Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 01:16 AM EDT

PDB ID	:	2YZD
Title	:	Crystal structure of uricase from Arthrobacter globiformis in complex with 8-azaxanthin (inhibitor)
Authors	:	Juan, E.C.M.; Hossain, M.T.; Hoque, M.M.; Suzuki, K.; Sekiguchi, T.; Takenaka, A.
Deposited on	:	2007-05-05
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

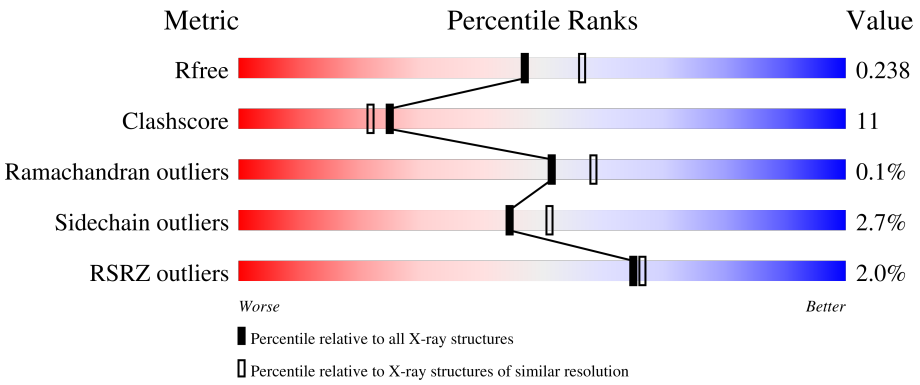
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	.% 75% 19% • 5%
1	B	302	3% 74% 20% • 5%
1	C	302	.% 77% 16% • 5%
1	D	302	.% 78% 14% • 5%
1	E	302	4% 71% 24% • 5%

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Mol	Chain	Length	Quality of chain
1	F	302	2% 75% 19% • 5%
1	G	302	2% 74% 21% • 5%
1	H	302	% 78% 16% • 5%

2 Entry composition (i)

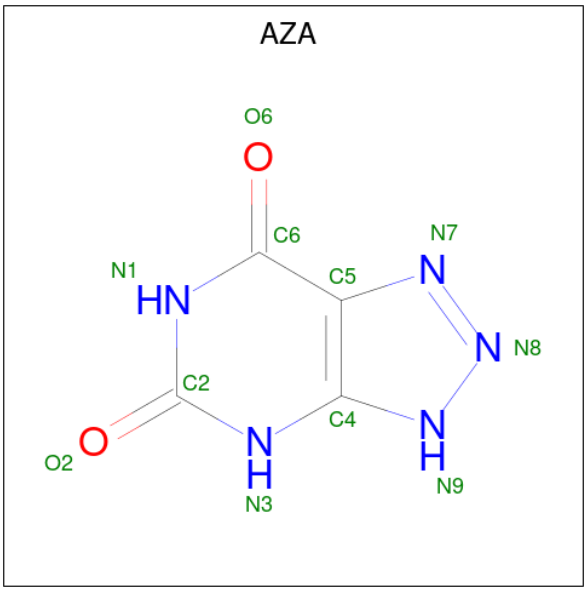
There are 3 unique types of molecules in this entry. The entry contains 19524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2284	1436	408	437	3	0	0	0
1	B	287	2284	1436	408	437	3	0	0	0
1	C	287	2284	1436	408	437	3	0	0	0
1	D	287	2284	1436	408	437	3	0	0	0
1	E	287	2284	1436	408	437	3	0	0	0
1	F	287	2288	1439	409	437	3	0	0	0
1	G	287	2284	1436	408	437	3	0	0	0
1	H	287	2284	1436	408	437	3	0	0	0

- Molecule 2 is 8-AZAXANTHINE (three-letter code: AZA) (formula: $C_4H_3N_5O_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	158	158	158	0	0
3	B	129	129	129	0	0
3	C	131	131	131	0	0
3	D	164	164	164	0	0

