



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:27 PM UTC

PDB ID : 2IOU / pdb_00002iou
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

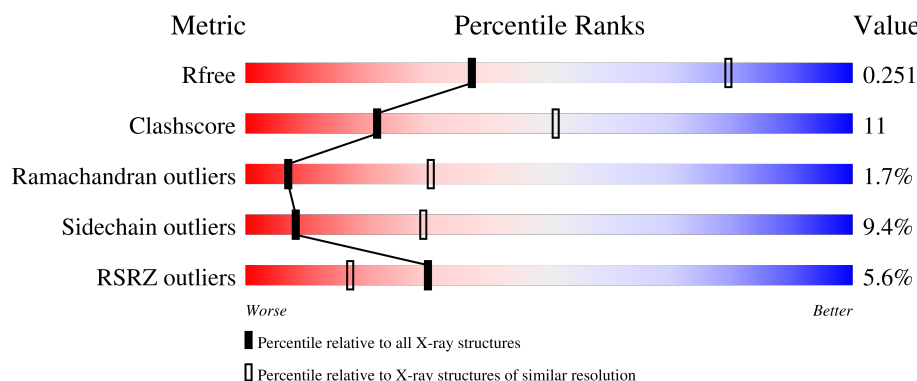
1 Overall quality at a glance

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	0% 79% 19% ..
1	B	376	0% 82% 16% ..
1	C	376	0% 83% 16% .
1	D	376	2% 83% 16% .
1	E	376	3% 82% 17% .

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Mol	Chain	Length	Quality of chain
1	F	376	7% 77% 21%
2	G	535	9% 62% 25% 6% 5%
2	H	535	15% 62% 25% 5% 5%

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			

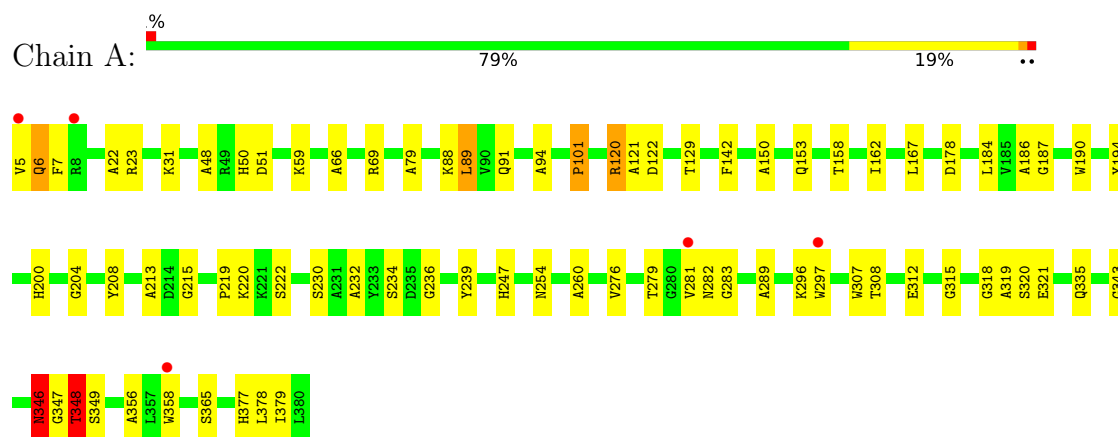
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

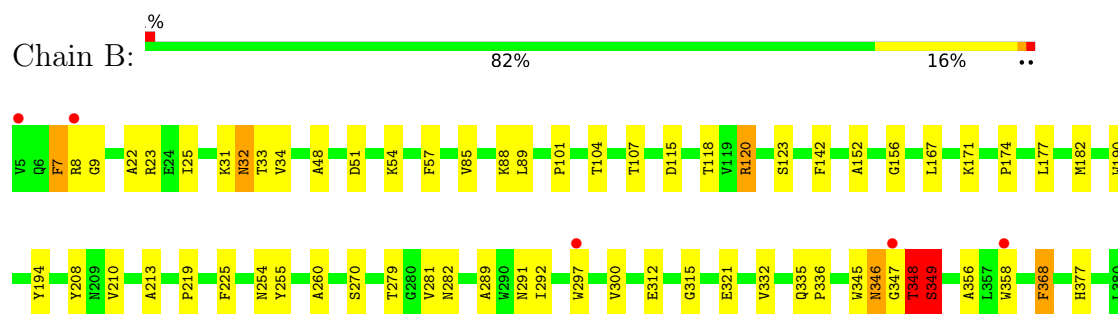
3 Residue-property plots [i](#)

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

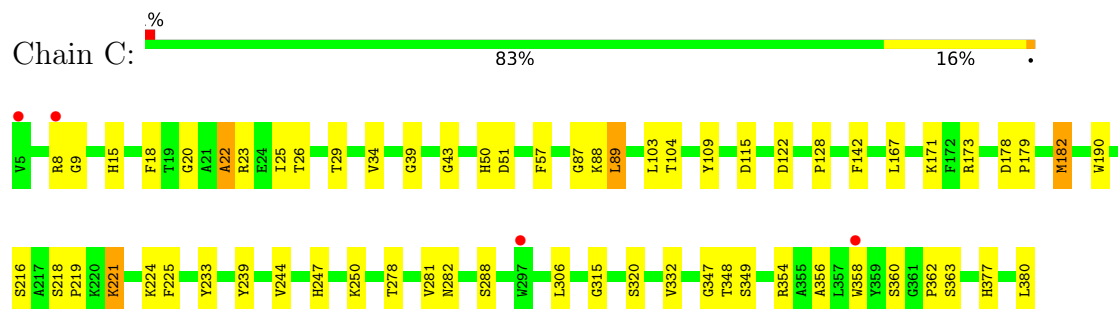
• Molecule 1: Major Tropism Determinant P1



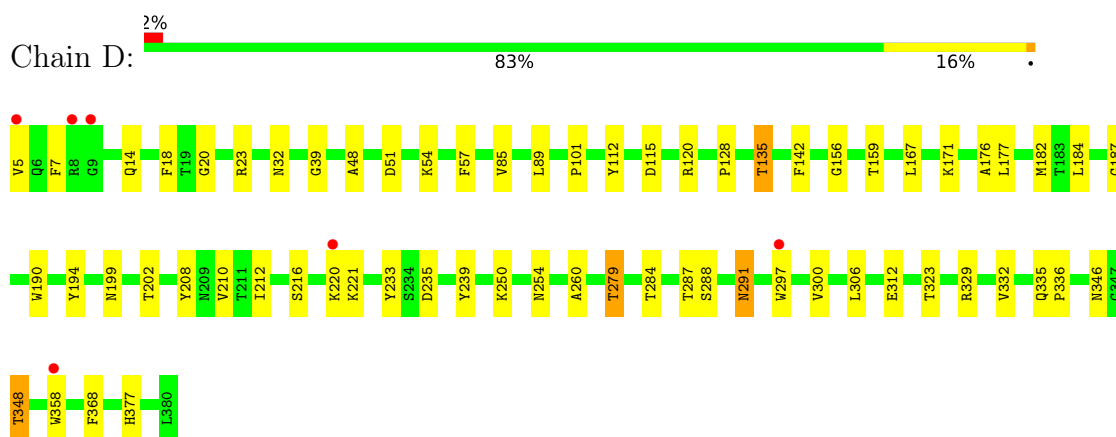
• Molecule 1: Major Tropism Determinant P1



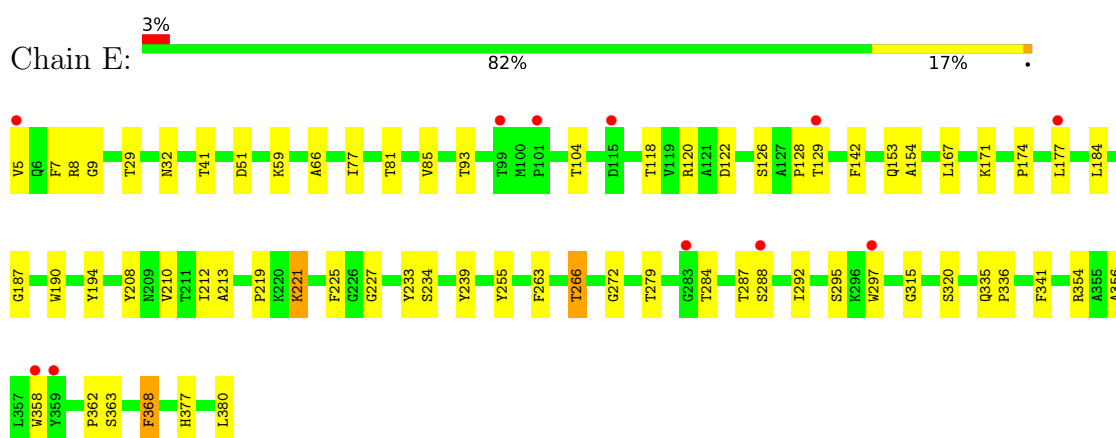
• Molecule 1: Major Tropism Determinant P1



