



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 08:18 PM GMT

PDB ID : 1VAY
Title : Crystal Structure of Uricase from *Arthrobacter globiformis* with inhibitor 8-azaxanthine
Authors : Hossain, M.T.; Suzuki, K.; Yamamoto, T.; Imamura, S.; Sekiguchi, T.; Takenaka, A.
Deposited on : 2004-02-19
Resolution : 2.24 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

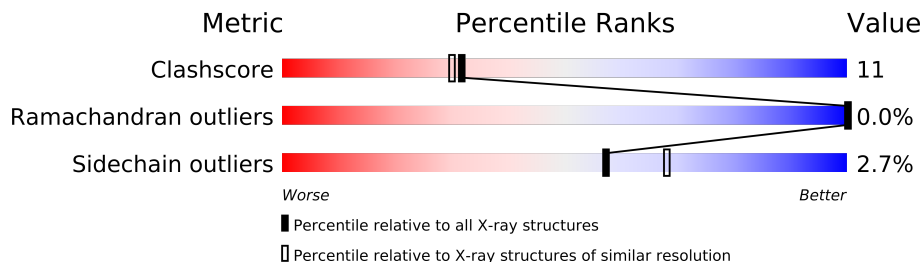
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.24 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	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	<div><div></div><div></div></div>
1	B	287	<div><div></div><div></div></div>
1	C	287	<div><div></div><div></div></div>
1	D	287	<div><div></div><div></div></div>
1	E	287	<div><div></div><div></div></div>
1	F	287	<div><div></div><div></div></div>
1	G	287	<div><div></div><div></div></div>
1	H	287	<div><div></div><div></div></div>

2 Entry composition

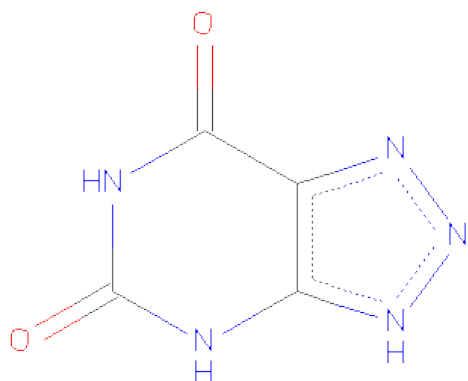
There are 3 unique types of molecules in this entry. The entry contains 19410 atoms, of which 0 are hydrogen and 0 are deuterium.

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 8-AZAXANTHINE (three-letter code: AZA) (formula: C₄H₃N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			11	4	5	2		
2	D	1	Total	C	N	O	0	0
			11	4	5	2		
2	B	1	Total	C	N	O	0	0
			11	4	5	2		
2	A	1	Total	C	N	O	0	0
			11	4	5	2		
2	H	1	Total	C	N	O	0	0
			11	4	5	2		
2	G	1	Total	C	N	O	0	0
			11	4	5	2		
2	F	1	Total	C	N	O	0	0
			11	4	5	2		
2	E	1	Total	C	N	O	0	0
			11	4	5	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	149	Total	O	0	0
			149	149		
3	C	107	Total	O	0	0
			107	107		
3	D	139	Total	O	0	0
			139	139		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	114	Total 114	O 114	0	0
3	F	146	Total 146	O 146	0	0
3	G	148	Total 148	O 148	0	0
3	H	113	Total 113	O 113	0	0

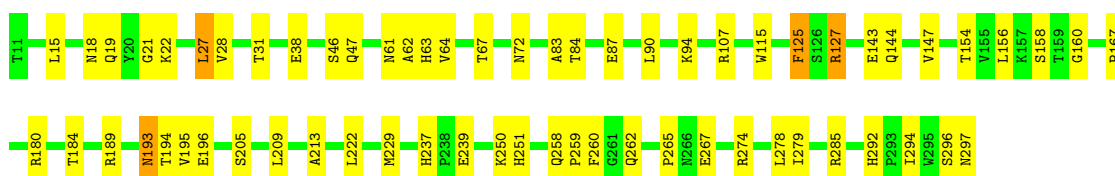
3 Residue-property plots

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

Note EDS was not executed.

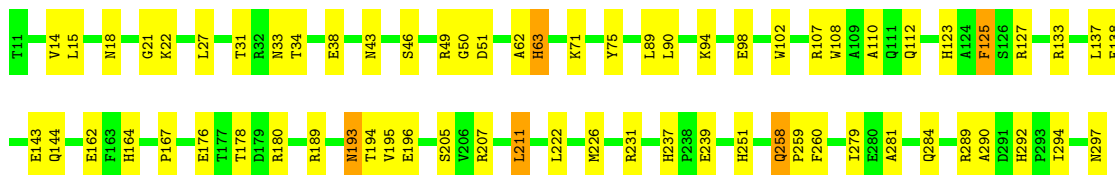
- Molecule 1: Uric acid oxidase

Chain A:



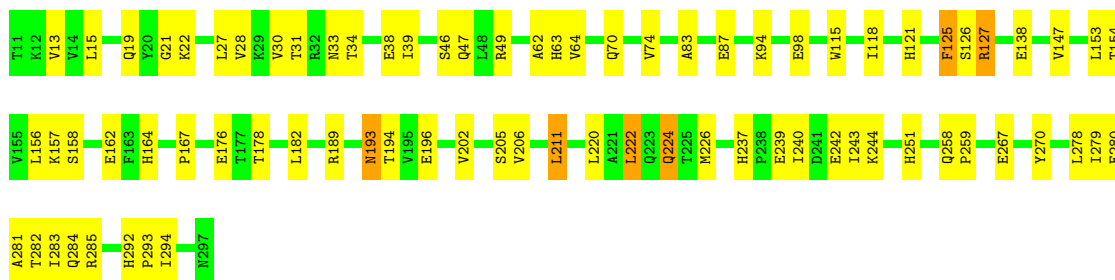
- Molecule 1: Uric acid oxidase

Chain B:



- Molecule 1: Uric acid oxidase

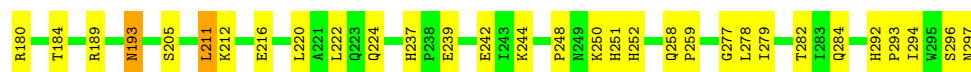
Chain C:



- Molecule 1: Uric acid oxidase

Chain D:





- Molecule 1: Uric acid oxidase

Chain E:



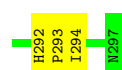
- Molecule 1: Uric acid oxidase

Chain F:



- Molecule 1: Uric acid oxidase

Chain G:



- Molecule 1: Uric acid oxidase

Chain H:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.33Å 122.28Å 283.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.24	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.24)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19410	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2334	0.62	0/3167
1	B	0.36	0/2334	0.63	0/3167
1	C	0.34	0/2334	0.61	0/3167
1	D	0.35	0/2334	0.61	0/3167
1	E	0.34	0/2334	0.61	0/3167
1	F	0.35	0/2334	0.62	0/3167
1	G	0.35	0/2334	0.63	0/3167
1	H	0.34	0/2334	0.59	0/3167
All	All	0.35	0/18672	0.62	0/25336

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2177	49	0
1	B	2282	0	2177	61	0
1	C	2282	0	2177	73	0
1	D	2282	0	2177	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2282	0	2177	54	0
1	F	2282	0	2177	50	0
1	G	2282	0	2177	72	0
1	H	2282	0	2177	52	0
2	A	11	0	3	1	0
2	B	22	0	6	1	0
2	D	11	0	3	1	0
2	E	11	0	3	1	0
2	F	11	0	3	1	0
2	G	11	0	3	2	0
2	H	11	0	3	2	0
3	A	150	0	0	2	0
3	B	149	0	0	2	0
3	C	107	0	0	0	0
3	D	139	0	0	3	0
3	E	114	0	0	0	0
3	F	146	0	0	2	0
3	G	148	0	0	3	0
3	H	113	0	0	1	0
All	All	19410	0	17440	411	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (411) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:15:LEU:HD21	1:E:18:ASN:ND2	1.89	0.88
1:H:162:GLU:HB3	1:H:178:THR:HA	1.59	0.82
1:E:292:HIS:HD2	1:E:294:ILE:H	1.28	0.82
1:B:289:ARG:HG3	1:G:143:GLU:OE2	1.80	0.82
1:F:22:LYS:HZ2	1:G:251:HIS:HE1	1.27	0.82
1:G:292:HIS:HD2	1:G:294:ILE:H	1.30	0.79
1:C:147:VAL:HG23	1:C:294:ILE:HD13	1.62	0.79
1:B:289:ARG:HA	1:G:143:GLU:HG2	1.64	0.79
1:C:118:ILE:HD11	1:C:126:SER:HB3	1.63	0.79
1:D:292:HIS:HD2	1:D:294:ILE:H	1.28	0.79
1:C:31:THR:HB	1:C:38:GLU:HB2	1.62	0.78
1:H:153:LEU:HD21	1:H:211:LEU:HD11	1.65	0.78
1:H:147:VAL:HG23	1:H:294:ILE:HD13	1.67	0.77
1:E:147:VAL:HG23	1:E:294:ILE:HD13	1.66	0.76
1:G:258:GLN:HA	1:G:258:GLN:HE21	1.52	0.75
1:E:180:ARG:HH12	2:E:1308:AZA:HN3	1.35	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:HIS:HD2	1:B:294:ILE:H	1.33	0.74
1:F:162:GLU:HB3	1:F:178:THR:HA	1.68	0.73
1:H:193:ASN:C	1:H:193:ASN:HD22	1.91	0.73
1:E:162:GLU:HB3	1:E:178:THR:HA	1.70	0.73
1:F:292:HIS:HD2	1:F:294:ILE:H	1.36	0.73
1:C:193:ASN:HD22	1:C:193:ASN:C	1.93	0.71
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.53	0.71
1:G:31:THR:HB	1:G:38:GLU:HB2	1.73	0.71
1:H:189:ARG:HH11	1:H:189:ARG:HG3	1.56	0.70
1:G:153:LEU:HD21	1:G:211:LEU:HD11	1.73	0.70
1:E:31:THR:HB	1:E:38:GLU:HB2	1.74	0.70
1:C:239:GLU:HG2	1:C:240:ILE:HD12	1.74	0.69
1:A:292:HIS:HD2	1:A:294:ILE:H	1.40	0.69
1:F:62:ALA:O	1:G:167:PRO:HG3	1.93	0.69
1:D:189:ARG:HH11	1:D:189:ARG:HG3	1.59	0.68
1:B:94:LYS:HG3	1:B:98:GLU:OE2	1.94	0.68
1:G:237:HIS:CB	1:G:240:ILE:HD13	2.24	0.68
1:A:180:ARG:HH12	2:A:1304:AZA:HN3	1.41	0.67
1:F:147:VAL:HG23	1:F:294:ILE:HD13	1.76	0.67
1:G:239:GLU:HG2	1:G:240:ILE:HD12	1.75	0.67
1:E:15:LEU:HD21	1:E:18:ASN:HD22	1.59	0.67
1:F:180:ARG:HH12	2:F:1307:AZA:HN3	1.41	0.67
1:H:193:ASN:ND2	1:H:194:THR:HG22	2.11	0.65
1:B:162:GLU:HB3	1:B:178:THR:HA	1.75	0.65
1:E:162:GLU:CB	1:E:178:THR:HA	2.26	0.65
1:E:193:ASN:HD22	1:E:193:ASN:C	1.99	0.65
1:D:147:VAL:HG23	1:D:294:ILE:HD13	1.79	0.65
1:D:31:THR:HB	1:D:38:GLU:HB2	1.78	0.65
1:H:260:PHE:HB2	1:H:262:GLN:HE21	1.62	0.64
