



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:52 pm BST

PDB ID : 5J3D  
Title : Crystal structure of human Fab 14N4 in complex with post-fusion RSV F  
Authors : Mousa, J.J.; Crowe, J.E.  
Deposited on : 2016-03-30  
Resolution : 4.08 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

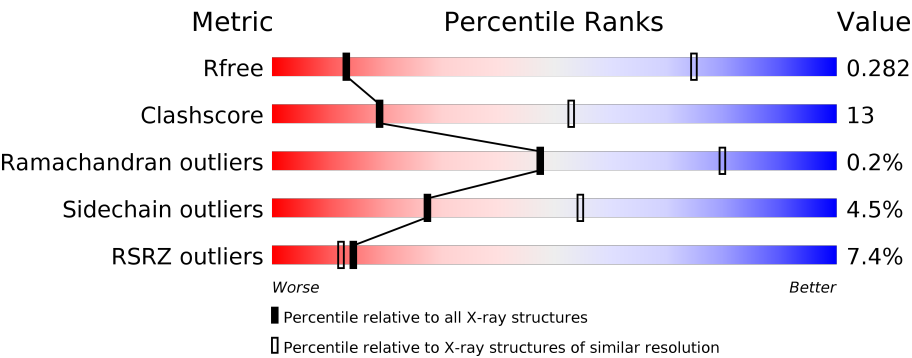
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.08 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	1133 (4.46-3.70)
Clashscore	141614	1013 (4.42-3.74)
Ramachandran outliers	138981	1151 (4.46-3.70)
Sidechain outliers	138945	1139 (4.46-3.70)
RSRZ outliers	127900	1012 (4.48-3.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	224	<div><div>7%</div><div><div></div><div>72%</div><div>25%</div><div></div></div><div></div></div>
1	C	224	<div><div>2%</div><div><div></div><div>72%</div><div>24%</div><div></div></div><div></div></div>
1	H	224	<div><div>28%</div><div><div></div><div>73%</div><div>25%</div><div></div></div><div></div></div>
2	B	218	<div><div>5%</div><div><div></div><div>69%</div><div>28%</div><div></div></div><div></div></div>
2	D	218	<div><div>2%</div><div><div></div><div>71%</div><div>26%</div><div></div></div><div></div></div>
2	L	218	<div><div>39%</div><div><div></div><div>79%</div><div>19%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	E	73	<div><div></div><div>64%34%</div><div></div></div>
3	G	73	<div><div></div><div>77%22%</div><div></div></div>
3	J	73	<div><div></div><div>60%36%</div><div></div></div>
4	F	394	<div><div>%</div><div></div><div>60%27%9%</div><div></div></div>
4	I	394	<div><div>%</div><div></div><div>61%27%9%</div><div></div></div>
4	K	394	<div><div></div><div>60%27%9%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19902 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 14N4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1624	1020	275	322	7			
1	C	220	Total	C	N	O	S	0	0	0
			1624	1020	275	322	7			
1	H	220	Total	C	N	O	S	0	0	0
			1624	1020	275	322	7			

- Molecule 2 is a protein called 14N4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1665	1044	276	339	6			
2	D	215	Total	C	N	O	S	0	0	0
			1665	1044	276	339	6			
2	L	215	Total	C	N	O	S	0	0	0
			1665	1044	276	339	6			

- Molecule 3 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	73	Total	C	N	O	S	0	0	0
			580	366	95	116	3			
3	G	73	Total	C	N	O	S	0	0	0
			580	366	95	116	3			
3	J	73	Total	C	N	O	S	0	0	0
			580	366	95	116	3			

- Molecule 4 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	358	Total	C	N	O	S	0	0	0
			2765	1744	458	545	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	358	Total	C	N	O	S	0	0	0
			2765	1744	458	545	18			
4	K	358	Total	C	N	O	S	0	0	0
			2765	1744	458	545	18			

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	VAL	ILE	conflict	UNP P03420
F	447	VAL	MET	conflict	UNP P03420
F	514	GLY	-	expression tag	UNP P03420
F	515	LEU	-	expression tag	UNP P03420
F	516	GLU	-	expression tag	UNP P03420
F	517	VAL	-	expression tag	UNP P03420
F	518	LEU	-	expression tag	UNP P03420
F	519	PHE	-	expression tag	UNP P03420
F	520	GLN	-	expression tag	UNP P03420
F	521	GLY	-	expression tag	UNP P03420
F	522	PRO	-	expression tag	UNP P03420
F	523	HIS	-	expression tag	UNP P03420
F	524	HIS	-	expression tag	UNP P03420
F	525	HIS	-	expression tag	UNP P03420
F	526	HIS	-	expression tag	UNP P03420
F	527	HIS	-	expression tag	UNP P03420
F	528	HIS	-	expression tag	UNP P03420
F	529	HIS	-	expression tag	UNP P03420
F	530	HIS	-	expression tag	UNP P03420
F	531	SER	-	expression tag	UNP P03420
F	532	ALA	-	expression tag	UNP P03420
F	533	TRP	-	expression tag	UNP P03420
F	534	SER	-	expression tag	UNP P03420
F	535	HIS	-	expression tag	UNP P03420
F	536	PRO	-	expression tag	UNP P03420
F	537	GLN	-	expression tag	UNP P03420
F	538	PHE	-	expression tag	UNP P03420
F	539	GLU	-	expression tag	UNP P03420
F	540	LYS	-	expression tag	UNP P03420
I	379	VAL	ILE	conflict	UNP P03420
I	447	VAL	MET	conflict	UNP P03420
I	514	GLY	-	expression tag	UNP P03420
I	515	LEU	-	expression tag	UNP P03420
I	516	GLU	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
I	517	VAL	-	expression tag	UNP P03420
I	518	LEU	-	expression tag	UNP P03420
I	519	PHE	-	expression tag	UNP P03420
I	520	GLN	-	expression tag	UNP P03420
I	521	GLY	-	expression tag	UNP P03420
I	522	PRO	-	expression tag	UNP P03420
I	523	HIS	-	expression tag	UNP P03420
I	524	HIS	-	expression tag	UNP P03420
I	525	HIS	-	expression tag	UNP P03420
I	526	HIS	-	expression tag	UNP P03420
I	527	HIS	-	expression tag	UNP P03420
I	528	HIS	-	expression tag	UNP P03420
I	529	HIS	-	expression tag	UNP P03420
I	530	HIS	-	expression tag	UNP P03420
I	531	SER	-	expression tag	UNP P03420
I	532	ALA	-	expression tag	UNP P03420
I	533	TRP	-	expression tag	UNP P03420
I	534	SER	-	expression tag	UNP P03420
I	535	HIS	-	expression tag	UNP P03420
I	536	PRO	-	expression tag	UNP P03420
I	537	GLN	-	expression tag	UNP P03420
I	538	PHE	-	expression tag	UNP P03420
I	539	GLU	-	expression tag	UNP P03420
I	540	LYS	-	expression tag	UNP P03420
K	379	VAL	ILE	conflict	UNP P03420
K	447	VAL	MET	conflict	UNP P03420
K	514	GLY	-	expression tag	UNP P03420
K	515	LEU	-	expression tag	UNP P03420
K	516	GLU	-	expression tag	UNP P03420
K	517	VAL	-	expression tag	UNP P03420
K	518	LEU	-	expression tag	UNP P03420
K	519	PHE	-	expression tag	UNP P03420
K	520	GLN	-	expression tag	UNP P03420
K	521	GLY	-	expression tag	UNP P03420
K	522	PRO	-	expression tag	UNP P03420
K	523	HIS	-	expression tag	UNP P03420
K	524	HIS	-	expression tag	UNP P03420
K	525	HIS	-	expression tag	UNP P03420
K	526	HIS	-	expression tag	UNP P03420
K	527	HIS	-	expression tag	UNP P03420
K	528	HIS	-	expression tag	UNP P03420
K	529	HIS	-	expression tag	UNP P03420

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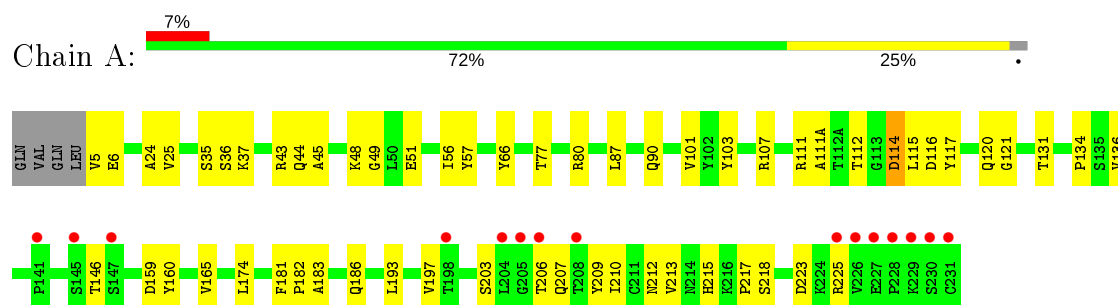
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Chain	Residue	Modelled	Actual	Comment	Reference
K	530	HIS	-	expression tag	UNP P03420
K	531	SER	-	expression tag	UNP P03420
K	532	ALA	-	expression tag	UNP P03420
K	533	TRP	-	expression tag	UNP P03420
K	534	SER	-	expression tag	UNP P03420
K	535	HIS	-	expression tag	UNP P03420
K	536	PRO	-	expression tag	UNP P03420
K	537	GLN	-	expression tag	UNP P03420
K	538	PHE	-	expression tag	UNP P03420
K	539	GLU	-	expression tag	UNP P03420
K	540	LYS	-	expression tag	UNP P03420

