



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:49 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

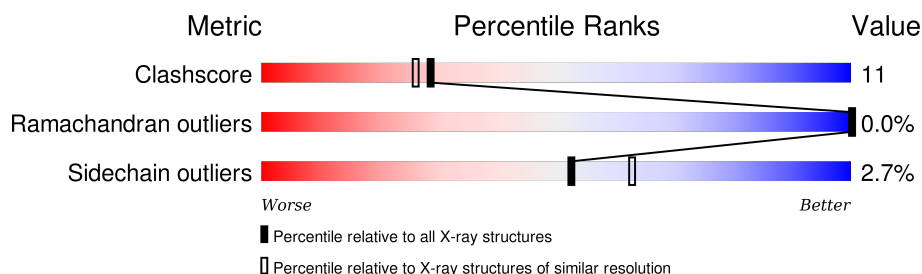
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	 78% 21% .
1	B	287	 77% 22% .
1	C	287	 73% 25% .
1	D	287	 78% 21% .
1	E	287	 78% 21% .
1	F	287	 82% 16% .
1	G	287	 75% 23% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	287	 A horizontal bar chart showing the quality of the chain. The bar is divided into two segments: a green segment representing 79% and a yellow segment representing 20%. A small red dot is at the end of the bar. The text '79%' is centered under the green segment and '20%' is centered under the yellow segment.

2 Entry composition

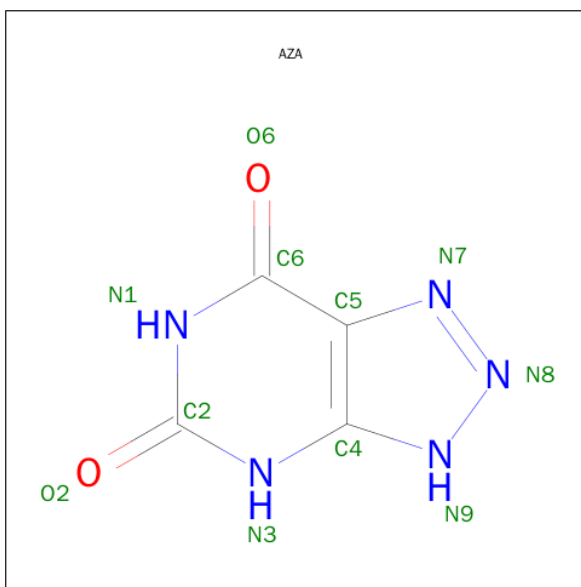
There are 3 unique types of molecules in this entry. The entry contains 19410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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		

Continued on next page...

Continued from previous page...

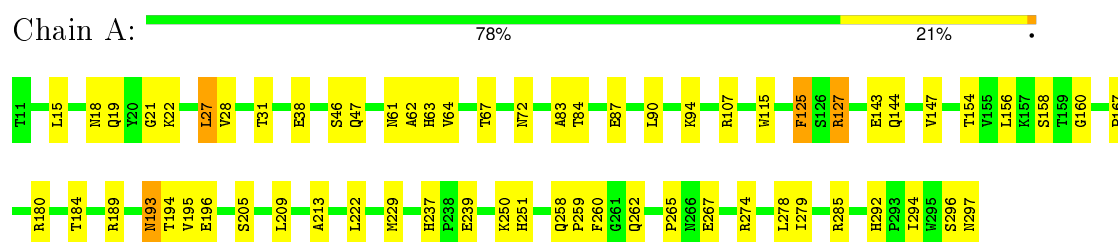
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	114	Total 114	O 114	0	0
3	F	146	Total 146	O 146	0	0
3	G	148	Total 148	O 148	0	0
3	H	113	Total 113	O 113	0	0

3 Residue-property plots

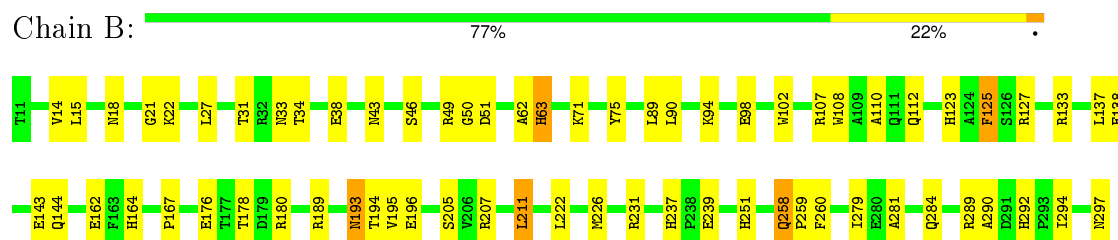
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