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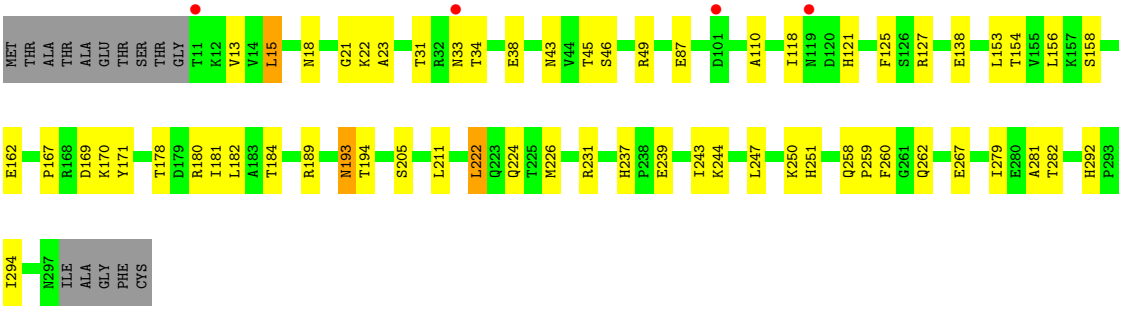
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	115	115	115	0	0
			Total	O		
3	F	148	148	148	0	0
			Total	O		
3	G	155	155	155	0	0
			Total	O		
3	H	160	160	160	0	0

3 Residue-property plots (i)

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

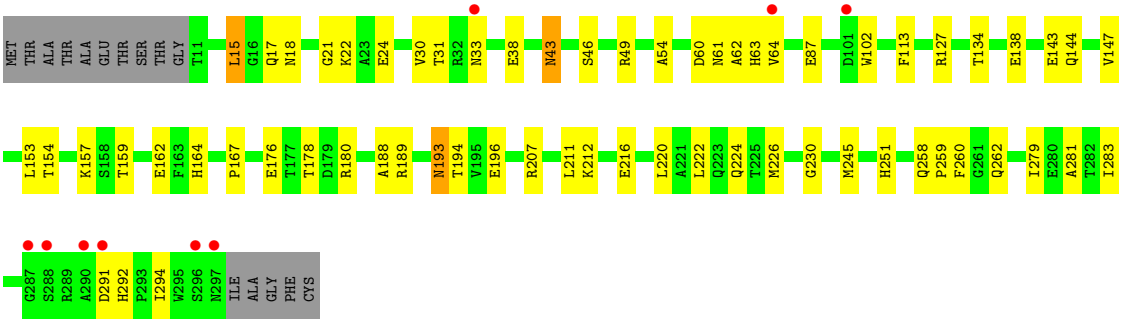
- Molecule 1: Uricase

Chain A:



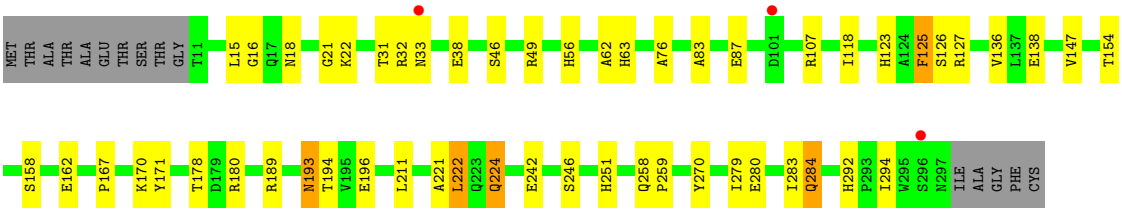
- Molecule 1: Uricase

Chain B:



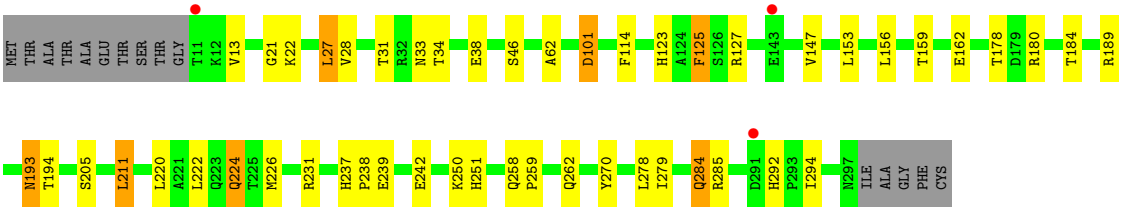
- Molecule 1: Uricase

Chain C:



