



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:41 am GMT

PDB ID : 3WLW  
Title : Molecular Architecture of the ErbB2 Extracellular Domain Homodimer  
Authors : Hu, S.; Lou, Z.Y.; Guo, Y.J.  
Deposited on : 2013-11-15  
Resolution : 3.09 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

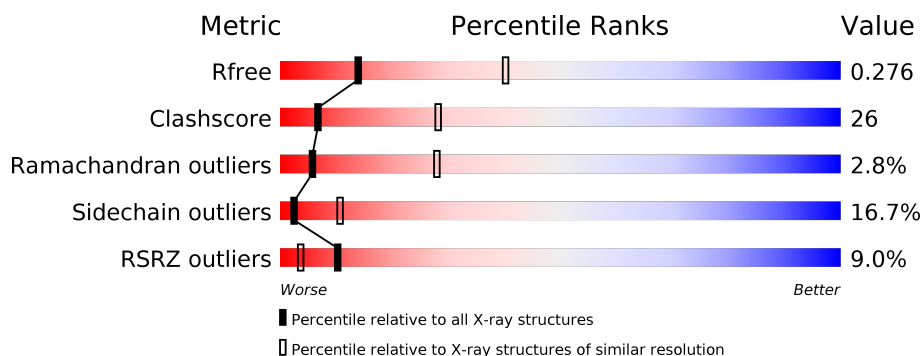
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 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))
$R_{free}$	100719	1116 (3.10-3.06)
Clashscore	112137	1220 (3.10-3.06)
Ramachandran outliers	110173	1176 (3.10-3.06)
Sidechain outliers	110143	1176 (3.10-3.06)
RSRZ outliers	101464	1123 (3.10-3.06)

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	564	<div> <div>3%</div> <div>60%</div> <div>30%</div> <div>7%</div> <div>..</div> </div>
1	B	564	<div> <div>2%</div> <div>55%</div> <div>34%</div> <div>9%</div> <div>..</div> </div>
2	C	217	<div> <div>24%</div> <div>43%</div> <div>46%</div> <div>10%</div> <div>.</div> </div>
2	H	217	<div> <div>4%</div> <div>54%</div> <div>35%</div> <div>9%</div> <div>.</div> </div>
3	D	217	<div> <div>33%</div> <div>43%</div> <div>37%</div> <div>16%</div> <div>.</div> </div>
3	L	217	<div> <div>10%</div> <div>53%</div> <div>36%</div> <div>8%</div> <div>.</div> </div>

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
4	NAG	A	1001	X	-	X	-
5	NAG	B	1001	X	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15155 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			
1	B	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			

- Molecule 2 is a protein called Antibody H Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1624	1021	269	327	7			
2	C	217	Total	C	N	O	S	0	0	0
			1624	1021	269	327	7			

- Molecule 3 is a protein called Antibody L Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1616	1001	269	340	6			
3	D	217	Total	C	N	O	S	0	0	0
			1616	1001	269	340	6			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	14	Total	O	0	0
			14	14		
6	H	2	Total	O	0	0
			2	2		
6	L	5	Total	O	0	0
			5	5		
6	C	12	Total	O	0	0
			12	12		
6	D	19	Total	O	0	0
			19	19		

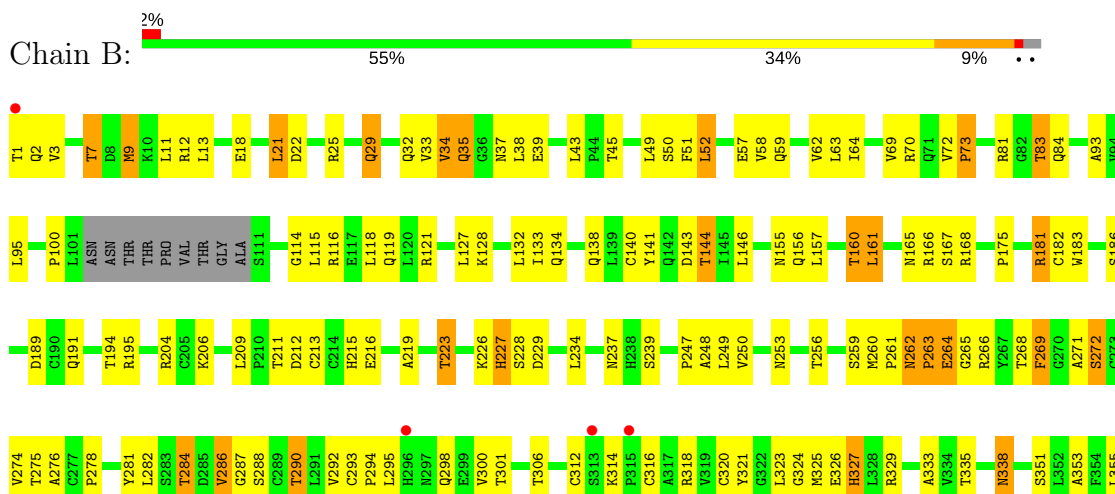
### 3 Residue-property plots

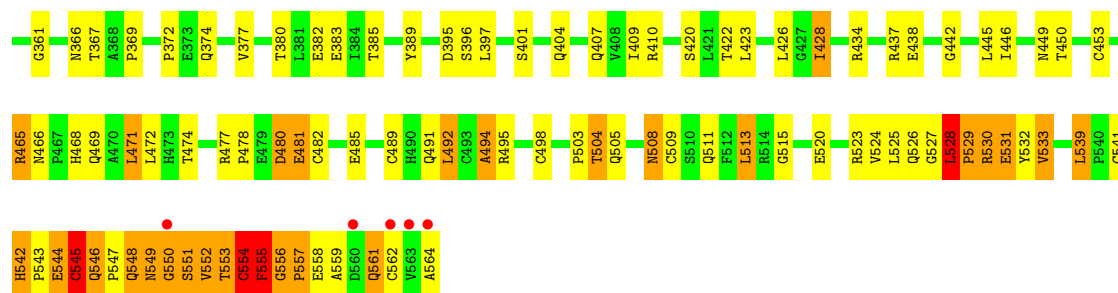
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Receptor tyrosine-protein kinase erbB-2

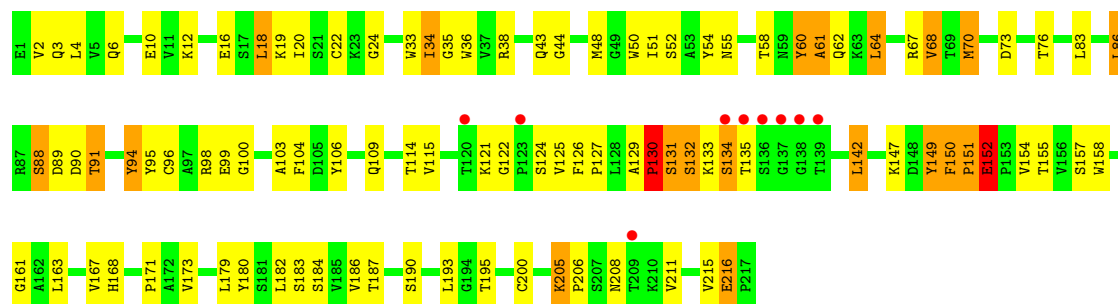


- Molecule 1: Receptor tyrosine-protein kinase erbB-2

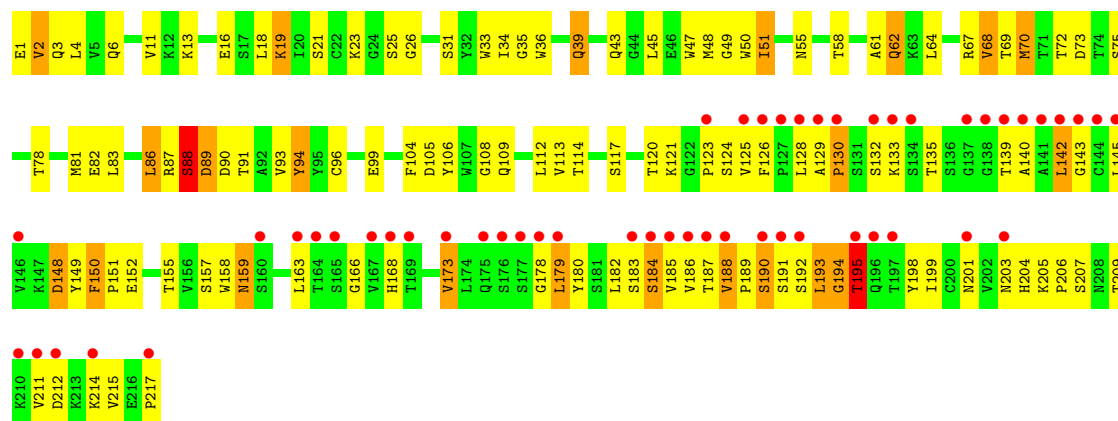
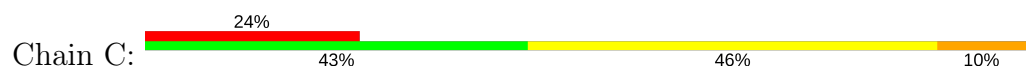




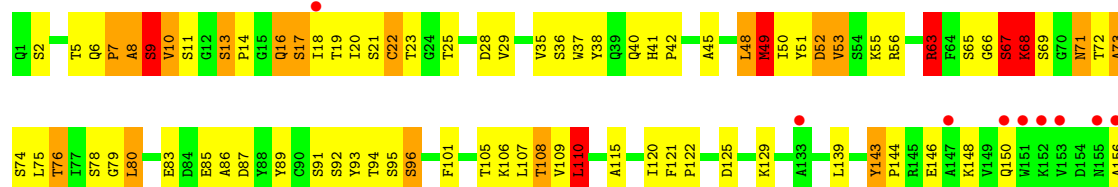
• Molecule 2: Antibody H Chain

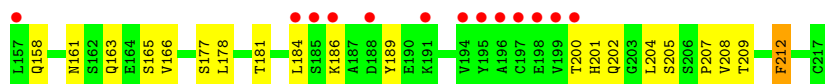


• Molecule 2: Antibody H Chain

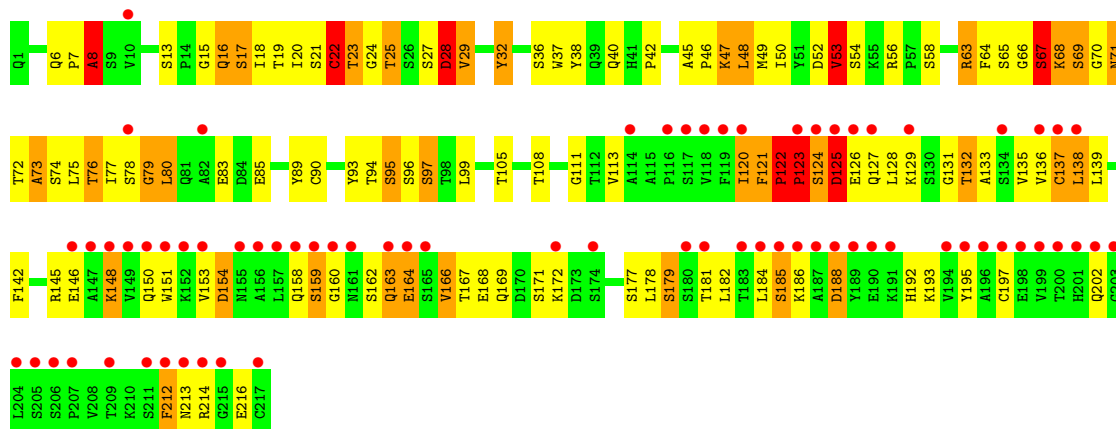
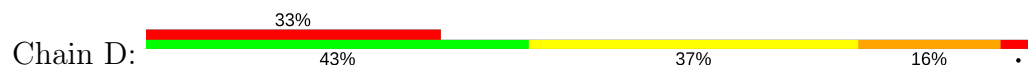


• Molecule 3: Antibody L Chain





### ● Molecule 3: Antibody L Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.72Å 104.19Å 116.71Å 106.89° 99.65° 111.12°	Depositor
Resolution (Å)	32.26 – 3.09 48.29 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.26-3.09) 80.7 (48.29-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.232 , 0.269 0.240 , 0.276	Depositor DCC
$R_{free}$ test set	3053 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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

### 5.1 Standard geometry

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

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	0.58	3/4374 (0.1%)	0.91	24/5950 (0.4%)
1	B	0.59	2/4374 (0.0%)	0.88	13/5950 (0.2%)
2	C	0.46	0/1664	0.78	5/2268 (0.2%)
2	H	0.50	1/1664 (0.1%)	0.91	10/2268 (0.4%)
3	D	0.60	0/1649	1.08	18/2241 (0.8%)
3	L	0.55	0/1649	1.02	12/2241 (0.5%)
All	All	0.56	6/15374 (0.0%)	0.92	82/20918 (0.4%)

