



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 AM GMT

PDB ID : 2IOU  
Title : Major Tropism Determinant P1 (Mtd-P1) Variant Complexed with Bordetella  
brochiseptica Virulence Factor Pertactin extracellular domain (Prn-E).  
Authors : Miller, J.L.; Ghosh, P.  
Deposited on : 2006-10-10  
Resolution : 3.16 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

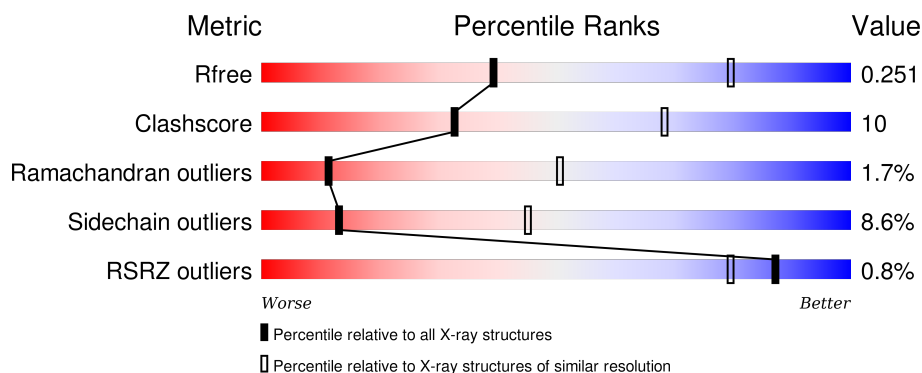
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	376	<div> <div>80%</div> <div>19%</div> <div>..</div> </div>
1	B	376	<div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	C	376	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	D	376	<div> <div>85%</div> <div>15%</div> <div>.</div> </div>
1	E	376	<div> <div>%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	376	
2	G	535	
2	H	535	

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	MG	A	3	-	-	-	X
3	MG	D	4	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23900 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 Major Tropism Determinant P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	B	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	C	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	D	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	E	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			
1	F	376	Total	C	N	O	S	0	0	0
			2758	1736	477	539	6			

- Molecule 2 is a protein called Pertactin Extracellular Domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	508	Total	C	N	O	S	54	0	0
			3674	2265	686	717	6			
2	H	508	Total	C	N	O	S	54	0	0
			3674	2265	686	717	6			

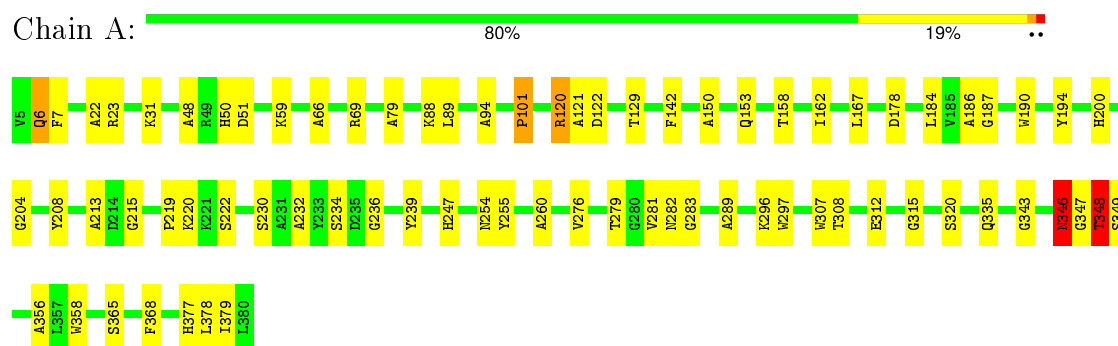
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		

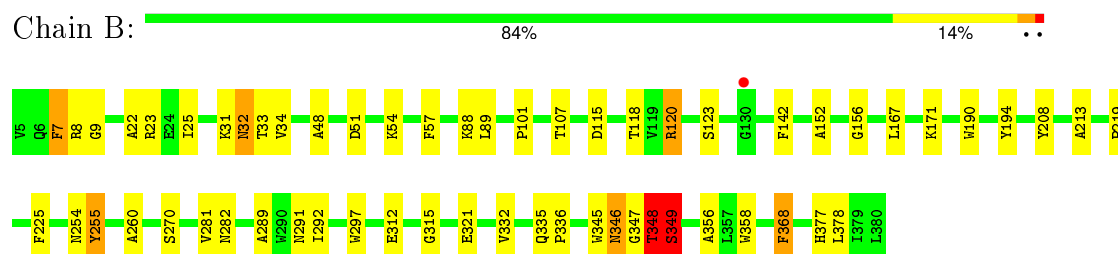
### 3 Residue-property plots

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

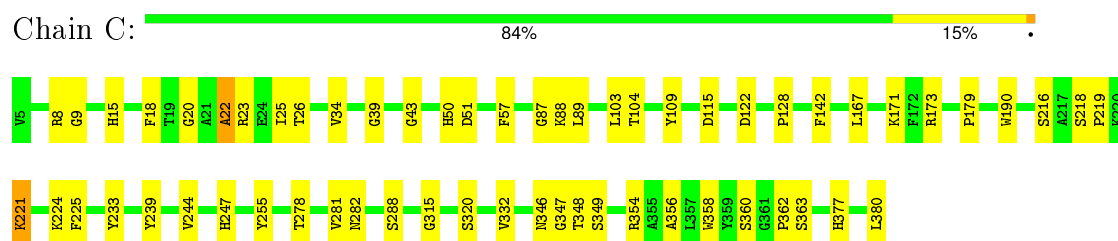
#### • Molecule 1: Major Tropism Determinant P1



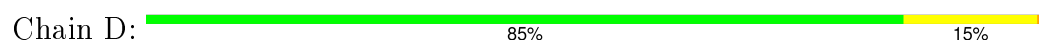
#### • Molecule 1: Major Tropism Determinant P1



#### • Molecule 1: Major Tropism Determinant P1



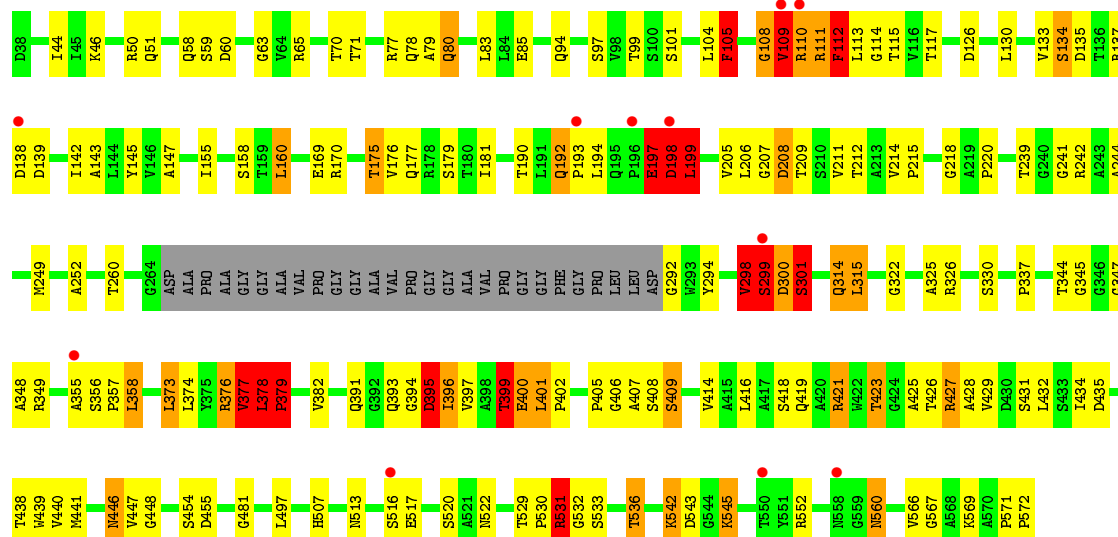
#### • Molecule 1: Major Tropism Determinant P1







● Molecule 2: Pertactin Extracellular Domain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	413.46 Å   413.46 Å   98.86 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	49.63 – 3.16 49.60 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.63-3.16) 99.9 (49.60-3.16)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.224 , 0.249 0.227 , 0.251	Depositor DCC
$R_{free}$ test set	8334 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.9	EDS
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 166223 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.45	2/2828 (0.1%)	0.59	1/3856 (0.0%)
1	B	1.67	4/2828 (0.1%)	0.79	7/3856 (0.2%)
1	C	0.44	0/2828	0.55	0/3856
1	D	0.44	0/2828	0.57	2/3856 (0.1%)
1	E	0.43	0/2828	0.54	0/3856
1	F	0.87	5/2828 (0.2%)	0.83	8/3856 (0.2%)
2	G	1.57	12/3731 (0.3%)	1.31	26/5073 (0.5%)
2	H	3.57	23/3731 (0.6%)	1.64	48/5073 (0.9%)
All	All	1.68	46/24430 (0.2%)	0.98	92/33282 (0.3%)

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	B	0	2
1	F	1	0
2	G	0	9
2	H	0	7
All	All	1	18

