



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 5XAZ / pdb_00005xaz
Title : Crystal structure of full length native tylp, a tetracycline resistance regulator from *Streptomyces fradiae*
Authors : Ray, S.; Panjikar, S.; Anand, R.
Deposited on : 2017-03-15
Resolution : 2.30 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

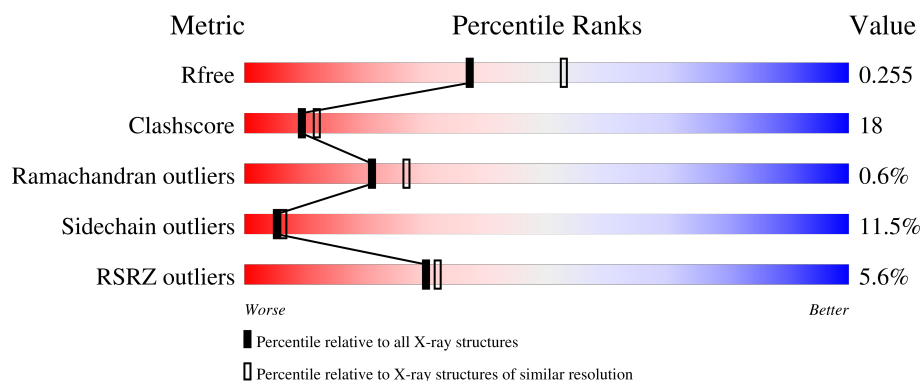
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	228	5% 66% 25% 6% .
1	B	228	5% 68% 19% 10% .
1	C	228	7% 63% 25% 5% 7%
1	D	228	3% 70% 21% . .
1	E	228	8% 58% 26% 9% . 7%

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Mol	Chain	Length	Quality of chain
1	F	228	4% 72% 19% 6%
1	G	228	6% 62% 24% 6% 7%
1	H	228	6% 66% 20% 6% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13820 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 Gamma-butyrolactone receptor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1709	1067	318	319	5			
1	H	211	Total	C	N	O	S	0	0	0
			1620	1015	296	304	5			
1	B	223	Total	C	N	O	S	0	0	0
			1709	1067	318	319	5			
1	C	213	Total	C	N	O	S	0	0	0
			1634	1024	299	306	5			
1	D	220	Total	C	N	O	S	0	1	0
			1702	1062	318	316	6			
1	E	213	Total	C	N	O	S	0	1	0
			1643	1030	304	304	5			
1	F	222	Total	C	N	O	S	0	0	0
			1701	1063	317	316	5			
1	G	213	Total	C	N	O	S	0	1	0
			1643	1030	304	304	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	ARG	engineered mutation	UNP Q9XCC7
A	227	LEU	-	expression tag	UNP Q9XCC7
A	228	GLU	-	expression tag	UNP Q9XCC7
A	229	HIS	-	expression tag	UNP Q9XCC7
H	113	ALA	ARG	engineered mutation	UNP Q9XCC7
H	227	LEU	-	expression tag	UNP Q9XCC7
H	228	GLU	-	expression tag	UNP Q9XCC7
H	229	HIS	-	expression tag	UNP Q9XCC7
B	113	ALA	ARG	engineered mutation	UNP Q9XCC7
B	227	LEU	-	expression tag	UNP Q9XCC7
B	228	GLU	-	expression tag	UNP Q9XCC7
B	229	HIS	-	expression tag	UNP Q9XCC7
C	113	ALA	ARG	engineered mutation	UNP Q9XCC7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	227	LEU	-	expression tag	UNP Q9XCC7
C	228	GLU	-	expression tag	UNP Q9XCC7
C	229	HIS	-	expression tag	UNP Q9XCC7
D	113	ALA	ARG	engineered mutation	UNP Q9XCC7
D	227	LEU	-	expression tag	UNP Q9XCC7
D	228	GLU	-	expression tag	UNP Q9XCC7
D	229	HIS	-	expression tag	UNP Q9XCC7
E	113	ALA	ARG	engineered mutation	UNP Q9XCC7
E	227	LEU	-	expression tag	UNP Q9XCC7
E	228	GLU	-	expression tag	UNP Q9XCC7
E	229	HIS	-	expression tag	UNP Q9XCC7
F	113	ALA	ARG	engineered mutation	UNP Q9XCC7
F	227	LEU	-	expression tag	UNP Q9XCC7
F	228	GLU	-	expression tag	UNP Q9XCC7
F	229	HIS	-	expression tag	UNP Q9XCC7
G	113	ALA	ARG	engineered mutation	UNP Q9XCC7
G	227	LEU	-	expression tag	UNP Q9XCC7
G	228	GLU	-	expression tag	UNP Q9XCC7
G	229	HIS	-	expression tag	UNP Q9XCC7

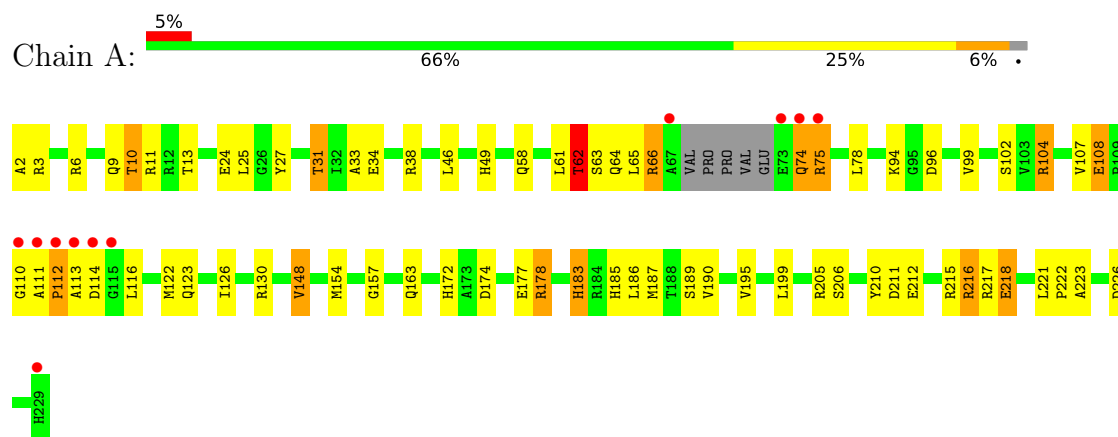
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	H	58	Total O 58 58	0	0
2	B	68	Total O 68 68	0	0
2	C	57	Total O 57 57	0	0
2	D	62	Total O 62 62	0	0
2	E	45	Total O 45 45	0	0
2	F	62	Total O 62 62	0	0
2	G	49	Total O 49 49	0	0

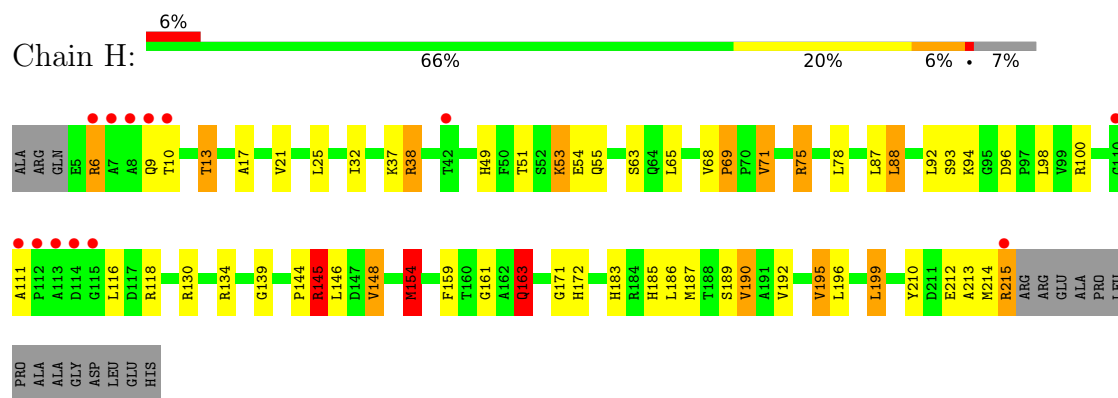
3 Residue-property plots [i](#)

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.

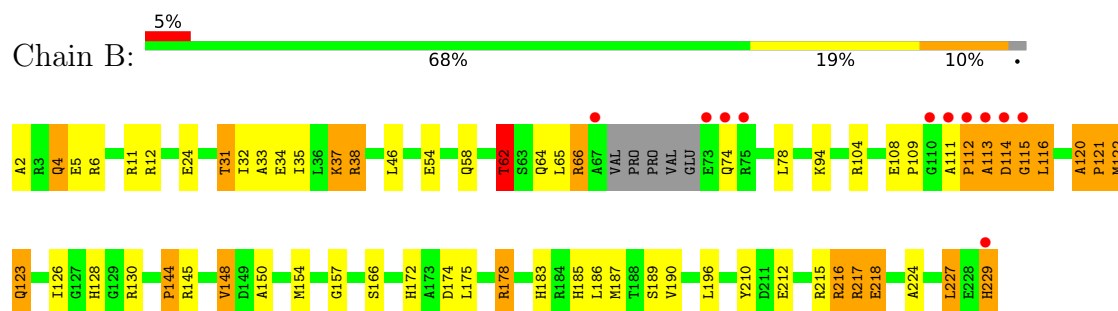
- Molecule 1: Gamma-butyrolactone receptor protein