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	3
1	B	0	1
2	C	0	2
2	H	0	1
3	D	0	6
3	L	0	4
4	A	1	0
All	All	1	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	LEU	C-N	10.37	1.53	1.34
1	A	265	GLY	C-N	8.59	1.53	1.34
1	A	247	PRO	C-N	6.51	1.49	1.34
1	B	557	PRO	N-CD	5.63	1.55	1.47
1	A	529	PRO	N-CD	5.28	1.55	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	130	PRO	N-CD	5.18	1.55	1.47

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	GLU	CB-CA-C	-11.98	86.43	110.40
1	B	269	PHE	CB-CA-C	11.84	134.09	110.40
2	H	62	GLN	N-CA-CB	-10.85	91.07	110.60
1	A	510	SER	CB-CA-C	-10.46	90.22	110.10
3	L	48	LEU	N-CA-CB	-10.30	89.81	110.40
1	A	546	GLN	N-CA-CB	-10.10	92.42	110.60
3	L	53	VAL	N-CA-CB	9.46	132.31	111.50
3	D	67	SER	CB-CA-C	-9.11	92.79	110.10
3	D	7	PRO	N-CA-C	8.94	135.34	112.10
1	A	240	GLY	N-CA-C	-8.92	90.81	113.10
2	H	132	SER	N-CA-C	-8.29	88.63	111.00
3	D	7	PRO	CB-CA-C	-8.23	91.42	112.00
3	L	9	SER	CB-CA-C	-8.12	94.67	110.10
2	H	60	TYR	CB-CA-C	-8.08	94.23	110.40
3	D	125	ASP	CB-CA-C	-7.81	94.78	110.40
3	D	79	GLY	N-CA-C	-7.76	93.70	113.10
1	B	494	ALA	CB-CA-C	-7.75	98.48	110.10
2	H	132	SER	N-CA-CB	7.68	122.03	110.50
3	D	53	VAL	N-CA-CB	7.64	128.32	111.50
1	A	325	MET	CB-CA-C	7.53	125.47	110.40
1	A	197	VAL	N-CA-CB	-7.46	95.09	111.50
2	H	61	ALA	CB-CA-C	-7.46	98.92	110.10
3	L	17	SER	N-CA-C	-7.35	91.14	111.00
1	A	546	GLN	N-CA-C	7.34	130.83	111.00
3	L	110	LEU	CA-CB-CG	7.13	131.70	115.30
3	D	23	THR	N-CA-C	-7.13	91.75	111.00
1	A	511	GLN	N-CA-CB	7.04	123.27	110.60
1	A	545	CYS	N-CA-CB	-7.03	97.94	110.60
1	A	387	TYR	N-CA-CB	-6.94	98.10	110.60
2	H	90	ASP	N-CA-C	-6.80	92.63	111.00
1	B	100	PRO	N-CA-C	6.75	129.65	112.10
1	B	161	LEU	CA-CB-CG	6.73	130.77	115.30
2	C	62	GLN	CB-CA-C	-6.61	97.19	110.40
1	B	428	ILE	CB-CA-C	-6.56	98.48	111.60
2	C	195	THR	N-CA-CB	-6.54	97.87	110.30
2	C	89	ASP	N-CA-C	-6.52	93.39	111.00
1	A	313	SER	CB-CA-C	-6.40	97.95	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ARG	N-CA-C	6.38	128.22	111.00
1	B	7	THR	CB-CA-C	-6.37	94.41	111.60
2	H	61	ALA	N-CA-CB	-6.27	101.32	110.10
3	L	9	SER	CA-C-N	-6.27	103.40	117.20
3	D	28	ASP	CB-CA-C	-6.17	98.07	110.40
1	A	177	CYS	CB-CA-C	6.08	122.56	110.40
3	L	49	MET	N-CA-C	-6.08	94.58	111.00
3	L	53	VAL	N-CA-C	-6.01	94.78	111.00
3	D	28	ASP	N-CA-C	5.99	127.18	111.00
2	C	88	SER	N-CA-C	-5.94	94.95	111.00
3	L	67	SER	CB-CA-C	-5.93	98.84	110.10
3	D	121	PHE	C-N-CD	-5.91	107.60	120.60
3	L	68	LYS	N-CA-C	5.78	126.61	111.00
3	D	69	SER	CB-CA-C	5.76	121.04	110.10
3	D	122	PRO	C-N-CD	5.75	140.48	128.40
3	D	123	PRO	CA-N-CD	-5.72	103.49	111.50
2	H	129	ALA	C-N-CD	5.70	140.37	128.40
1	A	511	GLN	N-CA-C	-5.69	95.63	111.00
2	H	94	TYR	N-CA-C	5.68	126.33	111.00
1	A	100	PRO	N-CA-C	5.63	126.73	112.10
3	D	8	ALA	CB-CA-C	-5.56	101.76	110.10
1	A	314	LYS	N-CA-C	-5.51	96.13	111.00
3	L	52	ASP	CB-CA-C	5.49	121.38	110.40
1	A	386	GLY	N-CA-C	-5.45	99.47	113.10
1	B	531	GLU	N-CA-C	5.38	125.53	111.00
2	C	94	TYR	N-CA-C	5.35	125.45	111.00
1	A	431	LEU	CB-CA-C	-5.35	100.03	110.20
3	D	22	CYS	N-CA-C	5.31	125.34	111.00
1	B	271	ALA	N-CA-CB	5.23	117.43	110.10
1	B	29	GLN	N-CA-C	5.22	125.09	111.00
1	A	100	PRO	CB-CA-C	-5.20	99.01	112.00
1	A	528	LEU	C-N-CD	5.20	139.31	128.40
3	D	160	GLY	N-CA-C	-5.19	100.13	113.10
1	B	556	GLY	C-N-CD	5.19	139.29	128.40
2	H	142	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	78	ARG	NE-CZ-NH2	-5.14	117.73	120.30
3	D	29	VAL	N-CA-C	-5.13	97.16	111.00
1	A	432	GLY	N-CA-C	5.11	125.87	113.10
1	A	195	ARG	CB-CA-C	-5.10	100.21	110.40
3	D	32	TYR	N-CA-C	5.08	124.72	111.00
1	B	269	PHE	N-CA-C	-5.06	97.34	111.00
1	A	101	LEU	N-CA-CB	5.05	120.49	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	GLU	CB-CA-C	-5.03	100.35	110.40
1	B	539	LEU	O-C-N	5.02	130.64	121.10
3	L	143	TYR	N-CA-C	-5.01	97.47	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	NAG	C1

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	SER	Peptide
1	A	247	PRO	Mainchain
1	A	77	LEU	Peptide
1	B	529	PRO	Peptide
2	C	190	SER	Peptide
2	C	88	SER	Peptide
3	D	121	PHE	Mainchain
3	D	159	SER	Peptide
3	D	22	CYS	Peptide
3	D	63	ARG	Peptide
3	D	67	SER	Peptide
3	D	8	ALA	Peptide
2	H	152	GLU	Peptide
3	L	16	GLN	Peptide
3	L	22	CYS	Peptide
3	L	63	ARG	Peptide
3	L	67	SER	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	4277	0	4106	142	0
1	B	4277	0	4108	216	3
2	C	1624	0	1567	110	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1624	0	1567	81	1
3	D	1616	0	1548	148	0
3	L	1616	0	1548	89	0
4	A	28	0	25	8	0
5	B	14	0	13	10	0
6	A	27	0	0	4	0
6	B	14	0	0	1	0
6	C	12	0	0	7	0
6	D	19	0	0	4	0
6	H	2	0	0	0	0
6	L	5	0	0	1	0
All	All	15155	0	14482	766	3

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 26.

All (766) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:GLN:CG	1:B:548:GLN:HG3	1.37	1.53
3:D:123:PRO:HB2	3:D:127:GLN:CD	1.29	1.48
1:A:237:ASN:HD21	4:A:1001:NAG:C1	1.21	1.47
3:D:123:PRO:CB	3:D:127:GLN:NE2	1.79	1.44
1:B:250:VAL:CB	1:B:260:MET:O	1.69	1.39
1:B:546:GLN:HG2	1:B:548:GLN:CG	1.52	1.36
2:H:131:SER:OG	2:H:133:LYS:HB3	1.23	1.33
3:D:123:PRO:HB2	3:D:127:GLN:NE2	1.01	1.32
2:H:131:SER:OG	2:H:133:LYS:CB	1.77	1.31
1:A:553:THR:HG22	6:A:1114:HOH:O	1.36	1.24
1:B:250:VAL:HG12	1:B:261:PRO:CA	1.67	1.23
1:B:250:VAL:HB	1:B:260:MET:O	1.12	1.23
1:A:238:HIS:HB2	1:A:273:CYS:SG	1.79	1.22
2:H:131:SER:OG	2:H:133:LYS:CA	1.88	1.21
2:H:131:SER:OG	2:H:133:LYS:N	1.73	1.21
3:D:23:THR:CG2	3:D:72:THR:HG22	1.69	1.20
1:B:549:ASN:O	1:B:550:GLY:O	1.60	1.20
3:D:22:CYS:CB	3:D:73:ALA:HB1	1.71	1.19
1:B:250:VAL:CG1	1:B:261:PRO:HA	1.76	1.16
2:C:128:LEU:HD22	3:D:122:PRO:O	1.43	1.15
3:L:94:THR:HG22	3:L:96:SER:H	1.12	1.15
3:D:22:CYS:HB2	3:D:73:ALA:CB	1.74	1.15