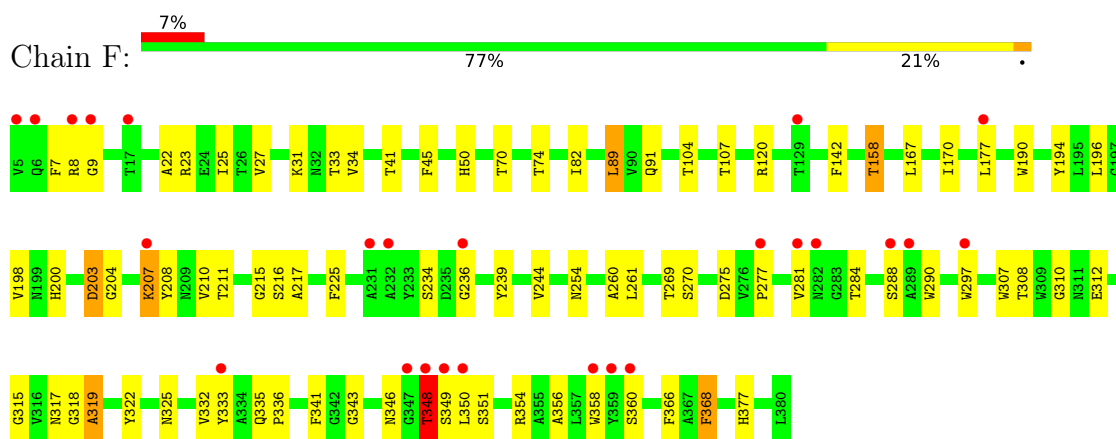
• Molecule 1: Major Tropism Determinant P1



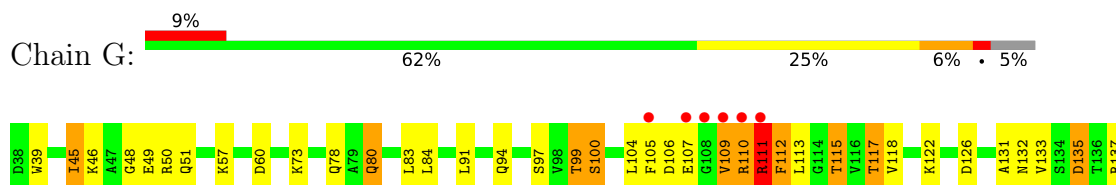
• Molecule 1: Major Tropism Determinant P1

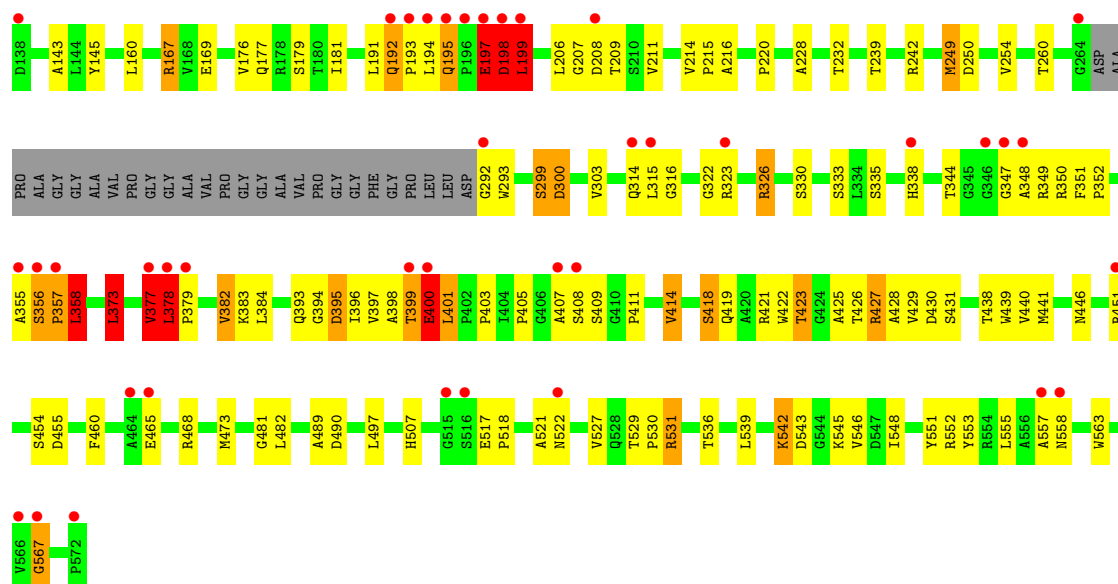


• Molecule 1: Major Tropism Determinant P1

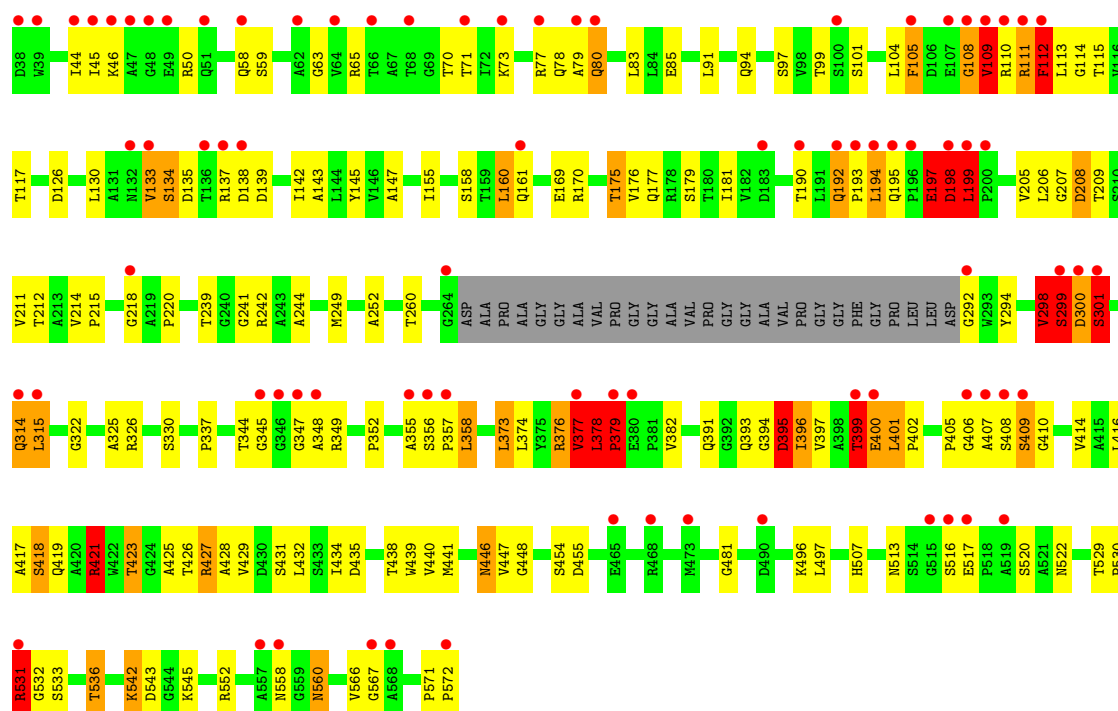


• Molecule 2: Pertactin Extracellular Domain





• Molecule 2: Pertactin Extracellular Domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	413.46Å 413.46Å 98.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.63 – 3.16 49.63 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.63-3.16) 99.9 (49.63-3.16)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.249 0.227 , 0.251	Depositor DCC
R_{free} test set	8362 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23900	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.59	2/2828 (0.1%)	0.82	6/3856 (0.2%)
1	B	1.57	4/2828 (0.1%)	1.06	5/3856 (0.1%)
1	C	0.55	0/2828	0.77	0/3856
1	D	0.55	0/2828	0.82	4/3856 (0.1%)
1	E	0.54	0/2828	0.79	0/3856
1	F	1.05	6/2828 (0.2%)	0.97	8/3856 (0.2%)
2	G	1.30	15/3731 (0.4%)	1.40	31/5073 (0.6%)
2	H	2.67	25/3731 (0.7%)	1.73	64/5073 (1.3%)
All	All	1.38	52/24430 (0.2%)	1.14	118/33282 (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	B	0	2
1	F	1	0
2	G	0	9
2	H	0	7
All	All	1	18