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	408	SER	CB-OG	153.18	3.41	1.42
2	H	299	SER	CB-OG	96.94	2.68	1.42
1	B	349	SER	CB-OG	-67.15	0.55	1.42
2	G	377	VAL	CB-CG2	64.35	2.88	1.52
2	H	379	PRO	N-CD	63.04	2.36	1.47
2	H	409	SER	CB-OG	-57.05	0.68	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	377	VAL	CB-CG2	54.54	2.67	1.52
2	G	377	VAL	CB-CG1	51.97	2.62	1.52
1	B	348	THR	CB-OG1	49.10	2.41	1.43
2	H	300	ASP	CB-CG	-27.32	0.94	1.51
2	H	377	VAL	CB-CG1	-24.66	1.01	1.52
1	F	349	SER	CA-CB	-24.18	1.16	1.52
2	H	112	PHE	CB-CG	-20.39	1.16	1.51
2	G	400	GLU	CB-CG	-19.42	1.15	1.52
1	B	348	THR	CB-CG2	19.10	2.15	1.52
2	H	197	GLU	CB-CG	-19.03	1.16	1.52
1	F	346	ASN	C-N	-18.75	0.99	1.33
2	H	108	GLY	C-N	-18.47	0.91	1.34
1	F	348	THR	CB-CG2	18.13	2.12	1.52
2	H	298	VAL	C-N	-16.12	0.96	1.34
1	F	348	THR	CB-OG1	15.44	1.74	1.43
2	G	399	THR	CB-CG2	14.38	1.99	1.52
2	G	197	GLU	C-N	-13.54	1.02	1.34
2	H	111	ARG	C-N	-13.51	1.02	1.34
2	G	198	ASP	CB-CG	-12.93	1.24	1.51
2	G	400	GLU	C-N	-12.64	1.04	1.34
2	H	379	PRO	CB-CG	12.45	2.12	1.50
2	G	111	ARG	C-N	-11.20	1.08	1.34
2	H	401	LEU	CB-CG	11.13	1.84	1.52
2	G	111	ARG	CB-CG	-11.09	1.22	1.52
2	H	377	VAL	C-N	10.25	1.57	1.34
2	H	405	PRO	C-N	9.85	1.50	1.33
2	G	378	LEU	CB-CG	-8.71	1.27	1.52
2	H	399	THR	C-N	-8.25	1.15	1.34
2	H	109	VAL	CB-CG1	7.79	1.69	1.52
2	G	399	THR	CB-OG1	7.30	1.57	1.43
2	H	378	LEU	CB-CG	6.55	1.71	1.52
1	A	348	THR	C-N	-6.55	1.19	1.34
1	B	349	SER	C-N	-6.46	1.19	1.34
1	F	350	LEU	C-N	-6.23	1.19	1.34
2	H	401	LEU	C-N	-6.20	1.22	1.34
2	H	198	ASP	CB-CG	-6.15	1.38	1.51
2	G	110	ARG	C-N	6.11	1.48	1.34
1	A	348	THR	CA-CB	5.55	1.67	1.53
2	H	377	VAL	C-O	-5.53	1.12	1.23
2	H	407	ALA	C-N	5.02	1.45	1.34

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	ASP	CB-CG-OD1	-39.30	82.93	118.30
2	H	300	ASP	CB-CG-OD2	38.97	153.38	118.30
2	G	377	VAL	CG1-CB-CG2	-35.82	53.59	110.90
2	H	378	LEU	C-N-CD	-33.40	47.13	120.60
2	G	377	VAL	CA-CB-CG2	-29.63	66.46	110.90
2	G	198	ASP	CB-CG-OD2	-25.91	94.98	118.30
2	G	377	VAL	CA-CB-CG1	-25.83	72.16	110.90
2	H	377	VAL	CG1-CB-CG2	-25.07	70.79	110.90
2	H	111	ARG	CA-CB-CG	21.46	160.62	113.40
2	G	400	GLU	CA-CB-CG	21.00	159.60	113.40
2	H	399	THR	O-C-N	-20.22	90.34	122.70
1	F	348	THR	CA-CB-CG2	-20.14	84.20	112.40
2	H	377	VAL	CA-CB-CG2	-20.06	80.81	110.90
1	B	348	THR	OG1-CB-CG2	-20.02	63.96	110.00
2	H	198	ASP	CB-CG-OD2	-19.48	100.77	118.30
2	G	111	ARG	O-C-N	-18.04	93.83	122.70
2	G	198	ASP	CB-CG-OD1	17.93	134.44	118.30
2	H	399	THR	C-N-CA	17.57	165.61	121.70
1	B	349	SER	CA-CB-OG	17.43	158.25	111.20
1	F	349	SER	N-CA-CB	16.93	135.90	110.50
2	H	379	PRO	CA-N-CD	-16.83	87.94	111.50
2	G	197	GLU	O-C-N	-16.25	96.70	122.70
1	F	350	LEU	CA-CB-CG	15.93	151.93	115.30
2	H	198	ASP	CB-CG-OD1	15.82	132.54	118.30
2	H	112	PHE	CB-CG-CD2	-15.19	110.17	120.80
2	H	376	ARG	O-C-N	14.64	146.12	122.70
2	H	108	GLY	C-N-CA	14.43	157.78	121.70
2	H	399	THR	CA-C-N	14.33	148.72	117.20
2	H	409	SER	CA-CB-OG	14.20	149.54	111.20
1	B	346	ASN	O-C-N	-13.86	99.64	123.20
2	G	399	THR	CA-CB-CG2	-13.86	93.00	112.40
2	H	110	ARG	N-CA-CB	13.69	135.25	110.60
1	F	348	THR	OG1-CB-CG2	-13.65	78.60	110.00
2	H	299	SER	CA-CB-OG	-13.25	75.43	111.20
2	H	197	GLU	CA-CB-CG	13.21	142.45	113.40
2	H	110	ARG	CB-CA-C	-13.07	84.25	110.40
2	G	378	LEU	CB-CG-CD2	-12.96	88.96	111.00
2	H	377	VAL	CA-CB-CG1	12.28	129.32	110.90
2	H	408	SER	CA-CB-OG	-12.11	78.51	111.20
2	H	112	PHE	CB-CG-CD1	12.07	129.25	120.80
2	G	111	ARG	CA-CB-CG	11.85	139.46	113.40
2	H	409	SER	O-C-N	-11.84	103.07	123.20
2	H	409	SER	CA-C-N	11.82	139.85	116.20

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	378	LEU	CA-CB-CG	-11.81	88.13	115.30
2	G	399	THR	OG1-CB-CG2	-11.56	83.42	110.00
2	G	400	GLU	O-C-N	-11.36	104.53	122.70
2	H	400	GLU	CB-CG-CD	-11.33	83.62	114.20
2	G	111	ARG	C-N-CA	11.22	149.76	121.70
2	G	197	GLU	C-N-CA	11.22	149.75	121.70
2	H	300	ASP	CA-CB-CG	11.20	138.03	113.40
2	H	376	ARG	CA-C-N	-10.59	93.90	117.20
1	B	346	ASN	CA-C-N	10.55	137.30	116.20
2	G	111	ARG	CA-C-N	10.50	140.31	117.20
2	G	197	GLU	CA-C-N	10.33	139.92	117.20
1	F	350	LEU	CB-CG-CD1	10.25	128.42	111.00
2	H	378	LEU	CB-CG-CD1	-9.89	94.18	111.00
2	G	378	LEU	O-C-N	-9.78	102.51	121.10
1	B	348	THR	CA-CB-OG1	-9.77	88.47	109.00
2	H	112	PHE	CA-CB-CG	9.46	136.61	113.90
2	H	108	GLY	O-C-N	-9.31	107.80	122.70
2	H	298	VAL	O-C-N	-9.12	108.11	122.70
2	G	400	GLU	CB-CG-CD	-8.99	89.94	114.20
2	H	379	PRO	N-CA-CB	8.96	114.05	103.30
2	G	378	LEU	CB-CG-CD1	8.95	126.21	111.00
2	G	400	GLU	C-N-CA	8.81	143.73	121.70
2	H	377	VAL	C-N-CA	-8.15	101.33	121.70
2	G	198	ASP	CA-CB-CG	7.82	130.61	113.40
2	H	110	ARG	CA-CB-CG	7.71	130.36	113.40
2	H	377	VAL	CA-C-O	7.66	136.19	120.10
2	H	377	VAL	CA-C-N	-7.38	100.96	117.20
2	H	110	ARG	CB-CG-CD	6.61	128.78	111.60
2	G	378	LEU	CA-CB-CG	6.61	130.50	115.30
2	H	108	GLY	CA-C-N	6.39	131.26	117.20
1	D	346	ASN	C-N-CA	-6.37	108.93	122.30
2	G	400	GLU	CA-C-N	6.30	131.06	117.20
2	H	301	SER	CA-CB-OG	6.27	128.14	111.20
1	A	346	ASN	C-N-CA	-6.10	109.48	122.30
2	H	111	ARG	CB-CG-CD	-6.06	95.85	111.60
1	B	349	SER	O-C-N	-6.03	113.06	122.70
2	H	405	PRO	O-C-N	-5.98	113.03	123.20
2	H	379	PRO	CB-CG-CD	-5.85	83.68	106.50
2	H	377	VAL	N-CA-C	-5.82	95.29	111.00
1	F	350	LEU	O-C-N	5.78	131.95	122.70
2	H	401	LEU	CB-CG-CD2	5.60	120.52	111.00
2	G	315	LEU	CA-CB-CG	5.57	128.11	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	346	ASN	O-C-N	-5.55	113.76	123.20
1	D	348	THR	N-CA-CB	5.53	120.80	110.30
1	F	350	LEU	CB-CG-CD2	-5.47	101.71	111.00
1	B	378	LEU	CA-CB-CG	5.33	127.55	115.30
2	H	405	PRO	CA-C-N	5.30	126.79	116.20
2	G	378	LEU	CA-C-N	5.23	131.75	117.10
2	H	378	LEU	CB-CA-C	-5.03	100.64	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	349	SER	CA

