



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 07:55 AM EST

PDB ID : 2IAE  
Title : Crystal structure of a protein phosphatase 2A (PP2A) holoenzyme.  
Authors : Cho, U.S.; Xu, W.  
Deposited on : 2006-09-07  
Resolution : 3.50 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.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

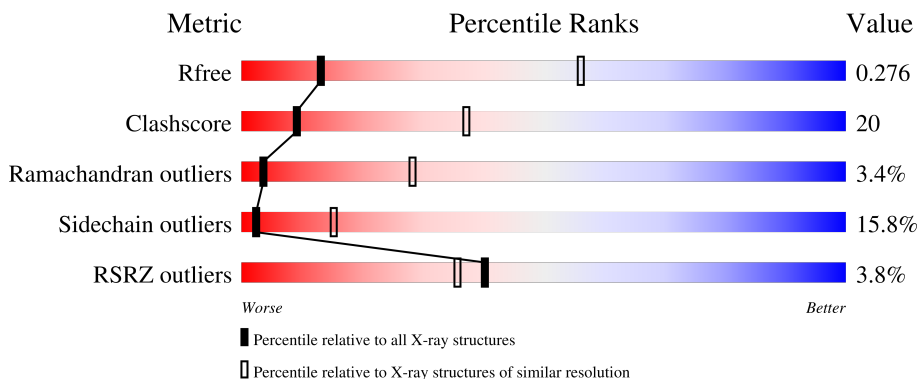
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	589	
1	D	589	
2	B	407	
2	E	407	
3	C	309	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	309	
4	M	7	
4	N	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLL	C	309	-	X	-	X
4	DAM	M	7	-	-	X	-
4	ACB	N	3	-	-	X	-
4	DAM	N	7	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19955 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	Total	C	N	O	S	0	0	0
			4541	2885	765	864	27			
1	D	583	Total	C	N	O	S	0	0	0
			4541	2885	765	864	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	376	Total	C	N	O	S	0	0	0
			2974	1945	486	533	10			
2	E	377	Total	C	N	O	S	0	0	0
			2987	1958	487	531	11			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	306	Total	C	N	O	S	0	0	0
			2430	1538	415	462	15			
3	F	291	Total	C	N	O	S	0	0	0
			2336	1479	402	440	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	ASN	ASP	engineered mutation	UNP P67775
F	88	ASN	ASP	engineered mutation	UNP P67775

- Molecule 4 is a protein called microcystin-LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	N	7	Total	C	N	O	0	0	0
			71	49	10	12			

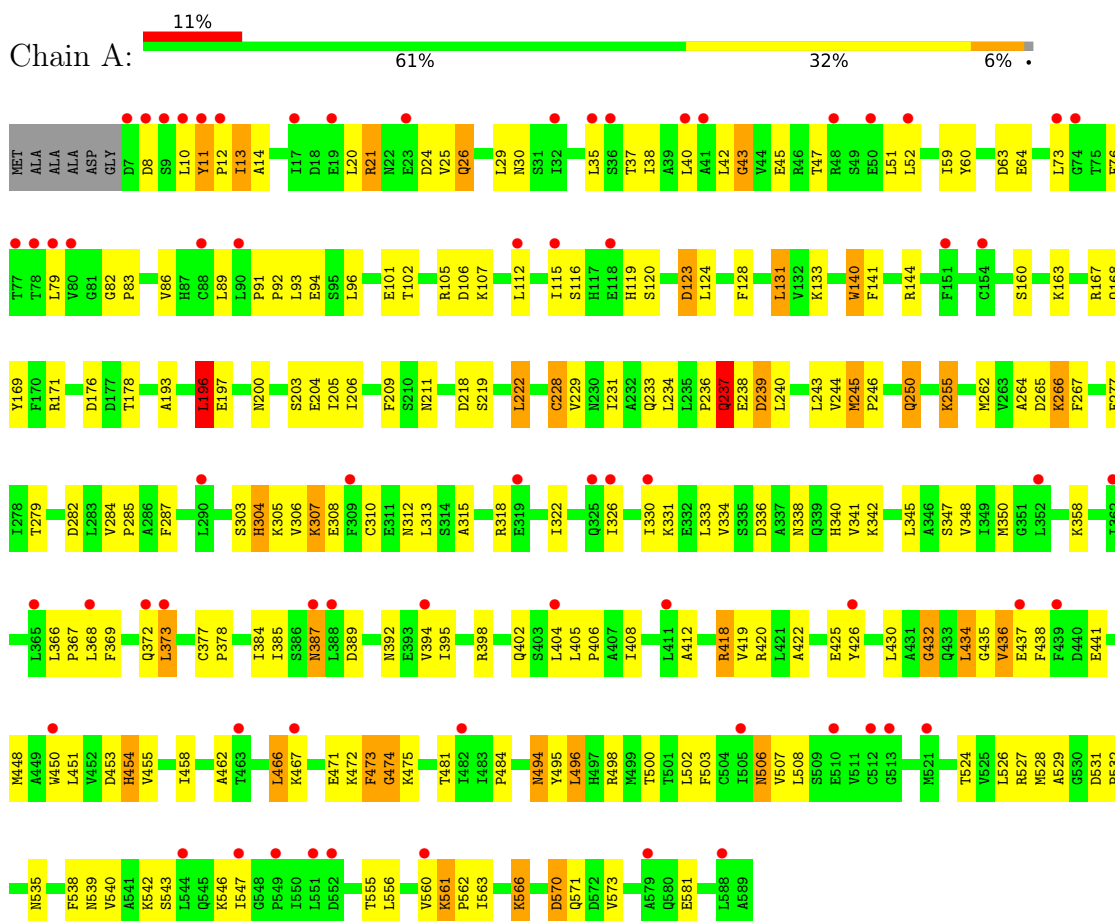
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		

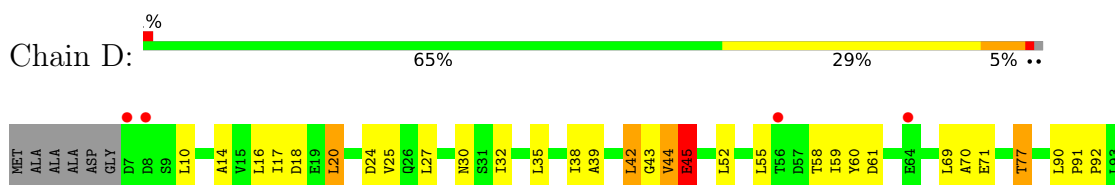
### 3 Residue-property plots

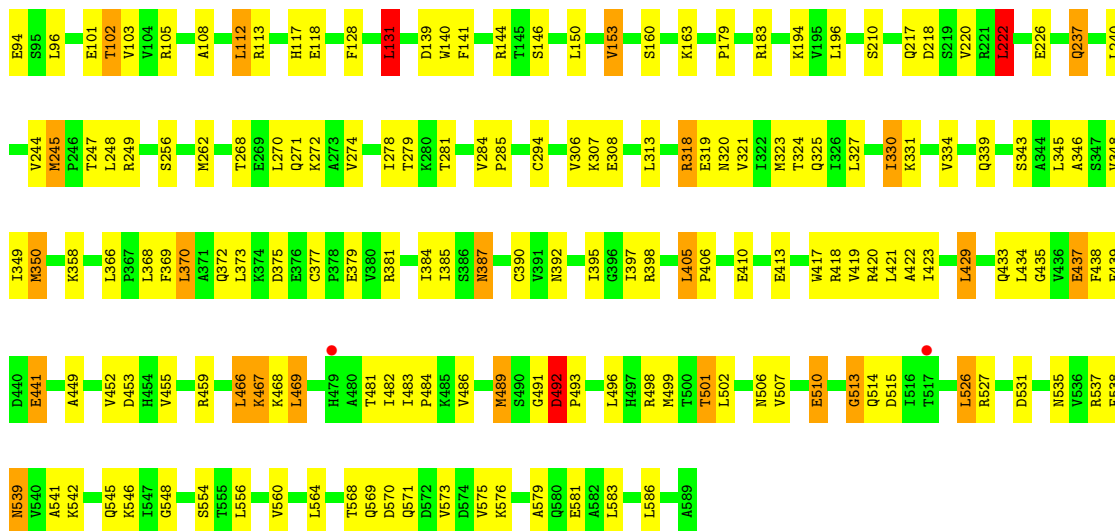
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