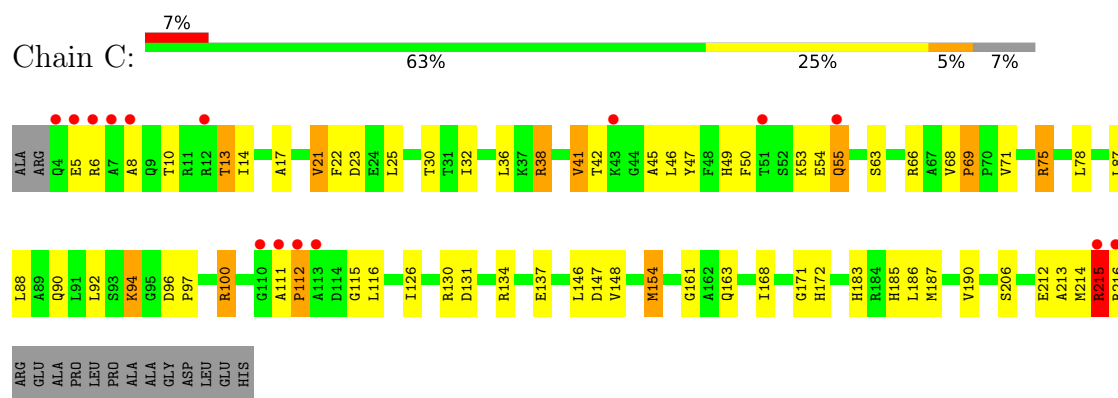
- Molecule 1: Gamma-butyrolactone receptor protein



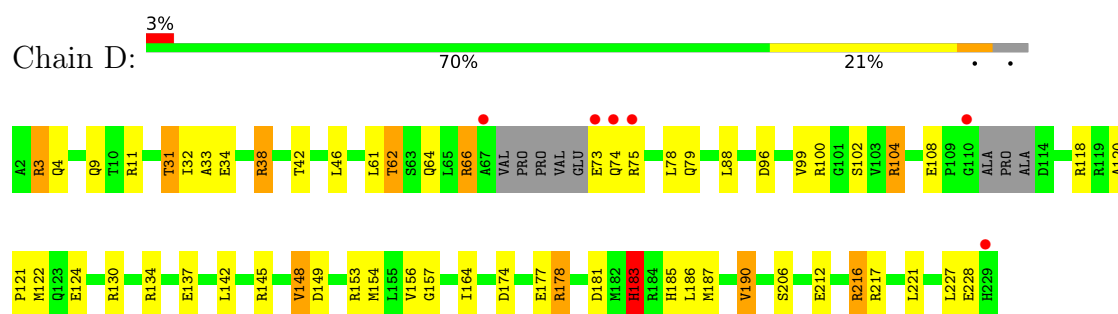
- Molecule 1: Gamma-butyrolactone receptor protein



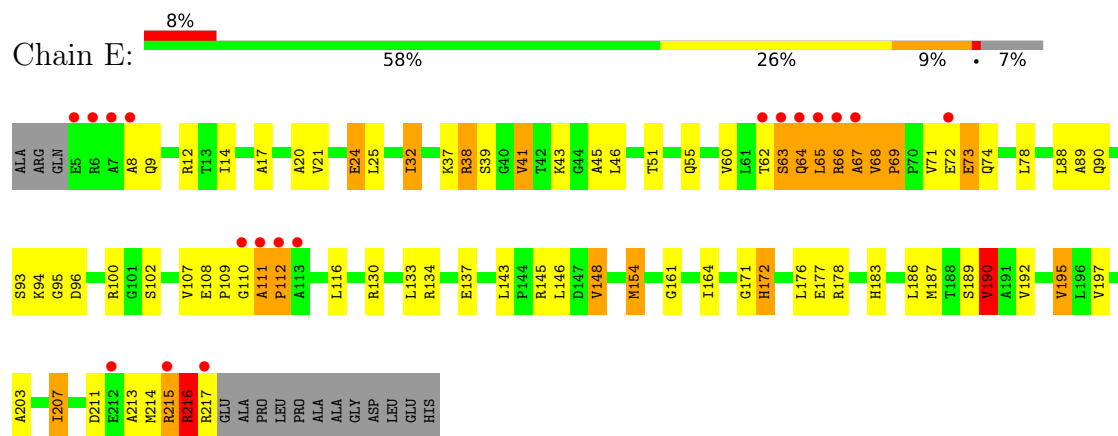
- Molecule 1: Gamma-butyrolactone receptor protein



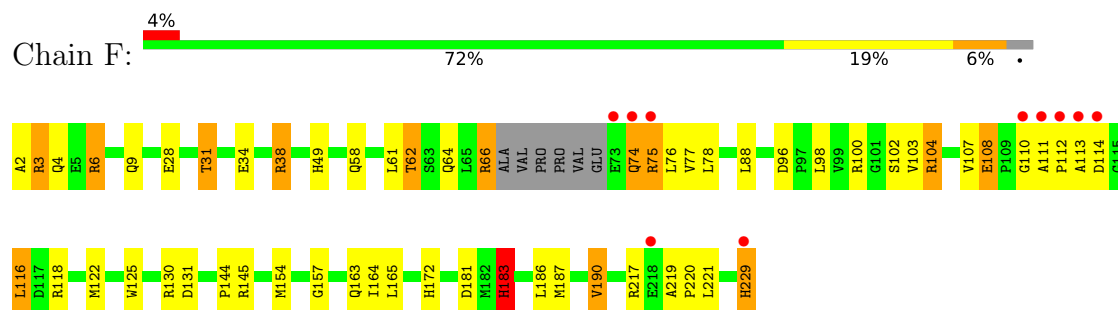
- Molecule 1: Gamma-butyrolactone receptor protein



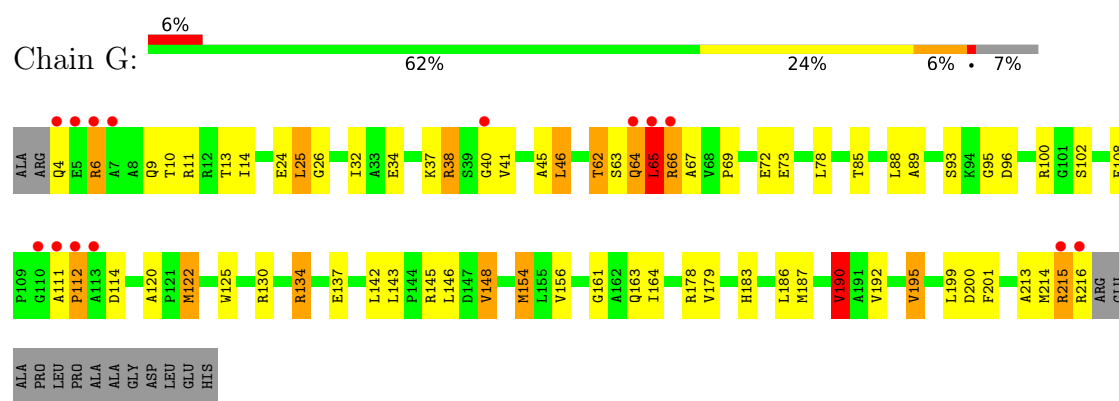
- Molecule 1: Gamma-butyrolactone receptor protein