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	346	ASN	Mainchain
1	B	349	SER	Mainchain
2	G	111	ARG	Mainchain,Peptide
2	G	197	GLU	Mainchain,Peptide
2	G	198	ASP	Sidechain
2	G	378	LEU	Mainchain,Peptide
2	G	400	GLU	Mainchain,Peptide
2	H	108	GLY	Peptide
2	H	112	PHE	Sidechain
2	H	199	LEU	Peptide
2	H	298	VAL	Mainchain
2	H	301	SER	Mainchain
2	H	379	PRO	Peptide
2	H	399	THR	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	2758	0	2615	51	0
1	B	2758	0	2614	52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2758	0	2615	40	0
1	D	2758	0	2615	37	0
1	E	2758	0	2615	45	0
1	F	2758	0	2614	66	0
2	G	3674	0	3666	120	0
2	H	3674	0	3665	128	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
All	All	23900	0	23019	487	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (487) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:401:LEU:CB	2:H:401:LEU:CG	1.84	1.51
2:G:399:THR:CB	2:G:399:THR:CG2	1.99	1.39
1:F:348:THR:CB	1:F:348:THR:OG1	1.74	1.35
2:H:379:PRO:CB	2:H:379:PRO:CG	2.12	1.28
1:F:348:THR:CB	1:F:348:THR:CG2	2.12	1.27
2:H:377:VAL:CG2	2:H:377:VAL:HG13	1.67	1.25
1:B:348:THR:CB	1:B:348:THR:CG2	2.15	1.25
2:G:377:VAL:HG13	2:G:377:VAL:HG22	1.26	1.11
2:G:400:GLU:O	2:G:401:LEU:HG	1.47	1.10
2:G:377:VAL:O	2:G:399:THR:OG1	1.67	1.10
2:H:409:SER:OG	2:H:409:SER:HB2	1.27	1.05
2:H:409:SER:OG	2:H:409:SER:HB3	1.27	1.04
1:B:349:SER:CA	1:B:349:SER:OG	2.06	1.03
2:G:377:VAL:CG2	2:G:377:VAL:HG13	1.90	1.00
1:D:190:TRP:HE1	1:D:377:HIS:CD2	1.79	1.00
2:G:377:VAL:HA	2:G:377:VAL:CG1	1.93	0.98
1:B:349:SER:OG	1:B:349:SER:HB2	1.17	0.98
2:H:409:SER:OG	2:H:409:SER:CB	0.68	0.97
2:H:409:SER:OG	2:H:409:SER:CA	2.11	0.97
1:B:349:SER:OG	1:B:349:SER:HB3	1.16	0.97
2:H:299:SER:O	2:H:325:ALA:HB2	1.66	0.96
1:E:315:GLY:HA2	1:F:317:ASN:HD21	1.25	0.96
2:G:490:ASP:HB3	2:G:518:PRO:HA	1.48	0.95
2:G:426:THR:HG21	2:G:429:VAL:HG23	1.48	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:379:PRO:CD	2:H:379:PRO:CB	2.47	0.93
1:D:190:TRP:HE1	1:D:377:HIS:HD2	1.12	0.93
2:G:377:VAL:CG2	2:G:377:VAL:CG1	2.49	0.91
2:H:426:THR:HG21	2:H:429:VAL:HG23	1.53	0.91
2:G:426:THR:HG22	2:G:428:ALA:H	1.36	0.91
1:F:348:THR:CG2	1:F:348:THR:CA	2.49	0.89
2:H:542:LYS:HA	2:H:542:LYS:HE3	1.52	0.89
2:G:400:GLU:O	2:G:401:LEU:CG	2.22	0.86
2:H:377:VAL:CG1	2:H:377:VAL:CG2	2.52	0.86
1:F:348:THR:HG23	1:F:348:THR:O	1.75	0.86
1:F:348:THR:CG2	1:F:348:THR:N	2.39	0.85
1:D:260:ALA:O	1:D:297:TRP:HZ3	1.60	0.84
2:G:111:ARG:HH22	2:G:193:PRO:HG3	1.42	0.84
1:B:349:SER:OG	1:B:349:SER:CB	0.55	0.84
1:D:199:ASN:HA	1:D:220:LYS:HE2	1.62	0.82
2:G:48:GLY:HA3	2:G:51:GLN:HG3	1.60	0.82
1:C:190:TRP:HE1	1:C:377:HIS:HD2	1.28	0.81
2:H:344:THR:O	2:H:377:VAL:CB	2.29	0.81
2:G:399:THR:CG2	2:G:399:THR:CA	2.58	0.81
1:B:348:THR:H	1:B:348:THR:CG2	1.94	0.80
2:G:377:VAL:CA	2:G:377:VAL:CG1	2.60	0.79
1:B:254:ASN:ND2	1:B:312:GLU:HB2	1.96	0.79
1:F:348:THR:HG22	1:F:348:THR:N	1.98	0.79
2:H:252:ALA:N	2:H:301:SER:HB3	1.97	0.78
1:C:142:PHE:HB3	1:C:167:LEU:HD23	1.66	0.78
1:B:260:ALA:O	1:B:297:TRP:HZ3	1.66	0.78
1:C:218:SER:HB2	1:C:219:PRO:HD2	1.64	0.78
1:C:190:TRP:HE1	1:C:377:HIS:CD2	2.02	0.77
2:G:377:VAL:CB	2:G:377:VAL:CG1	2.62	0.77
1:B:190:TRP:HE1	1:B:377:HIS:CD2	2.02	0.77
2:H:426:THR:CG2	2:H:428:ALA:H	1.97	0.77
1:F:348:THR:HG22	1:F:348:THR:H	1.50	0.77
1:E:190:TRP:HE1	1:E:377:HIS:CD2	2.04	0.76
2:G:179:SER:H	2:G:209:THR:HG22	1.51	0.76
1:E:221:LYS:HD2	1:E:227:GLY:HA2	1.67	0.75
2:H:80:GLN:HE21	2:H:83:LEU:HD22	1.50	0.75
2:G:344:THR:O	2:G:377:VAL:CB	2.34	0.75
1:F:254:ASN:HD21	1:F:312:GLU:HG2	1.52	0.75
2:G:545:LYS:HD3	2:G:552:ARG:HH11	1.52	0.75
1:E:190:TRP:HE1	1:E:377:HIS:HD2	1.33	0.74
1:C:348:THR:HG23	1:C:349:SER:H	1.52	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:344:THR:O	2:H:377:VAL:HB	1.87	0.74
1:E:59:LYS:HD3	1:E:66:ALA:HB2	1.70	0.73
2:H:426:THR:HG22	2:H:428:ALA:H	1.52	0.73
2:G:192:GLN:NE2	2:G:192:GLN:O	2.22	0.73
2:G:377:VAL:CG2	2:G:377:VAL:CA	2.67	0.73
2:H:377:VAL:CG2	2:H:377:VAL:CB	2.67	0.73
2:G:377:VAL:O	2:G:378:LEU:CB	2.37	0.73
2:H:218:GLY:HA2	2:H:242:ARG:HH21	1.54	0.72
2:H:113:LEU:HB3	2:H:117:THR:HG21	1.71	0.72
2:G:558:ASN:HB3	2:H:402:PRO:HD2	1.71	0.71
1:E:7:PHE:HZ	1:F:7:PHE:HE1	1.38	0.71
1:B:142:PHE:HB3	1:B:167:LEU:HD23	1.70	0.71
2:H:176:VAL:HB	2:H:206:LEU:HD22	1.71	0.71
2:G:377:VAL:O	2:G:378:LEU:HB3	1.90	0.71
2:H:542:LYS:HD3	2:H:543:ASP:H	1.56	0.70
2:G:552:ARG:O	2:G:567:GLY:HA2	1.91	0.70
2:H:192:GLN:OE1	2:H:194:LEU:HA	1.90	0.70
1:E:315:GLY:HA2	1:F:317:ASN:ND2	2.04	0.70
2:G:399:THR:OG1	2:G:399:THR:CG2	2.39	0.69
1:B:348:THR:CB	1:B:348:THR:OG1	2.41	0.68
1:E:358:TRP:CZ3	1:F:335:GLN:OE1	2.46	0.68
2:G:109:VAL:O	2:G:111:ARG:N	2.27	0.68
1:B:260:ALA:O	1:B:297:TRP:CZ3	2.47	0.68
2:G:192:GLN:OE1	2:G:194:LEU:HA	1.94	0.68
2:H:376:ARG:HG2	2:H:377:VAL:O	1.94	0.67
2:H:299:SER:HA	2:H:299:SER:OG	1.94	0.67
2:H:401:LEU:CD1	2:H:401:LEU:CB	2.70	0.67
1:B:348:THR:OG1	1:B:348:THR:CG2	2.42	0.67
2:G:373:LEU:HB2	2:G:394:GLY:HA3	1.77	0.66
2:G:300:ASP:HB3	2:G:323:ARG:O	1.94	0.66
2:G:377:VAL:CG2	2:G:377:VAL:HA	2.26	0.66
1:D:190:TRP:NE1	1:D:377:HIS:CD2	2.61	0.66
2:H:481:GLY:H	2:H:507:HIS:HD2	1.43	0.66
2:G:481:GLY:H	2:G:507:HIS:HD2	1.40	0.66
2:H:104:LEU:O	2:H:105:PHE:HB3	1.94	0.66
2:G:531:ARG:HB3	2:G:531:ARG:HH11	1.61	0.66
2:H:176:VAL:HG12	2:H:209:THR:HG21	1.78	0.65
2:H:393:GLN:HB3	2:H:423:THR:HG23	1.78	0.65
1:D:335:GLN:NE2	1:D:336:PRO:HD2	2.12	0.65
2:H:192:GLN:NE2	2:H:192:GLN:O	2.30	0.65
2:G:109:VAL:C	2:G:111:ARG:H	1.99	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLY:O	1:C:39:GLY:HA2	1.96	0.65
1:B:348:THR:HG23	1:B:348:THR:OG1	1.95	0.64
2:G:373:LEU:H	2:G:395:ASP:H	1.44	0.64
