



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 AM UTC

PDB ID : 1VAX / pdb_00001vax
Title : Crystal Structure of Uricase from *Arthrobacter globiformis*
Authors : Hossain, M.T.; Suzuki, K.; Yamamoto, T.; Imamura, S.; Sekiguchi, T.; Takenaka, A.
Deposited on : 2004-02-19
Resolution : 1.99 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

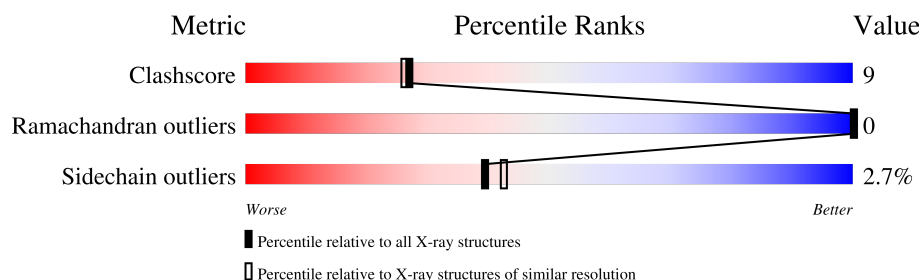
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	83% 15% .
1	B	287	80% 17% .
1	C	287	76% 21% .
1	D	287	81% 18% .
1	E	287	76% 22% .
1	F	287	80% 17% .
1	G	287	82% 17% .
1	H	287	80% 17% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20135 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 Uric acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	B	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	C	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	D	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	E	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	F	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	G	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			
1	H	287	Total	C	N	O	S	0	0	0
			2282	1435	408	436	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	245	Total	O	0	0
			245	245		
2	B	225	Total	O	0	0
			225	225		
2	C	239	Total	O	0	0
			239	239		
2	D	242	Total	O	0	0
			242	242		
2	E	222	Total	O	0	0
			222	222		
2	F	247	Total	O	0	0
			247	247		

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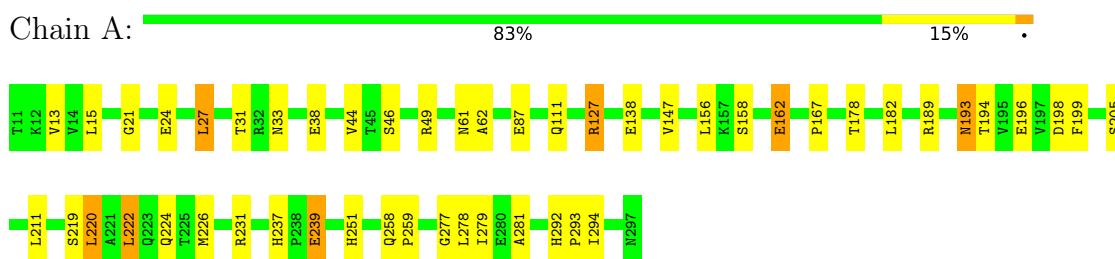
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	232	Total 232	O 232	0	0
2	H	227	Total 227	O 227	0	0

3 Residue-property plots [i](#)

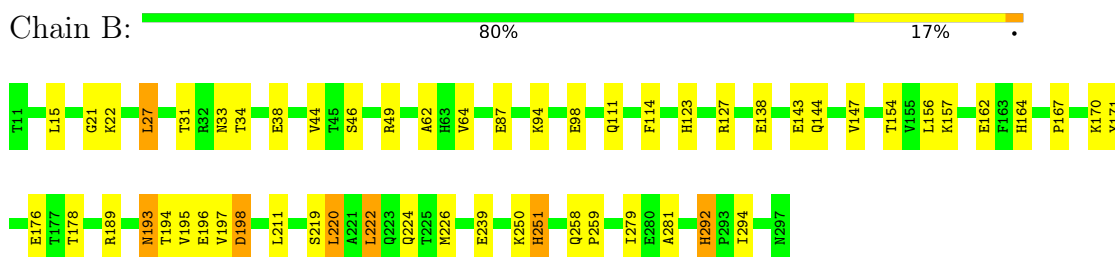
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

