD3	2.35	0.41
3:P:6196:LYS:C	3:P:6198:GLY:H	2.24	0.41
3:N:4048:THR:HG23	3:N:4204:GLN:HG2	2.02	0.41
3:P:6243:TRP:HZ3	3:P:6246:ASN:HB3	1.86	0.40
1:C:5248:ASN:C	1:C:5248:ASN:HD22	2.24	0.40
3:M:1048:THR:CG2	3:M:1204:GLN:HG2	2.50	0.40
3:N:4009:ASN:ND2	3:N:4166:ILE:HD13	2.31	0.40
1:A:1156:PHE:CB	1:A:1165:GLU:HG2	2.49	0.40
3:M:1029:LEU:HD22	3:M:1137:TYR:HE2	1.85	0.40
3:O:5203:ILE:HG12	3:O:5215:ALA:CB	2.50	0.40
3:P:6045:GLU:O	3:P:6046:TYR:HD2	2.05	0.40
3:M:1045:GLU:O	3:M:1046:TYR:HD2	2.05	0.40
3:M:1166:ILE:HG12	3:M:1276:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6180:HIS:O	3:P:6182:GLY:N	2.55	0.40
3:O:5196:LYS:C	3:O:5198:GLY:H	2.24	0.40
3:N:4046:TYR:HA	3:N:4205:ALA:O	2.20	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 PDB entries followed by that with respect to all EM entries.

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	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	B	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	C	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
1	D	149/264 (56%)	144 (97%)	5 (3%)	0	100	100
3	M	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
3	N	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
3	O	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
3	P	348/439 (79%)	270 (78%)	67 (19%)	11 (3%)	5	41
All	All	1988/2812 (71%)	1656 (83%)	288 (14%)	44 (2%)	13	49

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	1126	THR
3	M	1361	PRO
3	N	4126	THR
3	N	4361	PRO
3	O	5126	THR
3	O	5361	PRO
3	P	6126	THR

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Mol	Chain	Res	Type
3	P	6361	PRO
3	M	1156	SER
3	M	1201	GLY
3	M	1202	ASP
3	N	4156	SER
3	N	4201	GLY
3	N	4202	ASP
3	O	5156	SER
3	O	5201	GLY
3	O	5202	ASP
3	P	6156	SER
3	P	6201	GLY
3	P	6202	ASP
3	M	1075	ASP
3	M	1181	ARG
3	M	1324	ARG
3	N	4049	CYS
3	N	4075	ASP
3	N	4181	ARG
3	N	4324	ARG
3	O	5049	CYS
3	O	5075	ASP
3	O	5181	ARG
3	O	5324	ARG
3	P	6075	ASP
3	P	6181	ARG
3	P	6324	ARG
3	M	1049	CYS
3	P	6049	CYS
3	M	1293	ALA
3	M	1328	CYS
3	N	4293	ALA
3	N	4328	CYS
3	O	5293	ALA
3	O	5328	CYS
3	P	6293	ALA
3	P	6328	CYS

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 PDB entries followed by that with respect to all EM

entries.

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	122/218 (56%)	115 (94%)	7 (6%)	25	62
1	B	122/218 (56%)	115 (94%)	7 (6%)	25	62
1	C	122/218 (56%)	115 (94%)	7 (6%)	25	62
1	D	122/218 (56%)	115 (94%)	7 (6%)	25	62
3	M	299/370 (81%)	290 (97%)	9 (3%)	48	77
3	N	299/370 (81%)	290 (97%)	9 (3%)	48	77
3	O	299/370 (81%)	290 (97%)	9 (3%)	48	77
3	P	299/370 (81%)	290 (97%)	9 (3%)	48	77
All	All	1684/2352 (72%)	1620 (96%)	64 (4%)	44	73

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1143	LYS
1	A	1155	LYS
1	A	1183	GLU
1	A	1191	TRP
1	A	1207	ARG
1	A	1248	ASN
1	A	1253	THR
1	B	4143	LYS
1	B	4155	LYS
1	B	4183	GLU
1	B	4191	TRP
1	B	4207	ARG
1	B	4248	ASN
1	B	4253	THR
1	C	5143	LYS
1	C	5155	LYS
1	C	5183	GLU
1	C	5191	TRP
1	C	5207	ARG
1	C	5248	ASN
1	C	5253	THR
1	D	6143	LYS
1	D	6155	LYS

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Mol	Chain	Res	Type
1	D	6183	GLU
1	D	6191	TRP
1	D	6207	ARG
1	D	6248	ASN
1	D	6253	THR
3	M	1035	SER
3	M	1049	CYS
3	M	1118	HIS
3	M	1188	ASP
3	M	1192	TYR
3	M	1200	PHE
3	M	1212	ASP
3	M	1292	ASP
3	M	1334	SER
3	N	4035	SER
3	N	4049	CYS
3	N	4118	HIS
3	N	4188	ASP
3	N	4192	TYR
3	N	4200	PHE
3	N	4212	ASP
3	N	4292	ASP
3	N	4334	SER
3	O	5035	SER
3	O	5049	CYS
3	O	5118	HIS
3	O	5188	ASP
3	O	5192	TYR
3	O	5200	PHE
3	O	5212	ASP
3	O	5292	ASP
3	O	5334	SER
3	P	6035	SER
3	P	6049	CYS
3	P	6118	HIS
3	P	6188	ASP
3	P	6192	TYR
3	P	6200	PHE
3	P	6212	ASP
3	P	6292	ASP
3	P	6334	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1190	ASN
1	A	1197	GLN
1	A	1248	ASN
1	B	4128	HIS
1	B	4190	ASN
1	B	4197	GLN
1	B	4248	ASN
1	C	5128	HIS
1	C	5190	ASN
1	C	5197	GLN
1	C	5248	ASN
1	D	6128	HIS
1	D	6190	ASN
1	D	6197	GLN
1	D	6248	ASN
3	M	1073	HIS
3	M	1100	ASN
3	M	1331	HIS
3	M	1345	HIS
3	M	1355	HIS
3	N	4073	HIS
3	N	4100	ASN
3	N	4331	HIS
3	N	4345	HIS
3	N	4355	HIS
3	O	5073	HIS
3	O	5100	ASN
3	O	5331	HIS
3	O	5345	HIS
3	O	5355	HIS
3	P	6073	HIS
3	P	6100	ASN
3	P	6331	HIS
3	P	6345	HIS
3	P	6355	HIS

5.3.3 RNA ⓘ

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 32 ligands modelled in this entry, 32 are unknown - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.