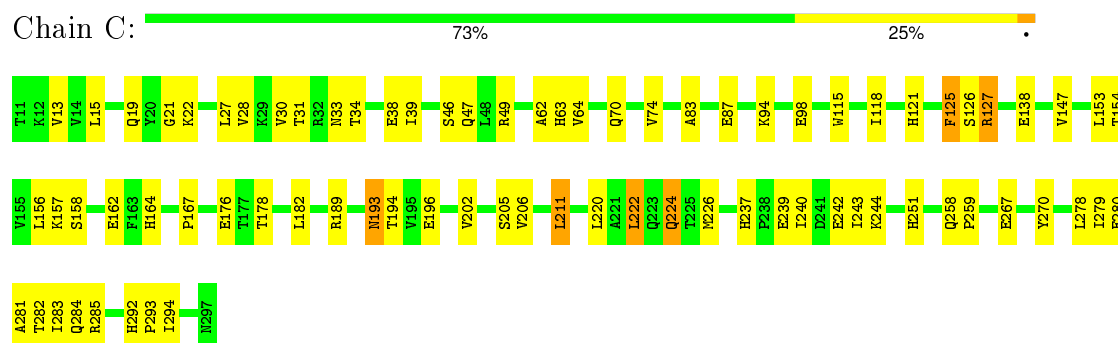
- Molecule 1: Uric acid oxidase



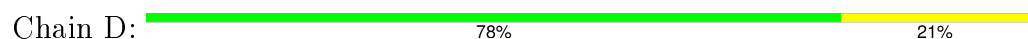
- Molecule 1: Uric acid oxidase

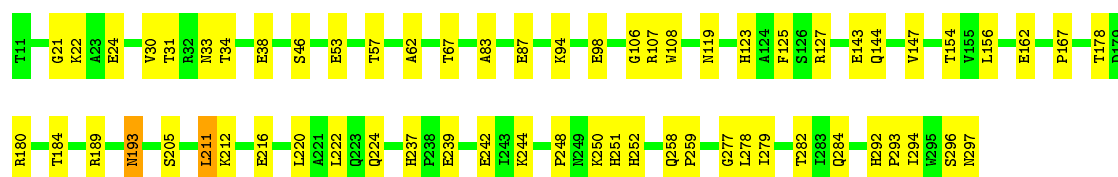


- Molecule 1: Uric acid oxidase

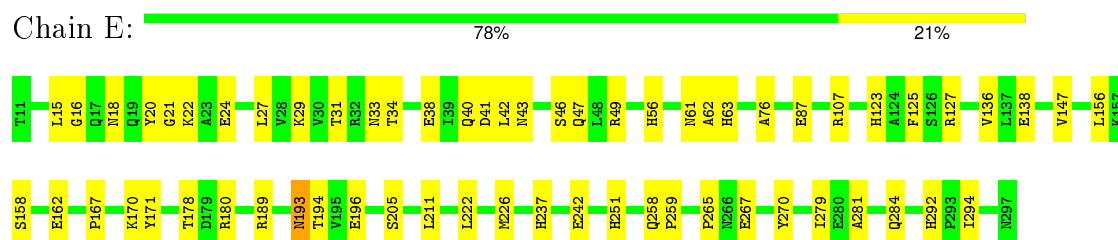


- Molecule 1: Uric acid oxidase

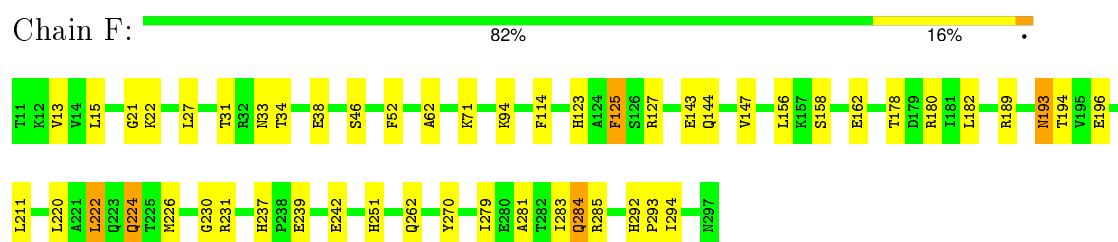




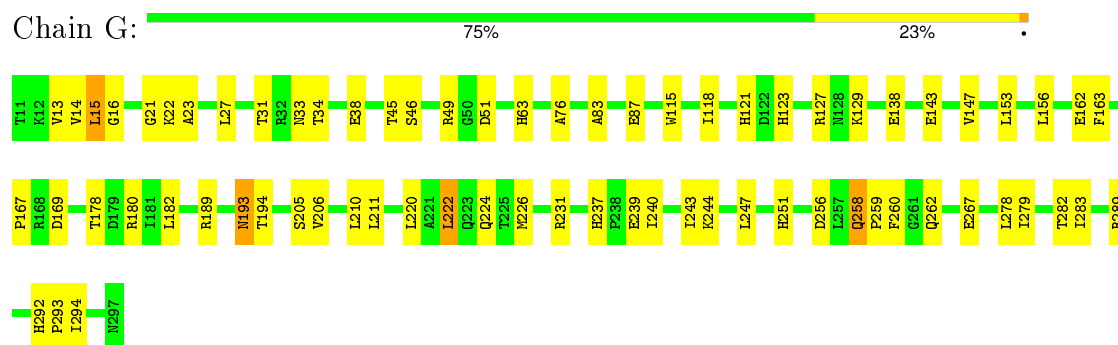
- Molecule 1: Uric acid oxidase



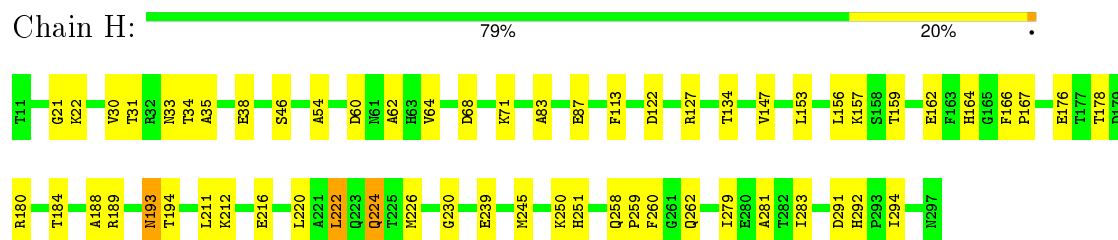
- Molecule 1: Uric acid oxidase



- Molecule 1: Uric acid oxidase



- Molecule 1: Uric acid oxidase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.33 Å 122.28 Å 283.92 Å 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 [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	49	0
1	B	2282	0	2177	61	0
1	C	2282	0	2177	73	0
1	D	2282	0	2177	54	0
1	E	2282	0	2177	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (411) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:ARG:HH12	2:E:1308:AZA:HN3	1.35	0.75