1:G:258:GLN:HB2	1:G:259:PRO:HD3	1.79	0.64
1:G:83:ALA:HB3	1:G:87:GLU:OE2	1.97	0.64
1:H:292:HIS:HD2	1:H:294:ILE:H	1.45	0.64
1:B:31:THR:HB	1:B:38:GLU:HB2	1.80	0.64
1:C:162:GLU:HB3	1:C:178:THR:HA	1.79	0.64
1:A:147:VAL:HG23	1:A:294:ILE:HD13	1.79	0.63
1:G:33:ASN:OD1	1:G:34:THR:HG23	1.98	0.63
1:D:242:GLU:HB3	1:D:284:GLN:HB3	1.78	0.63
1:F:22:LYS:HZ2	1:G:251:HIS:CE1	2.15	0.63
1:G:180:ARG:HH12	2:G:1306:AZA:HN3	1.47	0.62
1:F:231:ARG:HG3	1:G:13:VAL:HG21	1.81	0.62
1:C:83:ALA:HB3	1:C:87:GLU:OE2	1.98	0.62
1:F:251:HIS:HE1	1:G:22:LYS:NZ	1.97	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:31:THR:HB	1:F:38:GLU:HB2	1.82	0.62
1:G:237:HIS:HB2	1:G:240:ILE:HD13	1.82	0.62
1:G:256:ASP:OD1	1:G:258:GLN:HG2	1.99	0.62
1:C:196:GLU:O	1:C:196:GLU:HG3	1.99	0.61
1:E:292:HIS:CD2	1:E:294:ILE:H	2.15	0.61
1:C:127:ARG:HB2	1:D:154:THR:HB	1.83	0.61
1:C:21:GLY:HA3	1:C:46:SER:O	2.01	0.61
1:D:83:ALA:HB3	1:D:87:GLU:OE2	2.01	0.60
1:D:220:LEU:H	1:D:224:GLN:NE2	1.99	0.60
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.66	0.60
1:G:193:ASN:HD21	1:G:239:GLU:HA	1.67	0.60
1:C:189:ARG:HH11	1:C:189:ARG:HG3	1.67	0.60
1:E:21:GLY:HA3	1:E:46:SER:O	2.02	0.60
1:A:27:LEU:HD22	1:A:28:VAL:N	2.17	0.60
1:F:189:ARG:HH11	1:F:189:ARG:HG3	1.67	0.60
1:G:162:GLU:HB3	1:G:178:THR:HA	1.83	0.60
1:C:292:HIS:HD2	1:C:294:ILE:H	1.49	0.59
1:H:83:ALA:N	1:H:87:GLU:OE2	2.30	0.59
1:E:15:LEU:C	1:E:15:LEU:HD23	2.22	0.59
1:A:21:GLY:HA3	1:A:46:SER:O	2.02	0.59
1:F:22:LYS:NZ	1:G:251:HIS:HE1	1.98	0.59
1:H:180:ARG:HH12	2:H:1305:AZA:HN3	1.50	0.59
1:F:94:LYS:HE2	3:F:1376:HOH:O	2.01	0.59
1:C:237:HIS:HB3	1:C:240:ILE:HD13	1.85	0.59
1:C:239:GLU:HG2	1:C:240:ILE:CD1	2.33	0.59
1:F:193:ASN:HD22	1:F:193:ASN:C	2.06	0.59
1:E:242:GLU:HB3	1:E:284:GLN:HB3	1.82	0.59
1:D:94:LYS:HG3	1:D:98:GLU:OE2	2.03	0.59
1:B:226:MET:HE2	1:B:279:ILE:HG22	1.85	0.59
1:G:292:HIS:CD2	1:G:294:ILE:H	2.18	0.58
1:E:107:ARG:NH1	1:E:136:VAL:HG11	2.18	0.58
1:H:31:THR:HB	1:H:38:GLU:HB2	1.86	0.58
1:B:21:GLY:HA3	1:B:46:SER:O	2.04	0.58
1:B:226:MET:HE3	1:B:281:ALA:HB3	1.86	0.58
1:E:251:HIS:HE1	1:H:22:LYS:NZ	2.02	0.57
1:H:220:LEU:H	1:H:224:GLN:NE2	2.03	0.57
1:B:162:GLU:CB	1:B:178:THR:HA	2.35	0.57
1:A:83:ALA:HB3	1:A:87:GLU:OE2	2.05	0.57
1:E:15:LEU:HD23	1:E:16:GLY:O	2.05	0.57
1:B:22:LYS:NZ	1:C:251:HIS:CE1	2.72	0.57
1:C:202:VAL:O	1:C:206:VAL:HG23	2.04	0.57
1:F:13:VAL:HG11	1:G:231:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:PRO:HG3	1:C:62:ALA:O	2.05	0.57
1:E:193:ASN:ND2	1:E:194:THR:HG22	2.21	0.56
1:B:226:MET:CE	1:B:279:ILE:HG22	2.35	0.56
1:F:285:ARG:HH11	1:F:285:ARG:HG3	1.71	0.56
1:C:267:GLU:HG2	1:D:30:VAL:O	2.06	0.56
1:A:167:PRO:HG3	1:D:62:ALA:O	2.06	0.56
1:B:237:HIS:HB3	1:B:239:GLU:OE2	2.06	0.56
1:C:240:ILE:HD12	1:C:240:ILE:N	2.21	0.56
1:H:162:GLU:CB	1:H:178:THR:HA	2.32	0.55
1:F:27:LEU:HD13	1:F:27:LEU:C	2.27	0.55
1:D:180:ARG:HH12	2:D:1302:AZA:HN3	1.53	0.55
1:B:180:ARG:HH12	2:B:1301:AZA:HN3	1.54	0.55
1:B:22:LYS:NZ	1:C:251:HIS:HE1	2.05	0.55
1:A:194:THR:OG1	1:A:196:GLU:HG2	2.06	0.55
1:H:21:GLY:HA3	1:H:46:SER:O	2.05	0.55
1:B:189:ARG:HG3	1:B:189:ARG:NH1	2.22	0.55
1:E:194:THR:OG1	1:E:196:GLU:HG2	2.07	0.55
1:A:196:GLU:O	1:A:196:GLU:HG3	2.06	0.55
1:B:144:GLN:HG3	1:B:195:VAL:HG11	1.88	0.55
1:E:62:ALA:O	1:H:167:PRO:HG3	2.06	0.55