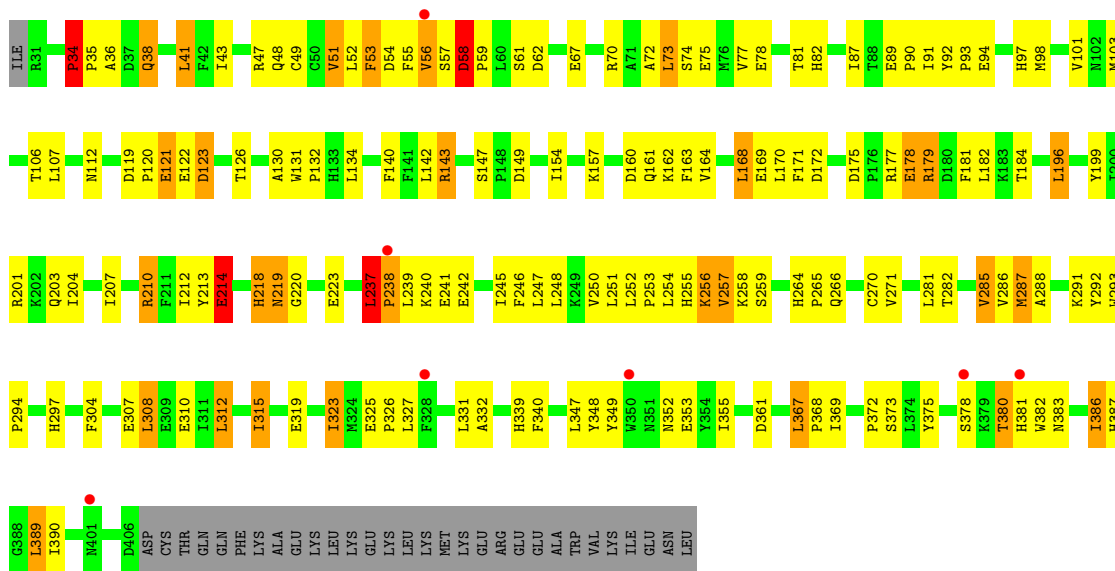


- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

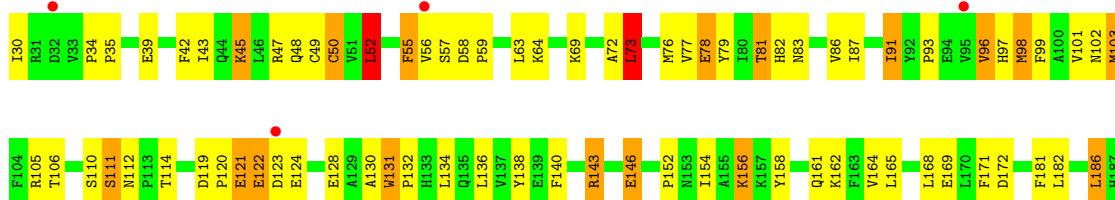


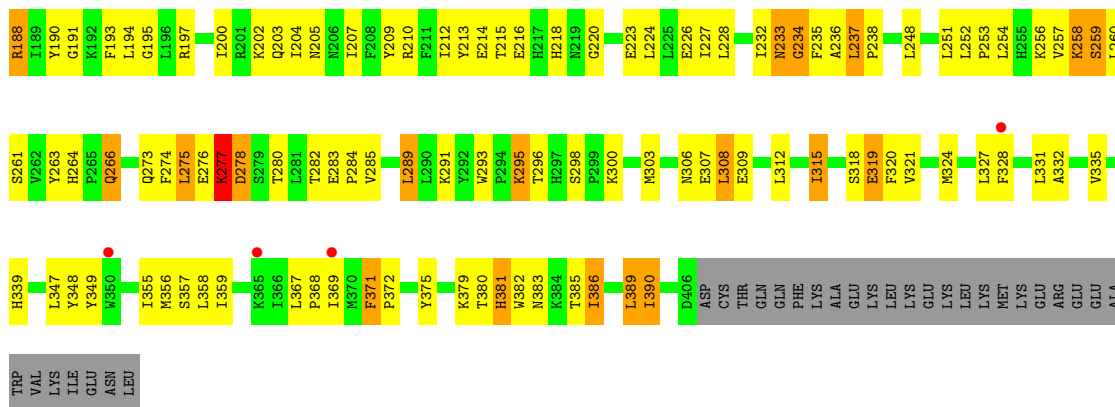


- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

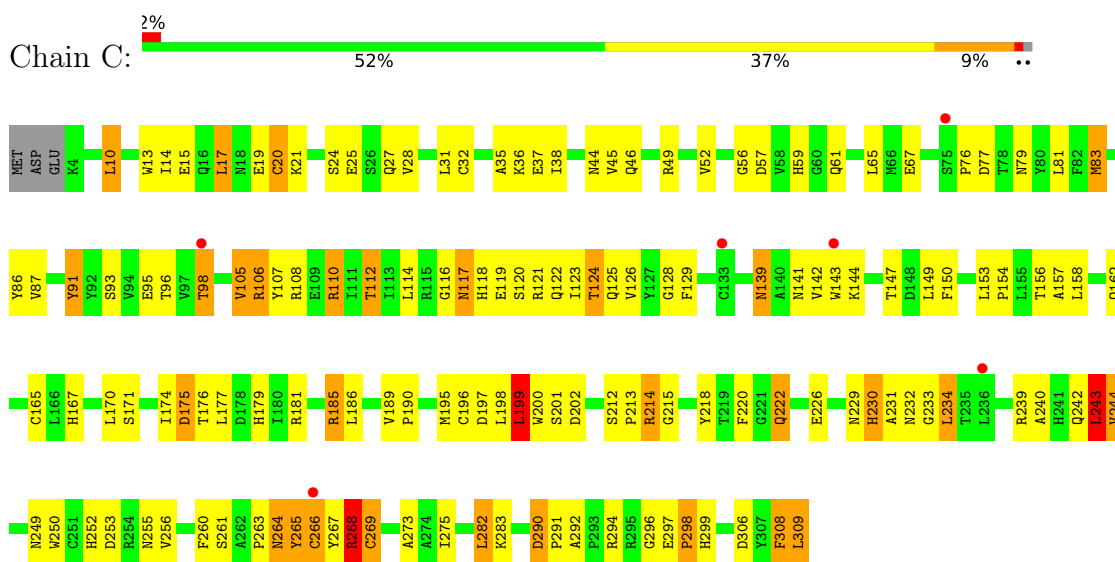


- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

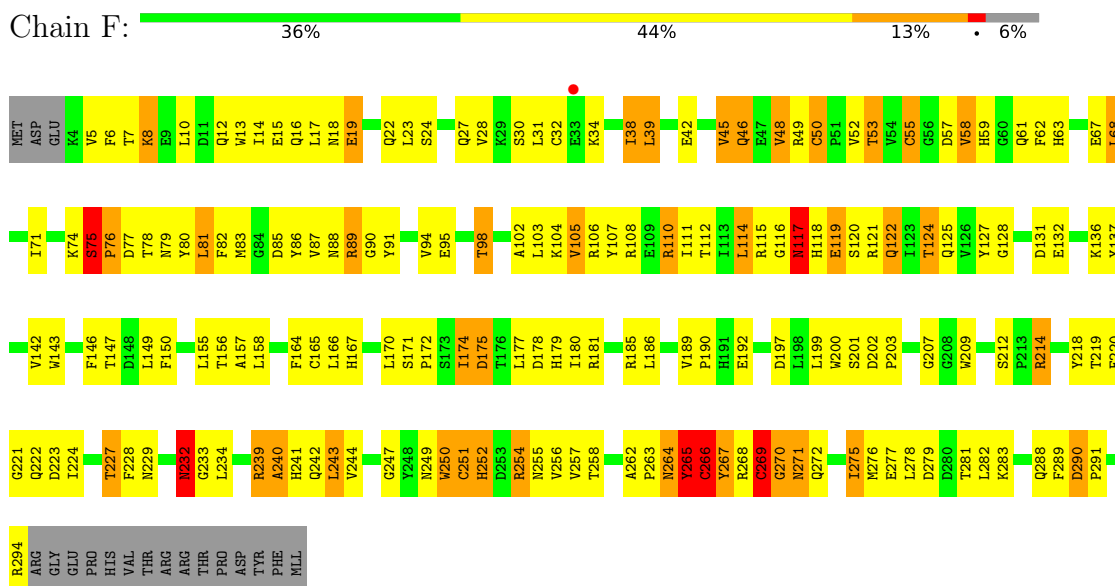




• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform





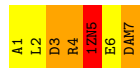
- Molecule 4: microcystin-LR

Chain M:  14% 43% 43%



- Molecule 4: microcystin-LR

Chain N:  43% 43% 14%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	265.30Å 265.30Å 265.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 49.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.50) 97.4 (49.27-3.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.257 , 0.316 0.233 , 0.276	Depositor DCC
$R_{free}$ test set	3853 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.3	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 190.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.037 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, DAM, FGA, DAL, MN, MLL, ACB

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	0.40	0/4615	0.61	3/6266 (0.0%)
1	D	0.44	0/4615	0.63	2/6266 (0.0%)
2	B	0.46	0/3056	0.64	2/4170 (0.0%)
2	E	0.47	0/3073	0.64	2/4195 (0.0%)
3	C	0.44	0/2480	0.70	3/3371 (0.1%)
3	F	0.53	0/2393	0.75	1/3247 (0.0%)
4	M	0.69	0/17	0.98	0/19
4	N	1.49	0/17	1.81	0/19
All	All	0.45	0/20266	0.65	13/27553 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
2	B	0	1
2	E	0	2
3	C	0	4
3	F	0	2
4	M	0	4
4	N	0	1
All	All	0	17

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	298	PRO	N-CA-CB	6.44	111.03	103.30
2	E	52	LEU	CA-CB-CG	6.18	129.51	115.30
2	B	34	PRO	N-CA-CB	5.86	110.33	103.30
1	A	434	LEU	CA-CB-CG	5.72	128.46	115.30
2	E	73	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	496	LEU	CA-CB-CG	5.56	128.10	115.30
1	D	131	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	131	LEU	CA-CB-CG	5.41	127.73	115.30
3	C	199	LEU	CA-CB-CG	5.30	127.49	115.30
3	C	243	LEU	CA-CB-CG	5.30	127.49	115.30
3	F	90	GLY	N-CA-C	-5.14	100.25	113.10
1	D	222	LEU	CA-CB-CG	5.08	126.97	115.30
2	B	41	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	LEU	Peptide
2	B	214	GLU	Peptide
3	C	233	GLY	Peptide
3	C	266	CYS	Peptide
3	C	296	GLY	Peptide
3	C	308	PHE	Peptide
1	D	492	ASP	Peptide
1	D	59	ILE	Peptide
2	E	234	GLY	Peptide
2	E	277	LYS	Peptide
3	F	266	CYS	Peptide
3	F	75	SER	Peptide
4	M	2	LEU	Mainchain
4	M	4	ARG	Peptide
4	M	5	1ZN	Mainchain,Peptide
4	N	5	1ZN	Peptide

## 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	4541	0	4641	135	0
1	D	4541	0	4641	122	0
2	B	2974	0	2849	119	0
2	E	2987	0	2858	132	0
3	C	2430	0	2273	108	2
3	F	2336	0	2229	179	4
4	M	71	0	61	16	2
4	N	71	0	63	28	4
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	19955	0	19615	790	6

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 20.