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:THR:CG2	6:A:1114:HOH:O	1.90	1.13
1:A:528:LEU:O	1:A:530:ARG:N	1.83	1.11
1:B:237:ASN:CG	5:B:1001:NAG:C1	2.19	1.08
1:B:546:GLN:O	1:B:548:GLN:N	1.86	1.08
1:B:250:VAL:CG1	1:B:260:MET:O	2.02	1.08
1:A:326:GLU:O	1:A:327:HIS:HB3	1.54	1.07
1:B:545:CYS:SG	1:B:562:CYS:SG	1.31	1.07
3:D:23:THR:HG22	3:D:72:THR:HG22	1.35	1.06
1:A:528:LEU:HB2	1:A:529:PRO:HD3	1.37	1.05
1:B:247:PRO:HB2	1:B:265:GLY:HA2	1.32	1.04
2:C:128:LEU:CD2	3:D:122:PRO:O	2.05	1.04
2:C:130:PRO:HG2	2:C:193:LEU:HD11	1.38	1.04
3:D:131:GLY:HA2	3:D:186:LYS:HB2	1.40	1.04
1:B:542:HIS:CE1	1:B:543:PRO:HD2	1.92	1.04
1:B:546:GLN:CG	1:B:548:GLN:CG	2.23	1.03
2:C:130:PRO:HG3	2:C:142:LEU:HB3	1.38	1.02
1:A:528:LEU:C	1:A:530:ARG:H	1.63	1.01
3:D:24:GLY:O	3:D:71:ASN:HB3	1.63	0.99
1:B:553:THR:HG22	1:B:554:CYS:H	1.24	0.99
3:D:67:SER:O	3:D:68:LYS:HB2	1.58	0.98
1:B:545:CYS:O	1:B:546:GLN:HB2	1.61	0.98
3:L:9:SER:C	3:L:11:SER:H	1.66	0.98
2:C:189:PRO:HB3	2:C:191:SER:HB3	1.42	0.98
1:B:237:ASN:ND2	5:B:1001:NAG:O5	1.94	0.97
3:L:9:SER:O	3:L:11:SER:N	1.96	0.97
3:D:123:PRO:CB	3:D:127:GLN:CD	2.19	0.96
1:A:384:ILE:HG22	1:A:386:GLY:O	1.65	0.95
3:D:94:THR:HG22	3:D:96:SER:H	1.28	0.95
1:B:546:GLN:HE21	1:B:548:GLN:CB	1.79	0.95
1:B:541:CYS:O	1:B:542:HIS:O	1.84	0.95
1:B:553:THR:HG22	1:B:554:CYS:N	1.82	0.95
3:D:23:THR:CG2	3:D:72:THR:CG2	2.46	0.94
3:D:123:PRO:CA	3:D:127:GLN:NE2	2.31	0.94
1:A:554:CYS:SG	1:A:555:PHE:N	2.35	0.94
2:H:131:SER:HG	2:H:133:LYS:HB3	1.12	0.94
1:B:546:GLN:C	1:B:548:GLN:H	1.69	0.93
1:A:528:LEU:HB2	1:A:529:PRO:CD	1.98	0.93
3:D:16:GLN:HA	3:D:17:SER:HB3	1.51	0.93
3:L:72:THR:HA	3:L:73:ALA:HB3	1.48	0.93
1:B:250:VAL:HG12	1:B:261:PRO:HA	0.94	0.92
3:D:23:THR:CB	3:D:72:THR:HG22	1.98	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:HD21	4:A:1001:NAG:C2	1.82	0.91
3:D:69:SER:O	3:D:72:THR:O	1.87	0.91
3:L:9:SER:OG	3:L:10:VAL:N	1.98	0.91
1:B:237:ASN:HD21	5:B:1001:NAG:C1	1.56	0.91
3:L:35:VAL:O	3:L:52:ASP:O	1.91	0.89
1:B:545:CYS:CB	1:B:562:CYS:SG	2.61	0.88
3:D:72:THR:HA	3:D:73:ALA:HB3	1.56	0.87
1:B:545:CYS:O	1:B:546:GLN:CB	2.22	0.87
2:H:131:SER:HG	2:H:133:LYS:CB	1.73	0.87
2:C:51:ILE:HG12	2:C:58:THR:HG22	1.54	0.86
1:B:327:HIS:O	1:B:327:HIS:CD2	2.28	0.86
3:D:16:GLN:CA	3:D:17:SER:HB3	2.05	0.86
1:A:510:SER:O	1:A:511:GLN:OE1	1.94	0.86
2:C:203:ASN:HD21	2:C:205:LYS:HG3	1.40	0.86
1:B:546:GLN:NE2	1:B:548:GLN:HB2	1.89	0.86
4:A:1001:NAG:O3	4:A:1002:NAG:O5	1.93	0.85
1:B:528:LEU:HB2	1:B:529:PRO:HD3	1.56	0.85
3:L:13:SER:HA	3:L:110:LEU:HB2	1.56	0.85
1:A:238:HIS:HB2	1:A:273:CYS:CB	2.06	0.85
3:L:72:THR:HA	3:L:73:ALA:CB	2.07	0.84
1:B:250:VAL:HA	1:B:262:ASN:H	1.42	0.83
1:B:553:THR:O	1:B:554:CYS:O	1.95	0.83
1:A:532:TYR:HB3	1:A:554:CYS:SG	2.17	0.83
3:D:23:THR:HB	3:D:72:THR:CG2	2.08	0.83
2:C:142:LEU:HD22	2:C:193:LEU:HD12	1.60	0.83
2:H:131:SER:CB	2:H:133:LYS:HB3	2.09	0.83
1:B:546:GLN:NE2	1:B:548:GLN:CB	2.41	0.82
1:B:83:THR:HG22	1:B:84:GLN:HG3	1.61	0.82
1:B:546:GLN:HG3	1:B:548:GLN:HG3	1.58	0.82
3:D:72:THR:HA	3:D:73:ALA:CB	2.10	0.82
3:L:29:VAL:HG21	3:L:73:ALA:HB2	1.59	0.82
1:A:144:THR:HG21	1:A:182:CYS:H	1.44	0.81
1:B:546:GLN:HE21	1:B:548:GLN:CD	1.83	0.81
3:D:123:PRO:HB2	3:D:127:GLN:HE21	1.41	0.81
1:B:250:VAL:HG12	1:B:260:MET:O	1.76	0.81
2:C:139:THR:O	6:C:308:HOH:O	1.98	0.81
1:B:272:SER:HB3	5:B:1001:NAG:O7	1.81	0.81
3:D:123:PRO:C	3:D:127:GLN:HE21	1.84	0.81
1:A:524:VAL:HG11	1:A:533:VAL:HG22	1.61	0.81
1:B:553:THR:CG2	1:B:554:CYS:H	1.82	0.81
2:H:131:SER:CB	2:H:133:LYS:H	1.94	0.81