1:F:193:ASN:ND2	1:F:194:THR:HG22	2.22	0.55
1:A:160:GLY:HA3	3:B:1416:HOH:O	2.07	0.55
1:A:19:GLN:HE21	1:A:47:GLN:NE2	2.05	0.55
1:G:163:PHE:CZ	2:G:1306:AZA:C5	2.90	0.54
1:G:237:HIS:HB3	1:G:240:ILE:HD13	1.89	0.54
1:B:284:GLN:OE1	1:B:290:ALA:HB2	2.07	0.54
1:D:184:THR:HA	1:D:250:LYS:HG3	1.90	0.54
1:F:251:HIS:CE1	1:G:22:LYS:NZ	2.76	0.54
1:B:62:ALA:O	1:C:167:PRO:HG3	2.07	0.54
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.72	0.54
1:B:279:ILE:HD12	1:B:279:ILE:N	2.23	0.54
1:B:15:LEU:HD11	1:B:18:ASN:ND2	2.22	0.54
1:B:194:THR:OG1	1:B:196:GLU:HG2	2.07	0.54
1:G:15:LEU:HD22	1:G:16:GLY:O	2.08	0.53
1:A:143:GLU:HG2	1:A:144:GLN:N	2.23	0.53
1:E:189:ARG:HG3	1:E:189:ARG:NH1	2.24	0.53
1:B:292:HIS:CD2	1:B:294:ILE:H	2.22	0.53
1:G:279:ILE:N	1:G:279:ILE:HD12	2.24	0.53
1:H:113:PHE:HB3	1:H:127:ARG:CZ	2.38	0.53
1:E:251:HIS:CE1	1:H:22:LYS:NZ	2.77	0.53
1:A:72:ASN:HB3	1:B:260:PHE:CZ	2.44	0.53
1:H:292:HIS:CD2	1:H:294:ILE:H	2.25	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:156:LEU:C	1:C:156:LEU:HD23	2.30	0.53
1:D:279:ILE:N	1:D:279:ILE:HD12	2.24	0.53
1:E:170:LYS:HE3	1:E:171:TYR:CE2	2.44	0.53
1:F:162:GLU:HG3	1:F:220:LEU:HD23	1.91	0.53
1:E:251:HIS:HE1	1:H:22:LYS:HZ3	1.57	0.53
1:B:22:LYS:HZ3	1:C:251:HIS:HE1	1.57	0.53
1:F:193:ASN:HD22	1:F:194:THR:HG22	1.75	0.52
1:D:87:GLU:HB2	3:D:1401:HOH:O	2.08	0.52
1:B:193:ASN:HD21	1:B:239:GLU:HA	1.75	0.52
1:C:237:HIS:CB	1:C:240:ILE:HD13	2.38	0.52
1:E:167:PRO:HD2	1:H:64:VAL:O	2.09	0.52
1:G:169:ASP:HB2	3:G:1418:HOH:O	2.10	0.52
1:A:296:SER:O	1:A:297:ASN:OXT	2.28	0.52
1:H:230:GLY:HA3	1:H:283:ILE:HG13	1.91	0.52
1:F:237:HIS:HB3	1:F:239:GLU:OE2	2.10	0.51
1:F:251:HIS:HE1	1:G:22:LYS:HZ3	1.57	0.51
1:B:51:ASP:O	1:B:63:HIS:HD2	1.94	0.51
1:D:53:GLU:O	1:D:57:THR:HG23	2.10	0.51
1:G:21:GLY:HA3	1:G:46:SER:O	2.11	0.51
1:D:205:SER:HG	1:D:237:HIS:CE1	2.28	0.51
1:H:193:ASN:ND2	1:H:193:ASN:C	2.64	0.51
1:E:49:ARG:HH12	1:E:138:GLU:CD	2.12	0.51
1:F:292:HIS:CD2	1:F:293:PRO:HD2	2.46	0.51
1:F:127:ARG:HG2	1:F:127:ARG:HH11	1.76	0.51
1:G:49:ARG:HH12	1:G:138:GLU:CD	2.14	0.51
1:G:162:GLU:CB	1:G:178:THR:HA	2.40	0.51
1:E:27:LEU:HD13	1:E:27:LEU:C	2.30	0.51
1:G:226:MET:CE	1:G:279:ILE:HG22	2.42	0.50
1:G:244:LYS:HE2	1:G:282:THR:OG1	2.11	0.50
1:G:76:ALA:HB1	1:H:262:GLN:HE22	1.76	0.50
1:A:19:GLN:HE21	1:A:47:GLN:HE22	1.58	0.50
1:C:226:MET:HE3	1:C:281:ALA:HB3	1.93	0.50
1:H:188:ALA:HB2	1:H:245:MET:HG2	1.93	0.50
1:C:19:GLN:NE2	1:C:47:GLN:NE2	2.59	0.50
1:A:62:ALA:O	1:D:167:PRO:HG3	2.11	0.50
1:A:195:VAL:HG22	3:A:1382:HOH:O	2.11	0.50
1:B:49:ARG:HH12	1:B:138:GLU:CD	2.14	0.50
1:D:21:GLY:HA3	1:D:46:SER:O	2.12	0.50
1:C:237:HIS:HB3	1:C:239:GLU:OE2	2.11	0.50
1:E:76:ALA:HB1	1:F:262:GLN:HE22	1.76	0.50
1:C:242:GLU:HB3	1:C:284:GLN:HB3	1.94	0.50
1:B:164:HIS:HB3	1:B:176:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:158:SER:OG	1:F:123:HIS:HB2	2.11	0.49
1:C:189:ARG:NH1	1:C:189:ARG:HG3	2.27	0.49
1:G:127:ARG:NH2	3:G:1312:HOH:O	2.45	0.49
1:C:118:ILE:O	1:C:121:HIS:HB2	2.12	0.49
1:F:292:HIS:CD2	1:F:294:ILE:H	2.25	0.49
1:A:84:THR:OG1	1:A:87:GLU:HG3	2.13	0.49
1:A:193:ASN:ND2	1:A:194:THR:HG22	2.27	0.49
1:F:21:GLY:HA3	1:F:46:SER:O	2.13	0.49
1:H:222:LEU:HB2	2:H:1305:AZA:O2	2.11	0.49
1:G:23:ALA:HA	1:G:45:THR:HG23	1.94	0.49
1:F:196:GLU:HG3	1:F:196:GLU:O	2.12	0.49