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	408	SER	CB-OG	99.61	3.41	1.42
2	H	379	PRO	N-CD	63.11	2.36	1.47
2	H	299	SER	CB-OG	63.06	2.68	1.42
1	B	348	THR	CB-OG1	61.06	2.41	1.43
1	B	349	SER	CB-OG	-43.60	0.55	1.42
2	G	377	VAL	CB-CG2	41.04	2.88	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	409	SER	CB-OG	-37.03	0.68	1.42
2	H	377	VAL	CB-CG2	34.80	2.67	1.52
2	G	377	VAL	CB-CG1	33.16	2.62	1.52
2	H	108	GLY	C-N	-30.93	0.91	1.33
1	F	349	SER	CA-CB	-28.59	1.16	1.54
2	H	298	VAL	C-N	-26.23	0.96	1.33
1	F	346	ASN	C-N	-23.43	0.99	1.33
2	H	300	ASP	CB-CG	-23.07	0.94	1.52
2	G	197	GLU	C-N	-21.98	1.02	1.33
2	H	111	ARG	C-N	-21.36	1.02	1.33
1	B	348	THR	CB-CG2	19.04	2.15	1.52
1	F	348	THR	CB-OG1	18.99	1.74	1.43
2	G	111	ARG	C-N	-18.14	1.08	1.33
1	F	348	THR	CB-CG2	18.07	2.12	1.52
2	H	401	LEU	CB-CG	15.70	1.84	1.53
2	H	377	VAL	C-N	15.61	1.57	1.33
2	H	377	VAL	CB-CG1	-15.60	1.01	1.52
2	H	112	PHE	CB-CG	-14.77	1.16	1.50
2	G	399	THR	CB-CG2	14.32	1.99	1.52
2	G	400	GLU	C-N	-13.80	1.04	1.33
2	H	399	THR	C-N	-13.30	1.15	1.33
2	G	378	LEU	CB-CG	-13.08	1.27	1.53
2	H	379	PRO	CB-CG	12.51	2.12	1.49
2	G	400	GLU	CB-CG	-12.40	1.15	1.52
2	H	405	PRO	C-N	12.22	1.50	1.33
2	H	197	GLU	CB-CG	-12.15	1.16	1.52
2	G	198	ASP	CB-CG	-10.98	1.24	1.52
1	A	348	THR	C-N	-10.92	1.19	1.33
1	F	350	LEU	C-N	-10.48	1.19	1.33
2	G	110	ARG	C-N	10.30	1.48	1.33
1	B	349	SER	C-N	-10.07	1.19	1.33
2	G	111	ARG	CB-CG	-9.95	1.22	1.52
2	H	377	VAL	C-O	-9.42	1.12	1.24
2	H	401	LEU	C-N	-9.23	1.22	1.33
2	H	407	ALA	C-N	9.19	1.45	1.33
2	H	378	LEU	CB-CG	9.05	1.71	1.53
2	G	399	THR	CB-OG1	8.82	1.57	1.43
1	A	348	THR	CA-CB	8.47	1.67	1.53
2	H	378	LEU	N-CA	8.38	1.55	1.46
2	G	398	ALA	C-N	-6.71	1.24	1.33
2	G	352	PRO	CA-C	5.91	1.57	1.52
1	F	350	LEU	CB-CG	5.90	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	198	ASP	CB-CG	-5.29	1.38	1.52
2	H	352	PRO	CA-C	5.28	1.57	1.52
2	H	109	VAL	CB-CG1	5.05	1.69	1.52
2	G	198	ASP	CA-C	5.04	1.59	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	377	VAL	CG1-CB-CG2	-26.00	53.59	110.80
2	G	377	VAL	CA-CB-CG2	-25.85	66.46	110.40
2	H	300	ASP	CA-CB-CG	25.43	138.03	112.60
1	B	349	SER	CA-CB-OG	23.57	158.25	111.10
2	H	111	ARG	CA-CB-CG	23.26	160.62	114.10
2	H	399	THR	O-C-N	-23.21	90.34	122.37
2	H	399	THR	CA-C-N	23.07	165.61	121.54
2	H	399	THR	C-N-CA	23.07	165.61	121.54
2	H	112	PHE	CA-CB-CG	22.81	136.61	113.80
2	G	400	GLU	CA-CB-CG	22.75	159.60	114.10
1	B	348	THR	OG1-CB-CG2	-22.67	63.96	109.30
2	G	377	VAL	CA-CB-CG1	-22.50	72.16	110.40
2	G	111	ARG	O-C-N	-21.62	93.83	122.59
2	H	376	ARG	O-C-N	20.09	146.12	123.22
2	H	108	GLY	CA-C-N	19.89	157.78	121.97
2	H	108	GLY	C-N-CA	19.89	157.78	121.97
2	H	409	SER	CA-CB-OG	19.22	149.54	111.10
2	H	378	LEU	C-N-CD	-18.99	47.13	125.00
1	B	346	ASN	O-C-N	-18.92	99.64	122.34
2	H	377	VAL	CG1-CB-CG2	-18.18	70.79	110.80
2	G	198	ASP	CA-CB-CG	18.01	130.61	112.60
2	H	299	SER	CA-CB-OG	-17.84	75.43	111.10
2	H	110	ARG	CB-CA-C	-17.71	84.25	112.06
2	H	377	VAL	CA-CB-CG2	-17.40	80.81	110.40
2	G	197	GLU	O-C-N	-17.38	96.70	122.08
2	H	379	PRO	CA-N-CD	-17.19	87.94	112.00
2	H	400	GLU	CB-CG-CD	-17.05	83.62	112.60
2	G	378	LEU	O-C-N	-16.35	102.51	121.32
2	H	408	SER	CA-CB-OG	-16.30	78.51	111.10
2	H	110	ARG	N-CA-CB	15.48	135.25	111.71
1	F	348	THR	CA-CB-CG2	-15.47	84.20	110.50
2	H	300	ASP	CB-CG-OD1	-15.42	82.93	118.40
1	F	348	THR	OG1-CB-CG2	-15.35	78.60	109.30
2	H	300	ASP	CB-CG-OD2	15.21	153.38	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	409	SER	O-C-N	-15.19	103.07	123.12
2	G	111	ARG	CA-C-N	14.78	149.76	121.54
2	G	111	ARG	C-N-CA	14.78	149.76	121.54
2	G	197	GLU	CA-C-N	14.77	149.75	121.54
2	G	197	GLU	C-N-CA	14.77	149.75	121.54
2	H	197	GLU	CA-CB-CG	14.18	142.45	114.10
1	B	348	THR	CA-CB-OG1	-14.08	88.47	109.60
2	H	377	VAL	CA-C-O	13.99	136.19	121.23
2	G	400	GLU	O-C-N	-13.35	104.53	122.41
2	G	400	GLU	CB-CG-CD	-13.33	89.94	112.60
1	F	349	SER	N-CA-CB	13.19	135.90	114.27
2	H	377	VAL	CA-C-N	-13.06	101.33	122.48
2	H	377	VAL	C-N-CA	-13.06	101.33	122.48
2	G	399	THR	OG1-CB-CG2	-12.94	83.42	109.30
2	G	111	ARG	CA-CB-CG	12.68	139.46	114.10
2	H	298	VAL	O-C-N	-11.57	108.11	122.57
2	H	108	GLY	O-C-N	-11.46	107.80	122.70
2	H	198	ASP	CA-CB-CG	11.16	123.77	112.60
2	H	377	VAL	CA-CB-CG1	11.13	129.32	110.40
2	H	377	VAL	N-CA-C	-11.08	95.29	109.58
2	G	399	THR	CA-CB-CG2	-10.30	93.00	110.50
2	H	379	PRO	N-CA-CB	10.28	114.05	103.25
1	F	350	LEU	CA-CB-CG	10.18	151.93	116.30
2	G	198	ASP	CB-CG-OD2	-10.18	94.98	118.40
2	G	400	GLU	CA-C-N	8.99	143.73	121.80
2	G	400	GLU	C-N-CA	8.99	143.73	121.80
2	H	301	SER	CA-CB-OG	8.52	128.14	111.10
2	H	110	ARG	CA-CB-CG	8.13	130.36	114.10
2	H	378	LEU	CA-CB-CG	-8.05	88.13	116.30
2	H	378	LEU	N-CA-C	7.97	119.30	110.13
1	F	346	ASN	O-C-N	-7.78	113.76	122.55
2	H	198	ASP	CB-CG-OD2	-7.67	100.77	118.40
2	H	110	ARG	CB-CG-CD	7.60	128.78	111.30
2	H	195	GLN	N-CA-C	7.48	114.95	108.22
2	G	378	LEU	CB-CG-CD2	-7.25	88.96	110.70
1	F	350	LEU	O-C-N	7.15	131.95	122.36
2	H	405	PRO	O-C-N	-7.12	113.03	122.64
2	H	379	PRO	CB-CG-CD	-7.00	83.68	106.10
1	B	349	SER	O-C-N	-6.99	113.06	122.43
2	G	198	ASP	CB-CG-OD1	6.97	134.44	118.40
2	H	111	ARG	CB-CG-CD	-6.72	95.85	111.30
1	A	348	THR	CB-CA-C	6.32	122.99	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	558	ASN	N-CA-C	6.28	118.64	108.34
2	H	352	PRO	N-CA-C	6.20	118.27	110.70
2	H	112	PHE	CB-CG-CD2	-6.20	110.17	120.70
2	H	111	ARG	CA-C-N	6.17	130.63	122.42
2	H	111	ARG	C-N-CA	6.17	130.63	122.42
2	G	348	ALA	N-CA-C	6.17	118.99	110.35
2	H	198	ASP	CB-CG-OD1	6.15	132.54	118.40
1	D	348	THR	N-CA-CB	6.10	120.80	110.49
2	G	352	PRO	N-CA-C	6.05	118.08	110.70
1	D	348	THR	CA-CB-OG1	-5.95	100.67	109.60
1	F	350	LEU	CB-CG-CD1	5.91	128.42	110.70
2	H	110	ARG	N-CA-C	5.76	119.30	111.17
2	H	405	PRO	CA-C-N	5.62	131.75	121.85
2	H	405	PRO	C-N-CA	5.62	131.75	121.85
1	D	346	ASN	CA-C-N	-5.61	108.93	121.82
1	D	346	ASN	C-N-CA	-5.61	108.93	121.82
2	H	378	LEU	N-CA-CB	-5.57	103.20	109.49
2	H	378	LEU	CA-C-N	5.56	126.79	119.84
2	H	378	LEU	C-N-CA	5.56	126.79	119.84
2	H	378	LEU	CB-CA-C	-5.55	100.64	110.47
2	H	378	LEU	CB-CG-CD1	-5.51	94.18	110.70
2	G	110	ARG	O-C-N	5.45	129.84	122.59
1	F	349	SER	CA-CB-OG	-5.44	100.22	111.10
1	A	346	ASN	O-C-N	5.44	130.37	122.43
1	A	346	ASN	CA-C-N	-5.25	109.48	121.19
1	A	346	ASN	C-N-CA	-5.25	109.48	121.19
2	H	407	ALA	CA-C-N	5.22	128.28	120.87
2	H	407	ALA	C-N-CA	5.22	128.28	120.87
2	H	298	VAL	CA-C-N	5.18	131.44	121.54
2	H	298	VAL	C-N-CA	5.18	131.44	121.54
2	H	421	ARG	N-CA-C	5.17	115.99	107.20
2	G	378	LEU	CB-CG-CD1	5.17	126.21	110.70
2	G	169	GLU	N-CA-C	5.14	115.32	108.38
2	G	373	LEU	N-CA-C	-5.12	106.19	112.90
2	G	104	LEU	N-CA-C	5.10	119.03	112.41
1	A	348	THR	CA-C-N	-5.09	114.51	122.65
1	A	348	THR	C-N-CA	-5.09	114.51	122.65
2	H	300	ASP	N-CA-C	-5.06	104.02	111.81
2	H	161	GLN	N-CA-C	5.03	116.64	109.14
2	H	112	PHE	CB-CG-CD1	5.03	129.25	120.70
2	G	378	LEU	CA-C-N	5.00	126.09	119.84
2	G	378	LEU	C-N-CA	5.00	126.09	119.84