- Molecule 1: Gamma-butyrolactone receptor protein



- Molecule 1: Gamma-butyrolactone receptor protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.48Å 71.57Å 158.58Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.81-2.30) 99.2 (19.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.253 0.208 , 0.255	Depositor DCC
R_{free} test set	992 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4642e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.39	6/1731 (0.3%)	1.37	11/2343 (0.5%)
1	B	1.43	11/1731 (0.6%)	1.30	7/2343 (0.3%)
1	C	1.32	4/1656 (0.2%)	1.32	8/2245 (0.4%)
1	D	1.33	5/1722 (0.3%)	1.30	4/2326 (0.2%)
1	E	1.38	4/1669 (0.2%)	1.38	19/2262 (0.8%)
1	F	1.32	10/1723 (0.6%)	1.30	6/2332 (0.3%)
1	G	1.36	5/1669 (0.3%)	1.39	14/2262 (0.6%)
1	H	1.25	2/1642 (0.1%)	1.29	10/2227 (0.4%)
All	All	1.35	47/13543 (0.3%)	1.33	79/18340 (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	G	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	PRO	C-O	-6.55	1.16	1.24
1	C	69	PRO	CA-C	6.51	1.56	1.52
1	D	124	GLU	C-O	-6.44	1.16	1.24
1	A	49	HIS	CE1-NE2	6.37	1.39	1.32
1	D	206	SER	C-O	6.33	1.31	1.24
1	F	190	VAL	C-O	6.26	1.31	1.24
1	B	120	ALA	CA-C	6.25	1.60	1.52
1	B	6	ARG	C-O	-6.16	1.17	1.24
1	B	229	HIS	CG-CD2	6.06	1.42	1.35
1	G	190	VAL	CA-C	6.05	1.60	1.52
1	G	120	ALA	N-CA	5.98	1.52	1.46
1	B	128	HIS	CG-CD2	5.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	125	TRP	CD2-CE2	5.84	1.51	1.41
1	F	183	HIS	CE1-NE2	5.73	1.38	1.32
1	A	177	GLU	CA-C	5.71	1.60	1.52
1	G	179	VAL	N-CA	-5.68	1.39	1.46
1	F	190	VAL	CA-C	5.64	1.59	1.52
1	D	227	LEU	C-O	-5.52	1.17	1.23
1	F	77	VAL	C-O	-5.48	1.17	1.24
1	E	133	LEU	C-O	-5.46	1.17	1.24
1	A	49	HIS	CG-CD2	5.46	1.41	1.35
1	A	183	HIS	CE1-NE2	5.43	1.38	1.32
1	F	229	HIS	CG-CD2	5.41	1.41	1.35
1	H	154	MET	C-O	-5.41	1.17	1.24
1	A	96	ASP	CA-C	5.38	1.59	1.53
1	B	123	GLN	C-O	-5.38	1.17	1.24
1	B	144	PRO	C-O	-5.37	1.17	1.23
1	G	200	ASP	C-O	5.37	1.30	1.24
1	F	163	GLN	CA-C	5.35	1.59	1.52
1	F	108	GLU	CA-C	-5.30	1.46	1.52
1	A	172	HIS	CG-CD2	5.22	1.41	1.35
1	D	183	HIS	CE1-NE2	5.22	1.37	1.32
1	H	49	HIS	CD2-NE2	-5.21	1.32	1.37
1	B	4	GLN	C-O	-5.19	1.18	1.24
1	B	183	HIS	CG-CD2	5.16	1.41	1.35
1	C	147	ASP	C-O	-5.13	1.17	1.24
1	E	73	GLU	C-O	-5.12	1.17	1.23
1	F	172	HIS	CE1-NE2	5.12	1.37	1.32
1	E	172	HIS	CG-CD2	5.12	1.41	1.35
1	F	49	HIS	CE1-NE2	5.08	1.37	1.32
1	B	183	HIS	CE1-NE2	5.07	1.37	1.32
1	D	190	VAL	CA-C	5.07	1.59	1.52
1	E	74	GLN	C-O	-5.05	1.17	1.23
1	G	26	GLY	N-CA	5.04	1.51	1.45
1	C	49	HIS	CG-CD2	5.04	1.41	1.35
1	B	196	LEU	CA-C	5.01	1.59	1.52
1	C	206	SER	CA-C	5.01	1.59	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25	LEU	CA-C-N	-12.40	108.90	122.55
1	G	25	LEU	C-N-CA	-12.40	108.90	122.55
1	C	6	ARG	N-CA-C	-11.16	100.19	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	111	ALA	N-CA-C	-8.63	98.67	109.64
1	E	8	ALA	N-CA-C	-8.62	102.32	112.92
1	G	24	GLU	N-CA-C	8.09	119.72	111.07
1	A	99	VAL	N-CA-C	-7.97	103.14	111.58
1	G	25	LEU	N-CA-C	-7.69	99.08	110.46
1	C	75	ARG	CG-CD-NE	-7.33	95.89	112.00
1	E	68	VAL	CA-C-N	7.30	124.92	119.66
1	E	68	VAL	C-N-CA	7.30	124.92	119.66
1	D	75	ARG	N-CA-C	-7.17	100.58	111.56
1	B	113	ALA	N-CA-C	-7.09	99.71	109.71
1	G	122	MET	CG-SD-CE	-6.86	85.80	100.90
1	H	54	GLU	N-CA-C	6.67	119.40	111.33
1	H	96	ASP	CA-C-N	6.66	126.10	118.85
1	H	96	ASP	C-N-CA	6.66	126.10	118.85
1	E	69	PRO	CA-C-O	-6.60	115.52	120.73
1	A	63	SER	N-CA-C	6.57	119.00	111.11
1	F	114	ASP	N-CA-C	6.49	119.48	107.99
1	E	64	GLN	N-CA-C	-6.31	97.36	110.80
1	H	145	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	G	65	LEU	N-CA-C	-6.30	99.73	109.24
1	E	67	ALA	N-CA-C	-6.28	105.52	113.43
1	E	69	PRO	O-C-N	6.27	124.10	121.15
1	E	72	GLU	N-CA-C	6.25	118.39	110.33
1	E	14	ILE	N-CA-C	-6.24	104.66	110.53
1	H	163	GLN	N-CA-CB	-6.20	100.98	110.16
1	G	62	THR	CB-CA-C	-6.19	103.60	111.22
1	B	175	LEU	N-CA-C	6.17	117.67	111.07
1	C	215	ARG	N-CA-C	-6.05	107.13	114.75
1	B	62	THR	N-CA-CB	-6.04	102.54	110.88
1	B	150	ALA	N-CA-C	-5.95	104.80	111.28
1	G	72	GLU	N-CA-C	5.92	117.53	110.19
1	A	163	GLN	N-CA-C	-5.90	104.76	111.14
1	G	190	VAL	N-CA-CB	-5.89	101.51	111.23
1	B	114	ASP	N-CA-C	-5.83	98.39	110.80
1	F	108	GLU	CB-CA-C	-5.82	100.14	109.69
1	C	163	GLN	N-CA-CB	-5.82	101.58	110.01
1	E	111	ALA	CA-C-N	5.78	127.06	119.84
1	E	111	ALA	C-N-CA	5.78	127.06	119.84
1	E	111	ALA	C-N-CD	-5.75	101.43	125.00
1	F	6	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	C	63	SER	N-CA-C	5.69	117.56	111.36
1	H	63	SER	N-CA-C	5.68	118.40	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	VAL	N-CA-CB	-5.67	101.87	111.23
1	H	69	PRO	CA-C-N	-5.59	114.50	120.03
1	H	69	PRO	C-N-CA	-5.59	114.50	120.03
1	F	96	ASP	CA-C-N	5.57	124.77	118.97
1	F	96	ASP	C-N-CA	5.57	124.77	118.97
1	A	195	VAL	N-CA-C	-5.47	105.78	111.58
1	B	4	GLN	N-CA-C	5.45	116.91	111.07
1	H	6	ARG	N-CA-C	5.38	118.16	110.68
1	F	103	VAL	N-CA-C	5.33	116.06	110.62
1	B	12	ARG	CG-CD-NE	-5.32	100.30	112.00
1	E	68	VAL	N-CA-C	5.31	113.20	108.63
1	G	201	PHE	N-CA-C	-5.31	106.39	112.92
1	G	143	LEU	CA-C-N	-5.29	114.51	119.85
1	G	143	LEU	C-N-CA	-5.29	114.51	119.85
1	C	131	ASP	CB-CA-C	-5.28	102.60	110.88
1	G	163	GLN	N-CA-CB	-5.26	102.39	110.12
1	D	96	ASP	CA-C-N	5.25	124.70	119.24
1	D	96	ASP	C-N-CA	5.25	124.70	119.24
1	A	108	GLU	CB-CA-C	-5.25	101.47	109.50
1	E	216	ARG	N-CA-C	-5.24	99.64	110.80
1	C	21	VAL	N-CA-C	5.23	115.44	110.42
1	G	145	ARG	CG-CD-NE	-5.15	100.67	112.00
1	C	168	ILE	N-CA-C	5.14	115.76	110.36
1	D	148	VAL	N-CA-CB	-5.12	103.58	110.54
1	A	25	LEU	CA-C-N	-5.11	115.51	121.85
1	A	25	LEU	C-N-CA	-5.11	115.51	121.85
1	E	32	ILE	CB-CA-C	5.11	119.03	112.14
1	A	63	SER	CB-CA-C	-5.08	102.68	110.81
1	A	62	THR	N-CA-CB	-5.04	102.99	110.61
1	E	43	LYS	CA-C-N	5.04	125.43	119.94
1	E	43	LYS	C-N-CA	5.04	125.43	119.94
1	E	24	GLU	N-CA-C	5.01	116.55	111.14
1	A	107	VAL	CA-C-N	5.01	127.99	120.83
1	A	107	VAL	C-N-CA	5.01	127.99	120.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	40	GLY	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	1709	0	1741	105	0
1	B	1709	0	1741	72	0
1	C	1634	0	1669	43	0
1	D	1702	0	1736	52	0
1	E	1643	0	1684	65	1
1	F	1701	0	1734	48	0
1	G	1643	0	1683	64	0
1	H	1620	0	1655	56	0
2	A	58	0	0	7	0
2	B	68	0	0	19	0
2	C	57	0	0	3	0
2	D	62	0	0	11	0
2	E	45	0	0	4	0
2	F	62	0	0	12	0
2	G	49	0	0	5	0
2	H	58	0	0	8	1
All	All	13820	0	13643	483	1

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 18.