1:H:156:LEU:C	1:H:156:LEU:HD23	2.33	0.49
1:H:162:GLU:HB3	1:H:178:THR:CA	2.38	0.49
1:G:267:GLU:HG2	1:H:30:VAL:O	2.13	0.49
1:C:193:ASN:ND2	1:C:194:THR:HG22	2.28	0.48
1:B:162:GLU:HB3	1:B:178:THR:CA	2.43	0.48
1:D:251:HIS:HD2	3:D:1355:HOH:O	1.95	0.48
1:B:27:LEU:HD23	1:B:75:TYR:CD1	2.47	0.48
1:H:258:GLN:N	1:H:259:PRO:CD	2.76	0.48
1:F:33:ASN:OD1	1:F:34:THR:HG23	2.14	0.48
1:F:22:LYS:NZ	1:G:251:HIS:CE1	2.79	0.48
1:A:64:VAL:O	1:D:167:PRO:HD2	2.14	0.48
1:F:114:PHE:O	1:F:127:ARG:HD2	2.14	0.48
1:D:193:ASN:HD21	1:D:239:GLU:HA	1.79	0.48
1:G:193:ASN:ND2	1:G:194:THR:HG22	2.29	0.47
1:D:220:LEU:HB2	1:D:224:GLN:NE2	2.29	0.47
1:G:226:MET:HE2	1:G:279:ILE:HG22	1.95	0.47
1:E:258:GLN:N	1:E:259:PRO:CD	2.78	0.47
1:H:212:LYS:O	1:H:216:GLU:HG3	2.14	0.47
1:C:193:ASN:ND2	1:C:193:ASN:C	2.66	0.47
1:D:220:LEU:H	1:D:224:GLN:HE21	1.62	0.47
1:C:19:GLN:HE21	1:C:47:GLN:HE22	1.62	0.47
1:C:19:GLN:HE21	1:C:47:GLN:NE2	2.12	0.47
1:H:164:HIS:HB3	1:H:176:GLU:HB3	1.96	0.47
1:D:292:HIS:CD2	1:D:293:PRO:HD2	2.50	0.47
1:E:107:ARG:HH12	1:E:136:VAL:HG11	1.78	0.47
1:D:292:HIS:CD2	1:D:294:ILE:H	2.19	0.47
1:G:193:ASN:HD22	1:G:194:THR:HG22	1.80	0.47
1:C:162:GLU:CB	1:C:178:THR:HA	2.44	0.47
1:D:94:LYS:HD3	3:D:1429:HOH:O	2.14	0.47
1:B:27:LEU:HD13	1:B:27:LEU:C	2.35	0.47
1:H:239:GLU:CD	1:H:239:GLU:H	2.17	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:265:PRO:HG2	1:E:267:GLU:OE2	2.14	0.47
1:A:19:GLN:NE2	1:A:47:GLN:NE2	2.63	0.47
1:C:279:ILE:HD12	1:C:279:ILE:N	2.30	0.47
1:C:153:LEU:HD21	1:C:211:LEU:HD11	1.96	0.47
1:E:162:GLU:HB3	1:E:178:THR:CA	2.44	0.47
1:F:156:LEU:HD23	1:F:156:LEU:C	2.35	0.47
1:F:226:MET:HE3	1:F:281:ALA:HB3	1.97	0.47
1:C:83:ALA:CB	1:C:87:GLU:OE2	2.64	0.46
1:E:22:LYS:NZ	1:H:251:HIS:CE1	2.84	0.46
1:A:292:HIS:CD2	1:A:294:ILE:H	2.27	0.46
1:A:154:THR:HB	1:B:127:ARG:HB3	1.98	0.46
1:E:123:HIS:HB2	1:F:158:SER:OG	2.15	0.46
1:B:112:GLN:HB3	1:B:133:ARG:HB3	1.98	0.46
1:G:282:THR:C	1:G:283:ILE:HD12	2.35	0.46
1:D:156:LEU:HD23	1:D:156:LEU:C	2.36	0.46
1:D:162:GLU:HB3	1:D:178:THR:HA	1.97	0.46
1:G:260:PHE:HB2	1:G:262:GLN:HE21	1.80	0.46
1:B:207:ARG:O	1:B:211:LEU:HD22	2.16	0.46
1:B:125:PHE:N	1:B:125:PHE:CD1	2.84	0.46
1:A:258:GLN:N	1:A:259:PRO:CD	2.78	0.46
1:B:143:GLU:HB2	1:G:289:ARG:HA	1.97	0.46
1:G:118:ILE:O	1:G:121:HIS:HB2	2.16	0.46
1:A:15:LEU:HD11	1:A:18:ASN:ND2	2.31	0.46
1:C:118:ILE:HD12	1:D:211:LEU:HG	1.96	0.46
1:G:258:GLN:N	1:G:259:PRO:CD	2.79	0.46
1:E:170:LYS:HE3	1:E:171:TYR:HE2	1.81	0.46
1:A:205:SER:O	1:A:209:LEU:HG	2.16	0.46
1:G:51:ASP:O	1:G:63:HIS:HD2	1.99	0.45
1:F:125:PHE:CD1	1:F:125:PHE:N	2.84	0.45
1:F:52:PHE:HA	3:F:1354:HOH:O	2.16	0.45
1:D:125:PHE:N	1:D:125:PHE:CD1	2.85	0.45
1:A:158:SER:OG	1:B:123:HIS:HB2	2.16	0.45
1:E:193:ASN:HD22	1:E:194:THR:N	2.15	0.45
1:B:22:LYS:HZ2	1:C:251:HIS:CE1	2.34	0.45
1:B:107:ARG:NH1	1:B:297:ASN:HA	2.31	0.45
1:F:251:HIS:CE1	1:G:22:LYS:HZ2	2.33	0.45
1:D:193:ASN:HD22	1:D:193:ASN:C	2.20	0.45
1:G:226:MET:HB2	1:G:247:LEU:HD12	1.99	0.45
1:D:239:GLU:H	1:D:239:GLU:CD	2.19	0.45
1:H:193:ASN:HD22	1:H:194:THR:HG22	1.82	0.45
1:H:134:THR:HG21	1:H:189:ARG:HH22	1.82	0.45
1:H:189:ARG:HH11	1:H:189:ARG:CG	2.28	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:239:GLU:CD	1:C:239:GLU:H	2.20	0.45
1:C:27:LEU:HD13	1:C:27:LEU:C	2.36	0.45
1:E:226:MET:CE	1:E:279:ILE:HG22	2.47	0.45
