



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3BZE / pdb_00003bze
Title : The human non-classical major histocompatibility complex molecule HLA-E
Authors : Hoare, H.L.; Sullivan, L.C.; Ely, L.K.; Beddoe, T.; Henderson, K.N.; Lin, J.; Clements, C.S.; Reid, H.H.; Brooks, A.G.; Rossjohn, J.
Deposited on : 2008-01-17
Resolution : 2.50 Å(reported)

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

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

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

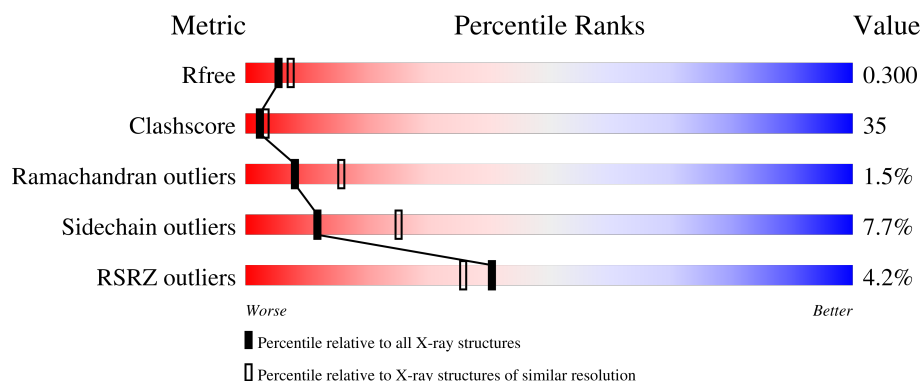
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	273	3% 59% 33% 7% .
1	C	273	8% 39% 45% 15% .
1	E	273	% 53% 37% 8% .
1	G	273	3% 56% 36% 7% .
2	B	100	67% 28% 5%

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Mol	Chain	Length	Quality of chain
2	D	100	
2	F	100	
2	H	100	
3	P	9	
3	Q	9	
3	R	9	
3	S	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12744 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			
1	C	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			
1	E	267	Total	C	N	O	S	0	0	0
			2187	1370	392	418	7			
1	G	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called leader peptide of HLA class I histocompatibility antigen, alpha chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			
3	Q	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			
3	R	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			
3	S	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			

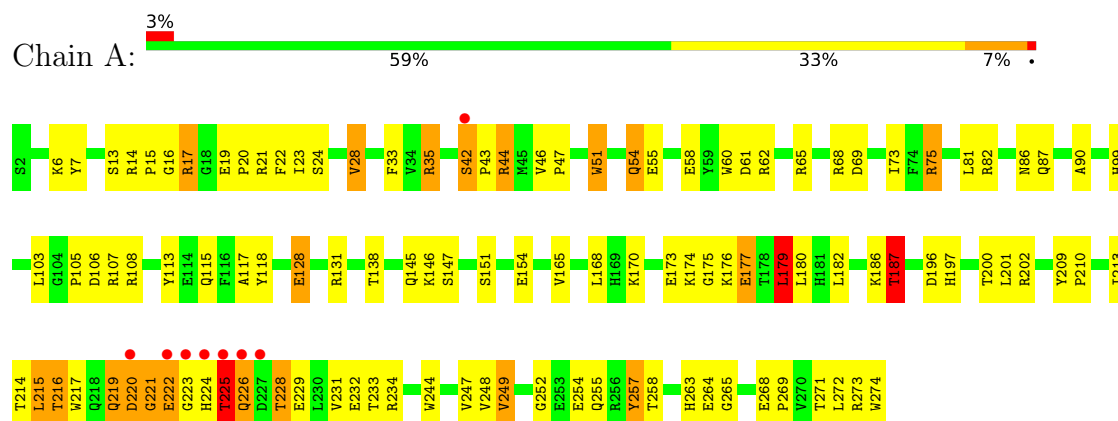
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	20	Total	O	0	0
			20	20		
4	C	48	Total	O	0	0
			48	48		
4	D	11	Total	O	0	0
			11	11		
4	E	20	Total	O	0	0
			20	20		
4	F	10	Total	O	0	0
			10	10		
4	G	44	Total	O	0	0
			44	44		
4	H	12	Total	O	0	0
			12	12		
4	P	3	Total	O	0	0
			3	3		
4	Q	1	Total	O	0	0
			1	1		
4	R	1	Total	O	0	0
			1	1		
4	S	1	Total	O	0	0
			1	1		

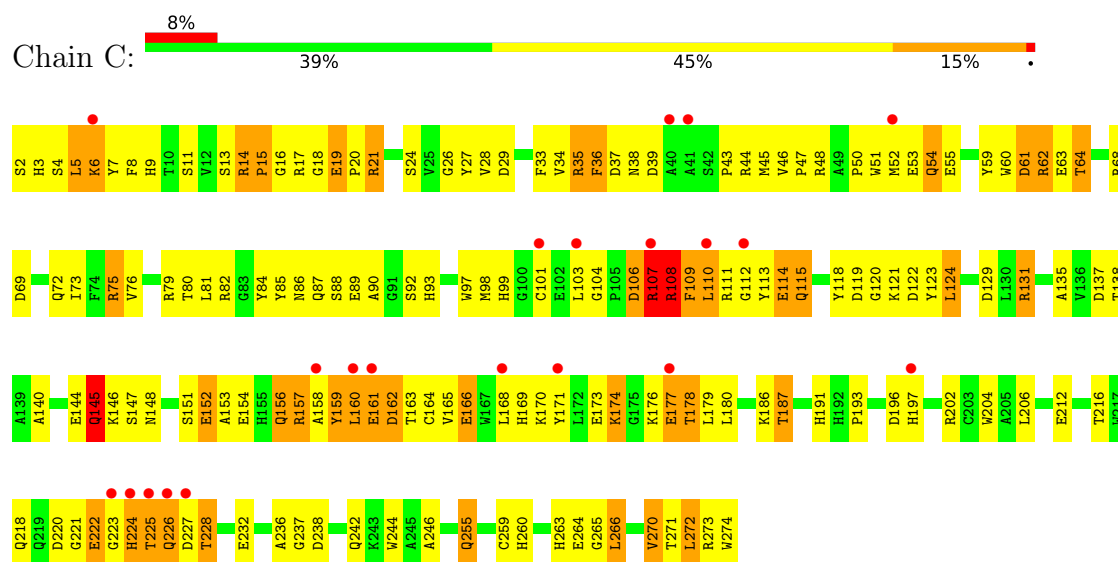
3 Residue-property plots [i](#)

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.

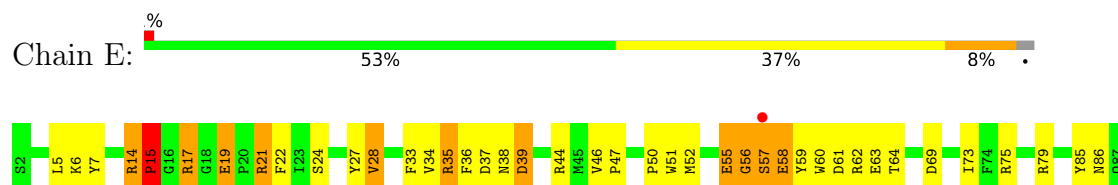
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

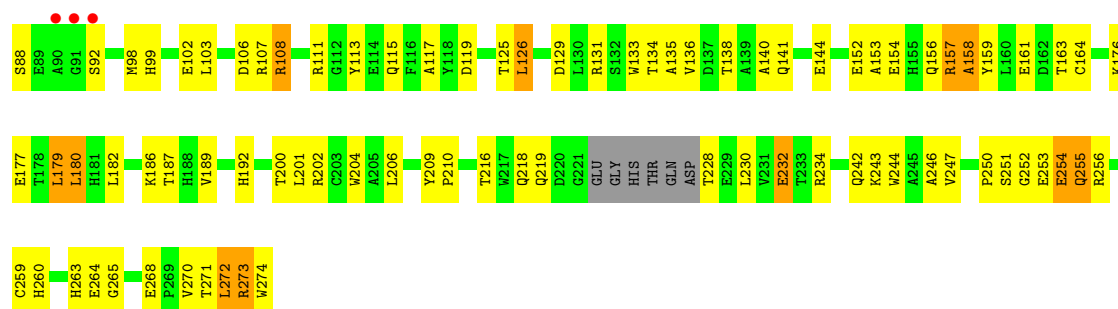


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

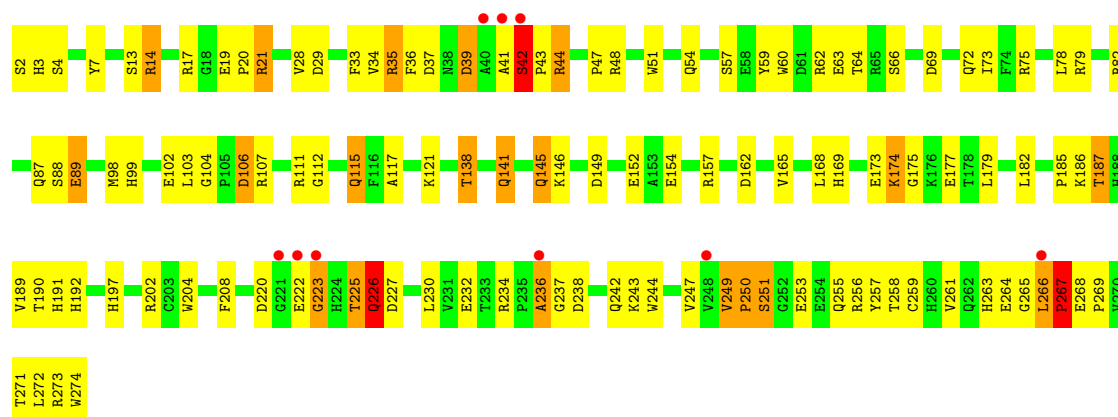


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E





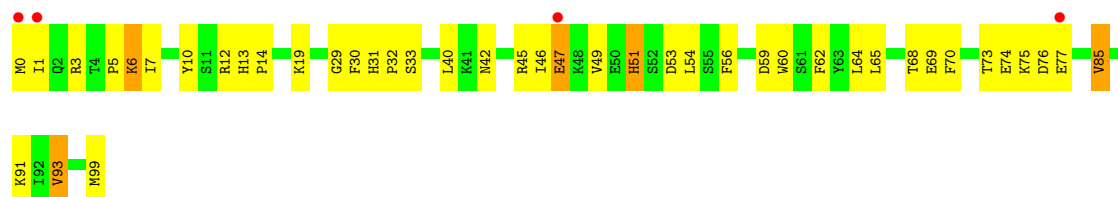
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 2: Beta-2-microglobulin

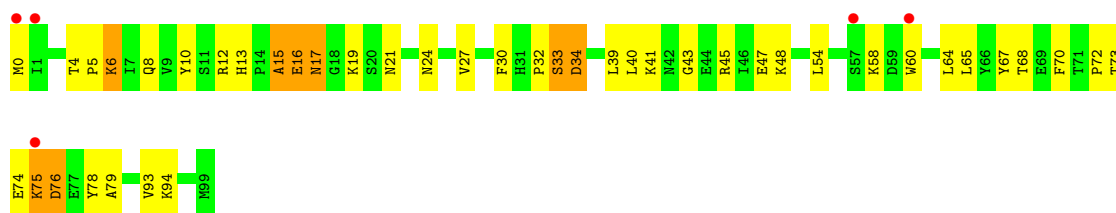


- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

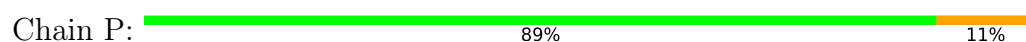




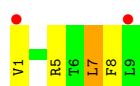
● Molecule 2: Beta-2-microglobulin



● Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



● Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



● Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



● Molecule 3: leader peptide of HLA class I histocompatibility antigen, alpha chain G



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.78Å 73.35Å 131.53Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.50) 98.1 (15.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.296 0.255 , 0.300	Depositor DCC
R_{free} test set	3195 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12744	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

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	0.86	10/2300 (0.4%)	1.32	29/3127 (0.9%)
1	C	0.69	6/2300 (0.3%)	1.25	24/3127 (0.8%)
1	E	0.64	5/2251 (0.2%)	1.13	20/3059 (0.7%)
1	G	0.73	5/2300 (0.2%)	1.23	26/3127 (0.8%)
2	B	0.55	0/860	0.94	2/1162 (0.2%)
2	D	0.49	0/860	0.96	4/1162 (0.3%)
2	F	0.80	3/860 (0.3%)	1.03	4/1162 (0.3%)
2	H	0.80	4/860 (0.5%)	1.05	4/1162 (0.3%)
3	P	0.73	0/74	1.03	1/98 (1.0%)
3	Q	0.62	0/74	1.22	2/98 (2.0%)
3	R	0.65	0/74	1.09	1/98 (1.0%)
3	S	0.71	0/74	1.25	1/98 (1.0%)
All	All	0.72	33/12887 (0.3%)	1.17	118/17480 (0.7%)