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	Peptide,Mainchain
2	G	197	GLU	Peptide,Mainchain
2	G	198	ASP	Sidechain
2	G	378	LEU	Peptide,Mainchain
2	G	400	GLU	Peptide,Mainchain
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	54	0
1	B	2758	0	2615	55	0
1	C	2758	0	2615	42	0
1	D	2758	0	2615	39	0
1	E	2758	0	2615	45	0
1	F	2758	0	2614	67	0
2	G	3674	0	3666	123	0
2	H	3674	0	3665	132	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	23020	504	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 11.

All (504) 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:CG	2:H:401:LEU:CB	1.84	1.51
2:G:399:THR:CG2	2:G:399:THR:CB	1.99	1.39
1:F:348:THR:OG1	1:F:348:THR:CB	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:HG13	2:H:377:VAL:CG2	1.67	1.25
1:B:348:THR:CB	1:B:348:THR:CG2	2.15	1.25
2:G:377:VAL:HG22	2:G:377:VAL:HG13	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:OG	1:B:349:SER:CA	2.06	1.03
2:G:377:VAL:HG13	2:G:377:VAL:CG2	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:426:THR:HG21	2:G:429:VAL:HG23	1.48	0.95
2:G:490:ASP:HB3	2:G:518:PRO:HA	1.48	0.95
2:H:379:PRO:CB	2:H:379:PRO:CD	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:CG2	2:H:377:VAL:CG1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:B:348:THR:H	1.94	0.80
2:G:377:VAL:CG1	2:G:377:VAL:CA	2.60	0.79
1:B:254:ASN:ND2	1:B:312:GLU:HB2	1.96	0.79
1:F:348:THR:N	1:F:348:THR:HG22	1.98	0.79
2:H:252:ALA:N	2:H:301:SER:HB3	1.97	0.78
1:B:260:ALA:O	1:B:297:TRP:HZ3	1.66	0.78
1:C:142:PHE:HB3	1:C:167:LEU:HD23	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:CG1	2:G:377:VAL:CB	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:C:348:THR:HG23	1:C:349:SER:H	1.52	0.74
1:E:190:TRP:HE1	1:E:377:HIS:HD2	1.33	0.74
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:O	2:G:192:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:VAL:C	2:G:111:ARG:H	1.99	0.70
2:G:399:THR:CG2	2:G:399:THR:OG1	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:OG	2:H:299:SER:HA	1.94	0.67
2:H:401:LEU:CB	2:H:401:LEU:CD1	2.70	0.67
1:B:348:THR:CG2	1:B:348:THR:OG1	2.42	0.67
2:G:300:ASP:HB3	2:G:323:ARG:O	1.94	0.66
2:G:373:LEU:HB2	2:G:394:GLY:HA3	1.77	0.66
1:D:190:TRP:NE1	1:D:377:HIS:CD2	2.61	0.66
2:G:377:VAL:CG2	2:G:377:VAL:HA	2.26	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:G:531:ARG:HH11	2:G:531:ARG:HB3	1.61	0.66
2:H:104:LEU:O	2:H:105:PHE:HB3	1.94	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:O	2:H:192:GLN:NE2	2.30	0.65
1:C:20:GLY:O	1:C:39:GLY:HA2	1.96	0.65
1:B:348:THR:OG1	1:B:348:THR:HG23	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
2:H:314:GLN:CD	2:H:314:GLN:H	2.05	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:OG1	1:F:348:THR:CG2	2.46	0.62
2:H:529:THR:HB	2:H:530:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:B:348:THR:N	2.64	0.61
2:H:299:SER:O	2:H:325:ALA:CB	2.44	0.61
2:H:379:PRO:CD	2:H:379:PRO:CA	2.75	0.60
2:H:401:LEU:CG	2:H:401:LEU: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
1:C:122:ASP:OD1	1:C:128:PRO:HA	2.00	0.60
1:C:57:PHE:HD2	1:C:171:LYS:HD2	1.66	0.60
2:G:521:ALA:HB2	2:G:551:TYR:CE2	2.36	0.60
2:G:558:ASN:HB2	2:H:401:LEU:HD23	1.84	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:A:6:GLN:N	1:A:6:GLN:HE21	2.00	0.59
1:F:82:ILE:HG12	1:F:91:GLN:HG3	1.85	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
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:H:373:LEU:H	2:H:395:ASP:H	1.51	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:346:ASN:HD22	1:A:346:ASN:C	2.11	0.58
2:H:409:SER:CB	2:H:409:SER:HG	1.24	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:G:454:SER:O	2:G:455:ASP:HB2	2.04	0.57
2:H:423:THR:HB	2:H:440:VAL:HB	1.86	0.57
1:E:356:ALA:HB3	1:F:332:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:399:THR:CG2	2:G:399:THR:HA	2.35	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
1:A:142:PHE:HB3	1:A:167:LEU:HD23	1.88	0.56
2:H:135:ASP:HB3	2:H:138:ASP:HB2	1.88	0.56
2:H:252:ALA:H	2:H:301:SER:CB	2.19	0.56
2:G:521:ALA:HB2	2:G:551:TYR:HE2	1.68	0.56
2:H:112:PHE:O	2:H:142:ILE:HD12	2.05	0.56
1:A:59:LYS:HD3	1:A:66:ALA:HB2	1.88	0.56
2:G:531:ARG:HB3	2:G:531:ARG:NH1	2.19	0.56
2:H:356:SER:O	2:H:357:PRO:C	2.48	0.56
1:D:20:GLY:O	1:D:39:GLY:HA2	2.06	0.56
2:H:249:MET:HA	2:H:299:SER:HB2	1.86	0.56
1:A:377:HIS:CE1	1:A:379:ILE:HD11	2.42	0.55
1:C:348:THR:HG23	1:C:349:SER:N	2.19	0.55
2:G:109:VAL:C	2:G:111:ARG:N	2.64	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:175:THR:HG23	2:H:205:VAL:HB	1.89	0.55
2:H:345:GLY:HA3	2:H:377:VAL:HB	1.87	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:G:115:THR:CG2	2:G:132:ASN:HB2	2.37	0.55
2:H:298:VAL:HG11	2:H:301:SER:O	2.07	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
1:E:221:LYS:HD2	1:E:227:GLY:CA	2.36	0.55
2:H:58:GLN:HE21	2:H:85:GLU:HG2	1.72	0.54
1:B:88:LYS:HD2	1:B:115:ASP:HB2	1.88	0.54
2:H:298:VAL:CG1	2:H:301:SER:O	2.55	0.54
1:E:221:LYS:HA	1:E:233:TYR:CE2	2.42	0.54
2:G:422:TRP:HH2	2:G:426:THR:HG1	1.55	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
2:H:314:GLN:H	2:H:314:GLN:NE2	2.04	0.54
1:E:356:ALA:HB1	1:E:358:TRP:CZ3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HG2	1:A:89:LEU:H	1.73	0.54
1:E:297:TRP:HH2	1:F:225:PHE:CE1	2.26	0.54
1:A:190:TRP:HE1	1:A:377:HIS:CD2	2.27	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
1:B:118:THR:OG1	1:B:120:ARG:NH1	2.41	0.53
2:H:181:ILE:HD12	2:H:211:VAL:HG22	1.91	0.53
