



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:38 AM GMT

PDB ID : 2XNX  
Title : BC1 FRAGMENT OF STREPTOCOCCAL M1 PROTEIN IN COMPLEX  
WITH HUMAN FIBRINOGEN  
Authors : Macheboeuf, P.; Y Fu, C.; Zinkernagel, A.S.; Johnson, J.E.; Nizet, V.; Ghosh,  
P.  
Deposited on : 2010-08-06  
Resolution : 3.30 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

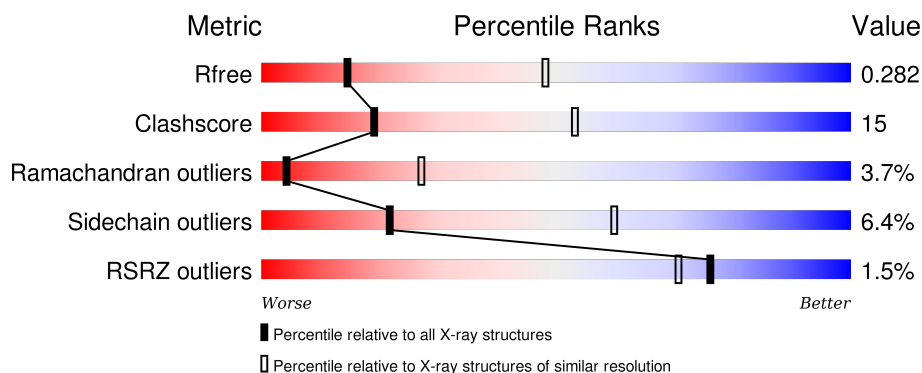
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. 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	87	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>6%</div> <div>14%</div> </div> </div>
1	D	87	<div> <div>55%</div> <div>28%</div> <div>5%</div> <div>13%</div> </div>
1	G	87	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>21%</div> <div>7%</div> <div>16%</div> </div> </div>
1	J	87	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>24%</div> <div>7%</div> <div>17%</div> </div> </div>
2	B	328	<div> <div>57%</div> <div>35%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	328	
2	H	328	
2	K	328	
3	C	319	
3	F	319	
3	I	319	
3	L	319	
4	M	146	
4	N	146	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23867 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 FIBRINOGEN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	75	Total	C	N	O	S	0	0	1
			609	377	116	113	3			
1	D	76	Total	C	N	O	S	0	0	0
			628	388	123	114	3			
1	G	73	Total	C	N	O	S	0	0	1
			591	366	113	109	3			
1	J	72	Total	C	N	O	S	0	0	0
			591	366	113	109	3			

- Molecule 2 is a protein called FIBRINOGEN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	313	Total	C	N	O	S	0	0	1
			2509	1565	443	479	22			
2	E	310	Total	C	N	O	S	0	0	1
			2483	1549	437	475	22			
2	H	313	Total	C	N	O	S	0	0	0
			2517	1571	444	480	22			
2	K	309	Total	C	N	O	S	0	0	1
			2474	1544	435	473	22			

- Molecule 3 is a protein called FIBRINOGEN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	1
			2428	1540	408	468	12			
3	F	304	Total	C	N	O	S	0	0	1
			2436	1546	409	469	12			
3	I	300	Total	C	N	O	S	0	0	0
			2409	1530	405	462	12			
3	L	305	Total	C	N	O	S	0	0	1
			2444	1551	410	470	13			

- Molecule 4 is a protein called M PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	108	Total	C	N	O	0	0	1
			874	536	153	185			
4	N	108	Total	C	N	O	0	0	1
			874	536	153	185			

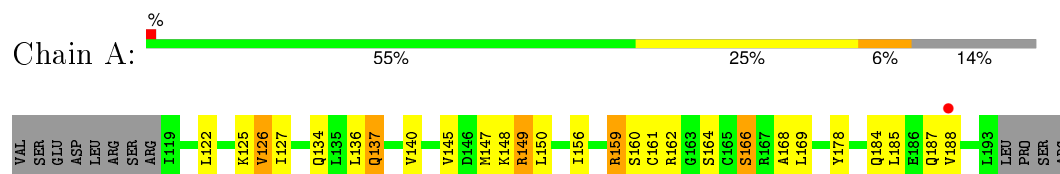
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	126	MET	-	EXPRESSION TAG	UNP Q48WD8
M	127	VAL	-	EXPRESSION TAG	UNP Q48WD8
M	264	LEU	-	EXPRESSION TAG	UNP Q48WD8
M	265	GLU	-	EXPRESSION TAG	UNP Q48WD8
M	266	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	267	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	268	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	269	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	270	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	271	HIS	-	EXPRESSION TAG	UNP Q48WD8
M	195	ALA	THR	CONFLICT	UNP Q48WD8
N	126	MET	-	EXPRESSION TAG	UNP Q48WD8
N	127	VAL	-	EXPRESSION TAG	UNP Q48WD8
N	264	LEU	-	EXPRESSION TAG	UNP Q48WD8
N	265	GLU	-	EXPRESSION TAG	UNP Q48WD8
N	266	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	267	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	268	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	269	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	270	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	271	HIS	-	EXPRESSION TAG	UNP Q48WD8
N	195	ALA	THR	CONFLICT	UNP Q48WD8

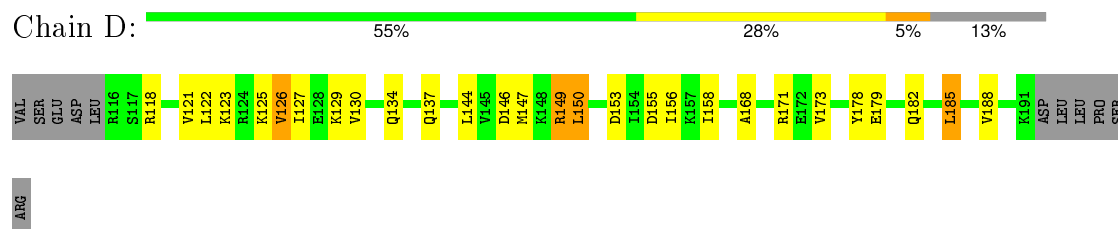
### 3 Residue-property plots [i](#)

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 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.