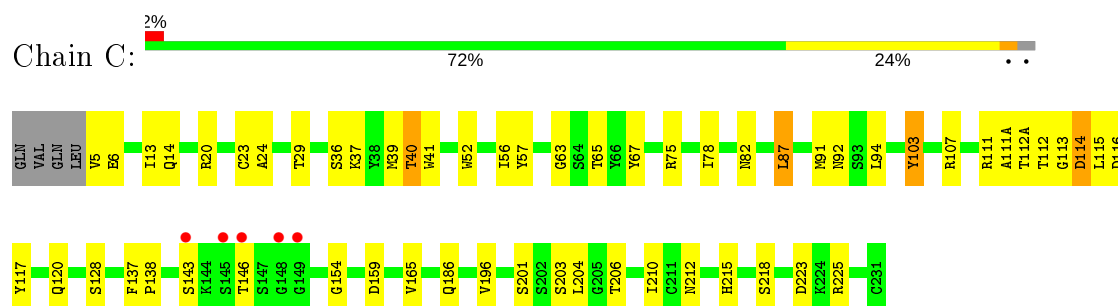
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

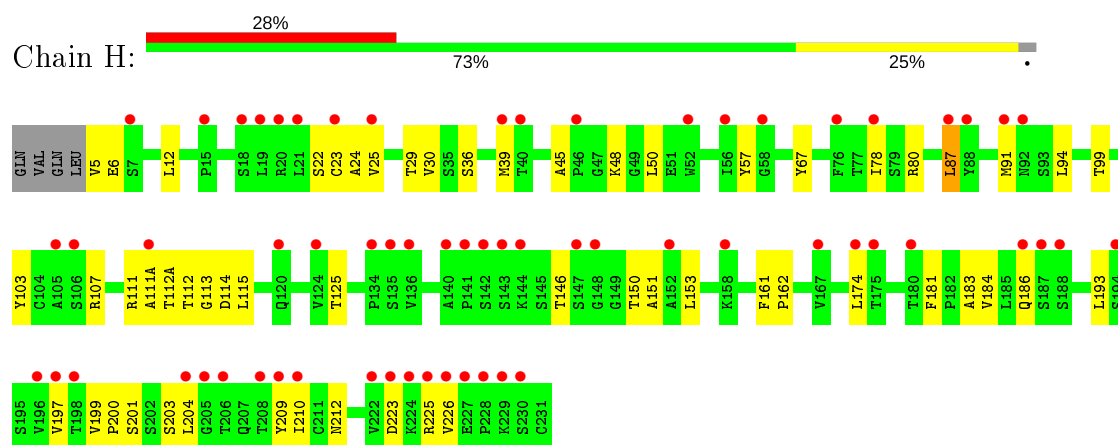
- Molecule 1: 14N4 heavy chain



- Molecule 1: 14N4 heavy chain

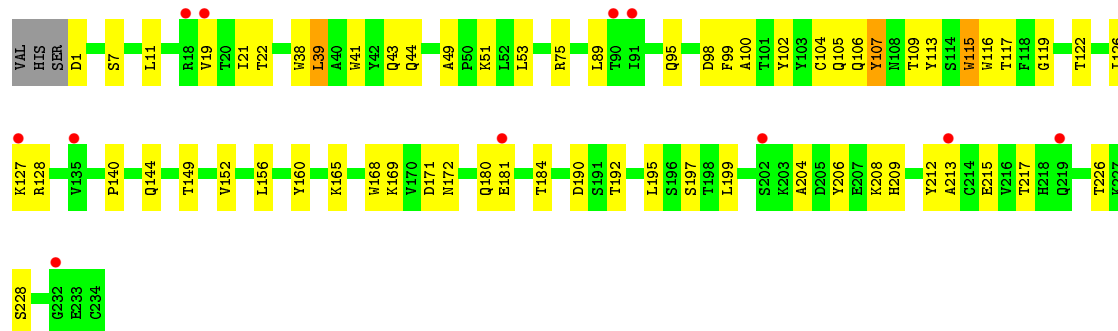


- Molecule 1: 14N4 heavy chain

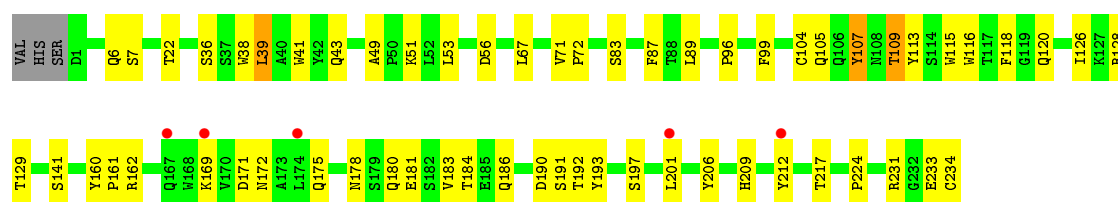


- Molecule 2: 14N4 light chain

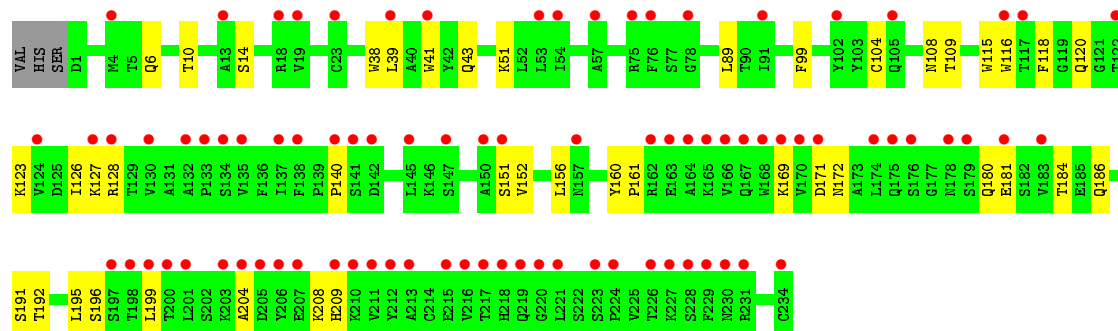
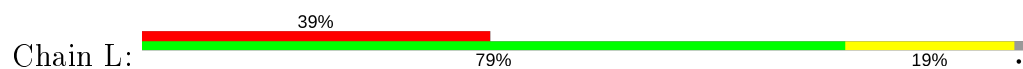




- Molecule 2: 14N4 light chain



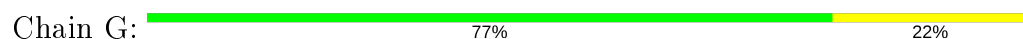
- Molecule 2: 14N4 light chain



- Molecule 3: Fusion glycoprotein F0



- Molecule 3: Fusion glycoprotein F0





V452	ILE	M251	A147
T455	C333	L282	S150
L456	L334	T253	G151
	T335		V152
K461	R336	E256	A153
	T337		
G464	D338	L261	L158
K465	R339	M262	H159
	G340	D263	L160
V469	W341	M264	E161
	Y342	P265	
I474	C343	L266	V164
I475	D344	T267	
N476	N345	M268	K168
F477	A346	D269	
		Q270	L172
L481	F352		
		L273	A177
S485	Q361	M277	V178
	S362		
D489	N363	R282	L181
	R364	Q283	
L503	S372		V185
A504	L373	I288	K191
F505	T374	M289	
		S290	L195
K508	S377	I291	Y198
		I292	I199
L512	N383	K293	
L513		E294	
G514	I386		
LEU		L297	Q202
GLU	I395	A298	L203
VAL		Y299	L204
LEU	S398	V300	P205
PHE	K399	V301	I206
GLN	T400		
GLY	D401	I309	S211
PRO	V402	D310	
HIS	S403	T311	I214
HIS	S404	P312	
HIS		C313	I217
HIS	L410	R314	E218
HIS		K315	T219
HIS	C416		
HIS		T318	
HIS	C422	S319	L230
SER		P320	L231
ALA	N426	L321	E232
TRP	K427	C322	I233
SER		THR	T234
HIS	N437	THR	R235
PRO	G438	ASN	V243
GLN	C439	THR	T244
PHE		LYS	T245
GLU	N444	GLU	P246
LYS	T449	GLY	
		SER	T249
		ASN	Y250

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.13Å 235.13Å 220.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 4.08 49.50 – 4.08	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.50-4.08) 84.8 (49.50-4.08)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.257 , 0.282 0.257 , 0.282	Depositor DCC
$R_{free}$ test set	1999 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 105.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	19902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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)

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	0.34	0/1660	0.56	0/2262
1	C	0.45	0/1660	0.63	0/2262
1	H	0.27	0/1660	0.51	0/2262
2	B	0.34	0/1704	0.55	0/2317
2	D	0.42	0/1704	0.59	0/2317
2	L	0.29	0/1704	0.50	0/2317
3	E	0.50	0/586	0.75	0/789
3	G	0.64	0/586	0.85	1/789 (0.1%)
3	J	0.50	0/586	0.73	0/789
4	F	0.50	0/2805	0.74	2/3803 (0.1%)
4	I	0.54	0/2805	0.81	4/3803 (0.1%)
4	K	0.56	1/2805 (0.0%)	0.80	5/3803 (0.1%)
All	All	0.46	1/20265 (0.0%)	0.68	12/27513 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	439	CYS	CB-SG	-6.17	1.71	1.82