All (483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:THR:HG22	1:H:55:GLN:NE2	1.07	1.38
1:A:111:ALA:HB3	1:A:114:ASP:CB	1.51	1.38
1:H:51:THR:CG2	1:H:55:GLN:NE2	1.91	1.34
1:B:35:ILE:HA	2:B:304:HOH:O	1.20	1.34
1:H:51:THR:CG2	1:H:55:GLN:HE22	1.44	1.24
1:G:64:GLN:OE1	1:G:102:SER:OG	1.56	1.23
1:D:62:THR:HG22	2:D:303:HOH:O	1.41	1.21
1:A:111:ALA:CA	1:A:114:ASP:HB2	1.71	1.20
1:B:64:GLN:HE22	1:B:217:ARG:NH2	1.41	1.18
1:B:172:HIS:HD2	2:B:306:HOH:O	1.26	1.18
1:A:31:THR:HG22	1:A:34:GLU:H	1.09	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLN:NE2	1:E:102:SER:OG	1.77	1.16
1:H:214:MET:O	1:H:215:ARG:HB3	1.45	1.16
1:A:111:ALA:HB3	1:A:114:ASP:CG	1.71	1.14
1:A:110:GLY:C	1:A:112:PRO:CD	2.21	1.13
1:G:6:ARG:HG2	1:G:6:ARG:HH11	1.15	1.12
1:A:111:ALA:N	1:A:114:ASP:HB2	1.64	1.11
1:D:122[A]:MET:HE1	1:D:156:VAL:HG11	1.31	1.11
1:B:31:THR:HG22	1:B:34:GLU:H	1.10	1.10
1:A:111:ALA:CB	1:A:114:ASP:CB	2.29	1.10
1:B:64:GLN:NE2	1:B:217:ARG:HH22	1.51	1.07
1:A:110:GLY:C	1:A:112:PRO:HD2	1.77	1.06
1:E:62:THR:HB	1:E:66:ARG:NH1	1.68	1.06
1:C:90:GLN:O	1:C:94:LYS:HG2	1.52	1.05
1:E:62:THR:HB	1:E:66:ARG:HH11	1.12	1.05
1:A:111:ALA:HB3	1:A:114:ASP:CA	1.85	1.04
1:B:64:GLN:NE2	1:B:217:ARG:NH2	2.05	1.03
1:A:111:ALA:CB	1:A:114:ASP:HB2	1.89	1.02
1:E:63:SER:O	1:E:64:GLN:C	1.96	1.01
1:A:111:ALA:CB	1:A:114:ASP:CG	2.34	0.99
1:E:63:SER:O	1:E:67:ALA:CB	2.10	0.99
1:H:145:ARG:NH1	1:H:145:ARG:HB3	1.78	0.98
1:A:110:GLY:CA	1:A:112:PRO:HD2	1.94	0.97
1:G:65:LEU:HD21	1:G:125:TRP:HA	1.47	0.97
1:A:31:THR:CG2	1:A:34:GLU:H	1.77	0.97
1:A:111:ALA:N	1:A:112:PRO:HD3	1.80	0.95
1:G:122:MET:HE1	1:G:156:VAL:HG11	1.47	0.94
1:H:214:MET:HA	1:H:214:MET:HE2	1.48	0.93
1:B:172:HIS:CD2	2:B:306:HOH:O	2.07	0.92
1:F:6:ARG:NH2	2:F:301:HOH:O	2.02	0.92
1:A:110:GLY:CA	1:A:112:PRO:CD	2.47	0.92
1:A:110:GLY:HA3	1:A:112:PRO:HD2	1.50	0.91
1:F:116:LEU:HD13	1:F:118:ARG:HG3	1.51	0.91
1:E:63:SER:O	1:E:67:ALA:HB2	1.69	0.90
1:A:62:THR:CG2	1:A:66:ARG:HH22	1.84	0.90
1:B:31:THR:CG2	1:B:34:GLU:H	1.86	0.87
1:A:111:ALA:N	1:A:112:PRO:CD	2.30	0.87
1:H:51:THR:HG22	1:H:55:GLN:CD	2.00	0.86
1:F:31:THR:HG22	1:F:34:GLU:H	1.41	0.86
1:G:62:THR:CG2	2:G:308:HOH:O	2.23	0.85
1:F:6:ARG:NE	2:F:301:HOH:O	1.90	0.85
1:A:64:GLN:NE2	1:A:217:ARG:HH22	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122[A]:MET:HE1	1:D:156:VAL:CG1	2.05	0.85
1:D:122[A]:MET:CE	1:D:156:VAL:HG11	2.06	0.85
1:C:38:ARG:HH11	1:C:38:ARG:CG	1.89	0.85
1:A:111:ALA:HB3	1:A:114:ASP:OD1	1.76	0.85
1:F:6:ARG:CZ	2:F:301:HOH:O	2.21	0.85
1:B:64:GLN:CD	1:B:217:ARG:HH22	1.85	0.85
1:A:31:THR:HG22	1:A:34:GLU:N	1.92	0.84
1:A:64:GLN:HE22	1:A:217:ARG:NH2	1.75	0.84
1:A:111:ALA:C	1:A:113:ALA:C	2.45	0.83
1:A:112:PRO:HA	1:A:114:ASP:N	1.93	0.83
1:B:62:THR:HG23	1:B:66:ARG:NH2	1.94	0.83
1:E:63:SER:O	1:E:64:GLN:O	1.97	0.83
1:A:78:LEU:HD13	1:A:187:MET:HE1	1.60	0.83
1:A:112:PRO:CA	1:A:114:ASP:N	2.42	0.83
1:D:74:GLN:CB	1:D:79:GLN:HB3	2.08	0.82
1:F:110:GLY:HA3	2:F:339:HOH:O	1.78	0.82
1:A:111:ALA:HB3	1:A:114:ASP:HA	1.60	0.82
1:A:112:PRO:HA	1:A:114:ASP:H	1.43	0.82
1:E:183[B]:HIS:CD2	2:E:323:HOH:O	2.32	0.82
1:B:62:THR:CG2	1:B:66:ARG:HH22	1.93	0.82
1:A:110:GLY:HA3	1:A:112:PRO:CD	2.09	0.81
1:A:110:GLY:C	1:A:112:PRO:HD3	2.02	0.81
1:A:112:PRO:N	1:A:114:ASP:N	2.29	0.81
1:H:38:ARG:HH11	1:H:38:ARG:CG	1.95	0.80
1:B:78:LEU:HD13	1:B:187:MET:HE1	1.61	0.80
1:C:38:ARG:HH11	1:C:38:ARG:HG2	1.44	0.80
1:E:38:ARG:HH11	1:E:38:ARG:HB3	1.46	0.80
1:H:145:ARG:CB	1:H:145:ARG:HH11	1.94	0.80
1:B:123:GLN:HG2	2:B:366:HOH:O	1.82	0.79
1:A:111:ALA:CB	1:A:114:ASP:OD1	2.29	0.79
1:G:6:ARG:HG2	1:G:6:ARG:NH1	1.88	0.79
1:A:111:ALA:C	1:A:114:ASP:HB2	2.07	0.79
1:H:145:ARG:NH1	1:H:145:ARG:CB	2.46	0.78
1:G:183[A]:HIS:CE1	1:G:187:MET:HE2	2.19	0.78
1:A:111:ALA:N	1:A:114:ASP:CB	2.47	0.78
1:D:73:GLU:O	1:D:74:GLN:CB	2.30	0.77
1:D:183:HIS:ND1	2:D:301:HOH:O	2.02	0.77
1:A:64:GLN:HE22	1:A:217:ARG:HH22	1.30	0.77
1:A:78:LEU:HD13	1:A:187:MET:CE	2.15	0.77
1:B:31:THR:HG22	1:B:34:GLU:N	1.94	0.77
1:B:166:SER:HB3	2:B:306:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:VAL:CG2	1:H:195:VAL:HG13	2.15	0.77
1:B:64:GLN:HE22	1:B:217:ARG:HH21	1.29	0.76
1:D:122[B]:MET:HE2	1:D:122[B]:MET:HA	1.67	0.76
1:A:111:ALA:H	1:A:114:ASP:HB2	1.50	0.76
1:F:78:LEU:HD13	1:F:187:MET:HE1	1.67	0.76
1:H:75:ARG:NH1	2:H:301:HOH:O	2.09	0.76
1:F:74:GLN:O	1:F:75:ARG:CB	2.30	0.75
1:A:62:THR:CG2	1:A:66:ARG:NH2	2.50	0.75
1:B:78:LEU:HD13	1:B:187:MET:CE	2.16	0.75
1:G:154:MET:HE3	1:G:186:LEU:HD22	1.69	0.75
1:A:111:ALA:O	1:A:113:ALA:C	2.30	0.74
1:D:154:MET:HE3	1:D:186:LEU:HD22	1.69	0.74
1:B:111:ALA:H	1:B:114:ASP:CB	1.99	0.74
1:A:110:GLY:CA	1:A:112:PRO:HD3	2.17	0.74
1:H:71:VAL:HG13	2:H:315:HOH:O	1.86	0.74
1:C:183:HIS:HD2	2:C:326:HOH:O	1.70	0.73
1:D:31:THR:HG22	1:D:34:GLU:H	1.51	0.73
1:A:6:ARG:NE	2:A:301:HOH:O	2.00	0.73
1:D:130:ARG:HH11	1:D:130:ARG:HG2	1.53	0.73
1:H:51:THR:CG2	1:H:55:GLN:CD	2.59	0.73
1:G:122:MET:CE	1:G:156:VAL:HG11	2.19	0.73
1:A:62:THR:HG23	1:A:66:ARG:NH2	2.03	0.73
1:F:62:THR:HG22	2:F:307:HOH:O	1.89	0.73
1:A:189:SER:OG	1:H:185:HIS:HD2	1.72	0.72
1:A:112:PRO:CA	1:A:113:ALA:C	2.62	0.72
1:C:10:THR:HA	1:C:13:THR:HG23	1.71	0.72
1:B:62:THR:HG23	1:B:66:ARG:HH22	1.52	0.72
1:H:189:SER:CB	2:H:302:HOH:O	2.37	0.72
1:E:63:SER:O	1:E:67:ALA:HB3	1.89	0.72
1:C:111:ALA:O	1:C:112:PRO:C	2.32	0.72
1:G:95:GLY:HA2	1:G:100:ARG:HD2	1.71	0.72
1:A:111:ALA:O	1:A:112:PRO:C	2.33	0.71
1:D:66:ARG:NH1	2:D:303:HOH:O	2.23	0.71
1:A:10:THR:HG22	1:A:223:ALA:H	1.53	0.71
1:F:31:THR:CG2	1:F:34:GLU:H	2.03	0.71
1:G:111:ALA:HB1	1:G:112:PRO:HD2	1.71	0.71
1:D:130:ARG:HD3	1:D:149:ASP:OD2	1.91	0.71
1:A:111:ALA:H	1:A:114:ASP:CB	2.04	0.70
1:F:154:MET:HE3	1:F:186:LEU:HD22	1.71	0.70
1:G:65:LEU:HD21	1:G:125:TRP:CA	2.21	0.70
1:D:38:ARG:HB2	1:D:38:ARG:HH11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLU:CD	2:C:307:HOH:O	2.33	0.70
1:F:130:ARG:NH1	1:F:131:ASP:OD1	2.24	0.70
1:G:11:ARG:NE	2:G:301:HOH:O	1.97	0.70
1:A:112:PRO:CA	1:A:114:ASP:H	2.01	0.69
1:A:218:GLU:O	1:A:218:GLU:CD	2.34	0.69
1:A:24:GLU:CD	1:A:38:ARG:HH22	2.01	0.69
1:E:215:ARG:O	1:E:216:ARG:HB2	1.92	0.69
1:E:211:ASP:O	1:E:215:ARG:HG2	1.93	0.69
1:B:62:THR:HG22	1:B:66:ARG:HH12	1.57	0.69
1:F:2:ALA:O	1:F:6:ARG:HG3	1.93	0.69
1:H:189:SER:OG	2:H:302:HOH:O	2.10	0.68
1:H:38:ARG:HH11	1:H:38:ARG:HG2	1.59	0.68
1:B:111:ALA:H	1:B:114:ASP:HB2	1.59	0.68
1:G:214:MET:HE2	1:G:214:MET:HA	1.74	0.68
1:E:111:ALA:HB1	1:E:112:PRO:HD2	1.77	0.67
1:E:183[A]:HIS:CE1	1:E:187:MET:HE2	2.28	0.67
1:A:112:PRO:N	1:A:114:ASP:HB2	2.09	0.67
1:F:38:ARG:HH11	1:F:38:ARG:HB2	1.60	0.67
1:B:224:ALA:HA	1:B:227:LEU:HD22	1.77	0.66
1:D:164:ILE:CD1	1:E:164:ILE:CD1	2.73	0.66
1:F:111:ALA:O	1:F:113:ALA:O	2.13	0.66
1:G:63:SER:O	1:G:65:LEU:N	2.29	0.65
1:E:62:THR:CG2	2:E:304:HOH:O	2.45	0.65
1:E:154:MET:HE3	1:E:186:LEU:HD22	1.79	0.65
1:F:78:LEU:HD13	1:F:187:MET:CE	2.25	0.65
1:H:10:THR:HA	1:H:13:THR:HG23	1.77	0.65
1:A:111:ALA:O	1:A:113:ALA:N	2.29	0.65
1:G:38:ARG:HH11	1:G:38:ARG:CG	2.09	0.65
1:B:189:SER:OG	1:C:185:HIS:HD2	1.80	0.65
1:D:31:THR:CG2	1:D:34:GLU:H	2.10	0.64
1:G:63:SER:C	1:G:65:LEU:N	2.53	0.64
1:D:145:ARG:HD3	2:D:360:HOH:O	1.97	0.64
1:G:65:LEU:CD2	1:G:125:TRP:HA	2.26	0.64
1:A:111:ALA:C	1:A:114:ASP:N	2.56	0.64
1:H:154:MET:HE3	1:H:186:LEU:HD22	1.80	0.64
1:A:10:THR:HG21	1:A:226:ASP:OD2	1.97	0.64
1:F:61:LEU:HA	1:F:102:SER:HB2	1.79	0.64
1:B:157:GLY:O	1:C:161:GLY:HA3	1.97	0.63
1:C:38:ARG:HG2	1:C:38:ARG:NH1	2.09	0.63
1:G:183[A]:HIS:HE1	1:G:187:MET:HE2	1.63	0.63
1:C:8:ALA:HA	2:C:352:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ARG:HD2	2:F:356:HOH:O	1.98	0.63
1:A:6:ARG:NH2	2:A:301:HOH:O	2.26	0.63
1:A:64:GLN:CD	1:A:217:ARG:HH22	2.06	0.63
1:A:154:MET:HE3	1:A:186:LEU:HD22	1.79	0.63
1:D:64:GLN:HG3	1:D:99:VAL:HG22	1.79	0.63
1:A:62:THR:HG22	1:A:66:ARG:HH12	1.64	0.62
1:A:64:GLN:NE2	1:A:217:ARG:NH2	2.40	0.62
1:E:95:GLY:HA2	1:E:100:ARG:HD2	1.82	0.62
1:B:114:ASP:O	1:B:116:LEU:N	2.30	0.62
1:B:166:SER:CB	2:B:306:HOH:O	2.44	0.62
1:C:54:GLU:OE1	1:C:115:GLY:O	2.18	0.61
1:E:46:LEU:C	1:E:46:LEU:HD23	2.24	0.61
1:B:111:ALA:HB1	1:B:112:PRO:HD2	1.81	0.61
1:B:154:MET:HE3	1:B:186:LEU:HD22	1.81	0.61
1:C:214:MET:O	1:C:215:ARG:HD3	2.00	0.61
1:D:78:LEU:HD13	1:D:187:MET:HE1	1.82	0.61
1:E:65:LEU:C	1:E:67:ALA:H	2.09	0.61
1:B:229:HIS:HE1	2:B:349:HOH:O	1.82	0.61
1:H:183:HIS:HD2	2:H:332:HOH:O	1.81	0.60
1:G:130:ARG:HG3	1:G:148:VAL:HG13	1.82	0.60
1:E:60:VAL:O	1:E:63:SER:HB3	2.01	0.60
1:G:41:VAL:HG13	1:G:45:ALA:HB3	1.84	0.60
1:H:183:HIS:CE1	1:H:187:MET:HE2	2.36	0.60
1:G:38:ARG:HH11	1:G:38:ARG:HG2	1.66	0.60
1:F:28:GLU:OE1	1:F:111:ALA:HB3	2.02	0.60
1:C:90:GLN:O	1:C:94:LYS:CG	2.40	0.59
1:E:134:ARG:NH1	1:E:137:GLU:HB3	2.17	0.59
1:E:192:VAL:CG2	1:E:195:VAL:HG13	2.31	0.59
1:H:196:LEU:HA	1:H:199:LEU:HD22	1.85	0.59
1:E:9:GLN:HG2	1:E:12:ARG:NH1	2.17	0.59
1:F:111:ALA:O	1:F:113:ALA:C	2.46	0.58
1:B:37:LYS:HE3	2:B:325:HOH:O	2.02	0.58
1:E:108:GLU:CG	1:E:108:GLU:O	2.50	0.58
1:G:63:SER:HB3	1:G:67:ALA:CB	2.33	0.58
1:B:111:ALA:HB3	1:B:114:ASP:HB2	1.85	0.58
1:E:203:ALA:O	1:E:207:ILE:HG23	2.03	0.58
1:F:104:ARG:O	1:F:108:GLU:HG3	2.02	0.58
1:G:38:ARG:HH11	1:G:38:ARG:HB3	1.67	0.58
1:F:183:HIS:ND1	2:F:303:HOH:O	2.24	0.58
1:E:38:ARG:HB3	1:E:38:ARG:NH1	2.18	0.58
1:A:111:ALA:HB2	1:A:114:ASP:CG	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:NH2	2:B:301:HOH:O	2.31	0.58
1:E:64:GLN:NE2	1:E:102:SER:HG	2.00	0.58
1:H:38:ARG:CG	1:H:38:ARG:NH1	2.62	0.57
1:C:50:PHE:HB3	1:C:55:GLN:CG	2.34	0.57
1:G:215:ARG:O	1:G:216:ARG:HG3	2.04	0.57
1:G:62:THR:HG21	2:G:308:HOH:O	1.95	0.57
1:A:189:SER:OG	1:H:185:HIS:CD2	2.57	0.57
1:D:130:ARG:CD	1:D:149:ASP:OD2	2.53	0.57
1:F:164:ILE:CD1	1:G:164:ILE:CD1	2.83	0.57
1:A:157:GLY:O	1:H:161:GLY:HA3	2.05	0.57
1:H:51:THR:H	1:H:55:GLN:NE2	2.02	0.57
1:A:215:ARG:O	1:A:216:ARG:CB	2.53	0.56
1:B:185:HIS:HE1	2:B:363:HOH:O	1.87	0.56
1:E:17:ALA:CB	1:E:39:SER:HB3	2.35	0.56
1:G:137:GLU:HB2	1:G:142:LEU:HD12	1.87	0.56
1:A:174:ASP:OD2	1:A:178:ARG:HD2	2.06	0.56
1:H:38:ARG:HH11	1:H:38:ARG:HG3	1.70	0.56
1:H:214:MET:HE2	1:H:214:MET:CA	2.29	0.56
1:C:41:VAL:HG13	1:C:42:THR:N	2.21	0.56
1:D:174:ASP:OD2	1:D:178:ARG:HD2	2.05	0.56
1:H:38:ARG:HG2	1:H:38:ARG:NH1	2.17	0.56
1:D:157:GLY:O	1:E:161:GLY:HA3	2.06	0.56
1:D:120:ALA:N	1:D:121:PRO:CD	2.68	0.56
1:H:192:VAL:HG22	1:H:195:VAL:HG13	1.88	0.56
1:B:24:GLU:OE2	1:B:38:ARG:NH2	2.39	0.56
1:E:38:ARG:HH11	1:E:38:ARG:CB	2.16	0.56