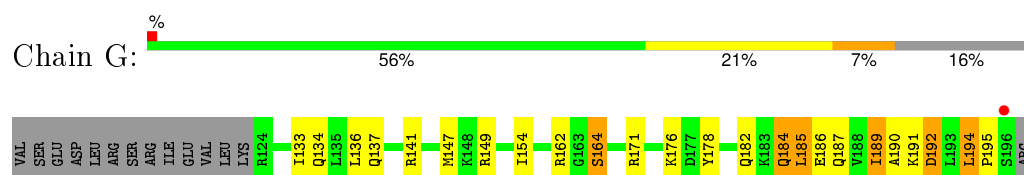
- Molecule 1: FIBRINOGEN ALPHA CHAIN



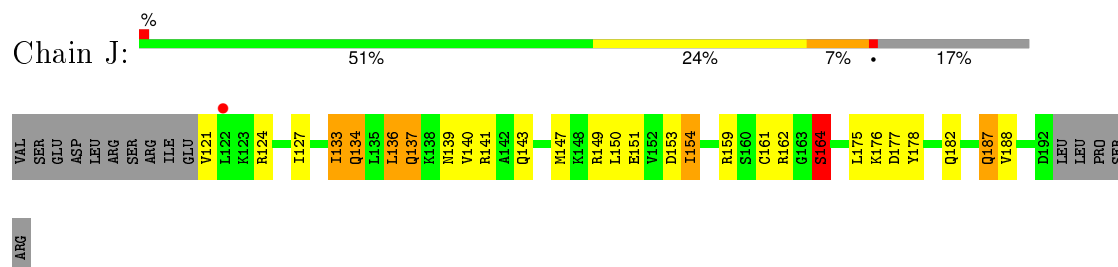
- Molecule 1: FIBRINOGEN ALPHA CHAIN



- Molecule 1: FIBRINOGEN ALPHA CHAIN

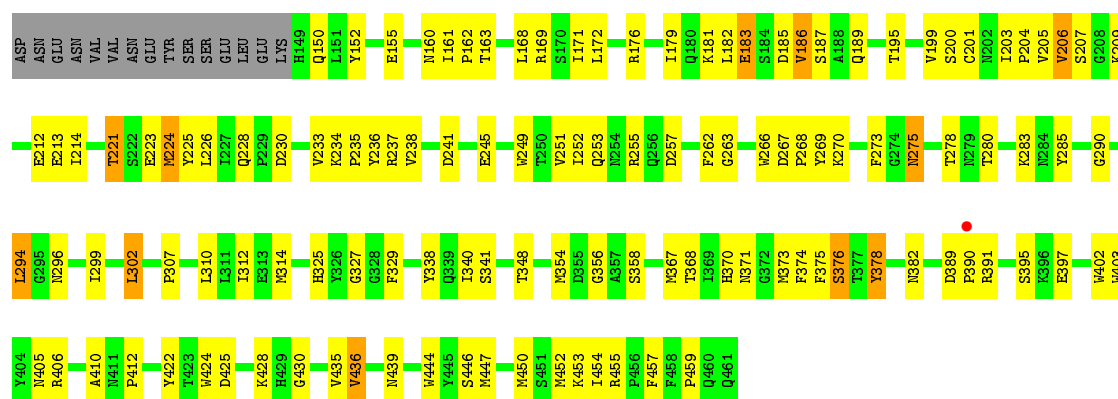


- Molecule 1: FIBRINOGEN ALPHA CHAIN

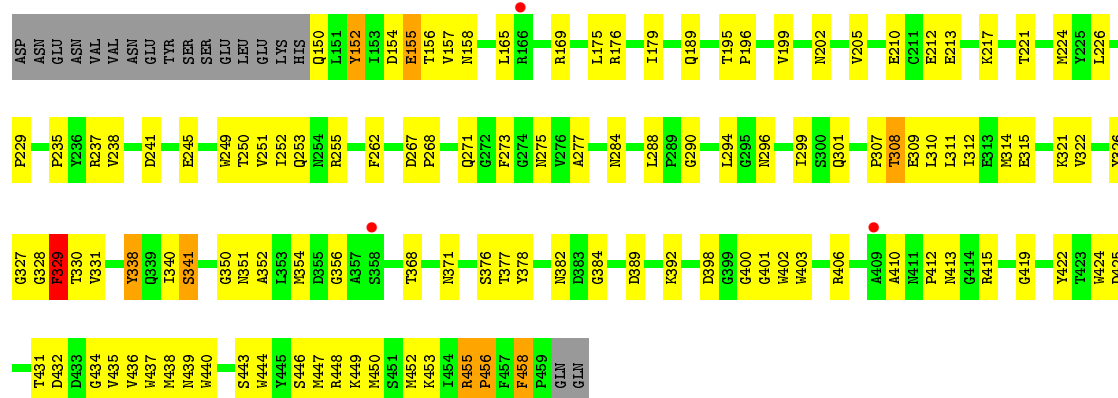


- Molecule 2: FIBRINOGEN BETA CHAIN

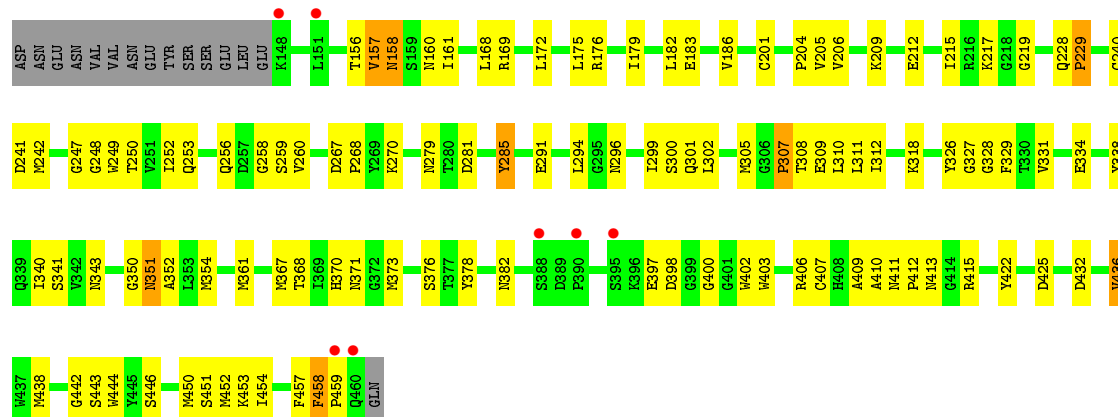




• Molecule 2: FIBRINOGEN BETA CHAIN



• Molecule 2: FIBRINOGEN BETA CHAIN

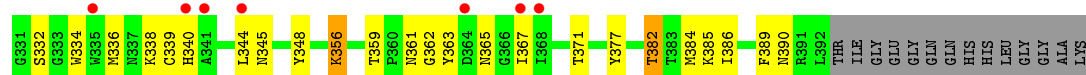


• Molecule 2: FIBRINOGEN BETA CHAIN

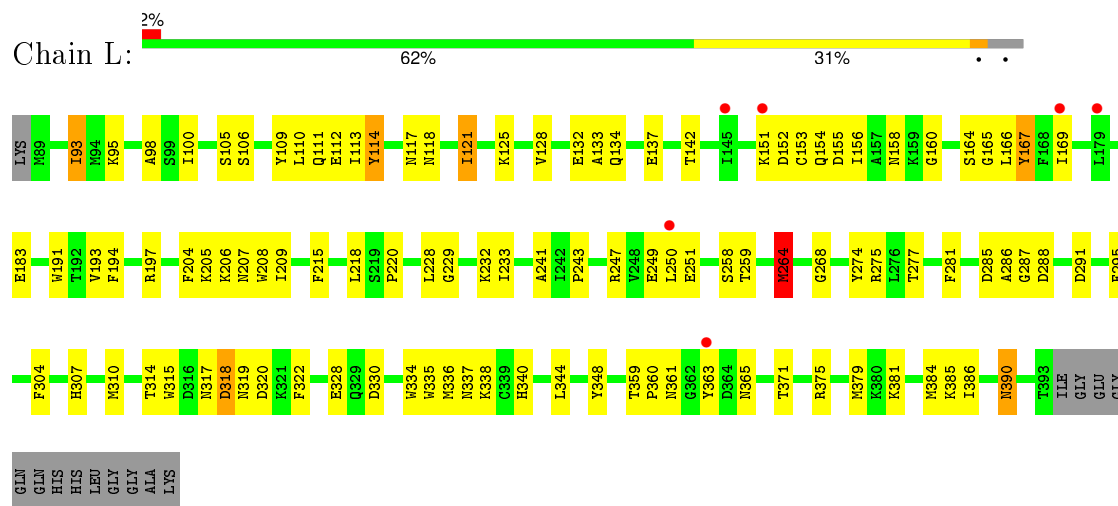




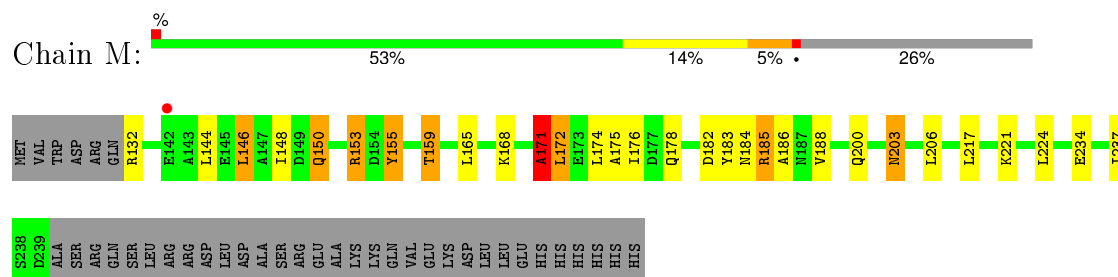




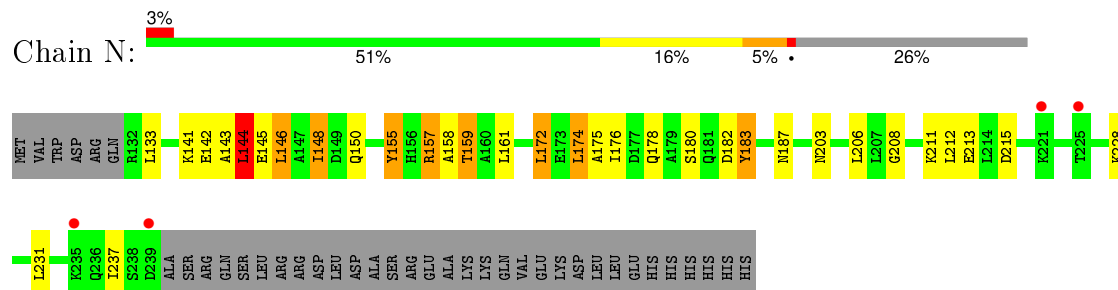
### • Molecule 3: FIBRINOGEN GAMMA CHAIN



### • Molecule 4: M PROTEIN



### • Molecule 4: M PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.72Å 216.87Å 140.81Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	116.25 – 3.30 116.09 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (116.25-3.30) 96.5 (116.09-3.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.277 , 0.325 0.241 , 0.282	Depositor DCC
$R_{free}$ test set	4832 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.6	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 95538 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	23867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.41	0/610	0.59	0/813
1	D	0.39	0/629	0.57	0/836
1	G	0.41	0/593	0.55	0/792
1	J	0.38	0/592	0.58	0/788
2	B	0.43	0/2573	0.62	0/3478
2	E	0.44	1/2545 (0.0%)	0.62	0/3439
2	H	0.41	0/2581	0.58	0/3487
2	K	0.44	1/2536 (0.0%)	0.59	0/3427
3	C	0.46	0/2494	0.57	0/3372
3	F	0.45	0/2502	0.59	0/3383
3	I	0.41	0/2475	0.53	0/3346
3	L	0.45	0/2510	0.57	0/3393
4	M	0.40	0/876	0.64	1/1169 (0.1%)
4	N	0.39	0/876	0.62	0/1169
All	All	0.43	2/24392 (0.0%)	0.59	1/32892 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	458	PHE	C-N	-5.67	1.23	1.34
2	E	458	PHE	C-N	-5.61	1.23	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	171	ALA	C-N-CA	5.07	134.38	121.70