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	212	CYS	CA-CB-SG	12.46	136.43	114.00
4	K	172	LEU	CA-CB-CG	-6.41	100.56	115.30
4	I	231	LEU	CA-CB-CG	-6.26	100.91	115.30
4	I	373	LEU	CA-CB-CG	-6.26	100.90	115.30
4	I	305	LEU	CB-CG-CD1	-5.41	101.80	111.00
4	K	172	LEU	CB-CG-CD2	-5.39	101.83	111.00
4	F	333	CYS	CA-CB-SG	5.34	123.61	114.00
4	K	373	LEU	CA-CB-CG	-5.31	103.09	115.30
4	K	333	CYS	CA-CB-SG	5.22	123.39	114.00
4	F	193	LEU	CB-CG-CD1	-5.19	102.17	111.00
3	G	61	LEU	CB-CG-CD2	-5.14	102.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	151	GLY	N-CA-C	5.07	125.78	113.10

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	1624	0	1599	43	0
1	C	1624	0	1599	45	1
1	H	1624	0	1599	36	0
2	B	1665	0	1600	48	0
2	D	1665	0	1600	65	0
2	L	1665	0	1600	33	0
3	E	580	0	589	25	0
3	G	580	0	589	13	0
3	J	580	0	589	26	0
4	F	2765	0	2798	112	0
4	I	2765	0	2798	122	0
4	K	2765	0	2798	109	0
All	All	19902	0	19758	514	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (514) 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)
2:D:38:TRP:CE2	4:I:268:ASN:HB3	1.81	1.15
2:D:38:TRP:HH2	4:I:269:ASP:HA	1.35	0.89
1:A:35:SER:O	4:I:465:LYS:NZ	2.09	0.86
2:D:109:THR:HG23	4:I:267:THR:HA	1.55	0.85
4:F:345:ASN:HD22	4:I:455:THR:HG21	1.42	0.84
4:F:272:LYS:O	4:F:276:ASN:ND2	2.12	0.82
2:B:109:THR:O	2:B:116:TRP:NE1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASN:ND2	1:C:223:ASP:OD1	2.13	0.80
3:E:59:ILE:HG23	4:I:469:VAL:HB	1.64	0.79
4:K:318:THR:HG21	4:K:336:ARG:HB2	1.65	0.78
4:F:261:ILE:HG12	4:F:264:MET:HE1	1.65	0.77
4:I:152:VAL:HG11	4:K:152:VAL:HB	1.67	0.77
4:K:270:GLN:HG2	4:K:309:ILE:HD12	1.67	0.76
2:D:107:TYR:O	4:I:268:ASN:ND2	2.18	0.76
4:F:290:SER:OG	4:F:291:ILE:N	2.19	0.75
4:F:171:LEU:HD23	4:I:513:LEU:HD11	1.68	0.75
2:D:38:TRP:CZ2	4:I:268:ASN:C	2.61	0.74
2:D:38:TRP:CH2	4:I:269:ASP:HA	2.22	0.74
1:C:36:SER:HA	4:K:465:LYS:NZ	2.03	0.73
4:F:270:GLN:HG2	4:F:309:ILE:HD12	1.69	0.73
2:D:38:TRP:CZ2	4:I:268:ASN:HB3	2.23	0.73
2:B:107:TYR:O	4:F:268:ASN:ND2	2.22	0.72
4:K:252:LEU:O	4:K:282:ARG:NH1	2.23	0.71
2:D:38:TRP:CH2	4:I:268:ASN:C	2.64	0.71
4:F:318:THR:HG21	4:F:336:ARG:HB2	1.73	0.71
1:A:212:ASN:ND2	1:A:223:ASP:OD1	2.23	0.70
2:L:6:GLN:HB2	2:L:120:GLN:HE22	1.56	0.70
1:H:5:VAL:N	1:H:24:ALA:O	2.24	0.70
4:F:166:LYS:NZ	4:K:514:GLY:HA3	2.06	0.70
4:I:270:GLN:HG2	4:I:309:ILE:HD12	1.73	0.70
2:D:43:GLN:HB2	2:D:53:LEU:HD11	1.73	0.69
2:D:96:PRO:HA	2:D:99:PHE:CD2	2.28	0.69
4:I:266:ILE:HD12	4:I:270:GLN:HB2	1.75	0.69
2:D:38:TRP:CD2	4:I:268:ASN:HB3	2.28	0.68
1:C:186:GLN:HA	2:D:180:GLN:HE22	1.58	0.68
1:A:174:LEU:HD21	1:A:197:VAL:HG21	1.74	0.68
2:D:38:TRP:CZ2	4:I:268:ASN:O	2.47	0.68
4:K:449:THR:HG23	4:K:456:LEU:HD11	1.76	0.68
1:C:39:MET:HE3	1:C:87:LEU:HD22	1.75	0.68
2:D:38:TRP:HH2	4:I:269:ASP:CA	2.05	0.68
4:F:148:ILE:HB	4:F:154:VAL:HG12	1.74	0.68
4:K:261:ILE:HG12	4:K:264:MET:HE1	1.75	0.68
4:K:334:LEU:HD22	4:K:395:ILE:HD13	1.75	0.67
4:K:230:LEU:O	4:K:234:THR:HG23	1.95	0.66
1:C:23:CYS:HB3	1:C:87:LEU:HD23	1.78	0.66
2:B:43:GLN:O	2:B:51:LYS:N	2.27	0.66
4:F:266:ILE:HD12	4:F:270:GLN:HB2	1.78	0.66
2:D:171:ASP:OD2	2:D:209:HIS:ND1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:277:ASN:OD1	4:F:361:GLN:HG2	1.94	0.66
1:A:77:THR:HB	1:A:90:GLN:HB3	1.77	0.66
1:A:43:ARG:NE	1:A:51:GLU:OE1	2.24	0.66
1:A:183:ALA:HA	1:A:193:LEU:HB3	1.79	0.65
4:F:149:ALA:HB3	4:K:152:VAL:HG22	1.78	0.65
1:H:151:ALA:HB3	1:H:204:LEU:HD21	1.78	0.65
4:K:290:SER:OG	4:K:291:ILE:N	2.29	0.65
4:I:318:THR:HG21	4:I:336:ARG:HB2	1.77	0.65
2:B:171:ASP:OD2	2:B:209:HIS:ND1	2.21	0.65
1:A:5:VAL:N	1:A:24:ALA:O	2.30	0.65
3:J:66:GLU:HA	3:J:79:ILE:HG21	1.78	0.65
3:G:52:TRP:HB2	4:K:461:LYS:HG2	1.80	0.64
1:C:5:VAL:N	1:C:117:TYR:HH	1.95	0.64
2:D:41:TRP:CZ3	2:D:104:CYS:HB3	2.32	0.64
2:L:171:ASP:OD2	2:L:209:HIS:ND1	2.29	0.64
1:A:114:ASP:N	1:A:114:ASP:OD1	2.31	0.64
2:D:169:LYS:HE2	2:D:172:ASN:HA	1.79	0.64
4:F:345:ASN:ND2	4:I:455:THR:HG21	2.12	0.64
2:B:41:TRP:CE2	2:B:89:LEU:HB2	2.32	0.64
4:I:351:PHE:CE2	4:I:353:PRO:HB3	2.32	0.63
3:E:46:SER:HB3	4:F:313:CYS:SG	2.38	0.63
3:E:64:ILE:HG22	4:I:474:ILE:HG13	1.80	0.63
1:C:107:ARG:HD3	1:C:114:ASP:OD1	1.99	0.63
3:E:64:ILE:HD12	3:E:79:ILE:HG23	1.81	0.63
1:A:210:ILE:HG12	1:A:225:ARG:HG2	1.80	0.63
1:A:36:SER:HA	4:I:465:LYS:NZ	2.13	0.62
4:F:251:MET:HG3	4:F:299:TYR:CE1	2.35	0.62
1:C:210:ILE:HG12	1:C:225:ARG:HG2	1.82	0.62
3:E:28:ILE:HD11	4:F:363:ASN:HA	1.80	0.62
4:F:199:ILE:HD11	4:I:199:ILE:HD11	1.81	0.62
4:F:199:ILE:HD11	4:K:199:ILE:HD11	1.82	0.62
1:A:57:TYR:HE1	1:A:112:THR:HG21	1.64	0.61
4:I:264:MET:HE3	4:I:266:ILE:HD11	1.82	0.61
2:D:105:GLN:HB2	2:D:118:PHE:CE1	2.34	0.61
4:F:152:VAL:HG11	4:I:152:VAL:HG21	1.81	0.61
1:A:182:PRO:HD3	2:B:184:THR:HG22	1.82	0.61
2:D:6:GLN:H	2:D:120:GLN:HE22	1.49	0.61
4:F:166:LYS:HZ1	4:K:514:GLY:HA3	1.65	0.61
1:C:114:ASP:N	1:C:114:ASP:OD1	2.27	0.61
1:C:40:THR:OG1	1:C:41:TRP:N	2.33	0.61
4:F:253:THR:OG1	4:F:256:GLU:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:246:PRO:HB3	4:K:283:GLN:HA	1.81	0.61
4:K:336:ARG:NH1	4:K:383:ASN:OD1	2.34	0.61
1:H:30:VAL:O	1:H:80:ARG:NH1	2.34	0.61
2:B:169:LYS:HE2	2:B:172:ASN:HA	1.83	0.61
4:F:229:ARG:NH2	4:F:256:GLU:OE1	2.29	0.61
2:D:56:ASP:OD1	2:D:107:TYR:OH	2.17	0.60
2:L:126:ILE:O	2:L:160:TYR:OH	2.17	0.60
4:K:277:ASN:OD1	4:K:361:GLN:HG2	2.02	0.60
2:D:38:TRP:CH2	4:I:269:ASP:CA	2.83	0.60
4:I:345:ASN:OD1	4:K:455:THR:HG21	2.01	0.60
4:I:251:MET:HG3	4:I:299:TYR:CE1	2.37	0.60
4:K:252:LEU:HD22	4:K:301:VAL:HG21	1.82	0.60
1:C:5:VAL:N	1:C:117:TYR:OH	2.35	0.60
4:F:469:VAL:HB	3:J:59:ILE:HG23	1.83	0.59
4:I:426:ASN:ND2	4:I:446:GLY:O	2.36	0.59
4:F:474:ILE:HG13	3:J:64:ILE:HG22	1.84	0.59
4:I:199:ILE:HD11	4:K:199:ILE:HD11	1.83	0.59
2:L:156:LEU:HB2	2:L:195:LEU:HB3	1.84	0.59
1:A:57:TYR:CE1	1:A:112:THR:HG21	2.36	0.59
4:I:252:LEU:HD23	4:I:256:GLU:HB2	1.83	0.59
2:B:11:LEU:HD23	2:B:19:VAL:HG13	1.82	0.59
4:F:465:LYS:NZ	1:H:36:SER:HA	2.18	0.59
4:I:246:PRO:HB3	4:I:283:GLN:HA	1.83	0.59
4:K:164:VAL:O	4:K:168:LYS:HB2	2.03	0.58
4:I:253:THR:OG1	4:I:256:GLU:HG3	2.03	0.58
2:L:43:GLN:HB3	2:L:51:LYS:HB3	1.84	0.58
1:C:112(A):THR:CG2	2:D:38:TRP:HE1	2.17	0.58
4:K:253:THR:OG1	4:K:256:GLU:HG3	2.04	0.58
1:A:35:SER:HA	1:A:80:ARG:NH1	2.19	0.58
1:C:107:ARG:NH1	1:C:111:ARG:HG3	2.18	0.58
2:D:175:GLN:OE1	2:D:178:ASN:ND2	2.35	0.57
4:F:278:VAL:HG22	3:J:98:GLN:NE2	2.20	0.57
2:B:1:ASP:HB3	2:B:115:TRP:CE2	2.39	0.57
3:J:46:SER:HB3	4:K:313:CYS:SG	2.45	0.57
4:F:152:VAL:HB	4:K:152:VAL:HG21	1.86	0.57
3:G:40:VAL:HG11	3:G:42:LYS:HE2	1.86	0.57
1:C:36:SER:HA	4:K:465:LYS:HZ2	1.69	0.57
4:K:426:ASN:OD1	4:K:427:LYS:N	2.38	0.57
1:C:114:ASP:O	1:C:115:LEU:HD13	2.05	0.57
2:D:38:TRP:CH2	4:I:269:ASP:N	2.73	0.57
2:B:99:PHE:CE1	2:B:126:ILE:HG12	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TYR:CE1	1:C:112:THR:HG21	2.39	0.57
3:G:46:SER:HB3	4:I:313:CYS:SG	2.46	0.56
1:A:165:VAL:HG23	1:A:215:HIS:HB2	1.87	0.56
1:A:5:VAL:N	1:A:117:TYR:HH	2.03	0.56
4:I:374:THR:HG21	4:K:404:SER:HB3	1.86	0.56
4:I:171:LEU:HD23	4:K:513:LEU:HD11	1.87	0.56
4:I:297:LEU:HD12	4:I:298:ALA:H	1.70	0.56
4:F:226:LYS:HE2	3:J:81:GLN:NE2	2.21	0.56
4:K:251:MET:HG3	4:K:299:TYR:CE1	2.40	0.56
3:J:36:THR:HB	4:K:336:ARG:HD2	1.87	0.56
4:I:261:ILE:HG12	4:I:264:MET:HE1	1.87	0.56
2:D:38:TRP:CH2	4:I:269:ASP:OD1	2.59	0.56
3:J:90:VAL:HG11	4:K:294:GLU:HG2	1.88	0.56
1:C:103:TYR:HE1	2:D:49:ALA:HA	1.71	0.55
2:L:10:THR:HG22	2:L:123:LYS:HB3	1.87	0.55
1:H:186:GLN:HA	2:L:180:GLN:HE22	1.71	0.55
4:I:334:LEU:HB3	4:I:395:ILE:HD11	1.88	0.55
2:B:156:LEU:HD22	2:B:195:LEU:HD13	1.87	0.55
4:F:161:GLU:HA	4:K:160:LEU:HD21	1.88	0.55
4:K:269:ASP:OD1	2:L:38:TRP:CH2	2.60	0.55
1:A:186:GLN:HA	2:B:180:GLN:HE22	1.72	0.55
1:C:111(A):ALA:HB2	4:I:258:LEU:HD22	1.89	0.55
1:A:134:PRO:HB3	1:A:160:TYR:HB3	1.89	0.55
2:B:156:LEU:HB2	2:B:195:LEU:HB3	1.89	0.55
1:C:91:MET:HB3	1:C:94:LEU:HD21	1.88	0.54