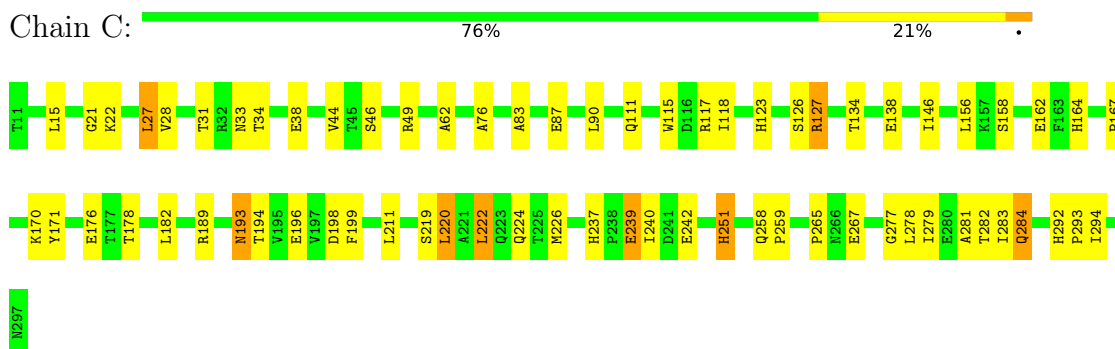
• Molecule 1: Uric acid oxidase



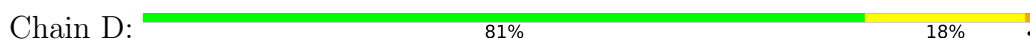
• Molecule 1: Uric acid oxidase

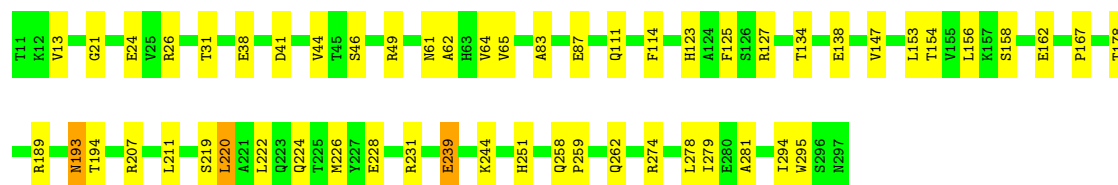


• Molecule 1: Uric acid oxidase

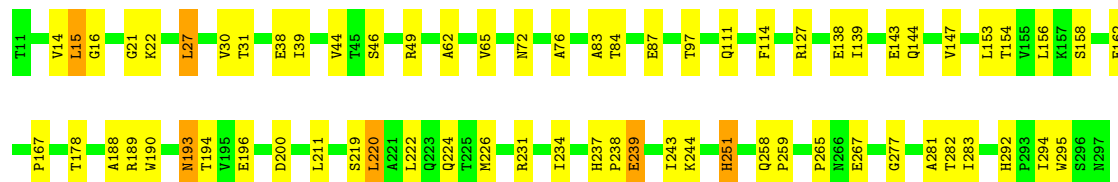


• Molecule 1: Uric acid oxidase

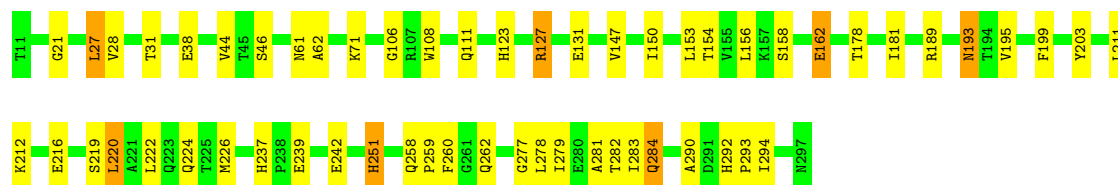
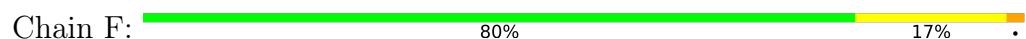




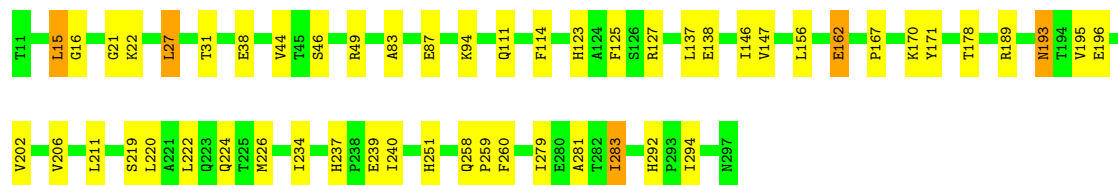
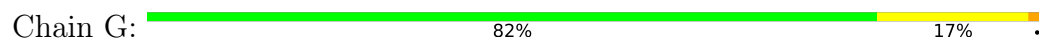
- Molecule 1: Uric acid oxidase



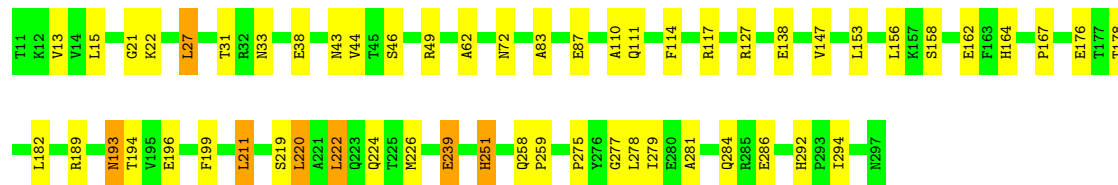
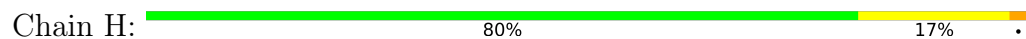
- Molecule 1: Uric acid oxidase