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	609	0	649	18	0
1	D	628	0	676	23	0
1	G	591	0	628	16	0
1	J	591	0	632	25	0
2	B	2509	0	2367	98	0
2	E	2483	0	2345	94	0
2	H	2517	0	2380	85	0
2	K	2474	0	2337	79	0
3	C	2428	0	2273	72	0
3	F	2436	0	2284	74	0
3	I	2409	0	2261	56	0
3	L	2444	0	2293	82	0
4	M	874	0	886	32	0
4	N	874	0	886	43	0
All	All	23867	0	22897	712	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 (712) 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)
4:M:171:ALA:HB3	4:M:172:LEU:HB2	1.24	1.14
2:B:169:ARG:HD3	4:N:155:TYR:CE2	1.97	0.97
4:M:171:ALA:HB3	4:M:172:LEU:CB	1.96	0.95
4:N:143:ALA:O	4:N:146:LEU:HB2	1.66	0.93
2:K:412:PRO:HB3	2:K:450:MET:HG2	1.55	0.87
4:N:143:ALA:H	4:N:144:LEU:HB2	1.38	0.86
2:B:252:ILE:HG22	2:B:294:LEU:HD23	1.58	0.86
2:K:422:TYR:OH	2:K:432:ASP:OD1	1.93	0.84
3:C:165:GLY:O	3:C:167:TYR:HD1	1.61	0.84
2:E:277:ALA:HB1	2:E:288:LEU:O	1.76	0.84
2:H:412:PRO:HB3	2:H:450:MET:CE	2.09	0.82
2:K:226:LEU:HD11	2:K:235:PRO:HB2	1.61	0.81
2:E:169:ARG:HG2	4:N:183:TYR:HE2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HD3	4:N:155:TYR:HE2	1.43	0.80
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.47	0.79
2:H:398:ASP:O	2:H:415:ARG:HD2	1.82	0.79
2:K:329:PHE:HE2	2:K:454:ILE:HD11	1.48	0.79
4:M:153:ARG:HH11	4:M:153:ARG:HG3	1.49	0.78
2:B:302:LEU:HD22	2:B:454:ILE:HD11	1.64	0.78
2:H:240:CYS:HB3	2:H:242:MET:CE	2.13	0.78
2:E:310:LEU:HD22	2:E:329:PHE:CE2	2.19	0.78
1:G:136:LEU:HD12	2:H:168:LEU:HD21	1.66	0.78
3:C:165:GLY:O	3:C:167:TYR:CD1	2.37	0.78
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.67	0.76
2:E:329:PHE:HE1	2:E:331:VAL:HG23	1.51	0.76
3:I:109:TYR:HB2	4:N:174:LEU:HD22	1.67	0.76
1:D:134:GLN:HA	1:D:137:GLN:HG2	1.67	0.75
4:N:143:ALA:H	4:N:144:LEU:CB	1.99	0.75
2:E:340:ILE:HG12	2:E:341:SER:N	2.02	0.75
2:E:377:THR:HG22	2:E:401:GLY:HA3	1.68	0.75
3:F:179:LEU:HD23	3:F:218:LEU:HD12	1.67	0.75
3:F:191:TRP:HB3	3:F:385:LYS:HD2	1.69	0.74
2:K:432:ASP:OD2	2:K:443:SER:O	2.06	0.73
2:E:310:LEU:HD22	2:E:329:PHE:CD2	2.23	0.73
1:D:185:LEU:HA	1:D:188:VAL:HG22	1.69	0.73
3:L:304:PHE:HB3	3:L:338:LYS:HB3	1.71	0.72
3:L:228:LEU:O	3:L:232:LYS:HD2	1.89	0.72
4:M:172:LEU:O	4:M:176:ILE:HG13	1.90	0.72
2:B:340:ILE:HG12	2:B:341:SER:N	2.04	0.72
3:L:268:GLY:O	3:L:274:TYR:HA	1.90	0.71
2:H:354:MET:HG2	2:H:371:ASN:HD22	1.56	0.71
2:H:351:ASN:HD21	2:H:354:MET:CE	2.03	0.70
4:N:157:ARG:O	4:N:161:LEU:HD12	1.89	0.70
2:K:207:SER:O	2:K:214:ILE:HG12	1.91	0.70
4:N:144:LEU:O	4:N:148:ILE:HG12	1.91	0.70
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.72	0.70
3:I:154:GLN:HG3	3:I:158:ASN:HD21	1.55	0.69
2:H:412:PRO:HB3	2:H:450:MET:SD	2.33	0.69
3:C:178:PHE:HE2	3:C:232:LYS:HB3	1.57	0.69
3:I:260:ALA:HB2	3:I:286:ALA:HB3	1.73	0.69
2:H:242:MET:HE2	2:H:248:GLY:H	1.58	0.69
2:B:155:GLU:HA	3:C:96:TYR:OH	1.92	0.69
1:D:147:MET:SD	3:F:121:ILE:HD11	2.32	0.69
2:H:412:PRO:HB3	2:H:450:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:109:TYR:CE2	4:N:178:GLN:HG2	2.28	0.69
2:E:310:LEU:HB2	2:E:329:PHE:HD2	1.56	0.69
4:N:143:ALA:N	4:N:144:LEU:HB2	2.09	0.68
1:J:188:VAL:O	1:J:188:VAL:CG1	2.42	0.68
2:B:209:LYS:HA	2:B:228:GLN:O	1.93	0.68
2:E:340:ILE:HG12	2:E:341:SER:H	1.59	0.68
2:E:354:MET:HG2	2:E:371:ASN:HD22	1.59	0.68
2:K:294:LEU:HD23	2:K:299:ILE:HG13	1.76	0.68
2:H:240:CYS:HB3	2:H:242:MET:HE1	1.75	0.68
2:B:354:MET:HG2	2:B:371:ASN:HD22	1.59	0.68
2:B:370:HIS:O	2:B:373:MET:HB2	1.93	0.68
1:J:151:GLU:OE1	2:K:182:LEU:HD21	1.94	0.68
2:H:209:LYS:HA	2:H:228:GLN:O	1.93	0.68
3:L:105:SER:O	4:N:146:LEU:HD21	1.94	0.68
1:G:185:LEU:O	1:G:189:ILE:HG12	1.94	0.68
2:E:389:ASP:OD1	2:E:392:LYS:HB2	1.94	0.67
3:I:268:GLY:O	3:I:274:TYR:HA	1.93	0.67
2:E:376:SER:HB3	2:E:382:ASN:H	1.59	0.67
2:B:251:VAL:HG22	2:B:453:LYS:HG2	1.75	0.67
4:N:155:TYR:HE1	4:N:159:THR:CG2	2.06	0.67
2:H:240:CYS:HB3	2:H:242:MET:HE3	1.77	0.67
2:B:237:ARG:HH11	2:B:237:ARG:HG3	1.58	0.67
2:E:155:GLU:HB3	3:F:96:TYR:CE2	2.29	0.67
1:A:136:LEU:HD12	2:B:168:LEU:HD21	1.76	0.67
2:K:237:ARG:O	2:K:238:VAL:HG23	1.94	0.67
2:H:310:LEU:HD12	2:H:311:LEU:N	2.10	0.67
2:B:340:ILE:HG12	2:B:341:SER:H	1.60	0.66
3:I:344:LEU:HD12	3:I:384:MET:SD	2.35	0.66
2:E:329:PHE:HD1	2:E:330:THR:N	1.94	0.66
1:G:154:ILE:HG22	1:G:171:ARG:HH12	1.58	0.66
2:B:376:SER:HB3	2:B:382:ASN:H	1.60	0.66
2:H:176:ARG:HD3	3:I:117:ASN:OD1	1.96	0.66
1:J:188:VAL:O	1:J:188:VAL:HG12	1.96	0.65
2:K:171:ILE:HG13	2:K:172:LEU:N	2.09	0.65
2:E:176:ARG:NH2	3:F:116:SER:OG	2.30	0.65
3:C:359:THR:HG21	3:C:365:ASN:HD21	1.62	0.65
2:B:354:MET:HG2	2:B:371:ASN:ND2	2.12	0.65
3:F:310:MET:SD	3:F:337:ASN:ND2	2.68	0.65
3:I:334:TRP:HB3	3:I:336:MET:SD	2.37	0.65
2:K:422:TYR:O	2:K:444:TRP:HB3	1.97	0.64
1:G:134:GLN:HA	1:G:137:GLN:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:GLU:HB3	3:F:96:TYR:HE2	1.61	0.64
2:K:176:ARG:HH11	2:K:176:ARG:CG	2.10	0.64
3:L:204:PHE:CD1	3:L:215:PHE:HZ	2.15	0.64
2:H:458:PHE:H	2:H:459:PRO:CD	2.11	0.64
2:B:169:ARG:HG3	3:C:110:LEU:HD21	1.80	0.64
3:F:372:TRP:CD2	3:F:373:LYS:HE3	2.33	0.63
4:N:155:TYR:C	4:N:155:TYR:HD1	2.01	0.63
4:N:143:ALA:N	4:N:144:LEU:CB	2.60	0.63
3:I:263:ALA:HB1	3:I:264:MET:HE3	1.78	0.63
3:F:344:LEU:HD12	3:F:384:MET:SD	2.38	0.63
1:G:141:ARG:HB3	1:G:185:LEU:HD21	1.78	0.63
2:K:412:PRO:HB3	2:K:450:MET:CG	2.28	0.63
3:I:361:ASN:HB3	3:I:363:TYR:CD2	2.33	0.62
4:M:153:ARG:NH1	4:M:153:ARG:HG3	2.14	0.62
3:L:204:PHE:CD1	3:L:215:PHE:CZ	2.87	0.62
2:B:207:SER:O	2:B:214:ILE:HG12	2.00	0.62
3:C:315:TRP:HB2	3:C:328:GLU:HG3	1.80	0.62
2:B:310:LEU:HD22	2:B:329:PHE:CD1	2.35	0.62
1:A:150:LEU:HD13	3:C:125:LYS:HE2	1.80	0.62
2:H:376:SER:HB3	2:H:382:ASN:H	1.65	0.62
2:K:367:MET:HB2	2:K:406:ARG:HB2	1.82	0.62
3:F:180:VAL:HG12	3:F:228:LEU:HD11	1.81	0.62
2:E:398:ASP:O	2:E:415:ARG:HD3	1.99	0.62
1:J:164:SER:OG	3:L:137:GLU:O	2.18	0.62
4:N:155:TYR:HE1	4:N:159:THR:HG21	1.64	0.61
3:F:191:TRP:CB	3:F:385:LYS:HD2	2.31	0.61
2:K:206:VAL:HG22	2:K:214:ILE:HG23	1.83	0.61
3:L:250:LEU:HD22	3:L:379:MET:HG3	1.82	0.61
3:F:287:GLY:HA3	3:F:371:THR:OG1	2.01	0.61
2:E:400:GLY:HA3	2:E:413:ASN:O	2.01	0.61
2:H:252:ILE:HB	2:H:299:ILE:HD11	1.83	0.60
2:E:412:PRO:HB3	2:E:450:MET:SD	2.41	0.60
3:I:169:ILE:HD12	3:I:180:VAL:CG2	2.32	0.60
3:C:390:ASN:OD1	3:C:390:ASN:N	2.33	0.60
2:K:176:ARG:HH11	2:K:176:ARG:HG2	1.66	0.60
2:H:204:PRO:HA	3:I:217:HIS:HA	1.83	0.60
2:E:422:TYR:O	2:E:444:TRP:HB3	2.01	0.60
3:I:169:ILE:HD12	3:I:180:VAL:HG22	1.84	0.59
1:D:144:LEU:HD12	2:E:175:LEU:HD21	1.83	0.59
3:F:288:ASP:H	3:F:371:THR:HG21	1.67	0.59
4:M:184:ASN:O	4:M:186:ALA:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:208:GLY:HA2	4:N:211:LYS:HE3	1.84	0.59
2:K:241:ASP:HB3	2:K:249:TRP:HB2	1.82	0.59
4:M:185:ARG:HH21	4:N:182:ASP:HA	1.67	0.59
2:B:307:PRO:O	2:B:457:PHE:N	2.34	0.59
3:C:330:ASP:OD2	3:C:340:HIS:NE2	2.35	0.59
3:C:167:TYR:O	3:C:179:LEU:HD12	2.03	0.59
2:K:224:MET:SD	2:K:237:ARG:HD3	2.43	0.59
1:A:185:LEU:HA	1:A:188:VAL:HG22	1.84	0.59
2:E:179:ILE:HG21	3:F:120:LYS:HG2	1.83	0.59
4:M:168:LYS:O	4:M:171:ALA:CB	2.50	0.59
2:B:172:LEU:HD22	3:C:113:ILE:HG22	1.85	0.58
2:K:329:PHE:CE2	2:K:454:ILE:HD11	2.35	0.58
3:F:228:LEU:O	3:F:232:LYS:HD2	2.03	0.58
3:F:232:LYS:O	3:F:236:ILE:HG13	2.03	0.58
2:E:329:PHE:HE1	2:E:331:VAL:CG2	2.16	0.58
3:L:193:VAL:HG22	3:L:385:LYS:HB3	1.85	0.58
2:E:384:GLY:HA3	2:E:406:ARG:HG3	1.85	0.58
2:H:370:HIS:O	2:H:373:MET:HB2	2.04	0.58
2:E:329:PHE:CE1	2:E:331:VAL:HG23	2.37	0.58
1:D:129:LYS:HE3	3:F:104:ASP:HB2	1.86	0.58
2:E:356:GLY:HA2	2:E:368:THR:O	2.03	0.58
3:F:197:ARG:O	3:F:198:LEU:HD23	2.03	0.58
1:J:139:ASN:O	3:L:114:TYR:HE2	1.86	0.57
2:B:435:VAL:CG1	2:B:447:MET:HB2	2.35	0.57
2:K:374:PHE:O	2:K:403:TRP:HA	2.04	0.57
3:L:275:ARG:O	3:L:277:THR:HG23	2.04	0.57
1:A:149:ARG:HG2	2:B:425:ASP:O	2.04	0.57
3:L:307:HIS:CE1	3:L:340:HIS:HA	2.39	0.57
2:H:367:MET:HE1	2:H:406:ARG:HH12	1.69	0.57
3:L:208:TRP:HE3	3:L:314:THR:CG2	2.17	0.57
3:C:178:PHE:CE2	3:C:232:LYS:HB3	2.39	0.57
3:C:292:GLY:HA2	3:C:305:THR:O	2.04	0.57
2:B:252:ILE:HB	2:B:299:ILE:HD11	1.87	0.57
2:H:351:ASN:HD21	2:H:354:MET:HE3	1.68	0.57
3:F:239:GLN:O	3:F:240:SER:O	2.23	0.57
2:H:253:GLN:HB3	2:H:452:MET:HB2	1.86	0.57
3:L:132:GLU:O	3:L:134:GLN:N	2.36	0.57
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.86	0.57
2:E:309:GLU:HG2	2:E:455:ARG:O	2.05	0.57
3:L:307:HIS:HE1	3:L:340:HIS:HA	1.70	0.56
2:K:402:TRP:CD1	2:K:403:TRP:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:236:ILE:O	3:F:239:GLN:HG3	2.04	0.56
1:D:122:LEU:HD23	1:D:123:LYS:HZ3	1.69	0.56
2:H:179:ILE:HG21	3:I:120:LYS:HG2	1.87	0.56
2:K:221:THR:O	2:K:225:TYR:OH	2.18	0.56
2:H:412:PRO:HG3	2:H:450:MET:HE1	1.86	0.56
2:B:435:VAL:HG12	2:B:447:MET:HB2	1.88	0.56
3:L:208:TRP:HA	3:L:314:THR:HG21	1.87	0.56
3:L:208:TRP:HE3	3:L:314:THR:HG23	1.70	0.56
4:N:155:TYR:CD1	4:N:155:TYR:C	2.75	0.56
3:C:236:ILE:HA	3:C:239:GLN:HE21	1.71	0.56
2:E:448:ARG:HH11	2:E:448:ARG:HG3	1.71	0.56
3:L:204:PHE:HD1	3:L:215:PHE:HZ	1.53	0.56
2:H:312:ILE:HG12	2:H:452:MET:HG2	1.86	0.56
3:L:132:GLU:C	3:L:134:GLN:H	2.09	0.56
3:L:165:GLY:O	3:L:167:TYR:CD1	2.59	0.56
4:N:172:LEU:HD22	4:N:176:ILE:HD11	1.88	0.56
3:L:100:ILE:O	3:L:100:ILE:HG22	2.05	0.56
1:J:159:ARG:HB2	1:J:159:ARG:HH11	1.71	0.55
2:E:402:TRP:CZ3	2:E:412:PRO:HD2	2.41	0.55
3:C:250:LEU:HD22	3:C:379:MET:HG3	1.87	0.55
1:D:126:VAL:O	1:D:126:VAL:HG12	2.06	0.55
2:H:176:ARG:NH1	3:I:116:SER:OG	2.40	0.55
1:G:133:ILE:HD11	3:I:107:ILE:HG12	1.89	0.55
3:C:208:TRP:HA	3:C:314:THR:HG21	1.88	0.55
3:C:168:PHE:HE1	3:C:179:LEU:HB2	1.70	0.55
3:C:152:ASP:HA	3:C:169:ILE:HG21	1.87	0.55
1:G:149:ARG:HH21	2:H:425:ASP:HA	1.70	0.55
3:I:264:MET:H	3:I:264:MET:CE	2.20	0.55
3:L:249:GLU:HG2	3:L:259:THR:HG22	1.88	0.55
3:L:344:LEU:HD12	3:L:384:MET:SD	2.47	0.55
3:C:356:LYS:HG3	3:C:362:GLY:HA3	1.89	0.55
3:L:264:MET:H	3:L:264:MET:CE	2.20	0.55
2:E:402:TRP:CG	2:E:403:TRP:N	2.74	0.55
1:G:133:ILE:O	1:G:133:ILE:HG22	2.06	0.55
2:E:432:ASP:CG	2:E:443:SER:O	2.45	0.55
2:E:237:ARG:O	2:E:238:VAL:HG23	2.06	0.55
1:A:148:LYS:HE3	1:A:178:TYR:HB3	1.90	0.54
1:J:154:ILE:HD11	3:L:128:VAL:HG21	1.89	0.54
3:L:166:LEU:HD22	3:L:218:LEU:HB3	1.88	0.54
3:C:286:ALA:O	3:C:372:TRP:HB2	2.08	0.54
4:M:200:GLN:NE2	4:M:203:ASN:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:203:ASN:HD22	4:M:206:LEU:HD12	1.72	0.54
2:B:150:GLN:C	2:B:152:TYR:H	2.10	0.54
2:B:253:GLN:HB3	2:B:452:MET:HB2	1.89	0.54
3:I:191:TRP:HB3	3:I:385:LYS:HD2	1.89	0.54
3:C:232:LYS:O	3:C:236:ILE:HG13	2.07	0.54
3:F:295:PHE:CD1	3:F:375:ARG:HD3	2.43	0.54
3:I:204:PHE:HE2	3:I:227:TRP:HB2	1.72	0.54
4:M:182:ASP:C	4:M:184:ASN:HB3	2.29	0.54
2:K:402:TRP:CZ3	2:K:412:PRO:HD2	2.43	0.54
3:C:228:LEU:O	3:C:232:LYS:HD2	2.08	0.54
3:F:264:MET:O	3:F:278:TYR:HA	2.07	0.54
2:H:400:GLY:HA3	2:H:413:ASN:O	2.07	0.54
4:M:221:LYS:HA	4:M:224:LEU:HD12	1.90	0.54
4:M:146:LEU:HD23	4:M:146:LEU:H	1.72	0.54
2:B:171:ILE:HG23	2:B:172:LEU:N	2.23	0.53
1:A:159:ARG:C	1:A:161:CYS:H	2.12	0.53
2:E:268:PRO:O	2:E:273:PHE:HD2	1.91	0.53