4:I:311:THR:HG23	4:I:344:ASP:HB2	1.90	0.54
4:I:422:CYS:HB3	4:I:452:VAL:HG22	1.89	0.54
2:D:160:TYR:CD2	2:D:161:PRO:HA	2.42	0.54
2:B:38:TRP:HH2	4:F:269:ASP:OD1	1.90	0.54
2:D:99:PHE:CE1	2:D:126:ILE:HG12	2.42	0.54
2:D:38:TRP:CZ3	4:I:269:ASP:OD1	2.59	0.54
4:F:475:ILE:CD1	3:J:65:LYS:HE2	2.37	0.54
1:H:107:ARG:NH1	1:H:111:ARG:HG3	2.22	0.54
3:J:28:ILE:HD11	4:K:363:ASN:HA	1.88	0.54
1:C:36:SER:O	1:C:37:LYS:HG3	2.07	0.54
3:G:64:ILE:HD12	3:G:79:ILE:HG23	1.90	0.54
1:A:215:HIS:CE1	1:A:218:SER:HG	2.23	0.54
1:A:103:TYR:HE1	2:B:49:ALA:HA	1.73	0.53
1:A:203:SER:HB2	1:A:206:THR:HB	1.90	0.53
4:K:338:ASP:HB2	4:K:342:TYR:OH	2.08	0.53
3:E:40:VAL:HG22	4:F:316:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:ARG:NH1	2:B:190:ASP:O	2.41	0.53
4:I:204:LEU:HD22	4:K:481:LEU:O	2.08	0.53
3:E:46:SER:OG	4:F:311:THR:HB	2.08	0.53
1:H:114:ASP:N	1:H:114:ASP:OD1	2.41	0.53
2:L:41:TRP:CZ3	2:L:104:CYS:HB3	2.43	0.53
2:D:178:ASN:HD22	2:D:201:LEU:HD21	1.74	0.53
1:A:6:GLU:OE1	1:A:120:GLN:N	2.42	0.53
1:A:136:VAL:HG21	1:A:213:VAL:HG21	1.89	0.53
4:F:374:THR:HG21	4:I:404:SER:HB3	1.91	0.53
1:H:91:MET:HB3	1:H:94:LEU:HD21	1.91	0.53
4:I:505:PHE:HB2	4:K:177:ALA:HB2	1.91	0.53
4:K:266:ILE:HD12	4:K:270:GLN:HB2	1.91	0.53
2:B:75:ARG:CZ	2:B:95:GLN:HG3	2.38	0.52
1:C:113:GLY:HA2	2:D:116:TRP:CZ2	2.44	0.52
4:F:182:SER:OG	4:K:181:LEU:HD13	2.09	0.52
2:B:7:SER:OG	2:B:22:THR:OG1	2.27	0.52
1:C:159:ASP:OD1	1:C:186:GLN:NE2	2.42	0.52
4:K:269:ASP:OD1	2:L:38:TRP:HH2	1.92	0.52
4:F:318:THR:CG2	4:F:336:ARG:HB2	2.38	0.52
2:D:99:PHE:CD1	2:D:126:ILE:HG12	2.45	0.52
3:E:51:GLY:HA3	4:I:458:TYR:HB2	1.91	0.52
2:L:128:ARG:NH1	2:L:192:THR:HG23	2.25	0.52
2:L:169:LYS:HE2	2:L:172:ASN:HA	1.92	0.52
1:A:159:ASP:OD1	1:A:186:GLN:NE2	2.43	0.52
4:F:336:ARG:NH1	4:F:383:ASN:OD1	2.39	0.52
2:D:109:THR:HG22	2:D:113:TYR:CD2	2.45	0.51
4:F:152:VAL:HG13	4:I:149:ALA:HB3	1.92	0.51
4:F:219:THR:OG1	4:I:476:ASN:HB3	2.10	0.51
4:I:290:SER:OG	4:I:291:ILE:N	2.43	0.51
1:C:112(A):THR:HG22	2:D:38:TRP:HE1	1.75	0.51
1:A:112:THR:CB	4:F:271:LYS:HZ3	2.24	0.51
4:F:416:CYS:O	4:F:437:ASN:HA	2.10	0.51
2:D:160:TYR:CG	2:D:161:PRO:HA	2.45	0.51
4:K:321:LEU:O	4:K:333:CYS:HA	2.11	0.51
3:G:59:ILE:HG23	4:K:469:VAL:HB	1.92	0.51
4:F:426:ASN:OD1	4:F:427:LYS:N	2.44	0.51
1:H:99:THR:HG23	1:H:125:THR:HA	1.92	0.51
3:E:65:LYS:HE2	4:I:475:ILE:CD1	2.41	0.51
1:C:154:GLY:HA3	1:C:196:VAL:HG12	1.93	0.51
1:C:113:GLY:HA3	2:D:107:TYR:CD1	2.45	0.51
4:I:410:LEU:HA	4:I:444:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:470:LYS:HE2	3:J:60:GLU:OE2	2.10	0.51
2:B:113:TYR:H	2:B:113:TYR:HD2	1.59	0.51
1:C:203:SER:HB2	1:C:206:THR:HB	1.93	0.51
3:E:53:TYR:HB2	4:F:305:LEU:HD11	1.91	0.51
1:H:113:GLY:HA2	2:L:116:TRP:CZ2	2.46	0.51
4:F:193:LEU:HD13	4:I:492:ILE:HG21	1.92	0.51
4:F:232:GLU:OE1	4:K:235:ARG:NH1	2.44	0.51
4:F:273:LEU:HD11	4:F:364:ARG:HG2	1.92	0.50
3:G:46:SER:OG	4:I:311:THR:HB	2.11	0.50
4:I:426:ASN:OD1	4:I:427:LYS:N	2.44	0.50
2:B:126:ILE:O	2:B:160:TYR:OH	2.29	0.50
4:F:246:PRO:HB3	4:F:283:GLN:HA	1.93	0.50
4:F:311:THR:HG23	4:F:344:ASP:HB2	1.93	0.50
4:I:152:VAL:CG1	4:K:152:VAL:HB	2.40	0.50
3:J:84:ASP:O	3:J:88:ASN:HB3	2.11	0.50
3:J:38:SER:HB3	4:K:318:THR:HG22	1.93	0.50
4:F:214:ILE:HD11	4:K:214:ILE:HD11	1.93	0.50
2:B:38:TRP:CH2	4:F:269:ASP:OD1	2.64	0.50
4:K:311:THR:HG23	4:K:344:ASP:HB2	1.94	0.50
4:K:264:MET:HE3	4:K:266:ILE:HD11	1.94	0.50
4:I:233:ILE:HD13	4:I:299:TYR:CE2	2.47	0.50
4:K:266:ILE:HD12	4:K:270:GLN:CB	2.41	0.50
2:B:144:GLN:HG2	2:B:149:THR:O	2.12	0.50
4:F:352:PHE:CD1	4:F:372:SER:HB3	2.46	0.50
3:J:49:ARG:NH1	3:J:52:TRP:CE2	2.80	0.50
2:B:140:PRO:HD3	2:B:152:VAL:HG22	1.94	0.49
2:D:181:GLU:HG2	2:D:197:SER:HB2	1.95	0.49
4:F:177:ALA:HB2	4:K:505:PHE:HB2	1.94	0.49
2:D:36:SER:HB2	2:D:38:TRP:CE3	2.47	0.49
2:D:96:PRO:HA	2:D:99:PHE:HD2	1.75	0.49
4:K:320:PRO:HA	4:K:334:LEU:O	2.11	0.49
2:B:204:ALA:O	2:B:208:LYS:HG3	2.12	0.49
1:C:201:SER:HA	1:C:204:LEU:HG	1.94	0.49
4:I:297:LEU:HD12	4:I:298:ALA:N	2.27	0.49
4:I:321:LEU:HB3	4:I:334:LEU:HB2	1.95	0.49
4:I:449:THR:HG23	4:I:456:LEU:HD11	1.94	0.49
4:K:318:THR:H	4:K:339:ARG:HD3	1.78	0.49
4:K:334:LEU:HD22	4:K:395:ILE:CD1	2.42	0.49
1:A:101:VAL:HG12	1:A:103:TYR:HE2	1.77	0.49
2:D:126:ILE:HD12	2:D:191:SER:HB3	1.95	0.49
4:K:318:THR:CG2	4:K:336:ARG:HB2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:SER:OG	2:D:234:CYS:SG	2.71	0.49
4:F:465:LYS:HZ1	1:H:36:SER:HA	1.78	0.49
1:C:63:GLY:O	1:C:65:THR:HG23	2.12	0.49
4:I:346:ALA:HB2	4:K:455:THR:HG23	1.95	0.49
2:L:160:TYR:CG	2:L:161:PRO:HA	2.48	0.49
2:B:41:TRP:CZ3	2:B:104:CYS:HB3	2.47	0.48
2:D:162:ARG:HB2	2:D:193:TYR:CZ	2.48	0.48
3:E:32:PHE:CE2	3:E:34:GLN:HG2	2.48	0.48
1:C:112(A):THR:O	4:I:262:ASN:ND2	2.46	0.48
1:H:174:LEU:HD21	1:H:197:VAL:HG21	1.95	0.48
4:I:206:ILE:HD13	4:I:209:LYS:HD2	1.93	0.48
1:C:111(A):ALA:HA	4:I:262:ASN:OD1	2.14	0.48
4:F:252:LEU:O	4:F:282:ARG:NH1	2.43	0.48
3:J:97:MET:SD	4:K:292:ILE:HG22	2.52	0.48
4:F:426:ASN:ND2	4:F:429:ARG:HD2	2.28	0.48
1:H:39:MET:HE2	1:H:87:LEU:HB3	1.95	0.48
4:K:416:CYS:O	4:K:437:ASN:HA	2.14	0.48
3:E:92:GLU:HA	3:E:95:LEU:HD12	1.94	0.48
4:K:243:VAL:HG22	4:K:288:ILE:HG23	1.95	0.48
4:K:400:THR:HG22	4:K:401:ASP:N	2.29	0.48
2:D:105:GLN:HB2	2:D:118:PHE:CD1	2.49	0.48
3:E:64:ILE:HG12	3:E:83:LEU:HD21	1.95	0.48
1:H:201:SER:HA	1:H:204:LEU:HG	1.96	0.48
4:I:314:TRP:HZ2	4:I:380:ASN:HD21	1.58	0.48
1:A:5:VAL:N	1:A:117:TYR:OH	2.47	0.48
4:F:297:LEU:HD12	4:F:298:ALA:H	1.79	0.48
4:F:368:ASP:OD2	4:F:370:MET:HE2	2.13	0.48
2:L:99:PHE:CD1	2:L:126:ILE:HG12	2.49	0.48
3:E:36:THR:HB	4:F:336:ARG:HD2	1.96	0.47
4:F:338:ASP:HB3	4:F:394:LYS:HE3	1.95	0.47
4:I:425:SER:HA	4:I:431:ILE:HA	1.95	0.47
1:A:107:ARG:NH1	1:A:111:ARG:HG3	2.30	0.47
2:B:104:CYS:O	2:B:119:GLY:N	2.36	0.47
2:L:156:LEU:HD22	2:L:195:LEU:HD13	1.97	0.47
2:D:67:LEU:HD21	2:D:71:VAL:HB	1.95	0.47
3:G:60:GLU:HA	4:I:296:VAL:HG23	1.97	0.47
3:G:66:GLU:HA	3:G:79:ILE:HG21	1.95	0.47
1:H:111(A):ALA:HA	4:K:262:ASN:OD1	2.13	0.47
2:D:39:LEU:HA	2:D:105:GLN:O	2.15	0.47
4:I:238:SER:HB3	4:K:249:THR:OG1	2.14	0.47
1:C:5:VAL:N	1:C:24:ALA:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:90:VAL:HG22	4:F:292:ILE:HD11	1.96	0.47
4:F:150:SER:HB2	4:F:151:GLY:HA2	1.97	0.47
3:E:36:THR:HG22	4:F:386:ILE:CG1	2.45	0.47
4:K:422:CYS:HB3	4:K:452:VAL:HG22	1.97	0.47
1:H:210:ILE:HG12	1:H:225:ARG:HG2	1.97	0.47
4:I:321:LEU:O	4:I:334:LEU:N	2.39	0.47
4:I:341:TRP:CZ2	4:I:360:VAL:HG21	2.50	0.47
4:F:506:ILE:HD11	4:K:178:VAL:HG11	1.97	0.47
4:K:267:THR:HB	2:L:109:THR:HG22	1.97	0.47
2:B:206:TYR:O	2:B:212:TYR:OH	2.30	0.47
4:F:337:THR:HG21	4:F:396:MET:HB2	1.97	0.47
4:I:231:LEU:HD23	4:I:231:LEU:HA	1.67	0.47
4:I:481:LEU:HD22	4:K:206:ILE:HG13	1.96	0.47
2:B:165:LYS:HB3	2:B:217:THR:OG1	2.15	0.47
4:F:153:ALA:HB1	4:F:156:LYS:HB3	1.97	0.46
1:C:107:ARG:HA	1:C:116:ASP:OD1	2.15	0.46
3:E:50:THR:HB	4:I:457:TYR:HA	1.98	0.46
4:K:485:SER:O	4:K:489:ASP:N	2.42	0.46
2:D:206:TYR:O	2:D:212:TYR:OH	2.31	0.46
4:I:160:LEU:HD21	4:K:161:GLU:HB2	1.96	0.46
2:L:14:SER:OG	2:L:127:LYS:HB2	2.16	0.46
2:D:99:PHE:CZ	2:D:126:ILE:HG23	2.50	0.46
3:E:44:TYR:HB2	4:F:313:CYS:HB2	1.98	0.46
4:F:226:LYS:HE2	3:J:81:GLN:HE22	1.79	0.46
4:I:171:LEU:HG	4:I:171:LEU:O	2.15	0.46
4:I:318:THR:CG2	4:I:336:ARG:HB2	2.45	0.46
4:I:334:LEU:HD22	4:I:395:ILE:HD13	1.97	0.46
4:K:268:ASN:HB2	2:L:108:ASN:O	2.16	0.46
4:F:404:SER:HB3	4:K:374:THR:HG21	1.97	0.46
2:B:127:LYS:HA	2:B:160:TYR:OH	2.16	0.46
2:B:215:GLU:HG2	2:B:226:THR:OG1	2.16	0.46
4:F:266:ILE:HD12	4:F:270:GLN:CB	2.46	0.46
4:K:474:ILE:HG12	4:K:474:ILE:H	1.52	0.46
4:F:152:VAL:HG11	4:I:152:VAL:CG2	2.45	0.46
3:E:37:CYS:SG	4:F:319:SER:HB3	2.55	0.46
4:I:195:LEU:HD23	4:I:195:LEU:HA	1.68	0.45
4:I:252:LEU:O	4:I:282:ARG:NH1	2.45	0.45
3:J:36:THR:HG22	4:K:386:ILE:HG12	1.97	0.45
1:H:181:PHE:CZ	2:L:196:SER:HB3	2.51	0.45
2:L:41:TRP:CE2	2:L:89:LEU:HB2	2.50	0.45