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:TYR:HE1	2:H:70:MET:HG3	1.45	0.80
1:B:140:CYS:HA	1:B:166:ARG:HH21	1.45	0.80
3:L:40:GLN:O	3:L:86:ALA:HB1	1.81	0.80
1:B:523:ARG:HG2	1:B:527:GLY:HA3	1.62	0.80
2:C:51:ILE:HG13	2:C:70:MET:HB2	1.62	0.80
3:D:23:THR:HB	3:D:72:THR:HG22	1.62	0.79
2:C:142:LEU:CD2	2:C:193:LEU:HD12	2.12	0.79
1:B:428:ILE:HG13	1:B:428:ILE:O	1.81	0.79
3:D:120:ILE:HD12	3:D:212:PHE:HB3	1.62	0.79
1:A:253:ASN:ND2	1:A:256:THR:OG1	2.13	0.79
3:L:23:THR:HB	3:L:72:THR:OG1	1.82	0.79
1:B:545:CYS:SG	1:B:562:CYS:CB	2.72	0.78
1:B:546:GLN:HE21	1:B:548:GLN:CG	1.96	0.78
2:C:128:LEU:HD23	3:D:123:PRO:HA	1.64	0.78
1:B:250:VAL:HB	1:B:260:MET:C	2.05	0.77
2:H:91:THR:HG23	2:H:114:THR:HA	1.68	0.76
1:A:362:ASP:HB3	1:A:367:THR:HG23	1.66	0.76
2:C:193:LEU:HA	2:C:198:TYR:HE2	1.50	0.76
3:L:20:ILE:HD12	3:L:20:ILE:H	1.50	0.76
2:C:133:LYS:HZ1	3:D:212:PHE:HB2	1.51	0.76
3:D:123:PRO:CB	3:D:127:GLN:HE22	1.94	0.75
1:A:18:GLU:N	1:A:18:GLU:OE1	2.18	0.75
1:A:238:HIS:CB	1:A:273:CYS:SG	2.69	0.75
2:H:190:SER:HA	2:H:193:LEU:HD13	1.67	0.75
1:B:546:GLN:HG3	1:B:548:GLN:HE21	1.49	0.75
3:L:20:ILE:HD12	3:L:20:ILE:N	2.02	0.75
1:B:237:ASN:HD21	5:B:1001:NAG:H61	1.52	0.75
3:D:123:PRO:C	3:D:127:GLN:NE2	2.40	0.75
2:C:142:LEU:HD22	2:C:193:LEU:CD1	2.16	0.75
1:B:250:VAL:CA	1:B:260:MET:O	2.34	0.74
2:H:48:MET:HG2	2:H:64:LEU:HD21	1.68	0.74
1:B:541:CYS:C	1:B:542:HIS:O	2.23	0.74
1:A:250:VAL:HG21	1:A:259:SER:HB3	1.70	0.73
2:C:158:TRP:HZ3	2:C:198:TYR:HB3	1.50	0.73
3:L:94:THR:HG22	3:L:96:SER:N	1.97	0.73
1:B:81:ARG:HG2	1:B:127:LEU:HD12	1.70	0.73
1:A:326:GLU:O	1:A:327:HIS:CB	2.34	0.73
2:H:89:ASP:CG	2:H:89:ASP:O	2.24	0.73
1:B:438:GLU:OE2	1:B:465:ARG:NH1	2.22	0.73
1:B:542:HIS:NE2	1:B:543:PRO:HD2	2.03	0.72
1:B:546:GLN:HG3	1:B:548:GLN:NE2	2.04	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:N	1:A:528:LEU:HD23	2.05	0.72
1:A:256:THR:HB	1:A:258:GLU:HG3	1.71	0.71
1:B:530:ARG:O	1:B:530:ARG:HG3	1.88	0.71
1:A:453:CYS:SG	1:A:477:ARG:NH1	2.63	0.71
2:C:194:GLY:HA3	2:C:217:PRO:HG2	1.72	0.71
3:L:83:GLU:HA	3:L:85:GLU:HG3	1.73	0.71
1:B:22:ASP:OD1	1:B:25:ARG:NH1	2.23	0.71
3:D:123:PRO:O	3:D:124:SER:OG	2.07	0.71
3:L:14:PRO:HD3	3:L:110:LEU:H	1.56	0.71
1:A:140:CYS:HA	1:A:166:ARG:HH21	1.54	0.71
3:L:41:HIS:HB3	3:L:42:PRO:HD2	1.71	0.71
3:L:16:GLN:HB2	3:L:17:SER:OG	1.91	0.71
1:B:237:ASN:HD21	5:B:1001:NAG:C6	2.04	0.70
1:B:546:GLN:HG2	1:B:548:GLN:CB	2.21	0.70
3:D:50:ILE:HG21	3:D:56:ARG:HG2	1.73	0.70
1:A:529:PRO:O	1:A:530:ARG:O	2.10	0.69
3:L:22:CYS:HB3	3:L:23:THR:HA	1.74	0.69
3:L:5:THR:O	3:L:22:CYS:O	2.11	0.69
2:H:16:GLU:O	2:H:86:LEU:HB2	1.92	0.69
1:A:279:TYR:OH	1:A:438:GLU:OE2	2.11	0.69
1:B:524:VAL:HG11	1:B:533:VAL:HG22	1.76	0.68
1:A:347:LYS:HE2	1:A:349:PHE:CZ	2.28	0.68
1:B:237:ASN:OD1	5:B:1001:NAG:C1	2.42	0.68
3:D:133:ALA:N	3:D:184:LEU:O	2.26	0.68
1:B:237:ASN:HD21	5:B:1001:NAG:C5	2.05	0.68
2:H:131:SER:O	2:H:135:THR:HG23	1.94	0.68
3:L:5:THR:O	3:L:22:CYS:C	2.33	0.68
3:L:67:SER:O	3:L:68:LYS:HB2	1.92	0.68
1:B:541:CYS:O	1:B:542:HIS:C	2.32	0.68
1:B:33:VAL:HG13	1:B:57:GLU:HB2	1.76	0.68
2:H:51:ILE:HG12	2:H:58:THR:HG22	1.75	0.67
1:B:542:HIS:CG	1:B:543:PRO:CD	2.77	0.67
3:D:124:SER:C	3:D:126:GLU:H	1.98	0.67
1:A:249:LEU:HD11	1:A:267:TYR:CZ	2.28	0.67
2:C:151:PRO:HD2	2:C:206:PRO:HB3	1.77	0.67
3:D:111:GLY:O	6:D:314:HOH:O	2.12	0.67
1:B:494:ALA:HB3	1:B:508:ASN:HB3	1.76	0.67
2:H:64:LEU:HB3	2:H:68:VAL:HG22	1.76	0.66
1:B:263:PRO:O	1:B:264:GLU:HG2	1.96	0.66
2:H:150:PHE:HD2	2:H:179:LEU:HD23	1.60	0.66
3:D:52:ASP:O	3:D:53:VAL:HG22	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:18:ILE:HG22	3:D:19:THR:H	1.59	0.66
3:D:67:SER:O	3:D:68:LYS:CB	2.41	0.66
3:L:143:TYR:O	3:L:201:HIS:NE2	2.29	0.66
1:B:374:GLN:O	1:B:377:VAL:HG13	1.94	0.66
2:C:91:THR:HG23	2:C:114:THR:HA	1.77	0.66
3:D:150:GLN:O	6:D:307:HOH:O	2.13	0.66
1:B:247:PRO:CB	1:B:265:GLY:HA2	2.19	0.66
3:D:8:ALA:HA	3:D:105:THR:HA	1.78	0.66
3:D:94:THR:HG22	3:D:96:SER:N	2.07	0.65
2:C:183:SER:OG	2:C:184:SER:N	2.29	0.65
3:D:16:GLN:HA	3:D:17:SER:CB	2.26	0.65
1:A:407:GLN:HA	1:A:435:SER:O	1.97	0.65
3:D:23:THR:HG21	3:D:72:THR:CG2	2.25	0.65
1:B:284:THR:HG22	1:B:287:GLY:H	1.62	0.65
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.62	0.65
3:D:139:LEU:HD22	3:D:178:LEU:HB3	1.79	0.65
2:H:130:PRO:O	2:H:131:SER:HB3	1.96	0.65
1:A:22:ASP:OD1	1:A:25:ARG:NH1	2.29	0.65
1:B:546:GLN:NE2	1:B:548:GLN:CD	2.50	0.65
2:C:139:THR:HA	2:C:190:SER:H	1.60	0.65
1:B:284:THR:HG22	1:B:288:SER:H	1.62	0.64
1:B:144:THR:HG21	1:B:182:CYS:H	1.62	0.64
3:D:139:LEU:HB3	3:D:142:PHE:CE2	2.33	0.64
2:H:125:VAL:HG21	2:H:211:VAL:HG11	1.79	0.64
1:A:404:GLN:OE1	1:A:434:ARG:NH1	2.30	0.64
1:A:51:PHE:CE1	1:A:52:LEU:HD13	2.32	0.64
3:L:8:ALA:HA	3:L:106:LYS:H	1.61	0.64
1:A:528:LEU:C	1:A:530:ARG:N	2.33	0.64
1:B:132:LEU:HD13	1:B:161:LEU:HD23	1.80	0.64
1:B:250:VAL:CG1	1:B:260:MET:C	2.64	0.64
1:B:542:HIS:HB2	1:B:557:PRO:O	1.97	0.64
3:D:25:THR:N	3:D:28:ASP:OD2	2.28	0.64
1:B:325:MET:O	1:B:329:ARG:HB3	1.98	0.63
3:D:23:THR:HB	3:D:72:THR:HG23	1.80	0.63
3:D:139:LEU:HB3	3:D:142:PHE:HE2	1.61	0.63
1:B:324:GLY:HA2	1:B:329:ARG:HA	1.81	0.63
1:B:542:HIS:CD2	1:B:543:PRO:HD2	2.32	0.63
2:C:51:ILE:HG21	2:C:72:THR:HG23	1.81	0.63
3:D:17:SER:HB3	3:D:78:SER:O	1.98	0.63
1:A:459:PRO:HB2	1:A:462:GLN:HG3	1.81	0.63
3:D:23:THR:CB	3:D:72:THR:CG2	2.67	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASN:ND2	5:B:1001:NAG:H61	2.14	0.62
1:B:546:GLN:NE2	1:B:548:GLN:CG	2.61	0.62
1:A:265:GLY:O	1:A:266:ARG:HD3	1.99	0.62
3:D:22:CYS:HB2	3:D:73:ALA:HB1	0.81	0.62
3:D:132:THR:HA	3:D:185:SER:HA	1.82	0.62
2:C:135:THR:HA	6:C:308:HOH:O	1.98	0.62
3:D:24:GLY:O	3:D:71:ASN:CB	2.44	0.62
1:B:327:HIS:O	1:B:327:HIS:CG	2.48	0.62
1:B:383:GLU:OE1	1:B:410:ARG:NE	2.27	0.62
1:A:238:HIS:HB2	1:A:273:CYS:HB2	1.80	0.62
1:B:250:VAL:HA	1:B:262:ASN:N	2.13	0.62
1:B:335:THR:N	1:B:338:ASN:OD1	2.29	0.62
2:H:6:GLN:H	2:H:109:GLN:HE22	1.47	0.62
1:B:478:PRO:HB2	1:B:481:GLU:HB2	1.81	0.62
3:D:182:LEU:HG	3:D:184:LEU:HG	1.82	0.62
3:D:16:GLN:CB	3:D:17:SER:HB3	2.30	0.62
3:L:7:PRO:HG2	3:L:105:THR:HG21	1.82	0.62
3:L:78:SER:OG	3:L:79:GLY:N	2.29	0.62
1:A:335:THR:HG23	1:A:337:ALA:H	1.65	0.61
1:A:175:PRO:O	3:D:32:TYR:OH	2.13	0.61
1:B:144:THR:CG2	1:B:182:CYS:H	2.13	0.61
1:B:7:THR:O	1:B:39:GLU:OE1	2.18	0.61
2:C:194:GLY:CA	2:C:217:PRO:HD2	2.30	0.61
3:D:8:ALA:H	3:D:105:THR:HG22	1.65	0.61
2:H:51:ILE:HD11	2:H:70:MET:C	2.22	0.61
1:A:141:TYR:OH	1:A:185:GLU:HG2	2.00	0.61
3:D:123:PRO:HB2	3:D:127:GLN:CG	2.25	0.61
2:C:189:PRO:HB2	2:C:192:SER:H	1.66	0.60
3:L:143:TYR:O	3:L:201:HIS:CE1	2.54	0.60
1:A:298:GLN:HG2	1:A:312:CYS:SG	2.41	0.60
1:A:94:VAL:HG22	1:A:133:ILE:HG23	1.83	0.60
3:L:71:ASN:OD1	3:L:71:ASN:N	2.32	0.60
2:H:171:PRO:HG2	3:L:166:VAL:H	1.66	0.60
3:D:108:THR:OG1	3:D:169:GLN:NE2	2.33	0.60
1:B:546:GLN:HG2	1:B:548:GLN:HG3	0.64	0.60
1:B:542:HIS:ND1	1:B:543:PRO:HD2	2.16	0.60
1:B:552:VAL:HG13	1:B:552:VAL:O	2.01	0.60
2:C:188:VAL:HG11	2:C:198:TYR:HE1	1.66	0.60
3:D:15:GLY:O	3:D:16:GLN:HB3	2.02	0.60
1:B:284:THR:HG23	1:B:286:VAL:HG13	1.83	0.59
1:B:542:HIS:CD2	1:B:543:PRO:CD	2.86	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:VAL:HB	3:D:182:LEU:HD23	1.85	0.59
3:D:19:THR:HG22	3:D:76:THR:HB	1.85	0.59
1:B:300:VAL:HG12	1:B:301:THR:H	1.67	0.59
2:H:60:TYR:CE1	2:H:70:MET:HG3	2.32	0.59
3:L:9:SER:C	3:L:11:SER:N	2.33	0.58
1:A:144:THR:CG2	1:A:182:CYS:H	2.13	0.58
2:C:193:LEU:HA	2:C:198:TYR:CE2	2.35	0.58
3:D:42:PRO:HG3	3:D:168:GLU:HG3	1.84	0.58
3:L:19:THR:HG22	3:L:76:THR:HB	1.83	0.58
1:B:7:THR:OG1	1:B:39:GLU:OE1	2.19	0.58
2:C:18:LEU:HB2	2:C:86:LEU:HD21	1.86	0.58
1:A:523:ARG:HB2	1:A:531:GLU:HB2	1.85	0.58
1:B:209:LEU:HB3	1:B:211:THR:HG22	1.85	0.58
1:B:250:VAL:HG12	1:B:260:MET:C	2.23	0.58
1:B:51:PHE:CE1	1:B:52:LEU:HD13	2.38	0.58
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.39	0.58
3:D:128:LEU:HA	3:D:132:THR:O	2.03	0.58
1:A:141:TYR:O	1:A:144:THR:HG22	2.04	0.57
1:A:237:ASN:ND2	4:A:1001:NAG:C7	2.67	0.57
1:B:274:VAL:HG12	1:B:276:ALA:H	1.69	0.57
3:L:35:VAL:HB	3:L:53:VAL:HG12	1.86	0.57
3:L:16:GLN:HA	3:L:78:SER:O	2.05	0.57
2:H:89:ASP:OD2	2:H:89:ASP:O	2.23	0.57
1:A:238:HIS:HA	1:A:273:CYS:HB2	1.84	0.57
1:B:58:VAL:HG11	1:B:62:VAL:HG22	1.86	0.57
3:D:17:SER:CB	3:D:78:SER:O	2.52	0.57
2:C:125:VAL:HG11	2:C:211:VAL:HG11	1.87	0.57
2:C:193:LEU:O	2:C:195:THR:CB	2.53	0.57
1:B:9:MET:O	1:B:12:ARG:HB2	2.05	0.56
3:D:72:THR:CA	3:D:73:ALA:HB3	2.32	0.56
2:H:149:TYR:CE1	2:H:180:TYR:HB2	2.40	0.56
1:A:352:LEU:HD12	1:A:384:ILE:HD11	1.87	0.56
3:D:123:PRO:HD2	3:D:124:SER:H	1.70	0.56
1:A:284:THR:HG22	1:A:288:SER:H	1.70	0.56
1:B:248:ALA:O	1:B:262:ASN:HB3	2.06	0.56
2:H:51:ILE:HG22	2:H:52:SER:N	2.20	0.56
3:D:145:ARG:NH2	3:D:166:VAL:HG11	2.20	0.56
1:B:194:THR:OG1	1:B:204:ARG:NH1	2.36	0.56
1:B:544:GLU:O	1:B:545:CYS:HB2	2.05	0.56
2:C:61:ALA:O	2:C:62:GLN:HB2	2.06	0.56
3:L:8:ALA:HA	3:L:105:THR:HB	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:PHE:CD2	2:H:179:LEU:HD23	2.40	0.56
2:C:193:LEU:O	2:C:195:THR:N	2.38	0.56
3:L:22:CYS:HB3	3:L:23:THR:CA	2.35	0.56
1:B:64:ILE:HD13	1:B:72:VAL:HG21	1.87	0.56
3:D:16:GLN:HG3	3:D:16:GLN:O	2.03	0.56
3:L:9:SER:C	3:L:10:VAL:HG12	2.26	0.56
1:B:141:TYR:O	1:B:144:THR:HG22	2.07	0.55
1:B:215:HIS:CD2	1:B:227:HIS:HB3	2.41	0.55
3:D:124:SER:O	3:D:127:GLN:N	2.38	0.55
3:D:54:SER:HB3	3:D:66:GLY:O	2.07	0.55
2:H:6:GLN:H	2:H:109:GLN:NE2	2.03	0.55
2:H:131:SER:HG	2:H:133:LYS:CA	1.99	0.55
1:B:494:ALA:O	1:B:495:ARG:HB2	2.06	0.55
2:C:157:SER:HB3	2:C:201:ASN:HB2	1.89	0.55
2:H:18:LEU:HD11	2:H:20:ILE:HG13	1.88	0.55
3:D:16:GLN:HB2	3:D:17:SER:HB3	1.88	0.55
1:B:546:GLN:C	1:B:548:GLN:N	2.40	0.55
3:L:22:CYS:H	3:L:37:TRP:HH2	1.54	0.55
1:B:35:GLN:HG2	1:B:59:GLN:NE2	2.22	0.55
3:D:70:GLY:HA2	3:D:72:THR:N	2.22	0.55
1:B:559:ALA:HA	1:B:562:CYS:SG	2.47	0.55
3:D:50:ILE:HD13	3:D:53:VAL:O	2.06	0.55
3:L:6:GLN:HB2	3:L:7:PRO:HD2	1.88	0.55
1:A:1:THR:OG1	1:A:2:GLN:N	2.39	0.55
1:B:489:CYS:SG	1:B:498:CYS:N	2.80	0.55
2:C:166:GLY:HA3	2:C:187:THR:HB	1.88	0.55
2:H:38:ARG:HB3	2:H:48:MET:HE1	1.87	0.55
1:B:333:ALA:HB2	1:B:355:LEU:HG	1.88	0.55
1:B:503:PRO:HD2	1:B:504:THR:HG22	1.89	0.55
1:B:63:LEU:HD13	1:B:93:ALA:HB3	1.89	0.54
1:A:248:ALA:O	1:A:262:ASN:ND2	2.37	0.54
1:A:553:THR:HG23	6:A:1114:HOH:O	1.78	0.54
2:C:124:SER:HB3	2:C:126:PHE:CE2	2.42	0.54
2:C:159:ASN:OD1	2:C:199:ILE:N	2.41	0.54
3:D:70:GLY:HA2	3:D:72:THR:H	1.72	0.54
2:C:158:TRP:CZ3	2:C:198:TYR:HB3	2.39	0.54
1:B:249:LEU:O	1:B:262:ASN:N	2.40	0.54
3:D:123:PRO:CA	3:D:127:GLN:HE22	2.10	0.54
1:B:542:HIS:ND1	1:B:543:PRO:CD	2.71	0.54
1:B:557:PRO:HD2	1:B:561:GLN:NE2	2.22	0.54
2:C:204:HIS:CE1	2:C:206:PRO:HB2	2.43	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:50:ILE:HG22	3:L:56:ARG:HA	1.89	0.54
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.43	0.54
1:B:542:HIS:CG	1:B:543:PRO:N	2.75	0.54
1:A:237:ASN:CG	4:A:1001:NAG:C1	2.74	0.53
2:C:4:LEU:O	2:C:108:GLY:HA2	2.08	0.53
2:C:128:LEU:HD23	3:D:122:PRO:O	2.06	0.53
2:H:18:LEU:HD23	2:H:86:LEU:HD11	1.89	0.53
2:C:189:PRO:CB	2:C:191:SER:HB3	2.26	0.53
2:C:45:LEU:HG	3:D:89:TYR:CZ	2.44	0.53
1:A:554:CYS:SG	1:A:556:GLY:N	2.82	0.53
3:L:23:THR:CB	3:L:72:THR:OG1	2.55	0.53
1:A:450:THR:O	1:A:477:ARG:HB2	2.07	0.53
1:B:250:VAL:CG1	1:B:261:PRO:CA	2.57	0.53
1:B:95:LEU:HD23	1:B:134:GLN:HB3	1.90	0.53
1:B:183:TRP:N	1:B:189:ASP:O	2.31	0.53
2:C:159:ASN:N	2:C:199:ILE:O	2.35	0.52
3:D:6:GLN:HB2	3:D:105:THR:CG2	2.39	0.52
1:A:253:ASN:HD22	1:A:256:THR:HG1	1.51	0.52
1:A:443:LEU:HD23	1:A:469:GLN:HA	1.91	0.52
1:B:143:ASP:OD1	1:B:143:ASP:N	2.40	0.52
2:H:157:SER:OG	2:H:161:GLY:N	2.41	0.52
1:B:248:ALA:O	1:B:265:GLY:HA3	2.10	0.52
1:B:555:PHE:HB2	1:B:562:CYS:HA	1.90	0.52
1:B:249:LEU:HD11	1:B:287:GLY:HA2	1.92	0.52
1:B:35:GLN:HG2	1:B:59:GLN:HE21	1.74	0.52
3:L:200:THR:HG23	3:L:207:PRO:HD3	1.92	0.52
1:A:14:PRO:O	1:A:17:PRO:HD3	2.09	0.52
1:B:253:ASN:HB2	1:B:260:MET:HE3	1.90	0.52
1:B:262:ASN:O	1:B:264:GLU:N	2.38	0.52
2:C:39:GLN:OE1	3:D:40:GLN:NE2	2.37	0.52
3:D:72:THR:CA	3:D:73:ALA:CB	2.84	0.52
1:B:128:LYS:HA	1:B:155:ASN:OD1	2.10	0.52
1:B:29:GLN:HA	1:B:51:PHE:HB2	1.92	0.52
2:H:167:VAL:O	2:H:168:HIS:ND1	2.43	0.52
2:H:95:TYR:CE1	3:L:45:ALA:HB2	2.44	0.52
3:L:148:LYS:HB3	3:L:200:THR:HB	1.91	0.52
1:B:542:HIS:CE1	1:B:543:PRO:CD	2.81	0.52
1:B:542:HIS:ND1	1:B:543:PRO:N	2.57	0.52
2:C:142:LEU:HD13	6:C:306:HOH:O	2.09	0.52
2:C:193:LEU:O	2:C:195:THR:HB	2.10	0.52
3:D:164:GLU:OE1	3:D:178:LEU:HD21	2.10	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:LYS:HG3	3:D:48:LEU:N	2.24	0.52
2:H:2:VAL:HB	2:H:106:TYR:CE2	2.45	0.52
1:B:223:THR:OG1	1:B:223:THR:O	2.25	0.51
2:H:67:ARG:NH1	2:H:83:LEU:HD21	2.25	0.51
2:C:185:VAL:HG21	3:D:138:LEU:HD22	1.91	0.51
3:D:145:ARG:HH21	3:D:166:VAL:HG11	1.76	0.51
3:L:115:ALA:HB1	3:L:204:LEU:HG	1.92	0.51
3:L:53:VAL:O	3:L:66:GLY:O	2.28	0.51
1:A:533:VAL:HB	6:A:1111:HOH:O	2.10	0.51
3:D:37:TRP:HB2	3:D:50:ILE:H	1.75	0.51
1:A:444:ALA:HB3	1:A:471:LEU:HD23	1.93	0.51
3:L:49:MET:O	3:L:49:MET:HG2	2.09	0.51
1:B:140:CYS:HA	1:B:166:ARG:NH2	2.22	0.51
1:B:528:LEU:HB2	1:B:529:PRO:CD	2.35	0.51
1:B:209:LEU:HB2	1:B:212:ASP:OD2	2.10	0.51
1:B:262:ASN:C	1:B:264:GLU:H	2.12	0.51
2:H:121:LYS:HG3	2:H:122:GLY:H	1.76	0.51
3:D:123:PRO:HG2	3:D:127:GLN:HB3	1.93	0.50
3:D:53:VAL:HG23	3:D:54:SER:N	2.26	0.50
3:D:71:ASN:OD1	3:D:71:ASN:N	2.40	0.50
2:C:123:PRO:HA	2:C:149:TYR:HB3	1.92	0.50
2:C:64:LEU:HB3	2:C:68:VAL:HG22	1.93	0.50
1:A:8:ASP:OD1	1:A:10:LYS:NZ	2.44	0.50
1:A:23:MET:HG3	1:A:419:TYR:OH	2.11	0.50
1:A:390:ILE:HG22	1:A:426:LEU:HD21	1.93	0.50
1:B:543:PRO:O	1:B:544:GLU:HB2	2.12	0.50
1:B:385:THR:OG1	1:B:385:THR:O	2.26	0.50
1:B:542:HIS:CG	1:B:543:PRO:HD2	2.43	0.50
2:C:73:ASP:OD1	2:C:75:SER:OG	2.28	0.50
3:D:124:SER:C	3:D:126:GLU:N	2.65	0.50
3:L:83:GLU:HB3	6:L:301:HOH:O	2.12	0.50
3:D:135:VAL:HG12	3:D:151:TRP:CH2	2.46	0.50
2:H:158:TRP:CH2	2:H:200:CYS:HB3	2.46	0.50
2:H:61:ALA:HB3	2:H:64:LEU:HB2	1.93	0.50
3:L:9:SER:O	3:L:10:VAL:HG12	2.10	0.50
1:A:560:ASP:HB3	1:A:561:GLN:OE1	2.11	0.50
1:B:546:GLN:CG	1:B:548:GLN:CD	2.79	0.50
2:H:205:LYS:HA	2:H:208:ASN:H	1.76	0.50
3:L:72:THR:CA	3:L:73:ALA:HB3	2.33	0.50
1:A:344:GLY:HA2	1:A:380:THR:OG1	2.11	0.50
1:B:2:GLN:HG3	1:B:3:VAL:HG23	1.94	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:THR:HB	1:B:292:VAL:H	1.77	0.50
1:B:29:GLN:HG3	1:B:29:GLN:O	2.07	0.50
3:D:153:VAL:HG13	3:D:195:TYR:CE1	2.47	0.50
3:L:9:SER:O	3:L:10:VAL:CG1	2.60	0.50
1:A:323:LEU:HD23	1:A:328:LEU:HD13	1.93	0.49