- Molecule 1: Uric acid oxidase



- Molecule 1: Uric acid oxidase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.43Å 122.54Å 284.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.99	Depositor
% Data completeness (in resolution range)	93.9 (10.00-1.99)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20135	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/2334	0.88	9/3167 (0.3%)
1	B	0.35	0/2334	0.86	9/3167 (0.3%)
1	C	0.35	0/2334	0.86	8/3167 (0.3%)
1	D	0.35	0/2334	0.87	9/3167 (0.3%)
1	E	0.35	0/2334	0.85	7/3167 (0.2%)
1	F	0.36	0/2334	0.88	9/3167 (0.3%)
1	G	0.36	0/2334	0.86	4/3167 (0.1%)
1	H	0.35	0/2334	0.88	9/3167 (0.3%)
All	All	0.36	0/18672	0.86	64/25336 (0.3%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	VAL	N-CA-C	7.63	117.62	106.55
1	B	219	SER	N-CA-C	6.86	119.67	109.59
1	H	33	ASN	N-CA-C	-6.76	103.84	111.14
1	H	199	PHE	N-CA-C	6.36	118.75	111.11
1	B	64	VAL	N-CA-C	6.24	116.70	107.15
1	E	220	LEU	N-CA-C	-6.19	105.68	113.72
1	F	44	VAL	N-CA-C	6.16	117.89	108.71
1	D	44	VAL	N-CA-C	6.09	117.79	108.71
1	C	220	LEU	N-CA-C	-6.07	105.91	113.38
1	E	65	VAL	N-CA-C	-6.07	100.82	108.84
1	D	111	GLN	N-CA-C	-6.06	99.83	109.59
1	C	44	VAL	N-CA-C	6.05	117.73	108.71
1	D	251	HIS	N-CA-C	6.02	118.93	109.96
1	H	219	SER	N-CA-C	5.97	118.38	109.25
1	E	251	HIS	N-CA-C	5.95	118.97	110.10
1	B	44	VAL	N-CA-C	5.94	117.56	108.71
1	A	111	GLN	N-CA-C	-5.85	100.17	109.59
1	H	277	GLY	N-CA-C	-5.82	104.63	112.14
1	H	111	GLN	N-CA-C	-5.79	100.27	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	44	VAL	N-CA-C	5.77	117.30	108.71
1	H	220	LEU	N-CA-C	-5.76	106.29	113.38
1	G	44	VAL	N-CA-C	5.72	117.24	108.71
1	A	199	PHE	N-CA-C	5.71	117.96	111.11
1	E	111	GLN	N-CA-C	-5.60	100.57	109.59
1	D	220	LEU	N-CA-C	-5.59	106.50	113.38
1	D	61	ASN	N-CA-C	5.59	119.19	112.93
1	H	251	HIS	N-CA-C	5.54	118.21	109.96
1	A	44	VAL	N-CA-C	5.54	116.96	108.71
1	F	219	SER	N-CA-C	5.53	117.72	109.59
1	E	44	VAL	N-CA-C	5.51	116.92	108.71
1	A	219	SER	N-CA-C	5.46	118.44	109.76
1	A	198	ASP	N-CA-C	-5.45	99.08	108.56
1	D	219	SER	N-CA-C	5.42	118.38	109.76
1	F	111	GLN	N-CA-C	-5.41	100.89	109.59
1	B	251	HIS	N-CA-C	5.40	118.15	110.10
1	A	220	LEU	N-CA-C	-5.40	106.70	113.72
1	B	111	GLN	N-CA-C	-5.39	100.91	109.59
1	C	251	HIS	N-CA-C	5.38	118.12	110.10
1	C	199	PHE	N-CA-C	5.38	117.56	111.11
1	C	111	GLN	N-CA-C	-5.37	100.94	109.59
1	G	111	GLN	N-CA-C	-5.33	101.01	109.59
1	C	277	GLY	N-CA-C	-5.29	105.31	112.14
1	F	277	GLY	N-CA-C	-5.28	105.33	112.14
1	C	198	ASP	N-CA-C	-5.26	99.40	108.56
1	G	219	SER	N-CA-C	5.25	118.11	109.76
1	D	24	GLU	N-CA-C	5.23	118.46	111.24
1	A	61	ASN	N-CA-C	5.22	118.77	112.93
1	B	292	HIS	CA-C-N	5.20	125.00	119.28
1	B	292	HIS	C-N-CA	5.20	125.00	119.28
1	E	219	SER	N-CA-C	5.19	118.01	109.76
1	G	251	HIS	N-CA-C	5.18	117.82	110.10
1	F	199	PHE	N-CA-C	5.17	117.32	111.11
1	A	251	HIS	N-CA-C	5.17	117.67	109.96
1	B	198	ASP	N-CA-C	-5.15	101.89	109.62
1	H	284	GLN	N-CA-C	5.14	117.22	109.41
1	D	65	VAL	N-CA-C	-5.12	102.08	108.84
1	C	219	SER	N-CA-C	5.11	117.10	109.59
1	F	251	HIS	N-CA-C	5.10	117.70	110.10
1	F	220	LEU	N-CA-C	-5.09	106.75	113.17
1	F	290	ALA	N-CA-C	5.09	116.64	111.14
1	F	61	ASN	N-CA-C	5.09	118.52	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	N-CA-C	-5.08	107.13	113.38
1	A	277	GLY	N-CA-C	-5.06	105.61	112.14
1	E	277	GLY	N-CA-C	-5.05	105.62	112.14

There are no chirality outliers.

There are no planarity outliers.