2:B:213:ALA:HB2	2:B:228:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:THR:HG22	2:D:113:TYR:HD2	1.82	0.45
2:L:43:GLN:O	2:L:51:LYS:N	2.41	0.45
4:F:346:ALA:HB2	4:I:455:THR:HG23	1.97	0.45
4:K:297:LEU:HD12	4:K:298:ALA:H	1.82	0.45
4:K:352:PHE:CE1	4:K:372:SER:HB3	2.52	0.45
2:D:128:ARG:NH1	2:D:192:THR:HG23	2.31	0.45
4:F:334:LEU:HD22	4:F:395:ILE:HD13	1.99	0.45
1:H:183:ALA:HA	1:H:193:LEU:HB3	1.98	0.45
2:B:39:LEU:HA	2:B:105:GLN:O	2.16	0.45
4:F:161:GLU:HG3	4:K:160:LEU:HD11	1.99	0.45
4:F:476:ASN:ND2	3:J:67:ASN:HB2	2.32	0.45
4:K:191:LYS:HA	4:K:191:LYS:HD3	1.59	0.45
3:G:64:ILE:HG22	4:K:474:ILE:HG13	1.98	0.45
2:B:128:ARG:NH1	2:B:192:THR:HG23	2.32	0.45
2:D:96:PRO:HA	2:D:99:PHE:CE2	2.51	0.45
1:C:6:GLU:OE2	1:C:103:TYR:HA	2.17	0.45
4:I:219:THR:OG1	4:K:476:ASN:HB3	2.17	0.45
3:E:97:MET:O	3:E:98:GLN:HG3	2.17	0.45
4:K:508:LYS:O	4:K:512:LEU:HD13	2.15	0.45
4:I:351:PHE:O	4:I:353:PRO:HD3	2.17	0.44
3:J:44:TYR:HB2	4:K:313:CYS:HB2	1.99	0.44
4:K:352:PHE:CD1	4:K:372:SER:HB3	2.52	0.44
1:H:184:VAL:HG11	2:L:180:GLN:HB3	1.99	0.44
2:L:151:SER:HA	2:L:199:LEU:O	2.16	0.44
4:F:252:LEU:CD2	4:F:301:VAL:HG11	2.48	0.44
1:H:45:ALA:HB3	1:H:48:LYS:HB2	1.99	0.44
4:F:476:ASN:HB3	4:K:219:THR:OG1	2.16	0.44
1:A:66:TYR:CE1	2:B:113:TYR:HD1	2.36	0.44
1:H:181:PHE:HA	2:L:184:THR:HG22	1.99	0.44
1:A:44:GLN:HG3	1:A:49:GLY:O	2.17	0.44
1:A:103:TYR:CE1	2:B:49:ALA:HA	2.53	0.44
1:C:67:TYR:OH	1:C:78:ILE:HG22	2.17	0.44
1:H:12:LEU:HA	1:H:125:THR:O	2.16	0.44
1:C:75:ARG:HB3	1:C:92:ASN:O	2.17	0.44
4:I:266:ILE:HD12	4:I:270:GLN:CB	2.45	0.44
4:I:386:ILE:HD13	4:I:395:ILE:CD1	2.48	0.44
1:H:186:GLN:HG2	2:L:180:GLN:OE1	2.18	0.44
1:H:150:THR:HB	1:H:199:VAL:O	2.18	0.44
4:F:150:SER:HB3	4:F:154:VAL:HG11	2.00	0.44
4:I:196:LYS:C	4:I:196:LYS:HD3	2.38	0.44
4:K:150:SER:HB2	4:K:151:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:455:THR:HG21	4:K:345:ASN:OD1	2.18	0.44
4:I:407:ILE:HD11	4:I:457:TYR:HB3	1.99	0.44
4:F:252:LEU:HD22	4:F:301:VAL:HG21	1.99	0.43
4:F:497:GLU:O	4:F:497:GLU:HG2	2.17	0.43
4:I:290:SER:HB3	4:I:300:VAL:HG23	2.00	0.43
1:A:36:SER:HA	4:I:465:LYS:HZ2	1.81	0.43
1:C:57:TYR:HE1	1:C:112:THR:HG21	1.83	0.43
2:D:67:LEU:CD2	2:D:71:VAL:HB	2.48	0.43
4:F:499:ILE:HD11	4:K:185:VAL:HG12	2.00	0.43
4:I:309:ILE:CG2	4:I:310:ASP:N	2.80	0.43
3:J:68:LYS:O	3:J:69:CYS:HB3	2.17	0.43
2:B:43:GLN:HB2	2:B:53:LEU:HD21	2.00	0.43
4:F:235:ARG:NH1	4:I:232:GLU:OE2	2.51	0.43
4:I:416:CYS:O	4:I:437:ASN:HA	2.18	0.43
1:C:116:ASP:OD1	1:C:116:ASP:N	2.51	0.43
1:C:165:VAL:HG23	1:C:215:HIS:HB2	2.00	0.43
3:J:49:ARG:NH1	3:J:52:TRP:NE1	2.67	0.43
3:J:48:LEU:O	3:J:50:THR:HG23	2.18	0.43
1:A:183:ALA:HB2	1:A:193:LEU:HD23	1.99	0.43
2:D:38:TRP:HZ2	4:I:268:ASN:O	1.97	0.43
1:H:212:ASN:ND2	1:H:223:ASP:OD1	2.51	0.43
4:F:161:GLU:CA	4:K:160:LEU:HD21	2.49	0.43
1:A:6:GLU:CD	1:A:121:GLY:H	2.22	0.43
4:F:195:LEU:HA	4:F:195:LEU:HD23	1.57	0.43
3:G:38:SER:HB3	4:I:318:THR:HG22	2.00	0.43
1:H:57:TYR:HE1	1:H:112:THR:HG21	1.83	0.43
4:K:252:LEU:HA	4:K:252:LEU:HD12	1.81	0.43
2:B:44:GLN:O	2:B:100:ALA:HB1	2.18	0.43
2:B:109:THR:HG22	4:F:267:THR:HA	2.01	0.43
2:B:1:ASP:HB3	2:B:115:TRP:CD2	2.54	0.43
1:C:13:ILE:HD12	1:C:14:GLN:H	1.84	0.43
4:I:477:PHE:CD2	4:I:477:PHE:C	2.91	0.43
1:A:207:GLN:HB3	1:A:209:TYR:CZ	2.54	0.43
4:F:217:ILE:HD13	4:I:217:ILE:CG2	2.49	0.43
1:A:111(A):ALA:HA	4:F:262:ASN:OD1	2.18	0.43
4:F:217:ILE:HD11	4:I:218:GLU:HG3	2.00	0.43
3:J:46:SER:OG	4:K:311:THR:HB	2.19	0.43
2:B:128:ARG:HH12	2:B:192:THR:HG23	1.84	0.43
2:D:43:GLN:O	2:D:51:LYS:N	2.45	0.43
3:E:81:GLN:HE22	4:I:226:LYS:HE2	1.84	0.42
4:F:364:ARG:HD3	4:F:364:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:481:LEU:HD12	4:K:481:LEU:HA	1.70	0.42
1:C:6:GLU:OE1	1:C:120:GLN:N	2.53	0.42
2:D:175:GLN:HB3	2:D:178:ASN:OD1	2.19	0.42
3:E:83:LEU:HA	3:E:83:LEU:HD23	1.84	0.42
1:A:114:ASP:O	1:A:115:LEU:HD13	2.19	0.42
4:F:483:PHE:HD1	4:I:198:TYR:CE2	2.38	0.42
3:E:93:LEU:HD11	4:F:238:SER:OG	2.20	0.42
4:K:181:LEU:O	4:K:181:LEU:HG	2.20	0.42
4:K:410:LEU:HA	4:K:444:ASN:ND2	2.34	0.42
3:G:30:GLU:HG3	3:G:40:VAL:O	2.20	0.42
1:H:67:TYR:CE1	1:H:78:ILE:HG22	2.54	0.42
1:H:161:PHE:HA	1:H:162:PRO:HA	1.81	0.42
1:H:50:LEU:O	2:L:118:PHE:HB2	2.20	0.42
2:L:160:TYR:CD2	2:L:161:PRO:HA	2.55	0.42
2:L:204:ALA:O	2:L:208:LYS:HG3	2.19	0.42
4:F:375:LEU:HD13	4:F:379:VAL:HG11	2.02	0.42
1:A:116:ASP:OD1	1:A:116:ASP:N	2.50	0.42
1:H:23:CYS:HB3	1:H:87:LEU:HD23	2.00	0.42
4:I:217:ILE:HD13	4:K:217:ILE:HG21	2.02	0.42
4:I:273:LEU:HD11	4:I:364:ARG:HG2	2.02	0.42
2:L:99:PHE:CZ	2:L:126:ILE:HG23	2.55	0.42
2:D:71:VAL:HG12	2:D:72:PRO:HD2	2.01	0.42
1:H:114:ASP:O	1:H:115:LEU:HD13	2.20	0.42
4:I:203:LEU:HG	4:I:203:LEU:O	2.19	0.42
4:I:264:MET:O	4:I:266:ILE:N	2.53	0.42
1:H:39:MET:HB2	1:H:87:LEU:HD13	2.02	0.41
4:I:264:MET:HE3	4:I:266:ILE:CD1	2.49	0.41
4:I:334:LEU:HA	4:I:334:LEU:HD23	1.65	0.41
3:J:83:LEU:HA	3:J:83:LEU:HD23	1.85	0.41
1:A:37:LYS:HD3	1:A:107:ARG:O	2.19	0.41
2:B:181:GLU:HG2	2:B:197:SER:HB2	2.02	0.41
1:H:200:PRO:HG2	1:H:203:SER:OG	2.21	0.41
4:I:150:SER:HB2	4:I:151:GLY:HA2	2.02	0.41
4:I:400:THR:HG22	4:I:401:ASP:N	2.35	0.41
4:F:455:THR:HG23	4:K:346:ALA:HB2	2.02	0.41
4:F:191:LYS:HA	4:F:191:LYS:HD3	1.68	0.41
4:F:503:LEU:HA	4:F:503:LEU:HD23	1.85	0.41
3:E:65:LYS:HE2	4:I:475:ILE:HD11	2.02	0.41
3:J:33:TYR:O	3:J:37:CYS:N	2.53	0.41
4:K:400:THR:HG22	4:K:401:ASP:H	1.85	0.41
2:D:41:TRP:CD2	2:D:89:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:37:CYS:SG	4:I:319:SER:HB3	2.61	0.41
4:I:505:PHE:CB	4:K:177:ALA:HB2	2.50	0.41
2:B:41:TRP:CD2	2:B:89:LEU:HB2	2.55	0.41
2:D:6:GLN:HB2	2:D:120:GLN:NE2	2.35	0.41
2:D:217:THR:HG22	2:D:224:PRO:HG3	2.02	0.41
4:F:208:ASN:HD21	4:I:481:LEU:H	1.69	0.41
4:K:198:TYR:O	4:K:202:GLN:HB2	2.20	0.41
2:B:21:ILE:HD13	2:B:122:THR:HB	2.03	0.41
4:K:232:GLU:O	4:K:233:ILE:C	2.59	0.41
4:K:315:LYS:HD2	4:K:341:TRP:CZ2	2.55	0.41
4:I:204:LEU:CD2	4:K:481:LEU:HB3	2.51	0.41
4:K:158:LEU:HD23	4:K:161:GLU:OE2	2.21	0.41
3:J:45:LEU:HA	4:K:311:THR:O	2.20	0.41
4:F:166:LYS:HZ2	4:K:514:GLY:HA3	1.83	0.41
3:E:53:TYR:CD2	4:F:264:MET:HG2	2.56	0.41
4:F:400:THR:HG22	4:F:401:ASP:N	2.36	0.41
1:A:45:ALA:HB3	1:A:48:LYS:HB2	2.03	0.41
1:C:137:PHE:HB3	2:D:141:SER:OG	2.21	0.41
2:D:190:ASP:OD1	2:D:191:SER:N	2.54	0.41
4:F:252:LEU:HD22	4:F:301:VAL:HG11	2.02	0.41
2:L:140:PRO:HD3	2:L:152:VAL:HG22	2.02	0.41
2:L:126:ILE:HD12	2:L:191:SER:HB3	2.03	0.41
1:A:131:THR:HG21	1:A:217:PRO:O	2.21	0.41
4:F:261:ILE:HA	4:F:264:MET:HE2	2.03	0.41
1:H:153:LEU:HB2	1:H:226:VAL:HG11	2.03	0.41
4:K:321:LEU:HB3	4:K:334:LEU:HB2	2.03	0.41
4:K:334:LEU:HD13	4:K:386:ILE:HD12	2.03	0.41
2:B:98:ASP:HB3	2:B:102:TYR:OH	2.20	0.41
1:C:138:PRO:O	2:D:141:SER:HB3	2.21	0.41
1:H:153:LEU:HD21	1:H:209:TYR:CD2	2.56	0.41
4:K:273:LEU:HD11	4:K:364:ARG:HG2	2.03	0.41
2:B:168:TRP:CE2	2:B:199:LEU:HB2	2.57	0.40
4:F:334:LEU:HD23	4:F:334:LEU:HA	1.82	0.40
4:F:505:PHE:CB	4:I:177:ALA:HB2	2.51	0.40
4:I:191:LYS:HD3	4:I:191:LYS:HA	1.78	0.40
4:F:181:LEU:HD23	4:K:181:LEU:CD2	2.51	0.40
1:A:181:PHE:CD2	2:B:184:THR:HG23	2.57	0.40
2:D:128:ARG:NH2	2:D:129:THR:O	2.51	0.40
2:D:83:SER:HA	2:D:87:PHE:CE1	2.56	0.40
4:F:378:GLU:OE1	4:I:400:THR:HG21	2.22	0.40
4:K:503:LEU:HD23	4:K:503:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HA	1:A:116:ASP:OD1	2.21	0.40
2:B:38:TRP:CE2	4:F:268:ASN:HB3	2.56	0.40
1:C:215:HIS:ND1	1:C:218:SER:OG	2.49	0.40
2:D:7:SER:OG	2:D:22:THR:OG1	2.39	0.40
4:F:341:TRP:CZ3	4:F:365:VAL:HG21	2.56	0.40
4:I:167:ILE:CD1	4:K:164:VAL:HG13	2.52	0.40
4:I:386:ILE:HD13	4:I:395:ILE:HD12	2.04	0.40
2:L:181:GLU:CD	2:L:195:LEU:HD21	2.41	0.40
1:H:6:GLU:HA	1:H:22:SER:O	2.21	0.40
4:I:320:PRO:HA	4:I:334:LEU:O	2.21	0.40
2:B:106:GLN:HE21	2:B:117:THR:N	2.19	0.40
1:C:52:TRP:HB3	2:D:116:TRP:O	2.22	0.40
4:F:160:LEU:HD21	4:I:161:GLU:HB2	2.03	0.40
4:F:477:PHE:CD2	4:F:477:PHE:C	2.94	0.40
3:G:53:TYR:CE1	4:K:464:GLY:HA3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLN:OE1	1:C:20:ARG:NH1[8_554]	2.13	0.07