1:D:248:PRO:HA	1:D:277:GLY:O	2.17	0.45
1:H:157:LYS:HE3	1:H:159:THR:O	2.16	0.45
1:H:33:ASN:OD1	1:H:34:THR:HG23	2.17	0.45
1:B:33:ASN:OD1	1:B:34:THR:HG23	2.16	0.45
1:C:28:VAL:HG21	1:D:252:HIS:CD2	2.52	0.45
1:B:205:SER:OG	1:B:237:HIS:HE1	1.99	0.45
1:B:258:GLN:N	1:B:259:PRO:CD	2.80	0.45
1:D:244:LYS:HG2	1:D:282:THR:OG1	2.17	0.45
1:E:33:ASN:OD1	1:E:34:THR:HG23	2.16	0.44
1:E:167:PRO:HG3	1:H:62:ALA:O	2.18	0.44
1:G:243:ILE:HG23	1:G:243:ILE:O	2.16	0.44
1:D:106:GLY:HA3	1:D:108:TRP:CH2	2.52	0.44
1:C:193:ASN:HD22	1:C:194:THR:HG22	1.82	0.44
1:C:49:ARG:HH12	1:C:138:GLU:CD	2.21	0.44
1:A:279:ILE:HD12	1:A:279:ILE:N	2.32	0.44
1:F:182:LEU:HD11	1:F:222:LEU:HG	1.99	0.44
1:C:224:GLN:HB3	1:C:224:GLN:HE21	1.63	0.44
1:C:283:ILE:N	1:C:283:ILE:HD12	2.32	0.44
1:D:189:ARG:HG3	1:D:189:ARG:NH1	2.29	0.44
1:C:33:ASN:OD1	1:C:34:THR:HG23	2.16	0.44
1:H:134:THR:HG21	1:H:189:ARG:NH2	2.31	0.44
1:A:125:PHE:CD1	1:A:125:PHE:N	2.86	0.44
1:H:226:MET:HE3	1:H:281:ALA:HB3	2.00	0.44
1:D:296:SER:O	1:D:297:ASN:OXT	2.36	0.44
1:F:279:ILE:N	1:F:279:ILE:HD12	2.33	0.44
1:E:22:LYS:NZ	1:H:251:HIS:HE1	2.16	0.44
1:G:189:ARG:HH11	1:G:189:ARG:HG3	1.81	0.44
1:A:193:ASN:C	1:A:193:ASN:HD22	2.22	0.44
1:C:30:VAL:HG22	1:C:39:ILE:CD1	2.48	0.44
1:G:292:HIS:CD2	1:G:293:PRO:HD2	2.53	0.43
1:F:13:VAL:HG21	1:G:231:ARG:HG3	1.99	0.43
1:H:226:MET:CE	1:H:279:ILE:HG22	2.48	0.43
1:B:251:HIS:CE1	1:C:22:LYS:NZ	2.86	0.43
1:F:242:GLU:HB3	1:F:284:GLN:HB3	2.00	0.43
1:E:193:ASN:C	1:E:193:ASN:ND2	2.71	0.43
1:D:107:ARG:NH1	1:D:297:ASN:HA	2.34	0.43
1:E:61:ASN:O	1:H:166:PHE:HA	2.18	0.43
1:A:184:THR:HA	1:A:250:LYS:HG3	1.99	0.43
1:C:158:SER:OG	1:D:123:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:156:LEU:HD23	1:E:156:LEU:C	2.39	0.43
1:D:33:ASN:OD1	1:D:34:THR:HG23	2.17	0.43
1:C:205:SER:OG	1:C:237:HIS:HE1	2.01	0.43
1:H:184:THR:HA	1:H:250:LYS:HG3	2.01	0.43
1:D:258:GLN:N	1:D:259:PRO:CD	2.82	0.43
1:A:22:LYS:HE2	1:A:67:THR:O	2.18	0.43
1:A:90:LEU:O	1:A:94:LYS:HG3	2.17	0.43
1:B:279:ILE:CD1	1:B:279:ILE:N	2.82	0.43
1:A:278:LEU:C	1:A:279:ILE:HD12	2.39	0.43
1:C:182:LEU:HD11	1:C:222:LEU:HG	2.01	0.43
1:G:182:LEU:HD11	1:G:222:LEU:HG	1.98	0.43
1:E:15:LEU:HD12	1:E:56:HIS:HB2	2.01	0.43
1:H:189:ARG:NH1	1:H:189:ARG:HG3	2.29	0.43
1:G:162:GLU:HG3	1:G:220:LEU:HD23	2.00	0.43
1:A:107:ARG:NH1	3:A:1348:HOH:O	2.51	0.43
1:B:14:VAL:HG12	1:B:15:LEU:N	2.33	0.43
1:C:278:LEU:C	1:C:279:ILE:HD12	2.39	0.43
1:B:90:LEU:HA	1:B:137:LEU:HD22	2.01	0.43
1:C:258:GLN:N	1:C:259:PRO:CD	2.81	0.43
1:G:156:LEU:HD23	1:G:156:LEU:C	2.39	0.43
1:B:144:GLN:NE2	3:B:1320:HOH:O	2.40	0.43
1:B:107:ARG:CZ	1:B:297:ASN:HA	2.49	0.43
1:B:43:ASN:O	1:B:110:ALA:HA	2.18	0.43
1:C:292:HIS:CD2	1:C:294:ILE:H	2.33	0.43
1:B:167:PRO:HD2	1:C:64:VAL:O	2.18	0.43
1:A:156:LEU:C	1:A:156:LEU:HD23	2.39	0.43
1:G:206:VAL:O	1:G:210:LEU:HG	2.19	0.43
1:G:193:ASN:C	1:G:193:ASN:HD22	2.22	0.42
1:E:20:TYR:O	1:E:47:GLN:HA	2.18	0.42
1:G:278:LEU:C	1:G:279:ILE:HD12	2.40	0.42
1:C:220:LEU:H	1:C:224:GLN:NE2	2.17	0.42
1:G:14:VAL:HG12	1:G:15:LEU:N	2.34	0.42
1:A:274:ARG:HD2	1:D:24:GLU:HB3	2.01	0.42
1:C:292:HIS:CD2	1:C:293:PRO:HD2	2.54	0.42
1:G:239:GLU:CD	1:G:239:GLU:H	2.23	0.42
1:F:226:MET:CE	1:F:279:ILE:HG22	2.50	0.42
1:A:115:TRP:CD2	1:A:127:ARG:HG2	2.54	0.42
1:E:24:GLU:HB3	1:E:43:ASN:HD21	1.83	0.42