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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%)	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%)	39	42
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%)	55	65
1	B	236/240 (98%)	230 (98%)	6 (2%)	55	65
1	C	236/240 (98%)	226 (96%)	10 (4%)	36	41
1	D	236/240 (98%)	231 (98%)	5 (2%)	61	71
1	E	236/240 (98%)	228 (97%)	8 (3%)	44	53
1	F	236/240 (98%)	228 (97%)	8 (3%)	44	53
1	G	236/240 (98%)	231 (98%)	5 (2%)	61	71
1	H	236/240 (98%)	233 (99%)	3 (1%)	76	85
All	All	1888/1920 (98%)	1837 (97%)	51 (3%)	52	63

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	7,12,12	1.71	2 (28%)	4,17,17	7.48	3 (75%)
2	AZA	B	1301	-	7,12,12	1.72	2 (28%)	4,17,17	7.50	3 (75%)
2	AZA	B	1303	-	7,12,12	1.72	2 (28%)	4,17,17	7.45	3 (75%)
2	AZA	D	1302	-	7,12,12	1.71	2 (28%)	4,17,17	7.47	3 (75%)
2	AZA	E	1308	-	7,12,12	1.72	2 (28%)	4,17,17	7.47	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AZA	F	1307	-	7,12,12	1.73	2 (28%)	4,17,17	7.46	3 (75%)
2	AZA	G	1306	-	7,12,12	1.71	2 (28%)	4,17,17	7.50	3 (75%)
2	AZA	H	1305	-	7,12,12	1.73	2 (28%)	4,17,17	7.48	3 (75%)