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	2282	0	2177	29	0
1	B	2282	0	2177	42	0
1	C	2282	0	2177	60	0
1	D	2282	0	2177	43	0
1	E	2282	0	2177	53	0
1	F	2282	0	2177	51	0
1	G	2282	0	2177	43	0
1	H	2282	0	2177	46	0
2	A	245	0	0	0	0
2	B	225	0	0	1	0
2	C	239	0	0	0	0
2	D	242	0	0	0	0
2	E	222	0	0	1	0
2	F	247	0	0	2	0
2	G	232	0	0	1	0
2	H	227	0	0	0	0
All	All	20135	0	17416	329	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (329) 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:F:131:GLU:HB2	1:F:150:ILE:HD11	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:HIS:HD2	1:A:294:ILE:H	1.25	0.83
1:F:150:ILE:HD13	1:F:203:TYR:OH	1.79	0.82
1:C:292:HIS:HD2	1:C:294:ILE:H	1.28	0.81
1:E:194:THR:OG1	1:E:196:GLU:HG2	1.80	0.80
1:H:162:GLU:HB3	1:H:178:THR:HA	1.66	0.77
1:C:237:HIS:HB3	1:C:240:ILE:HD13	1.67	0.76
1:A:62:ALA:O	1:D:167:PRO:HG3	1.85	0.76
1:E:147:VAL:HG23	1:E:294:ILE:HD13	1.67	0.76
1:E:292:HIS:HD2	1:E:294:ILE:H	1.33	0.76
1:G:239:GLU:HG2	1:G:240:ILE:HD12	1.66	0.76
1:C:118:ILE:HD11	1:C:126:SER:HB3	1.69	0.74
1:B:144:GLN:HE21	1:B:195:VAL:HG11	1.51	0.74
1:A:162:GLU:HB3	1:A:178:THR:HA	1.70	0.73
1:E:231:ARG:HG3	1:H:13:VAL:HG21	1.68	0.73
1:H:292:HIS:HD2	1:H:294:ILE:H	1.34	0.73
1:C:239:GLU:HG2	1:C:240:ILE:HD12	1.70	0.73
1:F:162:GLU:HB3	1:F:178:THR:HA	1.71	0.73
1:F:292:HIS:HD2	1:F:294:ILE:H	1.36	0.73
1:H:194:THR:OG1	1:H:196:GLU:HG2	1.92	0.70
1:E:234:ILE:HD12	1:E:283:ILE:HG22	1.73	0.69
1:F:153:LEU:HD21	1:F:211:LEU:HD11	1.72	0.69
1:C:193:ASN:C	1:C:193:ASN:HD22	2.01	0.69
1:C:237:HIS:CB	1:C:240:ILE:HD13	2.23	0.69
1:F:31:THR:HB	1:F:38:GLU:HB2	1.73	0.69
1:D:207:ARG:O	1:D:211:LEU:HD13	1.92	0.68
1:G:220:LEU:H	1:G:224:GLN:NE2	1.92	0.68
1:B:21:GLY:HA3	1:B:46:SER:O	1.93	0.68
1:E:21:GLY:HA3	1:E:46:SER:O	1.94	0.66
1:G:234:ILE:HD12	1:G:283:ILE:HG22	1.77	0.66
1:F:158:SER:HA	1:F:181:ILE:HD13	1.77	0.66
1:G:147:VAL:HG23	1:G:294:ILE:HD13	1.78	0.66
1:G:162:GLU:HB3	1:G:178:THR:HA	1.77	0.66
1:D:226:MET:HE3	1:D:281:ALA:HB3	1.78	0.66
1:G:226:MET:HE3	1:G:281:ALA:HB3	1.79	0.66
1:A:167:PRO:HG3	1:D:62:ALA:O	1.96	0.65
1:C:226:MET:HE3	1:C:281:ALA:HB3	1.77	0.65
1:D:153:LEU:HD21	1:D:211:LEU:HD11	1.78	0.65
1:F:220:LEU:H	1:F:224:GLN:NE2	1.94	0.65
1:E:153:LEU:HD21	1:E:211:LEU:HD21	1.78	0.65
1:H:220:LEU:H	1:H:224:GLN:NE2	1.95	0.64
1:D:162:GLU:HB3	1:D:178:THR:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ASN:C	1:F:193:ASN:HD22	2.03	0.64
1:G:189:ARG:HG3	1:G:189:ARG:HH11	1.62	0.64
1:E:22:LYS:NZ	1:H:251:HIS:HE1	1.95	0.64
1:B:292:HIS:HD2	1:B:294:ILE:H	1.46	0.64
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.64	0.63
1:B:220:LEU:H	1:B:224:GLN:NE2	1.96	0.63
1:H:49:ARG:HH12	1:H:138:GLU:CD	2.07	0.63
1:C:220:LEU:H	1:C:224:GLN:NE2	1.96	0.63
1:E:31:THR:HB	1:E:38:GLU:HB2	1.79	0.63
1:F:226:MET:HE3	1:F:281:ALA:HB3	1.80	0.63
1:C:33:ASN:OD1	1:C:34:THR:HG23	1.98	0.62
1:C:170:LYS:HE3	1:C:171:TYR:CZ	2.35	0.62
1:D:220:LEU:H	1:D:224:GLN:NE2	1.98	0.62
1:B:33:ASN:OD1	1:B:34:THR:HG23	2.00	0.62
1:H:83:ALA:HB3	1:H:87:GLU:OE2	2.00	0.62
1:B:144:GLN:NE2	1:B:195:VAL:HG11	2.14	0.61
1:B:226:MET:HE3	1:B:281:ALA:HB3	1.81	0.61
1:E:143:GLU:HG2	1:E:144:GLN:N	2.15	0.61
1:F:21:GLY:HA3	1:F:46:SER:O	2.00	0.61
1:A:226:MET:HE3	1:A:281:ALA:HB3	1.81	0.61
1:D:193:ASN:C	1:D:193:ASN:HD22	2.08	0.61
1:G:283:ILE:HD12	1:G:283:ILE:N	2.15	0.61
1:C:162:GLU:HB3	1:C:178:THR:HA	1.83	0.61
1:F:189:ARG:HG3	1:F:189:ARG:HH11	1.66	0.61
1:B:147:VAL:HG23	1:B:294:ILE:HD13	1.83	0.61
1:H:31:THR:HB	1:H:38:GLU:HB2	1.83	0.61
1:A:49:ARG:HH12	1:A:138:GLU:CD	2.08	0.60
1:A:220:LEU:H	1:A:224:GLN:NE2	1.99	0.60
1:B:162:GLU:HB3	1:B:178:THR:HA	1.82	0.60
1:F:62:ALA:O	1:G:167:PRO:HG3	2.01	0.60
1:G:193:ASN:C	1:G:193:ASN:HD22	2.08	0.60
1:E:220:LEU:H	1:E:224:GLN:NE2	1.99	0.59
1:G:137:LEU:HD13	1:G:146:ILE:HD11	1.84	0.59
1:B:27:LEU:C	1:B:27:LEU:HD13	2.28	0.59
1:E:83:ALA:HB3	1:E:87:GLU:OE2	2.02	0.59
1:A:239:GLU:CD	1:A:239:GLU:H	2.08	0.59
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.66	0.59
1:F:158:SER:HA	1:F:181:ILE:CD1	2.33	0.59
1:G:196:GLU:O	1:G:196:GLU:HG3	2.03	0.59
1:E:76:ALA:HA	1:F:262:GLN:HE22	1.68	0.58
1:A:21:GLY:HA3	1:A:46:SER:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:GLY:HA3	1:H:46:SER:O	2.03	0.58
1:B:194:THR:OG1	1:B:196:GLU:HG2	2.03	0.58
1:B:156:LEU:HD23	1:B:156:LEU:C	2.29	0.58
1:E:27:LEU:HD13	1:E:27:LEU:C	2.28	0.58
1:E:62:ALA:O	1:H:167:PRO:HG3	2.04	0.58
1:D:244:LYS:HZ2	1:D:295:TRP:CG	2.21	0.58
1:B:143:GLU:HG2	1:B:144:GLN:N	2.18	0.57
1:C:189:ARG:HG3	1:C:189:ARG:HH11	1.70	0.57
1:F:237:HIS:HB3	1:F:239:GLU:OE2	2.05	0.57
1:B:193:ASN:C	1:B:193:ASN:HD22	2.13	0.57
1:E:189:ARG:O	1:E:243:ILE:HD12	2.05	0.57
1:C:239:GLU:HG2	1:C:240:ILE:CD1	2.35	0.56
1:G:226:MET:HE3	1:G:281:ALA:CB	2.34	0.56
1:C:21:GLY:HA3	1:C:46:SER:O	2.04	0.56
1:D:31:THR:HB	1:D:38:GLU:HB2	1.86	0.56
1:E:162:GLU:HB3	1:E:178:THR:HA	1.87	0.56
1:B:31:THR:HB	1:B:38:GLU:HB2	1.86	0.56
1:G:31:THR:HB	1:G:38:GLU:HB2	1.88	0.56
1:E:22:LYS:NZ	1:H:251:HIS:CE1	2.72	0.56
1:E:158:SER:OG	1:F:123:HIS:HB2	2.06	0.55
1:B:22:LYS:HZ2	1:C:251:HIS:CE1	2.23	0.55
1:C:283:ILE:N	1:C:283:ILE:HD12	2.21	0.55
1:E:22:LYS:HZ3	1:H:251:HIS:HE1	1.54	0.55
1:H:189:ARG:HG3	1:H:189:ARG:HH11	1.71	0.55
1:A:193:ASN:C	1:A:193:ASN:HD22	2.15	0.55