3:L:207:ASN:OD1	3:L:207:ASN:C	2.47	0.53
1:D:149:ARG:HH21	2:E:425:ASP:HA	1.74	0.53
2:K:172:LEU:HG	3:L:113:ILE:HG21	1.91	0.53
1:D:158:ILE:HD12	1:D:171:ARG:HH11	1.71	0.53
1:A:122:LEU:HD22	3:C:96:TYR:HD2	1.73	0.53
4:M:168:LYS:O	4:M:171:ALA:HB2	2.09	0.53
4:N:183:TYR:C	4:N:183:TYR:CD1	2.82	0.53
4:M:237:ILE:HD12	4:N:237:ILE:HG21	1.91	0.53
2:H:183:GLU:HG3	3:I:124:LEU:HD13	1.91	0.53
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.90	0.53
1:D:125:LYS:C	1:D:127:ILE:H	2.11	0.53
3:F:197:ARG:NH2	3:F:348:TYR:HB2	2.23	0.53
3:C:174:ALA:HB2	3:C:235:LEU:HD22	1.90	0.53
2:B:224:MET:O	2:B:224:MET:HG3	2.07	0.53
3:C:191:TRP:CE3	3:C:385:LYS:HD2	2.44	0.53
2:K:309:GLU:HG2	2:K:455:ARG:O	2.09	0.53
3:L:334:TRP:HB3	3:L:336:MET:SD	2.49	0.53
3:F:208:TRP:HA	3:F:314:THR:HG21	1.91	0.53
2:E:224:MET:SD	2:E:237:ARG:HB3	2.50	0.52
2:B:283:LYS:HD2	2:B:285:TYR:HE1	1.74	0.52
2:H:156:THR:C	2:H:158:ASN:H	2.13	0.52
2:E:169:ARG:HG2	4:N:183:TYR:CE2	2.35	0.52
2:E:238:VAL:HG11	2:E:250:THR:HG23	1.91	0.52
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:432:ASP:OD2	2:E:443:SER:O	2.27	0.52
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.91	0.52
2:H:318:LYS:HA	2:H:318:LYS:HE2	1.90	0.52
2:E:277:ALA:CB	2:E:288:LEU:O	2.55	0.52
2:K:267:ASP:CB	2:K:268:PRO:HD3	2.38	0.52
4:M:183:TYR:HA	4:M:184:ASN:C	2.30	0.52
2:H:258:GLY:N	2:H:291:GLU:OE2	2.39	0.52
2:H:267:ASP:HB3	2:H:268:PRO:HD3	1.90	0.52
2:E:340:ILE:CG1	2:E:341:SER:N	2.72	0.52
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.92	0.52
3:F:153:CYS:HA	3:F:156:ILE:HD12	1.92	0.52
4:M:171:ALA:CB	4:M:172:LEU:CB	2.80	0.52
3:C:149:THR:OG1	3:C:168:PHE:O	2.10	0.52
1:D:122:LEU:HD23	1:D:123:LYS:NZ	2.25	0.52
3:F:334:TRP:HB2	3:F:343:HIS:CE1	2.45	0.52
2:H:351:ASN:ND2	2:H:354:MET:CE	2.73	0.52
2:H:212:GLU:O	2:H:215:ILE:HG22	2.10	0.52
4:N:145:GLU:CD	4:N:145:GLU:H	2.14	0.52
2:H:169:ARG:NH1	4:M:183:TYR:CD2	2.77	0.52
2:K:186:VAL:HG12	2:K:186:VAL:O	2.09	0.52
3:C:289:ALA:O	3:C:341:ALA:HB3	2.10	0.51
4:M:171:ALA:CB	4:M:172:LEU:HB2	2.16	0.51
2:B:235:PRO:HG2	3:C:168:PHE:CE2	2.45	0.51
3:L:281:PHE:HB2	3:L:288:ASP:OD2	2.10	0.51
2:K:169:ARG:HG3	3:L:110:LEU:HD21	1.90	0.51
3:F:281:PHE:CZ	3:F:287:GLY:O	2.64	0.51
3:L:361:ASN:HB3	3:L:363:TYR:HD2	1.75	0.51
2:B:422:TYR:O	2:B:444:TRP:HB3	2.10	0.51
2:B:226:LEU:HD11	2:B:235:PRO:HB2	1.91	0.51
3:I:179:LEU:HD23	3:I:218:LEU:HD12	1.92	0.51
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.91	0.51
2:H:285:TYR:H	2:H:285:TYR:HD1	1.58	0.51
2:H:310:LEU:HD12	2:H:311:LEU:H	1.76	0.51
1:G:194:LEU:H	1:G:195:PRO:HD2	1.75	0.51
3:L:390:ASN:OD1	3:L:390:ASN:N	2.43	0.51
2:B:186:VAL:O	2:B:186:VAL:HG12	2.11	0.51
4:N:183:TYR:C	4:N:183:TYR:HD1	2.14	0.51
4:M:171:ALA:HB1	4:N:172:LEU:HG	1.93	0.51
2:B:236:TYR:OH	2:B:302:LEU:HD12	2.11	0.51
3:I:359:THR:HG21	3:I:365:ASN:HD21	1.76	0.51
2:K:400:GLY:HA3	2:K:413:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:GLU:HG2	3:C:96:TYR:OH	2.11	0.51
2:E:226:LEU:HD11	2:E:235:PRO:HB2	1.93	0.51
2:E:438:MET:O	2:E:440:TRP:N	2.43	0.51
3:C:301:ASP:C	3:C:303:PHE:H	2.12	0.50
2:E:205:VAL:HG23	3:F:216:GLY:O	2.12	0.50
3:I:281:PHE:HB2	3:I:288:ASP:OD2	2.11	0.50
3:C:264:MET:O	3:C:278:TYR:HA	2.10	0.50
3:L:191:TRP:HB3	3:L:385:LYS:HB2	1.93	0.50
2:E:376:SER:HB3	2:E:382:ASN:N	2.25	0.50
3:F:289:ALA:C	3:F:291:ASP:H	2.14	0.50
2:B:185:ASP:C	2:B:187:SER:H	2.14	0.50
2:B:171:ILE:CG2	2:B:172:LEU:N	2.74	0.50
2:B:179:ILE:HD11	3:C:121:ILE:HG13	1.92	0.50
1:J:147:MET:HG2	3:L:121:ILE:HD11	1.94	0.50
3:I:197:ARG:HH21	3:I:348:TYR:HB2	1.77	0.50
3:L:95:LYS:HA	3:L:98:ALA:HB3	1.93	0.50
3:L:114:TYR:C	3:L:114:TYR:CD1	2.84	0.50
2:H:422:TYR:O	2:H:444:TRP:HB3	2.11	0.50
2:B:181:LYS:C	2:B:183:GLU:H	2.15	0.50
2:E:152:TYR:C	2:E:152:TYR:CD1	2.85	0.50
2:B:205:VAL:HG23	3:C:216:GLY:O	2.12	0.50
2:B:314:MET:HB3	2:B:450:MET:HE2	1.93	0.50
4:M:172:LEU:H	4:M:175:ALA:H	1.60	0.50
2:H:204:PRO:HB3	3:I:217:HIS:ND1	2.26	0.50
3:L:320:ASP:HB3	3:L:336:MET:HB2	1.94	0.50
4:M:155:TYR:C	4:M:155:TYR:CD1	2.85	0.50
2:B:230:ASP:HB3	2:B:233:VAL:HG23	1.93	0.50
1:J:187:GLN:HG2	1:J:187:GLN:O	2.12	0.50
3:I:264:MET:HE2	3:I:264:MET:H	1.77	0.49
3:F:338:LYS:N	3:F:339:CYS:HA	2.26	0.49
3:L:197:ARG:HH21	3:L:348:TYR:HB2	1.78	0.49
2:K:230:ASP:HB2	2:K:301:GLN:HE21	1.77	0.49
2:H:242:MET:HA	2:H:247:GLY:HA2	1.94	0.49
2:H:241:ASP:HB3	2:H:249:TRP:HB2	1.94	0.49
1:G:184:GLN:O	1:G:186:GLU:N	2.44	0.49
2:H:229:PRO:HB2	2:H:301:GLN:HE22	1.77	0.49
2:K:162:PRO:HB3	2:K:166:ARG:HH21	1.77	0.49
1:J:159:ARG:HB2	1:J:159:ARG:NH1	2.27	0.49
2:B:358:SER:HB3	2:B:439:ASN:OD1	2.12	0.49
3:L:165:GLY:O	3:L:167:TYR:HD1	1.96	0.49
2:H:307:PRO:HB2	2:H:457:PHE:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:GLN:HA	3:F:190:GLY:HA3	1.95	0.49
2:B:402:TRP:CG	2:B:403:TRP:N	2.80	0.49
2:E:150:GLN:C	2:E:152:TYR:H	2.15	0.49
1:D:118:ARG:HA	1:D:121:VAL:HG22	1.94	0.49
4:M:146:LEU:O	4:M:150:GLN:HB2	2.12	0.49
2:H:411:ASN:N	2:H:436:VAL:O	2.43	0.49
2:K:210:GLU:OE1	2:K:212:GLU:HB3	2.13	0.49
3:I:332:SER:HB2	3:I:345:ASN:O	2.12	0.49
2:B:169:ARG:HD3	4:N:155:TYR:CD2	2.45	0.49
3:I:154:GLN:HG3	3:I:158:ASN:ND2	2.26	0.49
2:H:310:LEU:HA	2:H:454:ILE:HG22	1.94	0.49
4:M:206:LEU:HD23	4:N:206:LEU:HD21	1.95	0.49
3:F:367:ILE:O	3:F:378:SER:HA	2.13	0.49
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.77	0.49
3:L:315:TRP:HE3	3:L:328:GLU:OE2	1.96	0.49
3:I:100:ILE:O	3:I:104:ASP:HB2	2.12	0.49
3:C:166:LEU:HD11	3:C:218:LEU:O	2.13	0.48
2:B:340:ILE:CG1	2:B:341:SER:N	2.74	0.48
2:B:435:VAL:HG12	2:B:435:VAL:O	2.13	0.48
2:E:255:ARG:CZ	2:E:262:PHE:CD1	2.96	0.48
2:E:340:ILE:CG1	2:E:341:SER:H	2.24	0.48
3:F:227:TRP:CD1	3:F:229:GLY:N	2.81	0.48
3:F:212:LYS:HG3	3:F:274:TYR:OH	2.13	0.48
2:E:312:ILE:HG12	2:E:452:MET:HG2	1.95	0.48
4:N:172:LEU:O	4:N:175:ALA:HB3	2.14	0.48
2:K:268:PRO:O	2:K:273:PHE:HD2	1.97	0.48
3:I:108:ARG:HB3	4:N:174:LEU:HD11	1.95	0.48
3:L:330:ASP:OD2	3:L:340:HIS:CE1	2.66	0.48
3:F:278:TYR:OH	3:F:290:PHE:O	2.31	0.48
2:H:410:ALA:HA	2:H:436:VAL:O	2.13	0.48
1:G:154:ILE:HD12	2:H:182:LEU:HD13	1.94	0.48
3:C:325:ASN:HB3	3:C:328:GLU:HB3	1.94	0.48
2:B:161:ILE:N	2:B:162:PRO:CD	2.76	0.48
3:C:276:LEU:HB2	3:C:335:TRP:NE1	2.29	0.48
4:N:212:LEU:HA	4:N:215:ASP:HB2	1.96	0.48
2:K:226:LEU:HD11	2:K:235:PRO:CB	2.37	0.48
1:G:133:ILE:O	1:G:133:ILE:CG2	2.62	0.48
4:N:228:LYS:HA	4:N:231:LEU:HB2	1.93	0.48
4:N:143:ALA:N	4:N:144:LEU:HB3	2.28	0.48
2:K:402:TRP:CG	2:K:403:TRP:N	2.82	0.48
2:E:154:ASP:C	2:E:156:THR:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:CYS:HB2	3:C:141:ASP:OD2	2.14	0.48
2:K:253:GLN:O	2:K:451:SER:HA	2.14	0.48
2:E:199:VAL:O	3:F:141:ASP:HA	2.13	0.48
3:C:178:PHE:CD1	3:C:178:PHE:N	2.81	0.48
2:E:275:ASN:O	2:E:290:GLY:HA3	2.13	0.48
3:I:245:ALA:HB2	3:I:389:PHE:HD1	1.78	0.48
2:K:324:ALA:HB2	2:K:349:ALA:HB3	1.96	0.48
2:H:205:VAL:HG23	3:I:216:GLY:C	2.34	0.48
3:L:258:SER:HB2	3:L:286:ALA:HB2	1.96	0.48
2:H:175:LEU:O	2:H:179:ILE:HG13	2.14	0.47
2:E:448:ARG:NH1	2:E:448:ARG:HG3	2.29	0.47
3:C:276:LEU:HB2	3:C:335:TRP:CD1	2.49	0.47
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.13	0.47
2:E:410:ALA:HA	2:E:436:VAL:O	2.14	0.47
2:E:321:LYS:O	2:E:322:VAL:HG13	2.14	0.47
3:F:250:LEU:HD22	3:F:379:MET:HG3	1.96	0.47
2:E:213:GLU:HG2	2:E:217:LYS:HE3	1.95	0.47
4:M:132:ARG:HH22	4:N:133:LEU:HD13	1.79	0.47
1:D:123:LYS:HE3	2:E:154:ASP:OD1	2.14	0.47
2:E:156:THR:C	2:E:158:ASN:H	2.17	0.47
1:A:125:LYS:C	1:A:127:ILE:H	2.18	0.47
3:L:251:GLU:HB3	3:L:381:LYS:HB2	1.95	0.47
2:B:179:ILE:CD1	3:C:121:ILE:HG13	2.44	0.47
2:B:252:ILE:HB	2:B:299:ILE:CD1	2.44	0.47
2:K:328:GLY:O	2:K:329:PHE:HB2	2.15	0.47
1:J:140:VAL:CG1	2:K:171:ILE:HD11	2.45	0.47
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.13	0.47
2:E:157:VAL:O	2:E:157:VAL:CG1	2.63	0.47
2:H:422:TYR:OH	2:H:432:ASP:OD1	2.14	0.47
1:J:178:TYR:O	1:J:182:GLN:HB2	2.15	0.47
2:E:435:VAL:HG12	2:E:447:MET:HB2	1.97	0.47
4:N:155:TYR:HD1	4:N:155:TYR:O	1.95	0.47
3:I:367:ILE:HG21	3:I:382:THR:HG21	1.96	0.47
3:I:245:ALA:HB2	3:I:389:PHE:CD1	2.49	0.47
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.97	0.47
3:C:387:ILE:HG13	3:C:388:PRO:HD2	1.97	0.47
2:H:458:PHE:H	2:H:459:PRO:HD2	1.80	0.47
1:D:156:ILE:HG21	2:E:415:ARG:NH1	2.30	0.47
2:H:296:ASN:HB3	2:H:338:TYR:CE2	2.50	0.47
2:K:377:THR:HG22	2:K:401:GLY:HA3	1.97	0.47
2:E:202:ASN:ND2	2:E:284:ASN:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:267:ASP:HB3	2:K:268:PRO:CD	2.42	0.47
1:J:139:ASN:HB3	3:L:114:TYR:CE2	2.50	0.47
1:D:158:ILE:HD12	1:D:171:ARG:NH1	2.29	0.47
2:B:430:GLY:O	2:B:444:TRP:HH2	1.98	0.47
1:G:176:LYS:H	1:G:176:LYS:HD2	1.79	0.47
3:F:229:GLY:O	3:F:232:LYS:HB2	2.15	0.47
2:B:185:ASP:O	2:B:187:SER:N	2.48	0.47
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.96	0.47
2:K:368:THR:HB	2:K:409:ALA:HB2	1.97	0.47
2:K:169:ARG:HD3	4:M:155:TYR:CE2	2.50	0.46
2:B:206:VAL:HG22	2:B:206:VAL:O	2.14	0.46
3:L:275:ARG:HG3	3:L:310:MET:O	2.15	0.46
3:L:330:ASP:HA	3:L:365:ASN:HB3	1.97	0.46
2:H:157:VAL:O	2:H:157:VAL:HG12	2.14	0.46
2:K:161:ILE:N	2:K:162:PRO:HD2	2.30	0.46
2:K:409:ALA:O	2:K:438:MET:HB2	2.16	0.46
3:C:306:SER:O	3:C:337:ASN:ND2	2.48	0.46
1:J:121:VAL:HA	1:J:124:ARG:HB3	1.96	0.46
2:B:275:ASN:O	2:B:290:GLY:HA3	2.15	0.46
3:L:153:CYS:HA	3:L:156:ILE:HD12	1.96	0.46
3:F:250:LEU:HD13	3:F:379:MET:SD	2.55	0.46
2:B:412:PRO:HB3	2:B:450:MET:HG2	1.97	0.46
2:K:157:VAL:O	2:K:157:VAL:HG12	2.16	0.46
3:C:178:PHE:HD1	3:C:178:PHE:N	2.14	0.46
2:E:435:VAL:O	2:E:446:SER:HA	2.15	0.46
1:J:175:LEU:C	1:J:177:ASP:H	2.19	0.46
1:J:140:VAL:HG12	2:K:171:ILE:HD11	1.98	0.46
3:F:372:TRP:CE3	3:F:373:LYS:HE3	2.51	0.46
2:H:432:ASP:CG	2:H:443:SER:O	2.54	0.46
2:K:253:GLN:HA	2:K:292:TYR:O	2.15	0.46
1:J:134:GLN:HA	1:J:137:GLN:HG2	1.98	0.46
2:B:160:ASN:O	2:B:163:THR:HB	2.16	0.46
2:K:410:ALA:HB1	2:K:437:TRP:CE3	2.51	0.46
3:L:191:TRP:CZ3	3:L:247:ARG:HB3	2.51	0.46
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.97	0.46
3:I:209:ILE:H	3:I:209:ILE:HG13	1.63	0.46
2:E:308:THR:HA	2:E:456:PRO:HA	1.98	0.46
1:J:159:ARG:CB	1:J:159:ARG:HH11	2.29	0.45
2:B:268:PRO:O	2:B:273:PHE:HD2	1.99	0.45
2:B:340:ILE:CG1	2:B:341:SER:H	2.26	0.45
3:F:307:HIS:O	3:F:310:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:PRO:HB3	2:B:450:MET:CG	2.46	0.45
3:C:240:SER:O	3:C:242:ILE:N	2.40	0.45
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.97	0.45
3:F:318:ASP:C	3:F:318:ASP:OD1	2.54	0.45
3:F:191:TRP:CZ2	3:F:387:ILE:HG21	2.51	0.45
2:K:252:ILE:HB	2:K:299:ILE:HD11	1.97	0.45
2:H:438:MET:HG2	2:H:442:GLY:O	2.16	0.45
3:L:322:PHE:CD1	3:L:338:LYS:HG3	2.52	0.45
2:E:376:SER:CB	2:E:382:ASN:H	2.27	0.45
3:L:206:LYS:HG3	3:L:215:PHE:CE2	2.51	0.45
2:H:252:ILE:HG22	2:H:294:LEU:HD13	1.99	0.45
2:E:402:TRP:CD1	2:E:403:TRP:N	2.84	0.45
2:K:402:TRP:CH2	2:K:412:PRO:HD2	2.52	0.45
2:H:351:ASN:HD21	2:H:354:MET:HE2	1.78	0.45
2:H:351:ASN:ND2	2:H:354:MET:HE3	2.30	0.45
2:K:172:LEU:HG	3:L:113:ILE:CG2	2.46	0.45
3:L:243:PRO:CB	3:L:264:MET:HG3	2.46	0.45