1:G:147:VAL:HG23	1:G:294:ILE:HD13	2.02	0.42
1:E:196:GLU:O	1:E:196:GLU:HG3	2.19	0.42
1:B:226:MET:HE2	1:B:279:ILE:CG2	2.49	0.42
1:B:22:LYS:HZ3	1:C:251:HIS:CE1	2.32	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:284:GLN:HE22	1:B:290:ALA:CB	2.32	0.42
1:C:156:LEU:HD23	1:C:157:LYS:N	2.34	0.42
1:A:260:PHE:HB2	1:A:262:GLN:HE21	1.84	0.42
1:A:265:PRO:HG2	1:A:267:GLU:HG3	2.01	0.42
1:C:244:LYS:HE2	1:C:282:THR:OG1	2.19	0.42
1:D:127:ARG:HH11	1:D:127:ARG:HG2	1.84	0.42
1:C:70:GLN:O	1:C:74:VAL:HG23	2.19	0.42
1:A:251:HIS:CE1	1:D:22:LYS:HZ2	2.38	0.42
1:C:19:GLN:NE2	1:C:47:GLN:HE22	2.18	0.42
1:C:243:ILE:O	1:C:243:ILE:HG23	2.20	0.42
1:A:285:ARG:HG3	1:A:285:ARG:HH11	1.85	0.42
1:A:213:ALA:CB	1:A:229:MET:HA	2.50	0.42
1:D:242:GLU:CB	1:D:284:GLN:HB3	2.49	0.42
1:F:189:ARG:HH11	1:F:189:ARG:CG	2.33	0.42
1:E:41:ASP:O	1:E:42:LEU:HD23	2.20	0.42
1:G:205:SER:OG	1:G:237:HIS:HE1	2.03	0.41
1:A:61:ASN:HA	1:A:64:VAL:HG23	2.02	0.41
1:G:115:TRP:CE2	1:G:127:ARG:HG2	2.55	0.41
1:H:279:ILE:N	1:H:279:ILE:HD12	2.35	0.41
1:D:212:LYS:O	1:D:216:GLU:HG3	2.20	0.41
1:A:193:ASN:HD21	1:A:239:GLU:HA	1.85	0.41
1:D:22:LYS:HE2	1:D:67:THR:C	2.40	0.41
1:E:205:SER:OG	1:E:237:HIS:CE1	2.73	0.41
1:B:89:LEU:HD22	1:B:108:TRP:HB3	2.02	0.41
1:A:205:SER:OG	1:A:237:HIS:CE1	2.74	0.41
1:C:94:LYS:O	1:C:98:GLU:HG3	2.20	0.41
1:F:71:LYS:HB3	1:F:71:LYS:HE2	1.79	0.41
1:F:143:GLU:HG2	1:F:144:GLN:N	2.35	0.41
1:B:50:GLY:HA3	1:B:102:TRP:O	2.19	0.41
1:C:285:ARG:HG3	1:C:285:ARG:HH11	1.85	0.41
1:C:125:PHE:CD1	1:C:125:PHE:N	2.89	0.41
1:G:27:LEU:C	1:G:27:LEU:HD13	2.41	0.41
1:F:224:GLN:HB3	1:F:224:GLN:HE21	1.66	0.41
1:E:226:MET:HE2	1:E:279:ILE:HG22	2.01	0.41
1:C:164:HIS:HB3	1:C:176:GLU:HB3	2.02	0.41
1:C:115:TRP:CE2	1:C:127:ARG:HG2	2.56	0.41
1:G:123:HIS:CG	1:H:159:THR:HG22	2.56	0.41
1:E:29:LYS:HB3	1:E:40:GLN:HB2	2.03	0.41
1:D:143:GLU:OE2	1:D:292:HIS:HE1	2.04	0.41
1:E:162:GLU:HB2	1:E:178:THR:HA	2.02	0.41
1:G:240:ILE:HD12	1:G:240:ILE:N	2.36	0.41
1:D:279:ILE:CD1	1:D:279:ILE:N	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:154:THR:HB	1:D:127:ARG:HB3	2.03	0.41
1:B:231:ARG:HG3	1:C:13:VAL:HG11	2.03	0.41
1:H:35:ALA:O	1:H:122:ASP:HB3	2.20	0.41
1:D:83:ALA:N	1:D:87:GLU:OE2	2.50	0.41
1:A:205:SER:OG	1:A:237:HIS:HE1	2.04	0.41
1:F:230:GLY:HA3	1:F:283:ILE:HG13	2.03	0.41
1:F:285:ARG:NH1	1:F:285:ARG:HG3	2.35	0.40
1:A:31:THR:HB	1:A:38:GLU:HB2	2.01	0.40
1:H:54:ALA:HB1	1:H:60:ASP:HB3	2.03	0.40
1:E:226:MET:HE3	1:E:281:ALA:HB3	2.02	0.40
1:B:71:LYS:HE2	1:B:71:LYS:HB3	1.95	0.40
1:G:87:GLU:HB2	3:G:1314:HOH:O	2.21	0.40
1:C:226:MET:CE	1:C:281:ALA:HB3	2.51	0.40
1:B:284:GLN:HE22	1:B:290:ALA:HB2	1.86	0.40
1:D:278:LEU:C	1:D:279:ILE:HD12	2.41	0.40
1:G:129:LYS:HE3	3:H:1307:HOH:O	2.22	0.40
1:H:68:ASP:O	1:H:71:LYS:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/287 (99%)	276 (97%)	9 (3%)	0	100	100
1	B	285/287 (99%)	277 (97%)	8 (3%)	0	100	100
1	C	285/287 (99%)	278 (98%)	7 (2%)	0	100	100
1	D	285/287 (99%)	276 (97%)	9 (3%)	0	100	100
1	E	285/287 (99%)	273 (96%)	12 (4%)	0	100	100
1	F	285/287 (99%)	278 (98%)	7 (2%)	0	100	100
1	G	285/287 (99%)	280 (98%)	5 (2%)	0	100	100
1	H	285/287 (99%)	275 (96%)	9 (3%)	1 (0%)	43	46
All	All	2280/2296 (99%)	2213 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	291	ASP