1:B:356:ALA:HB3	1:C:332:VAL:HG12	1.91	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:89:LEU:HD11	1:C:51:ASP:HB2	1.89	0.53
2:H:252:ALA:N	2:H:301:SER:CB	2.72	0.53
2:G:395:ASP:O	2:G:425:ALA:O	2.27	0.53
2:G:356:SER:O	2:G:357:PRO:C	2.51	0.53
1:F:25:ILE:HG23	1:F:34:VAL:HG13	1.90	0.52
2:G:249:MET:HG3	2:G:299:SER:HB2	1.91	0.52
2:G:427:ARG:O	2:G:427:ARG:HG2	2.10	0.52
2:G:106:ASP:CG	2:G:107:GLU:H	2.17	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
1:A:51:ASP:HB2	1:C:89:LEU:HD11	1.92	0.52
1:A:315:GLY:N	1:B:336:PRO:HG3	2.25	0.52
2:H:373:LEU:HB2	2:H:394:GLY:HA3	1.92	0.52
1:B:213:ALA:HB1	1:B:219:PRO:HG3	1.92	0.52
1:E:142:PHE:HB3	1:E:167:LEU:HD23	1.92	0.52
2:G:377:VAL:CG2	2:G:377:VAL:CB	2.88	0.52
1:B:270:SER:OG	1:B:347:GLY:O	2.27	0.52
2:G:314:GLN:H	2:G:314:GLN:CD	2.17	0.52
2:H:377:VAL:CG2	2:H:377:VAL:CA	2.87	0.52
2:H:419:GLN:HA	2:H:419:GLN:HE21	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
1:D:48:ALA:HB2	1:F:50:HIS:HA	1.92	0.51
1:F:198:VAL:HG23	1:F:211:THR:O	2.10	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:117:THR:HG22	2:H:145:TYR:HB3	1.91	0.51
2:H:315:LEU:HD23	2:H:315:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:89:LEU:HD11	1:B:51:ASP:HB2	1.92	0.51
2:G:400:GLU:O	2:G:401:LEU:CD1	2.59	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:G:357:PRO:O	2:G:358:LEU:C	2.54	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:318:GLY:O	1:F:319:ALA:C	2.54	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
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
2:G:191:LEU:O	2:G:193:PRO:HD3	2.12	0.50
1:A:356:ALA:HB1	1:A:358:TRP:CZ3	2.46	0.50
1:B:32:ASN:N	1:B:32:ASN:HD22	2.10	0.50
1:A:200:HIS:HA	1:A:204:GLY:O	2.11	0.50
1:C:15:HIS:O	1:C:43:GLY:HA2	2.12	0.49
1:F:194:TYR:CZ	1:F:208:TYR:HB2	2.48	0.49
2:H:379:PRO:CG	2:H:379:PRO:CA	2.87	0.49
1:F:196:LEU:HD21	1:F:244:VAL:HG11	1.95	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: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
1:E:234:SER:HB2	2:H:572:PRO:HB2	1.95	0.49
2:G:322:GLY:HA2	2:G:358:LEU:HD22	1.95	0.49
2:H:218:GLY:HA2	2:H:242:ARG:NH2	2.26	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:G:299:SER:O	2:G:300:ASP:C	2.56	0.48
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
1:B:25:ILE:HG23	1:B:34:VAL:HG13	1.95	0.48
2:G:558:ASN:CB	2:H:402:PRO:HD2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:MET:HE1	2:H:496:LYS:NZ	2.28	0.48
1:B:281:VAL:HG12	1:B:282:ASN:N	2.29	0.48
1:D:57:PHE:HB3	1:D:171:LYS:HE3	1.96	0.48
1:F:9:GLY:HA3	1:F:27:VAL:O	2.13	0.48
2:G:181:ILE:HD12	2:G:211:VAL:HG22	1.95	0.48
1:A:178:ASP:C	1:A:178:ASP:OD1	2.57	0.47
1:F:348:THR:CG2	1:F:348:THR:C	2.87	0.47
2:G:465:GLU:HG2	2:G:468:ARG:CZ	2.44	0.47
2:G:314:GLN:HE21	2:G:315:LEU:HD22	1.79	0.47
2:H:80:GLN:HG3	2:H:83:LEU:HB2	1.96	0.47
1:D:235:ASP:OD1	1:D:235:ASP:C	2.57	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: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
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
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: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
1:B:22:ALA:C	1:B:23:ARG:HG3	2.40	0.47
1:C:103:LEU:HA	1:C:109:TYR:OH	2.14	0.47
1:C:182:MET:HE2	1:C:250:LYS:HE2	1.97	0.47
2:H:435:ASP:OD1	2:H:435:ASP:C	2.58	0.47
2:H:552:ARG:HE	2:H:571:PRO:HD2	1.78	0.47
1:D:254:ASN:ND2	1:D:312:GLU:HB2	2.30	0.47
1:D:358:TRP:HZ3	1:E:335:GLN:OE1	1.97	0.47
2:H:198:ASP:O	2:H:199:LEU:HG	2.15	0.47
1:A:79:ALA:HB2	1:A:94:ALA:HA	1.95	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:C:239:TYR:CE2	1:C:362:PRO:HB2	2.50	0.47
2:G:254:VAL:HB	2:G:303:VAL:HG22	1.96	0.47
2:H:244:ALA:HA	2:H:294:TYR:O	2.15	0.47
2:G:48:GLY:HA3	2:G:51:GLN:CG	2.38	0.47
2:H:426:THR:HG22	2:H:428:ALA:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:HG12	1:C:282:ASN:H	1.80	0.46
1:E:154:ALA:HA	1:E:266:THR:HG23	1.96	0.46
1:F:366:PHE:HB3	1:F:368:PHE:CE2	2.50	0.46
1:D:89:LEU:C	1:D:89:LEU:HD23	2.41	0.46
1:A:307:TRP:CZ2	1:A:343:GLY:HA2	2.51	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:C:315:GLY:HA3	1:C:358:TRP:HB3	1.97	0.46
1:D:182:MET:HE2	1:D:250:LYS:NZ	2.30	0.46
2:G:546:VAL:HG13	2:G:553:TYR:HB2	1.96	0.46
1:F:269:THR:HG22	1:F:270:SER:N	2.30	0.46
2:H:147:ALA:HA	2:H:169:GLU:O	2.16	0.46
1:F:203:ASP:OD2	1:F:210:VAL:HG11	2.16	0.46
2:H:207:GLY:O	2:H:208:ASP:C	2.57	0.46
1:B:270:SER:HB3	1:B:345:TRP:O	2.16	0.46
1:A:254:ASN:HD21	1:A:312:GLU:HG2	1.81	0.46
1:A:260:ALA:O	1:A:297:TRP:HZ3	1.98	0.46
1:D:51:ASP:HB2	1:F:89:LEU:HD11	1.98	0.46
2:G:45:ILE:HA	2:G:73:LYS:O	2.16	0.46
2:H:212:THR:HA	2:H:239:THR:O	2.16	0.46
2:H:378:LEU:HB3	2:H:379:PRO:HD3	1.98	0.46
1:A:239:TYR:HB3	1:C:354:ARG:NH2	2.31	0.45
1:D:332:VAL:HB	1:D:335:GLN:HB2	1.97	0.45
2:H:249:MET:HG2	2:H:299:SER:HB2	1.98	0.45
1:B:254:ASN:HD21	1:B:312:GLU:HB2	1.74	0.45
2:H:543:ASP:HB2	2:H:545:LYS:HE3	1.96	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
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: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:B:174:PRO:CB	1:B:182:MET:HE3	2.47	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:B:31:LYS:HB2	1:B:33:THR:HG22	1.99	0.45
1:D:18:PHE:CZ	1:D:20:GLY:HA2	2.51	0.45
1:D:358:TRP:CE3	1:E:336:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:TRP:HZ3	1:F:335:GLN:OE1	1.97	0.45
2:H:378:LEU:CB	2:H:379:PRO:CD	2.93	0.45
1:A:101:PRO:HD3	1:A:121:ALA:HB3	1.99	0.44
1:B:174:PRO:HB3	1:B:182:MET:HE3	1.99	0.44