## 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	218/224 (97%)	198 (91%)	20 (9%)	0	100	100
1	C	218/224 (97%)	199 (91%)	19 (9%)	0	100	100
1	H	218/224 (97%)	199 (91%)	19 (9%)	0	100	100
2	B	213/218 (98%)	198 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	213/218 (98%)	198 (93%)	13 (6%)	2 (1%)	17	55
2	L	213/218 (98%)	198 (93%)	15 (7%)	0	100	100
3	E	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	11	46
3	G	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	11	46
3	J	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	11	46
4	F	354/394 (90%)	333 (94%)	21 (6%)	0	100	100
4	I	354/394 (90%)	334 (94%)	20 (6%)	0	100	100
4	K	354/394 (90%)	332 (94%)	21 (6%)	1 (0%)	41	75
All	All	2568/2727 (94%)	2384 (93%)	178 (7%)	6 (0%)	47	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	69	CYS
3	J	69	CYS
3	E	69	CYS
4	K	153	ALA
2	D	233	GLU
2	D	231	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/187 (98%)	178 (97%)	5 (3%)	44	66
1	C	183/187 (98%)	174 (95%)	9 (5%)	25	52
1	H	183/187 (98%)	177 (97%)	6 (3%)	38	62
2	B	190/193 (98%)	187 (98%)	3 (2%)	62	79
2	D	190/193 (98%)	183 (96%)	7 (4%)	34	60
2	L	190/193 (98%)	187 (98%)	3 (2%)	62	79
3	E	66/66 (100%)	63 (96%)	3 (4%)	27	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	66/66 (100%)	63 (96%)	3 (4%)	27	54
3	J	66/66 (100%)	63 (96%)	3 (4%)	27	54
4	F	329/362 (91%)	309 (94%)	20 (6%)	18	47
4	I	329/362 (91%)	306 (93%)	23 (7%)	15	42
4	K	329/362 (91%)	310 (94%)	19 (6%)	20	48
All	All	2304/2424 (95%)	2200 (96%)	104 (4%)	27	54