1:B:167:PRO:HG3	1:C:62:ALA:O	2.07	0.55
1:E:193:ASN:C	1:E:193:ASN:HD22	2.14	0.55
1:D:226:MET:HE3	1:D:281:ALA:CB	2.36	0.55
1:D:21:GLY:HA3	1:D:46:SER:O	2.07	0.54
1:A:27:LEU:HD13	1:A:27:LEU:C	2.32	0.54
1:E:167:PRO:HG3	1:H:62:ALA:O	2.08	0.54
1:E:190:TRP:HB3	1:E:243:ILE:HD13	1.90	0.54
1:C:170:LYS:HE3	1:C:171:TYR:CE2	2.42	0.54
1:D:189:ARG:HG3	1:D:189:ARG:HH11	1.71	0.54
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.73	0.53
1:E:188:ALA:HB1	1:E:243:ILE:HD11	1.89	0.53
1:F:242:GLU:HB3	1:F:284:GLN:HB3	1.90	0.53
1:A:158:SER:OG	1:B:123:HIS:HB2	2.09	0.53
1:B:49:ARG:HH12	1:B:138:GLU:CD	2.16	0.53
1:D:193:ASN:HD22	1:D:194:THR:HG22	1.74	0.53
1:F:147:VAL:HG23	1:F:294:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:HIS:CE1	1:G:22:LYS:HZ2	2.27	0.53
1:D:83:ALA:HB3	1:D:87:GLU:OE2	2.09	0.53
1:C:83:ALA:N	1:C:87:GLU:OE2	2.38	0.52
1:C:90:LEU:HD21	1:C:146:ILE:HD11	1.90	0.52
1:E:283:ILE:N	1:E:283:ILE:HD12	2.24	0.52
1:F:156:LEU:C	1:F:156:LEU:HD23	2.34	0.52
1:C:220:LEU:HB2	1:C:224:GLN:NE2	2.25	0.52
1:B:170:LYS:HE3	1:B:171:TYR:CZ	2.45	0.52
1:C:182:LEU:HD11	1:C:222:LEU:HG	1.91	0.52
1:F:278:LEU:C	1:F:279:ILE:HD12	2.35	0.52
1:B:196:GLU:O	1:B:196:GLU:HG3	2.09	0.52
1:C:258:GLN:NE2	1:C:258:GLN:HA	2.25	0.52
1:C:118:ILE:CD1	1:C:126:SER:HB3	2.39	0.52
1:C:189:ARG:HG3	1:C:189:ARG:NH1	2.25	0.52
1:F:226:MET:HE3	1:F:281:ALA:CB	2.39	0.52
1:C:76:ALA:HB1	1:D:262:GLN:HE22	1.76	0.51
1:C:226:MET:HE3	1:C:281:ALA:CB	2.39	0.51
1:E:193:ASN:HD21	1:E:239:GLU:HA	1.76	0.51
1:B:292:HIS:CD2	1:B:294:ILE:H	2.25	0.51
1:F:239:GLU:CD	1:F:239:GLU:H	2.19	0.51
1:H:127:ARG:HH11	1:H:127:ARG:HG2	1.75	0.51
1:H:226:MET:HE3	1:H:281:ALA:HB3	1.92	0.51
1:C:240:ILE:HD12	1:C:240:ILE:N	2.26	0.51
1:G:21:GLY:HA3	1:G:46:SER:O	2.11	0.51
1:H:156:LEU:C	1:H:156:LEU:HD23	2.36	0.50
1:F:212:LYS:HZ1	1:F:216:GLU:CD	2.20	0.50
1:E:244:LYS:HZ2	1:E:295:TRP:CG	2.29	0.50
1:G:239:GLU:HG2	1:G:240:ILE:CD1	2.37	0.50
1:F:283:ILE:N	1:F:283:ILE:HD12	2.26	0.50
1:B:22:LYS:NZ	1:C:251:HIS:CE1	2.79	0.50
1:H:162:GLU:CB	1:H:178:THR:HA	2.39	0.50
1:A:156:LEU:C	1:A:156:LEU:HD23	2.37	0.49
1:E:226:MET:HE3	1:E:281:ALA:HB3	1.93	0.49
1:H:162:GLU:HB3	1:H:178:THR:CA	2.39	0.49
1:G:94:LYS:HD2	2:G:6136:HOH:O	2.11	0.49
1:G:237:HIS:HB3	1:G:239:GLU:OE2	2.13	0.49
1:B:193:ASN:HD21	1:B:239:GLU:HA	1.77	0.49
1:D:114:PHE:O	1:D:127:ARG:HD2	2.12	0.49
1:D:193:ASN:ND2	1:D:194:THR:HG22	2.28	0.49
1:A:226:MET:HE3	1:A:281:ALA:CB	2.43	0.49
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:HG3	1:B:189:ARG:NH1	2.28	0.49
1:D:127:ARG:HG2	1:D:127:ARG:HH11	1.77	0.49
1:F:153:LEU:CD2	1:F:211:LEU:HD11	2.39	0.49
1:H:27:LEU:HD13	1:H:27:LEU:C	2.38	0.49
1:B:87:GLU:HB2	2:B:338:HOH:O	2.12	0.49
1:C:265:PRO:HG2	1:C:267:GLU:OE2	2.12	0.49
1:D:147:VAL:HG23	1:D:294:ILE:HD13	1.95	0.49
1:G:83:ALA:HB3	1:G:87:GLU:OE2	2.12	0.49
1:C:242:GLU:HB3	1:C:284:GLN:HB3	1.95	0.49
1:F:226:MET:HE1	1:F:279:ILE:HG22	1.95	0.48
1:C:134:THR:HG21	1:C:189:ARG:NH2	2.28	0.48
1:A:13:VAL:HG21	1:D:231:ARG:HG3	1.96	0.48
1:B:94:LYS:HG3	1:B:98:GLU:OE2	2.11	0.48
1:G:292:HIS:HD2	1:G:294:ILE:H	1.60	0.48
1:B:226:MET:HE3	1:B:281:ALA:CB	2.43	0.48
1:C:158:SER:OG	1:D:123:HIS:HB2	2.13	0.48
1:G:195:VAL:HG12	1:G:195:VAL:O	2.14	0.48
1:H:164:HIS:HB3	1:H:176:GLU:HB3	1.96	0.48
1:C:38:GLU:OE2	1:C:117:ARG:NH2	2.47	0.48
1:E:156:LEU:HD23	1:E:156:LEU:C	2.39	0.47
1:H:162:GLU:HG3	1:H:220:LEU:HD23	1.95	0.47
1:B:114:PHE:O	1:B:127:ARG:HD2	2.14	0.47
1:E:237:HIS:HB3	1:E:239:GLU:OE2	2.14	0.47
1:G:234:ILE:HD11	1:G:283:ILE:O	2.15	0.47
1:D:156:LEU:C	1:D:156:LEU:HD23	2.39	0.47
1:G:127:ARG:HG2	1:G:127:ARG:HH11	1.79	0.47
1:D:228:GLU:OE2	1:D:231:ARG:NH2	2.47	0.47
1:E:189:ARG:HG3	1:E:189:ARG:NH1	2.30	0.47
1:F:226:MET:CE	1:F:279:ILE:HG22	2.45	0.47
1:B:62:ALA:O	1:C:167:PRO:HG3	2.15	0.47
1:H:153:LEU:HD21	1:H:211:LEU:HD11	1.96	0.47
1:C:278:LEU:C	1:C:279:ILE:HD12	2.39	0.47
1:F:162:GLU:HB3	1:F:178:THR:CA	2.43	0.47
1:G:202:VAL:O	1:G:206:VAL:HG23	2.14	0.47
1:F:251:HIS:CE1	1:G:22:LYS:NZ	2.84	0.46
1:A:194:THR:OG1	1:A:196:GLU:HG2	2.16	0.46
1:G:27:LEU:C	1:G:27:LEU:HD13	2.41	0.46
1:C:49:ARG:HH12	1:C:138:GLU:CD	2.24	0.46
1:H:147:VAL:HG23	1:H:294:ILE:HD13	1.98	0.46
1:D:162:GLU:HG3	1:D:220:LEU:HD23	1.97	0.46
1:E:30:VAL:HG22	1:E:39:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:ILE:HD12	1:F:279:ILE:N	2.30	0.45
1:E:22:LYS:HZ3	1:H:251:HIS:CE1	2.31	0.45
1:E:154:THR:HB	1:F:127:ARG:HB2	1.98	0.45
1:E:15:LEU:HD22	1:E:16:GLY:O	2.16	0.45
1:E:251:HIS:CE1	1:H:22:LYS:NZ	2.85	0.45
1:E:258:GLN:N	1:E:259:PRO:CD	2.80	0.45
1:G:162:GLU:HG3	1:G:220:LEU:HD23	1.98	0.45
1:D:134:THR:HG21	1:D:189:ARG:NH2	2.31	0.45
1:F:189:ARG:HG3	1:F:189:ARG:NH1	2.29	0.45
1:A:147:VAL:HG23	1:A:294:ILE:HD13	1.99	0.45
1:F:27:LEU:C	1:F:27:LEU:HD13	2.42	0.45
1:H:193:ASN:HD22	1:H:193:ASN:C	2.24	0.45
1:A:127:ARG:HB2	1:B:154:THR:HB	1.98	0.45
1:G:49:ARG:HH12	1:G:138:GLU:CD	2.24	0.45
1:E:22:LYS:HZ2	1:H:251:HIS:CE1	2.34	0.45
1:B:162:GLU:CB	1:B:178:THR:HA	2.46	0.45
1:C:279:ILE:HD12	1:C:279:ILE:N	2.32	0.45
1:C:115:TRP:CE2	1:C:127:ARG:HG2	2.52	0.44
1:G:226:MET:CE	1:G:279:ILE:HG22	2.48	0.44
1:H:278:LEU:C	1:H:279:ILE:HD12	2.42	0.44
1:A:24:GLU:HB3	1:D:274:ARG:HD2	2.00	0.44
1:C:258:GLN:N	1:C:259:PRO:CD	2.80	0.44
1:B:222:LEU:HD13	1:B:279:ILE:HB	1.99	0.44