2:G:177:GLN:NE2	2:G:207:GLY:HA3	2.32	0.44
1:C:50:HIS:CE1	1:C:87:GLY:HA2	2.52	0.44
1:F:260:ALA:O	1:F:297:TRP:CZ3	2.71	0.44
2:H:322:GLY:HA2	2:H:358:LEU:HD22	1.99	0.44
2:H:409:SER:O	2:H:410:GLY:C	2.59	0.44
2:G:377:VAL:O	2:G:378:LEU:HB2	2.17	0.44
2:H:71:THR:HG22	2:H:97:SER:HB3	1.99	0.44
2:H:192:GLN:HA	2:H:197:GLU:OE1	2.18	0.44
2:H:357:PRO:O	2:H:358:LEU:C	2.60	0.44
2:H:377:VAL:HG13	2:H:377:VAL:HG21	1.82	0.44
1:A:358:TRP:CZ3	1:B:335:GLN:OE1	2.71	0.44
1:F:89:LEU:CD2	1:F:91:GLN:HB2	2.47	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:F:356:ALA:HB1	1:F:358:TRP:CZ3	2.53	0.44
1:A:220:LYS:HA	1:A:232:ALA:HA	1.99	0.44
1:A:347:GLY:O	1:A:348:THR:CG2	2.66	0.44
1:C:88:LYS:HG3	1:C:115:ASP:HB2	2.00	0.44
2:G:314:GLN:CD	2:G:314:GLN:N	2.76	0.44
2:G:411:PRO:HA	2:G:430:ASP:OD2	2.18	0.44
2:H:427:ARG:HB2	2:H:446:ASN:HB2	1.99	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
1:C:173:ARG:HH22	1:C:179:PRO:HD3	1.83	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
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
1:A:254:ASN:ND2	1:A:312:GLU:HG2	2.33	0.43
1:B:89:LEU:C	1:B:89:LEU:HD23	2.43	0.43
2:G:100:SER:HB3	2:G:115:THR:HB	2.01	0.43
2:G:383:LYS:HA	2:G:383:LYS:HD2	1.88	0.43
1:A:150:ALA:HB3	1:A:296:LYS:HA	2.00	0.43
1:A:213:ALA:HB1	1:A:219:PRO:HD3	2.00	0.43
1:A:222:SER:OG	1:A:247:HIS:HD2	2.02	0.43
1:A:276:VAL:HG22	1:A:283:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:TYR:CZ	1:D:208:TYR:HB2	2.54	0.43
2:G:115:THR:HG21	2:G:132:ASN:HB2	2.00	0.43
2:G:293:TRP:O	2:G:316:GLY:HA3	2.18	0.43
2:G:326:ARG:NH1	2:G:326:ARG:HB3	2.34	0.43
1:E:255:TYR:CD2	1:E:341:PHE:CE1	3.06	0.43
1:E:358:TRP:CD2	1:F:336:PRO:HD2	2.54	0.43
1:F:307:TRP:CZ2	1:F:343:GLY:HA2	2.54	0.43
2:H:112:PHE:O	2:H:142:ILE:CD1	2.65	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:89:LEU:C	1:A:89:LEU:HD23	2.43	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
2:H:417:ALA:O	2:H:418:SER:C	2.62	0.43
2:G:220:PRO:HA	2:G:242:ARG:HB3	2.00	0.42
2:G:403:PRO:O	2:G:405:PRO:HD3	2.19	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: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: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:B:332:VAL:HB	1:B:335:GLN:HB2	2.00	0.42
1:E:358:TRP:CE3	1:F:336:PRO:HD2	2.54	0.42
1:F:158:THR:HG22	1:F:290:TRP:CZ2	2.55	0.42
1:F:200:HIS:HA	1:F:204:GLY:O	2.20	0.42
2:G:373:LEU:N	2:G:395:ASP:H	2.13	0.42
1:A:120:ARG:HH11	1:A:120:ARG:HB3	1.85	0.42
1:B:348:THR:CG2	1:B:348:THR:CA	2.94	0.42
1:E:32:ASN:OD1	1:F:45:PHE:CE2	2.73	0.42
2:G:117:THR:HG23	2:G:145:TYR:HB3	2.02	0.42
1:A:222:SER:OG	1:A:247:HIS:CD2	2.73	0.42
1:C:22:ALA:O	1:C:23:ARG:HB2	2.20	0.42
1:D:287:THR:HG21	2:H:536:THR:HG21	2.01	0.42
1:E:213:ALA:HB1	1:E:219:PRO:HD3	2.01	0.42
1:F:261:LEU:HD12	1:F:261:LEU:C	2.45	0.42
2:H:299:SER:OG	2:H:299:SER:CB	2.68	0.42
1:F:31:LYS:HB2	1:F:33:THR:HG22	2.01	0.42
1:A:319:ALA:C	1:A:321:GLU:H	2.27	0.42
2:G:80:GLN:HE21	2:G:83:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:531:ARG:HB3	2:H:532:GLY:H	1.57	0.42
1:E:263:PHE:O	1:E:295:SER:HB2	2.20	0.41
2:G:84:LEU:HD23	2:G:118:VAL:HG13	2.01	0.41
2:G:393:GLN:HB3	2:G:423:THR:HG23	2.02	0.41
1:E:239:TYR:CE2	1:E:362:PRO:HB2	2.55	0.41
1:F:269:THR:O	1:F:351:SER:HB2	2.20	0.41
2:G:527:VAL:HB	2:G:563:TRP:HB2	2.01	0.41
1:D:115:ASP:OD2	1:D:135:THR:HG22	2.20	0.41
1:F:203:ASP:HB3	1:F:207:LYS:HG2	2.03	0.41
2:H:214:VAL:HG13	2:H:215:PRO:HD2	2.03	0.41
1:E:212:ILE:HG12	1:E:279:THR:HG23	2.03	0.41
1:E:368:PHE:N	1:E:368:PHE:CD2	2.88	0.41
2:H:105:PHE:HB2	2:H:112:PHE:HA	2.03	0.41
1:A:260:ALA:O	1:A:297:TRP:CZ3	2.73	0.41
1:A:282:ASN:OD1	1:A:289:ALA:HA	2.21	0.41
1:B:57:PHE:HB3	1:B:171:LYS:HE3	2.02	0.41
1:D:184:LEU:HD21	1:D:187:GLY:HA2	2.03	0.41
2:G:378:LEU:HD12	2:G:378:LEU:O	2.20	0.41
1:A:69:ARG:HD2	1:A:162:ILE:HB	2.02	0.41
1:A:220:LYS:NZ	1:A:230:SER:O	2.53	0.41
1:B:8:ARG:HA	1:C:23:ARG:HE	1.85	0.41
1:D:212:ILE:HG12	1:D:279:THR:HG23	2.03	0.41
2:G:193:PRO:HD2	2:G:197:GLU:CD	2.45	0.41
2:H:193:PRO:HD3	2:H:197:GLU:OE2	2.21	0.41
1:D:112:TYR:CD1	1:D:128:PRO:HD3	2.55	0.41
1:D:176:ALA:HB3	1:D:182:MET:HE1	2.03	0.41
2:G:481:GLY:H	2:G:507:HIS:CD2	2.30	0.41
2:H:545:LYS:HD3	2:H:552:ARG:HH11	1.86	0.41
1:A:22:ALA:O	1:A:23:ARG:HB2	2.21	0.41
1:B:348:THR:H	1:B:348:THR:HG23	1.79	0.41
1:A:48:ALA:HB2	1:C:50:HIS:HA	2.02	0.41
1:E:174:PRO:HG3	1:E:190:TRP:CD2	2.55	0.41
2:G:382:VAL:HG12	2:G:383:LYS:H	1.85	0.41
2:H:198:ASP:O	2:H:199:LEU:CB	2.65	0.41
1:A:318:GLY:O	1:A:319:ALA:C	2.64	0.41
1:A:215:GLY:HA2	1:A:236:GLY:HA3	2.04	0.40
1:A:348:THR:OG1	1:A:349:SER:N	2.54	0.40
1:B:194:TYR:CZ	1:B:208:TYR:HB2	2.56	0.40
1:C:178:ASP:C	1:C:178:ASP:OD1	2.64	0.40
1:E:77:ILE:HD11	1:E:81:THR:HG21	2.02	0.40
1:F:348:THR:CB	1:F:348:THR:HG1	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:460:PHE:H	2:G:460:PHE:HD1	1.69	0.40
2:H:299:SER:O	2:H:325:ALA:CA	2.68	0.40
1:A:307:TRP:CE2	1:A:343:GLY:HA2	2.56	0.40
1:C:347:GLY:O	1:C:348:THR:HG22	2.22	0.40
1:C:356:ALA:HB1	1:C:358:TRP:CZ3	2.56	0.40
1:F:89:LEU:HD21	1:F:91:GLN:HB2	2.03	0.40
1:F:310:GLY:HA3	1:F:341:PHE:HE2	1.86	0.40
2:G:552:ARG:O	2:G:567:GLY:CA	2.66	0.40
2:H:513:ASN:HD21	2:H:516:SER:HB3	1.86	0.40
1:C:25:ILE:HG23	1:C:34:VAL:HG13	2.03	0.40
1:D:7:PHE:HZ	1:E:7:PHE:HE1	1.68	0.40
2:G:418:SER:O	2:G:419:GLN:HB2	2.20	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:18:PHE:CE2	1:C:26:THR:HG21	2.56	0.40
2:G:518:PRO:HD3	2:G:548:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