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	C	0	2
1	G	1	3
All	All	1	5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ARG	CA-C	-12.19	1.36	1.52
1	A	220	ASP	CA-C	-9.60	1.40	1.52
1	A	44	ARG	N-CA	-9.50	1.33	1.46
1	E	158	ALA	N-CA	-9.11	1.35	1.46
1	E	56	GLY	CA-C	-8.97	1.44	1.52
1	C	159	TYR	C-N	-8.52	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	15	ALA	N-CA	-8.47	1.35	1.46
1	G	226	GLN	N-CA	-8.28	1.34	1.45
1	A	220	ASP	N-CA	-7.78	1.36	1.46
1	G	220	ASP	N-CA	-7.58	1.36	1.46
1	E	157	ARG	CA-C	-7.35	1.43	1.52
1	G	234	ARG	C-N	7.19	1.42	1.33
1	G	227	ASP	C-N	-7.19	1.23	1.33
2	F	76	ASP	C-N	7.17	1.43	1.33
1	A	249	VAL	CA-CB	-7.03	1.45	1.54
1	A	219	GLN	CA-C	-7.02	1.43	1.52
1	C	61	ASP	C-N	-7.02	1.24	1.33
2	H	45	ARG	C-N	-6.32	1.26	1.33
2	H	46	ILE	N-CA	-6.18	1.38	1.46
2	H	77	GLU	C-N	-5.69	1.26	1.33
1	E	56	GLY	N-CA	-5.66	1.38	1.45
1	C	162	ASP	CA-C	-5.65	1.45	1.52
1	A	226	GLN	C-O	-5.52	1.19	1.23
1	G	267	PRO	C-N	5.46	1.39	1.33
1	A	249	VAL	N-CA	-5.42	1.40	1.46
1	A	215	LEU	N-CA	5.35	1.52	1.46
2	H	77	GLU	CA-C	-5.31	1.46	1.52
1	C	228	THR	CA-CB	-5.31	1.46	1.53
1	A	44	ARG	C-N	-5.26	1.26	1.33
1	E	57	SER	C-N	-5.22	1.26	1.33
1	C	160	LEU	CA-C	-5.06	1.46	1.52
2	F	75	LYS	N-CA	-5.05	1.39	1.46
1	C	160	LEU	N-CA	-5.02	1.40	1.46

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	234	ARG	O-C-N	-21.82	104.53	121.55
1	C	108	ARG	N-CA-C	19.42	134.29	110.41
1	A	219	GLN	CA-C-N	-18.13	86.91	121.54
1	A	219	GLN	C-N-CA	-18.13	86.91	121.54
1	C	110	LEU	N-CA-C	-17.98	90.65	113.12
1	C	107	ARG	N-CA-C	15.65	131.67	112.58
1	A	215	LEU	N-CA-CB	-15.20	85.15	110.68
1	A	220	ASP	CA-CB-CG	-14.80	97.80	112.60
1	E	273	ARG	CB-CA-C	13.84	137.96	110.42
1	C	228	THR	N-CA-CB	-12.61	89.56	110.37
1	G	234	ARG	CA-C-N	12.35	136.92	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	234	ARG	C-N-CA	12.35	136.92	120.25
1	A	219	GLN	OE1-CD-NE2	-10.72	111.88	122.60
1	A	214	THR	CB-CA-C	-10.61	94.76	110.24
1	E	156	GLN	OE1-CD-NE2	-10.56	112.04	122.60
1	G	226	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	C	109	PHE	N-CA-C	-9.66	90.23	110.80
1	E	158	ALA	N-CA-C	-9.54	95.72	111.37
1	E	56	GLY	N-CA-C	-9.53	100.98	111.93
1	E	254	GLU	N-CA-C	9.23	122.33	111.71
1	A	213	ILE	CA-C-N	-9.23	107.28	121.86
1	A	213	ILE	C-N-CA	-9.23	107.28	121.86
1	C	108	ARG	N-CA-CB	-9.13	97.87	110.38
1	A	222	GLU	CA-C-N	9.06	129.13	120.98
1	A	222	GLU	C-N-CA	9.06	129.13	120.98
1	A	44	ARG	N-CA-C	-8.96	91.71	110.80
2	D	47	GLU	CB-CA-C	8.61	128.95	110.19
1	G	42	SER	CB-CA-C	8.59	127.10	110.17
1	A	221	GLY	N-CA-C	-8.43	93.21	113.18
1	G	249	VAL	CB-CA-C	-8.36	96.14	111.36
1	G	115	GLN	N-CA-C	8.30	121.88	108.76
1	A	44	ARG	CA-C-N	-8.26	109.24	121.05
1	A	44	ARG	C-N-CA	-8.26	109.24	121.05
2	D	47	GLU	N-CA-C	-7.87	100.73	110.41
1	G	220	ASP	N-CA-C	7.80	127.41	110.80
1	G	249	VAL	CA-C-N	7.80	127.81	119.78
1	G	249	VAL	C-N-CA	7.80	127.81	119.78
2	H	33	SER	N-CA-C	7.69	119.44	111.14
1	E	55	GLU	CA-C-N	7.65	127.36	120.10
1	E	55	GLU	C-N-CA	7.65	127.36	120.10
1	C	107	ARG	CA-C-N	7.41	134.99	121.06
1	C	107	ARG	C-N-CA	7.41	134.99	121.06
1	A	219	GLN	CG-CD-NE2	7.33	127.40	116.40
1	C	114	GLU	CB-CA-C	7.31	122.61	110.03
1	G	223	GLY	O-C-N	-7.29	113.22	122.70
1	C	16	GLY	N-CA-C	7.29	121.46	112.64
1	E	273	ARG	N-CA-C	-7.26	95.33	110.80
1	A	220	ASP	N-CA-C	7.24	126.22	110.80
1	C	61	ASP	O-C-N	7.14	131.20	121.92
1	E	156	GLN	CG-CD-NE2	7.08	127.01	116.40
1	A	75	ARG	N-CA-C	-7.05	103.53	111.14
2	F	16	GLU	CB-CA-C	-7.03	101.76	111.95
1	G	223	GLY	N-CA-C	6.94	129.62	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	GLU	O-C-N	6.81	131.04	123.01
1	C	159	TYR	O-C-N	6.72	129.02	122.03
1	C	266	LEU	CA-C-N	6.71	126.21	119.24
1	C	266	LEU	C-N-CA	6.71	126.21	119.24
1	G	226	GLN	CG-CD-NE2	6.65	126.38	116.40
2	D	75	LYS	N-CA-C	6.60	119.81	111.69
1	A	228	THR	N-CA-CB	-6.54	100.38	110.85
1	E	46	VAL	CA-C-N	6.50	126.26	119.76
1	E	46	VAL	C-N-CA	6.50	126.26	119.76
3	P	8	PHE	N-CA-C	-6.41	98.09	108.41
1	G	226	GLN	CA-C-N	-6.35	114.33	122.77
1	G	226	GLN	C-N-CA	-6.35	114.33	122.77
1	G	44	ARG	N-CA-C	6.34	117.86	108.60
1	G	29	ASP	CB-CA-C	-6.32	108.64	117.23
1	A	147	SER	N-CA-C	6.30	118.23	111.36
1	G	220	ASP	CB-CA-C	-6.27	97.95	110.42
2	F	76	ASP	N-CA-C	6.26	120.09	110.20
1	A	186	LYS	N-CA-C	-6.25	99.08	109.46
1	G	267	PRO	O-C-N	-6.25	114.20	122.64
1	E	157	ARG	O-C-N	6.21	130.85	122.59
3	Q	7	LEU	N-CA-C	6.19	119.49	109.40
1	G	28	VAL	N-CA-C	-6.17	97.46	107.28
2	F	33	SER	N-CA-C	6.08	118.70	111.71
1	E	126	LEU	N-CA-C	-6.04	101.54	110.48
2	D	6	LYS	N-CA-C	-5.98	100.81	110.32
1	A	187	THR	N-CA-C	5.88	119.14	109.85
1	A	265	GLY	N-CA-C	5.82	121.07	114.67
1	E	28	VAL	N-CA-C	-5.79	98.08	107.28
1	E	115	GLN	N-CA-C	5.76	117.28	108.42
2	H	17	ASN	N-CA-C	5.71	122.97	110.80
1	A	42	SER	CB-CA-C	-5.69	98.95	110.17
2	B	6	LYS	N-CA-C	-5.69	101.21	110.20
1	G	226	GLN	CA-C-O	5.65	127.84	121.51
3	S	8	PHE	N-CA-C	-5.63	99.34	108.41
1	E	157	ARG	CA-C-O	5.56	128.46	120.51
2	B	67	TYR	N-CA-C	5.53	117.20	108.96
1	C	187	THR	N-CA-C	5.52	118.40	109.40
3	R	8	PHE	N-CA-C	-5.52	99.52	108.41
1	C	147	SER	N-CA-C	-5.52	105.17	112.34
1	E	186	LYS	N-CA-C	-5.51	100.20	108.96
1	C	61	ASP	CA-C-N	-5.48	112.87	120.38
1	C	61	ASP	C-N-CA	-5.48	112.87	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	N-CA-C	-5.47	98.01	106.72
1	G	250	PRO	CB-CA-C	-5.46	104.24	111.23
1	A	257	TYR	N-CA-C	5.41	117.72	108.90
2	F	6	LYS	N-CA-C	-5.37	101.78	110.32
2	H	6	LYS	N-CA-C	-5.36	101.79	110.32
1	C	27	TYR	N-CA-C	5.34	117.79	108.76
3	Q	8	PHE	N-CA-C	-5.28	99.91	108.41
1	C	29	ASP	CB-CA-C	-5.26	110.07	117.23
1	C	75	ARG	N-CA-C	-5.25	105.56	111.28
1	A	234	ARG	CA-C-N	5.22	126.03	120.13
1	A	234	ARG	C-N-CA	5.22	126.03	120.13
1	G	186	LYS	N-CA-C	-5.20	100.69	108.96
1	G	75	ARG	N-CA-C	-5.18	105.72	111.36
1	C	270	VAL	N-CA-C	5.13	116.69	108.89
1	A	223	GLY	N-CA-C	-5.11	103.00	110.97
1	G	266	LEU	C-N-CD	-5.07	104.23	125.00
1	E	75	ARG	N-CA-C	-5.06	105.77	111.28
1	C	64	THR	N-CA-C	-5.06	105.85	111.36
1	G	236	ALA	N-CA-C	-5.04	107.10	113.20
1	A	220	ASP	CB-CA-C	-5.03	100.41	110.42
1	E	79	ARG	N-CA-C	-5.02	105.50	110.97
1	C	156	GLN	N-CA-C	-5.01	106.01	111.82
2	H	44	GLU	O-C-N	-5.01	117.30	122.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	42	SER	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	ARG	Peptide
1	C	227	ASP	Mainchain
1	G	223	GLY	Peptide
1	G	226	GLN	Mainchain
1	G	267	PRO	Mainchain

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	2234	0	2072	124	0
1	C	2234	0	2066	298	2
1	E	2187	0	2035	115	0
1	G	2234	0	2072	134	1
2	B	837	0	803	46	2
2	D	837	0	803	47	0
2	F	837	0	803	52	0
2	H	837	0	803	76	0
3	P	73	0	83	1	0
3	Q	73	0	83	4	0
3	R	73	0	83	6	0
3	S	73	0	83	7	0
4	A	44	0	0	14	0
4	B	20	0	0	12	0
4	C	48	0	0	46	0
4	D	11	0	0	6	0
4	E	20	0	0	9	0
4	F	10	0	0	10	0
4	G	44	0	0	24	4
4	H	12	0	0	4	0
4	P	3	0	0	0	0
4	Q	1	0	0	2	0
4	R	1	0	0	4	0
4	S	1	0	0	0	0
All	All	12744	0	11789	863	5

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 35.