3:C:372:TRP:CZ3	3:C:373:LYS:HE2	2.51	0.45
3:I:307:HIS:CE1	3:I:340:HIS:HA	2.52	0.45
1:A:184:GLN:HA	1:A:187:GLN:HG3	1.96	0.45
2:E:154:ASP:C	2:E:156:THR:N	2.69	0.45
2:H:250:THR:HG21	2:H:302:LEU:HD21	1.99	0.45
1:J:136:LEU:HD21	3:L:111:GLN:HG3	1.98	0.45
2:H:402:TRP:CG	2:H:403:TRP:N	2.84	0.45
4:N:158:ALA:O	4:N:161:LEU:HB2	2.17	0.45
3:F:200:GLY:N	3:F:225:GLU:OE2	2.35	0.45
3:L:318:ASP:C	3:L:319:ASN:HD22	2.21	0.45
2:H:334:GLU:HA	2:H:338:TYR:CE1	2.51	0.45
2:H:258:GLY:O	2:H:260:VAL:N	2.50	0.45
2:K:435:VAL:O	2:K:446:SER:HA	2.16	0.45
2:K:234:LYS:HG2	2:K:235:PRO:HD2	1.99	0.45
1:A:169:LEU:HB2	2:B:189:GLN:OE1	2.17	0.45
3:L:322:PHE:HD1	3:L:338:LYS:HG3	1.82	0.45
3:I:225:GLU:O	3:I:226:PHE:HB3	2.16	0.45
3:C:329:GLN:C	3:C:331:GLY:H	2.19	0.45
3:F:325:ASN:ND2	3:F:328:GLU:HG2	2.32	0.45
2:B:307:PRO:HB2	2:B:457:PHE:HB3	1.99	0.44
1:A:184:GLN:O	1:A:185:LEU:HB2	2.17	0.44
2:K:230:ASP:HB3	2:K:233:VAL:HB	1.99	0.44
3:I:356:LYS:HD2	3:I:362:GLY:HA3	1.99	0.44
3:L:154:GLN:NE2	3:L:158:ASN:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:432:ASP:CG	2:K:443:SER:O	2.55	0.44
3:L:191:TRP:HB3	3:L:385:LYS:HD2	1.99	0.44
3:I:204:PHE:CE2	3:I:227:TRP:HB2	2.52	0.44
2:K:230:ASP:HB2	2:K:301:GLN:NE2	2.31	0.44
3:F:263:ALA:O	3:F:278:TYR:HB2	2.17	0.44
3:I:338:LYS:N	3:I:339:CYS:HA	2.33	0.44
2:K:174:ASN:O	2:K:178:LYS:HG2	2.18	0.44
2:E:310:LEU:HD12	2:E:311:LEU:H	1.82	0.44
3:C:359:THR:HG21	3:C:365:ASN:ND2	2.31	0.44
3:F:387:ILE:CG1	3:F:388:PRO:HD2	2.47	0.44
2:E:412:PRO:HB3	2:E:450:MET:CG	2.48	0.44
2:H:215:ILE:HA	2:H:219:GLY:O	2.17	0.44
3:I:281:PHE:CG	3:I:288:ASP:HB2	2.52	0.44
3:L:193:VAL:HG12	3:L:194:PHE:N	2.32	0.44
2:H:406:ARG:N	2:H:407:CYS:HA	2.32	0.44
2:B:312:ILE:HG12	2:B:452:MET:HG2	1.99	0.44
4:M:171:ALA:O	4:M:174:LEU:HB3	2.18	0.44
2:H:412:PRO:CB	2:H:450:MET:CE	2.90	0.44
3:L:197:ARG:NH2	3:L:348:TYR:HB2	2.33	0.44
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.18	0.44
2:H:350:GLY:O	2:H:352:ALA:N	2.51	0.44
3:L:109:TYR:CE2	4:N:150:GLN:HG2	2.53	0.44
1:D:178:TYR:O	1:D:182:GLN:HB2	2.17	0.44
3:C:207:ASN:OD1	3:C:209:ILE:N	2.51	0.44
2:H:252:ILE:HB	2:H:299:ILE:CD1	2.47	0.44
3:C:301:ASP:C	3:C:303:PHE:N	2.71	0.44
1:J:133:ILE:O	1:J:133:ILE:HG22	2.18	0.44
2:B:237:ARG:HG3	2:B:237:ARG:NH1	2.30	0.44
2:B:160:ASN:C	2:B:160:ASN:OD1	2.56	0.44
2:B:204:PRO:HG3	2:B:223:GLU:OE2	2.17	0.44
3:C:128:VAL:C	3:C:130:GLN:H	2.21	0.44
3:C:304:PHE:CG	3:C:338:LYS:HE3	2.53	0.44
3:I:234:HIS:CE1	3:I:269:PRO:HG3	2.53	0.44
3:I:390:ASN:N	3:I:390:ASN:OD1	2.51	0.44
3:L:194:PHE:HB2	3:L:228:LEU:HB3	2.00	0.43
2:B:378:TYR:CD1	2:B:378:TYR:C	2.91	0.43
1:J:127:ILE:HG22	1:J:127:ILE:O	2.18	0.43
3:I:287:GLY:HA3	3:I:371:THR:HB	1.98	0.43
2:E:251:VAL:HG22	2:E:453:LYS:HG2	2.00	0.43
4:N:141:LYS:O	4:N:143:ALA:N	2.51	0.43
2:H:343:ASN:HA	2:H:354:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:344:LEU:HA	3:I:367:ILE:HG23	2.00	0.43
1:J:150:LEU:HD13	3:L:125:LYS:HE2	1.99	0.43
1:D:155:ASP:HB2	1:D:173:VAL:HG21	1.99	0.43
2:E:326:TYR:O	2:E:328:GLY:N	2.52	0.43
4:N:155:TYR:CE1	4:N:159:THR:CG2	2.95	0.43
3:C:191:TRP:HZ3	3:C:247:ARG:CB	2.31	0.43
2:E:310:LEU:HD12	2:E:311:LEU:N	2.33	0.43
2:B:435:VAL:O	2:B:446:SER:HA	2.19	0.43
2:H:438:MET:HA	2:H:442:GLY:O	2.18	0.43
3:I:234:HIS:HE1	3:I:269:PRO:HG3	1.83	0.43
3:C:153:CYS:HB2	3:C:192:THR:OG1	2.18	0.43
1:G:154:ILE:CG2	1:G:171:ARG:HH12	2.30	0.43
2:B:172:LEU:HB3	3:C:113:ILE:HG21	2.00	0.43
2:K:435:VAL:HG12	2:K:447:MET:HB2	2.00	0.43
3:L:229:GLY:O	3:L:233:ILE:HG13	2.18	0.43
2:H:240:CYS:CB	2:H:242:MET:HE3	2.44	0.43
1:J:159:ARG:C	1:J:161:CYS:H	2.22	0.43
2:B:410:ALA:HA	2:B:436:VAL:O	2.19	0.43
2:K:429:HIS:C	2:K:431:THR:H	2.22	0.43
2:B:389:ASP:C	2:B:391:ARG:H	2.22	0.43
2:K:310:LEU:HD22	2:K:329:PHE:CE2	2.53	0.43
1:D:130:VAL:O	1:D:134:GLN:HG2	2.19	0.43
3:L:197:ARG:CD	3:L:204:PHE:CE2	3.01	0.43
1:A:147:MET:HG2	3:C:121:ILE:HD11	2.01	0.43
1:J:175:LEU:C	1:J:177:ASP:N	2.72	0.43
2:B:378:TYR:HA	2:B:395:SER:O	2.17	0.43
3:C:275:ARG:NH2	3:C:311:GLN:NE2	2.67	0.43
3:F:169:ILE:HG12	3:F:180:VAL:HG22	2.00	0.43
2:B:255:ARG:CZ	2:B:262:PHE:CD1	3.02	0.43
1:A:126:VAL:HG12	1:A:126:VAL:O	2.19	0.43
4:N:145:GLU:HA	4:N:148:ILE:HG13	2.01	0.43
2:K:374:PHE:HB2	2:K:382:ASN:HB3	2.01	0.43
3:F:166:LEU:HG	3:F:220:PRO:HB3	2.01	0.43
2:B:203:ILE:CD1	3:C:145:ILE:HD11	2.49	0.43
2:K:307:PRO:HB2	2:K:457:PHE:HB3	1.99	0.43
2:E:329:PHE:C	2:E:329:PHE:CD1	2.93	0.42
2:E:415:ARG:H	2:E:434:GLY:HA2	1.84	0.42
3:L:264:MET:H	3:L:264:MET:HE2	1.82	0.42
2:B:185:ASP:C	2:B:187:SER:N	2.72	0.42
3:L:295:PHE:CD2	3:L:375:ARG:HD3	2.54	0.42
3:I:252:ASP:HB2	3:I:377:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:ASP:O	3:C:206:LYS:HE2	2.19	0.42
3:F:240:SER:O	3:F:241:ALA:HB3	2.20	0.42
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.54	0.42
3:F:264:MET:H	3:F:264:MET:HE2	1.84	0.42
2:B:374:PHE:O	2:B:403:TRP:HA	2.19	0.42
2:E:195:THR:HA	2:E:196:PRO:HD3	1.93	0.42
1:A:166:SER:HG	2:B:195:THR:HG1	1.58	0.42
3:F:131:LEU:HG	3:F:131:LEU:O	2.19	0.42
2:B:252:ILE:HD12	2:B:299:ILE:HD13	2.02	0.42
2:H:402:TRP:CH2	2:H:412:PRO:HG2	2.55	0.42
3:I:154:GLN:O	3:I:157:ALA:N	2.52	0.42
3:I:195:GLN:HB3	3:I:384:MET:HB2	2.02	0.42
2:B:161:ILE:N	2:B:162:PRO:HD2	2.35	0.42
3:F:225:GLU:O	3:F:226:PHE:HB3	2.19	0.42
3:F:207:ASN:OD1	3:F:207:ASN:C	2.58	0.42
3:L:166:LEU:HG	3:L:220:PRO:HB3	2.01	0.42
2:B:230:ASP:HB3	2:B:233:VAL:CG2	2.50	0.42
3:F:128:VAL:C	3:F:130:GLN:H	2.22	0.42
2:H:172:LEU:HD22	3:I:113:ILE:HG22	2.02	0.42
3:C:166:LEU:HB3	3:C:179:LEU:HD11	2.02	0.42
3:I:197:ARG:HB2	3:I:382:THR:HG23	2.00	0.42
2:H:179:ILE:O	2:H:183:GLU:HB2	2.20	0.42
1:D:149:ARG:HG2	2:E:425:ASP:O	2.19	0.42
4:M:155:TYR:HD1	4:M:155:TYR:O	2.02	0.42
2:B:314:MET:CB	2:B:450:MET:HE2	2.50	0.42
2:K:212:GLU:O	2:K:215:ILE:HG22	2.20	0.42
2:B:199:VAL:HG11	2:B:278:THR:HG22	2.00	0.42
2:K:312:ILE:HG12	2:K:452:MET:HG2	2.02	0.42
2:H:351:ASN:ND2	2:H:354:MET:HE2	2.34	0.42
2:K:159:SER:HA	2:K:162:PRO:HG2	2.02	0.42
2:K:410:ALA:HA	2:K:436:VAL:O	2.19	0.42
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.84	0.42
2:B:310:LEU:CD2	2:B:329:PHE:CD1	3.03	0.42
1:D:179:GLU:HA	1:D:182:GLN:HB2	2.02	0.42
3:I:236:ILE:O	3:I:239:GLN:NE2	2.49	0.42
2:K:176:ARG:CG	2:K:176:ARG:NH1	2.75	0.42
3:F:196:LYS:O	3:F:225:GLU:HA	2.20	0.42
2:H:340:ILE:HG12	2:H:341:SER:N	2.34	0.42
2:B:356:GLY:HA2	2:B:368:THR:O	2.20	0.42
2:H:300:SER:HA	2:H:331:VAL:HB	2.01	0.42
1:G:147:MET:HG3	2:H:175:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:165:GLY:O	3:L:167:TYR:CE1	2.72	0.42
3:L:100:ILE:CG2	3:L:100:ILE:O	2.68	0.42
2:K:435:VAL:O	2:K:447:MET:N	2.52	0.42
3:I:230:ASN:HA	3:I:233:ILE:HG12	2.01	0.42
2:K:238:VAL:CG1	2:K:239:TYR:N	2.82	0.41
3:F:278:TYR:CZ	3:F:308:ASN:HB2	2.55	0.41
3:C:191:TRP:HB3	3:C:385:LYS:HD2	2.02	0.41
3:I:278:TYR:CZ	3:I:308:ASN:HB2	2.55	0.41
3:I:194:PHE:HE2	3:I:386:ILE:HG23	1.84	0.41
3:F:110:LEU:C	3:F:112:GLU:H	2.23	0.41
3:F:370:ALA:HA	3:F:373:LYS:O	2.20	0.41
3:F:287:GLY:HA3	3:F:371:THR:HG1	1.85	0.41
3:C:250:LEU:HD13	3:C:379:MET:SD	2.60	0.41
2:E:438:MET:C	2:E:440:TRP:H	2.24	0.41
2:E:410:ALA:HB1	2:E:437:TRP:CE3	2.55	0.41
2:K:209:LYS:HA	2:K:228:GLN:O	2.19	0.41
1:D:144:LEU:HA	2:E:175:LEU:HD11	2.02	0.41
3:L:110:LEU:C	3:L:112:GLU:H	2.23	0.41
4:M:155:TYR:HE1	4:M:159:THR:CG2	2.33	0.41
2:K:200:SER:HA	3:L:142:THR:OG1	2.19	0.41
2:H:368:THR:HB	2:H:409:ALA:HB2	2.01	0.41
3:C:370:ALA:HA	3:C:373:LYS:O	2.20	0.41
3:L:207:ASN:OD1	3:L:209:ILE:N	2.52	0.41
3:L:334:TRP:CZ3	3:L:335:TRP:HZ3	2.39	0.41
2:K:152:TYR:CD2	2:K:153:ILE:N	2.83	0.41
3:C:185:ASP:OD1	3:C:185:ASP:C	2.59	0.41
2:H:242:MET:HA	2:H:247:GLY:CA	2.51	0.41
1:A:161:CYS:O	1:A:162:ARG:C	2.58	0.41
3:C:191:TRP:CZ3	3:C:247:ARG:HB3	2.56	0.41
2:E:350:GLY:O	2:E:352:ALA:N	2.54	0.41
3:F:109:TYR:CD2	4:M:178:GLN:HG3	2.55	0.41
1:A:168:ALA:HA	2:B:189:GLN:NE2	2.26	0.41
3:F:154:GLN:HG3	3:F:158:ASN:ND2	2.36	0.41
2:E:252:ILE:HD12	2:E:299:ILE:HD13	2.03	0.41
2:K:224:MET:SD	2:K:237:ARG:HB3	2.60	0.41
3:C:191:TRP:HZ3	3:C:247:ARG:HB3	1.86	0.41
2:H:326:TYR:O	2:H:328:GLY:N	2.54	0.41
3:C:281:PHE:CE1	3:C:288:ASP:HB2	2.55	0.41
2:H:186:VAL:O	2:H:186:VAL:HG12	2.21	0.41
3:L:93:ILE:O	3:L:93:ILE:HG22	2.21	0.41
2:E:315:GLU:OE1	2:E:449:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:176:ARG:HD2	3:L:117:ASN:OD1	2.20	0.41
4:M:234:GLU:HA	4:M:237:ILE:HG12	2.03	0.41
2:B:266:TRP:CZ3	2:B:375:PHE:HD2	2.38	0.41
1:A:134:GLN:HA	1:A:137:GLN:HG3	2.02	0.41
2:B:176:ARG:NH2	3:C:116:SER:OG	2.54	0.41
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.95	0.41
4:N:183:TYR:CE1	4:N:187:ASN:ND2	2.88	0.41
3:L:304:PHE:CB	3:L:338:LYS:HB3	2.48	0.41
4:M:183:TYR:HD1	4:M:185:ARG:HB3	1.85	0.41
2:E:238:VAL:HG22	2:E:294:LEU:HD11	2.02	0.41
2:E:352:ALA:HB3	2:E:437:TRP:CZ2	2.55	0.41
3:C:262:TYR:CE1	3:C:281:PHE:HD1	2.39	0.41
2:K:156:THR:C	2:K:158:ASN:H	2.24	0.41
3:F:354:TYR:O	3:F:376:TRP:HB3	2.21	0.41
3:F:217:HIS:CD2	3:F:217:HIS:N	2.88	0.41
2:B:224:MET:SD	2:B:237:ARG:HD3	2.61	0.41
3:F:154:GLN:HG3	3:F:158:ASN:HD21	1.86	0.41
2:E:296:ASN:HB3	2:E:338:TYR:CD1	2.57	0.41
4:N:148:ILE:H	4:N:148:ILE:HG12	1.71	0.40
2:B:294:LEU:HB3	2:B:299:ILE:HD11	2.03	0.40
2:B:249:TRP:CE3	2:B:455:ARG:HB2	2.57	0.40
3:C:326:CYS:SG	3:C:336:MET:HB3	2.61	0.40
3:C:197:ARG:O	3:C:198:LEU:HG	2.21	0.40
3:F:227:TRP:HD1	3:F:229:GLY:N	2.19	0.40
2:E:226:LEU:HD21	3:F:168:PHE:HZ	1.85	0.40
3:L:156:ILE:HD11	3:L:169:ILE:HD11	2.03	0.40
2:K:410:ALA:CB	2:K:437:TRP:CE3	3.04	0.40
2:E:329:PHE:C	2:E:329:PHE:HD1	2.24	0.40
3:L:197:ARG:O	3:L:381:LYS:HA	2.22	0.40
3:I:263:ALA:O	3:I:264:MET:C	2.60	0.40
2:E:314:MET:HB3	2:E:450:MET:HE2	2.04	0.40
2:H:422:TYR:O	2:H:444:TRP:HE3	2.05	0.40
3:F:325:ASN:HB3	3:F:328:GLU:HG2	2.03	0.40
2:B:212:GLU:O	2:B:213:GLU:C	2.59	0.40
4:N:145:GLU:HA	4:N:148:ILE:CG1	2.51	0.40
1:J:143:GLN:HE22	3:L:117:ASN:HB2	1.87	0.40
2:K:365:ARG:C	2:K:367:MET:H	2.24	0.40
2:E:212:GLU:O	2:E:213:GLU:C	2.59	0.40
3:L:287:GLY:HA3	3:L:371:THR:HB	2.02	0.40
1:G:178:TYR:O	1:G:182:GLN:HB2	2.22	0.40
3:L:151:LYS:H	3:L:155:ASP:HB3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:310:LEU:HD22	2:H:329:PHE:CE2	2.56	0.40
2:B:221:THR:O	2:B:225:TYR:OH	2.26	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	73/87 (84%)	53 (73%)	15 (20%)	5 (7%)	1	12
1	D	74/87 (85%)	58 (78%)	14 (19%)	2 (3%)	6	35
1	G	71/87 (82%)	54 (76%)	8 (11%)	9 (13%)	0	2
1	J	70/87 (80%)	52 (74%)	13 (19%)	5 (7%)	1	11
2	B	311/328 (95%)	248 (80%)	52 (17%)	11 (4%)	4	29
2	E	308/328 (94%)	244 (79%)	51 (17%)	13 (4%)	3	23
2	H	311/328 (95%)	255 (82%)	43 (14%)	13 (4%)	3	23
2	K	307/328 (94%)	248 (81%)	47 (15%)	12 (4%)	4	25
3	C	301/319 (94%)	235 (78%)	60 (20%)	6 (2%)	9	43
3	F	302/319 (95%)	244 (81%)	48 (16%)	10 (3%)	5	30
3	I	298/319 (93%)	243 (82%)	48 (16%)	7 (2%)	8	39
3	L	303/319 (95%)	245 (81%)	46 (15%)	12 (4%)	4	24
4	M	106/146 (73%)	93 (88%)	10 (9%)	3 (3%)	6	34
4	N	106/146 (73%)	97 (92%)	7 (7%)	2 (2%)	10	45
All	All	2941/3228 (91%)	2369 (81%)	462 (16%)	110 (4%)	4	27