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	56	ILE
1	A	87	LEU
1	A	114	ASP
1	A	146	THR
2	B	39	LEU
2	B	107	TYR
2	B	115	TRP
1	C	29	THR
1	C	40	THR
1	C	56	ILE
1	C	82	ASN
1	C	87	LEU
1	C	103	TYR
1	C	114	ASP
1	C	128	SER
1	C	146	THR
2	D	39	LEU
2	D	107	TYR
2	D	109	THR
2	D	115	TRP
2	D	183	VAL
2	D	184	THR
2	D	186	GLN
3	E	30	GLU
3	E	88	ASN
3	E	90	VAL
4	F	148	ILE
4	F	154	VAL
4	F	195	LEU

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Mol	Chain	Res	Type
4	F	211	SER
4	F	244	THR
4	F	252	LEU
4	F	338	ASP
4	F	345	ASN
4	F	361	GLN
4	F	377	SER
4	F	398	SER
4	F	401	ASP
4	F	403	SER
4	F	422	CYS
4	F	449	THR
4	F	472	GLU
4	F	474	ILE
4	F	476	ASN
4	F	477	PHE
4	F	485	SER
3	G	30	GLU
3	G	88	ASN
3	G	90	VAL
1	H	25	VAL
1	H	29	THR
1	H	87	LEU
1	H	103	TYR
1	H	112(A)	THR
1	H	146	THR
4	I	195	LEU
4	I	204	LEU
4	I	211	SER
4	I	244	THR
4	I	252	LEU
4	I	255	SER
4	I	288	ILE
4	I	289	MET
4	I	338	ASP
4	I	345	ASN
4	I	361	GLN
4	I	377	SER
4	I	398	SER
4	I	401	ASP
4	I	403	SER
4	I	416	CYS