All (863) 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:C:223:GLY:HA2	1:C:224:HIS:CG	1.45	1.46
1:A:224:HIS:HB2	1:A:225:THR:CB	1.54	1.37
2:F:4:THR:HG23	4:F:107:HOH:O	1.21	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:VAL:CG1	1:G:250:PRO:HD2	1.55	1.33
1:G:89:GLU:H	1:G:89:GLU:CD	1.35	1.32
1:G:146:LYS:HE2	4:G:285:HOH:O	1.18	1.31
1:G:169:HIS:HD2	4:G:307:HOH:O	0.96	1.30
1:E:113:TYR:HE1	4:E:314:HOH:O	0.94	1.28
1:G:98:MET:HG3	4:G:297:HOH:O	1.15	1.27
1:C:129:ASP:OD2	1:C:131:ARG:HG3	1.14	1.27
2:H:47:GLU:CD	2:H:48:LYS:H	1.41	1.25
1:C:34:VAL:HB	1:C:45:MET:CE	1.68	1.23
1:A:187:THR:CG2	4:A:305:HOH:O	1.84	1.23
3:Q:7:LEU:HD12	4:Q:204:HOH:O	1.38	1.21
1:C:14:ARG:NH2	1:C:39:ASP:OD2	1.72	1.20
1:E:232:GLU:HG3	4:E:323:HOH:O	1.38	1.20
1:A:224:HIS:CB	1:A:225:THR:HB	1.72	1.20
1:G:89:GLU:N	1:G:89:GLU:OE2	1.74	1.20
1:C:34:VAL:CB	1:C:45:MET:HE2	1.72	1.20
2:H:47:GLU:OE1	2:H:48:LYS:N	1.73	1.19
1:G:141:GLN:CG	4:G:310:HOH:O	1.87	1.19
1:C:8:PHE:HE2	4:C:296:HOH:O	1.22	1.19
1:C:171:TYR:CD1	4:C:297:HOH:O	1.92	1.19
1:C:169:HIS:HA	4:C:298:HOH:O	1.37	1.18
1:C:55:GLU:HG2	1:C:174:LYS:NZ	1.59	1.18
1:A:17:ARG:HG3	4:A:297:HOH:O	1.45	1.17
2:F:5:PRO:HD2	4:F:107:HOH:O	1.44	1.15
1:C:223:GLY:CA	1:C:224:HIS:CG	2.30	1.14
1:G:249:VAL:CG1	1:G:250:PRO:CD	2.26	1.14
2:B:3:ARG:HD3	4:B:112:HOH:O	1.47	1.13
1:C:223:GLY:HA2	1:C:224:HIS:ND1	1.63	1.13
1:C:157:ARG:HH11	1:C:157:ARG:CB	1.60	1.12
1:A:128:GLU:HA	1:A:128:GLU:OE1	1.49	1.12
1:A:219:GLN:HG3	1:A:220:ASP:N	1.36	1.10
1:C:35:ARG:H	1:C:45:MET:HE3	1.14	1.10
1:C:226:GLN:HB3	4:C:295:HOH:O	1.48	1.10
1:C:6:LYS:HA	4:C:285:HOH:O	1.51	1.09
1:C:35:ARG:N	1:C:45:MET:CE	2.16	1.09
1:A:219:GLN:CG	1:A:220:ASP:N	2.13	1.08
1:G:141:GLN:N	4:G:293:HOH:O	1.84	1.08
1:C:129:ASP:OD2	1:C:131:ARG:CG	2.02	1.07
1:A:224:HIS:HB3	1:A:225:THR:HA	1.31	1.07
1:G:141:GLN:HG2	4:G:310:HOH:O	1.49	1.07
1:A:224:HIS:CB	1:A:225:THR:CB	2.30	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:THR:CG2	1:G:226:GLN:OE1	2.04	1.06
1:A:226:GLN:HB3	1:A:228:THR:OG1	1.57	1.05
1:C:153:ALA:N	4:C:310:HOH:O	1.89	1.04
1:C:171:TYR:HD1	4:C:297:HOH:O	1.27	1.04
2:H:51:HIS:NE2	4:H:107:HOH:O	1.90	1.04
1:G:157:ARG:NH1	4:G:281:HOH:O	1.90	1.04
1:A:86:ASN:HB2	4:C:294:HOH:O	1.59	1.02
1:G:89:GLU:CD	1:G:89:GLU:N	2.13	1.02
1:G:249:VAL:HG12	1:G:250:PRO:HD2	1.04	1.02
1:A:19:GLU:HA	1:A:75:ARG:HH21	1.18	1.02
1:G:236:ALA:O	2:H:12:ARG:HD3	1.59	1.02
1:G:249:VAL:HG12	1:G:250:PRO:CD	1.86	1.00
1:C:176:LYS:HG3	1:C:180:LEU:HD12	1.41	1.00
2:B:75:LYS:HB3	4:B:101:HOH:O	1.58	0.99
1:C:8:PHE:CE2	4:C:296:HOH:O	2.04	0.99
1:C:159:TYR:CD2	1:C:160:LEU:HD23	1.98	0.98
1:C:162:ASP:O	1:C:166:GLU:HG2	1.64	0.97
1:G:225:THR:HG22	1:G:226:GLN:OE1	1.61	0.97
1:C:157:ARG:HH11	1:C:157:ARG:CG	1.77	0.97
1:A:224:HIS:CB	1:A:225:THR:CA	2.42	0.97
1:C:85:TYR:CE2	4:C:313:HOH:O	2.16	0.97
1:C:87:GLN:NE2	1:C:93:HIS:CE1	2.32	0.96
1:A:224:HIS:HB3	1:A:225:THR:CA	1.94	0.96
2:B:73:THR:HG22	2:B:74:GLU:H	1.30	0.96
1:C:55:GLU:CG	1:C:174:LYS:NZ	2.30	0.95
1:C:85:TYR:HE2	4:C:313:HOH:O	1.47	0.95
1:A:219:GLN:CG	1:A:220:ASP:H	1.75	0.95
2:H:47:GLU:CG	2:H:48:LYS:H	1.79	0.95
1:E:218:GLN:HG3	1:E:260:HIS:NE2	1.82	0.94
2:H:47:GLU:CG	2:H:48:LYS:N	2.29	0.94
1:C:255:GLN:HB3	4:C:284:HOH:O	1.67	0.94
2:D:49:VAL:HG22	2:D:68:THR:HB	1.50	0.94
1:A:187:THR:HB	4:A:305:HOH:O	1.67	0.94
1:A:13:SER:HA	1:A:20:PRO:HB3	1.50	0.93
1:G:187:THR:HG22	1:G:204:TRP:O	1.68	0.93
1:C:43:PRO:HG2	4:C:309:HOH:O	1.66	0.93
2:D:19:LYS:CE	4:D:111:HOH:O	2.14	0.93
1:G:141:GLN:HB2	4:G:293:HOH:O	1.66	0.93
2:B:73:THR:HG22	2:B:74:GLU:N	1.80	0.93
1:G:141:GLN:HG3	4:G:310:HOH:O	1.52	0.93
1:C:2:SER:HA	1:C:103:LEU:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:LYS:NZ	2:F:76:ASP:OD2	2.02	0.93
1:G:249:VAL:HG13	1:G:250:PRO:HD2	1.49	0.93
1:E:274:TRP:HZ2	4:E:311:HOH:O	1.51	0.92
1:A:219:GLN:HG3	1:A:220:ASP:H	1.10	0.92
2:D:51:HIS:NE2	4:D:108:HOH:O	2.03	0.91
1:G:141:GLN:CB	4:G:293:HOH:O	2.18	0.91
1:C:34:VAL:HB	1:C:45:MET:HE2	0.92	0.91
1:A:138:THR:HG22	4:C:305:HOH:O	1.70	0.90
1:C:35:ARG:N	1:C:45:MET:HE1	1.85	0.90
1:C:92:SER:HB3	4:C:312:HOH:O	1.71	0.90
1:G:249:VAL:HG13	1:G:250:PRO:CD	1.99	0.90
1:G:169:HIS:CD2	4:G:307:HOH:O	1.81	0.90
1:C:153:ALA:HB3	4:C:310:HOH:O	1.70	0.89
1:C:54:GLN:NE2	1:C:55:GLU:HG2	1.88	0.89
1:A:19:GLU:CA	1:A:75:ARG:HH21	1.85	0.89
1:E:113:TYR:CE1	4:E:314:HOH:O	1.82	0.89
1:E:187:THR:HG21	1:E:272:LEU:HD21	1.56	0.88
1:G:268:GLU:HG2	4:G:303:HOH:O	1.71	0.88
1:C:35:ARG:N	1:C:45:MET:HE3	1.81	0.87
2:H:47:GLU:HG3	2:H:48:LYS:N	1.89	0.87
1:A:17:ARG:H	1:A:17:ARG:NH1	1.71	0.87
1:G:146:LYS:CE	4:G:285:HOH:O	1.88	0.87
1:C:51:TRP:HB2	1:C:174:LYS:O	1.75	0.87
1:A:106:ASP:O	1:A:107:ARG:HB2	1.73	0.86
1:A:43:PRO:O	1:A:44:ARG:HG2	1.74	0.86
1:C:159:TYR:CD2	1:C:160:LEU:CD2	2.58	0.86
1:C:162:ASP:O	1:C:166:GLU:CG	2.23	0.86
1:C:103:LEU:HD22	1:C:107:ARG:O	1.76	0.86
1:C:43:PRO:CG	4:C:309:HOH:O	2.21	0.86
1:C:104:GLY:HA3	1:C:110:LEU:HD13	1.58	0.86
1:E:180:LEU:CD2	1:E:180:LEU:N	2.38	0.85
1:E:17:ARG:HH11	1:E:17:ARG:N	1.73	0.85
1:C:162:ASP:O	1:C:166:GLU:CD	2.19	0.85
1:C:5:LEU:HG	1:C:5:LEU:O	1.73	0.85
1:G:152:GLU:OE2	3:S:5:ARG:NH1	2.09	0.85
2:D:19:LYS:HE2	4:D:111:HOH:O	1.73	0.84
1:A:128:GLU:OE1	1:A:128:GLU:CA	2.24	0.84
1:C:226:GLN:OE1	4:C:295:HOH:O	1.94	0.84
1:G:202:ARG:HH12	2:H:99:MET:HE3	1.42	0.84
1:C:153:ALA:CA	4:C:310:HOH:O	2.22	0.84
1:G:66:SER:HB3	3:S:2:MET:HE2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:O	1:A:44:ARG:CG	2.27	0.83
1:E:157:ARG:O	1:E:158:ALA:C	2.18	0.83
1:C:157:ARG:CB	1:C:157:ARG:NH1	2.42	0.82
2:D:51:HIS:CE1	4:D:108:HOH:O	2.31	0.82
1:E:230:LEU:HD11	1:E:243:LYS:HE3	1.61	0.82
1:C:6:LYS:HB2	1:C:99:HIS:O	1.80	0.82
1:C:35:ARG:H	1:C:45:MET:CE	1.80	0.82
1:A:17:ARG:H	1:A:17:ARG:HH11	1.23	0.82
1:C:159:TYR:HD2	1:C:160:LEU:CD2	1.93	0.82
1:C:169:HIS:NE2	1:C:170:LYS:HG3	1.95	0.82
2:F:41:LYS:C	2:F:43:GLY:H	1.84	0.81
2:H:98:ASP:O	2:H:99:MET:CG	2.29	0.81
1:C:104:GLY:HA2	1:C:110:LEU:HD22	1.63	0.81
1:C:157:ARG:HH11	1:C:157:ARG:HB3	1.46	0.80
1:C:106:ASP:OD2	1:C:108:ARG:CD	2.30	0.80
2:B:75:LYS:CB	4:B:101:HOH:O	2.23	0.80
1:C:6:LYS:CD	1:C:113:TYR:OH	2.29	0.80
1:A:224:HIS:CA	1:A:225:THR:HG22	2.07	0.80
2:B:73:THR:CG2	2:B:74:GLU:H	1.95	0.80
1:E:263:HIS:CD2	1:E:265:GLY:H	1.98	0.79
1:C:55:GLU:CD	1:C:174:LYS:NZ	2.41	0.79
1:A:224:HIS:HB2	1:A:225:THR:HB	0.81	0.79
2:B:32:PRO:HB2	4:B:115:HOH:O	1.82	0.79
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.18	0.79
1:C:157:ARG:O	1:C:161:GLU:HB2	1.83	0.78
2:B:17:ASN:ND2	2:B:74:GLU:HG3	1.98	0.78
1:C:159:TYR:CE2	1:C:160:LEU:HD23	2.19	0.78
3:R:5:ARG:CA	4:R:181:HOH:O	2.29	0.78
1:C:111:ARG:HH12	1:C:113:TYR:HB3	1.49	0.78
1:C:6:LYS:HG3	4:C:296:HOH:O	1.84	0.78
1:A:62:ARG:NH1	4:A:311:HOH:O	1.91	0.77
2:H:45:ARG:HG2	2:H:45:ARG:HH11	1.49	0.77
2:H:47:GLU:CD	2:H:48:LYS:N	2.26	0.77
1:C:14:ARG:HH22	1:C:39:ASP:CG	1.91	0.77
3:R:5:ARG:N	4:R:181:HOH:O	2.18	0.77
1:C:263:HIS:CD2	1:C:265:GLY:H	2.03	0.77
2:F:4:THR:HA	4:F:107:HOH:O	1.85	0.77
1:A:224:HIS:C	1:A:225:THR:HG22	2.10	0.76
1:C:255:GLN:CB	4:C:284:HOH:O	2.27	0.76
2:H:40:LEU:HD11	2:H:81:ARG:HH21	1.51	0.76
2:B:73:THR:CG2	2:B:74:GLU:N	2.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:THR:CG2	2:B:75:LYS:HG2	2.15	0.75
2:B:73:THR:HG21	2:B:75:LYS:HG2	1.67	0.75
1:C:111:ARG:HG2	1:C:112:GLY:H	1.52	0.75
1:C:111:ARG:HD3	4:C:307:HOH:O	1.85	0.74
1:C:43:PRO:CD	4:C:309:HOH:O	2.34	0.74
1:C:55:GLU:HB2	1:C:60:TRP:HE1	1.52	0.74
1:C:98:MET:HE2	2:D:60:TRP:CZ3	2.22	0.74
1:C:157:ARG:CG	1:C:157:ARG:NH1	2.44	0.74
1:C:169:HIS:O	1:C:173:GLU:HG2	1.88	0.74
1:G:17:ARG:HD3	4:G:305:HOH:O	1.88	0.74
1:C:106:ASP:OD2	1:C:108:ARG:HD2	1.88	0.73
1:E:180:LEU:N	1:E:180:LEU:HD23	2.03	0.73
1:A:176:LYS:HG3	1:A:180:LEU:HD12	1.70	0.73
1:G:141:GLN:CA	4:G:293:HOH:O	2.30	0.73
1:A:7:TYR:HB2	1:A:99:HIS:CE1	2.24	0.73
1:E:129:ASP:O	1:E:131:ARG:HG3	1.89	0.73
1:C:34:VAL:CG2	1:C:45:MET:HE2	2.19	0.73
1:C:7:TYR:HD1	1:C:99:HIS:HE1	1.35	0.73
1:G:102:GLU:OE1	1:G:111:ARG:NH2	2.19	0.73
1:G:225:THR:CB	1:G:226:GLN:OE1	2.37	0.73
1:C:6:LYS:HD3	1:C:113:TYR:OH	1.88	0.73
1:E:274:TRP:CZ2	4:E:311:HOH:O	2.33	0.72
2:B:73:THR:HG21	2:B:75:LYS:CG	2.18	0.72
2:H:42:ASN:HD21	2:H:76:ASP:HA	1.53	0.72
2:H:58:LYS:HE3	4:H:109:HOH:O	1.89	0.72
1:C:44:ARG:CD	4:C:300:HOH:O	2.38	0.72
1:C:47:PRO:HG3	1:C:60:TRP:CZ2	2.25	0.72
1:C:87:GLN:HE22	1:C:93:HIS:CE1	2.08	0.72
1:C:48:ARG:NE	2:D:53:ASP:OD2	2.23	0.72
1:E:17:ARG:HH11	1:E:17:ARG:H	1.38	0.71
1:G:44:ARG:HB2	1:G:64:THR:OG1	1.89	0.71
1:G:21:ARG:HE	1:G:39:ASP:HB2	1.55	0.71
2:B:73:THR:HG22	2:B:75:LYS:H	1.55	0.71
1:C:104:GLY:HA3	4:C:275:HOH:O	1.89	0.71
1:C:103:LEU:HD21	1:C:165:VAL:HG13	1.73	0.71
1:C:113:TYR:O	1:C:114:GLU:HB2	1.89	0.71
1:C:129:ASP:CG	1:C:131:ARG:HG3	2.11	0.71
2:F:4:THR:CA	4:F:107:HOH:O	2.38	0.70
1:G:197:HIS:C	1:G:251:SER:OG	2.34	0.70
1:C:80:THR:HG22	1:C:84:TYR:CE2	2.27	0.70
1:G:250:PRO:HG2	1:G:253:GLU:OE1	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:LEU:O	1:G:268:GLU:N	2.24	0.70
1:G:225:THR:HB	1:G:226:GLN:OE1	1.91	0.70
2:H:70:PHE:HD2	2:H:78:TYR:CE2	2.08	0.70
1:A:19:GLU:HA	1:A:75:ARG:NH2	2.02	0.70
1:A:106:ASP:OD2	1:A:108:ARG:HB3	1.91	0.70
2:F:45:ARG:NH1	2:F:47:GLU:HG2	2.06	0.70
1:C:157:ARG:HH11	1:C:157:ARG:HG2	1.56	0.69
2:B:89:GLN:O	4:B:106:HOH:O	2.09	0.69
1:C:156:GLN:O	1:C:160:LEU:HG	1.92	0.69
1:E:22:PHE:HB3	1:E:38:ASN:ND2	2.07	0.69
1:A:17:ARG:HH11	1:A:17:ARG:N	1.90	0.69
1:C:103:LEU:HG	1:C:168:LEU:HD23	1.75	0.69
1:C:137:ASP:OD1	1:C:138:THR:N	2.25	0.69
1:G:17:ARG:CD	4:G:305:HOH:O	2.41	0.69
1:E:129:ASP:OD2	1:E:131:ARG:HB2	1.93	0.69
1:E:202:ARG:HG3	1:E:202:ARG:HH11	1.58	0.69
1:E:202:ARG:HD2	1:E:204:TRP:CZ2	2.28	0.68
1:G:249:VAL:HG13	1:G:250:PRO:HD3	1.74	0.68
1:C:223:GLY:HA2	1:C:224:HIS:CB	2.04	0.68
1:E:263:HIS:HD2	1:E:265:GLY:H	1.41	0.68
1:G:138:THR:O	4:G:293:HOH:O	2.10	0.68
1:G:98:MET:HE2	2:H:56:PHE:HE1	1.58	0.68
1:C:157:ARG:NH1	1:C:157:ARG:HG2	2.07	0.68
1:C:34:VAL:CB	1:C:45:MET:CE	2.51	0.68
1:C:62:ARG:HH11	1:C:62:ARG:HB3	1.59	0.68
2:F:75:LYS:HG3	2:F:76:ASP:OD2	1.94	0.68
1:C:35:ARG:O	1:C:45:MET:HE3	1.94	0.67
2:H:40:LEU:O	2:H:78:TYR:HD1	1.78	0.67
2:H:41:LYS:HG3	2:H:78:TYR:CE1	2.30	0.67
1:C:108:ARG:O	1:C:110:LEU:N	2.27	0.67
1:E:47:PRO:HG3	1:E:60:TRP:CZ2	2.30	0.67
1:E:206:LEU:HD23	1:E:242:GLN:HB2	1.77	0.67
4:C:301:HOH:O	2:D:32:PRO:HB2	1.93	0.67
2:H:40:LEU:CD1	2:H:81:ARG:HH21	2.07	0.67
1:G:106:ASP:O	1:G:107:ARG:HB2	1.93	0.67
2:H:98:ASP:O	2:H:99:MET:HG3	1.94	0.67
1:C:111:ARG:HG2	1:C:112:GLY:N	2.10	0.67
1:C:236:ALA:O	2:D:12:ARG:HD3	1.95	0.67
1:G:13:SER:HA	1:G:20:PRO:HB3	1.77	0.66
1:C:165:VAL:HB	1:C:166:GLU:OE2	1.96	0.66
1:A:6:LYS:HD3	1:A:113:TYR:OH	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NE	4:A:279:HOH:O	2.21	0.66
1:A:187:THR:HG21	4:A:305:HOH:O	1.69	0.66
2:H:98:ASP:O	2:H:99:MET:HG2	1.96	0.66
1:A:42:SER:O	1:A:43:PRO:C	2.37	0.66
2:H:39:LEU:O	2:H:40:LEU:HD23	1.96	0.66
1:C:223:GLY:CA	1:C:224:HIS:ND1	2.49	0.65
1:C:232:GLU:OE1	2:D:6:LYS:HE3	1.97	0.65
1:E:103:LEU:HD22	1:E:107:ARG:O	1.97	0.65
1:C:135:ALA:HB2	1:C:144:GLU:HB2	1.78	0.65
1:C:44:ARG:HD3	4:C:300:HOH:O	1.97	0.65
2:B:32:PRO:CB	4:B:115:HOH:O	2.42	0.65
1:C:224:HIS:C	1:C:226:GLN:H	2.03	0.65
1:G:185:PRO:HD2	1:G:266:LEU:HG	1.79	0.65
1:C:11:SER:HA	1:C:21:ARG:O	1.97	0.64
2:B:75:LYS:CA	4:B:101:HOH:O	2.45	0.64
1:C:98:MET:O	1:C:114:GLU:HA	1.97	0.64
2:B:39:LEU:HD12	2:B:68:THR:HG22	1.78	0.64
1:C:44:ARG:HD2	4:C:300:HOH:O	1.96	0.64
2:H:98:ASP:C	2:H:99:MET:HG3	2.22	0.64
1:A:106:ASP:OD2	1:A:108:ARG:CB	2.46	0.64
1:A:224:HIS:HB2	1:A:225:THR:CG2	2.25	0.64
2:F:41:LYS:C	2:F:43:GLY:N	2.50	0.64
1:G:267:PRO:HG2	4:G:303:HOH:O	1.98	0.64
1:A:176:LYS:N	1:A:177:GLU:OE1	2.31	0.64
1:G:226:GLN:NE2	1:G:257:TYR:HE2	1.96	0.64
1:G:253:GLU:HB3	1:G:256:ARG:HD2	1.80	0.64
1:C:5:LEU:HD23	1:C:101:CYS:SG	2.37	0.63
1:C:48:ARG:CZ	2:D:53:ASP:OD2	2.47	0.63
2:H:41:LYS:HB2	2:H:78:TYR:HE1	1.62	0.63
1:C:273:ARG:O	1:C:274:TRP:HB3	1.99	0.63
1:E:106:ASP:OD2	1:E:108:ARG:HG3	1.97	0.63
2:F:73:THR:HG21	2:F:75:LYS:HE3	1.80	0.63
1:A:15:PRO:HG2	1:A:90:ALA:O	1.98	0.63
1:C:228:THR:HA	1:C:246:ALA:O	1.99	0.63
2:F:4:THR:CG2	4:F:107:HOH:O	1.98	0.63
1:C:223:GLY:CA	1:C:224:HIS:CD2	2.82	0.63
1:E:180:LEU:N	1:E:180:LEU:HD22	2.12	0.62
1:C:60:TRP:O	1:C:64:THR:OG1	2.16	0.62
1:C:187:THR:HG22	1:C:272:LEU:HG	1.80	0.62
1:A:187:THR:HG22	4:A:305:HOH:O	1.73	0.62
1:A:210:PRO:O	1:A:263:HIS:HE1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:OD1	1:A:86:ASN:O	2.18	0.62
1:G:247:VAL:O	1:G:249:VAL:HG23	1.99	0.62
1:A:219:GLN:HB3	1:A:257:TYR:CE2	2.35	0.62
1:C:108:ARG:O	1:C:109:PHE:C	2.42	0.62
1:C:129:ASP:CG	1:C:131:ARG:CG	2.70	0.62
1:G:88:SER:N	4:G:309:HOH:O	1.87	0.61