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	0/2/2/2
2	AZA	B	1301	-	-	0/0/0/0	0/2/2/2
2	AZA	B	1303	-	-	0/0/0/0	0/2/2/2
2	AZA	D	1302	-	-	0/0/0/0	0/2/2/2
2	AZA	E	1308	-	-	0/0/0/0	0/2/2/2
2	AZA	F	1307	-	-	0/0/0/0	0/2/2/2
2	AZA	G	1306	-	-	0/0/0/0	0/2/2/2
2	AZA	H	1305	-	-	0/0/0/0	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1304	AZA	C6-N1	2.59	1.37	1.33
2	D	1302	AZA	C6-N1	2.60	1.37	1.33
2	B	1301	AZA	C6-N1	2.62	1.38	1.33
2	E	1308	AZA	C6-N1	2.62	1.38	1.33
2	G	1306	AZA	C6-N1	2.63	1.38	1.33
2	B	1303	AZA	C6-N1	2.64	1.38	1.33
2	F	1307	AZA	C6-N1	2.64	1.38	1.33
2	H	1305	AZA	C6-N1	2.66	1.38	1.33
2	G	1306	AZA	C6-C5	2.69	1.46	1.41
2	B	1301	AZA	C6-C5	2.71	1.46	1.41
2	A	1304	AZA	C6-C5	2.71	1.46	1.41
2	F	1307	AZA	C6-C5	2.72	1.46	1.41
2	D	1302	AZA	C6-C5	2.72	1.46	1.41
2	B	1303	AZA	C6-C5	2.72	1.46	1.41
2	H	1305	AZA	C6-C5	2.72	1.46	1.41
2	E	1308	AZA	C6-C5	2.74	1.46	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	AZA	C5-C6-N1	-8.59	111.84	123.59
2	G	1306	AZA	C5-C6-N1	-8.58	111.86	123.59
2	H	1305	AZA	C5-C6-N1	-8.57	111.87	123.59
2	A	1304	AZA	C5-C6-N1	-8.57	111.87	123.59
2	E	1308	AZA	C5-C6-N1	-8.56	111.89	123.59
2	B	1303	AZA	C5-C6-N1	-8.55	111.90	123.59
2	D	1302	AZA	C5-C6-N1	-8.55	111.90	123.59
2	F	1307	AZA	C5-C6-N1	-8.54	111.91	123.59
2	F	1307	AZA	N9-N8-N7	2.69	114.87	111.35
2	E	1308	AZA	N9-N8-N7	2.69	114.88	111.35
2	B	1301	AZA	N9-N8-N7	2.69	114.88	111.35
2	B	1303	AZA	N9-N8-N7	2.71	114.89	111.35
2	D	1302	AZA	N9-N8-N7	2.71	114.90	111.35
2	H	1305	AZA	N9-N8-N7	2.71	114.90	111.35
2	A	1304	AZA	N9-N8-N7	2.72	114.91	111.35
2	G	1306	AZA	N9-N8-N7	2.72	114.91	111.35
2	B	1303	AZA	C6-N1-C2	11.88	125.52	115.25
2	F	1307	AZA	C6-N1-C2	11.93	125.56	115.25
2	D	1302	AZA	C6-N1-C2	11.93	125.56	115.25
2	E	1308	AZA	C6-N1-C2	11.95	125.58	115.25
2	H	1305	AZA	C6-N1-C2	11.96	125.58	115.25
2	A	1304	AZA	C6-N1-C2	11.96	125.59	115.25
2	G	1306	AZA	C6-N1-C2	11.99	125.61	115.25
2	B	1301	AZA	C6-N1-C2	12.00	125.62	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1304	AZA	1	0
2	B	1301	AZA	1	0
2	D	1302	AZA	1	0
2	E	1308	AZA	1	0
2	F	1307	AZA	1	0
2	G	1306	AZA	2	0
2	H	1305	AZA	2	0

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.