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	236/240 (98%)	230 (98%)	6 (2%)	60	71
1	B	236/240 (98%)	230 (98%)	6 (2%)	60	71
1	C	236/240 (98%)	226 (96%)	10 (4%)	40	46
1	D	236/240 (98%)	231 (98%)	5 (2%)	66	76
1	E	236/240 (98%)	228 (97%)	8 (3%)	49	58
1	F	236/240 (98%)	228 (97%)	8 (3%)	49	58
1	G	236/240 (98%)	231 (98%)	5 (2%)	66	76
1	H	236/240 (98%)	233 (99%)	3 (1%)	80	89
All	All	1888/1920 (98%)	1837 (97%)	51 (3%)	57	68

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

Mol	Chain	Res	Type
1	A	27	LEU
1	A	63	HIS
1	A	125	PHE
1	A	127	ARG
1	A	193	ASN
1	A	222	LEU
1	B	63	HIS
1	B	125	PHE
1	B	193	ASN
1	B	211	LEU
1	B	222	LEU
1	B	258	GLN
1	C	15	LEU
1	C	63	HIS
1	C	125	PHE

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Mol	Chain	Res	Type
1	C	127	ARG
1	C	193	ASN
1	C	211	LEU
1	C	222	LEU
1	C	224	GLN
1	C	270	TYR
1	C	280	GLU
1	D	119	ASN
1	D	144	GLN
1	D	193	ASN
1	D	211	LEU
1	D	222	LEU
1	E	63	HIS
1	E	87	GLU
1	E	125	PHE
1	E	127	ARG
1	E	193	ASN
1	E	211	LEU
1	E	222	LEU
1	E	270	TYR
1	F	15	LEU
1	F	125	PHE
1	F	193	ASN
1	F	211	LEU
1	F	222	LEU
1	F	224	GLN
1	F	270	TYR
1	F	284	GLN
1	G	15	LEU
1	G	193	ASN
1	G	222	LEU
1	G	224	GLN
1	G	258	GLN
1	H	193	ASN
1	H	222	LEU
1	H	224	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	47	GLN

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Mol	Chain	Res	Type
1	A	63	HIS
1	A	111	GLN
1	A	193	ASN
1	A	237	HIS
1	A	251	HIS
1	A	258	GLN
1	A	262	GLN
1	A	292	HIS
1	B	43	ASN
1	B	47	GLN
1	B	63	HIS
1	B	111	GLN
1	B	144	GLN
1	B	193	ASN
1	B	224	GLN
1	B	237	HIS
1	B	251	HIS
1	B	258	GLN
1	B	262	GLN
1	B	284	GLN
1	B	292	HIS
1	C	40	GLN
1	C	43	ASN
1	C	47	GLN
1	C	111	GLN
1	C	193	ASN
1	C	224	GLN
1	C	237	HIS
1	C	251	HIS
1	C	258	GLN
1	C	292	HIS
1	D	43	ASN
1	D	47	GLN
1	D	111	GLN
1	D	144	GLN
1	D	193	ASN
1	D	224	GLN
1	D	251	HIS
1	D	262	GLN
1	D	292	HIS
1	E	18	ASN
1	E	43	ASN

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Mol	Chain	Res	Type
1	E	111	GLN
1	E	193	ASN
1	E	224	GLN
1	E	237	HIS
1	E	251	HIS
1	E	258	GLN
1	E	292	HIS
1	F	43	ASN
1	F	47	GLN
1	F	63	HIS
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	292	HIS
1	G	43	ASN
1	G	63	HIS
1	G	111	GLN
1	G	193	ASN
1	G	237	HIS
1	G	251	HIS
1	G	258	GLN
1	G	262	GLN
1	G	292	HIS
1	H	43	ASN
1	H	47	GLN
1	H	111	GLN
1	H	144	GLN
1	H	193	ASN
1	H	224	GLN
1	H	237	HIS
1	H	251	HIS
1	H	262	GLN
1	H	292	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AZA	A	1304	-	12,12,12	1.58	2 (16%)	7,17,17	1.63	2 (28%)
2	AZA	B	1301	-	12,12,12	1.59	2 (16%)	7,17,17	1.62	2 (28%)
2	AZA	B	1303	-	12,12,12	1.59	2 (16%)	7,17,17	1.62	2 (28%)
2	AZA	D	1302	-	12,12,12	1.58	2 (16%)	7,17,17	1.63	2 (28%)
2	AZA	E	1308	-	12,12,12	1.59	2 (16%)	7,17,17	1.62	2 (28%)
2	AZA	F	1307	-	12,12,12	1.59	2 (16%)	7,17,17	1.62	2 (28%)
2	AZA	G	1306	-	12,12,12	1.57	2 (16%)	7,17,17	1.63	2 (28%)
2	AZA	H	1305	-	12,12,12	1.58	2 (16%)	7,17,17	1.63	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AZA	A	1304	-	-	0/0/0/0	0/0/2/2
2	AZA	B	1301	-	-	0/0/0/0	0/0/2/2
2	AZA	B	1303	-	-	0/0/0/0	0/0/2/2
2	AZA	D	1302	-	-	0/0/0/0	0/0/2/2
2	AZA	E	1308	-	-	0/0/0/0	0/0/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AZA	F	1307	-	-	0/0/0/0	0/0/2/2
2	AZA	G	1306	-	-	0/0/0/0	0/0/2/2
2	AZA	H	1305	-	-	0/0/0/0	0/0/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	AZA	C4-N3	-3.46	1.32	1.37
2	A	1304	AZA	C4-N3	-3.44	1.32	1.37
2	F	1307	AZA	C4-N3	-3.44	1.32	1.37
2	B	1303	AZA	C4-N3	-3.43	1.32	1.37
2	E	1308	AZA	C4-N3	-3.41	1.33	1.37
2	H	1305	AZA	C4-N3	-3.41	1.33	1.37
2	D	1302	AZA	C4-N3	-3.39	1.33	1.37
2	E	1308	AZA	C6-C5	3.37	1.46	1.41
2	G	1306	AZA	C4-N3	-3.37	1.33	1.37
2	H	1305	AZA	C6-C5	3.35	1.46	1.41
2	B	1303	AZA	C6-C5	3.35	1.46	1.41
2	D	1302	AZA	C6-C5	3.34	1.46	1.41
2	F	1307	AZA	C6-C5	3.34	1.46	1.41
2	A	1304	AZA	C6-C5	3.34	1.46	1.41
2	B	1301	AZA	C6-C5	3.34	1.46	1.41
2	G	1306	AZA	C6-C5	3.31	1.46	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1304	AZA	N9-N8-N7	2.70	114.91	108.19
2	G	1306	AZA	N9-N8-N7	2.70	114.91	108.19
2	D	1302	AZA	N9-N8-N7	2.70	114.90	108.19
2	H	1305	AZA	N9-N8-N7	2.70	114.90	108.19
2	B	1303	AZA	N9-N8-N7	2.69	114.89	108.19
2	B	1301	AZA	N9-N8-N7	2.69	114.88	108.19
2	E	1308	AZA	N9-N8-N7	2.69	114.88	108.19
2	F	1307	AZA	N9-N8-N7	2.69	114.87	108.19
2	G	1306	AZA	C5-C4-N9	2.54	111.25	107.62
2	H	1305	AZA	C5-C4-N9	2.54	111.24	107.62
2	D	1302	AZA	C5-C4-N9	2.54	111.23	107.62
2	B	1303	AZA	C5-C4-N9	2.53	111.22	107.62
2	A	1304	AZA	C5-C4-N9	2.52	111.21	107.62
2	B	1301	AZA	C5-C4-N9	2.52	111.21	107.62
2	E	1308	AZA	C5-C4-N9	2.52	111.21	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1307	AZA	C5-C4-N9	2.52	111.20	107.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.