1:D:260:ALA:O	1:D:297:TRP:CZ3	2.48	0.64
2:G:557:ALA:HB2	2:G:563:TRP:CD2	2.33	0.64
1:B:315:GLY:HA3	1:B:358:TRP:HB3	1.80	0.63
2:H:114:GLY:O	2:H:117:THR:HG23	1.96	0.63
2:G:198:ASP:O	2:G:199:LEU:HB2	1.98	0.63
1:B:297:TRP:HH2	1:C:225:PHE:CE1	2.17	0.63
1:F:190:TRP:HE1	1:F:377:HIS:CD2	2.17	0.62
1:F:348:THR:CG2	1:F:348:THR:OG1	2.46	0.62
2:H:529:THR:HB	2:H:530:PRO:HD2	1.81	0.62
1:D:142:PHE:HB3	1:D:167:LEU:HD23	1.82	0.62
2:H:94:GLN:HG2	2:H:126:ASP:HB2	1.82	0.61
2:G:529:THR:HB	2:G:530:PRO:HD2	1.82	0.61
2:G:378:LEU:HD23	2:G:399:THR:H	1.65	0.61
2:G:176:VAL:HG12	2:G:209:THR:HG21	1.82	0.61
1:B:348:THR:N	1:B:348:THR:CG2	2.64	0.61
2:H:299:SER:O	2:H:325:ALA:CB	2.44	0.61
2:H:401:LEU:CA	2:H:401:LEU:CG	2.75	0.60
2:H:379:PRO:CD	2:H:379:PRO:CA	2.75	0.60
1:D:156:GLY:O	1:D:291:ASN:HB2	2.01	0.60
1:D:7:PHE:HE1	1:F:7:PHE:HZ	1.49	0.60
2:H:531:ARG:HH12	2:H:560:ASN:HB3	1.65	0.60
2:H:314:GLN:CD	2:H:314:GLN:H	2.05	0.60
1:C:122:ASP:OD1	1:C:128:PRO:HA	2.00	0.60
2:G:521:ALA:HB2	2:G:551:TYR:CE2	2.36	0.60
1:C:57:PHE:HD2	1:C:171:LYS:HD2	1.66	0.60
2:G:558:ASN:HB2	2:H:401:LEU:HD23	1.84	0.60
2:G:422:TRP:HH2	2:G:426:THR:HG1	1.50	0.60
2:H:542:LYS:HD3	2:H:543:ASP:N	2.16	0.60
2:H:416:LEU:HD12	2:H:434:ILE:HG12	1.83	0.60
1:F:315:GLY:HA3	1:F:358:TRP:HB3	1.85	0.59
2:G:426:THR:CG2	2:G:428:ALA:H	2.12	0.59
2:H:169:GLU:HG3	2:H:170:ARG:HG3	1.85	0.59
2:H:252:ALA:H	2:H:301:SER:HB3	1.67	0.59
1:F:82:ILE:HG12	1:F:91:GLN:HG3	1.85	0.59
1:A:6:GLN:HE21	1:A:6:GLN:N	2.00	0.59
1:E:7:PHE:CZ	1:F:7:PHE:HE1	2.21	0.59
2:G:57:LYS:O	2:G:60:ASP:HB2	2.03	0.59
2:H:409:SER:HG	2:H:409:SER:CB	1.24	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:373:LEU:H	2:H:395:ASP:H	1.51	0.58
1:E:184:LEU:HD21	1:E:187:GLY:HA2	1.84	0.58
2:H:115:THR:HG22	2:H:143:ALA:HA	1.85	0.58
2:G:94:GLN:HG2	2:G:126:ASP:HB2	1.85	0.58
1:A:315:GLY:HA3	1:A:358:TRP:HB3	1.85	0.58
1:E:266:THR:OG1	1:E:292:ILE:HG22	2.04	0.58
1:A:184:LEU:HD21	1:A:187:GLY:HA2	1.85	0.57
2:H:179:SER:H	2:H:209:THR:HG22	1.69	0.57
2:H:374:LEU:O	2:H:396:ILE:HA	2.04	0.57
2:H:50:ARG:HA	2:H:79:ALA:HB2	1.85	0.57
2:H:423:THR:HB	2:H:440:VAL:HB	1.86	0.57
2:G:454:SER:O	2:G:455:ASP:HB2	2.04	0.57
2:G:399:THR:HA	2:G:399:THR:CG2	2.35	0.57
1:E:356:ALA:HB3	1:F:332:VAL:HG12	1.85	0.57
1:F:348:THR:CG2	1:F:348:THR:H	2.08	0.57
1:A:50:HIS:HA	1:B:48:ALA:HB2	1.86	0.56
2:G:292:GLY:HA2	2:G:315:LEU:HG	1.87	0.56
2:H:252:ALA:H	2:H:301:SER:CB	2.19	0.56
2:H:135:ASP:HB3	2:H:138:ASP:HB2	1.88	0.56
1:A:142:PHE:HB3	1:A:167:LEU:HD23	1.88	0.56
2:H:112:PHE:O	2:H:142:ILE:HD12	2.05	0.56
2:G:521:ALA:HB2	2:G:551:TYR:HE2	1.68	0.56
2:G:531:ARG:NH1	2:G:531:ARG:HB3	2.19	0.56
1:A:59:LYS:HD3	1:A:66:ALA:HB2	1.88	0.56
2:H:249:MET:HA	2:H:299:SER:HB2	1.86	0.56
1:D:20:GLY:O	1:D:39:GLY:HA2	2.06	0.56
1:C:348:THR:HG23	1:C:349:SER:N	2.19	0.55
2:H:314:GLN:H	2:H:314:GLN:NE2	2.04	0.55
1:A:377:HIS:CE1	1:A:379:ILE:HD11	2.42	0.55
2:G:176:VAL:HB	2:G:206:LEU:HD22	1.88	0.55
2:G:314:GLN:HA	2:G:338:HIS:HB2	1.87	0.55
2:H:345:GLY:HA3	2:H:377:VAL:HB	1.87	0.55
2:H:175:THR:HG23	2:H:205:VAL:HB	1.89	0.55
1:E:315:GLY:CA	1:F:317:ASN:HD21	2.10	0.55
1:F:348:THR:CG2	1:F:348:THR:O	2.51	0.55
2:H:298:VAL:HG11	2:H:301:SER:O	2.07	0.55
2:G:115:THR:CG2	2:G:132:ASN:HB2	2.37	0.55
1:E:221:LYS:HD2	1:E:227:GLY:CA	2.36	0.55
1:A:23:ARG:HD2	1:C:9:GLY:HA3	1.88	0.55
1:C:281:VAL:HG12	1:C:282:ASN:N	2.22	0.55
2:H:58:GLN:HE21	2:H:85:GLU:HG2	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:298:VAL:CG1	2:H:301:SER:O	2.55	0.54
1:B:88:LYS:HD2	1:B:115:ASP:HB2	1.88	0.54
1:E:221:LYS:HA	1:E:233:TYR:CE2	2.42	0.54
2:G:539:LEU:HD13	2:G:555:LEU:HB2	1.89	0.54
2:G:113:LEU:HB3	2:G:117:THR:HG21	1.90	0.54
1:B:7:PHE:CD2	1:B:7:PHE:N	2.75	0.54
1:E:9:GLY:HA3	1:F:23:ARG:HD2	1.90	0.54
1:B:190:TRP:HE1	1:B:377:HIS:HD2	1.53	0.54
2:G:115:THR:HG23	2:G:143:ALA:HA	1.90	0.54
1:E:356:ALA:HB1	1:E:358:TRP:CZ3	2.43	0.54
1:E:297:TRP:HH2	1:F:225:PHE:CE1	2.26	0.54
1:A:88:LYS:HG2	1:A:89:LEU:H	1.73	0.54
1:A:190:TRP:HE1	1:A:377:HIS:CD2	2.27	0.53
1:A:346:ASN:HD22	1:A:346:ASN:C	2.11	0.53
2:G:377:VAL:HG22	2:G:377:VAL:CG1	2.12	0.53
2:H:220:PRO:HA	2:H:242:ARG:HB3	1.90	0.53
1:D:221:LYS:HA	1:D:233:TYR:CE2	2.43	0.53
2:H:181:ILE:HD12	2:H:211:VAL:HG22	1.91	0.53
1:B:118:THR:OG1	1:B:120:ARG:NH1	2.41	0.53
2:G:193:PRO:HD2	2:G:197:GLU:OE2	2.08	0.53
2:G:427:ARG:HB2	2:G:446:ASN:HB2	1.90	0.53
1:B:356:ALA:HB3	1:C:332:VAL:HG12	1.91	0.53
2:H:252:ALA:N	2:H:301:SER:CB	2.72	0.53
1:B:89:LEU:HD11	1:C:51:ASP:HB2	1.89	0.53
2:G:395:ASP:O	2:G:425:ALA:O	2.27	0.53
2:G:249:MET:HG3	2:G:299:SER:HB2	1.91	0.52
1:F:25:ILE:HG23	1:F:34:VAL:HG13	1.90	0.52
2:G:427:ARG:O	2:G:427:ARG:HG2	2.10	0.52
1:E:354:ARG:NH2	1:F:239:TYR:HB3	2.25	0.52
1:D:297:TRP:HH2	1:E:225:PHE:CE1	2.28	0.52
2:H:373:LEU:HB2	2:H:394:GLY:HA3	1.92	0.52
1:A:315:GLY:N	1:B:336:PRO:HG3	2.25	0.52
1:A:51:ASP:HB2	1:C:89:LEU:HD11	1.92	0.52
2:G:377:VAL:CG2	2:G:377:VAL:CB	2.88	0.52
1:E:142:PHE:HB3	1:E:167:LEU:HD23	1.92	0.52
1:B:213:ALA:HB1	1:B:219:PRO:HG3	1.92	0.52
2:H:377:VAL:CA	2:H:377:VAL:CG2	2.87	0.52
1:B:270:SER:OG	1:B:347:GLY:O	2.27	0.52
2:H:419:GLN:HE21	2:H:419:GLN:HA	1.74	0.51
1:D:89:LEU:HD11	1:E:51:ASP:HB2	1.91	0.51
1:A:297:TRP:HH2	1:B:225:PHE:CE1	2.28	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:VAL:HG23	1:F:211:THR:O	2.10	0.51
1:D:48:ALA:HB2	1:F:50:HIS:HA	1.92	0.51
2:G:214:VAL:HG12	2:G:216:ALA:H	1.76	0.51
1:C:57:PHE:HB3	1:C:171:LYS:HE3	1.92	0.51
2:H:356:SER:O	2:H:357:PRO:C	2.48	0.51
2:H:117:THR:HG22	2:H:145:TYR:HB3	1.91	0.51
2:H:315:LEU:H	2:H:315:LEU:HD23	1.75	0.51
1:E:171:LYS:HG2	1:E:380:LEU:HB2	1.93	0.51
2:G:105:PHE:HA	2:G:112:PHE:HA	1.92	0.51
1:F:254:ASN:ND2	1:F:312:GLU:HG2	2.24	0.51