3:D:136:VAL:HG13	3:D:181:THR:HG22	1.93	0.49
1:A:524:VAL:HG12	1:A:532:TYR:HA	1.94	0.49
2:H:18:LEU:HB3	2:H:86:LEU:HD21	1.93	0.49
1:A:19:THR:HB	1:A:472:LEU:HD13	1.93	0.49
1:B:545:CYS:SG	1:B:564:ALA:HB3	2.53	0.49
3:L:10:VAL:HG23	3:L:18:ILE:HG22	1.94	0.49
1:B:284:THR:CG2	1:B:286:VAL:HG13	2.42	0.49
2:C:36:TRP:CZ2	2:C:81:MET:HB2	2.48	0.49
2:H:171:PRO:HD2	3:L:165:SER:HB3	1.93	0.49
1:A:237:ASN:ND2	4:A:1001:NAG:C2	2.58	0.49
1:A:419:TYR:CE1	1:A:443:LEU:HD12	2.48	0.49
1:A:64:ILE:O	1:A:94:VAL:HA	2.13	0.49
1:B:268:THR:C	1:B:269:PHE:O	2.48	0.49
3:D:154:ASP:HB2	3:D:192:HIS:ND1	2.28	0.49
2:C:188:VAL:HG11	2:C:198:TYR:CE1	2.46	0.49
1:B:146:LEU:HB2	1:B:181:ARG:CZ	2.43	0.49
1:A:319:VAL:HG21	1:A:349:PHE:HE1	1.78	0.48
3:D:192:HIS:O	3:D:214:ARG:NH1	2.46	0.48
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.53	0.48
1:A:144:THR:O	1:A:181:ARG:HB3	2.13	0.48
1:A:237:ASN:ND2	4:A:1001:NAG:N2	2.61	0.48
1:B:372:PRO:HB3	1:B:397:LEU:HD11	1.95	0.48
2:C:23:LYS:HG3	2:C:78:THR:OG1	2.13	0.48
1:B:278:PRO:HG2	1:B:281:TYR:CD1	2.48	0.48
1:B:446:ILE:HG13	1:B:471:LEU:HD21	1.95	0.48
2:C:33:TRP:HB2	2:C:99:GLU:OE2	2.13	0.48
2:C:36:TRP:CZ3	2:C:96:CYS:HB3	2.48	0.48
1:B:250:VAL:HA	1:B:260:MET:O	2.13	0.48
1:B:250:VAL:CA	1:B:262:ASN:H	2.22	0.48
2:C:2:VAL:HG21	2:C:106:TYR:CZ	2.49	0.48
1:B:353:ALA:HA	1:B:389:TYR:O	2.14	0.48
1:B:551:SER:O	1:B:552:VAL:O	2.32	0.48
3:D:135:VAL:HG23	3:D:184:LEU:HD12	1.96	0.48
1:A:335:THR:HG22	1:A:338:ASN:ND2	2.29	0.48
1:A:128:LYS:HA	1:A:155:ASN:OD1	2.14	0.48
1:A:360:ASP:N	1:A:360:ASP:OD1	2.47	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:ASN:ND2	6:C:311:HOH:O	2.47	0.48
3:L:21:SER:O	3:L:22:CYS:C	2.50	0.48
3:D:163:GLN:HG3	3:D:164:GLU:H	1.79	0.48
1:A:325:MET:O	1:A:329:ARG:N	2.47	0.47
1:A:528:LEU:H	1:A:528:LEU:HD23	1.77	0.47
1:B:18:GLU:HG3	1:B:474:THR:HG21	1.96	0.47
1:A:514:ARG:HD2	1:A:531:GLU:OE1	2.14	0.47
1:B:1:THR:HG23	1:B:468:HIS:NE2	2.30	0.47
3:D:53:VAL:HG23	3:D:54:SER:H	1.78	0.47
3:D:50:ILE:HG22	3:D:56:ARG:HA	1.95	0.47
1:A:99:ASP:HA	1:A:100:PRO:HD3	1.73	0.47
1:A:300:VAL:HG12	1:A:301:THR:N	2.29	0.47
3:D:188:ASP:HB3	6:D:301:HOH:O	2.14	0.47
2:C:124:SER:HB3	2:C:126:PHE:CZ	2.50	0.47
2:H:127:PRO:HB3	2:H:215:VAL:HG22	1.97	0.47
2:H:44:GLY:HA2	3:L:89:TYR:OH	2.14	0.47
1:A:489:CYS:SG	1:A:498:CYS:N	2.88	0.47
3:D:45:ALA:HA	3:D:46:PRO:HD3	1.53	0.47
1:B:523:ARG:HD2	1:B:531:GLU:OE2	2.14	0.47
2:C:143:GLY:HA2	2:C:158:TRP:CZ2	2.49	0.47
1:A:116:ARG:NH2	1:A:168:ARG:HH12	2.12	0.47
2:C:19:LYS:HG2	2:C:82:GLU:HB2	1.96	0.47
3:D:137:CYS:HB2	3:D:151:TRP:CZ2	2.49	0.47
1:B:524:VAL:HG12	1:B:532:TYR:HA	1.97	0.47
2:C:35:GLY:HA3	2:C:104:PHE:HE2	1.79	0.47
3:D:123:PRO:CD	3:D:124:SER:H	2.27	0.46
3:D:23:THR:HG22	3:D:72:THR:CG2	2.22	0.46
1:A:140:CYS:HB2	1:A:168:ARG:HH21	1.80	0.46
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.63	0.46
1:B:119:GLN:OE1	1:B:121:ARG:NH2	2.49	0.46
1:B:144:THR:O	1:B:181:ARG:HB3	2.14	0.46
2:C:88:SER:HB2	2:C:89:ASP:HB3	1.97	0.46
3:D:6:GLN:HB3	3:D:21:SER:O	2.15	0.46
2:H:73:ASP:OD2	2:H:76:THR:HG23	2.16	0.46
3:L:23:THR:CG2	3:L:72:THR:OG1	2.63	0.46
3:L:72:THR:CA	3:L:73:ALA:CB	2.83	0.46
2:C:168:HIS:HB3	6:D:316:HOH:O	2.15	0.46
3:D:17:SER:O	3:D:18:ILE:HG12	2.15	0.46
2:H:131:SER:HG	2:H:133:LYS:C	2.19	0.46
3:L:91:SER:HB3	3:L:101:PHE:CD1	2.50	0.46
1:B:556:GLY:HA3	1:B:561:GLN:HG2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:LYS:HG2	3:D:69:SER:H	1.80	0.46
2:H:131:SER:C	2:H:133:LYS:N	2.58	0.46
1:A:168:ARG:HB2	2:C:31:SER:HB3	1.97	0.46
1:B:11:LEU:HA	1:B:11:LEU:HD23	1.76	0.46
2:C:130:PRO:CG	2:C:193:LEU:HD11	2.26	0.46
2:C:91:THR:HA	2:C:113:VAL:O	2.15	0.46
2:H:51:ILE:CG1	2:H:70:MET:HB2	2.45	0.46
1:A:29:GLN:HA	1:A:51:PHE:HB2	1.98	0.46
2:C:163:LEU:HD22	6:C:311:HOH:O	2.15	0.46
3:L:80:LEU:HD11	3:L:107:LEU:HD21	1.98	0.46
1:B:466:ASN:O	1:B:469:GLN:HB2	2.16	0.46
2:H:130:PRO:HA	2:H:134:SER:OG	2.15	0.46
3:D:20:ILE:HG22	3:D:21:SER:N	2.29	0.46
3:L:41:HIS:HB3	3:L:42:PRO:CD	2.44	0.46
3:D:148:LYS:HA	3:D:148:LYS:HE3	1.97	0.46
3:D:8:ALA:HA	3:D:105:THR:CA	2.45	0.46
3:D:6:GLN:HE21	3:D:105:THR:HG23	1.81	0.45
3:D:64:PHE:CE1	3:D:77:ILE:HG12	2.51	0.45
3:D:78:SER:OG	3:D:79:GLY:N	2.48	0.45
2:H:48:MET:HE1	2:H:94:TYR:CD2	2.51	0.45
3:L:8:ALA:HA	3:L:105:THR:CA	2.46	0.45
1:A:404:GLN:O	1:A:435:SER:OG	2.34	0.45
3:D:17:SER:C	3:D:18:ILE:HG12	2.36	0.45
3:D:80:LEU:HD13	3:D:80:LEU:HA	1.54	0.45
1:A:186:SER:OG	1:A:187:SER:N	2.50	0.45
3:D:18:ILE:HG22	3:D:19:THR:N	2.27	0.45
2:H:54:TYR:HD2	2:H:55:ASN:HD22	1.64	0.45
1:A:517:GLU:HG3	1:A:518:CYS:N	2.27	0.45
1:A:529:PRO:C	1:A:530:ARG:HG3	2.37	0.45
1:B:226:LYS:HB3	1:B:226:LYS:HE2	1.64	0.45
2:C:121:LYS:NZ	6:C:305:HOH:O	2.50	0.45
2:H:18:LEU:HD12	2:H:19:LYS:N	2.31	0.45
2:C:150:PHE:CD2	2:C:179:LEU:HD23	2.52	0.45
3:D:123:PRO:O	3:D:127:GLN:NE2	2.49	0.45
1:A:238:HIS:C	1:A:238:HIS:CD2	2.90	0.45
1:B:146:LEU:N	1:B:191:GLN:OE1	2.40	0.45
1:A:221:GLY:C	1:A:231:LEU:HG	2.37	0.45
1:A:393:TRP:HB2	1:A:426:LEU:HD22	1.98	0.45
1:B:239:SER:HA	5:B:1001:NAG:H83	1.97	0.45
1:B:59:GLN:O	1:B:83:THR:HB	2.17	0.45
1:B:274:VAL:HG12	1:B:276:ALA:N	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:O	1:A:239:SER:HB2	2.17	0.45
1:A:528:LEU:N	1:A:528:LEU:CD2	2.73	0.45
1:A:554:CYS:O	1:A:555:PHE:CD1	2.70	0.45
1:B:265:GLY:C	1:B:266:ARG:HG2	2.37	0.45
1:B:326:GLU:O	1:B:327:HIS:ND1	2.50	0.45
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.77	0.45
2:C:173:VAL:O	2:C:180:TYR:HA	2.17	0.45
3:D:124:SER:O	3:D:126:GLU:N	2.50	0.45
2:H:167:VAL:C	2:H:168:HIS:HD1	2.21	0.45
2:H:152:GLU:O	2:H:206:PRO:HG2	2.16	0.45
2:H:36:TRP:CZ3	2:H:96:CYS:HB3	2.51	0.45
1:A:13:LEU:HA	1:A:14:PRO:HD3	1.83	0.45
1:A:155:ASN:HD22	1:A:158:ALA:HB2	1.81	0.45
1:B:7:THR:O	1:B:37:ASN:HB2	2.16	0.45
2:C:16:GLU:O	2:C:86:LEU:HB2	2.17	0.45
3:D:164:GLU:HA	3:D:179:SER:O	2.17	0.45
3:L:17:SER:O	3:L:18:ILE:HG12	2.17	0.45
2:H:3:GLN:O	2:H:24:GLY:HA2	2.17	0.44
2:H:51:ILE:HG22	2:H:52:SER:O	2.16	0.44
1:A:140:CYS:HA	1:A:166:ARG:NH2	2.27	0.44
1:A:175:PRO:HB3	3:D:95:SER:HA	1.99	0.44
1:A:438:GLU:OE2	1:A:465:ARG:NH1	2.48	0.44
2:C:188:VAL:HG21	2:C:198:TYR:CE1	2.52	0.44
2:H:35:GLY:HA3	2:H:104:PHE:CE1	2.52	0.44
2:H:51:ILE:HD11	2:H:70:MET:O	2.16	0.44
3:L:63:ARG:HG2	3:L:78:SER:HB3	1.98	0.44
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.69	0.44
1:B:186:SER:HB3	1:B:189:ASP:OD2	2.17	0.44
1:B:21:LEU:HD12	1:B:43:LEU:HD22	2.00	0.44
1:A:297:ASN:OD1	1:A:311:LYS:HG2	2.17	0.44
2:C:129:ALA:HA	2:C:130:PRO:HD3	1.54	0.44
2:C:194:GLY:HA3	2:C:217:PRO:CG	2.45	0.44
2:H:131:SER:C	2:H:133:LYS:H	2.03	0.44
1:A:238:HIS:O	1:A:238:HIS:CD2	2.70	0.44
1:B:293:CYS:HA	1:B:294:PRO:HD3	1.87	0.44
1:B:551:SER:O	1:B:552:VAL:C	2.55	0.44
2:C:33:TRP:O	2:C:34:ILE:HD12	2.17	0.44
3:D:22:CYS:CB	3:D:73:ALA:CB	2.61	0.44
3:L:13:SER:CA	3:L:110:LEU:HB2	2.40	0.44
2:C:185:VAL:HG11	3:D:138:LEU:HD22	2.00	0.44
1:B:116:ARG:HA	1:B:138:GLN:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ASP:OD1	1:B:480:ASP:N	2.51	0.44
3:D:83:GLU:HG3	3:D:171:SER:HB2	2.00	0.44
1:A:41:THR:HA	1:A:65:ALA:O	2.17	0.44
1:B:553:THR:CG2	1:B:554:CYS:N	2.48	0.44
2:H:216:GLU:H	2:H:216:GLU:HG2	1.61	0.44
3:L:8:ALA:HA	3:L:105:THR:HA	1.99	0.44
1:A:319:VAL:HG22	1:A:320:CYS:N	2.33	0.43
1:A:353:ALA:HA	1:A:389:TYR:O	2.17	0.43
1:B:119:GLN:HA	1:B:183:TRP:HB3	2.00	0.43
2:C:150:PHE:HE2	2:C:178:GLY:O	2.01	0.43
2:C:204:HIS:O	2:C:207:SER:N	2.50	0.43
2:C:90:ASP:O	2:C:94:TYR:HE1	2.01	0.43
1:B:404:GLN:OE1	1:B:434:ARG:NH1	2.51	0.43
3:D:172:LYS:HA	3:D:172:LYS:HD2	1.93	0.43
1:A:238:HIS:CB	1:A:273:CYS:HB2	2.48	0.43
2:H:12:LYS:O	2:H:115:VAL:HA	2.18	0.43
2:H:158:TRP:CZ3	2:H:200:CYS:HB3	2.53	0.43
4:A:1002:NAG:C1	4:A:1002:NAG:C8	2.96	0.43
1:A:7:THR:O	1:A:37:ASN:HB2	2.18	0.43
1:A:401:SER:O	1:A:404:GLN:N	2.49	0.43
1:A:438:GLU:HB2	1:A:465:ARG:NH1	2.34	0.43
1:B:116:ARG:NH2	1:B:168:ARG:HH12	2.17	0.43
2:C:3:GLN:HB2	2:C:25:SER:OG	2.18	0.43
3:D:6:GLN:HB2	3:D:105:THR:HG23	2.00	0.43
3:L:28:ASP:O	3:L:92:SER:OG	2.36	0.43
1:A:215:HIS:CD2	1:A:227:HIS:HB3	2.53	0.43
1:A:374:GLN:O	1:A:377:VAL:HG13	2.18	0.43
1:B:219:ALA:HB2	1:B:234:LEU:HA	2.01	0.43
2:C:13:LYS:NZ	6:C:302:HOH:O	2.39	0.43
2:H:131:SER:OG	2:H:133:LYS:C	2.52	0.43
3:L:7:PRO:O	3:L:8:ALA:HB3	2.17	0.43
1:A:477:ARG:HA	1:A:478:PRO:HD3	1.83	0.43
1:B:70:ARG:HA	1:B:114:GLY:O	2.18	0.43
2:C:148:ASP:HA	2:C:179:LEU:HB2	2.00	0.43
2:C:36:TRP:HB3	2:C:48:MET:HE3	2.00	0.43
3:L:107:LEU:HD12	3:L:108:THR:N	2.32	0.43
1:B:34:VAL:HG22	1:B:34:VAL:O	2.18	0.43
1:B:43:LEU:HD13	1:B:49:LEU:HD21	2.00	0.43
1:B:555:PHE:HB3	1:B:561:GLN:O	2.18	0.43
2:C:6:GLN:O	2:C:109:GLN:NE2	2.52	0.43
2:C:143:GLY:HA2	2:C:158:TRP:CH2	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:5:THR:O	3:L:23:THR:N	2.52	0.43
1:A:527:GLY:HA2	1:A:528:LEU:HD23	2.01	0.43
1:B:361:GLY:HA2	1:B:369:PRO:HG3	2.00	0.43
1:B:442:GLY:O	1:B:469:GLN:HG2	2.18	0.43
3:D:164:GLU:HG2	3:D:178:LEU:HD21	2.01	0.43
3:L:91:SER:HB3	3:L:101:PHE:CE1	2.54	0.43
1:A:347:LYS:HD2	1:A:383:GLU:OE2	2.19	0.43
1:B:301:THR:HG23	1:B:306:THR:O	2.18	0.43
2:C:209:THR:O	2:C:211:VAL:HG23	2.19	0.43
2:C:199:ILE:HG12	2:C:214:LYS:CB	2.48	0.43
3:D:138:LEU:C	3:D:139:LEU:HD12	2.39	0.43
1:B:7:THR:C	1:B:39:GLU:OE1	2.57	0.43
3:L:14:PRO:HD3	3:L:110:LEU:N	2.29	0.43
1:A:249:LEU:HD11	1:A:267:TYR:CE2	2.54	0.42
1:A:464:PHE:CE2	1:A:470:ALA:HA	2.54	0.42
1:B:226:LYS:HG2	1:B:229:ASP:OD2	2.19	0.42
1:B:366:ASN:ND2	6:B:1113:HOH:O	2.45	0.42
2:H:124:SER:HB3	2:H:126:PHE:CZ	2.54	0.42
2:H:150:PHE:CD1	2:H:151:PRO:HA	2.54	0.42
3:L:66:GLY:HA3	3:L:75:LEU:HA	2.00	0.42
1:A:178:LYS:H	1:A:178:LYS:HG3	1.32	0.42
3:D:153:VAL:HG13	3:D:195:TYR:HE1	1.84	0.42
2:H:33:TRP:HB2	2:H:99:GLU:OE2	2.20	0.42
3:L:68:LYS:HB3	3:L:73:ALA:H	1.84	0.42
1:B:453:CYS:SG	1:B:477:ARG:HG2	2.58	0.42
1:B:546:GLN:CG	1:B:548:GLN:NE2	2.77	0.42
3:L:184:LEU:HD13	3:L:189:TYR:HD1	1.85	0.42
1:B:175:PRO:HD3	3:L:93:TYR:OH	2.20	0.42
1:B:115:LEU:HD21	1:B:118:LEU:HD23	2.00	0.42
2:C:140:ALA:HB2	2:C:190:SER:HB3	2.01	0.42
2:C:194:GLY:N	2:C:217:PRO:HD2	2.33	0.42
3:D:151:TRP:CZ3	3:D:197:CYS:HB2	2.54	0.42
1:A:81:ARG:HG2	1:A:127:LEU:HD12	2.00	0.42
1:B:546:GLN:HG2	1:B:546:GLN:O	2.19	0.42
2:C:120:THR:OG1	2:C:151:PRO:HD3	2.19	0.42
2:C:186:VAL:HG22	2:C:188:VAL:HG13	2.00	0.42
2:C:67:ARG:NH1	2:C:90:ASP:OD2	2.53	0.42
3:D:154:ASP:OD1	3:D:193:LYS:N	2.53	0.42
1:A:164:THR:HG22	1:A:166:ARG:HH12	1.84	0.42
1:B:546:GLN:CD	1:B:548:GLN:CG	2.85	0.42
1:B:423:LEU:HB2	1:B:446:ILE:HG23	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:SER:HA	2:C:135:THR:HG23	2.02	0.42
2:C:143:GLY:HA3	2:C:184:SER:O	2.19	0.42
3:L:121:PHE:HA	3:L:122:PRO:HD2	1.84	0.42
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.84	0.42
3:D:131:GLY:CA	3:D:186:LYS:HB2	2.30	0.42
3:D:94:THR:C	3:D:96:SER:H	2.23	0.42
3:L:8:ALA:HA	3:L:106:LYS:N	2.33	0.42
3:L:9:SER:C	3:L:10:VAL:CG1	2.87	0.42
2:H:6:GLN:HE21	2:H:6:GLN:HB3	1.73	0.42
1:B:250:VAL:HG12	1:B:261:PRO:N	2.26	0.42
1:B:321:TYR:CD2	1:B:326:GLU:HB3	2.54	0.42
1:B:509:CYS:SG	1:B:511:GLN:O	2.77	0.42
2:H:64:LEU:HB3	2:H:68:VAL:CG2	2.47	0.42
1:B:72:VAL:HA	1:B:73:PRO:HD2	1.90	0.41
1:A:175:PRO:HG2	3:D:97:SER:OG	2.20	0.41
3:L:51:TYR:CE2	3:L:55:LYS:HD2	2.55	0.41
3:L:8:ALA:N	3:L:105:THR:HG22	2.34	0.41
1:B:407:GLN:O	1:B:437:ARG:HG2	2.20	0.41
1:B:532:TYR:CZ	1:B:539:LEU:HB2	2.55	0.41
2:C:193:LEU:HG	2:C:194:GLY:H	1.84	0.41
2:C:90:ASP:O	2:C:91:THR:C	2.58	0.41
3:D:37:TRP:CD2	3:D:75:LEU:HB2	2.55	0.41
2:C:47:TRP:CG	3:D:99:LEU:HB3	2.55	0.41
3:L:122:PRO:HB3	3:L:212:PHE:CE1	2.55	0.41
3:L:38:TYR:N	3:L:89:TYR:O	2.53	0.41
1:B:480:ASP:C	1:B:482:CYS:H	2.23	0.41
2:C:140:ALA:HB2	2:C:190:SER:CB	2.50	0.41
2:C:64:LEU:O	2:C:67:ARG:HB2	2.20	0.41
3:D:131:GLY:C	3:D:186:LYS:H	2.24	0.41
2:H:183:SER:OG	2:H:184:SER:N	2.54	0.41
3:L:7:PRO:O	3:L:8:ALA:CB	2.69	0.41
1:A:163:ASP:OD1	1:A:164:THR:N	2.54	0.41
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.31	0.41
1:A:463:LEU:HD12	1:A:463:LEU:N	2.36	0.41
3:D:178:LEU:HD23	3:D:179:SER:N	2.35	0.41
1:A:384:ILE:CG2	1:A:386:GLY:O	2.51	0.41
1:B:426:LEU:N	1:B:449:ASN:OD1	2.29	0.41
1:A:525:LEU:HB2	1:A:526:GLN:HG3	2.01	0.41
1:B:445:LEU:HD12	1:B:472:LEU:O	2.20	0.41
2:C:105:ASP:C	3:D:48:LEU:HD22	2.41	0.41
3:D:75:LEU:HD12	3:D:76:THR:H	1.84	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186:VAL:HG22	2:H:187:THR:H	1.86	0.41
2:H:18:LEU:HB3	2:H:86:LEU:CD2	2.51	0.41
2:H:88:SER:HB2	2:H:89:ASP:H	1.44	0.41
3:L:156:ALA:O	3:L:158:GLN:HG2	2.20	0.41
3:L:166:VAL:HG23	3:L:177:SER:O	2.21	0.41
1:A:79:ILE:HB	1:A:125:GLU:HB3	2.02	0.41
1:A:209:LEU:HB2	1:A:211:THR:HG22	2.02	0.41
1:B:513:LEU:HD22	1:B:515:GLY:O	2.20	0.41
3:D:139:LEU:O	3:D:177:SER:HA	2.20	0.41
3:D:23:THR:HG21	3:D:72:THR:HG21	2.02	0.41
3:L:139:LEU:HD13	3:L:178:LEU:HB3	2.03	0.41
1:B:323:LEU:HB2	1:B:351:SER:O	2.20	0.41
2:C:18:LEU:HD22	2:C:113:VAL:HG11	2.03	0.41
2:C:142:LEU:HD22	2:C:193:LEU:HD11	1.98	0.41
2:C:166:GLY:HA3	2:C:187:THR:O	2.21	0.41
3:L:8:ALA:CA	3:L:105:THR:HB	2.51	0.41
3:L:80:LEU:HA	3:L:80:LEU:HD13	1.77	0.41
1:B:18:GLU:CD	1:B:18:GLU:H	2.23	0.41
2:C:155:THR:HB	2:C:203:ASN:HB3	2.03	0.41
3:D:49:MET:HA	3:D:50:ILE:HA	1.86	0.41
2:H:34:ILE:HA	2:H:34:ILE:HD12	1.86	0.41
3:L:10:VAL:HG13	3:L:107:LEU:HD13	2.03	0.41
1:A:340:GLN:HG2	1:A:340:GLN:H	1.43	0.41
1:A:352:LEU:HD12	1:A:384:ILE:CD1	2.50	0.41
1:A:378:PHE:O	1:A:381:LEU:HB3	2.21	0.41
3:D:213:ASN:HB2	3:D:216:GLU:CD	2.41	0.41
2:H:131:SER:OG	2:H:134:SER:N	2.54	0.41
1:A:319:VAL:HG21	1:A:349:PHE:CE1	2.56	0.40
1:B:492:LEU:HD11	1:B:520:GLU:OE1	2.22	0.40
2:C:105:ASP:O	3:D:48:LEU:HD22	2.21	0.40
2:C:1:GLU:O	2:C:26:GLY:HA3	2.22	0.40
1:A:443:LEU:HB3	1:A:470:ALA:O	2.21	0.40
1:B:397:LEU:H	1:B:397:LEU:HG	1.76	0.40
1:B:546:GLN:CD	1:B:548:GLN:HB2	2.38	0.40
2:C:151:PRO:HD2	2:C:206:PRO:CB	2.49	0.40
1:A:175:PRO:HD3	3:D:93:TYR:OH	2.22	0.40
1:A:155:ASN:ND2	1:A:158:ALA:HB2	2.36	0.40
1:A:80:VAL:HG22	1:A:126:ILE:HG12	2.03	0.40
3:D:67:SER:O	3:D:74:SER:HB2	2.22	0.40
2:H:100:GLY:N	2:H:103:ALA:O	2.43	0.40
2:H:98:ARG:O	2:H:104:PHE:HA	2.22	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:HA3	1:A:128:LYS:O	2.22	0.40
1:B:51:PHE:CD1	1:B:52:LEU:HD13	2.56	0.40
2:C:39:GLN:O	2:C:93:VAL:HG23	2.22	0.40
3:D:38:TYR:HD1	3:D:48:LEU:HA	1.87	0.40
2:H:131:SER:HG	2:H:134:SER:N	2.20	0.40
3:L:8:ALA:O	3:L:9:SER:CB	2.69	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:O	2:C:191:SER:O[1_654]	1.78	0.42
1:B:160:THR:C	2:C:191:SER:O[1_654]	2.02	0.18
1:B:532:TYR:OH	2:H:195:THR:O[1_566]	2.11	0.09