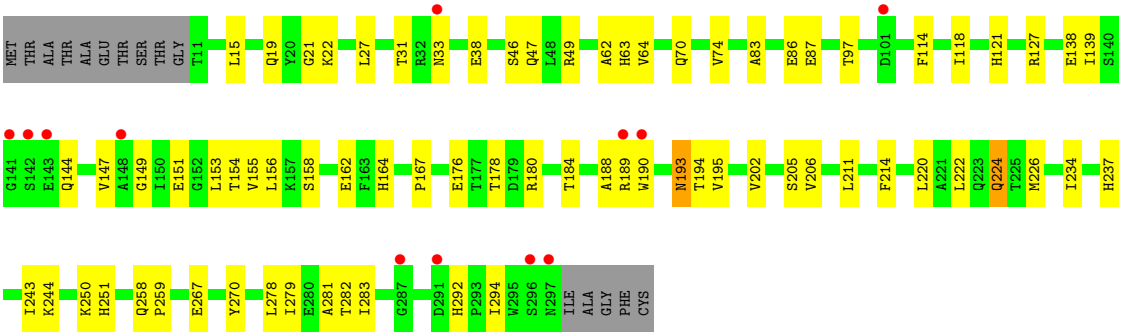
- Molecule 1: Uricase

Chain D:



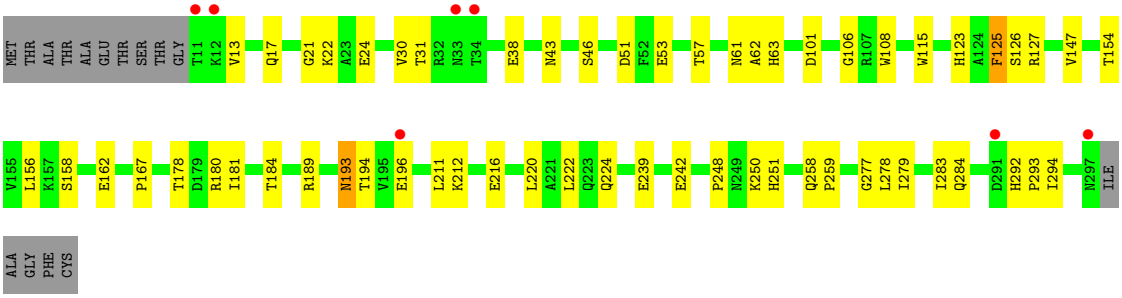
- Molecule 1: Uricase

Chain E:



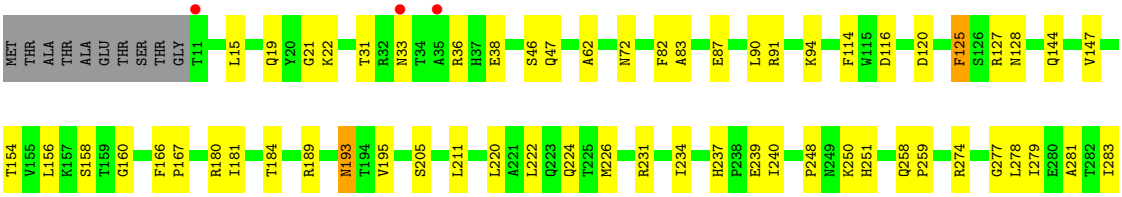
- Molecule 1: Uricase

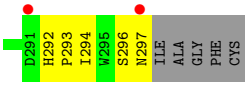
Chain F:



- Molecule 1: Uricase

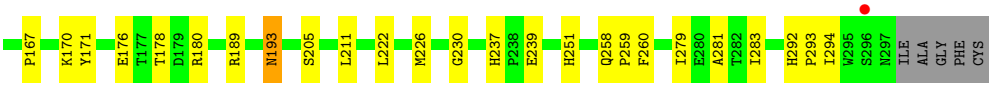
Chain G:





- Molecule 1: Uricase

Chain H:



4 Data and refinement statistics (i)

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 19.87 – 2.24	Depositor EDS
% Data completeness (in resolution range)	84.7 (20.00-2.24) 94.8 (19.87-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.23Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.239 0.191 , 0.238	Depositor DCC
R_{free} test set	13232 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19524	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0/2336	0.62	0/3171
1	B	0.34	0/2336	0.60	0/3171
1	C	0.33	0/2336	0.61	0/3171
1	D	0.35	0/2336	0.62	0/3171
1	E	0.34	0/2336	0.61	0/3171
1	F	0.34	0/2340	0.62	0/3175
1	G	0.34	0/2336	0.61	0/3171
1	H	0.36	0/2336	0.62	0/3171
All	All	0.34	0/18692	0.61	0/25372

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	2284	0	2179	58	0
1	B	2284	0	2179	54	0
1	C	2284	0	2179	48	0
1	D	2284	0	2179	53	0
1	E	2284	0	2179	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2288	0	2190	47	0
1	G	2284	0	2179	61	0
1	H	2284	0	2179	51	0
2	A	11	0	3	1	0
2	B	11	0	3	1	0
2	C	11	0	3	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	1	0
2	H	11	0	3	1	0
3	A	158	0	0	2	0
3	B	129	0	0	2	0
3	C	131	0	0	5	0
3	D	164	0	0	1	0
3	E	115	0	0	0	0
3	F	148	0	0	1	0
3	G	155	0	0	3	0
3	H	160	0	0	1	0
All	All	19524	0	17467	387	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 (387) 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:G:220:LEU:H	1:G:224:GLN:NE2	1.59	1.00
1:A:154:THR:HG23	1:A:250:LYS:NZ	1.85	0.91
1:C:292:HIS:HD2	1:C:294:ILE:H	1.24	0.83
1:D:180:ARG:HH12	2:D:1302:AZA:HN3	1.27	0.82
1:G:220:LEU:H	1:G:224:GLN:HE22	1.26	0.82
1:G:234:ILE:HD12	1:G:283:ILE:HG22	1.62	0.81
1:F:292:HIS:HD2	1:F:294:ILE:H	1.28	0.80
1:E:147:VAL:HG23	1:E:294:ILE:HD13	1.64	0.79
1:B:162:GLU:HB3	1:B:178:THR:HA	1.63	0.78
1:E:234:ILE:HD12	1:E:283:ILE:HG22	1.66	0.77
1:D:162:GLU:HB3	1:D:178:THR:HA	1.65	0.77
1:A:154:THR:HG23	1:A:250:LYS:HZ2	1.50	0.76
1:C:107:ARG:NH1	1:C:136:VAL:HG11	2.00	0.76
1:C:15:LEU:HD21	1:C:18:ASN:ND2	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:HIS:HD2	1:H:294:ILE:H	1.35	0.75
1:C:180:ARG:HH12	2:C:1304:AZA:HN3	1.33	0.74
1:A:292:HIS:HD2	1:A:294:ILE:H	1.33	0.74
1:C:147:VAL:HG23	1:C:294:ILE:HD13	1.69	0.72
1:G:292:HIS:HD2	1:G:294:ILE:H	1.37	0.72
1:H:189:ARG:HG3	1:H:189:ARG:HH11	1.54	0.71
1:B:193:ASN:C	1:B:193:ASN:HD22	1.92	0.71
1:E:180:ARG:HH12	2:E:1305:AZA:HN3	1.37	0.71
1:B:147:VAL:HG23	1:B:294:ILE:HD13	1.73	0.71
1:G:220:LEU:N	1:G:224:GLN:HE22	1.89	0.70
1:F:180:ARG:HH12	2:F:1307:AZA:HN3	1.39	0.70
1:A:153:LEU:HD21	1:A:211:LEU:HD11	1.73	0.70