2:H:114:GLY:H	2:H:117:THR:CG2	2.23	0.51
2:G:400:GLU:O	2:G:401:LEU:CD1	2.59	0.51
1:A:89:LEU:HD11	1:B:51:ASP:HB2	1.92	0.51
1:A:335:GLN:OE1	1:C:358:TRP:CZ3	2.64	0.50
1:B:282:ASN:OD1	1:B:289:ALA:HA	2.10	0.50
2:H:101:SER:HA	2:H:133:VAL:O	2.11	0.50
1:A:7:PHE:HZ	1:B:7:PHE:HE1	1.60	0.50
1:F:142:PHE:HB3	1:F:167:LEU:HD23	1.92	0.50
2:H:395:ASP:O	2:H:425:ALA:O	2.29	0.50
1:C:218:SER:HB2	1:C:219:PRO:CD	2.37	0.50
1:F:307:TRP:CE2	1:F:343:GLY:HA2	2.47	0.50
2:H:241:GLY:HA3	2:H:244:ALA:O	2.12	0.50
2:G:191:LEU:O	2:G:193:PRO:HD3	2.12	0.50
1:C:221:LYS:HA	1:C:233:TYR:CE2	2.46	0.50
1:D:23:ARG:HE	1:F:8:ARG:HA	1.77	0.50
1:E:272:GLY:HA3	1:E:287:THR:HG23	1.92	0.50
1:A:356:ALA:HB1	1:A:358:TRP:CZ3	2.46	0.50
1:B:32:ASN:HD22	1:B:32:ASN:N	2.10	0.50
1:A:200:HIS:HA	1:A:204:GLY:O	2.11	0.50
2:G:109:VAL:C	2:G:111:ARG:N	2.64	0.49
1:F:194:TYR:CZ	1:F:208:TYR:HB2	2.48	0.49
1:C:15:HIS:O	1:C:43:GLY:HA2	2.12	0.49
2:H:379:PRO:CG	2:H:379:PRO:CA	2.87	0.49
2:G:377:VAL:CG2	2:G:377:VAL:N	2.75	0.49
2:H:426:THR:HG23	2:H:428:ALA:H	1.76	0.49
1:F:196:LEU:HD21	1:F:244:VAL:HG11	1.95	0.49
1:D:336:PRO:HG3	1:F:315:GLY:N	2.28	0.49
1:F:22:ALA:O	1:F:23:ARG:HB2	2.11	0.49
2:H:292:GLY:N	2:H:315:LEU:HD12	2.28	0.49
2:H:218:GLY:HA2	2:H:242:ARG:NH2	2.26	0.49
2:G:322:GLY:HA2	2:G:358:LEU:HD22	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:SER:HB2	2:H:572:PRO:HB2	1.95	0.49
1:B:349:SER:CB	1:B:349:SER:HG	1.14	0.49
2:G:198:ASP:O	2:G:199:LEU:CB	2.61	0.49
2:H:130:LEU:HB2	2:H:160:LEU:HD12	1.95	0.48
1:E:122:ASP:OD2	1:E:128:PRO:HA	2.13	0.48
2:G:558:ASN:CB	2:H:402:PRO:HD2	2.41	0.48
1:B:25:ILE:HG23	1:B:34:VAL:HG13	1.95	0.48
2:G:192:GLN:HG2	2:G:195:GLN:H	1.78	0.48
2:G:542:LYS:HD3	2:G:543:ASP:N	2.29	0.48
1:B:255:TYR:CE2	1:B:358:TRP:HH2	2.32	0.48
1:A:194:TYR:CZ	1:A:208:TYR:HB2	2.49	0.48
2:G:356:SER:O	2:G:357:PRO:C	2.51	0.48
2:G:314:GLN:H	2:G:314:GLN:CD	2.17	0.48
1:B:281:VAL:HG12	1:B:282:ASN:N	2.29	0.48
2:G:181:ILE:HD12	2:G:211:VAL:HG22	1.95	0.48
1:F:9:GLY:HA3	1:F:27:VAL:O	2.13	0.48
1:D:57:PHE:HB3	1:D:171:LYS:HE3	1.96	0.48
2:G:465:GLU:HG2	2:G:468:ARG:CZ	2.44	0.47
2:H:80:GLN:HG3	2:H:83:LEU:HB2	1.96	0.47
2:G:314:GLN:HE21	2:G:315:LEU:HD22	1.79	0.47
2:H:378:LEU:HB3	2:H:379:PRO:CD	2.44	0.47
2:H:454:SER:O	2:H:455:ASP:HB2	2.13	0.47
2:G:106:ASP:CG	2:G:107:GLU:H	2.17	0.47
1:D:329:ARG:HD2	1:F:354:ARG:HD2	1.96	0.47
2:G:439:TRP:CZ2	2:G:441:MET:HG3	2.49	0.47
2:G:545:LYS:HD3	2:G:552:ARG:NH1	2.25	0.47
2:H:439:TRP:CZ2	2:H:441:MET:HG3	2.49	0.47
1:D:358:TRP:CZ3	1:E:335:GLN:OE1	2.68	0.47
2:G:167:ARG:HE	2:G:167:ARG:HB2	1.52	0.47
1:C:244:VAL:O	1:C:247:HIS:HB3	2.14	0.47
1:F:215:GLY:HA2	1:F:236:GLY:HA3	1.96	0.47
2:H:552:ARG:HE	2:H:571:PRO:HD2	1.78	0.47
1:C:103:LEU:HA	1:C:109:TYR:OH	2.14	0.47
1:D:358:TRP:HZ3	1:E:335:GLN:OE1	1.97	0.47
1:D:254:ASN:ND2	1:D:312:GLU:HB2	2.30	0.47
2:H:198:ASP:O	2:H:199:LEU:HG	2.15	0.47
1:B:156:GLY:O	1:B:291:ASN:HB2	2.15	0.47
2:H:109:VAL:HG12	2:H:109:VAL:O	2.14	0.47
1:A:79:ALA:HB2	1:A:94:ALA:HA	1.95	0.47
2:H:244:ALA:HA	2:H:294:TYR:O	2.15	0.47
1:C:239:TYR:CE2	1:C:362:PRO:HB2	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:254:VAL:HB	2:G:303:VAL:HG22	1.96	0.47
2:H:426:THR:HG22	2:H:428:ALA:N	2.26	0.47
2:G:48:GLY:HA3	2:G:51:GLN:CG	2.38	0.47
1:E:154:ALA:HA	1:E:266:THR:HG23	1.96	0.46
1:C:281:VAL:HG12	1:C:282:ASN:H	1.80	0.46
1:F:366:PHE:HB3	1:F:368:PHE:CE2	2.50	0.46
1:C:315:GLY:HA3	1:C:358:TRP:HB3	1.97	0.46
2:G:546:VAL:HG13	2:G:553:TYR:HB2	1.96	0.46
1:B:9:GLY:H	1:C:23:ARG:HD2	1.81	0.46
1:C:18:PHE:HE2	1:C:26:THR:HG21	1.79	0.46
1:A:307:TRP:CZ2	1:A:343:GLY:HA2	2.51	0.46
2:H:147:ALA:HA	2:H:169:GLU:O	2.16	0.46
1:F:269:THR:HG22	1:F:270:SER:N	2.30	0.46
1:F:203:ASP:OD2	1:F:210:VAL:HG11	2.16	0.46
1:B:270:SER:HB3	1:B:345:TRP:O	2.16	0.46
2:G:357:PRO:O	2:G:358:LEU:C	2.54	0.46
2:H:378:LEU:HB3	2:H:379:PRO:HD3	1.98	0.46
1:D:51:ASP:HB2	1:F:89:LEU:HD11	1.98	0.46
1:A:260:ALA:O	1:A:297:TRP:HZ3	1.98	0.46
2:G:45:ILE:HA	2:G:73:LYS:O	2.16	0.46
1:A:254:ASN:HD21	1:A:312:GLU:HG2	1.81	0.46
2:H:212:THR:HA	2:H:239:THR:O	2.16	0.46
2:H:249:MET:HG2	2:H:299:SER:HB2	1.98	0.45
1:D:332:VAL:HB	1:D:335:GLN:HB2	1.97	0.45
1:F:318:GLY:O	1:F:319:ALA:C	2.54	0.45
1:A:239:TYR:HB3	1:C:354:ARG:NH2	2.31	0.45
2:H:543:ASP:HB2	2:H:545:LYS:HE3	1.96	0.45
1:B:254:ASN:HD21	1:B:312:GLU:HB2	1.74	0.45
2:G:557:ALA:HB2	2:G:563:TRP:CE3	2.51	0.45
2:H:50:ARG:CA	2:H:79:ALA:HB2	2.45	0.45
1:C:224:LYS:HE3	1:C:247:HIS:O	2.16	0.45
2:G:99:THR:HB	2:G:131:ALA:HB3	1.98	0.45
1:D:239:TYR:HB3	1:F:354:ARG:NH2	2.32	0.45
1:E:194:TYR:CZ	1:E:208:TYR:HB2	2.52	0.45
1:E:297:TRP:CH2	1:F:225:PHE:CE1	3.04	0.45
2:H:112:PHE:HE2	2:H:139:ASP:HA	1.81	0.45
1:F:322:TYR:CD1	1:F:333:TYR:HB2	2.51	0.45
1:D:239:TYR:HB3	1:F:354:ARG:CZ	2.47	0.45
1:F:275:ASP:HB3	1:F:284:THR:OG1	2.17	0.45
1:D:18:PHE:CZ	1:D:20:GLY:HA2	2.51	0.45
1:B:31:LYS:HB2	1:B:33:THR:HG22	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:378:LEU:CB	2:H:379:PRO:CD	2.93	0.45
1:E:358:TRP:HZ3	1:F:335:GLN:OE1	1.97	0.45
1:D:358:TRP:CE3	1:E:336:PRO:HD2	2.52	0.45
2:G:177:GLN:NE2	2:G:207:GLY:HA3	2.32	0.44
1:A:101:PRO:HD3	1:A:121:ALA:HB3	1.99	0.44
1:C:50:HIS:CE1	1:C:87:GLY:HA2	2.52	0.44
2:H:322:GLY:HA2	2:H:358:LEU:HD22	1.99	0.44
1:F:260:ALA:O	1:F:297:TRP:CZ3	2.71	0.44
2:G:377:VAL:O	2:G:378:LEU:HB2	2.17	0.44
2:H:377:VAL:HG13	2:H:377:VAL:HG21	1.82	0.44
2:H:192:GLN:HA	2:H:197:GLU:OE1	2.18	0.44
2:H:71:THR:HG22	2:H:97:SER:HB3	1.99	0.44
1:F:89:LEU:CD2	1:F:91:GLN:HB2	2.47	0.44
1:A:358:TRP:CZ3	1:B:335:GLN:OE1	2.71	0.44
2:G:299:SER:O	2:G:300:ASP:C	2.56	0.44
1:F:356:ALA:HB1	1:F:358:TRP:CZ3	2.53	0.44
1:A:346:ASN:HD22	1:A:347:GLY:N	2.16	0.44