## 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	551/564 (98%)	453 (82%)	86 (16%)	12 (2%)	8	33
1	B	551/564 (98%)	445 (81%)	90 (16%)	16 (3%)	5	27
2	C	215/217 (99%)	176 (82%)	35 (16%)	4 (2%)	9	37
2	H	215/217 (99%)	192 (89%)	18 (8%)	5 (2%)	7	32
3	D	215/217 (99%)	164 (76%)	41 (19%)	10 (5%)	3	16
3	L	215/217 (99%)	165 (77%)	43 (20%)	7 (3%)	4	24
All	All	1962/1996 (98%)	1595 (81%)	313 (16%)	54 (3%)	6	28

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	LEU
1	A	530	ARG
1	A	555	PHE
1	B	262	ASN
1	B	528	LEU
1	B	545	CYS
1	B	546	GLN
1	B	548	GLN
1	B	550	GLY
1	B	552	VAL
1	B	553	THR
1	B	554	CYS
1	B	555	PHE
2	H	151	PRO
3	L	9	SER
3	L	10	VAL
3	L	73	ALA
2	C	130	PRO
2	C	194	GLY
3	D	53	VAL
3	D	68	LYS
3	D	123	PRO
3	D	124	SER
1	A	327	HIS
1	A	529	PRO
1	B	542	HIS
1	B	544	GLU
1	B	547	PRO
2	H	131	SER
3	L	7	PRO
2	C	195	THR
3	D	16	GLN
3	D	17	SER
3	D	73	ALA
3	D	125	ASP
1	A	239	SER
1	A	554	CYS
3	L	8	ALA
3	L	95	SER
2	C	193	LEU
3	D	95	SER
1	A	552	VAL
1	A	305	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	485	GLU
1	B	263	PRO
3	D	122	PRO
1	A	100	PRO
1	B	264	GLU
2	H	130	PRO
2	H	205	LYS
1	B	73	PRO
2	H	152	GLU
1	A	247	PRO
3	L	144	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	478/485 (99%)	401 (84%)	77 (16%)	3	12
1	B	478/485 (99%)	404 (84%)	74 (16%)	3	13
2	C	180/181 (99%)	149 (83%)	31 (17%)	2	10
2	H	180/181 (99%)	155 (86%)	25 (14%)	4	18
3	D	185/186 (100%)	144 (78%)	41 (22%)	1	4
3	L	185/186 (100%)	152 (82%)	33 (18%)	2	9
All	All	1686/1704 (99%)	1405 (83%)	281 (17%)	2	11