1:C:164:HIS:HB3	1:C:176:GLU:HB3	1.99	0.44
1:C:282:THR:C	1:C:283:ILE:HD12	2.43	0.44
1:D:189:ARG:HG3	1:D:189:ARG:NH1	2.32	0.44
1:E:49:ARG:HH12	1:E:138:GLU:CD	2.25	0.44
1:C:156:LEU:C	1:C:156:LEU:HD23	2.43	0.44
1:D:49:ARG:HH12	1:D:138:GLU:CD	2.26	0.44
1:D:258:GLN:N	1:D:259:PRO:CD	2.80	0.44
1:E:84:THR:HG22	1:E:200:ASP:OD2	2.17	0.44
1:E:265:PRO:HG2	1:E:267:GLU:OE2	2.18	0.44
1:C:220:LEU:HB2	1:C:224:GLN:HE22	1.83	0.43
1:B:22:LYS:NZ	1:C:251:HIS:HE1	2.16	0.43
1:F:162:GLU:CB	1:F:178:THR:HA	2.42	0.43
1:A:278:LEU:C	1:A:279:ILE:HD12	2.43	0.43
1:C:27:LEU:HD22	1:C:28:VAL:N	2.33	0.43
1:D:239:GLU:H	1:D:239:GLU:CD	2.26	0.43
1:D:278:LEU:C	1:D:279:ILE:HD12	2.43	0.43
1:E:14:VAL:HG11	1:H:286:GLU:HG3	2.01	0.43
1:E:114:PHE:O	1:E:127:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HB	1:A:38:GLU:HB2	2.00	0.43
1:C:226:MET:CE	1:C:279:ILE:HG22	2.49	0.43
1:F:193:ASN:C	1:F:193:ASN:ND2	2.75	0.43
1:G:156:LEU:HD23	1:G:156:LEU:C	2.43	0.43
1:A:258:GLN:N	1:A:259:PRO:CD	2.82	0.43
1:C:194:THR:OG1	1:C:196:GLU:HG2	2.18	0.43
1:F:162:GLU:HG3	1:F:220:LEU:HD23	2.00	0.43
1:C:258:GLN:HA	1:C:258:GLN:HE21	1.83	0.43
1:E:189:ARG:C	1:E:243:ILE:HD12	2.43	0.43
1:E:251:HIS:CE1	1:H:22:LYS:HZ2	2.36	0.43
1:G:15:LEU:HD22	1:G:16:GLY:O	2.18	0.43
1:H:114:PHE:O	1:H:127:ARG:HD2	2.17	0.43
1:B:258:GLN:N	1:B:259:PRO:CD	2.82	0.42
1:H:258:GLN:N	1:H:259:PRO:CD	2.81	0.42
1:F:195:VAL:HG22	2:F:8025:HOH:O	2.18	0.42
1:H:182:LEU:HD11	1:H:222:LEU:HG	2.01	0.42
1:H:226:MET:CE	1:H:279:ILE:HG22	2.50	0.42
1:H:279:ILE:HD12	1:H:279:ILE:N	2.35	0.42
1:D:162:GLU:CB	1:D:178:THR:HA	2.47	0.42
1:B:156:LEU:HD23	1:B:157:LYS:N	2.34	0.42
1:B:164:HIS:HB3	1:B:176:GLU:HB3	2.02	0.42
1:C:193:ASN:HD21	1:C:239:GLU:HA	1.85	0.42
1:F:106:GLY:HA3	1:F:108:TRP:CH2	2.55	0.42
1:D:26:ARG:NH2	1:D:41:ASP:OD1	2.44	0.42
1:D:153:LEU:CD2	1:D:211:LEU:HD11	2.49	0.42
1:F:251:HIS:HD2	2:F:6158:HOH:O	2.02	0.42
1:F:282:THR:C	1:F:283:ILE:HD12	2.45	0.42
1:H:127:ARG:HG2	1:H:127:ARG:NH1	2.34	0.42
1:A:231:ARG:HG3	1:D:13:VAL:HG21	2.01	0.41
1:F:193:ASN:HD21	1:F:239:GLU:HA	1.85	0.41
1:G:125:PHE:CD1	1:G:125:PHE:N	2.88	0.41
1:C:31:THR:HB	1:C:38:GLU:HB2	2.01	0.41
1:G:123:HIS:HB2	1:H:158:SER:OG	2.20	0.41
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.35	0.41
1:C:162:GLU:CB	1:C:178:THR:HA	2.49	0.41
1:D:125:PHE:CD1	1:D:125:PHE:N	2.88	0.41
1:G:114:PHE:O	1:G:127:ARG:HD2	2.19	0.41
1:E:237:HIS:HA	1:E:238:PRO:HD3	1.93	0.41
1:F:292:HIS:HA	1:F:293:PRO:HD3	1.94	0.41
1:G:237:HIS:CB	1:G:240:ILE:HD13	2.50	0.41
1:G:258:GLN:N	1:G:259:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:GLN:N	1:F:259:PRO:CD	2.84	0.41
1:G:137:LEU:HD13	1:G:146:ILE:CD1	2.48	0.41
1:G:170:LYS:HE3	1:G:171:TYR:CE2	2.55	0.41
1:F:27:LEU:HD22	1:F:28:VAL:N	2.36	0.41
1:H:193:ASN:HD21	1:H:239:GLU:HA	1.85	0.41
1:C:123:HIS:HB2	1:D:158:SER:OG	2.20	0.41
1:D:258:GLN:NE2	1:D:258:GLN:HA	2.36	0.41
1:H:38:GLU:OE2	1:H:117:ARG:NH2	2.54	0.41
1:E:139:ILE:HG12	1:E:144:GLN:HB3	2.02	0.41
1:G:220:LEU:H	1:G:224:GLN:HE21	1.66	0.41
1:A:182:LEU:HD11	1:A:222:LEU:HG	2.03	0.41
1:A:292:HIS:HA	1:A:293:PRO:HD3	1.94	0.41
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.36	0.41
1:B:197:VAL:HG12	1:B:198:ASP:N	2.35	0.41
1:B:251:HIS:CE1	1:C:22:LYS:NZ	2.89	0.41
1:C:127:ARG:HB2	1:D:154:THR:HB	2.03	0.41
1:C:193:ASN:C	1:C:193:ASN:ND2	2.73	0.41
1:C:258:GLN:HE21	1:C:258:GLN:CA	2.33	0.41
1:D:127:ARG:HG2	1:D:127:ARG:NH1	2.35	0.41
1:H:43:ASN:O	1:H:110:ALA:HA	2.21	0.41
1:E:97:THR:HG21	1:E:139:ILE:HG21	2.03	0.41
1:F:220:LEU:H	1:F:224:GLN:HE21	1.68	0.41
1:F:292:HIS:CD2	1:F:294:ILE:H	2.27	0.41
1:D:162:GLU:HB3	1:D:178:THR:CA	2.51	0.40
1:E:234:ILE:CD1	1:E:283:ILE:HG22	2.47	0.40
1:G:283:ILE:N	1:G:283:ILE:CD1	2.83	0.40
1:H:292:HIS:CD2	1:H:294:ILE:H	2.25	0.40
1:A:196:GLU:O	1:A:196:GLU:HG3	2.21	0.40
2:E:7199:HOH:O	1:H:275:PRO:HD3	2.22	0.40
1:C:170:LYS:HE3	1:C:171:TYR:OH	2.21	0.40
1:D:226:MET:CE	1:D:279:ILE:HG22	2.51	0.40
1:E:282:THR:C	1:E:283:ILE:HD12	2.46	0.40
1:C:27:LEU:C	1:C:27:LEU:HD13	2.46	0.40
1:E:127:ARG:HB3	1:F:154:THR:HB	2.04	0.40
1:F:71:LYS:HE2	1:F:71:LYS:HB3	1.96	0.40
1:G:220:LEU:H	1:G:224:GLN:HE22	1.68	0.40
1:G:260:PHE:CZ	1:H:72:ASN:HB3	2.56	0.40
1:A:205:SER:OG	1:A:237:HIS:CE1	2.74	0.40
1:C:292:HIS:HA	1:C:293:PRO:HD3	1.95	0.40
1:E:72:ASN:HB3	1:F:260:PHE:CZ	2.57	0.40
1:H:189:ARG:HG3	1:H:189:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/287 (99%)	282 (99%)	3 (1%)	0	100	100
1	B	285/287 (99%)	281 (99%)	4 (1%)	0	100	100
1	C	285/287 (99%)	278 (98%)	7 (2%)	0	100	100
1	D	285/287 (99%)	281 (99%)	4 (1%)	0	100	100
1	E	285/287 (99%)	280 (98%)	5 (2%)	0	100	100
1	F	285/287 (99%)	281 (99%)	4 (1%)	0	100	100
1	G	285/287 (99%)	281 (99%)	4 (1%)	0	100	100
1	H	285/287 (99%)	282 (99%)	3 (1%)	0	100	100
All	All	2280/2296 (99%)	2246 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	236/240 (98%)	226 (96%)	10 (4%)	26	25
1	B	236/240 (98%)	230 (98%)	6 (2%)	42	45
1	C	236/240 (98%)	228 (97%)	8 (3%)	32	33
1	D	236/240 (98%)	233 (99%)	3 (1%)	61	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	236/240 (98%)	231 (98%)	5 (2%)	47	52
1	F	236/240 (98%)	230 (98%)	6 (2%)	42	45
1	G	236/240 (98%)	229 (97%)	7 (3%)	36	38
1	H	236/240 (98%)	230 (98%)	6 (2%)	42	45
All	All	1888/1920 (98%)	1837 (97%)	51 (3%)	39	42