1:A:347:GLY:O	1:A:348:THR:HG23	2.18	0.44
1:B:368:PHE:HZ	2:H:406:GLY:O	2.01	0.44
1:A:347:GLY:O	1:A:348:THR:CG2	2.66	0.44
2:H:427:ARG:HB2	2:H:446:ASN:HB2	1.99	0.44
1:A:220:LYS:HA	1:A:232:ALA:HA	1.99	0.44
1:C:88:LYS:HG3	1:C:115:ASP:HB2	2.00	0.44
2:G:411:PRO:HA	2:G:430:ASP:OD2	2.18	0.44
1:A:101:PRO:HG3	1:A:122:ASP:HA	1.99	0.44
2:H:542:LYS:HA	2:H:542:LYS:CE	2.32	0.43
2:H:377:VAL:CG2	2:H:377:VAL:HA	2.48	0.43
2:H:531:ARG:HH22	2:H:560:ASN:HD22	1.66	0.43
2:G:214:VAL:HG13	2:G:215:PRO:HD2	2.00	0.43
2:G:384:LEU:O	2:G:414:VAL:HA	2.18	0.43
1:C:173:ARG:HH22	1:C:179:PRO:HD3	1.83	0.43
2:G:100:SER:HB3	2:G:115:THR:HB	2.01	0.43
2:H:198:ASP:O	2:H:199:LEU:CB	2.65	0.43
1:A:254:ASN:ND2	1:A:312:GLU:HG2	2.33	0.43
2:G:383:LYS:HA	2:G:383:LYS:HD2	1.88	0.43
2:G:115:THR:HG21	2:G:132:ASN:HB2	2.00	0.43
1:D:194:TYR:CZ	1:D:208:TYR:HB2	2.54	0.43
1:A:213:ALA:HB1	1:A:219:PRO:HD3	2.00	0.43
1:A:276:VAL:HG22	1:A:283:GLY:HA3	2.00	0.43
2:G:293:TRP:O	2:G:316:GLY:HA3	2.18	0.43
1:A:150:ALA:HB3	1:A:296:LYS:HA	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:326:ARG:HB3	2:G:326:ARG:NH1	2.34	0.43
1:A:222:SER:OG	1:A:247:HIS:HD2	2.02	0.43
1:E:358:TRP:CD2	1:F:336:PRO:HD2	2.54	0.43
2:H:112:PHE:O	2:H:142:ILE:CD1	2.65	0.43
1:F:307:TRP:CZ2	1:F:343:GLY:HA2	2.54	0.43
1:E:255:TYR:CD2	1:E:341:PHE:CE1	3.06	0.43
1:F:348:THR:CG2	1:F:348:THR:C	2.87	0.43
1:B:270:SER:HB2	1:B:348:THR:HA	2.01	0.43
2:G:423:THR:HB	2:G:440:VAL:HB	2.01	0.43
1:A:178:ASP:OD1	1:A:178:ASP:C	2.57	0.43
2:H:105:PHE:HA	2:H:112:PHE:HA	2.00	0.43
2:H:299:SER:O	2:H:322:GLY:O	2.36	0.43
1:D:235:ASP:C	1:D:235:ASP:OD1	2.57	0.42
2:H:155:ILE:HG23	2:H:158:SER:HB2	2.01	0.42
2:H:432:LEU:HB3	2:H:447:VAL:HG11	2.01	0.42
2:G:403:PRO:O	2:G:405:PRO:HD3	2.19	0.42
2:G:220:PRO:HA	2:G:242:ARG:HB3	2.00	0.42
1:B:22:ALA:C	1:B:23:ARG:HG3	2.40	0.42
2:H:435:ASP:OD1	2:H:435:ASP:C	2.58	0.42
2:G:135:ASP:OD1	2:G:137:ARG:HB2	2.19	0.42
1:B:254:ASN:HD22	1:B:312:GLU:HB2	1.81	0.42
2:H:391:GLN:HG2	2:H:421:ARG:HB3	2.00	0.42
1:B:332:VAL:HB	1:B:335:GLN:HB2	2.00	0.42
1:A:23:ARG:HD2	1:C:9:GLY:CA	2.49	0.42
1:A:254:ASN:OD1	1:A:312:GLU:HG2	2.19	0.42
1:E:358:TRP:CE3	1:F:336:PRO:HD2	2.54	0.42
2:G:373:LEU:N	2:G:395:ASP:H	2.13	0.42
1:F:200:HIS:HA	1:F:204:GLY:O	2.20	0.42
1:F:158:THR:HG22	1:F:290:TRP:CZ2	2.55	0.42
1:B:348:THR:CA	1:B:348:THR:CG2	2.94	0.42
2:G:117:THR:HG23	2:G:145:TYR:HB3	2.02	0.42
1:E:32:ASN:OD1	1:F:45:PHE:CE2	2.73	0.42
1:A:120:ARG:HH11	1:A:120:ARG:HB3	1.85	0.42
2:H:299:SER:OG	2:H:299:SER:CB	2.68	0.42
1:C:22:ALA:O	1:C:23:ARG:HB2	2.20	0.42
1:A:222:SER:OG	1:A:247:HIS:CD2	2.73	0.42
1:E:213:ALA:HB1	1:E:219:PRO:HD3	2.01	0.42
1:D:287:THR:HG21	2:H:536:THR:HG21	2.01	0.42
1:F:31:LYS:HB2	1:F:33:THR:HG22	2.01	0.42
2:H:531:ARG:HB3	2:H:532:GLY:H	1.57	0.42
1:D:89:LEU:HD23	1:D:89:LEU:C	2.41	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:80:GLN:HE21	2:G:83:LEU:HD22	1.84	0.42
2:G:393:GLN:HB3	2:G:423:THR:HG23	2.02	0.41
2:G:84:LEU:HD23	2:G:118:VAL:HG13	2.01	0.41
1:E:263:PHE:O	1:E:295:SER:HB2	2.20	0.41
2:G:527:VAL:HB	2:G:563:TRP:HB2	2.01	0.41
1:F:269:THR:O	1:F:351:SER:HB2	2.20	0.41
1:E:239:TYR:CE2	1:E:362:PRO:HB2	2.55	0.41
1:F:203:ASP:HB3	1:F:207:LYS:HG2	2.03	0.41
1:D:115:ASP:OD2	1:D:135:THR:HG22	2.20	0.41
2:H:207:GLY:O	2:H:208:ASP:C	2.57	0.41
2:H:214:VAL:HG13	2:H:215:PRO:HD2	2.03	0.41
2:H:105:PHE:HB2	2:H:112:PHE:HA	2.03	0.41
1:E:368:PHE:CD2	1:E:368:PHE:N	2.88	0.41
1:E:212:ILE:HG12	1:E:279:THR:HG23	2.03	0.41
2:G:378:LEU:HD12	2:G:378:LEU:O	2.20	0.41
1:A:260:ALA:O	1:A:297:TRP:CZ3	2.73	0.41
1:B:57:PHE:HB3	1:B:171:LYS:HE3	2.02	0.41
1:A:282:ASN:OD1	1:A:289:ALA:HA	2.21	0.41
1:D:184:LEU:HD21	1:D:187:GLY:HA2	2.03	0.41
2:H:193:PRO:HD3	2:H:197:GLU:OE2	2.21	0.41
1:B:8:ARG:HA	1:C:23:ARG:HE	1.85	0.41
1:A:220:LYS:NZ	1:A:230:SER:O	2.53	0.41
1:A:69:ARG:HD2	1:A:162:ILE:HB	2.02	0.41
1:D:212:ILE:HG12	1:D:279:THR:HG23	2.03	0.41
2:H:545:LYS:HD3	2:H:552:ARG:HH11	1.86	0.41
2:G:481:GLY:H	2:G:507:HIS:CD2	2.30	0.41
1:D:112:TYR:CD1	1:D:128:PRO:HD3	2.55	0.41
1:F:348:THR:CB	1:F:348:THR:HG1	2.17	0.41
1:B:348:THR:HG23	1:B:348:THR:H	1.79	0.41
1:A:22:ALA:O	1:A:23:ARG:HB2	2.21	0.41
1:E:174:PRO:HG3	1:E:190:TRP:CD2	2.55	0.41
1:A:48:ALA:HB2	1:C:50:HIS:HA	2.02	0.41
2:G:382:VAL:HG12	2:G:383:LYS:H	1.85	0.41
2:H:299:SER:O	2:H:325:ALA:CA	2.68	0.40
1:A:348:THR:OG1	1:A:349:SER:N	2.54	0.40
1:E:77:ILE:HD11	1:E:81:THR:HG21	2.02	0.40
1:A:215:GLY:HA2	1:A:236:GLY:HA3	2.04	0.40
1:B:194:TYR:CZ	1:B:208:TYR:HB2	2.56	0.40
2:G:460:PHE:H	2:G:460:PHE:HD1	1.69	0.40
2:G:552:ARG:O	2:G:567:GLY:CA	2.66	0.40
1:C:347:GLY:O	1:C:348:THR:HG22	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:LEU:HD21	1:F:91:GLN:HB2	2.03	0.40
1:C:356:ALA:HB1	1:C:358:TRP:CZ3	2.56	0.40
1:A:307:TRP:CE2	1:A:343:GLY:HA2	2.56	0.40
2:H:513:ASN:HD21	2:H:516:SER:HB3	1.86	0.40
1:F:310:GLY:HA3	1:F:341:PHE:HE2	1.86	0.40
1:D:7:PHE:HZ	1:E:7:PHE:HE1	1.68	0.40
2:G:542:LYS:HD3	2:G:543:ASP:H	1.86	0.40
2:H:63:GLY:H	2:H:65:ARG:HH12	1.69	0.40
1:C:25:ILE:HG23	1:C:34:VAL:HG13	2.03	0.40
2:G:418:SER:O	2:G:419:GLN:HB2	2.20	0.40
2:G:518:PRO:HD3	2:G:548:ILE:HG22	2.03	0.40
1:C:18:PHE:CE2	1:C:26:THR:HG21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/376 (100%)	350 (94%)	22 (6%)	2 (0%)	34	76
1	B	374/376 (100%)	350 (94%)	21 (6%)	3 (1%)	24	67
1	C	374/376 (100%)	352 (94%)	20 (5%)	2 (0%)	34	76
1	D	374/376 (100%)	348 (93%)	24 (6%)	2 (0%)	34	76
1	E	374/376 (100%)	346 (92%)	28 (8%)	0	100	100
1	F	374/376 (100%)	348 (93%)	23 (6%)	3 (1%)	24	67
2	G	504/535 (94%)	439 (87%)	42 (8%)	23 (5%)	3	21
2	H	504/535 (94%)	444 (88%)	41 (8%)	19 (4%)	4	26
All	All	3252/3326 (98%)	2977 (92%)	221 (7%)	54 (2%)	11	50