1:C:159:TYR:O	1:C:164:CYS:HB2	2.00	0.61
2:H:40:LEU:HD11	2:H:81:ARG:NH2	2.15	0.61
2:B:75:LYS:HA	4:B:101:HOH:O	2.00	0.61
1:C:218:GLN:NE2	1:C:221:GLY:O	2.33	0.61
1:A:197:HIS:CD2	1:G:42:SER:OG	2.54	0.61
2:B:74:GLU:HG2	4:B:117:HOH:O	1.99	0.61
1:C:13:SER:HA	1:C:20:PRO:HB3	1.81	0.61
1:C:112:GLY:N	4:C:278:HOH:O	2.34	0.61
1:C:35:ARG:CA	1:C:45:MET:HE1	2.29	0.61
2:F:4:THR:CB	4:F:107:HOH:O	2.42	0.61
1:G:89:GLU:OE2	1:G:89:GLU:CA	2.47	0.61
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.35	0.61
1:C:28:VAL:HG21	1:C:51:TRP:HH2	1.63	0.61
2:D:73:THR:HG22	2:D:74:GLU:N	2.15	0.61
1:C:48:ARG:NH2	2:D:53:ASP:OD2	2.33	0.61
1:E:133:TRP:NE1	1:E:153:ALA:HB2	2.16	0.61
1:A:14:ARG:HH11	1:A:21:ARG:HB2	1.66	0.60
1:C:24:SER:O	1:C:35:ARG:HA	2.01	0.60
1:G:182:LEU:HD13	1:G:264:GLU:HG2	1.82	0.60
1:A:216:THR:HG22	1:A:226:GLN:NE2	2.16	0.60
1:C:7:TYR:CD2	1:C:26:GLY:HA2	2.37	0.60
2:H:53:ASP:OD2	2:H:53:ASP:N	2.30	0.60
1:G:103:LEU:HG	1:G:168:LEU:HD23	1.83	0.60
1:C:9:HIS:CD2	1:C:97:TRP:CE3	2.90	0.60
1:C:264:GLU:HG3	4:C:305:HOH:O	2.00	0.60
2:D:42:ASN:HD21	2:D:76:ASP:HA	1.67	0.60
1:A:54:GLN:HG2	1:A:54:GLN:O	2.00	0.59
1:C:111:ARG:HB3	4:C:307:HOH:O	2.02	0.59
1:C:129:ASP:O	1:C:131:ARG:HG2	2.02	0.59
2:H:41:LYS:HA	2:H:78:TYR:CD1	2.37	0.59
1:E:254:GLU:HB2	1:E:255:GLN:HE21	1.67	0.59
1:E:57:SER:O	1:E:58:GLU:C	2.42	0.59
2:H:54:LEU:HA	2:H:64:LEU:HD21	1.84	0.59
1:C:224:HIS:O	1:C:226:GLN:N	2.36	0.59
1:E:69:ASP:O	1:E:73:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:HIS:CD2	1:G:265:GLY:H	2.21	0.59
1:E:189:VAL:HG11	1:E:274:TRP:HB2	1.84	0.59
2:H:98:ASP:C	2:H:99:MET:CG	2.75	0.59
1:C:158:ALA:O	1:C:162:ASP:HB2	2.02	0.59
1:C:187:THR:HG21	1:C:272:LEU:HD21	1.85	0.59
1:E:125:THR:HG22	1:E:126:LEU:O	2.03	0.59
1:C:6:LYS:CD	1:C:113:TYR:HH	2.16	0.58
1:A:145:GLN:HG3	1:A:146:LYS:N	2.17	0.58
1:C:158:ALA:O	1:C:162:ASP:N	2.36	0.58
1:E:17:ARG:H	1:E:17:ARG:NH1	2.01	0.58
2:H:41:LYS:HB2	2:H:46:ILE:HD11	1.85	0.58
2:F:16:GLU:O	2:F:17:ASN:C	2.45	0.58
2:H:23:LEU:HD23	2:H:39:LEU:HD13	1.84	0.58
1:C:169:HIS:CG	1:C:170:LYS:H	2.21	0.58
1:C:224:HIS:C	1:C:226:GLN:N	2.61	0.58
2:H:73:THR:CG2	2:H:75:LYS:HG2	2.33	0.58
1:C:6:LYS:HD2	1:C:113:TYR:HH	1.69	0.58
1:G:42:SER:HB3	1:G:43:PRO:HD2	1.86	0.58
1:G:69:ASP:O	1:G:73:ILE:HG12	2.04	0.58
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.69	0.58
1:A:202:ARG:HH12	2:B:99:MET:HE3	1.68	0.58
2:B:49:VAL:HG13	2:B:67:TYR:O	2.03	0.58
1:E:187:THR:HG23	1:E:204:TRP:O	2.04	0.57
1:A:247:VAL:HG22	1:A:248:VAL:N	2.20	0.57
1:C:151:SER:HA	4:C:282:HOH:O	2.04	0.57
1:E:180:LEU:HD23	1:E:180:LEU:H	1.70	0.57
1:A:87:GLN:NE2	1:A:118:TYR:OH	2.34	0.57
1:E:218:GLN:HG3	1:E:260:HIS:CD2	2.39	0.57
1:G:273:ARG:O	1:G:274:TRP:HB3	2.04	0.57
1:A:220:ASP:O	1:A:222:GLU:HG3	2.04	0.57
1:C:104:GLY:CA	1:C:110:LEU:HD22	2.34	0.57
1:C:169:HIS:CD2	1:C:170:LYS:HG3	2.40	0.57
2:H:41:LYS:HD2	2:H:78:TYR:OH	2.05	0.57
1:A:69:ASP:O	1:A:73:ILE:HG12	2.04	0.57
1:G:226:GLN:NE2	1:G:257:TYR:CE2	2.73	0.57
3:R:5:ARG:C	4:R:181:HOH:O	2.45	0.57
1:C:103:LEU:HG	1:C:168:LEU:CD2	2.35	0.57
1:C:106:ASP:CG	1:C:108:ARG:HD2	2.30	0.57
1:E:33:PHE:CD2	1:E:34:VAL:HG13	2.39	0.57
1:E:63:GLU:OE1	1:E:63:GLU:HA	2.05	0.57
1:G:177:GLU:CD	1:G:177:GLU:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:HB2	1:A:269:PRO:HD2	1.87	0.56
1:C:28:VAL:HG23	1:C:33:PHE:CD1	2.39	0.56
1:E:98:MET:HE1	2:F:58:LYS:HG2	1.87	0.56
1:C:154:GLU:O	1:C:157:ARG:HB3	2.05	0.56
1:G:273:ARG:O	1:G:274:TRP:CB	2.52	0.56
1:E:57:SER:C	1:E:59:TYR:N	2.59	0.56
1:A:273:ARG:O	1:A:274:TRP:HB3	2.06	0.56
1:E:135:ALA:HB1	1:E:140:ALA:HB3	1.88	0.56
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.40	0.56
1:A:224:HIS:C	1:A:225:THR:CG2	2.78	0.56
1:A:170:LYS:O	1:A:174:LYS:HG3	2.06	0.56
4:A:287:HOH:O	1:C:216:THR:HG23	2.06	0.56
1:G:87:GLN:HA	4:G:309:HOH:O	2.05	0.56
1:G:230:LEU:HD11	1:G:243:LYS:HE3	1.88	0.56
1:G:255:GLN:H	1:G:255:GLN:CD	2.14	0.56
1:C:33:PHE:HD2	1:C:52:MET:HG3	1.71	0.56
1:C:171:TYR:CE1	4:C:297:HOH:O	2.33	0.56
1:C:255:GLN:CA	4:C:284:HOH:O	2.53	0.56
1:A:175:GLY:HA3	1:A:179:LEU:HD22	1.87	0.55
1:A:216:THR:HG22	1:A:226:GLN:HE22	1.72	0.55
1:C:89:GLU:O	1:C:89:GLU:HG2	2.06	0.55
1:G:47:PRO:HG3	1:G:60:TRP:CH2	2.41	0.55
1:C:87:GLN:CD	1:C:93:HIS:CE1	2.85	0.55
1:C:157:ARG:HH11	1:C:157:ARG:HB2	1.65	0.55
1:C:177:GLU:H	1:C:177:GLU:CD	2.13	0.55
1:C:226:GLN:CB	4:C:295:HOH:O	2.24	0.55
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.41	0.55
1:A:202:ARG:NH1	2:B:99:MET:HE3	2.22	0.55
2:H:47:GLU:HG3	2:H:48:LYS:HG3	1.87	0.55
1:C:14:ARG:HD2	1:C:21:ARG:N	2.21	0.55
1:G:191:HIS:HB2	1:G:274:TRP:CE2	2.41	0.55
1:C:14:ARG:O	1:C:15:PRO:C	2.50	0.55
2:H:94:LYS:NZ	2:H:94:LYS:HB3	2.20	0.55
2:F:41:LYS:HE3	2:F:78:TYR:OH	2.07	0.55
2:D:54:LEU:HA	2:D:64:LEU:HD21	1.88	0.55
1:E:219:GLN:HA	1:E:256:ARG:O	2.06	0.55
1:G:14:ARG:NH2	1:G:39:ASP:OD1	2.38	0.55
1:C:255:GLN:HA	4:C:284:HOH:O	2.07	0.55
2:H:45:ARG:HH12	2:H:47:GLU:HA	1.72	0.55
1:A:224:HIS:CB	1:A:225:THR:HA	2.09	0.54
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:GLY:N	1:E:254:GLU:OE1	2.40	0.54
1:E:255:GLN:H	1:E:255:GLN:NE2	2.05	0.54
2:D:12:ARG:NH1	4:D:102:HOH:O	2.39	0.54
2:F:13:HIS:C	2:F:21:ASN:HD21	2.14	0.54
1:G:82:ARG:HA	1:G:87:GLN:HE21	1.71	0.54
2:H:41:LYS:CB	2:H:78:TYR:HE1	2.20	0.54
2:B:47:GLU:O	2:B:48:LYS:HB2	2.05	0.54
2:F:54:LEU:HA	2:F:64:LEU:HD21	1.89	0.54
1:G:250:PRO:CG	1:G:253:GLU:OE1	2.55	0.54
1:A:220:ASP:CG	1:A:221:GLY:N	2.53	0.54
1:G:41:ALA:O	1:G:43:PRO:CD	2.56	0.54
1:G:41:ALA:O	1:G:43:PRO:HD3	2.08	0.54
1:G:202:ARG:HH12	2:H:99:MET:CE	2.19	0.54
2:B:12:ARG:HB2	2:B:22:PHE:HB2	1.89	0.54
2:F:17:ASN:H	2:F:17:ASN:ND2	2.05	0.54
1:E:17:ARG:NH1	4:E:304:HOH:O	2.40	0.54
1:G:190:THR:HB	1:G:192:HIS:CE1	2.43	0.54
1:C:6:LYS:HD2	1:C:113:TYR:OH	2.06	0.54
1:G:191:HIS:HB2	1:G:274:TRP:NE1	2.23	0.54
2:B:73:THR:HG22	2:B:75:LYS:HG2	1.89	0.54
1:E:129:ASP:O	1:E:131:ARG:CG	2.55	0.54
1:G:266:LEU:O	1:G:267:PRO:C	2.50	0.54
2:H:41:LYS:CB	2:H:78:TYR:CE1	2.90	0.54
1:E:134:THR:HA	1:E:144:GLU:OE2	2.07	0.53
1:C:35:ARG:CA	1:C:45:MET:CE	2.87	0.53
1:G:20:PRO:HD3	4:G:279:HOH:O	2.08	0.53
2:H:45:ARG:O	2:H:46:ILE:C	2.50	0.53
2:H:73:THR:HG21	2:H:75:LYS:HG2	1.91	0.53
2:H:45:ARG:HG2	2:H:45:ARG:NH1	2.20	0.53
2:H:46:ILE:HD11	2:H:78:TYR:HE1	1.73	0.53
1:C:92:SER:C	1:C:93:HIS:CD2	2.86	0.53
1:G:111:ARG:HG2	1:G:112:GLY:N	2.21	0.53
1:C:191:HIS:ND1	1:C:193:PRO:HD3	2.23	0.53
1:E:57:SER:O	1:E:59:TYR:N	2.42	0.53
2:B:45:ARG:NH1	2:B:81:ARG:HH12	2.07	0.53
1:E:5:LEU:HD12	1:E:27:TYR:O	2.09	0.53
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.44	0.53
1:G:103:LEU:HD21	1:G:165:VAL:HG13	1.91	0.53
1:G:13:SER:HB3	1:G:78:LEU:HD13	1.90	0.53
2:H:41:LYS:CG	2:H:78:TYR:CE1	2.91	0.53
1:C:47:PRO:HG3	1:C:60:TRP:CH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:HIS:CG	1:C:170:LYS:N	2.77	0.52
1:G:59:TYR:HE1	3:S:1:VAL:HG12	1.74	0.52
1:C:114:GLU:C	1:C:115:GLN:HG2	2.35	0.52
1:C:55:GLU:HA	1:C:55:GLU:OE1	2.07	0.52
1:A:232:GLU:O	1:A:233:THR:C	2.52	0.52
2:D:69:GLU:HG2	2:D:70:PHE:N	2.24	0.52
1:G:243:LYS:HG2	1:G:244:TRP:N	2.25	0.52
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.92	0.52
1:A:226:GLN:HB3	1:A:228:THR:HG1	1.70	0.52
1:E:202:ARG:HH11	1:E:202:ARG:CG	2.23	0.52
1:E:272:LEU:N	1:E:272:LEU:HD22	2.24	0.52
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.44	0.52
1:C:6:LYS:HG3	1:C:8:PHE:CE2	2.45	0.52
1:E:234:ARG:HE	1:E:242:GLN:HG3	1.74	0.52
2:F:79:ALA:CB	2:F:94:LYS:HA	2.40	0.52
1:A:58:GLU:HB2	4:A:277:HOH:O	2.10	0.52
1:C:46:VAL:C	1:C:60:TRP:CZ3	2.87	0.52
2:H:12:ARG:HG2	2:H:13:HIS:CD2	2.44	0.52
1:E:202:ARG:HD2	1:E:204:TRP:CE2	2.45	0.52
1:C:160:LEU:O	1:C:164:CYS:HB3	2.09	0.52
1:A:249:VAL:HG11	1:A:254:GLU:HA	1.92	0.52
1:C:14:ARG:NH2	1:C:39:ASP:CG	2.58	0.52
1:C:156:GLN:O	1:C:160:LEU:CG	2.58	0.51
2:F:48:LYS:NZ	2:F:48:LYS:HB3	2.25	0.51
1:C:146:LYS:C	1:C:148:ASN:N	2.66	0.51
2:B:69:GLU:CD	2:B:70:PHE:N	2.68	0.51
2:F:4:THR:CG2	4:F:102:HOH:O	2.58	0.51
1:G:237:GLY:C	2:H:12:ARG:NH1	2.69	0.51
1:C:260:HIS:HA	1:C:270:VAL:O	2.11	0.51
2:H:23:LEU:O	2:H:67:TYR:HA	2.11	0.51
1:E:182:LEU:HD13	1:E:264:GLU:HB3	1.92	0.51
1:E:210:PRO:O	1:E:263:HIS:HE1	1.94	0.51
1:A:20:PRO:HD2	1:A:75:ARG:HE	1.75	0.51
1:C:50:PRO:HA	1:C:53:GLU:OE2	2.10	0.51
1:C:237:GLY:HA3	2:D:12:ARG:HH11	1.75	0.51
1:E:157:ARG:C	1:E:159:TYR:N	2.62	0.51
1:A:187:THR:CB	4:A:305:HOH:O	2.11	0.51
1:C:5:LEU:O	4:C:285:HOH:O	2.20	0.51
1:G:268:GLU:HB2	1:G:269:PRO:HD2	1.93	0.51
1:A:175:GLY:C	1:A:177:GLU:OE1	2.53	0.51
1:E:35:ARG:HD2	1:E:36:PHE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:GLU:O	1:G:175:GLY:N	2.44	0.51
2:H:54:LEU:HA	2:H:64:LEU:CD2	2.40	0.51
1:A:103:LEU:HG	1:A:168:LEU:CD2	2.42	0.50
1:C:159:TYR:HD2	1:C:160:LEU:HD21	1.74	0.50
1:C:176:LYS:C	1:C:178:THR:H	2.19	0.50
1:C:191:HIS:HB2	1:C:274:TRP:CE2	2.47	0.50
1:C:76:VAL:HA	1:C:79:ARG:HH21	1.76	0.50
1:C:106:ASP:OD1	1:C:106:ASP:N	2.30	0.50
2:D:42:ASN:ND2	2:D:77:GLU:H	2.08	0.50
1:E:234:ARG:HG2	1:E:242:GLN:O	2.12	0.50
1:C:114:GLU:O	1:C:115:GLN:HG2	2.12	0.50
1:E:202:ARG:NH1	1:E:246:ALA:HB2	2.27	0.50
2:F:41:LYS:HG3	2:F:78:TYR:CE1	2.47	0.50
1:G:7:TYR:CE2	3:S:2:MET:HB3	2.46	0.50
1:C:157:ARG:NH1	1:C:157:ARG:HB2	2.24	0.50
1:E:59:TYR:HE2	1:E:60:TRP:CZ3	2.30	0.50
2:F:47:GLU:O	2:F:48:LYS:HB2	2.11	0.50
1:A:43:PRO:O	1:A:44:ARG:HG3	2.11	0.50
1:C:238:ASP:OD1	1:C:238:ASP:C	2.54	0.50
1:C:273:ARG:O	1:C:274:TRP:CB	2.59	0.50
1:E:73:ILE:HD12	3:R:8:PHE:CE1	2.46	0.50
2:F:17:ASN:HA	2:F:72:PRO:O	2.11	0.50
1:C:223:GLY:HA3	1:C:224:HIS:CD2	2.47	0.50
1:E:254:GLU:HB2	1:E:255:GLN:NE2	2.25	0.50
2:B:69:GLU:CD	2:B:69:GLU:C	2.80	0.50
1:C:5:LEU:O	1:C:5:LEU:CG	2.53	0.50
1:C:119:ASP:HB3	2:D:0:MET:HG3	1.94	0.50
1:E:7:TYR:HB2	1:E:99:HIS:CE1	2.47	0.50
2:F:54:LEU:HA	2:F:64:LEU:CD2	2.41	0.50
2:H:12:ARG:NH2	2:H:22:PHE:CD2	2.80	0.50
1:G:37:ASP:OD1	1:G:39:ASP:HB2	2.11	0.50
3:Q:7:LEU:HB2	4:Q:204:HOH:O	2.11	0.50
4:C:317:HOH:O	2:D:99:MET:HE1	2.12	0.49
2:F:4:THR:HG22	4:F:102:HOH:O	2.11	0.49
1:G:82:ARG:HD2	1:G:88:SER:O	2.12	0.49
1:G:98:MET:CG	4:G:297:HOH:O	2.02	0.49
2:H:31:HIS:ND1	2:H:32:PRO:HA	2.27	0.49
2:F:65:LEU:HG	2:F:67:TYR:HD1	1.77	0.49
2:F:73:THR:HG21	2:F:75:LYS:CE	2.41	0.49
1:G:35:ARG:HG2	1:G:48:ARG:HD3	1.94	0.49
1:G:236:ALA:HB3	1:G:238:ASP:OD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PHE:CD1	1:C:36:PHE:C	2.90	0.49
1:E:152:GLU:C	1:E:154:GLU:H	2.20	0.49
1:C:69:ASP:O	1:C:73:ILE:HG12	2.12	0.49
1:E:250:PRO:O	1:E:251:SER:C	2.55	0.49
1:C:218:GLN:HA	1:C:223:GLY:HA3	1.95	0.49
1:G:87:GLN:CA	4:G:309:HOH:O	2.60	0.49
1:C:17:ARG:HD3	1:C:17:ARG:N	2.27	0.49
1:C:165:VAL:CB	1:C:166:GLU:OE2	2.57	0.49
2:D:46:ILE:HG22	2:D:47:GLU:O	2.12	0.49
2:H:46:ILE:HD11	2:H:78:TYR:CE1	2.48	0.49
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.47	0.49
1:C:54:GLN:H	1:C:54:GLN:CD	2.20	0.49
1:C:59:TYR:HD2	1:C:60:TRP:CD1	2.31	0.49
2:D:13:HIS:O	2:D:14:PRO:C	2.55	0.49
1:A:247:VAL:CG2	1:A:248:VAL:N	2.76	0.49
1:G:191:HIS:CG	1:G:274:TRP:CZ2	3.00	0.49
1:C:85:TYR:O	1:C:87:GLN:HG3	2.13	0.49
1:C:159:TYR:CE2	1:C:160:LEU:CD2	2.91	0.49
2:H:16:GLU:HB3	2:H:19:LYS:HG3	1.95	0.49
1:E:189:VAL:CG1	1:E:274:TRP:HB2	2.43	0.48
1:C:88:SER:C	1:C:90:ALA:H	2.19	0.48
1:C:144:GLU:C	1:C:146:LYS:H	2.21	0.48
1:E:21:ARG:NE	1:E:39:ASP:HB2	2.28	0.48
1:E:187:THR:HG21	1:E:272:LEU:CD2	2.34	0.48
2:H:41:LYS:HG2	2:H:42:ASN:OD1	2.13	0.48
2:B:20:SER:OG	2:B:69:GLU:OE1	2.29	0.48
1:C:72:GLN:O	1:C:75:ARG:HB3	2.13	0.48
2:D:73:THR:CG2	2:D:74:GLU:N	2.76	0.48
2:F:8:GLN:HA	4:F:100:HOH:O	2.12	0.48
2:H:67:TYR:CD1	2:H:67:TYR:N	2.81	0.48
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.78	0.48
2:F:27:VAL:HG23	2:F:27:VAL:O	2.12	0.48
1:A:106:ASP:O	1:A:107:ARG:CB	2.47	0.48
2:B:42:ASN:ND2	2:B:77:GLU:H	2.12	0.48
1:C:111:ARG:NH1	1:C:113:TYR:HB3	2.23	0.48
1:E:157:ARG:O	1:E:161:GLU:N	2.38	0.48
1:C:21:ARG:HG3	1:C:21:ARG:HH11	1.77	0.48
1:G:238:ASP:HB3	2:H:12:ARG:HD2	1.95	0.48
1:C:17:ARG:N	1:C:17:ARG:CD	2.77	0.48
1:C:177:GLU:CD	1:C:177:GLU:N	2.72	0.48
1:C:55:GLU:CB	1:C:60:TRP:HE1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:LYS:HG2	1:E:244:TRP:N	2.29	0.48
1:G:106:ASP:OD1	1:G:106:ASP:N	2.37	0.48
2:B:73:THR:CG2	2:B:75:LYS:CG	2.84	0.48
4:C:301:HOH:O	2:D:32:PRO:CB	2.58	0.48
1:A:224:HIS:CA	1:A:225:THR:CG2	2.85	0.47
2:B:67:TYR:CZ	4:B:116:HOH:O	2.55	0.47
1:C:14:ARG:HD3	1:C:19:GLU:O	2.14	0.47
1:C:35:ARG:O	1:C:45:MET:CE	2.62	0.47
1:E:98:MET:HB2	4:E:314:HOH:O	2.14	0.47
1:E:187:THR:HG22	1:E:272:LEU:HG	1.96	0.47
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.49	0.47
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.49	0.47
1:A:217:TRP:CZ3	1:A:257:TYR:HB3	2.49	0.47
1:C:44:ARG:HB3	1:C:64:THR:HG21	1.95	0.47