All (790) 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:N:2:LEU:HA	4:N:3:ACB:C4	1.12	1.53
4:N:2:LEU:CA	4:N:3:ACB:H43	1.04	1.51
4:N:2:LEU:O	4:N:3:ACB:N	1.74	1.18
4:N:2:LEU:CA	4:N:3:ACB:C4	1.86	1.17
4:N:2:LEU:HA	4:N:3:ACB:H42	1.29	1.12
4:N:2:LEU:N	4:N:3:ACB:C4	2.09	1.12
3:F:171:SER:HB2	3:F:197:ASP:HB3	1.33	1.08
3:C:269:CYS:SG	4:M:7:DAM:HB2	1.95	1.07
3:F:88:ASN:HB2	3:F:118:HIS:HD2	1.20	1.05
1:D:437:GLU:OE1	1:D:437:GLU:HA	1.52	1.03
3:F:46:GLN:HE21	3:F:46:GLN:HA	1.22	1.01
1:D:492:ASP:HA	1:D:498:ARG:HD3	1.38	1.00
4:N:2:LEU:N	4:N:3:ACB:H41	1.76	0.99
3:C:269:CYS:SG	4:M:7:DAM:CB	2.51	0.99
3:F:45:VAL:HG23	3:F:156:THR:HG23	1.43	0.98
4:N:2:LEU:C	4:N:3:ACB:H43	1.84	0.98
3:F:79:ASN:HD21	3:F:110:ARG:HE	1.12	0.97
3:C:185:ARG:HH21	3:C:185:ARG:HG3	1.28	0.95
2:E:237:LEU:HB3	2:E:238:PRO:HD2	1.49	0.94
3:C:124:THR:CG2	3:C:143:TRP:HE1	1.82	0.93
2:E:57:SER:HB2	2:E:59:PRO:HD2	1.52	0.92
2:B:352:ASN:HB2	2:B:355:ILE:HD12	1.53	0.91
3:F:244:VAL:HG11	3:F:249:ASN:HB2	1.51	0.91
3:F:243:LEU:CD2	4:N:7:DAM:HB1	2.00	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:2:LEU:N	4:N:3:ACB:H43	1.77	0.90
3:F:171:SER:HB2	3:F:197:ASP:CB	2.02	0.89
3:F:88:ASN:HB2	3:F:118:HIS:CD2	2.06	0.89
3:F:214:ARG:HG2	3:F:214:ARG:HH11	1.37	0.88
3:F:214:ARG:NE	3:F:241:HIS:HE1	1.70	0.88
4:N:2:LEU:H	4:N:3:ACB:H41	1.37	0.88
3:F:243:LEU:HD21	4:N:7:DAM:HB1	1.55	0.87
3:F:124:THR:HG21	3:F:143:TRP:HE1	1.38	0.87
2:B:87:ILE:HA	2:B:91:ILE:HD11	1.56	0.87
3:F:214:ARG:O	4:N:4:ARG:NH1	2.08	0.87
2:E:120:PRO:C	2:E:122:GLU:H	1.79	0.86
1:D:417:TRP:HZ3	1:D:421:LEU:HD12	1.41	0.85
1:D:245:MET:CE	1:D:245:MET:HA	2.06	0.85
3:F:124:THR:CG2	3:F:143:TRP:HE1	1.91	0.84
3:F:269:CYS:SG	4:N:7:DAM:CB	2.66	0.83
3:C:185:ARG:HH21	3:C:185:ARG:CG	1.92	0.82
2:B:367:LEU:H	2:B:368:PRO:HD2	1.44	0.82
3:C:171:SER:HB2	3:C:197:ASP:HB2	1.62	0.81
3:F:8:LYS:HE3	3:F:8:LYS:HA	1.61	0.81
3:F:98:THR:HB	3:F:146:PHE:HZ	1.45	0.81
1:D:492:ASP:HA	1:D:498:ARG:CD	2.10	0.80
3:F:229:ASN:HD22	3:F:255:ASN:HD22	1.29	0.80
3:F:79:ASN:ND2	3:F:110:ARG:HE	1.79	0.80
3:F:116:GLY:H	3:F:119:GLU:HG2	1.47	0.80
1:D:548:GLY:HA3	1:D:586:LEU:HD21	1.62	0.80
3:F:269:CYS:CB	4:N:7:DAM:HB2	2.12	0.79
2:B:256:LYS:HB2	3:C:309:MLL:HD22	1.64	0.79
3:C:17:LEU:HD12	3:C:98:THR:HG23	1.65	0.79
1:A:115:ILE:O	1:A:119:HIS:HD2	1.65	0.78
3:C:124:THR:HG23	3:C:143:TRP:HE1	1.46	0.78
3:F:171:SER:HB3	3:F:174:ILE:HD11	1.63	0.78
3:F:201:SER:HB2	3:F:218:TYR:O	1.83	0.78
2:E:190:TYR:CZ	2:E:197:ARG:HG3	2.19	0.78
3:C:201:SER:HB2	3:C:218:TYR:O	1.85	0.77
3:F:264:ASN:HA	3:F:267:TYR:O	1.85	0.77
3:C:243:LEU:HD21	4:M:7:DAM:HB1	1.65	0.77
2:B:237:LEU:HB2	2:B:238:PRO:HD2	1.67	0.77
3:F:269:CYS:SG	4:N:7:DAM:HB2	2.26	0.76
1:D:268:THR:HG21	1:D:308:GLU:HG2	1.68	0.75
1:D:435:GLY:HA2	1:D:438:PHE:HB3	1.68	0.75
3:F:24:SER:H	3:F:27:GLN:HE21	1.35	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:H	1:A:239:ASP:HB3	1.51	0.75
3:C:265:TYR:O	3:C:268:ARG:HB3	1.87	0.75
3:C:201:SER:HB3	3:C:218:TYR:H	1.52	0.74
3:F:147:THR:HA	3:F:150:PHE:CD1	2.22	0.74
2:B:52:LEU:HD11	2:B:97:HIS:CD2	2.22	0.74
2:B:121:GLU:OE1	4:M:2:LEU:CD1	2.36	0.74
3:F:88:ASN:CB	3:F:118:HIS:HD2	1.99	0.74
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.69	0.73
3:C:120:SER:O	3:C:124:THR:HB	1.87	0.73
3:F:38:ILE:HD12	3:F:108:ARG:HD3	1.70	0.73
1:A:418:ARG:CG	1:A:418:ARG:HH21	2.02	0.73
3:F:214:ARG:HH11	3:F:214:ARG:CG	2.01	0.73
1:A:244:VAL:O	1:A:244:VAL:HG22	1.87	0.72
1:A:500:THR:HA	1:A:503:PHE:HB2	1.70	0.72
3:F:45:VAL:HG11	3:F:181:ARG:NH1	2.03	0.72
3:F:45:VAL:HG23	3:F:156:THR:CG2	2.19	0.72
1:A:101:GLU:HG2	2:B:256:LYS:HE2	1.70	0.72
1:D:268:THR:HG21	1:D:308:GLU:CG	2.20	0.72
3:F:46:GLN:HE21	3:F:46:GLN:CA	2.01	0.72
1:A:418:ARG:HH21	1:A:418:ARG:HG3	1.54	0.71
1:D:455:VAL:HG23	3:F:71:ILE:HA	1.73	0.71
3:F:68:LEU:HD13	3:F:275:ILE:HG21	1.73	0.71
3:F:214:ARG:NE	3:F:241:HIS:CE1	2.56	0.71
1:A:11:TYR:N	1:A:12:PRO:HD3	2.06	0.71
2:B:252:LEU:HD22	2:B:288:ALA:HB3	1.73	0.71
2:B:332:ALA:HB1	2:B:372:PRO:HG2	1.73	0.71
2:B:168:LEU:HD21	2:B:204:ILE:HG22	1.73	0.71
3:F:24:SER:H	3:F:27:GLN:NE2	1.88	0.71
3:F:75:SER:O	3:F:77:ASP:N	2.23	0.71
4:M:3:ACB:O	4:M:6:FGA:HB3	1.91	0.71
1:D:324:THR:HG23	1:D:325:GLN:HG3	1.72	0.70
3:F:76:PRO:HG3	3:F:107:TYR:CE2	2.25	0.70
3:F:53:THR:HB	3:F:277:GLU:HG2	1.72	0.70
3:C:107:TYR:HB3	3:C:110:ARG:HB2	1.72	0.70
2:B:58:ASP:H	2:B:59:PRO:HD3	1.57	0.70
1:A:133:LYS:HE2	1:A:169:TYR:HE1	1.57	0.69
2:B:287:MET:O	2:B:291:LYS:HG2	1.93	0.69
2:B:52:LEU:HD11	2:B:97:HIS:HD2	1.55	0.69
1:D:499:MET:CE	1:D:539:ASN:HD22	2.06	0.69
2:B:74:SER:O	2:B:77:VAL:HG12	1.92	0.69
3:C:76:PRO:HB3	3:C:107:TYR:CE2	2.27	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:SER:C	1:A:305:LYS:H	1.95	0.69
2:E:381:HIS:CG	2:E:386:ILE:HD11	2.28	0.69
3:F:232:ASN:HB3	3:F:234:LEU:HG	1.75	0.68
1:D:222:LEU:HD23	1:D:262:MET:HG3	1.75	0.68
2:E:212:ILE:HD11	2:E:254:LEU:HG	1.75	0.68
3:F:17:LEU:HD13	3:F:23:LEU:HD23	1.75	0.68
3:C:65:LEU:HD22	3:C:96:THR:HG23	1.75	0.68
3:C:124:THR:HG21	3:C:143:TRP:HE1	1.59	0.68
3:C:150:PHE:HA	3:C:153:LEU:HD12	1.76	0.68
1:A:494:ASN:HD21	1:A:496:LEU:HD23	1.59	0.67
2:B:38:GLN:HA	2:B:38:GLN:HE21	1.59	0.67
1:D:274:VAL:CG1	1:D:278:ILE:HB	2.25	0.67
3:F:269:CYS:HB3	4:N:7:DAM:HB2	1.75	0.67
1:A:494:ASN:HD22	1:A:495:TYR:N	1.92	0.67
2:B:51:VAL:HG21	2:B:73:LEU:HB3	1.76	0.67
2:B:81:THR:HG21	2:B:143:ARG:HG2	1.76	0.67
2:E:228:LEU:O	2:E:232:ILE:HG12	1.95	0.67
3:F:247:GLY:HA2	3:F:272:GLN:O	1.95	0.67
2:E:248:LEU:HA	2:E:252:LEU:HD12	1.76	0.67
1:D:140:TRP:HZ3	2:E:209:TYR:HH	1.43	0.66
1:A:128:PHE:O	1:A:131:LEU:HB3	1.96	0.66
1:D:535:ASN:HA	1:D:538:PHE:CE1	2.30	0.66
3:F:243:LEU:HD23	4:N:7:DAM:HB1	1.77	0.66
2:B:81:THR:CG2	2:B:143:ARG:HG2	2.26	0.66
1:D:417:TRP:CZ3	1:D:421:LEU:HD12	2.28	0.66
3:F:264:ASN:HB2	3:F:270:GLY:HA2	1.78	0.66
4:N:2:LEU:H	4:N:3:ACB:C4	1.94	0.66
1:A:306:VAL:HG11	1:A:330:ILE:HD11	1.78	0.66
1:D:245:MET:HA	1:D:245:MET:HE3	1.77	0.66
2:E:57:SER:CB	2:E:59:PRO:HD2	2.25	0.66
1:A:561:LYS:H	1:A:562:PRO:HD2	1.61	0.65
2:E:320:PHE:CE2	2:E:324:MET:HG3	2.31	0.65
2:E:112:ASN:HD21	2:E:124:GLU:H	1.42	0.65
2:E:204:ILE:HA	2:E:207:ILE:HG12	1.77	0.65
2:B:160:ASP:HB3	2:B:163:PHE:H	1.60	0.65
1:A:529:ALA:HB2	1:A:540:VAL:HG11	1.79	0.65
3:F:31:LEU:HD11	3:F:102:ALA:HA	1.78	0.65
3:F:214:ARG:CZ	3:F:241:HIS:HE1	2.09	0.65
1:D:43:GLY:C	1:D:45:GLU:H	1.97	0.65
3:F:39:LEU:HD23	3:F:149:LEU:HD11	1.79	0.65
2:B:34:PRO:N	2:B:35:PRO:CD	2.60	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:237:LEU:HB3	2:E:238:PRO:CD	2.26	0.64
3:F:174:ILE:HG22	3:F:179:HIS:HB3	1.79	0.64
3:C:264:ASN:HA	3:C:267:TYR:O	1.97	0.64
4:M:3:ACB:O	4:M:6:FGA:CB	2.46	0.63
3:F:24:SER:HB3	3:F:27:GLN:HB2	1.80	0.63
3:C:243:LEU:CD2	4:M:7:DAM:HB1	2.29	0.63
1:D:496:LEU:CD2	3:F:78:THR:HG22	2.29	0.63
2:E:146:GLU:OE1	2:E:146:GLU:HA	1.97	0.63
3:F:46:GLN:HA	3:F:46:GLN:NE2	2.06	0.63
1:A:341:VAL:HG23	1:A:342:LYS:N	2.14	0.63
1:D:256:SER:HB3	2:E:106:THR:HG21	1.81	0.63
2:E:223:GLU:O	2:E:226:GLU:HB3	1.99	0.63
2:B:34:PRO:N	2:B:35:PRO:HD3	2.14	0.62
3:F:88:ASN:HD21	3:F:124:THR:HA	1.63	0.62
3:F:239:ARG:HG3	3:F:258:THR:HA	1.81	0.62
4:N:2:LEU:C	4:N:3:ACB:H2	2.02	0.62
2:B:130:ALA:O	2:B:134:LEU:HG	1.99	0.62
1:A:176:ASP:OD2	1:A:178:THR:HG22	1.99	0.62
3:F:78:THR:HG1	3:F:80:TYR:HE2	1.45	0.62
2:E:278:ASP:OD1	2:E:280:THR:HG22	2.00	0.62
3:F:164:PHE:HE2	3:F:166:LEU:HD21	1.64	0.62
2:B:218:HIS:HD2	2:B:220:GLY:H	1.48	0.62
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.80	0.62
3:F:75:SER:HB3	3:F:76:PRO:CD	2.30	0.62
4:M:3:ACB:O	4:M:6:FGA:N	2.32	0.62
1:D:372:GLN:HB3	1:D:384:ILE:HG13	1.82	0.62
2:E:103:MET:HA	2:E:103:MET:CE	2.30	0.62
1:D:346:ALA:HA	1:D:372:GLN:OE1	1.99	0.62
3:C:215:GLY:HA3	4:M:5:1ZN:H16	1.82	0.61
2:B:48:GLN:HA	2:B:51:VAL:HG12	1.83	0.61
1:A:338:ASN:HD22	1:A:340:HIS:H	1.49	0.61
1:D:538:PHE:HB3	1:D:575:VAL:HA	1.81	0.61
1:A:133:LYS:HG2	1:A:169:TYR:CE1	2.36	0.61
2:B:383:ASN:O	2:B:386:ILE:HD13	2.00	0.61
2:E:83:ASN:HB3	2:E:86:VAL:HG21	1.82	0.61
2:B:121:GLU:OE1	4:M:2:LEU:HD13	2.00	0.60
1:A:115:ILE:O	1:A:119:HIS:CD2	2.52	0.60
4:N:5:1ZN:H19	4:N:5:1ZN:H6	1.83	0.60
3:F:83:MET:HE3	3:F:240:ALA:HB2	1.84	0.60
3:F:120:SER:O	3:F:124:THR:HB	2.01	0.60
3:C:117:ASN:H	3:C:117:ASN:HD22	1.46	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:LEU:HB3	2:B:389:LEU:HD22	1.83	0.60
1:D:245:MET:HA	1:D:245:MET:HE2	1.82	0.60
2:B:58:ASP:N	2:B:59:PRO:CD	2.64	0.60
2:E:332:ALA:HB2	2:E:369:ILE:HG12	1.82	0.60
2:E:383:ASN:O	2:E:386:ILE:HD13	2.02	0.60
1:D:467:LYS:HB2	1:D:507:VAL:HG13	1.83	0.60
3:F:45:VAL:CG1	3:F:181:ARG:HH11	2.15	0.60
1:A:539:ASN:O	1:A:543:SER:HB2	2.02	0.60
2:B:52:LEU:HD21	2:B:101:VAL:HG21	1.84	0.60
2:B:72:ALA:O	2:B:75:GLU:HG2	2.02	0.60
2:E:168:LEU:HD21	2:E:204:ILE:HG22	1.82	0.60
3:C:24:SER:H	3:C:27:GLN:HE21	1.50	0.59
3:F:8:LYS:HA	3:F:8:LYS:CE	2.29	0.59
1:D:350:MET:HG2	1:D:387:ASN:O	2.00	0.59
2:E:263:TYR:O	2:E:266:GLN:HG2	2.02	0.59
2:B:281:LEU:O	2:B:285:VAL:HG13	2.02	0.59
1:A:13:ILE:HD12	1:A:14:ALA:H	1.66	0.59
2:E:332:ALA:HB1	2:E:372:PRO:HG2	1.83	0.59
3:C:222:GLN:O	3:C:226:GLU:HB2	2.02	0.59
3:F:209:TRP:CZ3	3:F:220:PHE:HB3	2.36	0.59
3:C:202:ASP:HB3	3:C:242:GLN:OE1	2.03	0.59
1:D:334:VAL:HG21	1:D:368:LEU:HD22	1.84	0.59
3:C:17:LEU:CD1	3:C:98:THR:HG23	2.32	0.59
2:E:58:ASP:N	2:E:59:PRO:HD2	2.18	0.59
1:A:120:SER:HB2	1:A:123:ASP:HB2	1.85	0.58
2:B:171:PHE:CE1	2:B:182:LEU:HB3	2.36	0.58
3:F:57:ASP:HB3	3:F:59:HIS:HD2	1.67	0.58
3:F:104:LYS:HA	3:F:111:ILE:HD11	1.85	0.58
1:A:451:LEU:HD12	1:A:462:ALA:HB1	1.85	0.58
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.37	0.58
1:A:307:LYS:HB3	1:A:348:VAL:HB	1.84	0.58
3:C:176:THR:H	3:C:179:HIS:HD2	1.49	0.58
2:E:355:ILE:HD12	2:E:355:ILE:H	1.69	0.58
3:F:104:LYS:CA	3:F:111:ILE:HD11	2.32	0.58
1:A:200:ASN:HA	1:A:203:SER:HB3	1.85	0.58
3:F:76:PRO:HG3	3:F:107:TYR:CZ	2.38	0.58
3:F:91:TYR:HB2	3:F:265:TYR:OH	2.03	0.58
3:F:266:CYS:HA	3:F:268:ARG:HB2	1.86	0.58
1:D:307:LYS:HB3	1:D:348:VAL:HB	1.86	0.58
3:F:250:TRP:CD1	3:F:257:VAL:HG22	2.39	0.58
2:B:304:PHE:O	2:B:308:LEU:HB2	2.03	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:VAL:HG21	3:C:249:ASN:HB2	1.86	0.57
1:D:499:MET:HE1	1:D:539:ASN:HD22	1.67	0.57
3:F:16:GLN:O	3:F:19:GLU:HG3	2.03	0.57
3:F:98:THR:HB	3:F:146:PHE:CZ	2.33	0.57
1:A:543:SER:O	1:A:547:ILE:HG12	2.04	0.57
2:B:77:VAL:HG23	2:B:140:PHE:HA	1.86	0.57
1:D:39:ALA:O	1:D:43:GLY:HA3	2.04	0.57
2:E:112:ASN:ND2	2:E:123:ASP:HA	2.19	0.57
3:C:76:PRO:HB3	3:C:107:TYR:CZ	2.39	0.57
2:B:286:VAL:HG11	2:B:323:ILE:HG13	1.85	0.57
3:C:230:HIS:HA	3:C:234:LEU:HD13	1.87	0.57
2:E:146:GLU:HG2	2:E:188:ARG:HH21	1.68	0.57
2:E:321:VAL:HA	2:E:324:MET:HE3	1.85	0.57
2:B:120:PRO:O	2:B:122:GLU:N	2.32	0.57
2:B:282:THR:HB	2:B:319:GLU:HG2	1.86	0.57
3:C:121:ARG:O	3:C:124:THR:HG22	2.05	0.57
1:D:366:LEU:HD12	1:D:369:PHE:HD2	1.69	0.57
2:E:335:VAL:HG22	2:E:347:LEU:HG	1.86	0.57
1:D:499:MET:HE3	1:D:535:ASN:HB3	1.85	0.57
2:E:283:GLU:HB3	2:E:284:PRO:HD3	1.87	0.57
1:A:467:LYS:HB2	1:A:507:VAL:HG12	1.86	0.56
3:F:57:ASP:HB3	3:F:59:HIS:CD2	2.40	0.56
2:B:168:LEU:HG	2:B:207:ILE:HD11	1.86	0.56
2:B:339:HIS:CD2	3:C:125:GLN:HB2	2.40	0.56
3:C:116:GLY:HA2	3:C:167:HIS:CG	2.41	0.56
3:F:214:ARG:CZ	3:F:241:HIS:CE1	2.88	0.56
2:B:97:HIS:O	2:B:101:VAL:HG23	2.05	0.56
1:A:412:ALA:HB1	1:A:450:TRP:HZ2	1.71	0.56
1:D:284:VAL:HB	1:D:285:PRO:HD3	1.87	0.56
3:F:62:PHE:HD1	3:F:63:HIS:HD2	1.53	0.56
3:C:185:ARG:HG3	3:C:185:ARG:NH2	2.08	0.56
3:C:201:SER:CB	3:C:218:TYR:H	2.18	0.56
3:F:167:HIS:CD2	3:F:241:HIS:HB2	2.40	0.56
3:C:149:LEU:HD23	3:C:149:LEU:O	2.06	0.56
1:D:369:PHE:O	1:D:373:LEU:HB2	2.06	0.56
2:B:212:ILE:CD1	2:B:253:PRO:HB2	2.36	0.56
1:D:483:ILE:N	1:D:484:PRO:HD2	2.20	0.56
3:F:265:TYR:O	3:F:268:ARG:HG3	2.06	0.56
3:F:13:TRP:CG	3:F:23:LEU:HD11	2.41	0.56
3:F:290:ASP:OD2	3:F:290:ASP:N	2.38	0.55
1:A:91:PRO:HB2	1:A:92:PRO:HD3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:SER:C	2:E:112:ASN:H	2.09	0.55
2:E:381:HIS:ND1	2:E:386:ILE:HD11	2.22	0.55
2:E:291:LYS:C	2:E:293:TRP:H	2.10	0.55
3:F:212:SER:HA	3:F:219:THR:HG23	1.88	0.55
1:A:524:THR:O	1:A:528:MET:HG3	2.07	0.55
2:E:78:GLU:HA	2:E:81:THR:OG1	2.07	0.55
1:A:366:LEU:HB3	1:A:367:PRO:HD3	1.88	0.55
1:A:435:GLY:HA2	1:A:438:PHE:HB3	1.89	0.55
2:E:143:ARG:HH11	2:E:143:ARG:HB2	1.72	0.55
3:F:79:ASN:HD21	3:F:110:ARG:NE	1.94	0.55
3:F:95:GLU:OE2	3:F:136:LYS:HE3	2.07	0.55
1:D:222:LEU:HD23	1:D:262:MET:CG	2.37	0.55
2:E:58:ASP:N	2:E:59:PRO:CD	2.70	0.55
3:F:276:MET:CE	3:F:278:LEU:HD21	2.36	0.55
1:A:303:SER:O	1:A:305:LYS:N	2.39	0.54
3:C:117:ASN:HB3	3:C:199:LEU:O	2.07	0.54
1:A:140:TRP:HD1	1:A:141:PHE:H	1.55	0.54
2:B:179:ARG:HB2	2:B:223:GLU:HG2	1.88	0.54
2:E:264:HIS:HE1	2:E:307:GLU:OE2	1.91	0.54
3:F:172:PRO:HG3	3:F:209:TRP:CD2	2.42	0.54
3:C:171:SER:HB2	3:C:197:ASP:CB	2.36	0.54
1:D:94:GLU:HB2	1:D:131:LEU:HD21	1.90	0.54
2:E:328:PHE:HA	2:E:331:LEU:HB2	1.90	0.54
3:F:91:TYR:N	3:F:265:TYR:OH	2.39	0.54
3:C:19:GLU:O	3:C:21:LYS:N	2.41	0.54
2:E:103:MET:HE1	2:E:134:LEU:HB3	1.88	0.54
3:F:214:ARG:HE	3:F:241:HIS:CE1	2.26	0.54
1:D:306:VAL:HG11	1:D:330:ILE:HD11	1.90	0.54
2:E:164:VAL:HG21	2:E:200:ILE:HG12	1.89	0.54
1:A:366:LEU:C	1:A:368:LEU:H	2.11	0.54
2:B:246:PHE:O	2:B:250:VAL:HB	2.08	0.54
3:C:265:TYR:CD1	3:C:266:CYS:N	2.76	0.54
2:E:72:ALA:O	2:E:76:MET:HG3	2.07	0.54
2:E:253:PRO:O	2:E:256:LYS:HG2	2.07	0.54
2:B:121:GLU:OE1	4:M:2:LEU:HD11	2.07	0.54
1:D:237:GLN:HA	1:D:240:LEU:HD12	1.89	0.54
4:M:5:1ZN:H6	4:M:5:1ZN:H19	1.90	0.54
3:C:185:ARG:CG	3:C:185:ARG:NH2	2.60	0.54
3:C:114:LEU:HD23	3:C:154:PRO:HG2	1.89	0.53
2:E:119:ASP:CG	2:E:120:PRO:HD2	2.29	0.53
2:E:260:LEU:HG	2:E:264:HIS:HB2	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:ND2	1:A:340:HIS:H	2.07	0.53
1:D:320:ASN:O	1:D:324:THR:HG22	2.09	0.53
1:D:397:ILE:HG21	1:D:434:LEU:HB2	1.90	0.53
3:F:157:ALA:HB3	3:F:165:CYS:HB2	1.90	0.53
1:D:531:ASP:O	1:D:537:ARG:HD3	2.09	0.53
2:E:194:LEU:O	2:E:197:ARG:HB3	2.08	0.53
3:F:58:VAL:HG12	3:F:86:TYR:HA	1.89	0.53
3:F:171:SER:HB3	3:F:174:ILE:CD1	2.35	0.53
3:F:264:ASN:O	3:F:265:TYR:HB3	2.08	0.53
3:C:229:ASN:O	3:C:234:LEU:HB3	2.09	0.53
3:F:132:GLU:OE1	3:F:136:LYS:HE2	2.09	0.53
3:F:174:ILE:HG21	3:F:180:ILE:HG22	1.91	0.53
3:F:75:SER:HB3	3:F:76:PRO:HD2	1.91	0.53
3:C:117:ASN:HD22	3:C:117:ASN:N	2.06	0.53
2:E:55:PHE:CD1	2:E:55:PHE:N	2.77	0.53
3:F:170:LEU:HD11	3:F:228:PHE:CD2	2.44	0.53
3:F:174:ILE:HG21	3:F:180:ILE:CG2	2.40	0.52
1:A:163:LYS:O	1:A:167:ARG:HG3	2.09	0.52
3:C:121:ARG:O	3:C:125:GLN:HG2	2.10	0.52
2:B:212:ILE:HD11	2:B:213:TYR:CZ	2.44	0.52
3:C:265:TYR:O	3:C:268:ARG:CB	2.57	0.52
1:A:93:LEU:HA	1:A:96:LEU:HB2	1.90	0.52
1:A:236:PRO:HB2	1:A:240:LEU:HG	1.91	0.52
1:A:303:SER:OG	1:A:333:LEU:HD13	2.10	0.52
3:F:45:VAL:HG11	3:F:181:ARG:HH11	1.70	0.52
3:F:240:ALA:O	3:F:242:GLN:N	2.42	0.52
2:E:79:TYR:CE2	2:E:86:VAL:HG11	2.44	0.52
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.91	0.52
1:A:418:ARG:CG	1:A:418:ARG:NH2	2.68	0.51
3:C:44:ASN:HB2	3:C:181:ARG:HA	1.92	0.51
3:C:212:SER:OG	3:C:214:ARG:HB2	2.10	0.51
2:E:152:PRO:O	2:E:156:LYS:HB3	2.10	0.51
2:E:273:GLN:O	2:E:276:GLU:HB2	2.09	0.51
3:F:229:ASN:ND2	3:F:255:ASN:HD22	2.04	0.51
2:B:89:GLU:HG2	2:B:154:ILE:HD13	1.92	0.51
3:F:45:VAL:CG1	3:F:181:ARG:NH1	2.72	0.51
3:F:50:CYS:SG	3:F:282:LEU:HD13	2.50	0.51
2:E:97:HIS:O	2:E:101:VAL:HG23	2.10	0.51
1:D:506:ASN:HB2	1:D:546:LYS:HG2	1.91	0.51
2:E:193:PHE:CE2	2:E:195:GLY:HA3	2.46	0.51
1:A:322:ILE:HA	1:A:326:ILE:HB	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:ARG:HA	3:C:110:ARG:HH21	1.75	0.51
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.93	0.51
2:B:52:LEU:CD1	2:B:98:MET:HA	2.40	0.51
2:B:168:LEU:C	2:B:170:LEU:H	2.13	0.51
1:D:278:ILE:HA	1:D:281:THR:HG22	1.93	0.51
2:E:232:ILE:HD12	2:E:274:PHE:CE1	2.46	0.51
2:E:386:ILE:O	2:E:390:ILE:HG22	2.11	0.51
3:C:215:GLY:HA3	4:M:5:1ZN:H14	1.92	0.50
1:A:264:ALA:HA	1:A:267:PHE:HB2	1.92	0.50
4:N:3:ACB:OXT	4:N:4:ARG:NE	2.44	0.50
3:F:239:ARG:NH2	3:F:242:GLN:OE1	2.44	0.50
1:A:494:ASN:HD22	1:A:494:ASN:C	2.14	0.50
3:C:35:ALA:HA	3:C:38:ILE:HG22	1.93	0.50
3:C:81:LEU:HA	3:C:112:THR:O	2.11	0.50
1:D:69:LEU:HD23	1:D:96:LEU:HD11	1.94	0.50
2:B:58:ASP:N	2:B:59:PRO:HD3	2.24	0.50
3:C:195:MET:O	3:C:198:LEU:HB2	2.10	0.50
3:C:266:CYS:HA	3:C:268:ARG:HG2	1.93	0.50
3:F:10:LEU:HD11	3:F:105:VAL:HG22	1.94	0.50
3:F:265:TYR:CD2	3:F:266:CYS:N	2.79	0.50
2:B:121:GLU:OE1	4:M:2:LEU:CD2	2.60	0.50
3:F:68:LEU:CD1	3:F:275:ILE:HG21	2.40	0.50
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.94	0.50
2:B:52:LEU:CD1	2:B:97:HIS:HD2	2.21	0.50
2:E:120:PRO:C	2:E:122:GLU:N	2.54	0.50
1:A:24:ASP:CG	1:A:25:VAL:H	2.15	0.50
1:A:466:LEU:HD23	1:A:508:LEU:HD11	1.94	0.50
1:A:11:TYR:H	1:A:12:PRO:HD3	1.76	0.50
1:A:229:VAL:O	1:A:233:GLN:HB2	2.11	0.50
1:A:369:PHE:O	1:A:373:LEU:HB2	2.12	0.50
1:D:439:PHE:CZ	1:D:469:LEU:HD11	2.47	0.50
2:E:52:LEU:HD12	2:E:98:MET:HB3	1.94	0.50
2:E:277:LYS:HA	2:E:277:LYS:CE	2.42	0.50
1:D:222:LEU:CD2	1:D:262:MET:HG3	2.42	0.49
3:C:297:GLU:C	3:C:299:HIS:H	2.15	0.49
1:D:319:GLU:O	1:D:323:MET:HB2	2.13	0.49
3:F:85:ASP:H	3:F:116:GLY:HA3	1.77	0.49
1:A:102:THR:O	1:A:106:ASP:HB2	2.12	0.49
3:C:24:SER:H	3:C:27:GLN:NE2	2.10	0.49
3:C:240:ALA:O	3:C:242:GLN:N	2.43	0.49
3:F:67:GLU:O	3:F:71:ILE:HG12	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ASN:ND2	2:B:219:ASN:H	2.09	0.49