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Mol	Chain	Res	Type
4	I	422	CYS
4	I	440	ASP
4	I	472	GLU
4	I	474	ILE
4	I	476	ASN
4	I	477	PHE
4	I	485	SER
3	J	30	GLU
3	J	88	ASN
3	J	90	VAL
4	K	195	LEU
4	K	204	LEU
4	K	211	SER
4	K	234	THR
4	K	244	THR
4	K	252	LEU
4	K	288	ILE
4	K	338	ASP
4	K	361	GLN
4	K	377	SER
4	K	398	SER
4	K	401	ASP
4	K	403	SER
4	K	422	CYS
4	K	449	THR
4	K	474	ILE
4	K	476	ASN
4	K	477	PHE
4	K	485	SER
2	L	39	LEU
2	L	115	TRP
2	L	186	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	GLN
2	D	180	GLN
3	E	26	GLN
3	E	81	GLN
4	F	345	ASN
4	F	380	ASN

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Mol	Chain	Res	Type
3	G	26	GLN
3	G	81	GLN
4	I	225	GLN
3	J	26	GLN
3	J	81	GLN
2	L	6	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 carbohydrates 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/224 (98%)	0.32	15 (6%) 17 14	125, 169, 259, 296	0
1	C	220/224 (98%)	-0.04	5 (2%) 60 51	71, 108, 207, 239	0
1	H	220/224 (98%)	1.56	63 (28%) 0 0	162, 259, 353, 380	0
2	B	215/218 (98%)	0.52	11 (5%) 28 24	130, 208, 264, 282	0
2	D	215/218 (98%)	0.04	5 (2%) 60 51	86, 143, 209, 223	0
2	L	215/218 (98%)	1.80	85 (39%) 0 0	167, 277, 375, 387	0
3	E	73/73 (100%)	-0.18	0 100 100	82, 108, 139, 163	0
3	G	73/73 (100%)	-0.22	0 100 100	79, 102, 128, 162	0
3	J	73/73 (100%)	-0.29	0 100 100	86, 110, 143, 169	0
4	F	358/394 (90%)	-0.06	5 (1%) 75 66	74, 109, 145, 185	0
4	I	358/394 (90%)	-0.13	4 (1%) 80 72	72, 97, 137, 195	0
4	K	358/394 (90%)	-0.17	0 100 100	76, 99, 133, 170	0
All	All	2598/2727 (95%)	0.28	193 (7%) 14 12	71, 125, 323, 387	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	147	ALA	7.2
4	I	149	ALA	6.5
1	H	228	PRO	6.5
2	L	216	VAL	5.7
2	L	142	ASP	5.7
1	A	205	GLY	5.6
1	H	148	GLY	5.6
1	H	229	LYS	5.6
2	L	134	SER	5.3
2	L	165	LYS	5.2
2	L	132	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	145	SER	5.2
1	H	227	GLU	5.1
2	L	166	VAL	5.0
2	L	210	LYS	5.0
2	L	176	SER	5.0
2	L	133	PRO	5.0
1	A	204	LEU	4.9
1	H	141	PRO	4.8
4	F	148	ILE	4.8
2	L	164	ALA	4.8
1	H	39	MET	4.6
2	L	220	GLY	4.5
1	A	229	LYS	4.5
2	L	147	SER	4.4
2	L	78	GLY	4.2
1	H	136	VAL	4.2
2	L	175	GLN	4.2
1	H	223	ASP	4.1
2	L	23	CYS	4.1
2	L	76	PHE	4.1
1	H	144	LYS	4.1
2	L	169	LYS	4.1
1	A	147	SER	4.0
1	H	106	SER	4.0
1	H	230	SER	4.0
2	L	219	GLN	4.0
2	L	217	THR	3.9
1	H	188	SER	3.8
1	H	91	MET	3.8
2	L	230	ASN	3.8
2	B	18	ARG	3.7
1	H	20	ARG	3.7
1	H	143	SER	3.6
4	I	148	ILE	3.6
2	B	127	LYS	3.6
2	L	13	ALA	3.6
1	H	167	VAL	3.6
2	L	229	PHE	3.6
2	L	204	ALA	3.6
1	A	226	VAL	3.6
2	B	19	VAL	3.5
2	L	178	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	137	ILE	3.5
1	C	148	GLY	3.4
1	H	225	ARG	3.4
2	L	198	THR	3.4
4	I	151	GLY	3.3
1	C	149	GLY	3.3
1	H	187	SER	3.3
2	L	221	LEU	3.3
1	H	140	ALA	3.3
2	L	212	TYR	3.3
1	H	135	SER	3.3
1	H	40	THR	3.3
2	L	227	LYS	3.2
1	H	25	VAL	3.2
2	L	170	VAL	3.2
4	I	150	SER	3.2
2	L	157	ASN	3.2
1	H	222	VAL	3.2
2	L	141	SER	3.2
1	H	92	ASN	3.1
4	F	150	SER	3.1
2	L	145	LEU	3.1
1	A	198	THR	3.1
1	H	206	THR	3.1
1	H	209	TYR	3.1
2	L	138	PHE	3.1
2	L	228	SER	3.1
2	B	202	SER	3.1
2	L	140	PRO	3.1
2	L	197	SER	3.1
1	H	174	LEU	3.1
1	H	158	LYS	3.0
2	L	201	LEU	3.0
1	H	196	VAL	3.0
1	H	152	ALA	3.0
1	H	134	PRO	3.0
1	H	197	VAL	3.0
1	H	194	SER	3.0
1	H	180	THR	3.0
2	B	91	ILE	3.0
2	L	183	VAL	2.9
2	L	167	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	102	TYR	2.9
1	H	76	PHE	2.9
2	L	215	GLU	2.9
1	A	230	SER	2.9
1	H	147	SER	2.9
1	H	226	VAL	2.9
2	B	232	GLY	2.9
1	A	206	THR	2.8
2	L	234	CYS	2.8
1	A	231	CYS	2.8
2	L	218	HIS	2.8
2	L	209	HIS	2.8
2	L	203	LYS	2.8
1	H	18	SER	2.7
4	F	149	ALA	2.7
2	L	162	ARG	2.7
2	D	169	LYS	2.7
2	L	122	THR	2.7
2	L	128	ARG	2.7
1	H	7	SER	2.6
1	H	210	ILE	2.6
1	C	146	THR	2.6
2	L	223	SER	2.6
1	H	56	ILE	2.6
2	L	211	VAL	2.6
2	D	174	LEU	2.6
1	H	15	PRO	2.6
2	L	39	LEU	2.5
2	L	206	TYR	2.5
1	H	19	LEU	2.5
2	B	213	ALA	2.5
2	L	130	VAL	2.5
2	L	150	ALA	2.5
2	L	205	ASP	2.5
2	L	200	THR	2.4
1	H	142	SER	2.4
2	L	75	ARG	2.4
1	A	208	THR	2.4
2	L	174	LEU	2.4
2	L	135	VAL	2.4
1	H	21	LEU	2.4
2	L	179	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	198	THR	2.4
1	H	52	TRP	2.3
1	H	105	ALA	2.3
2	L	124	VAL	2.3
2	L	226	THR	2.3
2	L	116	TRP	2.3
2	D	201	LEU	2.3
1	H	124	VAL	2.3
2	L	168	TRP	2.3
2	L	213	ALA	2.3
2	L	127	LYS	2.3
2	L	41	TRP	2.3
2	L	53	LEU	2.3
2	L	151	SER	2.3
1	H	88	TYR	2.3
1	A	228	PRO	2.3
1	H	120	GLN	2.3
1	A	145	SER	2.2
2	L	199	LEU	2.2
1	H	175	THR	2.2
1	H	186	GLN	2.2
2	L	163	GLU	2.2
2	B	135	VAL	2.2
1	H	46	PRO	2.2
1	H	78	ILE	2.2
1	A	141	PRO	2.2
1	H	224	LYS	2.2
2	L	54	ILE	2.2
1	H	204	LEU	2.2
2	B	90	THR	2.2
2	B	181	GLU	2.2
1	A	225	ARG	2.2
2	L	57	ALA	2.2
2	L	181	GLU	2.1
1	H	205	GLY	2.1
2	L	231	ARG	2.1
2	L	19	VAL	2.1
2	L	224	PRO	2.1
1	H	208	THR	2.1
1	C	143	SER	2.1
1	H	23	CYS	2.1
2	L	105	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	87	LEU	2.1
2	D	167	GLN	2.1
2	B	219	GLN	2.1
2	L	4	MET	2.1
2	L	171	ASP	2.1
2	L	91	ILE	2.1
2	L	18	ARG	2.0
1	H	58	GLY	2.0
2	D	212	TYR	2.0
1	A	227	GLU	2.0
2	L	207	GLU	2.0
1	H	111(A)	ALA	2.0
2	L	117	THR	2.0
4	F	414	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.