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	27	LEU
1	A	33	ASN
1	A	87	GLU
1	A	127	ARG
1	A	162	GLU
1	A	193	ASN
1	A	211	LEU
1	A	222	LEU
1	A	239	GLU
1	B	15	LEU
1	B	27	LEU
1	B	193	ASN
1	B	211	LEU
1	B	222	LEU
1	B	250	LYS
1	C	15	LEU
1	C	27	LEU
1	C	127	ARG
1	C	193	ASN
1	C	211	LEU
1	C	222	LEU
1	C	239	GLU
1	C	284	GLN
1	D	193	ASN
1	D	222	LEU
1	D	239	GLU
1	E	15	LEU
1	E	27	LEU
1	E	193	ASN
1	E	222	LEU
1	E	239	GLU

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Mol	Chain	Res	Type
1	F	27	LEU
1	F	127	ARG
1	F	162	GLU
1	F	193	ASN
1	F	222	LEU
1	F	284	GLN
1	G	15	LEU
1	G	27	LEU
1	G	162	GLU
1	G	193	ASN
1	G	211	LEU
1	G	222	LEU
1	G	283	ILE
1	H	15	LEU
1	H	27	LEU
1	H	193	ASN
1	H	211	LEU
1	H	222	LEU
1	H	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	63	HIS
1	A	111	GLN
1	A	193	ASN
1	A	224	GLN
1	A	237	HIS
1	A	251	HIS
1	A	258	GLN
1	A	262	GLN
1	A	292	HIS
1	B	40	GLN
1	B	43	ASN
1	B	47	GLN
1	B	72	ASN
1	B	111	GLN
1	B	144	GLN
1	B	193	ASN
1	B	224	GLN
1	B	237	HIS