2:B:367:LEU:H	2:B:368:PRO:CD	2.20	0.49
3:F:244:VAL:CG1	3:F:249:ASN:HB2	2.35	0.49
1:A:404:LEU:O	1:A:408:ILE:HG12	2.12	0.49
2:B:52:LEU:HD12	2:B:98:MET:HA	1.95	0.49
1:D:108:ALA:O	1:D:112:LEU:HB2	2.12	0.49
1:A:37:THR:HG22	1:A:40:LEU:HD21	1.94	0.49
1:A:246:PRO:O	1:A:250:GLN:HB2	2.13	0.49
1:A:535:ASN:HD21	3:C:79:ASN:ND2	2.10	0.49
1:D:339:GLN:NE2	1:D:377:CYS:HB2	2.28	0.49
1:D:556:LEU:HA	1:D:560:VAL:HB	1.95	0.49
3:F:115:ARG:HD2	3:F:119:GLU:HB2	1.93	0.49
1:D:438:PHE:HA	1:D:441:GLU:OE2	2.13	0.49
2:E:99:PHE:CZ	2:E:103:MET:HG2	2.48	0.49
2:B:219:ASN:H	2:B:219:ASN:HD22	1.60	0.49
3:C:147:THR:HA	3:C:150:PHE:CD1	2.48	0.48
2:B:120:PRO:C	2:B:122:GLU:N	2.67	0.48
2:B:251:LEU:O	2:B:254:LEU:HB2	2.13	0.48
1:D:429:LEU:O	1:D:433:GLN:HG2	2.12	0.48
3:F:89:ARG:HG3	3:F:128:GLY:CA	2.42	0.48
4:N:1:DAL:O	4:N:2:LEU:HG	2.13	0.48
3:C:20:CYS:O	3:C:95:GLU:HG2	2.13	0.48
1:D:128:PHE:O	1:D:131:LEU:HB3	2.13	0.48
1:D:513:GLY:O	1:D:515:ASP:N	2.46	0.48
1:D:541:ALA:HB1	1:D:579:ALA:HA	1.94	0.48
1:A:240:LEU:HD23	1:A:244:VAL:HG13	1.96	0.48
1:D:318:ARG:HA	1:D:321:VAL:HG12	1.95	0.48
2:E:52:LEU:HD12	2:E:98:MET:CB	2.43	0.48
1:D:44:VAL:O	1:D:45:GLU:HB2	2.13	0.48
3:F:48:VAL:HG21	3:F:81:LEU:HD22	1.94	0.48
3:F:251:CYS:HB3	3:F:256:VAL:O	2.13	0.48
3:C:14:ILE:HA	3:C:17:LEU:CD2	2.44	0.48
3:C:229:ASN:O	3:C:231:ALA:N	2.46	0.48
3:C:252:HIS:O	3:C:253:ASP:C	2.52	0.48
1:D:548:GLY:HA3	1:D:586:LEU:CD2	2.39	0.48
2:E:371:PHE:CG	2:E:372:PRO:HD3	2.49	0.48
3:F:34:LYS:O	3:F:38:ILE:HG23	2.13	0.48
1:A:240:LEU:HD23	1:A:244:VAL:CG1	2.44	0.48
1:A:436:VAL:HG13	1:A:437:GLU:H	1.79	0.48
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.44	0.48
1:A:495:TYR:HA	1:A:498:ARG:HG2	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:N	2:B:93:PRO:HD2	2.29	0.48
2:E:320:PHE:O	2:E:324:MET:HB2	2.12	0.48
3:F:265:TYR:CG	3:F:266:CYS:N	2.82	0.48
1:A:101:GLU:CG	2:B:256:LYS:HE2	2.43	0.48
1:A:307:LYS:HG3	1:A:308:GLU:N	2.28	0.48
2:B:55:PHE:O	2:B:57:SER:N	2.47	0.48
3:C:139:ASN:ND2	3:C:141:ASN:HB2	2.28	0.48
3:F:124:THR:HG21	3:F:143:TRP:NE1	2.19	0.48
1:A:341:VAL:HG23	1:A:342:LYS:H	1.79	0.47
2:B:255:HIS:CE1	2:B:271:VAL:HG21	2.49	0.47
1:A:10:LEU:HB3	1:A:12:PRO:HD3	1.96	0.47
2:E:218:HIS:CD2	2:E:220:GLY:H	2.32	0.47
3:F:74:LYS:HG3	3:F:75:SER:H	1.79	0.47
3:F:82:PHE:HB3	3:F:86:TYR:HE1	1.80	0.47
3:F:170:LEU:HB3	3:F:209:TRP:HH2	1.78	0.47
2:B:256:LYS:CB	3:C:309:MLL:HD22	2.41	0.47
3:C:91:TYR:HD2	3:C:91:TYR:O	1.97	0.47
1:D:449:ALA:O	1:D:452:VAL:HG12	2.14	0.47
2:E:49:CYS:O	2:E:52:LEU:HD22	2.14	0.47
3:F:50:CYS:O	3:F:52:VAL:HG12	2.14	0.47
3:F:114:LEU:HD21	3:F:157:ALA:HB2	1.96	0.47
2:B:123:ASP:OD1	4:M:2:LEU:HD21	2.14	0.47
1:D:52:LEU:HD12	1:D:92:PRO:HG3	1.96	0.47
2:E:257:VAL:HG12	2:E:259:SER:H	1.79	0.47
2:E:356:MET:HA	2:E:359:ILE:HD12	1.97	0.47
2:E:371:PHE:CD2	2:E:372:PRO:HD3	2.49	0.47
3:F:45:VAL:CG2	3:F:156:THR:HG23	2.29	0.47
4:N:2:LEU:HA	4:N:3:ACB:H43	0.61	0.47
1:A:244:VAL:O	1:A:244:VAL:CG2	2.58	0.47
1:A:560:VAL:HG12	1:A:560:VAL:O	2.14	0.47
3:C:45:VAL:HA	3:C:156:THR:HG23	1.96	0.47
3:C:57:ASP:HB2	3:C:260:PHE:CE2	2.49	0.47
3:C:123:ILE:HA	3:C:126:VAL:HG12	1.96	0.47
3:C:265:TYR:CG	3:C:266:CYS:N	2.82	0.47
1:D:499:MET:HE2	1:D:539:ASN:HD22	1.78	0.47
3:F:201:SER:HB3	3:F:218:TYR:H	1.79	0.47
3:F:232:ASN:C	3:F:234:LEU:H	2.17	0.47
2:B:218:HIS:HD2	2:B:220:GLY:N	2.09	0.47
1:A:116:SER:HB3	1:A:128:PHE:CE1	2.49	0.47
1:A:336:ASP:OD2	1:A:341:VAL:HG21	2.15	0.47
2:B:212:ILE:HD13	2:B:253:PRO:HB2	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:SER:O	2:B:387:HIS:HE1	1.98	0.47
1:D:14:ALA:HA	1:D:17:ILE:HG12	1.96	0.47
1:D:245:MET:O	1:D:249:ARG:HB2	2.13	0.47
2:E:382:TRP:HB2	3:F:121:ARG:HD3	1.97	0.47
3:F:251:CYS:SG	3:F:252:HIS:N	2.88	0.47
2:B:325:GLU:HB2	2:B:326:PRO:HD3	1.96	0.47
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.95	0.47
1:D:43:GLY:C	1:D:45:GLU:N	2.68	0.47
2:E:172:ASP:HB2	2:E:218:HIS:CE1	2.49	0.47
3:F:170:LEU:HD11	3:F:228:PHE:CE2	2.49	0.47
3:F:214:ARG:HG2	3:F:214:ARG:NH1	2.19	0.47
1:A:420:ARG:NH1	1:A:458:ILE:HG13	2.30	0.47
1:A:267:PHE:CE1	1:A:287:PHE:HB2	2.50	0.47
1:A:341:VAL:CG2	1:A:342:LYS:N	2.78	0.47
2:B:237:LEU:CB	2:B:238:PRO:HD2	2.41	0.47
2:B:47:ARG:O	2:B:51:VAL:N	2.45	0.46
3:F:243:LEU:C	3:F:243:LEU:HD12	2.35	0.46
3:C:195:MET:HA	3:C:198:LEU:HD12	1.97	0.46
3:F:281:THR:HG23	3:F:283:LYS:HG3	1.96	0.46
1:A:563:ILE:O	1:A:566:LYS:HG3	2.15	0.46
1:D:105:ARG:HD2	1:D:146:SER:OG	2.15	0.46
2:B:175:ASP:O	2:B:178:GLU:HB2	2.16	0.46
2:E:168:LEU:HD22	2:E:203:GLN:HG3	1.97	0.46
3:F:6:PHE:CZ	3:F:10:LEU:HD12	2.50	0.46
2:B:297:HIS:C	2:B:297:HIS:CD2	2.89	0.46
3:C:230:HIS:CG	3:C:230:HIS:O	2.68	0.46
1:D:489:MET:HB3	1:D:501:THR:OG1	2.16	0.46
2:E:77:VAL:HG23	2:E:140:PHE:HA	1.96	0.46
2:E:282:THR:HB	2:E:319:GLU:HG2	1.96	0.46
1:A:330:ILE:O	1:A:334:VAL:HG23	2.16	0.46
3:C:32:CYS:O	3:C:36:LYS:HB2	2.16	0.46
3:C:308:PHE:O	3:C:309:MLL:HD13	2.16	0.46
1:D:526:LEU:HD12	1:D:526:LEU:HA	1.83	0.46
2:E:295:LYS:HD3	2:E:295:LYS:H	1.80	0.46
3:F:137:TYR:CD1	3:F:142:VAL:HG11	2.51	0.46
1:A:20:LEU:HB2	1:A:21:ARG:HH11	1.81	0.46
2:B:81:THR:O	2:B:82:HIS:CD2	2.68	0.46
2:B:292:TYR:HA	3:C:309:MLL:HG	1.98	0.46
1:D:568:THR:O	1:D:576:LYS:HG3	2.15	0.46
1:A:47:THR:HG23	1:A:51:LEU:HD23	1.98	0.46
2:B:131:TRP:N	2:B:132:PRO:CD	2.78	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:ALA:HB3	3:C:165:CYS:HB2	1.98	0.46
1:D:373:LEU:HD13	1:D:384:ILE:CG2	2.46	0.46
1:A:160:SER:HA	1:A:163:LYS:HB2	1.98	0.46
2:B:168:LEU:HD21	2:B:204:ILE:CG2	2.44	0.46
2:B:247:LEU:HD21	2:B:285:VAL:HG11	1.98	0.46
2:B:307:GLU:HA	2:B:310:GLU:HB2	1.97	0.46
2:B:51:VAL:HG13	2:B:51:VAL:O	2.16	0.46
2:B:119:ASP:HA	2:B:120:PRO:HD3	1.83	0.46
2:B:170:LEU:C	2:B:172:ASP:H	2.19	0.46
2:E:171:PHE:CE1	2:E:182:LEU:HB3	2.50	0.46
1:A:11:TYR:N	1:A:12:PRO:CD	2.77	0.45
1:A:368:LEU:O	1:A:372:GLN:HB2	2.16	0.45
1:A:573:VAL:HG11	3:C:108:ARG:HH12	1.80	0.45
2:E:98:MET:O	2:E:102:ASN:ND2	2.47	0.45
2:E:191:GLY:HA2	2:E:197:ARG:HH11	1.80	0.45
3:F:232:ASN:O	3:F:234:LEU:N	2.49	0.45
3:F:288:GLN:O	3:F:289:PHE:HB3	2.16	0.45
3:C:157:ALA:N	3:C:165:CYS:O	2.45	0.45
1:D:306:VAL:CG1	1:D:330:ILE:HD11	2.45	0.45
2:E:202:LYS:O	2:E:205:ASN:HB2	2.16	0.45
1:A:102:THR:HG23	2:B:213:TYR:HB3	1.98	0.45
1:A:219:SER:HB2	2:B:210:ARG:HH22	1.80	0.45
1:A:467:LYS:O	1:A:471:GLU:HB2	2.16	0.45
1:D:248:LEU:HD11	1:D:270:LEU:HD13	1.98	0.45
1:D:274:VAL:HG13	1:D:278:ILE:HB	1.98	0.45
2:B:201:ARG:NE	2:B:242:GLU:OE1	2.49	0.45
3:C:118:HIS:HA	3:C:123:ILE:HG21	1.97	0.45
1:D:486:VAL:O	1:D:489:MET:HB2	2.15	0.45
1:D:535:ASN:O	1:D:539:ASN:HB2	2.16	0.45
2:E:347:LEU:C	2:E:349:TYR:N	2.70	0.45
1:A:310:CYS:HA	1:A:313:LEU:HD11	1.99	0.45
2:B:352:ASN:CB	2:B:355:ILE:HD12	2.35	0.45
3:F:209:TRP:CE2	3:F:224:ILE:HD13	2.51	0.45
1:A:193:ALA:HB2	1:A:205:ILE:HG21	1.97	0.45
2:E:47:ARG:HA	2:E:50:CYS:HB2	1.97	0.45
2:E:87:ILE:HG22	2:E:87:ILE:O	2.15	0.45
3:C:124:THR:HG21	3:C:143:TRP:NE1	2.29	0.45
2:E:132:PRO:O	2:E:136:LEU:HD12	2.16	0.45
3:F:116:GLY:H	3:F:119:GLU:CG	2.24	0.45
2:B:47:ARG:HH11	2:B:72:ALA:HB2	1.82	0.45
2:B:54:ASP:OD1	2:B:54:ASP:N	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:CYS:HA	2:E:52:LEU:HD13	1.99	0.45
2:E:200:ILE:O	2:E:204:ILE:HG23	2.16	0.45
1:D:349:ILE:HG21	1:D:372:GLN:OE1	2.17	0.45
1:D:419:VAL:O	1:D:420:ARG:C	2.55	0.45
1:D:564:LEU:O	1:D:568:THR:HG23	2.16	0.45
2:E:45:LYS:HE3	2:E:45:LYS:H	1.80	0.45
2:E:52:LEU:HB3	2:E:98:MET:HB2	1.98	0.45
2:E:120:PRO:O	2:E:122:GLU:N	2.49	0.45
2:B:248:LEU:HA	2:B:252:LEU:HD12	1.99	0.45
3:F:116:GLY:N	3:F:119:GLU:HG2	2.25	0.45
2:E:103:MET:HA	2:E:103:MET:HE3	1.99	0.44
3:F:55:CYS:SG	3:F:68:LEU:HD21	2.57	0.44
2:E:96:VAL:HG21	2:E:158:TYR:HB3	2.00	0.44
3:F:207:GLY:HA2	3:F:221:GLY:HA3	2.00	0.44
4:N:2:LEU:CA	4:N:3:ACB:H2	2.30	0.44
1:A:231:ILE:HA	1:A:234:LEU:HD12	1.98	0.44
1:A:419:VAL:O	1:A:422:ALA:HB3	2.17	0.44
1:D:101:GLU:HG3	1:D:103:VAL:HG23	1.99	0.44
1:D:141:PHE:CE2	2:E:209:TYR:CD2	3.05	0.44
2:E:300:LYS:HA	2:E:303:MET:HE3	1.99	0.44
3:F:167:HIS:CD2	3:F:241:HIS:CD2	3.06	0.44
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.99	0.44
2:B:251:LEU:HD11	2:B:270:CYS:HB3	1.98	0.44
1:D:112:LEU:HB3	1:D:150:LEU:HD21	2.00	0.44
1:A:209:PHE:CE1	1:A:228:CYS:HB2	2.53	0.44
2:B:41:LEU:HD21	2:B:90:PRO:HG2	2.00	0.44
3:C:261:SER:HA	3:C:273:ALA:HB1	2.00	0.44
3:F:78:THR:OG1	3:F:80:TYR:HE2	1.97	0.44
3:F:223:ASP:OD1	3:F:224:ILE:N	2.51	0.44
1:A:222:LEU:HD23	1:A:262:MET:CG	2.47	0.44
3:C:86:TYR:CD2	3:C:119:GLU:OE2	2.71	0.44
1:D:466:LEU:HG	1:D:482:ILE:HD13	1.99	0.44
3:F:263:PRO:HB2	3:F:291:PRO:HB3	1.99	0.44
1:A:206:ILE:HG13	1:A:243:LEU:HD23	2.00	0.44
1:D:496:LEU:HD21	3:F:78:THR:HG22	2.00	0.44
1:D:545:GLN:HA	1:D:586:LEU:HD11	2.00	0.44
3:F:202:ASP:O	3:F:219:THR:HA	2.18	0.44
1:D:535:ASN:ND2	3:F:76:PRO:O	2.51	0.44
1:A:82:GLY:HA3	1:A:83:PRO:HD2	1.77	0.43
1:D:271:GLN:HG3	1:D:279:THR:HG21	1.99	0.43
1:A:234:LEU:C	1:A:236:PRO:HD3	2.39	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HG23	1:A:345:LEU:HD11	2.00	0.43
2:B:252:LEU:HD22	2:B:288:ALA:CB	2.47	0.43
2:B:372:PRO:HA	2:B:375:TYR:CE1	2.53	0.43
2:E:119:ASP:HB3	2:E:121:GLU:CD	2.38	0.43
2:E:275:LEU:HD11	2:E:282:THR:HA	2.00	0.43
3:F:214:ARG:CG	3:F:214:ARG:NH1	2.67	0.43
1:A:43:GLY:C	1:A:45:GLU:H	2.22	0.43
1:D:313:LEU:HD13	1:D:321:VAL:HG13	2.01	0.43
1:D:370:LEU:HD12	1:D:370:LEU:HA	1.87	0.43
1:D:498:ARG:NE	1:D:531:ASP:OD2	2.45	0.43
3:F:203:PRO:HG3	3:F:256:VAL:HG11	1.99	0.43
2:B:252:LEU:HB2	2:B:253:PRO:HD3	2.01	0.43
2:B:369:ILE:HG22	2:B:369:ILE:O	2.18	0.43
2:E:252:LEU:HD11	2:E:285:VAL:HG12	1.99	0.43
2:E:347:LEU:C	2:E:349:TYR:H	2.21	0.43
3:F:178:ASP:OD2	3:F:178:ASP:N	2.51	0.43
1:A:373:LEU:HD13	1:A:384:ILE:HG21	2.00	0.43
3:C:189:VAL:HG11	3:C:199:LEU:HD21	2.00	0.43
3:C:196:CYS:O	3:C:200:TRP:HB2	2.18	0.43
1:D:420:ARG:NH1	1:D:453:ASP:OD1	2.50	0.43
2:E:204:ILE:HA	2:E:207:ILE:CG1	2.46	0.43
3:F:117:ASN:N	3:F:117:ASN:HD22	2.17	0.43
3:F:222:GLN:HB2	3:F:252:HIS:CD2	2.53	0.43
3:C:170:LEU:HD12	3:C:220:PHE:CE2	2.54	0.43
2:E:55:PHE:HB2	2:E:56:VAL:H	1.56	0.43
2:E:156:LYS:HD2	2:E:193:PHE:CZ	2.53	0.43
3:F:223:ASP:O	3:F:227:THR:HB	2.18	0.43
1:A:140:TRP:HA	1:A:144:ARG:NH1	2.33	0.43
1:A:350:MET:HG2	1:A:387:ASN:O	2.18	0.43
2:B:131:TRP:CZ3	2:B:178:GLU:HG2	2.53	0.43
2:B:293:TRP:HA	2:B:294:PRO:HD3	1.86	0.43
3:C:10:LEU:HD22	3:C:106:ARG:HB2	2.00	0.43
1:D:466:LEU:HA	1:D:469:LEU:CD2	2.48	0.43
2:E:121:GLU:CB	4:N:2:LEU:HD12	2.48	0.43
2:E:258:LYS:HG3	2:E:259:SER:N	2.33	0.43
2:E:382:TRP:CB	3:F:121:ARG:HD3	2.48	0.43
3:F:49:ARG:HG2	3:F:49:ARG:HH21	1.83	0.43
1:A:102:THR:HG22	1:A:105:ARG:CZ	2.49	0.43
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.54	0.43
2:E:81:THR:HB	2:E:82:HIS:CD2	2.53	0.43
1:A:171:ARG:HH12	1:A:204:GLU:HG2	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:THR:C	1:A:484:PRO:HD2	2.39	0.43
2:B:164:VAL:HG21	2:B:196:LEU:HG	2.00	0.43
3:C:56:GLY:HA2	3:C:83:MET:HB2	2.00	0.43
1:D:70:ALA:HB2	1:D:96:LEU:HD12	2.01	0.43
1:D:256:SER:CB	2:E:106:THR:HG21	2.47	0.43
1:D:387:ASN:ND2	1:D:390:CYS:HB2	2.33	0.43
3:F:88:ASN:ND2	3:F:124:THR:HA	2.32	0.43
3:F:290:ASP:HB2	3:F:291:PRO:CD	2.49	0.43
1:A:222:LEU:HD23	1:A:262:MET:HG3	2.00	0.43
1:A:336:ASP:HB3	1:A:341:VAL:HG21	1.99	0.43
1:A:426:TYR:HE1	1:A:430:LEU:HD12	1.84	0.43
2:B:380:THR:OG1	2:B:381:HIS:N	2.50	0.43
1:D:183:ARG:HG3	1:D:220:VAL:HG22	2.01	0.43
3:F:254:ARG:HD3	3:F:254:ARG:N	2.33	0.43
1:D:179:PRO:HB3	1:D:217:GLN:HG3	1.99	0.42
2:E:367:LEU:N	2:E:368:PRO:CD	2.82	0.42
2:B:120:PRO:C	2:B:122:GLU:H	2.17	0.42
2:B:212:ILE:CD1	2:B:253:PRO:CB	2.96	0.42
3:C:252:HIS:O	3:C:255:ASN:HB2	2.19	0.42
1:D:419:VAL:O	1:D:422:ALA:N	2.52	0.42
2:E:45:LYS:HE2	2:E:91:ILE:HG22	2.02	0.42
1:A:473:PHE:HD2	1:A:474:GLY:H	1.66	0.42
1:A:506:ASN:HB2	1:A:546:LYS:HG2	2.00	0.42
1:A:555:THR:HG22	1:A:555:THR:O	2.19	0.42
3:C:264:ASN:H	3:C:264:ASN:ND2	2.17	0.42
2:E:48:GLN:HE21	2:E:98:MET:HG2	1.84	0.42
3:F:232:ASN:HD22	3:F:232:ASN:HA	1.51	0.42
1:A:197:GLU:O	1:A:200:ASN:N	2.52	0.42
3:C:252:HIS:O	3:C:255:ASN:N	2.48	0.42
1:D:117:HIS:CE1	1:D:153:VAL:HG12	2.54	0.42
1:D:244:VAL:HG12	1:D:245:MET:HE3	2.00	0.42
2:E:210:ARG:HG2	2:E:214:GLU:HB3	2.01	0.42
3:F:28:VAL:HG11	3:F:142:VAL:HG23	2.01	0.42
3:F:167:HIS:CD2	3:F:241:HIS:HD2	2.37	0.42
3:F:271:ASN:CG	3:F:272:GLN:N	2.73	0.42
1:A:338:ASN:HD21	1:A:340:HIS:HB2	1.84	0.42
2:B:53:PHE:HD2	2:B:53:PHE:HA	1.75	0.42
2:B:257:VAL:HG23	2:B:259:SER:H	1.84	0.42
3:C:13:TRP:O	3:C:17:LEU:HD22	2.20	0.42
2:E:103:MET:HE3	2:E:134:LEU:HD22	2.00	0.42
3:F:85:ASP:HB2	3:F:167:HIS:HE1	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:177:LEU:O	3:F:180:ILE:HG12	2.19	0.42
1:A:73:LEU:HD23	1:A:89:LEU:HD22	2.02	0.42
1:A:466:LEU:HB3	1:A:508:LEU:HD21	2.01	0.42
2:B:238:PRO:HD3	2:E:42:PHE:CZ	2.55	0.42
2:B:264:HIS:N	2:B:265:PRO:HD2	2.35	0.42
3:C:171:SER:O	3:C:174:ILE:HG13	2.20	0.42
1:D:218:ASP:O	1:D:222:LEU:HD12	2.19	0.42
3:F:52:VAL:HG13	3:F:52:VAL:O	2.19	0.42
1:D:366:LEU:HD12	1:D:369:PHE:CD2	2.52	0.42
1:D:375:ASP:O	1:D:381:ARG:HD3	2.19	0.42
2:E:93:PRO:HB3	2:E:158:TYR:CE1	2.55	0.42
2:E:131:TRP:N	2:E:132:PRO:CD	2.82	0.42
3:F:189:VAL:HA	3:F:190:PRO:HD3	1.85	0.42
3:F:262:ALA:HA	3:F:263:PRO:HD3	1.84	0.42
1:A:377:CYS:HA	1:A:378:PRO:HD2	1.86	0.42
3:C:239:ARG:HH12	3:C:242:GLN:HB2	1.85	0.42
1:D:405:LEU:N	1:D:406:PRO:CD	2.83	0.42
1:D:482:ILE:HG22	1:D:483:ILE:N	2.35	0.42
3:F:290:ASP:CB	3:F:291:PRO:CD	2.97	0.42
1:A:453:ASP:OD2	1:A:454:HIS:N	2.53	0.42
2:B:241:GLU:O	2:B:245:ILE:HG12	2.20	0.42
2:B:253:PRO:O	2:B:256:LYS:HG2	2.20	0.42
2:E:130:ALA:O	2:E:134:LEU:HG	2.20	0.42
2:E:282:THR:HG21	2:E:315:ILE:HD11	2.02	0.42
3:F:119:GLU:OE1	3:F:119:GLU:N	2.53	0.42
1:A:119:HIS:HB3	1:A:120:SER:H	1.58	0.42
2:B:52:LEU:HD23	2:B:52:LEU:O	2.20	0.42
2:B:219:ASN:HD22	2:B:219:ASN:N	2.17	0.41
1:D:16:LEU:HB3	1:D:38:ILE:HD11	2.01	0.41
2:E:171:PHE:CD2	2:E:224:LEU:HG	2.54	0.41
3:F:200:TRP:HE3	3:F:214:ARG:HD3	1.83	0.41
2:E:339:HIS:CD2	3:F:125:GLN:HB3	2.55	0.41
3:C:114:LEU:HD21	3:C:157:ALA:HB2	2.03	0.41
3:C:212:SER:HA	3:C:213:PRO:HD3	1.94	0.41
3:C:215:GLY:HA3	4:M:5:1ZN:C12	2.50	0.41
1:D:32:ILE:O	1:D:35:LEU:HB2	2.20	0.41
1:D:217:GLN:HB2	1:D:220:VAL:HG23	2.01	0.41
1:D:385:ILE:HD12	1:D:423:ILE:HD11	2.02	0.41
1:D:343:SER:HB2	1:D:379:GLU:HG3	2.02	0.41
1:A:538:PHE:O	1:A:542:LYS:HB2	2.20	0.41
2:B:340:PHE:CE1	3:C:122:GLN:HG3	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:267:TYR:C	3:C:269:CYS:H	2.24	0.41
1:D:160:SER:HA	1:D:163:LYS:HB2	2.01	0.41
2:E:30:ILE:N	2:E:34:PRO:HG3	2.34	0.41
2:E:379:LYS:O	2:E:381:HIS:N	2.54	0.41
3:F:147:THR:HA	3:F:150:PHE:HD1	1.77	0.41
3:F:224:ILE:O	3:F:227:THR:N	2.54	0.41
1:A:245:MET:O	1:A:246:PRO:C	2.57	0.41
1:A:570:ASP:HB3	1:A:571:GLN:H	1.51	0.41
2:B:237:LEU:O	2:B:238:PRO:C	2.58	0.41
2:B:308:LEU:HB3	2:B:349:TYR:OH	2.21	0.41
2:B:308:LEU:HD11	2:B:327:LEU:HD11	2.02	0.41
3:F:240:ALA:C	3:F:242:GLN:H	2.23	0.41
3:C:174:ILE:C	3:C:174:ILE:HD12	2.40	0.41
2:E:356:MET:C	2:E:358:LEU:H	2.24	0.41
2:B:352:ASN:HB2	2:B:355:ILE:CD1	2.37	0.41
2:B:367:LEU:N	2:B:368:PRO:HD2	2.24	0.41
1:D:24:ASP:HB3	1:D:27:LEU:HD23	2.02	0.41
1:A:26:GLN:HA	1:A:29:LEU:HB3	2.03	0.41
1:A:35:LEU:HD12	1:A:38:ILE:HD12	2.03	0.41
1:A:279:THR:O	1:A:284:VAL:HG23	2.20	0.41
1:A:341:VAL:CG2	1:A:342:LYS:H	2.34	0.41
1:A:539:ASN:ND2	1:A:542:LYS:HD3	2.36	0.41
2:B:161:GLN:HG2	2:B:199:TYR:CG	2.56	0.41
2:B:312:LEU:HA	2:B:315:ILE:HB	2.03	0.41
3:C:114:LEU:HD13	3:C:156:THR:HA	2.03	0.41
3:C:117:ASN:HB2	3:C:200:TRP:CE2	2.56	0.41
1:D:467:LYS:NZ	1:D:510:GLU:OE2	2.48	0.41
1:D:564:LEU:HB3	1:D:583:LEU:HD21	2.03	0.41
2:E:69:LYS:O	2:E:73:LEU:HD22	2.21	0.41
2:E:128:GLU:O	2:E:131:TRP:HB2	2.21	0.41
2:E:291:LYS:C	2:E:293:TRP:N	2.74	0.41
3:F:155:LEU:HD23	3:F:155:LEU:HA	1.87	0.41
3:C:10:LEU:HD11	3:C:105:VAL:HG22	2.03	0.41
1:D:141:PHE:HZ	2:E:213:TYR:CD1	2.38	0.41
2:E:55:PHE:HD1	2:E:56:VAL:O	2.03	0.41
2:E:99:PHE:O	2:E:103:MET:HB2	2.20	0.41
2:E:138:TYR:CD2	2:E:181:PHE:HB3	2.56	0.41
2:E:186:LEU:HD12	2:E:227:ILE:HD13	2.02	0.41
3:F:117:ASN:HD22	3:F:117:ASN:H	1.68	0.41
3:F:122:GLN:OE1	4:N:5:1ZN:H7	2.21	0.41
1:A:338:ASN:ND2	1:A:340:HIS:HB2	2.36	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLN:HA	2:B:38:GLN:NE2	2.31	0.40
3:C:189:VAL:HA	3:C:190:PRO:HD3	1.89	0.40
2:E:190:TYR:CE2	2:E:197:ARG:HG3	2.56	0.40
1:A:237:GLN:HB3	1:A:238:GLU:H	1.80	0.40
1:A:432:GLY:HA3	1:A:472:LYS:HE2	2.02	0.40
1:D:38:ILE:O	1:D:42:LEU:HB3	2.22	0.40
2:E:131:TRP:O	2:E:132:PRO:C	2.59	0.40
2:E:295:LYS:HG2	2:E:296:THR:N	2.37	0.40
2:E:386:ILE:HA	2:E:389:LEU:HB2	2.03	0.40
3:F:14:ILE:HD13	3:F:103:LEU:HD23	2.02	0.40
1:A:255:LYS:O	2:B:106:THR:HG21	2.21	0.40
1:A:265:ASP:O	1:A:266:LYS:HD2	2.21	0.40
1:A:303:SER:C	1:A:305:LYS:N	2.63	0.40
1:A:310:CYS:HA	1:A:313:LEU:CD1	2.51	0.40
1:A:373:LEU:HD11	1:A:385:ILE:HD11	2.03	0.40
2:E:251:LEU:O	2:E:254:LEU:HB2	2.21	0.40
1:D:52:LEU:CD1	1:D:92:PRO:HG3	2.50	0.40
1:D:210:SER:HA	1:D:247:THR:HG21	2.04	0.40
2:E:289:LEU:HD23	2:E:308:LEU:CD2	2.52	0.40
3:F:59:HIS:CD2	3:F:267:TYR:HE2	2.40	0.40
1:A:94:GLU:HB2	1:A:131:LEU:CD2	2.51	0.40
1:A:531:ASP:HA	1:A:532:PRO:HD2	1.89	0.40
1:A:539:ASN:ND2	3:C:77:ASP:OD2	2.55	0.40
2:B:170:LEU:C	2:B:172:ASP:N	2.75	0.40
1:D:18:ASP:C	1:D:20:LEU:H	2.25	0.40
1:D:90:LEU:N	1:D:91:PRO:HD2	2.37	0.40
2:E:121:GLU:HB3	4:N:2:LEU:HD12	2.02	0.40
3:F:214:ARG:NH2	3:F:241:HIS:CE1	2.89	0.40