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	374/376 (100%)	350 (94%)	22 (6%)	2 (0%)	24	55
1	B	374/376 (100%)	350 (94%)	21 (6%)	3 (1%)	16	46
1	C	374/376 (100%)	352 (94%)	20 (5%)	2 (0%)	24	55
1	D	374/376 (100%)	348 (93%)	24 (6%)	2 (0%)	24	55
1	E	374/376 (100%)	346 (92%)	28 (8%)	0	100	100
1	F	374/376 (100%)	348 (93%)	23 (6%)	3 (1%)	16	46
2	G	504/535 (94%)	439 (87%)	42 (8%)	23 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	504/535 (94%)	444 (88%)	41 (8%)	19 (4%)	2	15
All	All	3252/3326 (98%)	2977 (92%)	221 (7%)	54 (2%)	7	30

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

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Mol	Chain	Res	Type
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
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%)	253 (93%)	18 (7%)	15	42
1	B	271/271 (100%)	256 (94%)	15 (6%)	19	47
1	C	271/271 (100%)	258 (95%)	13 (5%)	23	52
1	D	271/271 (100%)	251 (93%)	20 (7%)	13	38
1	E	271/271 (100%)	250 (92%)	21 (8%)	12	37
1	F	271/271 (100%)	250 (92%)	21 (8%)	12	37
2	G	375/388 (97%)	317 (84%)	58 (16%)	2	12
2	H	375/388 (97%)	317 (84%)	58 (16%)	2	12
All	All	2376/2402 (99%)	2152 (91%)	224 (9%)	8	29

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	GLN
1	A	31	LYS
1	A	89	LEU
1	A	91	GLN
1	A	120	ARG
1	A	129	THR
1	A	153	GLN
1	A	158	THR
1	A	234	SER
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	378	LEU
1	B	7	PHE
1	B	32	ASN
1	B	54	LYS
1	B	85	VAL
1	B	104	THR
1	B	107	THR
1	B	120	ARG
1	B	123	SER
1	B	177	LEU
1	B	210	VAL
1	B	279	THR
1	B	292	ILE
1	B	300	VAL
1	B	321	GLU
1	B	368	PHE
1	C	8	ARG
1	C	29	THR
1	C	89	LEU
1	C	104	THR
1	C	182	MET
1	C	221	LYS
1	C	278	THR
1	C	288	SER
1	C	306	LEU
1	C	320	SER

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Mol	Chain	Res	Type
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	85	VAL
1	D	120	ARG
1	D	135	THR
1	D	159	THR
1	D	177	LEU
1	D	202	THR
1	D	210	VAL
1	D	216	SER
1	D	279	THR
1	D	288	SER
1	D	291	ASN
1	D	300	VAL
1	D	306	LEU
1	D	323	THR
1	D	348	THR
1	D	368	PHE
1	E	5	VAL
1	E	8	ARG
1	E	29	THR
1	E	41	THR
1	E	85	VAL
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	177	LEU
1	E	210	VAL
1	E	221	LYS
1	E	266	THR
1	E	284	THR
1	E	288	SER
1	E	320	SER

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Mol	Chain	Res	Type
1	E	363	SER
1	E	368	PHE
1	F	41	THR
1	F	70	THR
1	F	74	THR
1	F	89	LEU
1	F	104	THR
1	F	107	THR
1	F	120	ARG
1	F	158	THR
1	F	170	ILE
1	F	177	LEU
1	F	203	ASP
1	F	207	LYS
1	F	216	SER
1	F	234	SER
1	F	281	VAL
1	F	288	SER
1	F	308	THR
1	F	325	ASN
1	F	348	THR
1	F	360	SER
1	F	368	PHE
2	G	39	TRP
2	G	46	LYS
2	G	49	GLU
2	G	50	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	109	VAL
2	G	115	THR
2	G	117	THR
2	G	122	LYS
2	G	133	VAL
2	G	135	ASP
2	G	160	LEU
2	G	167	ARG
2	G	192	GLN

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Mol	Chain	Res	Type
2	G	195	GLN
2	G	198	ASP
2	G	199	LEU
2	G	232	THR
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	358	LEU
2	G	373	LEU
2	G	377	VAL
2	G	378	LEU
2	G	382	VAL
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	451	ARG
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	H	45	ILE
2	H	46	LYS
2	H	59	SER

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Mol	Chain	Res	Type
2	H	70	THR
2	H	73	LYS
2	H	77	ARG
2	H	78	GLN
2	H	80	GLN
2	H	91	LEU
2	H	99	THR
2	H	111	ARG
2	H	133	VAL
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	194	LEU
2	H	197	GLU
2	H	198	ASP
2	H	199	LEU
2	H	260	THR
2	H	298	VAL
2	H	299	SER
2	H	300	ASP
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

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Mol	Chain	Res	Type
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	560	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	32	ASN
1	A	50	HIS
1	A	153	GLN
1	A	247	HIS
1	A	248	HIS
1	A	346	ASN
1	A	377	HIS
1	B	6	GLN
1	B	32	ASN
1	B	50	HIS
1	B	199	ASN
1	B	209	ASN
1	B	254	ASN
1	B	311	ASN
1	B	377	HIS
1	C	6	GLN
1	C	32	ASN
1	C	50	HIS
1	C	209	ASN
1	C	248	HIS
1	C	346	ASN
1	C	377	HIS
1	D	6	GLN
1	D	32	ASN

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Mol	Chain	Res	Type
1	D	50	HIS
1	D	209	ASN
1	D	248	HIS
1	D	311	ASN
1	D	377	HIS
1	E	32	ASN
1	E	50	HIS
1	E	248	HIS
1	E	311	ASN
1	E	377	HIS
1	F	6	GLN
1	F	32	ASN
1	F	91	GLN
1	F	149	ASN
1	F	209	ASN
1	F	317	ASN
1	F	325	ASN
1	F	377	HIS
2	G	40	ASN
2	G	52	HIS
2	G	173	ASN
2	G	177	GLN
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	40	ASN
2	H	52	HIS
2	H	58	GLN
2	H	78	GLN
2	H	80	GLN
2	H	103	GLN
2	H	173	ASN
2	H	177	GLN
2	H	187	HIS
2	H	314	GLN
2	H	363	GLN
2	H	369	GLN
2	H	419	GLN
2	H	507	HIS