1:E:192:HIS:HB2	1:E:200:THR:HB	1.97	0.47
1:C:7:TYR:HD1	1:C:99:HIS:CE1	2.23	0.47
1:C:88:SER:C	1:C:90:ALA:N	2.70	0.47
1:C:154:GLU:HA	1:C:157:ARG:HH12	1.78	0.47
2:D:85:VAL:O	2:D:85:VAL:HG22	2.15	0.47
1:E:157:ARG:O	1:E:158:ALA:O	2.32	0.47
1:A:14:ARG:O	1:A:15:PRO:C	2.56	0.47
1:C:55:GLU:OE1	1:C:174:LYS:NZ	2.47	0.47
1:A:65:ARG:NH2	4:A:313:HOH:O	2.48	0.47
1:C:153:ALA:CB	4:C:310:HOH:O	2.26	0.47
1:C:270:VAL:HG12	1:C:271:THR:N	2.30	0.47
2:D:69:GLU:O	2:D:70:PHE:HB3	2.15	0.47
1:E:106:ASP:O	1:E:107:ARG:HB2	2.13	0.47
2:F:45:ARG:HH11	2:F:47:GLU:HG2	1.79	0.47
1:G:14:ARG:HB2	1:G:17:ARG:HB3	1.96	0.47
1:G:79:ARG:HD2	4:G:284:HOH:O	2.15	0.47
1:G:104:GLY:O	1:G:107:ARG:N	2.32	0.47
2:H:12:ARG:HG2	2:H:13:HIS:NE2	2.30	0.47
1:A:182:LEU:CD1	1:A:264:GLU:HG2	2.45	0.47
2:D:54:LEU:HA	2:D:64:LEU:CD2	2.44	0.47
1:E:136:VAL:HG12	1:E:136:VAL:O	2.15	0.47
4:E:323:HOH:O	2:F:6:LYS:NZ	2.42	0.47
1:C:3:HIS:NE2	1:C:107:ARG:CZ	2.78	0.47
1:C:7:TYR:O	1:C:8:PHE:CD2	2.68	0.47
1:C:80:THR:HG22	1:C:84:TYR:CZ	2.49	0.47
1:C:148:ASN:HA	4:C:282:HOH:O	2.14	0.47
1:C:7:TYR:CE2	1:C:26:GLY:HA3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLU:OE1	3:Q:1:VAL:HB	2.15	0.47
1:C:92:SER:CB	4:C:312:HOH:O	2.43	0.47
1:G:182:LEU:CD1	1:G:264:GLU:HG2	2.45	0.47
1:C:223:GLY:CA	1:C:224:HIS:CB	2.75	0.46
1:C:169:HIS:CE1	1:C:170:LYS:HG3	2.48	0.46
1:G:63:GLU:OE1	1:G:63:GLU:HA	2.15	0.46
1:C:88:SER:OG	1:C:90:ALA:HB3	2.15	0.46
1:E:57:SER:C	1:E:59:TYR:H	2.24	0.46
2:H:25:CYS:HB2	2:H:39:LEU:HD21	1.97	0.46
1:A:68:ARG:HD3	4:A:310:HOH:O	2.15	0.46
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.50	0.46
1:C:121:LYS:HB2	2:D:1:ILE:HD12	1.97	0.46
2:D:51:HIS:HA	2:D:65:LEU:O	2.16	0.46
1:E:37:ASP:C	1:E:39:ASP:H	2.23	0.46
2:H:41:LYS:HA	2:H:78:TYR:CE1	2.50	0.46
1:A:17:ARG:CG	4:A:297:HOH:O	2.25	0.46
1:A:272:LEU:N	1:A:272:LEU:HD22	2.31	0.46
2:B:73:THR:HG21	2:B:75:LYS:HE3	1.97	0.46
1:G:145:GLN:HG3	1:G:146:LYS:N	2.30	0.46
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.50	0.46
1:C:103:LEU:HD13	1:C:107:ARG:HB3	1.98	0.46
1:C:129:ASP:C	1:C:131:ARG:HG2	2.41	0.46
1:C:144:GLU:O	1:C:148:ASN:ND2	2.49	0.46
1:C:187:THR:HG23	1:C:204:TRP:O	2.16	0.46
1:C:223:GLY:HA3	1:C:224:HIS:CG	2.41	0.46
1:A:54:GLN:NE2	1:A:55:GLU:HG2	2.31	0.45
1:A:73:ILE:HD12	3:P:8:PHE:CE1	2.52	0.45
2:B:67:TYR:CE2	4:B:116:HOH:O	2.69	0.45
1:G:4:SER:HB3	1:G:102:GLU:HG2	1.98	0.45
1:C:104:GLY:CA	1:C:110:LEU:HD13	2.36	0.45
1:A:224:HIS:CB	1:A:225:THR:CG2	2.91	0.45
1:C:196:ASP:HB2	1:C:197:HIS:CE1	2.51	0.45
1:A:44:ARG:O	1:A:46:VAL:HG13	2.16	0.45
1:C:191:HIS:CE1	1:C:193:PRO:HD3	2.50	0.45
1:C:220:ASP:C	1:C:222:GLU:H	2.25	0.45
2:F:39:LEU:HD12	2:F:68:THR:HG22	1.98	0.45
1:A:154:GLU:CD	1:A:154:GLU:N	2.75	0.45
2:F:73:THR:HG22	2:F:75:LYS:HG2	1.97	0.45
1:C:157:ARG:NH1	1:C:157:ARG:HB3	2.24	0.45
1:C:259:CYS:O	1:C:271:THR:HA	2.17	0.45
1:E:218:GLN:CG	1:E:260:HIS:CD2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:LEU:HD13	2:F:43:GLY:O	2.17	0.45
1:G:7:TYR:HB2	1:G:99:HIS:CE1	2.51	0.45
1:G:117:ALA:HB2	2:H:60:TRP:CZ2	2.52	0.45
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.51	0.45
1:C:98:MET:HE2	2:D:60:TRP:CH2	2.52	0.45
1:C:114:GLU:OE1	1:C:160:LEU:HD11	2.17	0.45
1:G:111:ARG:CG	1:G:112:GLY:N	2.79	0.45
2:H:73:THR:HG22	2:H:75:LYS:H	1.81	0.45
1:A:24:SER:O	1:A:35:ARG:HA	2.16	0.45
1:A:201:LEU:CD1	1:A:249:VAL:HG21	2.46	0.45
1:C:80:THR:CG2	1:C:84:TYR:CZ	3.00	0.45
1:C:154:GLU:N	4:C:310:HOH:O	2.49	0.45
1:C:187:THR:HG22	1:C:272:LEU:CG	2.46	0.45
1:C:202:ARG:HD2	1:C:244:TRP:CD2	2.52	0.45
2:H:19:LYS:HB2	4:H:105:HOH:O	2.16	0.45
1:A:42:SER:O	1:A:44:ARG:N	2.49	0.45
1:C:206:LEU:HD23	1:C:242:GLN:HB3	1.98	0.45
1:E:44:ARG:NH2	1:E:61:ASP:OD1	2.50	0.45
1:E:176:LYS:HG3	1:E:180:LEU:HG	1.99	0.45
1:G:237:GLY:C	2:H:12:ARG:HH11	2.24	0.45
2:B:94:LYS:NZ	2:B:94:LYS:HB3	2.32	0.44
1:C:109:PHE:CD1	1:C:161:GLU:HG3	2.51	0.44
1:E:201:LEU:HB2	1:E:247:VAL:HG12	1.98	0.44
1:G:98:MET:HE3	2:H:60:TRP:CZ3	2.52	0.44
1:A:220:ASP:HA	1:A:222:GLU:HG3	1.98	0.44
2:B:69:GLU:C	2:B:69:GLU:OE2	2.60	0.44
2:D:10:TYR:CD1	2:D:10:TYR:N	2.85	0.44
1:E:44:ARG:HB2	1:E:64:THR:OG1	2.17	0.44
2:F:10:TYR:N	2:F:10:TYR:CD1	2.86	0.44
3:R:4:PRO:C	4:R:181:HOH:O	2.53	0.44
1:C:104:GLY:N	1:C:110:LEU:HB2	2.31	0.44
1:C:159:TYR:CD2	1:C:160:LEU:HD21	2.48	0.44
1:C:111:ARG:NH1	4:C:291:HOH:O	2.51	0.44
1:E:6:LYS:HD3	1:E:113:TYR:OH	2.17	0.44
1:E:35:ARG:HG2	1:E:35:ARG:HH11	1.82	0.44
2:H:27:VAL:O	2:H:27:VAL:HG23	2.18	0.44
1:C:51:TRP:CE3	1:C:52:MET:HG2	2.53	0.44
1:E:202:ARG:CG	1:E:202:ARG:NH1	2.80	0.44
1:E:242:GLN:OE1	2:F:10:TYR:CD2	2.70	0.44
1:C:69:ASP:CG	3:S:5:ARG:HH22	2.24	0.44
1:C:87:GLN:CD	1:C:93:HIS:HE1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:THR:HG21	1:C:272:LEU:CD2	2.47	0.44
2:D:5:PRO:HB3	2:D:30:PHE:HB3	2.00	0.44
1:G:189:VAL:HG23	1:G:272:LEU:HB3	2.00	0.44
1:A:19:GLU:N	1:A:75:ARG:HH21	2.15	0.44
1:A:220:ASP:OD2	1:A:220:ASP:C	2.49	0.44
2:H:73:THR:HG22	2:H:75:LYS:HG2	1.98	0.44
1:A:182:LEU:HD11	1:A:264:GLU:HG2	1.99	0.44
1:C:123:TYR:HD1	1:C:124:LEU:HB2	1.83	0.44
1:E:117:ALA:HB2	2:F:60:TRP:CZ2	2.52	0.44
2:F:32:PRO:HB2	4:F:105:HOH:O	2.18	0.44
2:B:38:ASP:OD1	2:B:45:ARG:HD2	2.18	0.44
2:D:19:LYS:HE3	4:D:111:HOH:O	2.01	0.44
1:E:28:VAL:HG23	1:E:33:PHE:CD1	2.53	0.43
1:G:259:CYS:O	1:G:271:THR:HA	2.18	0.43
2:H:59:ASP:O	2:H:60:TRP:HB2	2.18	0.43
1:C:85:TYR:O	1:C:86:ASN:C	2.61	0.43
1:C:263:HIS:CD2	1:C:265:GLY:N	2.80	0.43
1:E:202:ARG:HB2	1:E:202:ARG:CZ	2.48	0.43
2:H:41:LYS:HG3	2:H:78:TYR:CZ	2.53	0.43
1:C:120:GLY:N	2:D:31:HIS:CE1	2.86	0.43
1:E:228:THR:HA	1:E:246:ALA:O	2.17	0.43
1:G:225:THR:HG21	1:G:226:GLN:OE1	2.09	0.43
1:G:226:GLN:HG2	1:G:247:VAL:HG23	1.99	0.43
2:D:7:ILE:HG21	2:D:93:VAL:HG11	2.00	0.43
1:E:14:ARG:HH22	1:E:39:ASP:CG	2.24	0.43
1:C:104:GLY:CA	4:C:275:HOH:O	2.57	0.43
2:F:33:SER:O	2:F:34:ASP:C	2.61	0.43
2:H:10:TYR:CD1	2:H:10:TYR:N	2.86	0.43
2:B:51:HIS:HD2	4:B:104:HOH:O	2.01	0.43
1:C:7:TYR:CD2	1:C:26:GLY:CA	3.01	0.43
1:C:43:PRO:O	1:C:68:ARG:NH2	2.52	0.43
1:C:62:ARG:HB3	1:C:62:ARG:NH1	2.28	0.43
1:E:106:ASP:OD2	1:E:108:ARG:HB2	2.19	0.43
1:G:258:THR:CG2	1:G:273:ARG:CZ	2.96	0.43
1:C:8:PHE:HB3	2:D:56:PHE:CE2	2.53	0.43
1:E:273:ARG:O	1:E:274:TRP:CB	2.67	0.43
2:F:16:GLU:HB3	2:F:19:LYS:HG2	2.01	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
1:A:197:HIS:CD2	1:G:42:SER:HG	2.33	0.43
1:A:229:GLU:HG3	1:C:131:ARG:HH21	1.83	0.43
1:C:158:ALA:O	1:C:162:ASP:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:ARG:HB3	2:D:29:GLY:O	2.19	0.43
2:H:73:THR:HG22	2:H:74:GLU:N	2.34	0.43
1:E:73:ILE:HD12	3:R:8:PHE:CZ	2.54	0.43
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.34	0.43
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.52	0.43
1:C:272:LEU:N	1:C:272:LEU:HD22	2.34	0.43
1:E:209:TYR:CD1	1:E:209:TYR:C	2.96	0.43
1:C:152:GLU:OE1	3:Q:5:ARG:HD3	2.19	0.42
1:E:216:THR:O	1:E:259:CYS:HA	2.19	0.42
1:G:173:GLU:O	1:G:174:LYS:C	2.61	0.42
2:D:7:ILE:CG2	2:D:93:VAL:HG11	2.49	0.42
1:E:24:SER:O	1:E:35:ARG:HA	2.18	0.42
1:E:50:PRO:C	1:E:52:MET:H	2.27	0.42
1:G:191:HIS:CD2	1:G:274:TRP:CZ2	3.07	0.42
1:C:135:ALA:HB1	1:C:140:ALA:HB3	2.01	0.42
1:E:14:ARG:NH1	1:E:19:GLU:O	2.41	0.42
1:G:2:SER:C	1:G:3:HIS:CD2	2.97	0.42
2:B:38:ASP:CG	2:B:45:ARG:HD2	2.44	0.42
1:C:69:ASP:OD2	3:S:5:ARG:NH2	2.52	0.42
1:G:14:ARG:HD3	1:G:19:GLU:O	2.19	0.42
1:A:82:ARG:CD	4:A:279:HOH:O	2.65	0.42
1:C:28:VAL:HG21	1:C:51:TRP:CH2	2.49	0.42
1:C:156:GLN:O	1:C:160:LEU:CD1	2.68	0.42
1:E:21:ARG:HE	1:E:39:ASP:HB2	1.84	0.42
2:F:16:GLU:HB3	2:F:19:LYS:CG	2.50	0.42
1:G:21:ARG:HG3	1:G:21:ARG:HH11	1.84	0.42
1:G:232:GLU:HB3	4:H:108:HOH:O	2.20	0.42
1:G:187:THR:HG21	1:G:261:VAL:HG21	2.01	0.42
2:H:39:LEU:C	2:H:40:LEU:HD23	2.44	0.42
1:E:119:ASP:CG	2:F:0:MET:HE2	2.44	0.42
1:E:152:GLU:C	1:E:154:GLU:N	2.77	0.42
1:E:255:GLN:NE2	1:E:255:GLN:N	2.68	0.42
1:A:209:TYR:CD1	1:A:209:TYR:C	2.98	0.42
1:A:273:ARG:O	1:A:274:TRP:CB	2.68	0.42
1:C:4:SER:OG	4:C:287:HOH:O	1.99	0.42
1:C:223:GLY:HA2	1:C:224:HIS:CE1	2.48	0.42
1:C:270:VAL:CG1	1:C:271:THR:N	2.83	0.42
2:D:40:LEU:CD2	2:D:45:ARG:HA	2.49	0.42
1:E:270:VAL:HG12	1:E:271:THR:N	2.35	0.42
1:A:105:PRO:C	1:A:107:ARG:N	2.77	0.42
1:A:258:THR:CG2	1:A:273:ARG:HH21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:C	1:C:45:MET:CE	2.92	0.42
1:C:129:ASP:CG	1:C:131:ARG:HG2	2.44	0.42
2:F:73:THR:HG21	2:F:75:LYS:HZ1	1.85	0.42
1:G:21:ARG:HG3	1:G:21:ARG:NH1	2.34	0.42
1:G:191:HIS:CD2	1:G:274:TRP:CH2	3.08	0.42
1:G:272:LEU:N	1:G:272:LEU:HD22	2.34	0.42
1:A:86:ASN:O	1:A:86:ASN:CG	2.62	0.42
1:A:176:LYS:O	1:A:177:GLU:C	2.62	0.42
1:C:121:LYS:O	1:C:122:ASP:C	2.63	0.42
1:G:247:VAL:O	1:G:247:VAL:HG13	2.20	0.42
1:A:22:PHE:CE1	1:A:24:SER:OG	2.73	0.41
2:B:40:LEU:CD2	2:B:45:ARG:HA	2.50	0.41
2:B:54:LEU:HA	2:B:64:LEU:HD21	2.02	0.41
1:C:34:VAL:C	1:C:45:MET:CE	2.89	0.41
1:C:44:ARG:NH2	1:C:61:ASP:OD1	2.52	0.41
1:C:82:ARG:HH11	1:C:89:GLU:HA	1.85	0.41
1:C:37:ASP:OD1	1:C:37:ASP:C	2.63	0.41
1:A:252:GLY:N	1:A:254:GLU:OE1	2.53	0.41
1:C:44:ARG:HA	1:C:64:THR:HG23	2.03	0.41
2:D:51:HIS:O	2:D:51:HIS:ND1	2.53	0.41
1:G:54:GLN:H	1:G:54:GLN:CD	2.27	0.41
1:C:33:PHE:CD2	1:C:52:MET:HG3	2.53	0.41
1:C:34:VAL:CG2	1:C:45:MET:CE	2.91	0.41
1:C:82:ARG:NH1	1:C:89:GLU:HA	2.35	0.41
1:C:176:LYS:C	1:C:178:THR:N	2.78	0.41
1:E:102:GLU:OE2	1:E:111:ARG:NH1	2.52	0.41
1:E:255:GLN:H	1:E:255:GLN:CD	2.28	0.41
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.01	0.41
1:C:5:LEU:HD23	1:C:164:CYS:SG	2.60	0.41
1:C:160:LEU:HG	1:C:160:LEU:H	1.55	0.41
2:D:33:SER:HB3	2:D:54:LEU:HD11	2.03	0.41
1:E:250:PRO:O	1:E:253:GLU:HB2	2.21	0.41
2:F:5:PRO:HB3	2:F:30:PHE:HB3	2.01	0.41
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.56	0.41
1:A:271:THR:C	1:A:272:LEU:HD22	2.45	0.41
2:B:73:THR:HG21	2:B:75:LYS:CE	2.51	0.41
1:C:106:ASP:HB2	1:C:108:ARG:HD2	2.02	0.41
1:C:145:GLN:HE21	1:C:145:GLN:HB2	1.62	0.41
1:C:218:GLN:OE1	1:C:260:HIS:CE1	2.74	0.41
1:E:56:GLY:O	1:E:59:TYR:HB3	2.20	0.41
1:G:257:TYR:CD1	1:G:257:TYR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:O	1:A:225:THR:OG1	2.31	0.41
1:C:51:TRP:CD1	1:C:51:TRP:H	2.39	0.41
2:F:41:LYS:O	2:F:43:GLY:N	2.52	0.41
1:G:7:TYR:CD2	3:S:2:MET:HB3	2.55	0.41
1:A:103:LEU:HD21	1:A:165:VAL:HG13	2.02	0.41
2:D:33:SER:HB3	2:D:62:PHE:CG	2.55	0.41
2:F:73:THR:HG21	2:F:75:LYS:NZ	2.36	0.41
1:C:106:ASP:CG	1:C:108:ARG:CD	2.90	0.41
1:C:263:HIS:HB3	1:C:266:LEU:HG	2.02	0.41
2:D:3:ARG:HG2	2:D:3:ARG:HH11	1.85	0.41
2:D:59:ASP:O	2:D:60:TRP:HB2	2.20	0.41
1:E:22:PHE:CB	1:E:38:ASN:ND2	2.81	0.41
1:E:179:LEU:C	1:E:180:LEU:HD22	2.45	0.41
1:G:197:HIS:O	1:G:251:SER:OG	2.38	0.41
1:E:126:LEU:HD13	1:E:133:TRP:CZ2	2.55	0.41
1:E:163:THR:O	1:E:164:CYS:C	2.62	0.41
1:G:208:PHE:CE1	1:G:242:GLN:HA	2.56	0.41
1:A:14:ARG:NH1	1:A:21:ARG:HB2	2.33	0.40
1:A:16:GLY:HA3	1:A:17:ARG:NH1	2.36	0.40
1:C:3:HIS:NE2	1:C:107:ARG:NH2	2.68	0.40
1:C:156:GLN:O	1:C:160:LEU:HD12	2.21	0.40
1:E:85:TYR:O	1:E:86:ASN:C	2.64	0.40
2:F:24:ASN:OD1	2:F:67:TYR:HB3	2.21	0.40
2:H:49:VAL:HG22	2:H:68:THR:HB	2.02	0.40
1:C:18:GLY:O	1:C:19:GLU:C	2.64	0.40
2:F:75:LYS:CG	2:F:76:ASP:OD2	2.67	0.40
2:H:39:LEU:HD23	2:H:39:LEU:HA	1.88	0.40
1:A:51:TRP:CD1	1:A:51:TRP:H	2.39	0.40
1:C:69:ASP:O	1:C:72:GLN:HB2	2.22	0.40
1:C:121:LYS:HB2	2:D:1:ILE:CD1	2.51	0.40
1:C:225:THR:O	1:C:226:GLN:O	2.39	0.40
1:G:36:PHE:CD1	1:G:36:PHE:C	2.99	0.40
1:C:98:MET:HE2	2:D:60:TRP:CE3	2.56	0.40
1:C:263:HIS:HD2	1:C:265:GLY:N	2.19	0.40
2:F:73:THR:HB	2:F:76:ASP:HB2	2.03	0.40
2:B:39:LEU:HD12	2:B:68:THR:CG2	2.47	0.40
1:C:162:ASP:O	1:C:163:THR:C	2.62	0.40
1:E:15:PRO:HB2	4:E:304:HOH:O	2.21	0.40
2:H:7:ILE:HG21	2:H:93:VAL:HG11	2.04	0.40
2:H:97:ARG:C	2:H:99:MET:H	2.30	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:GLU:OE2	4:G:309:HOH:O[2_646]	1.37	0.83
1:G:17:ARG:NH2	1:G:149:ASP:OD1[2_646]	1.50	0.70
1:C:145:GLN:CB	4:G:295:HOH:O[2_646]	1.56	0.64
1:C:145:GLN:NE2	4:G:295:HOH:O[2_646]	2.04	0.16
2:B:77:GLU:CD	4:G:309:HOH:O[2_646]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/273 (99%)	241 (89%)	26 (10%)	4 (2%)	8	16
1	C	271/273 (99%)	231 (85%)	32 (12%)	8 (3%)	3	5
1	E	263/273 (96%)	235 (89%)	24 (9%)	4 (2%)	8	16
1	G	271/273 (99%)	243 (90%)	24 (9%)	4 (2%)	8	16
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	D	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	12	24
2	F	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	12	24
2	H	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
3	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	S	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1496/1528 (98%)	1337 (89%)	137 (9%)	22 (2%)	8	16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	224	HIS