1:C:69:PRO:HG2	1:C:213:ALA:HB1	1.88	0.55
1:D:164:ILE:HD11	1:E:164:ILE:HD13	1.87	0.55
1:C:183:HIS:CE1	1:C:187:MET:HE2	2.42	0.55
1:B:62:THR:CG2	1:B:66:ARG:NH2	2.57	0.55
1:E:130:ARG:HG3	1:E:148:VAL:CG1	2.36	0.55
1:G:63:SER:O	1:G:64:GLN:C	2.48	0.55
1:G:63:SER:HB3	1:G:67:ALA:HB2	1.88	0.55
1:F:3:ARG:HB2	1:F:3:ARG:CZ	2.36	0.55
1:H:189:SER:HB3	2:H:302:HOH:O	2.03	0.55
1:H:68:VAL:HG13	1:H:87:LEU:HD23	1.89	0.54
1:B:111:ALA:O	1:B:112:PRO:C	2.50	0.54
1:A:62:THR:HG21	1:A:66:ARG:HH22	1.68	0.54
1:H:192:VAL:HG23	1:H:195:VAL:HG13	1.90	0.54
1:H:214:MET:O	1:H:215:ARG:CB	2.30	0.54
1:F:38:ARG:HB2	1:F:38:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:CD1	1:E:164:ILE:HD13	2.38	0.54
1:G:38:ARG:HH11	1:G:38:ARG:CB	2.21	0.54
1:H:214:MET:HA	1:H:214:MET:CE	2.30	0.54
1:B:11:ARG:NE	2:B:303:HOH:O	2.24	0.54
1:G:111:ALA:HB3	1:G:114:ASP:HB3	1.89	0.54
1:B:31:THR:HB	2:B:333:HOH:O	2.07	0.54
1:D:31:THR:HB	2:D:340:HOH:O	2.07	0.54
1:A:185:HIS:HD2	1:H:189:SER:OG	1.91	0.54
1:B:38:ARG:NE	2:B:301:HOH:O	2.04	0.53
1:D:104:ARG:HD3	1:E:109:PRO:HG2	1.89	0.53
1:G:192:VAL:CG2	1:G:195:VAL:HG13	2.37	0.53
1:A:123:GLN:HG2	2:A:355:HOH:O	2.07	0.53
1:D:130:ARG:HG2	1:D:130:ARG:NH1	2.23	0.53
1:A:111:ALA:CB	1:A:114:ASP:CA	2.73	0.53
1:A:183:HIS:ND1	2:A:303:HOH:O	2.19	0.53
1:D:42:THR:HA	1:D:228:GLU:HG2	1.90	0.53
1:F:66:ARG:NH1	2:F:307:HOH:O	2.41	0.53
1:F:157:GLY:O	1:G:161:GLY:HA3	2.09	0.53
1:G:10:THR:HG22	2:G:340:HOH:O	2.09	0.53
1:G:96:ASP:O	1:G:100:ARG:HG3	2.08	0.52
1:H:144:PRO:O	1:H:145:ARG:HG2	2.10	0.52
1:D:122[B]:MET:HA	1:D:122[B]:MET:CE	2.38	0.52
1:G:11:ARG:NH2	2:G:301:HOH:O	2.42	0.52
1:F:164:ILE:HD13	1:G:164:ILE:CD1	2.39	0.52
1:H:51:THR:HG23	1:H:55:GLN:NE2	2.11	0.52
1:B:94:LYS:HG3	1:B:210:TYR:OH	2.09	0.52
1:D:122[B]:MET:HE2	1:D:122[B]:MET:CA	2.36	0.52
1:A:74:GLN:NE2	1:A:205:ARG:NH2	2.58	0.52
1:C:68:VAL:HG13	1:C:87:LEU:HD23	1.92	0.52
1:C:154:MET:HE3	1:C:186:LEU:HD22	1.91	0.52
1:E:177:GLU:OE2	1:E:178:ARG:NH2	2.43	0.52
1:B:38:ARG:HB2	2:B:304:HOH:O	2.09	0.52
1:D:78:LEU:HD13	1:D:187:MET:CE	2.39	0.52
1:C:171:GLY:O	1:C:172:HIS:HB2	2.11	0.51
1:A:112:PRO:CD	1:A:114:ASP:HB2	2.40	0.51
1:E:192:VAL:HG22	1:E:195:VAL:HG13	1.91	0.51
1:B:31:THR:HG23	1:B:33:ALA:H	1.75	0.51
1:D:38:ARG:HB2	1:D:38:ARG:NH1	2.25	0.51
1:A:58:GLN:O	1:A:62:THR:HB	2.09	0.51
1:B:130:ARG:HG2	1:B:148:VAL:HG13	1.92	0.51
1:H:69:PRO:HG2	1:H:213:ALA:HB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ALA:H	1:B:114:ASP:HB3	1.75	0.51
1:E:64:GLN:O	1:E:67:ALA:HB3	2.11	0.51
1:F:3:ARG:NH1	1:F:3:ARG:HB3	2.26	0.51
1:B:113:ALA:C	1:B:115:GLY:N	2.68	0.51
1:C:214:MET:HA	1:C:214:MET:HE2	1.93	0.51
1:G:89:ALA:O	1:G:93:SER:HB2	2.10	0.51
1:H:139:GLY:HA3	2:H:320:HOH:O	2.11	0.50
1:A:112:PRO:N	1:A:114:ASP:CB	2.74	0.50
1:H:130:ARG:HE	1:H:134:ARG:NH2	2.10	0.50
1:E:108:GLU:O	1:E:108:GLU:HG2	2.11	0.50
1:F:3:ARG:CZ	1:F:3:ARG:CB	2.89	0.50
1:G:6:ARG:HH11	1:G:6:ARG:CG	2.03	0.50
1:A:61:LEU:HA	1:A:102:SER:HB2	1.93	0.50
1:B:24:GLU:CD	1:B:38:ARG:HH22	2.19	0.50
1:E:69:PRO:HG3	1:E:213:ALA:HB1	1.93	0.50
1:E:215:ARG:O	1:E:216:ARG:CB	2.59	0.50
1:A:111:ALA:HB2	1:A:114:ASP:OD1	2.10	0.50
1:B:114:ASP:O	1:B:114:ASP:OD2	2.30	0.50
1:B:218:GLU:OE1	1:B:218:GLU:O	2.30	0.50
1:C:111:ALA:O	1:C:112:PRO:O	2.30	0.50
1:F:164:ILE:CD1	1:G:164:ILE:HD13	2.42	0.50
1:H:171:GLY:O	1:H:172:HIS:HB2	2.10	0.50
1:A:13:THR:HG21	1:A:222:PRO:HG3	1.94	0.50
1:A:112:PRO:N	1:A:113:ALA:C	2.68	0.49
1:D:46:LEU:HD23	1:D:46:LEU:C	2.36	0.49
1:A:218:GLU:O	1:A:218:GLU:OE1	2.30	0.49
1:D:9:GLN:HG2	1:D:221:LEU:O	2.11	0.49
1:F:164:ILE:HD11	1:G:164:ILE:HD13	1.94	0.49
1:H:92:LEU:HD21	1:H:163:GLN:HG2	1.95	0.49
1:B:5:GLU:HG3	2:B:329:HOH:O	2.12	0.49
1:D:118:ARG:HD3	2:D:319:HOH:O	2.11	0.49
1:A:111:ALA:O	1:A:113:ALA:O	2.29	0.49
1:B:31:THR:HG23	1:B:33:ALA:N	2.27	0.49
1:A:11:ARG:NE	2:A:302:HOH:O	2.16	0.49
1:D:38:ARG:NH2	2:D:302:HOH:O	2.04	0.49
1:G:192:VAL:HG22	1:G:195:VAL:HG13	1.94	0.49
1:C:111:ALA:HB1	1:C:112:PRO:HD2	1.94	0.48
1:A:94:LYS:HG3	1:A:210:TYR:OH	2.14	0.48
1:H:118:ARG:NH2	2:H:304:HOH:O	2.30	0.48
1:D:32:ILE:HG12	2:D:333:HOH:O	2.13	0.48
1:G:62:THR:O	1:G:66:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG2	1:A:148:VAL:HG13	1.96	0.48
1:E:89:ALA:O	1:E:93:SER:HB2	2.13	0.48
1:A:6:ARG:CZ	2:A:301:HOH:O	2.44	0.48
1:B:144:PRO:O	1:B:145:ARG:HB2	2.14	0.48
1:G:85:THR:HG21	1:G:183[B]:HIS:CD2	2.49	0.48
1:B:62:THR:HG22	1:B:66:ARG:NH1	2.27	0.47
1:C:41:VAL:HG13	1:C:45:ALA:HB3	1.95	0.47
1:F:144:PRO:O	1:F:145:ARG:HB2	2.14	0.47
1:G:130:ARG:HG3	1:G:148:VAL:CG1	2.43	0.47
1:B:62:THR:HG21	1:B:66:ARG:HH22	1.78	0.47
1:E:62:THR:CB	1:E:66:ARG:NH1	2.60	0.47
1:E:110:GLY:O	1:E:111:ALA:C	2.55	0.47
1:A:104:ARG:O	1:A:108:GLU:HG3	2.15	0.47
1:E:130:ARG:HG3	1:E:148:VAL:HG13	1.96	0.47
1:G:214:MET:HE2	1:G:214:MET:CA	2.43	0.47
1:A:112:PRO:HD3	1:A:114:ASP:CB	2.44	0.47
1:G:69:PRO:HG3	1:G:213:ALA:HB1	1.96	0.47
1:A:2:ALA:O	1:A:6:ARG:HG3	2.15	0.47
1:E:65:LEU:N	1:E:65:LEU:HD23	2.29	0.47
1:H:88:LEU:HD13	1:H:159:PHE:CZ	2.50	0.47
1:C:50:PHE:HB3	1:C:55:GLN:HG2	1.96	0.47
1:E:41:VAL:HG13	1:E:45:ALA:HB3	1.96	0.47
1:E:90:GLN:OE1	1:E:94:LYS:HE2	2.15	0.47
1:B:58:GLN:O	1:B:62:THR:HB	2.15	0.46
1:D:164:ILE:HD13	1:E:164:ILE:CD1	2.44	0.46
1:B:35:ILE:CA	2:B:304:HOH:O	2.08	0.46
1:B:111:ALA:N	1:B:114:ASP:CB	2.74	0.46
1:B:215:ARG:O	1:B:216:ARG:CB	2.64	0.46
1:E:65:LEU:C	1:E:67:ALA:N	2.72	0.46
1:H:92:LEU:HD21	1:H:163:GLN:CG	2.45	0.46
1:B:120:ALA:HB3	1:B:121:PRO:HD3	1.96	0.46
1:A:112:PRO:HD3	1:A:114:ASP:HB2	1.96	0.46
1:G:65:LEU:HD23	1:G:125:TRP:CD1	2.51	0.46
1:B:2:ALA:HB3	2:B:329:HOH:O	2.15	0.46
1:B:189:SER:OG	1:C:185:HIS:CD2	2.65	0.46
1:C:32:ILE:HD11	1:C:53:LYS:N	2.30	0.46
1:G:62:THR:HB	1:G:66:ARG:HE	1.80	0.46
1:D:104:ARG:HD2	1:D:108:GLU:OE1	2.16	0.46
1:G:62:THR:O	1:G:62:THR:OG1	2.29	0.46
1:A:46:LEU:C	1:A:46:LEU:HD23	2.41	0.45
1:B:111:ALA:N	1:B:114:ASP:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:HE	1:C:134:ARG:NH2	2.14	0.45
1:D:177:GLU:HG2	2:D:355:HOH:O	2.16	0.45
1:A:74:GLN:NE2	1:A:205:ARG:HH22	2.14	0.45
1:C:130:ARG:HE	1:C:134:ARG:HH21	1.63	0.45
1:A:31:THR:HB	2:A:340:HOH:O	2.16	0.45
1:A:122:MET:HE2	1:A:122:MET:HA	1.99	0.45
1:B:154:MET:HE1	1:C:185:HIS:CD2	2.50	0.45
1:B:174:ASP:OD2	1:B:178:ARG:HD2	2.16	0.45
1:C:22:PHE:CE1	1:C:30:THR:HG21	2.51	0.45
1:G:63:SER:C	1:G:65:LEU:H	2.25	0.45
1:A:31:THR:HG23	1:A:33:ALA:H	1.81	0.45
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.75	0.45
1:B:46:LEU:C	1:B:46:LEU:HD23	2.42	0.45
1:E:183[A]:HIS:HE1	1:E:187:MET:HE2	1.80	0.45
1:A:111:ALA:CB	1:A:114:ASP:HA	2.39	0.45
1:E:96:ASP:O	1:E:100:ARG:HG3	2.17	0.44
1:B:54:GLU:HG3	1:B:116:LEU:HD23	2.00	0.44
1:D:3:ARG:CZ	1:D:3:ARG:HB3	2.47	0.44
1:E:63:SER:O	1:E:67:ALA:N	2.50	0.44
1:A:154:MET:HE1	1:H:185:HIS:CD2	2.51	0.44
1:C:23:ASP:OD2	1:C:100:ARG:HD3	2.18	0.44
1:F:62:THR:CG2	2:F:307:HOH:O	2.58	0.44
1:G:111:ALA:HB1	1:G:112:PRO:CD	2.46	0.44
1:C:5:GLU:O	1:C:5:GLU:HG3	2.16	0.44
1:C:41:VAL:CG1	1:C:42:THR:N	2.80	0.44
1:C:17:ALA:O	1:C:21:VAL:HG23	2.17	0.44
1:D:118:ARG:C	1:D:121:PRO:HD2	2.43	0.44
1:F:3:ARG:NH1	1:F:3:ARG:CB	2.80	0.44
1:F:112:PRO:HA	1:F:113:ALA:HA	1.57	0.44
1:A:31:THR:HG23	1:A:33:ALA:N	2.33	0.44
1:C:116:LEU:HD12	1:C:116:LEU:HA	1.84	0.44
1:D:118:ARG:O	1:D:121:PRO:HD2	2.17	0.44
1:E:62:THR:O	1:E:62:THR:OG1	2.29	0.44
1:E:146:LEU:HD13	1:E:190:VAL:HG22	2.00	0.44
1:G:38:ARG:HG2	1:G:38:ARG:NH1	2.31	0.44
1:D:11:ARG:NE	2:D:304:HOH:O	2.23	0.43
1:A:75:ARG:H	1:A:75:ARG:HG2	1.55	0.43
1:A:112:PRO:HA	1:A:113:ALA:HA	1.48	0.43
1:F:219:ALA:HA	1:F:220:PRO:HD3	1.78	0.43
1:F:229:HIS:HE1	2:F:353:HOH:O	2.00	0.43
1:C:14:ILE:HD11	1:C:41:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:HIS:HD2	1:E:189:SER:OG	2.01	0.43
1:E:214:MET:O	1:E:216:ARG:N	2.51	0.43
1:A:218:GLU:CD	1:A:218:GLU:C	2.87	0.43
1:G:178:ARG:HD3	1:G:178:ARG:HA	1.59	0.43
1:G:199:LEU:HA	1:G:199:LEU:HD23	1.76	0.43
1:A:62:THR:HG22	1:A:66:ARG:NH1	2.30	0.42
1:D:130:ARG:NH1	1:D:134:ARG:CZ	2.82	0.42
1:A:27:TYR:CD1	1:A:116:LEU:HD22	2.54	0.42
1:E:20:ALA:O	1:E:24:GLU:HG3	2.19	0.42
1:G:14:ILE:HD13	1:G:46:LEU:HA	2.01	0.42
1:D:212:GLU:HG3	1:D:216:ARG:NH1	2.35	0.42
1:B:62:THR:HG23	1:B:66:ARG:CZ	2.48	0.42
1:B:122:MET:HE2	1:B:122:MET:HA	2.00	0.42
1:E:21:VAL:HG22	1:E:38:ARG:HD3	2.02	0.42
1:E:171:GLY:O	1:E:172:HIS:HB2	2.19	0.42
1:A:185:HIS:CD2	1:H:189:SER:OG	2.71	0.42
1:C:96:ASP:HA	1:C:97:PRO:HD3	1.73	0.42
1:D:137:GLU:HB2	1:D:142:LEU:HD12	2.02	0.42
1:E:143:LEU:HD11	2:E:321:HOH:O	2.18	0.42
1:F:111:ALA:O	1:F:113:ALA:CA	2.68	0.42
1:E:214:MET:HE2	1:E:214:MET:HA	2.00	0.42
1:G:65:LEU:O	1:G:66:ARG:CB	2.66	0.42
1:H:92:LEU:CD2	1:H:163:GLN:HG2	2.49	0.41
1:E:51:THR:HG23	1:E:55:GLN:OE1	2.19	0.41
1:F:28:GLU:OE1	1:F:111:ALA:CB	2.67	0.41
1:F:58:GLN:O	1:F:62:THR:HB	2.20	0.41
1:G:46:LEU:CD1	1:G:46:LEU:C	2.93	0.41
1:C:36:LEU:HD21	1:C:46:LEU:HB2	2.01	0.41
1:E:111:ALA:CB	1:E:112:PRO:HD2	2.32	0.41
1:F:122:MET:CA	1:F:122:MET:HE3	2.51	0.41
1:C:47:TYR:HA	1:C:50:PHE:O	2.21	0.41
1:F:31:THR:HG22	1:F:34:GLU:CB	2.51	0.41
1:G:4:GLN:C	1:G:6:ARG:H	2.28	0.41
1:A:112:PRO:CD	1:A:114:ASP:CB	2.98	0.41
1:B:111:ALA:N	1:B:114:ASP:HB3	2.33	0.41
1:E:183[B]:HIS:HE1	2:E:324:HOH:O	2.02	0.41
1:H:17:ALA:O	1:H:21:VAL:HG23	2.20	0.41
1:H:146:LEU:HD11	1:H:190:VAL:HA	2.03	0.41
1:B:126:ILE:O	1:B:130:ARG:HB2	2.21	0.41
1:D:61:LEU:HA	1:D:102:SER:HB2	2.03	0.41
1:F:31:THR:HB	2:F:322:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:ARG:HD3	2:F:323:HOH:O	2.21	0.41
1:H:32:ILE:HD11	1:H:53:LYS:N	2.36	0.41
1:H:94:LYS:HE3	1:H:210:TYR:CE2	2.56	0.41
1:G:134:ARG:HA	1:G:134:ARG:HD2	1.81	0.41
1:H:130:ARG:HG3	1:H:148:VAL:HG13	2.02	0.41
1:G:34:GLU:OE2	1:G:38:ARG:HD2	2.20	0.41
1:G:146:LEU:HD13	1:G:190:VAL:HG22	2.03	0.41
1:D:183:HIS:CE1	2:D:301:HOH:O	2.60	0.41
1:F:9:GLN:HG3	1:F:221:LEU:O	2.21	0.41
1:A:126:ILE:O	1:A:130:ARG:HB2	2.20	0.41
1:G:6:ARG:HB2	1:G:9:GLN:HB2	2.02	0.41
1:B:32:ILE:HG12	2:B:343:HOH:O	2.20	0.40
1:A:9:GLN:HG2	1:A:221:LEU:O	2.20	0.40
1:H:116:LEU:HD12	1:H:116:LEU:HA	1.97	0.40
1:B:11:ARG:NH2	2:B:303:HOH:O	2.48	0.40
1:B:108:GLU:HA	1:B:109:PRO:HD3	1.91	0.40
1:F:98:LEU:HD12	1:F:217:ARG:HH12	1.86	0.40
1:C:38:ARG:CG	1:C:38:ARG:NH1	2.58	0.40
1:D:31:THR:HG23	1:D:33:ALA:N	2.36	0.40
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.91	0.40
1:F:64:GLN:OE1	1:F:217:ARG:NH2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ILE:CG2	2:H:352:HOH:O[2_645]	1.93	0.27