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	112	PHE
2	G	199	LEU
2	G	300	ASP
2	G	355	ALA
2	G	378	LEU
2	G	407	ALA
2	G	408	SER
2	G	409	SER
2	H	199	LEU
2	H	208	ASP
2	H	348	ALA
2	H	355	ALA
2	H	379	PRO
2	H	400	GLU
2	H	418	SER
2	H	531	ARG
1	A	186	ALA
2	G	377	VAL
2	H	44	ILE
1	B	348	THR
1	F	217	ALA
1	F	319	ALA
2	G	111	ARG
2	G	198	ASP
2	G	208	ASP
2	G	357	PRO
2	G	418	SER
2	G	489	ALA
2	G	567	GLY
2	H	105	PHE
2	H	134	SER
1	C	216	SER
1	D	284	THR
2	G	228	ALA
2	G	358	LEU
2	H	347	GLY
2	H	448	GLY
1	B	152	ALA
1	C	22	ALA
2	G	110	ARG
2	G	379	PRO
2	H	396	ILE
1	D	101	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	45	ILE
2	G	347	GLY
2	H	395	ASP
2	H	567	GLY
1	B	101	PRO
2	G	396	ILE
2	H	109	VAL
2	H	337	PRO
1	A	101	PRO
1	F	277	PRO
2	H	566	VAL