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Mol	Chain	Res	Type
1	C	226	GLN
1	G	267	PRO
1	A	225	THR
1	C	225	THR
1	G	174	LYS
1	A	51	TRP
1	A	179	LEU
1	A	255	GLN
1	C	177	GLU
1	C	222	GLU
1	E	51	TRP
1	E	138	THR
1	C	38	ASN
1	E	58	GLU
1	G	51	TRP
1	G	57	SER
1	C	15	PRO
1	C	145	GLN
2	F	15	ALA
1	E	15	PRO
2	D	85	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	236/236 (100%)	220 (93%)	16 (7%)	14	31
1	C	236/236 (100%)	210 (89%)	26 (11%)	6	13
1	E	231/236 (98%)	211 (91%)	20 (9%)	9	21
1	G	236/236 (100%)	215 (91%)	21 (9%)	9	20
2	B	95/95 (100%)	90 (95%)	5 (5%)	20	42
2	D	95/95 (100%)	92 (97%)	3 (3%)	34	62
2	F	95/95 (100%)	90 (95%)	5 (5%)	20	42
2	H	95/95 (100%)	87 (92%)	8 (8%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	8/8 (100%)	8 (100%)	0	100	100
3	Q	8/8 (100%)	8 (100%)	0	100	100
3	R	8/8 (100%)	8 (100%)	0	100	100
3	S	8/8 (100%)	8 (100%)	0	100	100
All	All	1351/1356 (100%)	1247 (92%)	104 (8%)	12	25