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	338	TYR
2	E	341	SER
2	E	439	ASN
3	F	240	SER
1	G	192	ASP
2	K	154	ASP
3	L	205	LYS
4	M	172	LEU
4	M	185	ARG
4	N	144	LEU
1	A	126	VAL
2	B	186	VAL
2	B	327	GLY
3	C	241	ALA
3	C	317	ASN
3	C	331	GLY
1	D	126	VAL
1	D	153	ASP
2	E	327	GLY
2	E	338	TYR
2	E	351	ASN
3	F	161	ALA
3	F	260	ALA
1	G	189	ILE
1	G	191	LYS
2	H	157	VAL
2	H	229	PRO
2	H	259	SER
2	H	305	MET
2	H	351	ASN
3	I	94	MET
3	I	264	MET
2	K	153	ILE
2	K	329	PHE
3	L	133	ALA
3	L	264	MET
3	L	318	ASP
4	M	171	ALA
1	A	160	SER
2	B	182	LEU
2	B	428	LYS
3	C	96	TYR
3	C	295	PHE

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Mol	Chain	Res	Type
2	E	329	PHE
1	G	162	ARG
2	H	279	ASN
2	H	458	PHE
1	J	164	SER
2	K	206	VAL
2	K	245	GLU
2	K	279	ASN
2	K	338	TYR
2	K	427	ALA
3	L	160	GLY
3	L	164	SER
1	A	166	SER
2	B	245	GLU
2	B	257	ASP
2	B	459	PRO
3	C	320	ASP
3	F	274	TYR
1	G	184	GLN
1	G	190	ALA
2	H	217	LYS
2	H	256	GLN
2	H	281	ASP
2	H	327	GLY
2	H	397	GLU
3	I	162	LYS
3	I	164	SER
1	J	134	GLN
1	J	153	ASP
2	K	359	GLN
2	K	458	PHE
3	L	241	ALA
3	L	337	ASN
1	A	164	SER
2	B	397	GLU
2	E	245	GLU
2	E	455	ARG
2	E	456	PRO
3	F	162	LYS
3	F	175	ASN
3	F	290	PHE
3	F	293	PHE