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	219/228 (96%)	211 (96%)	6 (3%)	2 (1%)	14	17
1	B	219/228 (96%)	212 (97%)	4 (2%)	3 (1%)	9	9
1	C	211/228 (92%)	199 (94%)	11 (5%)	1 (0%)	24	31
1	D	215/228 (94%)	209 (97%)	6 (3%)	0	100	100
1	E	212/228 (93%)	199 (94%)	11 (5%)	2 (1%)	14	17
1	F	218/228 (96%)	206 (94%)	11 (5%)	1 (0%)	24	31
1	G	212/228 (93%)	202 (95%)	8 (4%)	2 (1%)	14	17
1	H	209/228 (92%)	202 (97%)	7 (3%)	0	100	100
All	All	1715/1824 (94%)	1640 (96%)	64 (4%)	11 (1%)	21	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	B	112	PRO
1	B	216	ARG
1	C	112	PRO
1	E	112	PRO
1	E	216	ARG
1	B	115	GLY
1	F	75	ARG
1	G	64	GLN
1	G	112	PRO
1	A	112	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/182 (96%)	159 (91%)	16 (9%)	9	11
1	B	175/182 (96%)	157 (90%)	18 (10%)	7	8
1	C	170/182 (93%)	149 (88%)	21 (12%)	4	5
1	D	175/182 (96%)	158 (90%)	17 (10%)	8	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	171/182 (94%)	145 (85%)	26 (15%)	3	3
1	F	174/182 (96%)	157 (90%)	17 (10%)	7	10
1	G	171/182 (94%)	152 (89%)	19 (11%)	6	7
1	H	169/182 (93%)	145 (86%)	24 (14%)	3	3
All	All	1380/1456 (95%)	1222 (89%)	158 (11%)	5	6