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Mol	Chain	Res	Type
1	B	251	HIS
1	B	258	GLN
1	B	262	GLN
1	B	292	HIS
1	C	43	ASN
1	C	47	GLN
1	C	63	HIS
1	C	72	ASN
1	C	111	GLN
1	C	119	ASN
1	C	193	ASN
1	C	224	GLN
1	C	237	HIS
1	C	251	HIS
1	C	258	GLN
1	C	262	GLN
1	C	284	GLN
1	C	292	HIS
1	D	18	ASN
1	D	43	ASN
1	D	47	GLN
1	D	63	HIS
1	D	70	GLN
1	D	72	ASN
1	D	111	GLN
1	D	119	ASN
1	D	144	GLN
1	D	193	ASN
1	D	224	GLN
1	D	237	HIS
1	D	251	HIS
1	D	258	GLN
1	D	262	GLN
1	D	292	HIS
1	E	43	ASN
1	E	47	GLN
1	E	111	GLN
1	E	119	ASN
1	E	193	ASN
1	E	224	GLN
1	E	237	HIS
1	E	251	HIS

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Mol	Chain	Res	Type
1	E	258	GLN
1	E	262	GLN
1	E	292	HIS
1	F	43	ASN
1	F	63	HIS
1	F	72	ASN
1	F	111	GLN
1	F	193	ASN
1	F	224	GLN
1	F	237	HIS
1	F	251	HIS
1	F	262	GLN
1	F	284	GLN
1	F	292	HIS
1	G	33	ASN
1	G	43	ASN
1	G	47	GLN
1	G	63	HIS
1	G	111	GLN
1	G	193	ASN
1	G	224	GLN
1	G	237	HIS
1	G	251	HIS
1	G	258	GLN
1	G	262	GLN
1	G	284	GLN
1	G	292	HIS
1	H	33	ASN
1	H	40	GLN
1	H	43	ASN
1	H	63	HIS
1	H	111	GLN
1	H	119	ASN
1	H	193	ASN
1	H	224	GLN
1	H	237	HIS
1	H	251	HIS
1	H	262	GLN
1	H	284	GLN
1	H	292	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.