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Mol	Chain	Res	Type
3	F	338	LYS
1	G	164	SER
1	G	185	LEU
1	G	194	LEU
2	K	257	ASP
3	L	118	ASN
3	L	285	ASP
4	N	142	GLU
2	E	419	GLY
3	I	161	ALA
1	J	176	LYS
3	L	93	ILE
2	B	263	GLY
2	E	307	PRO
2	H	307	PRO
3	I	160	GLY
3	L	360	PRO
2	E	458	PHE
3	I	269	PRO
2	K	263	GLY
1	A	156	ILE
1	J	133	ILE
2	E	229	PRO
3	F	160	GLY
2	B	390	PRO

### 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	69/82 (84%)	64 (93%)	5 (7%)	18	54
1	D	71/82 (87%)	67 (94%)	4 (6%)	26	65
1	G	67/82 (82%)	64 (96%)	3 (4%)	34	72
1	J	67/82 (82%)	59 (88%)	8 (12%)	6	27
2	B	270/286 (94%)	252 (93%)	18 (7%)	20	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	267/286 (93%)	256 (96%)	11 (4%)	37	74
2	H	271/286 (95%)	257 (95%)	14 (5%)	29	67
2	K	266/286 (93%)	246 (92%)	20 (8%)	17	52
3	C	255/267 (96%)	239 (94%)	16 (6%)	22	60
3	F	256/267 (96%)	242 (94%)	14 (6%)	27	66
3	I	253/267 (95%)	238 (94%)	15 (6%)	24	63
3	L	257/267 (96%)	245 (95%)	12 (5%)	32	70
4	M	94/130 (72%)	83 (88%)	11 (12%)	7	28
4	N	94/130 (72%)	82 (87%)	12 (13%)	5	23
All	All	2557/2800 (91%)	2394 (94%)	163 (6%)	22	60