### 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	271/271 (100%)	254 (94%)	17 (6%)	22	61
1	B	271/271 (100%)	261 (96%)	10 (4%)	41	78
1	C	271/271 (100%)	260 (96%)	11 (4%)	37	75
1	D	271/271 (100%)	256 (94%)	15 (6%)	27	66
1	E	271/271 (100%)	252 (93%)	19 (7%)	19	57
1	F	271/271 (100%)	254 (94%)	17 (6%)	22	61
2	G	375/388 (97%)	316 (84%)	59 (16%)	3	14
2	H	375/388 (97%)	318 (85%)	57 (15%)	3	16
All	All	2376/2402 (99%)	2171 (91%)	205 (9%)	13	45

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	31	LYS
1	A	120	ARG
1	A	129	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	153	GLN
1	A	158	THR
1	A	234	SER
1	A	255	TYR
1	A	279	THR
1	A	281	VAL
1	A	308	THR
1	A	320	SER
1	A	346	ASN
1	A	348	THR
1	A	365	SER
1	A	368	PHE
1	A	378	LEU
1	B	7	PHE
1	B	32	ASN
1	B	54	LYS
1	B	107	THR
1	B	120	ARG
1	B	123	SER
1	B	255	TYR
1	B	292	ILE
1	B	321	GLU
1	B	368	PHE
1	C	8	ARG
1	C	104	THR
1	C	221	LYS
1	C	255	TYR
1	C	278	THR
1	C	288	SER
1	C	320	SER
1	C	346	ASN
1	C	360	SER
1	C	363	SER
1	C	380	LEU
1	D	5	VAL
1	D	14	GLN
1	D	32	ASN
1	D	54	LYS
1	D	120	ARG
1	D	159	THR
1	D	202	THR
1	D	210	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	216	SER
1	D	255	TYR
1	D	279	THR
1	D	291	ASN
1	D	323	THR
1	D	348	THR
1	D	368	PHE
1	E	8	ARG
1	E	29	THR
1	E	32	ASN
1	E	41	THR
1	E	93	THR
1	E	104	THR
1	E	118	THR
1	E	120	ARG
1	E	126	SER
1	E	129	THR
1	E	153	GLN
1	E	210	VAL
1	E	255	TYR
1	E	266	THR
1	E	291	ASN
1	E	320	SER
1	E	340	LEU
1	E	363	SER
1	E	368	PHE
1	F	41	THR
1	F	70	THR
1	F	104	THR
1	F	107	THR
1	F	120	ARG
1	F	203	ASP
1	F	207	LYS
1	F	216	SER
1	F	255	TYR
1	F	281	VAL
1	F	288	SER
1	F	308	THR
1	F	320	SER
1	F	333	TYR
1	F	348	THR
1	F	360	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	368	PHE
2	G	39	TRP
2	G	46	LYS
2	G	49	GLU
2	G	50	ARG
2	G	60	ASP
2	G	77	ARG
2	G	78	GLN
2	G	80	GLN
2	G	91	LEU
2	G	97	SER
2	G	99	THR
2	G	100	SER
2	G	105	PHE
2	G	111	ARG
2	G	115	THR
2	G	117	THR
2	G	122	LYS
2	G	133	VAL
2	G	135	ASP
2	G	167	ARG
2	G	192	GLN
2	G	195	GLN
2	G	198	ASP
2	G	199	LEU
2	G	232	THR
2	G	237	HIS
2	G	239	THR
2	G	249	MET
2	G	250	ASP
2	G	260	THR
2	G	299	SER
2	G	326	ARG
2	G	330	SER
2	G	333	SER
2	G	335	SER
2	G	349	ARG
2	G	350	ARG
2	G	351	PHE
2	G	356	SER
2	G	377	VAL
2	G	378	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	395	ASP
2	G	397	VAL
2	G	401	LEU
2	G	414	VAL
2	G	421	ARG
2	G	423	THR
2	G	427	ARG
2	G	431	SER
2	G	438	THR
2	G	482	LEU
2	G	497	LEU
2	G	517	GLU
2	G	522	ASN
2	G	531	ARG
2	G	536	THR
2	G	542	LYS
2	G	545	LYS
2	G	569	LYS
2	H	46	LYS
2	H	51	GLN
2	H	59	SER
2	H	60	ASP
2	H	70	THR
2	H	77	ARG
2	H	78	GLN
2	H	80	GLN
2	H	99	THR
2	H	105	PHE
2	H	110	ARG
2	H	111	ARG
2	H	134	SER
2	H	137	ARG
2	H	160	LEU
2	H	175	THR
2	H	177	GLN
2	H	190	THR
2	H	192	GLN
2	H	197	GLU
2	H	198	ASP
2	H	260	THR
2	H	299	SER
2	H	300	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	H	301	SER
2	H	314	GLN
2	H	315	LEU
2	H	326	ARG
2	H	330	SER
2	H	349	ARG
2	H	358	LEU
2	H	373	LEU
2	H	377	VAL
2	H	378	LEU
2	H	379	PRO
2	H	382	VAL
2	H	395	ASP
2	H	397	VAL
2	H	399	THR
2	H	414	VAL
2	H	421	ARG
2	H	423	THR
2	H	427	ARG
2	H	431	SER
2	H	438	THR
2	H	446	ASN
2	H	497	LEU
2	H	517	GLU
2	H	520	SER
2	H	522	ASN
2	H	531	ARG
2	H	533	SER
2	H	536	THR
2	H	542	LYS
2	H	545	LYS
2	H	560	ASN
2	H	569	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	32	ASN
1	A	50	HIS
1	A	91	GLN
1	A	153	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	247	HIS
1	A	248	HIS
1	A	346	ASN
1	A	377	HIS
1	B	32	ASN
1	B	254	ASN
1	B	377	HIS
1	C	32	ASN
1	C	50	HIS
1	C	248	HIS
1	C	346	ASN
1	C	377	HIS
1	D	32	ASN
1	D	50	HIS
1	D	91	GLN
1	D	248	HIS
1	D	377	HIS
1	E	32	ASN
1	E	248	HIS
1	E	377	HIS
1	F	32	ASN
1	F	209	ASN
1	F	247	HIS
1	F	317	ASN
1	F	377	HIS
2	G	52	HIS
2	G	173	ASN
2	G	187	HIS
2	G	340	ASN
2	G	363	GLN
2	G	369	GLN
2	G	419	GLN
2	G	507	HIS
2	H	52	HIS
2	H	58	GLN
2	H	80	GLN
2	H	187	HIS
2	H	314	GLN
2	H	363	GLN
2	H	419	GLN
2	H	507	HIS
2	H	513	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [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	376/376 (100%)	-0.20	0 100 100	47, 61, 75, 83	0
1	B	376/376 (100%)	-0.11	1 (0%) 94 92	46, 65, 75, 80	0
1	C	376/376 (100%)	-0.21	0 100 100	44, 58, 71, 80	0
1	D	376/376 (100%)	-0.11	1 (0%) 94 92	52, 66, 75, 80	0
1	E	376/376 (100%)	0.02	3 (0%) 87 79	58, 75, 89, 97	0
1	F	376/376 (100%)	-0.06	0 100 100	51, 69, 83, 91	0
2	G	502/535 (93%)	0.09	10 (1%) 68 52	57, 71, 92, 109	0
2	H	502/535 (93%)	0.20	11 (2%) 65 49	63, 81, 105, 120	0
All	All	3260/3326 (98%)	-0.03	26 (0%) 87 79	44, 68, 92, 120	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	193	PRO	3.8
2	G	558	ASN	3.8
2	H	550	THR	3.0
1	E	284	THR	2.8
2	G	198	ASP	2.7
2	G	516	SER	2.6
2	H	109	VAL	2.6
2	H	138	ASP	2.6
2	G	193	PRO	2.6
2	H	110	ARG	2.5
1	B	130	GLY	2.5
2	H	198	ASP	2.4
2	H	558	ASN	2.4
2	H	299	SER	2.3
2	G	355	ALA	2.2
1	D	102	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	196	PRO	2.2
2	H	516	SER	2.2
2	G	110	ARG	2.2
2	G	196	PRO	2.2
2	G	138	ASP	2.2
1	E	288	SER	2.1
2	G	572	PRO	2.1
2	G	550	THR	2.0
1	E	274	THR	2.0
2	H	355	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	MG	A	3	1/1	0.91	0.55	15.23	51,51,51,51	0
3	MG	D	4	1/1	0.96	0.59	14.53	57,57,57,57	0
3	MG	B	1	1/1	0.97	0.23	1.00	50,50,50,50	0
3	MG	D	2	1/1	0.97	0.23	0.28	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.