All (6) 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)
3:C:175:ASP:OD1	4:M:4:ARG:NE[11_466]	1.57	0.63
3:F:175:ASP:OD2	4:N:4:ARG:NE[12_664]	1.61	0.59
3:F:175:ASP:OD2	4:N:3:ACB:OXT[12_664]	1.65	0.55
3:C:175:ASP:CG	4:M:4:ARG:NE[11_466]	2.01	0.19
3:F:175:ASP:CG	4:N:4:ARG:NE[12_664]	2.05	0.15
3:F:175:ASP:OD1	4:N:4:ARG:NE[12_664]	2.19	0.01



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	581/589 (99%)	502 (86%)	63 (11%)	16 (3%)	5	32
1	D	581/589 (99%)	505 (87%)	65 (11%)	11 (2%)	8	40
2	B	374/407 (92%)	300 (80%)	60 (16%)	14 (4%)	3	26
2	E	375/407 (92%)	307 (82%)	53 (14%)	15 (4%)	3	24
3	C	304/309 (98%)	253 (83%)	40 (13%)	11 (4%)	3	26
3	F	289/309 (94%)	231 (80%)	41 (14%)	17 (6%)	1	15
4	M	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2505/2617 (96%)	2099 (84%)	322 (13%)	84 (3%)	3	28