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	35	ARG
1	A	54	GLN
1	A	115	GLN
1	A	128	GLU
1	A	151	SER
1	A	173	GLU
1	A	177	GLU
1	A	179	LEU
1	A	187	THR
1	A	196	ASP
1	A	200	THR
1	A	215	LEU
1	A	216	THR
1	A	225	THR
1	A	231	VAL
2	B	12	ARG
2	B	45	ARG
2	B	89	GLN
2	B	93	VAL
2	B	94	LYS
1	C	5	LEU
1	C	6	LYS
1	C	14	ARG
1	C	19	GLU
1	C	21	ARG
1	C	35	ARG
1	C	36	PHE
1	C	54	GLN
1	C	62	ARG
1	C	106	ASP
1	C	108	ARG

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Mol	Chain	Res	Type
1	C	115	GLN
1	C	124	LEU
1	C	131	ARG
1	C	145	GLN
1	C	152	GLU
1	C	157	ARG
1	C	161	GLU
1	C	166	GLU
1	C	174	LYS
1	C	178	THR
1	C	179	LEU
1	C	186	LYS
1	C	212	GLU
1	C	255	GLN
1	C	272	LEU
2	D	51	HIS
2	D	91	LYS
2	D	93	VAL
1	E	14	ARG
1	E	15	PRO
1	E	17	ARG
1	E	19	GLU
1	E	21	ARG
1	E	35	ARG
1	E	39	ASP
1	E	55	GLU
1	E	62	ARG
1	E	88	SER
1	E	92	SER
1	E	108	ARG
1	E	141	GLN
1	E	177	GLU
1	E	179	LEU
1	E	180	LEU
1	E	232	GLU
1	E	255	GLN
1	E	268	GLU
1	E	272	LEU
2	F	12	ARG
2	F	17	ASN
2	F	34	ASP
2	F	74	GLU