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	9	MET
1	A	13	LEU
1	A	18	GLU
1	A	35	GLN
1	A	45	THR
1	A	46	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	50	SER
1	A	52	LEU
1	A	69	VAL
1	A	74	LEU
1	A	78	ARG
1	A	80	VAL
1	A	134	GLN
1	A	153	LYS
1	A	156	GLN
1	A	159	LEU
1	A	160	THR
1	A	164	THR
1	A	178	LYS
1	A	181	ARG
1	A	192	SER
1	A	194	THR
1	A	206	LYS
1	A	216	GLU
1	A	223	THR
1	A	227	HIS
1	A	228	SER
1	A	238	HIS
1	A	247	PRO
1	A	250	VAL
1	A	256	THR
1	A	260	MET
1	A	264	GLU
1	A	266	ARG
1	A	272	SER
1	A	282	LEU
1	A	283	SER
1	A	284	THR
1	A	286	VAL
1	A	290	THR
1	A	295	LEU
1	A	298	GLN
1	A	312	CYS
1	A	318	ARG
1	A	320	CYS
1	A	329	ARG
1	A	335	THR
1	A	360	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	367	THR
1	A	382	GLU
1	A	396	SER
1	A	435	SER
1	A	443	LEU
1	A	450	THR
1	A	457	THR
1	A	471	LEU
1	A	474	THR
1	A	480	ASP
1	A	485	GLU
1	A	487	LEU
1	A	504	THR
1	A	505	GLN
1	A	509	CYS
1	A	511	GLN
1	A	513	LEU
1	A	517	GLU
1	A	525	LEU
1	A	528	LEU
1	A	529	PRO
1	A	530	ARG
1	A	533	VAL
1	A	546	GLN
1	A	549	ASN
1	A	553	THR
1	A	555	PHE
1	A	561	GLN
1	B	9	MET
1	B	13	LEU
1	B	21	LEU
1	B	32	GLN
1	B	34	VAL
1	B	35	GLN
1	B	45	THR
1	B	50	SER
1	B	52	LEU
1	B	69	VAL
1	B	83	THR
1	B	133	ILE
1	B	144	THR
1	B	156	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	160	THR
1	B	165	ASN
1	B	167	SER
1	B	181	ARG
1	B	195	ARG
1	B	206	LYS
1	B	213	CYS
1	B	216	GLU
1	B	223	THR
1	B	227	HIS
1	B	228	SER
1	B	256	THR
1	B	259	SER
1	B	272	SER
1	B	275	THR
1	B	282	LEU
1	B	284	THR
1	B	286	VAL
1	B	290	THR
1	B	295	LEU
1	B	298	GLN
1	B	312	CYS
1	B	314	LYS
1	B	316	CYS
1	B	318	ARG
1	B	320	CYS
1	B	327	HIS
1	B	338	ASN
1	B	367	THR
1	B	380	THR
1	B	382	GLU
1	B	395	ASP
1	B	396	SER
1	B	401	SER
1	B	409	ILE
1	B	420	SER
1	B	422	THR
1	B	450	THR
1	B	465	ARG
1	B	471	LEU
1	B	480	ASP
1	B	481	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	485	GLU
1	B	491	GLN
1	B	492	LEU
1	B	504	THR
1	B	505	GLN
1	B	508	ASN
1	B	513	LEU
1	B	525	LEU
1	B	526	GLN
1	B	528	LEU
1	B	533	VAL
1	B	545	CYS
1	B	549	ASN
1	B	551	SER
1	B	554	CYS
1	B	555	PHE
1	B	558	GLU
1	B	561	GLN
2	H	10	GLU
2	H	18	LEU
2	H	34	ILE
2	H	43	GLN
2	H	50	TRP
2	H	64	LEU
2	H	68	VAL
2	H	70	MET
2	H	86	LEU
2	H	88	SER
2	H	91	THR
2	H	130	PRO
2	H	132	SER
2	H	134	SER
2	H	142	LEU
2	H	147	LYS
2	H	149	TYR
2	H	150	PHE
2	H	152	GLU
2	H	154	VAL
2	H	155	THR
2	H	163	LEU
2	H	173	VAL
2	H	182	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	216	GLU
3	L	2	SER
3	L	13	SER
3	L	25	THR
3	L	36	SER
3	L	48	LEU
3	L	49	MET
3	L	63	ARG
3	L	65	SER
3	L	68	LYS
3	L	69	SER
3	L	71	ASN
3	L	74	SER
3	L	76	THR
3	L	80	LEU
3	L	87	ASP
3	L	96	SER
3	L	108	THR
3	L	109	VAL
3	L	110	LEU
3	L	120	ILE
3	L	125	ASP
3	L	129	LYS
3	L	146	GLU
3	L	150	GLN
3	L	161	ASN
3	L	163	GLN
3	L	181	THR
3	L	186	LYS
3	L	202	GLN
3	L	205	SER
3	L	208	VAL
3	L	209	THR
3	L	212	PHE
2	C	2	VAL
2	C	11	VAL
2	C	19	LYS
2	C	21	SER
2	C	39	GLN
2	C	43	GLN
2	C	50	TRP
2	C	51	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	C	55	ASN
2	C	68	VAL
2	C	69	THR
2	C	70	MET
2	C	83	LEU
2	C	86	LEU
2	C	87	ARG
2	C	112	LEU
2	C	117	SER
2	C	142	LEU
2	C	145	LEU
2	C	148	ASP
2	C	150	PHE
2	C	152	GLU
2	C	159	ASN
2	C	173	VAL
2	C	179	LEU
2	C	182	LEU
2	C	184	SER
2	C	188	VAL
2	C	195	THR
2	C	212	ASP
2	C	215	VAL
3	D	13	SER
3	D	22	CYS
3	D	25	THR
3	D	27	SER
3	D	28	ASP
3	D	29	VAL
3	D	36	SER
3	D	47	LYS
3	D	48	LEU
3	D	58	SER
3	D	63	ARG
3	D	65	SER
3	D	71	ASN
3	D	76	THR
3	D	80	LEU
3	D	85	GLU
3	D	90	CYS
3	D	97	SER
3	D	113	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	120	ILE
3	D	123	PRO
3	D	125	ASP
3	D	129	LYS
3	D	132	THR
3	D	137	CYS
3	D	138	LEU
3	D	146	GLU
3	D	148	LYS
3	D	154	ASP
3	D	158	GLN
3	D	159	SER
3	D	162	SER
3	D	163	GLN
3	D	164	GLU
3	D	166	VAL
3	D	167	THR
3	D	179	SER
3	D	185	SER
3	D	188	ASP
3	D	202	GLN
3	D	212	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	238	HIS
1	A	327	HIS
1	A	542	HIS
1	B	20	HIS
1	B	59	GLN
1	B	237	ASN
1	B	298	GLN
1	B	546	GLN
1	B	548	GLN
2	C	57	ASN
2	C	203	ASN
3	D	127	GLN
3	D	155	ASN
3	D	169	GLN