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	10	THR
1	A	31	THR
1	A	62	THR
1	A	65	LEU
1	A	66	ARG
1	A	74	GLN
1	A	75	ARG
1	A	104	ARG
1	A	148	VAL
1	A	178	ARG
1	A	190	VAL
1	A	206	SER
1	A	211	ASP
1	A	212	GLU
1	A	218	GLU
1	H	6	ARG
1	H	9	GLN
1	H	13	THR
1	H	25	LEU
1	H	37	LYS
1	H	38	ARG
1	H	53	LYS
1	H	65	LEU
1	H	71	VAL
1	H	75	ARG
1	H	78	LEU
1	H	88	LEU
1	H	93	SER
1	H	98	LEU
1	H	100	ARG
1	H	145	ARG

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Mol	Chain	Res	Type
1	H	148	VAL
1	H	154	MET
1	H	163	GLN
1	H	190	VAL
1	H	195	VAL
1	H	199	LEU
1	H	212	GLU
1	H	215	ARG
1	B	4	GLN
1	B	31	THR
1	B	37	LYS
1	B	38	ARG
1	B	62	THR
1	B	65	LEU
1	B	66	ARG
1	B	74	GLN
1	B	104	ARG
1	B	116	LEU
1	B	122	MET
1	B	148	VAL
1	B	178	ARG
1	B	190	VAL
1	B	212	GLU
1	B	217	ARG
1	B	218	GLU
1	B	227	LEU
1	C	13	THR
1	C	25	LEU
1	C	38	ARG
1	C	41	VAL
1	C	55	GLN
1	C	66	ARG
1	C	71	VAL
1	C	75	ARG
1	C	78	LEU
1	C	88	LEU
1	C	92	LEU
1	C	94	LYS
1	C	100	ARG
1	C	126	ILE
1	C	146	LEU
1	C	148	VAL