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	140	VAL
1	A	145	VAL
1	A	149	ARG
1	A	159	ARG
2	B	183	GLU
2	B	200	SER
2	B	206	VAL
2	B	221	THR
2	B	224	MET
2	B	238	VAL
2	B	269	TYR
2	B	275	ASN
2	B	280	THR
2	B	294	LEU
2	B	302	LEU
2	B	325	HIS
2	B	348	THR
2	B	376	SER
2	B	378	TYR
2	B	405	ASN
2	B	424	TRP
2	B	436	VAL
3	C	96	TYR
3	C	113	ILE

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Mol	Chain	Res	Type
3	C	121	ILE
3	C	128	VAL
3	C	132	GLU
3	C	144	GLN
3	C	178	PHE
3	C	183	GLU
3	C	226	PHE
3	C	285	ASP
3	C	315	TRP
3	C	339	CYS
3	C	340	HIS
3	C	359	THR
3	C	374	THR
3	C	390	ASN
1	D	146	ASP
1	D	149	ARG
1	D	150	LEU
1	D	185	LEU
2	E	152	TYR
2	E	155	GLU
2	E	165	LEU
2	E	221	THR
2	E	271	GLN
2	E	301	GLN
2	E	308	THR
2	E	329	PHE
2	E	378	TYR
2	E	424	TRP
2	E	431	THR
3	F	110	LEU
3	F	163	GLN
3	F	167	TYR
3	F	176	GLN
3	F	209	ILE
3	F	217	HIS
3	F	223	THR
3	F	228	LEU
3	F	239	GLN
3	F	242	ILE
3	F	302	LYS
3	F	315	TRP
3	F	340	HIS

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Mol	Chain	Res	Type
3	F	378	SER
1	G	164	SER
1	G	187	GLN
1	G	192	ASP
2	H	158	ASN
2	H	160	ASN
2	H	161	ILE
2	H	201	CYS
2	H	206	VAL
2	H	285	TYR
2	H	308	THR
2	H	309	GLU
2	H	361	MET
2	H	378	TYR
2	H	436	VAL
2	H	446	SER
2	H	451	SER
2	H	453	LYS
3	I	118	ASN
3	I	128	VAL
3	I	152	ASP
3	I	167	TYR
3	I	169	ILE
3	I	177	GLN
3	I	199	ASP
3	I	209	ILE
3	I	259	THR
3	I	303	PHE
3	I	314	THR
3	I	317	ASN
3	I	329	GLN
3	I	356	LYS
3	I	382	THR
1	J	136	LEU
1	J	137	GLN
1	J	141	ARG
1	J	149	ARG
1	J	154	ILE
1	J	162	ARG
1	J	164	SER
1	J	187	GLN
2	K	155	GLU

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Mol	Chain	Res	Type
2	K	163	THR
2	K	164	ASN
2	K	171	ILE
2	K	176	ARG
2	K	203	ILE
2	K	206	VAL
2	K	224	MET
2	K	227	ILE
2	K	267	ASP
2	K	269	TYR
2	K	276	VAL
2	K	280	THR
2	K	308	THR
2	K	330	THR
2	K	336	ASN
2	K	376	SER
2	K	383	ASP
2	K	421	GLN
2	K	448	ARG
3	L	106	SER
3	L	114	TYR
3	L	121	ILE
3	L	152	ASP
3	L	167	TYR
3	L	183	GLU
3	L	264	MET
3	L	291	ASP
3	L	317	ASN
3	L	359	THR
3	L	386	ILE
3	L	390	ASN
4	M	144	LEU
4	M	146	LEU
4	M	148	ILE
4	M	150	GLN
4	M	153	ARG
4	M	155	TYR
4	M	159	THR
4	M	165	LEU
4	M	188	VAL
4	M	203	ASN
4	M	217	LEU

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Mol	Chain	Res	Type
4	N	144	LEU
4	N	146	LEU
4	N	148	ILE
4	N	155	TYR
4	N	157	ARG
4	N	159	THR
4	N	172	LEU
4	N	174	LEU
4	N	180	SER
4	N	183	TYR
4	N	203	ASN
4	N	213	GLU

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	174	ASN
2	E	254	ASN
3	F	319	ASN
2	H	351	ASN
2	H	411	ASN
3	I	337	ASN
1	J	182	GLN
2	K	158	ASN
2	K	336	ASN
2	K	411	ASN
4	M	200	GLN
4	M	203	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	75/87 (86%)	0.27	1 (1%) 79 74	42, 82, 154, 183	0
1	D	76/87 (87%)	0.26	0 100 100	28, 72, 145, 164	0
1	G	73/87 (83%)	0.25	1 (1%) 78 73	36, 83, 157, 208	0
1	J	72/87 (82%)	0.19	1 (1%) 78 73	41, 87, 139, 162	0
2	B	313/328 (95%)	0.24	1 (0%) 94 94	21, 68, 147, 196	0
2	E	310/328 (94%)	0.32	3 (0%) 84 80	18, 60, 121, 187	0
2	H	313/328 (95%)	0.32	7 (2%) 65 59	21, 71, 140, 196	0
2	K	309/328 (94%)	0.22	2 (0%) 90 88	25, 77, 149, 196	0
3	C	303/319 (94%)	0.28	2 (0%) 89 86	15, 55, 105, 180	0
3	F	304/319 (95%)	0.33	2 (0%) 89 86	20, 61, 112, 208	0
3	I	300/319 (94%)	0.34	13 (4%) 39 32	30, 78, 149, 191	0
3	L	305/319 (95%)	0.31	6 (1%) 68 62	23, 69, 122, 187	0
4	M	108/146 (73%)	0.11	1 (0%) 85 82	38, 126, 180, 208	0
4	N	108/146 (73%)	0.24	4 (3%) 45 38	31, 111, 169, 201	0
All	All	2969/3228 (91%)	0.28	44 (1%) 76 71	15, 70, 150, 208	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	390	PRO	6.1
2	H	388	SER	6.1
4	N	239	ASP	5.5
2	H	148	LYS	5.1
2	K	390	PRO	4.9
3	I	295	PHE	4.4
1	G	196	SER	4.3
3	I	330	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	L	179	LEU	3.5
3	C	323	GLU	3.3
2	B	390	PRO	3.2
3	L	169	ILE	3.2
3	C	363	TYR	3.0
2	H	151	LEU	2.9
4	N	225	THR	2.9
3	I	368	ILE	2.8
4	M	142	GLU	2.8
2	H	460	GLN	2.8
3	I	226	PHE	2.7
3	I	367	ILE	2.6
3	F	297	ASP	2.5
2	K	324	ALA	2.5
3	I	290	PHE	2.5
2	H	459	PRO	2.5
4	N	221	LYS	2.4
3	I	335	TRP	2.4
3	F	330	ASP	2.4
3	L	151	LYS	2.4
3	L	145	ILE	2.4
1	A	188	VAL	2.4
4	N	235	LYS	2.3
3	L	250	LEU	2.3
3	I	344	LEU	2.3
2	E	409	ALA	2.2
3	I	340	HIS	2.2
1	J	122	LEU	2.2
2	E	358	SER	2.2
3	I	364	ASP	2.2
3	I	249	GLU	2.1
2	H	395	SER	2.1
3	L	363	TYR	2.1
3	I	341	ALA	2.1
2	E	166	ARG	2.0
3	I	204	PHE	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.