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Mol	Chain	Res	Type
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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	4
2	G	3

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Mol	Chain	Number of breaks
1	F	2
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	348:THR	C	349:SER	N	1.19
1	B	349:SER	C	350:LEU	N	1.19
1	F	350:LEU	C	351:SER	N	1.19
1	H	399:THR	C	400:GLU	N	1.15
1	G	111:ARG	C	112:PHE	N	1.08
1	G	400:GLU	C	401:LEU	N	1.05
1	H	111:ARG	C	112:PHE	N	1.03
1	G	197:GLU	C	198:ASP	N	1.02
1	F	346:ASN	C	347:GLY	N	0.99
1	H	298:VAL	C	299:SER	N	0.97
1	H	108:GLY	C	109:VAL	N	0.91

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, 95th 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 ²)	Q<0.9
1	A	376/376 (100%)	0.04	5 (1%) 75 55	47, 61, 75, 83	0
1	B	376/376 (100%)	0.12	5 (1%) 75 55	46, 65, 75, 80	0
1	C	376/376 (100%)	-0.15	4 (1%) 78 60	44, 58, 71, 80	0
1	D	376/376 (100%)	0.18	6 (1%) 70 50	52, 66, 75, 80	0
1	E	376/376 (100%)	0.44	11 (2%) 53 34	58, 75, 89, 97	0
1	F	376/376 (100%)	0.54	25 (6%) 24 14	51, 69, 83, 91	0
2	G	502/535 (93%)	0.67	46 (9%) 14 8	57, 71, 92, 109	0
2	H	502/535 (93%)	1.05	81 (16%) 4 3	63, 81, 105, 120	0
All	All	3260/3326 (98%)	0.40	183 (5%) 30 17	44, 68, 92, 120	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	109	VAL	9.7
2	G	348	ALA	9.7
2	H	348	ALA	8.4
2	H	299	SER	8.2
2	H	558	ASN	8.0
2	G	199	LEU	7.5
2	H	355	ALA	7.4
2	G	355	ALA	7.2
2	H	193	PRO	6.9
2	G	109	VAL	6.7
2	H	199	LEU	6.7
2	G	558	ASN	6.2
2	G	193	PRO	6.1
2	G	196	PRO	5.8
1	A	5	VAL	5.7
2	H	315	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	5	VAL	5.6
2	G	315	LEU	5.6
2	G	110	ARG	5.5
2	H	196	PRO	5.3
2	H	408	SER	5.2
2	H	110	ARG	5.2
1	F	8	ARG	5.1
1	E	5	VAL	5.1
1	F	348	THR	4.6
2	G	105	PHE	4.5
2	H	400	GLU	4.5
1	B	8	ARG	4.5
2	H	105	PHE	4.4
2	H	406	GLY	4.4
2	G	400	GLU	4.3
2	G	379	PRO	4.2
2	G	347	GLY	4.2
2	H	346	GLY	4.2
1	D	8	ARG	4.1
2	G	407	ALA	4.1
2	H	515	GLY	4.0
2	G	198	ASP	4.0
2	H	377	VAL	3.9
2	H	379	PRO	3.9
2	H	198	ASP	3.9
2	H	138	ASP	3.8
2	H	38	ASP	3.8
1	B	5	VAL	3.8
1	A	8	ARG	3.8
1	C	5	VAL	3.7
2	G	346	GLY	3.7
2	H	490	ASP	3.7
1	F	349	SER	3.7
2	H	567	GLY	3.5
2	H	347	GLY	3.5
2	H	531	ARG	3.5
2	G	195	GLN	3.5
1	E	177	LEU	3.5
2	H	111	ARG	3.4
2	H	356	SER	3.4
2	G	377	VAL	3.4
2	H	136	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	G	356	SER	3.4
1	E	288	SER	3.4
2	H	133	VAL	3.4
2	H	39	TRP	3.3
2	H	345	GLY	3.3
2	G	378	LEU	3.3
2	G	111	ARG	3.3
2	G	522	ASN	3.3
1	E	358	TRP	3.2
1	F	281	VAL	3.2
2	G	323	ARG	3.1
2	G	194	LEU	3.1
2	H	264	GLY	3.1
2	H	195	GLN	3.1
2	G	107	GLU	3.0
2	H	380	GLU	3.0
1	C	8	ARG	2.9
1	F	5	VAL	2.9
2	G	516	SER	2.9
2	H	77	ARG	2.9
2	H	292	GLY	2.9
2	H	47	ALA	2.9
1	F	289	ALA	2.9
1	E	297	TRP	2.8
2	G	464	ALA	2.8
2	G	138	ASP	2.8
2	H	48	GLY	2.8
1	E	283	GLY	2.8
2	H	161	GLN	2.8
2	H	407	ALA	2.8
2	H	46	LYS	2.8
1	C	358	TRP	2.7
2	G	264	GLY	2.7
2	H	62	ALA	2.7
2	G	338	HIS	2.7
1	C	297	TRP	2.7
2	H	137	ARG	2.7
2	G	197	GLU	2.7
2	G	557	ALA	2.7
2	H	572	PRO	2.6
2	H	557	ALA	2.6
1	F	207	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	282	ASN	2.6
2	G	465	GLU	2.6
2	H	473	MET	2.6
1	F	359	TYR	2.5
2	H	108	GLY	2.5
2	H	49	GLU	2.5
2	H	66	THR	2.5
2	H	468	ARG	2.5
2	H	517	GLU	2.5
2	G	399	THR	2.5
2	H	357	PRO	2.5
2	H	107	GLU	2.5
2	H	218	GLY	2.5
2	G	192	GLN	2.5
1	F	297	TRP	2.5
1	D	9	GLY	2.5
2	G	314	GLN	2.5
2	H	51	GLN	2.5
2	H	516	SER	2.4
2	H	183	ASP	2.4
1	F	350	LEU	2.4
1	E	359	TYR	2.4
2	H	79	ALA	2.4
2	H	45	ILE	2.4
2	H	194	LEU	2.4
1	B	297	TRP	2.4
1	F	277	PRO	2.4
1	B	347	GLY	2.4
1	F	231	ALA	2.4
2	H	112	PHE	2.4
2	H	301	SER	2.4
1	A	297	TRP	2.4
1	D	358	TRP	2.4
2	H	71	THR	2.4
2	H	568	ALA	2.4
2	H	409	SER	2.4
1	F	17	THR	2.4
2	H	58	GLN	2.4
2	H	314	GLN	2.4
2	H	465	GLU	2.4
1	F	288	SER	2.4
1	F	347	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	132	ASN	2.3
1	D	297	TRP	2.3
1	F	360	SER	2.3
2	G	357	PRO	2.3
1	F	232	ALA	2.3
1	F	358	TRP	2.3
2	H	399	THR	2.3
2	G	566	VAL	2.3
1	F	236	GLY	2.3
2	G	108	GLY	2.3
1	F	129	THR	2.3
2	G	408	SER	2.3
2	H	200	PRO	2.2
2	H	64	VAL	2.2
2	H	44	ILE	2.2
2	G	572	PRO	2.2
2	H	519	ALA	2.2
1	B	358	TRP	2.2
2	G	567	GLY	2.2
1	D	220	LYS	2.2
2	G	451	ARG	2.2
2	G	208	ASP	2.2
2	H	190	THR	2.2
1	F	333	TYR	2.2
2	H	300	ASP	2.2
2	H	68	THR	2.1
2	H	73	LYS	2.1
1	A	281	VAL	2.1
1	F	177	LEU	2.1
2	G	292	GLY	2.1
2	H	100	SER	2.1
1	A	358	TRP	2.1
1	E	129	THR	2.1
2	G	515	GLY	2.1
2	H	80	GLN	2.1
2	H	192	GLN	2.1
1	E	99	THR	2.0
1	F	9	GLY	2.0
1	E	101	PRO	2.0
1	E	115	ASP	2.0
1	F	6	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	3	1/1	0.85	0.20	51,51,51,51	0
3	MG	D	4	1/1	0.88	0.18	57,57,57,57	0
3	MG	D	2	1/1	1.00	0.03	49,49,49,49	0
3	MG	B	1	1/1	1.00	0.03	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.