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Mol	Chain	Res	Type
2	F	93	VAL
1	G	14	ARG
1	G	21	ARG
1	G	35	ARG
1	G	39	ASP
1	G	42	SER
1	G	62	ARG
1	G	72	GLN
1	G	89	GLU
1	G	106	ASP
1	G	115	GLN
1	G	121	LYS
1	G	138	THR
1	G	141	GLN
1	G	145	GLN
1	G	154	GLU
1	G	162	ASP
1	G	179	LEU
1	G	187	THR
1	G	222	GLU
1	G	225	THR
1	G	251	SER
2	H	1	ILE
2	H	33	SER
2	H	47	GLU
2	H	53	ASP
2	H	81	ARG
2	H	89	GLN
2	H	93	VAL
2	H	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	87	GLN
1	A	115	GLN
1	A	191	HIS
1	A	197	HIS
1	A	218	GLN
1	A	219	GLN
1	A	260	HIS

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Mol	Chain	Res	Type
1	A	263	HIS
2	B	17	ASN
2	B	42	ASN
2	B	51	HIS
2	B	89	GLN
1	C	87	GLN
1	C	93	HIS
1	C	115	GLN
1	C	127	ASN
1	C	145	GLN
1	C	226	GLN
1	C	263	HIS
2	D	42	ASN
1	E	87	GLN
1	E	169	HIS
1	E	255	GLN
1	E	263	HIS
2	F	17	ASN
2	F	89	GLN
1	G	3	HIS
1	G	72	GLN
1	G	87	GLN
1	G	99	HIS
1	G	115	GLN
1	G	155	HIS
1	G	156	GLN
1	G	191	HIS
1	G	192	HIS
1	G	219	GLN
1	G	242	GLN
1	G	263	HIS
2	H	2	GLN
2	H	17	ASN
2	H	42	ASN
2	H	89	GLN

5.3.3 RNA ⓘ

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](#)

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	273/273 (100%)	0.13	8 (2%) 53 49	13, 25, 48, 79	0
1	C	273/273 (100%)	0.57	21 (7%) 19 17	6, 27, 56, 72	0
1	E	267/273 (97%)	0.23	4 (1%) 72 68	11, 25, 47, 58	0
1	G	273/273 (100%)	0.34	9 (3%) 49 45	12, 26, 43, 63	0
2	B	100/100 (100%)	-0.15	0 100 100	14, 24, 43, 53	0
2	D	100/100 (100%)	0.20	4 (4%) 42 38	13, 26, 42, 82	0
2	F	100/100 (100%)	0.45	5 (5%) 34 30	14, 27, 42, 62	0
2	H	100/100 (100%)	0.88	11 (11%) 10 8	17, 27, 37, 44	0
3	P	9/9 (100%)	-0.35	0 100 100	23, 24, 28, 29	0
3	Q	9/9 (100%)	0.99	2 (22%) 2 2	19, 22, 25, 26	0
3	R	9/9 (100%)	0.28	0 100 100	12, 21, 25, 26	0
3	S	9/9 (100%)	0.49	0 100 100	14, 16, 21, 24	0
All	All	1522/1528 (99%)	0.33	64 (4%) 40 36	6, 26, 47, 82	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	THR	5.8
1	C	224	HIS	5.7
1	C	160	LEU	5.3
1	G	42	SER	5.3
1	G	222	GLU	4.5
1	C	223	GLY	4.4
1	C	227	ASP	4.2
2	F	0	MET	3.9
1	C	168	LEU	3.9
1	G	223	GLY	3.7
1	A	226	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	225	THR	3.6
1	G	40	ALA	3.6
2	H	1	ILE	3.6
1	A	227	ASP	3.5
1	A	223	GLY	3.5
1	C	158	ALA	3.3
1	C	6	LYS	3.3
1	A	224	HIS	3.2
1	C	226	GLN	3.2
1	G	41	ALA	3.1
2	D	77	GLU	2.9
2	H	57	SER	2.7
2	D	0	MET	2.7
1	A	42	SER	2.7
2	F	75	LYS	2.7
2	F	60	TRP	2.7
2	F	1	ILE	2.6
1	E	91	GLY	2.6
1	A	222	GLU	2.6
1	C	161	GLU	2.6
2	D	1	ILE	2.6
2	H	60	TRP	2.5
1	C	110	LEU	2.5
1	C	101	CYS	2.5
1	C	107	ARG	2.5
2	H	3	ARG	2.5
1	E	92	SER	2.5
1	C	40	ALA	2.4
2	H	85	VAL	2.4
2	H	4	THR	2.3
1	C	112	GLY	2.3
2	D	47	GLU	2.3
1	C	197	HIS	2.3
1	C	103	LEU	2.3
1	G	236	ALA	2.2
1	G	221	GLY	2.2
1	G	248	VAL	2.2
1	E	57	SER	2.2
2	H	61	SER	2.2
1	A	220	ASP	2.2
2	H	62	PHE	2.2
1	C	41	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	177	GLU	2.1
2	H	88	SER	2.1
2	H	90	PRO	2.1
1	C	52	MET	2.1
3	Q	1	VAL	2.1
3	Q	9	LEU	2.1
2	F	57	SER	2.1
1	G	266	LEU	2.1
1	C	171	TYR	2.0
1	E	90	ALA	2.0
2	H	48	LYS	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.