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Mol	Chain	Res	Type
1	C	154	MET
1	C	190	VAL
1	C	212	GLU
1	C	215	ARG
1	C	216	ARG
1	D	3	ARG
1	D	4	GLN
1	D	31	THR
1	D	38	ARG
1	D	62	THR
1	D	66	ARG
1	D	88	LEU
1	D	100	ARG
1	D	104	ARG
1	D	148	VAL
1	D	153	ARG
1	D	178	ARG
1	D	181	ASP
1	D	183	HIS
1	D	190	VAL
1	D	216	ARG
1	D	217	ARG
1	E	25	LEU
1	E	32	ILE
1	E	37	LYS
1	E	38	ARG
1	E	41	VAL
1	E	63	SER
1	E	65	LEU
1	E	66	ARG
1	E	68	VAL
1	E	71	VAL
1	E	73	GLU
1	E	78	LEU
1	E	88	LEU
1	E	107	VAL
1	E	116	LEU
1	E	145	ARG
1	E	148	VAL
1	E	154	MET
1	E	176	LEU
1	E	190	VAL

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Mol	Chain	Res	Type
1	E	195	VAL
1	E	197	VAL
1	E	207	ILE
1	E	215	ARG
1	E	216	ARG
1	E	217	ARG
1	F	3	ARG
1	F	4	GLN
1	F	31	THR
1	F	38	ARG
1	F	62	THR
1	F	66	ARG
1	F	74	GLN
1	F	76	LEU
1	F	88	LEU
1	F	100	ARG
1	F	104	ARG
1	F	107	VAL
1	F	116	LEU
1	F	165	LEU
1	F	181	ASP
1	F	183	HIS
1	F	190	VAL
1	G	6	ARG
1	G	13	THR
1	G	25	LEU
1	G	32	ILE
1	G	37	LYS
1	G	38	ARG
1	G	46	LEU
1	G	65	LEU
1	G	66	ARG
1	G	73	GLU
1	G	78	LEU
1	G	88	LEU
1	G	108	GLU
1	G	134	ARG
1	G	148	VAL
1	G	154	MET
1	G	190	VAL
1	G	195	VAL
1	G	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	74	GLN
1	A	163	GLN
1	A	185	HIS
1	H	49	HIS
1	H	55	GLN
1	H	64	GLN
1	H	90	GLN
1	H	163	GLN
1	H	183	HIS
1	H	185	HIS
1	B	4	GLN
1	B	64	GLN
1	B	185	HIS
1	B	229	HIS
1	C	163	GLN
1	C	183	HIS
1	C	185	HIS
1	D	185	HIS
1	E	64	GLN
1	E	74	GLN
1	E	163	GLN
1	F	74	GLN
1	F	163	GLN
1	F	185	HIS
1	F	229	HIS
1	G	64	GLN
1	G	74	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	223/228 (97%)	-0.32	11 (4%) 35 36	15, 24, 62, 138	0
1	B	223/228 (97%)	-0.36	11 (4%) 35 36	13, 24, 62, 129	0
1	C	213/228 (93%)	-0.06	15 (7%) 22 24	16, 31, 78, 130	0
1	D	220/228 (96%)	-0.41	6 (2%) 56 58	14, 24, 56, 96	1 (0%)
1	E	213/228 (93%)	-0.05	18 (8%) 16 18	12, 28, 70, 100	1 (0%)
1	F	222/228 (97%)	-0.33	10 (4%) 38 40	14, 24, 62, 134	0
1	G	213/228 (93%)	-0.09	14 (6%) 24 26	12, 30, 69, 104	1 (0%)
1	H	211/228 (92%)	-0.08	13 (6%) 26 28	16, 32, 71, 98	0
All	All	1738/1824 (95%)	-0.22	98 (5%) 30 32	12, 26, 69, 138	3 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	111	ALA	9.8
1	G	112	PRO	8.5
1	E	66	ARG	7.8
1	A	75	ARG	7.1
1	E	64	GLN	6.9
1	F	111	ALA	6.6
1	H	113	ALA	6.6
1	B	113	ALA	6.5
1	D	67	ALA	6.5
1	F	112	PRO	6.3
1	E	65	LEU	6.2
1	F	74	GLN	6.1
1	D	73	GLU	5.9
1	A	112	PRO	5.9
1	F	73	GLU	5.9
1	E	63	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	55	GLN	5.7
1	B	112	PRO	5.7
1	A	113	ALA	5.4
1	C	4	GLN	5.1
1	A	74	GLN	5.1
1	E	72	GLU	5.1
1	A	114	ASP	5.0
1	G	5	GLU	4.9
1	B	73	GLU	4.9
1	B	111	ALA	4.5
1	E	112	PRO	4.4
1	G	64	GLN	4.4
1	H	8	ALA	4.3
1	A	73	GLU	4.2
1	E	217	ARG	4.2
1	D	229	HIS	4.0
1	C	110	GLY	3.9
1	C	113	ALA	3.9
1	E	113	ALA	3.9
1	G	4	GLN	3.8
1	H	110	GLY	3.8
1	C	5	GLU	3.7
1	A	115	GLY	3.6
1	B	75	ARG	3.6
1	G	66	ARG	3.6
1	A	111	ALA	3.6
1	C	111	ALA	3.6
1	E	7	ALA	3.5
1	E	6	ARG	3.5
1	E	5	GLU	3.5
1	H	215	ARG	3.4
1	G	65	LEU	3.4
1	E	215	ARG	3.4
1	G	110	GLY	3.4
1	E	111	ALA	3.3
1	B	115	GLY	3.3
1	H	111	ALA	3.2
1	G	113	ALA	3.2
1	G	40	GLY	3.2
1	D	75	ARG	3.2
1	A	229	HIS	3.2
1	H	112	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	229	HIS	3.1
1	G	7	ALA	3.1
1	F	113	ALA	3.0
1	B	110	GLY	2.9
1	C	216	ARG	2.8
1	E	67	ALA	2.8
1	G	216	ARG	2.8
1	B	114	ASP	2.8
1	B	74	GLN	2.8
1	H	6	ARG	2.8
1	C	6	ARG	2.8
1	C	215	ARG	2.8
1	D	74	GLN	2.7
1	G	6	ARG	2.7
1	C	7	ALA	2.7
1	C	51	THR	2.6
1	H	7	ALA	2.6
1	E	110	GLY	2.5
1	A	67	ALA	2.4
1	D	110	GLY	2.4
1	F	75	ARG	2.3
1	H	42	THR	2.3
1	E	62	THR	2.3
1	F	110	GLY	2.3
1	C	112	PRO	2.2
1	A	110	GLY	2.2
1	H	10	THR	2.2
1	C	12	ARG	2.2
1	C	43	LYS	2.1
1	F	114	ASP	2.1
1	E	212	GLU	2.1
1	H	114	ASP	2.1
1	B	229	HIS	2.1
1	B	67	ALA	2.0
1	H	9	GLN	2.0
1	G	215	ARG	2.0
1	H	115	GLY	2.0
1	F	218	GLU	2.0
1	C	8	ALA	2.0
1	E	8	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.