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	304	HIS
2	B	34	PRO
2	B	56	VAL
2	B	121	GLU
2	B	382	TRP
3	C	269	CYS
3	C	298	PRO
1	D	493	PRO
1	D	514	GLN
2	E	121	GLU
2	E	161	GLN
2	E	380	THR
3	F	75	SER
3	F	76	PRO
3	F	94	VAL
3	F	252	HIS
3	F	265	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	239	ASP
2	B	238	PRO
2	B	380	THR
3	C	20	CYS
3	C	232	ASN
3	C	282	LEU
1	D	102	THR
1	D	491	GLY
1	D	510	GLU
1	D	513	GLY
1	D	573	VAL
2	E	234	GLY
3	F	232	ASN
3	F	233	GLY
3	F	251	CYS
1	A	43	GLY
1	A	237	GLN
1	A	315	ALA
1	A	475	LYS
2	B	61	SER
2	B	218	HIS
3	C	230	HIS
3	C	268	ARG
1	D	45	GLU
1	D	61	ASP
2	E	64	LYS
2	E	111	SER
2	E	237	LEU
2	E	348	TYR
3	F	240	ALA
3	F	271	ASN
1	A	76	PHE
1	A	196	LEU
1	A	245	MET
2	B	214	GLU
2	B	367	LEU
2	E	122	GLU
2	E	233	ASN
2	E	236	ALA
2	E	278	ASP
2	E	357	SER
1	A	79	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	432	GLY
1	A	561	LYS
2	B	36	ALA
3	C	263	PRO
1	D	492	ASP
3	F	89	ARG
3	F	127	TYR
3	F	269	CYS
3	F	270	GLY
1	A	474	GLY
3	C	59	HIS
3	C	129	PHE
2	E	35	PRO
2	E	371	PHE
3	F	117	ASN
1	A	11	TYR
1	A	436	VAL
2	B	58	ASP
1	D	44	VAL
2	B	51	VAL
2	B	237	LEU
3	C	128	GLY
3	F	50	CYS
3	F	5	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	509/512 (99%)	448 (88%)	61 (12%)	5 24
1	D	509/512 (99%)	445 (87%)	64 (13%)	4 22
2	B	310/379 (82%)	254 (82%)	56 (18%)	1 9
2	E	311/379 (82%)	257 (83%)	54 (17%)	2 11
3	C	257/273 (94%)	211 (82%)	46 (18%)	2 9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	253/273 (93%)	196 (78%)	57 (22%)	1	4
4	M	2/2 (100%)	0	2 (100%)	0	0
4	N	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	2153/2332 (92%)	1812 (84%)	341 (16%)	2	15