### 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 ⓘ

2 carbohydrates 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	NAG	A	1001	1,4	14,14,15	0.36	0	15,19,21	0.74	1 (6%)
4	NAG	A	1002	4	14,14,15	0.47	0	15,19,21	1.92	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAG	C3-C4-C5	2.08	113.89	110.22
4	A	1002	NAG	O5-C1-C2	2.14	114.44	111.47
4	A	1002	NAG	C4-C3-C2	3.06	115.50	111.02
4	A	1002	NAG	C1-O5-C5	5.99	120.42	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NAG	7	0
4	A	1002	NAG	2	0

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
5	NAG	B	1001	1	14,14,15	0.36	0	15,19,21	0.73	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1001	1	1/1/5/7	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	NAG	C3-C4-C5	2.05	113.83	110.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1001	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1001	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	NAG	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	555/564 (98%)	-0.21	16 (2%) 52 28	28, 52, 125, 178	0
1	B	555/564 (98%)	-0.25	9 (1%) 72 51	31, 54, 122, 152	0
2	C	217/217 (100%)	1.18	52 (23%) 1 0	39, 86, 170, 180	0
2	H	217/217 (100%)	0.06	9 (4%) 38 19	38, 70, 129, 178	0
3	D	217/217 (100%)	1.61	71 (32%) 0 0	45, 114, 187, 203	0
3	L	217/217 (100%)	0.33	22 (10%) 8 2	36, 102, 163, 185	0
All	All	1978/1996 (99%)	0.22	179 (9%) 10 4	28, 63, 166, 203	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	138	GLY	18.6
3	D	147	ALA	16.9
3	D	120	ILE	13.7
3	D	189	TYR	12.8
2	C	142	LEU	12.8
2	H	137	GLY	12.4
2	C	141	ALA	10.9
2	C	176	SER	10.5
1	A	559	ALA	10.3
2	C	130	PRO	10.3
2	C	125	VAL	9.8
3	D	159	SER	9.1
2	C	140	ALA	8.6
2	H	136	SER	8.1
2	H	135	THR	8.0
3	D	137	CYS	8.0
3	D	196	ALA	7.9
3	D	180	SER	7.5
3	D	213	ASN	7.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	164	THR	7.4
3	D	209	THR	7.3
1	B	564	ALA	7.1
2	C	139	THR	7.1
1	A	547	PRO	7.1
3	D	118	VAL	7.1
3	D	157	LEU	7.0
2	C	126	PHE	7.0
3	D	195	TYR	6.5
2	C	168	HIS	6.4
2	C	129	ALA	6.4
2	C	177	SER	6.4
3	D	190	GLU	6.2
3	D	124	SER	6.1
2	C	197	THR	6.1
3	D	205	SER	6.0
2	C	137	GLY	5.8
2	C	185	VAL	5.7
3	D	151	TRP	5.7
3	L	156	ALA	5.6
2	C	190	SER	5.6
3	D	149	VAL	5.6
3	D	199	VAL	5.4
3	D	187	ALA	5.2
2	C	178	GLY	5.2
3	D	194	VAL	5.2
3	D	206	SER	5.2
2	C	192	SER	5.1
3	D	161	ASN	5.1
3	D	202	GLN	5.0
1	A	543	PRO	5.0
2	C	214	LYS	4.9
3	D	214	ARG	4.9
1	A	544	GLU	4.9
2	C	175	GLN	4.9
3	D	156	ALA	4.8
3	D	200	THR	4.8
2	C	196	GLN	4.7
2	H	134	SER	4.7
2	C	201	ASN	4.7
3	D	201	HIS	4.6
3	D	134	SER	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	188	ASP	4.5
3	D	160	GLY	4.5
3	D	119	PHE	4.5
3	L	197	CYS	4.5
1	A	548	GLN	4.5
1	A	541	CYS	4.4
3	D	117	SER	4.4
2	C	179	LEU	4.4
3	L	199	VAL	4.3
1	B	563	VAL	4.3
3	D	138	LEU	4.3
2	C	128	LEU	4.2
1	A	540	PRO	4.2
1	B	550	GLY	4.2
3	D	129	LYS	4.2
3	L	157	LEU	4.1
3	D	197	CYS	4.0
3	D	204	LEU	4.0
3	D	207	PRO	4.0
3	L	198	GLU	3.9
3	D	155	ASN	3.9
3	D	185	SER	3.8
3	L	185	SER	3.8
2	C	188	VAL	3.8
1	A	542	HIS	3.7
2	C	145	LEU	3.7
2	C	212	ASP	3.6
3	L	195	TYR	3.6
3	D	148	LYS	3.5
3	L	152	LYS	3.5
3	D	136	VAL	3.4
3	L	184	LEU	3.4
3	D	186	LYS	3.4
1	A	528	LEU	3.4
2	H	138	GLY	3.4
3	D	165	SER	3.4
2	C	173	VAL	3.3
3	D	203	GLY	3.3
3	D	181	THR	3.3
3	L	196	ALA	3.3
2	C	143	GLY	3.2
2	C	187	THR	3.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	191	LYS	3.2
3	D	114	ALA	3.2
3	D	215	GLY	3.2
2	C	217	PRO	3.1
3	L	151	TRP	3.1
2	H	123	PRO	3.1
3	L	18	ILE	3.1
3	L	153	VAL	3.0
3	D	198	GLU	3.0
2	C	134	SER	3.0
3	D	174	SER	3.0
3	L	200	THR	3.0
3	D	116	PRO	2.9
3	D	158	GLN	2.9
3	L	155	ASN	2.9
2	C	165	SER	2.9
1	B	560	ASP	2.8
3	D	211	SER	2.8
2	C	203	ASN	2.7
3	D	10	VAL	2.7
2	C	169	THR	2.7
1	B	315	PRO	2.7
3	D	217	CYS	2.7
3	D	172	LYS	2.7
2	C	210	LYS	2.6
1	A	560	ASP	2.6
3	D	125	ASP	2.6
3	D	78	SER	2.6
2	C	211	VAL	2.6
3	D	184	LEU	2.6
2	C	133	LYS	2.6
2	C	184	SER	2.6
3	D	146	GLU	2.6
2	C	146	VAL	2.5
2	C	183	SER	2.5
1	A	564	ALA	2.5
3	L	133	ALA	2.5
3	L	147	ALA	2.5
3	L	191	LYS	2.5
2	C	160	SER	2.5
3	D	126	GLU	2.4
3	D	150	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	D	164	GLU	2.4
3	D	123	PRO	2.4
3	D	152	LYS	2.4
2	C	163	LEU	2.4
2	H	120	THR	2.4
3	L	186	LYS	2.4
2	C	191	SER	2.3
2	C	123	PRO	2.3
1	A	254	THR	2.3
2	C	195	THR	2.3
2	C	167	VAL	2.3
3	D	82	ALA	2.3
2	C	186	VAL	2.2
1	A	513	LEU	2.2
3	D	183	THR	2.2
1	B	1	THR	2.2
2	H	209	THR	2.2
1	B	562	CYS	2.2
3	L	188	ASP	2.2
2	C	132	SER	2.2
2	H	139	THR	2.2
3	L	150	GLN	2.2
3	D	163	GLN	2.2
3	D	212	PHE	2.2
1	B	296	HIS	2.2
2	C	144	CYS	2.1
2	C	127	PRO	2.1
1	A	313	SER	2.1
1	B	313	SER	2.1
3	D	127	GLN	2.1
3	L	194	VAL	2.0
3	D	153	VAL	2.0
1	A	545	CYS	2.0
1	A	563	VAL	2.0

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

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

### 6.3 Carbohydrates [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	1001	14/15	0.93	0.19	1.32	47,59,69,73	0
4	NAG	A	1002	14/15	0.82	0.24	-	80,88,108,108	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	1001	14/15	0.57	0.25	3.53	57,60,76,82	0

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

There are no such residues in this entry.