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	21	ARG
1	A	26	GLN
1	A	30	ASN
1	A	42	LEU
1	A	52	LEU
1	A	59	ILE
1	A	60	TYR
1	A	63	ASP
1	A	64	GLU
1	A	86	VAL
1	A	107	LYS
1	A	112	LEU
1	A	123	ASP
1	A	124	LEU
1	A	140	TRP
1	A	168	GLN
1	A	196	LEU
1	A	211	ASN
1	A	218	ASP
1	A	222	LEU
1	A	228	CYS
1	A	237	GLN
1	A	250	GLN
1	A	255	LYS
1	A	266	LYS
1	A	277	GLU
1	A	282	ASP
1	A	304	HIS
1	A	307	LYS
1	A	312	ASN
1	A	318	ARG
1	A	331	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	347	SER
1	A	358	LYS
1	A	373	LEU
1	A	387	ASN
1	A	389	ASP
1	A	392	ASN
1	A	394	VAL
1	A	395	ILE
1	A	398	ARG
1	A	402	GLN
1	A	418	ARG
1	A	425	GLU
1	A	434	LEU
1	A	441	GLU
1	A	448	MET
1	A	454	HIS
1	A	455	VAL
1	A	466	LEU
1	A	473	PHE
1	A	494	ASN
1	A	502	LEU
1	A	506	ASN
1	A	526	LEU
1	A	527	ARG
1	A	556	LEU
1	A	566	LYS
1	A	570	ASP
1	A	581	GLU
2	B	38	GLN
2	B	43	ILE
2	B	49	CYS
2	B	53	PHE
2	B	56	VAL
2	B	58	ASP
2	B	62	ASP
2	B	67	GLU
2	B	70	ARG
2	B	73	LEU
2	B	78	GLU
2	B	94	GLU
2	B	103	MET
2	B	107	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	112	ASN
2	B	123	ASP
2	B	126	THR
2	B	142	LEU
2	B	143	ARG
2	B	147	SER
2	B	149	ASP
2	B	157	LYS
2	B	162	LYS
2	B	168	LEU
2	B	169	GLU
2	B	177	ARG
2	B	178	GLU
2	B	179	ARG
2	B	181	PHE
2	B	184	THR
2	B	196	LEU
2	B	203	GLN
2	B	210	ARG
2	B	214	GLU
2	B	219	ASN
2	B	237	LEU
2	B	239	LEU
2	B	240	LYS
2	B	256	LYS
2	B	257	VAL
2	B	258	LYS
2	B	266	GLN
2	B	285	VAL
2	B	287	MET
2	B	308	LEU
2	B	312	LEU
2	B	315	ILE
2	B	323	ILE
2	B	331	LEU
2	B	348	TYR
2	B	353	GLU
2	B	361	ASP
2	B	373	SER
2	B	386	ILE
2	B	389	LEU
2	B	390	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	10	LEU
3	C	15	GLU
3	C	17	LEU
3	C	25	GLU
3	C	31	LEU
3	C	37	GLU
3	C	46	GLN
3	C	49	ARG
3	C	52	VAL
3	C	61	GLN
3	C	83	MET
3	C	87	VAL
3	C	91	TYR
3	C	93	SER
3	C	98	THR
3	C	105	VAL
3	C	106	ARG
3	C	110	ARG
3	C	112	THR
3	C	117	ASN
3	C	124	THR
3	C	139	ASN
3	C	144	LYS
3	C	158	LEU
3	C	162	GLN
3	C	175	ASP
3	C	177	LEU
3	C	185	ARG
3	C	186	LEU
3	C	199	LEU
3	C	214	ARG
3	C	222	GLN
3	C	234	LEU
3	C	243	LEU
3	C	244	VAL
3	C	250	TRP
3	C	256	VAL
3	C	264	ASN
3	C	265	TYR
3	C	268	ARG
3	C	275	ILE
3	C	282	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	283	LYS
3	C	290	ASP
3	C	294	ARG
3	C	306	ASP
1	D	10	LEU
1	D	20	LEU
1	D	25	VAL
1	D	30	ASN
1	D	42	LEU
1	D	45	GLU
1	D	55	LEU
1	D	58	THR
1	D	60	TYR
1	D	71	GLU
1	D	77	THR
1	D	102	THR
1	D	112	LEU
1	D	113	ARG
1	D	131	LEU
1	D	139	ASP
1	D	144	ARG
1	D	153	VAL
1	D	194	LYS
1	D	196	LEU
1	D	222	LEU
1	D	226	GLU
1	D	237	GLN
1	D	245	MET
1	D	272	LYS
1	D	294	CYS
1	D	318	ARG
1	D	327	LEU
1	D	330	ILE
1	D	331	LYS
1	D	345	LEU
1	D	350	MET
1	D	358	LYS
1	D	370	LEU
1	D	387	ASN
1	D	392	ASN
1	D	395	ILE
1	D	398	ARG

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	405	LEU
1	D	410	GLU
1	D	413	GLU
1	D	418	ARG
1	D	429	LEU
1	D	437	GLU
1	D	441	GLU
1	D	459	ARG
1	D	466	LEU
1	D	467	LYS
1	D	468	LYS
1	D	469	LEU
1	D	481	THR
1	D	489	MET
1	D	492	ASP
1	D	501	THR
1	D	502	LEU
1	D	526	LEU
1	D	527	ARG
1	D	539	ASN
1	D	542	LYS
1	D	554	SER
1	D	569	GLN
1	D	570	ASP
1	D	571	GLN
1	D	581	GLU
2	E	39	GLU
2	E	43	ILE
2	E	45	LYS
2	E	50	CYS
2	E	52	LEU
2	E	55	PHE
2	E	63	LEU
2	E	73	LEU
2	E	78	GLU
2	E	81	THR
2	E	91	ILE
2	E	96	VAL
2	E	98	MET
2	E	103	MET
2	E	105	ARG
2	E	111	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	114	THR
2	E	131	TRP
2	E	143	ARG
2	E	146	GLU
2	E	154	ILE
2	E	156	LYS
2	E	162	LYS
2	E	165	LEU
2	E	169	GLU
2	E	186	LEU
2	E	188	ARG
2	E	215	THR
2	E	216	GLU
2	E	233	ASN
2	E	235	PHE
2	E	258	LYS
2	E	259	SER
2	E	261	SER
2	E	266	GLN
2	E	275	LEU
2	E	277	LYS
2	E	289	LEU
2	E	295	LYS
2	E	298	SER
2	E	306	ASN
2	E	308	LEU
2	E	309	GLU
2	E	312	LEU
2	E	315	ILE
2	E	318	SER
2	E	319	GLU
2	E	327	LEU
2	E	375	TYR
2	E	381	HIS
2	E	385	THR
2	E	386	ILE
2	E	389	LEU
2	E	390	ILE
3	F	7	THR
3	F	8	LYS
3	F	12	GLN
3	F	15	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	F	18	ASN
3	F	19	GLU
3	F	22	GLN
3	F	30	SER
3	F	32	CYS
3	F	38	ILE
3	F	39	LEU
3	F	42	GLU
3	F	45	VAL
3	F	46	GLN
3	F	48	VAL
3	F	53	THR
3	F	55	CYS
3	F	58	VAL
3	F	61	GLN
3	F	68	LEU
3	F	75	SER
3	F	81	LEU
3	F	87	VAL
3	F	98	THR
3	F	105	VAL
3	F	106	ARG
3	F	110	ARG
3	F	112	THR
3	F	114	LEU
3	F	117	ASN
3	F	119	GLU
3	F	122	GLN
3	F	124	THR
3	F	131	ASP
3	F	158	LEU
3	F	174	ILE
3	F	175	ASP
3	F	185	ARG
3	F	186	LEU
3	F	192	GLU
3	F	199	LEU
3	F	214	ARG
3	F	227	THR
3	F	232	ASN
3	F	239	ARG
3	F	243	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	F	250	TRP
3	F	254	ARG
3	F	264	ASN
3	F	265	TYR
3	F	266	CYS
3	F	267	TYR
3	F	269	CYS
3	F	275	ILE
3	F	279	ASP
3	F	290	ASP
3	F	294	ARG
4	M	2	LEU
4	M	4	ARG
4	N	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	22	ASN
1	A	119	HIS
1	A	172	ASN
1	A	200	ASN
1	A	211	ASN
1	A	217	GLN
1	A	288	GLN
1	A	320	ASN
1	A	338	ASN
1	A	387	ASN
1	A	494	ASN
1	A	506	ASN
1	A	539	ASN
2	B	38	GLN
2	B	44	GLN
2	B	82	HIS
2	B	97	HIS
2	B	203	GLN
2	B	218	HIS
2	B	219	ASN
2	B	243	HIS
2	B	273	GLN
2	B	297	HIS
2	B	352	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	383	ASN
2	B	387	HIS
3	C	27	GLN
3	C	59	HIS
3	C	79	ASN
3	C	88	ASN
3	C	139	ASN
3	C	179	HIS
3	C	187	GLN
3	C	264	ASN
3	C	271	ASN
3	C	288	GLN
1	D	22	ASN
1	D	30	ASN
1	D	117	HIS
1	D	168	GLN
1	D	172	ASN
1	D	200	ASN
1	D	233	GLN
1	D	325	GLN
1	D	339	GLN
1	D	387	ASN
1	D	402	GLN
1	D	514	GLN
1	D	539	ASN
1	D	545	GLN
1	D	571	GLN
2	E	44	GLN
2	E	48	GLN
2	E	82	HIS
2	E	112	ASN
2	E	218	HIS
2	E	264	HIS
2	E	266	GLN
2	E	297	HIS
3	F	18	ASN
3	F	27	GLN
3	F	46	GLN
3	F	63	HIS
3	F	79	ASN
3	F	118	HIS
3	F	162	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
3	F	191	HIS
3	F	232	ASN
3	F	241	HIS
3	F	255	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1ZN	M	5	4	23,23,24	1.92	1 (4%)	24,29,31	1.60	6 (25%)
4	1ZN	N	5	4	23,23,24	2.11	2 (8%)	24,29,31	2.08	9 (37%)
4	FGA	N	6	4	7,8,9	1.55	1 (14%)	8,9,11	1.41	0
4	FGA	M	6	4	7,8,9	1.51	1 (14%)	8,9,11	1.33	1 (12%)
4	DAM	M	7	4	4,5,6	1.77	1 (25%)	3,5,7	3.56	3 (100%)
4	ACB	N	3	4	7,8,9	2.08	2 (28%)	8,10,12	1.66	1 (12%)
4	DAM	N	7	4	4,5,6	1.79	1 (25%)	3,5,7	5.02	3 (100%)
3	MLL	C	309	3	9,9,9	3.35	2 (22%)	11,11,11	2.26	2 (18%)
4	ACB	M	3	4	7,8,9	1.78	2 (28%)	8,10,12	1.84	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1ZN	M	5	4	-	4/22/25/27	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1ZN	N	5	4	-	2/22/25/27	0/1/1/1
4	FGA	N	6	4	-	4/8/8/9	-
4	FGA	M	6	4	-	3/8/8/9	-
4	DAM	M	7	4	-	0/0/4/6	-
4	ACB	N	3	4	-	3/9/10/12	-
4	DAM	N	7	4	-	0/0/4/6	-
3	MLL	C	309	3	-	9/10/10/10	-
4	ACB	M	3	4	-	1/9/10/12	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	5	1ZN	C15-C13	-9.20	1.26	1.45
3	C	309	MLL	O-C	9.06	1.44	1.21
4	M	5	1ZN	C15-C13	-8.56	1.27	1.45
3	C	309	MLL	OXT-C	4.18	1.43	1.33
4	N	3	ACB	O-C	4.13	1.34	1.22
4	M	3	ACB	O-C	3.56	1.33	1.22
4	M	6	FGA	OE2-CD	-3.48	1.24	1.42
4	N	6	FGA	OE2-CD	-3.44	1.24	1.42
4	N	7	DAM	C-CA	3.24	1.50	1.45
4	M	7	DAM	C-CA	2.97	1.49	1.45
4	N	3	ACB	CB-CG	2.41	1.54	1.50
4	N	5	1ZN	C15-C16	-2.07	1.27	1.32
4	M	3	ACB	OD1-CG	2.01	1.27	1.19

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	309	MLL	OXT-C-O	-6.54	111.04	123.84
4	N	7	DAM	O-C-CA	-6.52	116.85	125.22
4	N	5	1ZN	C18-CA-C16	-4.75	106.17	112.98
4	M	7	DAM	O-C-CA	-4.73	119.14	125.22
4	N	7	DAM	CM-N-CA	-4.59	116.47	123.45
4	N	5	1ZN	CA-C16-C15	3.91	129.57	123.59
4	N	5	1ZN	CA-C18-C	3.60	115.17	110.72
4	M	3	ACB	OD1-CG-CB	-3.56	115.44	124.91
4	N	3	ACB	CA-CB-CG	-3.54	106.29	110.75
4	N	7	DAM	CB-CA-N	-3.44	117.57	125.91
4	M	5	1ZN	C14-C13-C15	-3.24	112.97	118.08
4	N	5	1ZN	C11-C10-C2	-3.21	107.02	111.80

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	5	1ZN	C14-C13-C15	-3.19	113.05	118.08
3	C	309	MLL	O-C-CA	-3.05	110.93	120.95
4	M	7	DAM	CM-N-CA	-3.05	118.82	123.45
4	M	5	1ZN	C10-C12-C13	-2.91	117.46	126.67
4	M	5	1ZN	C18-CA-C16	-2.85	108.89	112.98
4	M	3	ACB	CA-CB-CG	-2.81	107.21	110.75
4	N	5	1ZN	C10-C12-C13	-2.70	118.11	126.67
4	N	5	1ZN	C2-C10-C12	2.61	114.95	110.24
4	M	5	1ZN	C15-C13-C12	2.59	127.94	119.42
4	M	7	DAM	CB-CA-N	-2.51	119.81	125.91
4	N	5	1ZN	C15-C13-C12	2.31	127.02	119.42
4	M	5	1ZN	C3-C2-C10	-2.14	110.46	115.45
4	M	6	FGA	CG-CB-CA	-2.04	106.80	113.35
4	M	5	1ZN	CA-C16-C15	2.01	126.67	123.59
4	N	5	1ZN	C16-CA-N	-2.01	105.27	109.86

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	309	MLL	O-C-CA-N
3	C	309	MLL	O-C-CA-CB
4	N	3	ACB	CA-CB-CG-OD1
4	N	5	1ZN	C12-C13-C15-C16
4	N	5	1ZN	C14-C13-C15-C16
3	C	309	MLL	CA-C-OXT-C10
4	M	5	1ZN	C14-C13-C15-C16
4	M	5	1ZN	C12-C13-C15-C16
4	N	6	FGA	CA-CB-CG-CD
4	N	6	FGA	OE2-CD-CG-CB
3	C	309	MLL	CA-CB-CG-CD2
4	N	3	ACB	OXT-C-CA-CB
3	C	309	MLL	CA-CB-CG-CD1
4	N	6	FGA	OXT-C-CA-N
4	M	6	FGA	OXT-C-CA-N
4	M	6	FGA	O-C-CA-N
4	N	6	FGA	O-C-CA-N
4	M	6	FGA	OE2-CD-CG-CB
3	C	309	MLL	OXT-C-CA-N
4	M	3	ACB	CA-CB-CG-OD1
4	M	5	1ZN	O-C-C18-CA
3	C	309	MLL	OXT-C-CA-CB

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	M	5	1ZN	C10-C2-C3-C4
4	N	3	ACB	O-C-CA-CB
3	C	309	MLL	C-CA-CB-CG
3	C	309	MLL	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	5	1ZN	4	0
4	N	5	1ZN	2	0
4	M	6	FGA	3	0
4	M	7	DAM	4	0
4	N	3	ACB	15	1
4	N	7	DAM	7	0
3	C	309	MLL	4	0
4	M	3	ACB	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	2:LEU	C	3:ACB	N	2.64

## 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	583/589 (98%)	0.56	67 (11%) 4 5	85, 114, 172, 203	0
1	D	583/589 (98%)	0.12	6 (1%) 82 77	96, 113, 129, 144	0
2	B	376/407 (92%)	-0.01	7 (1%) 66 61	77, 90, 126, 152	0
2	E	377/407 (92%)	0.05	8 (2%) 63 58	63, 76, 103, 139	0
3	C	305/309 (98%)	0.21	6 (1%) 65 60	81, 93, 112, 139	0
3	F	291/309 (94%)	0.25	1 (0%) 94 91	131, 149, 159, 166	0
4	M	2/7 (28%)	-0.05	0 100 100	86, 86, 86, 91	0
4	N	2/7 (28%)	-0.21	0 100 100	80, 80, 80, 85	0
All	All	2519/2624 (95%)	0.22	95 (3%) 40 36	63, 106, 153, 203	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	ASP	11.0
1	D	8	ASP	7.0
1	A	7	ASP	5.6
1	A	11	TYR	4.9
1	A	352	LEU	4.7
1	A	365	LEU	4.3
1	A	19	GLU	4.2
1	A	512	CYS	4.1
1	A	437	GLU	4.1
1	A	36	SER	4.0
1	A	372	GLN	4.0
2	E	56	VAL	3.7
1	A	9	SER	3.7
1	D	517	THR	3.6
2	B	401	ASN	3.6
2	E	32	ASP	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	17	ILE	3.5
1	A	40	LEU	3.5
1	A	8	ASP	3.4
2	E	369	ILE	3.3
1	A	118	GLU	3.3
1	A	551	LEU	3.3
1	A	482	ILE	3.2
1	D	64	GLU	3.1
1	A	10	LEU	3.0
2	B	350	TRP	3.0
1	A	547	ILE	3.0
1	A	330	ILE	3.0
1	A	326	ILE	3.0
1	A	12	PRO	2.9
1	A	426	TYR	2.9
1	A	112	LEU	2.9
1	A	35	LEU	2.8
1	A	77	THR	2.8
1	A	154	CYS	2.8
1	A	73	LEU	2.7
3	C	236	LEU	2.7
1	A	32	ILE	2.7
1	A	74	GLY	2.7
1	A	80	VAL	2.7
1	A	505	ILE	2.7
1	A	79	LEU	2.6
1	A	404	LEU	2.6
2	B	378	SER	2.6
3	C	75	SER	2.6
2	E	328	PHE	2.6
1	A	151	PHE	2.5
2	B	381	HIS	2.5
1	A	560	VAL	2.5
3	C	98	THR	2.5
1	A	463	THR	2.4
1	A	544	LEU	2.4
3	C	143	TRP	2.4
1	A	325	GLN	2.4
1	A	388	LEU	2.4
3	C	133	CYS	2.4
1	A	368	LEU	2.4
1	D	56	THR	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	95	VAL	2.4
1	A	48	ARG	2.4
2	E	365	LYS	2.4
3	F	33	GLU	2.3
3	C	266	CYS	2.3
2	B	56	VAL	2.3
1	A	90	LEU	2.3
1	A	23	GLU	2.3
1	A	41	ALA	2.3
1	A	50	GLU	2.3
1	A	309	PHE	2.3
2	B	238	PRO	2.3
1	A	387	ASN	2.3
2	E	350	TRP	2.2
1	A	411	LEU	2.2
1	A	467	LYS	2.2
1	A	579	ALA	2.2
1	A	290	LEU	2.2
1	A	394	VAL	2.2
1	A	513	GLY	2.2
1	A	549	PRO	2.2
2	B	328	PHE	2.2
1	A	88	CYS	2.1
1	A	362	ILE	2.1
1	A	552	ASP	2.1
1	A	319	GLU	2.1
1	A	521	MET	2.1
1	A	450	TRP	2.1
1	D	479	HIS	2.1
1	A	373	LEU	2.1
2	E	123	ASP	2.0
1	A	52	LEU	2.0
1	A	588	LEU	2.0
1	A	78	THR	2.0
1	A	510	GLU	2.0
1	A	115	ILE	2.0
1	A	439	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MLL	C	309	10/10	0.63	0.51	139,139,139,140	0
4	ACB	N	3	9/10	0.80	0.42	82,83,85,86	0
4	DAM	M	7	6/7	0.86	0.42	93,93,93,93	0
4	FGA	N	6	9/10	0.89	0.33	78,82,83,84	0
4	FGA	M	6	9/10	0.89	0.36	87,90,91,92	0
4	1ZN	M	5	23/24	0.91	0.40	85,85,89,90	0
4	ACB	M	3	9/10	0.91	0.35	87,88,90,90	0
4	DAM	N	7	6/7	0.91	0.29	84,84,84,85	0
4	DAL	N	1	5/6	0.94	0.20	84,84,84,84	0
4	1ZN	N	5	23/24	0.94	0.34	63,66,76,77	0
4	DAL	M	1	5/6	0.95	0.26	91,91,91,91	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MN	F	310	1/1	0.95	0.13	86,86,86,86	0
5	MN	C	310	1/1	0.96	0.09	119,119,119,119	0
5	MN	F	311	1/1	0.96	0.15	33,33,33,33	0
5	MN	C	311	1/1	0.97	0.12	63,63,63,63	0

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

There are no such residues in this entry.