1:C:31:THR:HB	1:C:38:GLU:HB2	1.73	0.70
1:H:180:ARG:HH12	2:H:1306:AZA:HN3	1.40	0.70
1:E:162:GLU:HB3	1:E:178:THR:HA	1.74	0.70
1:E:31:THR:HB	1:E:38:GLU:HB2	1.71	0.70
1:D:147:VAL:HG23	1:D:294:ILE:HD13	1.73	0.69
1:C:292:HIS:CD2	1:C:294:ILE:H	2.10	0.69
1:G:144:GLN:NE2	1:G:195:VAL:HG21	2.08	0.69
1:A:180:ARG:HH12	2:A:1301:AZA:HN3	1.38	0.69
1:C:162:GLU:HB3	1:C:178:THR:HA	1.75	0.69
1:E:193:ASN:C	1:E:193:ASN:HD22	1.98	0.67
1:G:220:LEU:N	1:G:224:GLN:NE2	2.40	0.67
1:B:180:ARG:HH12	2:B:1303:AZA:HN3	1.41	0.67
1:A:22:LYS:HZ2	1:D:251:HIS:HE1	1.42	0.67
1:B:220:LEU:H	1:B:224:GLN:NE2	1.92	0.67
1:A:184:THR:HA	1:A:250:LYS:HE2	1.77	0.67
1:D:292:HIS:HD2	1:D:294:ILE:H	1.43	0.66
1:G:234:ILE:CD1	1:G:283:ILE:HG22	2.26	0.66
1:A:31:THR:HB	1:A:38:GLU:HB2	1.79	0.65
1:E:21:GLY:HA3	1:E:46:SER:O	1.96	0.65
1:D:193:ASN:C	1:D:193:ASN:HD22	2.00	0.65
1:C:118:ILE:HD11	1:C:126:SER:HB3	1.78	0.65
1:A:251:HIS:HE1	1:D:22:LYS:HZ2	1.44	0.64
1:E:234:ILE:HD11	1:E:283:ILE:O	1.97	0.64
1:G:239:GLU:HG2	1:G:240:ILE:HD12	1.80	0.64
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.63	0.64
1:G:180:ARG:HH12	2:G:1308:AZA:HN3	1.46	0.63
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.64	0.63
1:G:147:VAL:HG23	1:G:294:ILE:HD13	1.81	0.63
1:B:193:ASN:ND2	1:B:194:THR:HG22	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ASN:ND2	1:D:194:THR:HG22	2.14	0.62
1:A:22:LYS:NZ	1:D:251:HIS:HE1	1.97	0.62
1:F:189:ARG:HG3	1:F:189:ARG:HH11	1.65	0.62
1:A:13:VAL:HG21	1:D:231:ARG:HG3	1.80	0.62
1:G:237:HIS:CB	1:G:240:ILE:HD13	2.29	0.62
1:H:15:LEU:HD11	1:H:18:ASN:ND2	2.14	0.62
1:G:234:ILE:HD11	1:G:283:ILE:O	1.99	0.61
1:A:231:ARG:HG3	1:D:13:VAL:HG11	1.81	0.61
1:C:193:ASN:C	1:C:193:ASN:HD22	2.02	0.61
1:D:193:ASN:HD22	1:D:194:THR:HG22	1.66	0.61
1:A:193:ASN:HD21	1:A:239:GLU:HA	1.66	0.61
1:C:107:ARG:HH12	1:C:136:VAL:HG11	1.66	0.61
1:A:167:PRO:HG3	1:D:62:ALA:O	2.01	0.61
1:C:162:GLU:CB	1:C:178:THR:HA	2.30	0.60
1:A:33:ASN:OD1	1:A:34:THR:HG23	2.01	0.60
1:B:292:HIS:HD2	1:B:294:ILE:H	1.48	0.60
1:F:31:THR:HB	1:F:38:GLU:HB2	1.83	0.60
1:G:21:GLY:HA3	1:G:46:SER:O	2.01	0.60
1:A:184:THR:CA	1:A:250:LYS:HE2	2.31	0.60
1:H:237:HIS:HB3	1:H:239:GLU:OE2	2.01	0.60
1:H:83:ALA:HB3	1:H:87:GLU:OE2	2.02	0.59
1:C:246:SER:HA	1:C:280:GLU:HG2	1.82	0.59
1:H:31:THR:HB	1:H:38:GLU:HB2	1.84	0.59
1:E:153:LEU:HD21	1:E:211:LEU:HD21	1.84	0.59
1:A:15:LEU:HD11	1:A:18:ASN:ND2	2.18	0.59
1:A:154:THR:HG23	1:A:250:LYS:HZ1	1.63	0.58
1:A:292:HIS:CD2	1:A:294:ILE:H	2.17	0.58
1:C:32:ARG:HD3	3:C:1330:HOH:O	2.03	0.58
1:A:267:GLU:HG2	1:B:30:VAL:O	2.03	0.58
1:C:158:SER:OG	1:D:123:HIS:HB2	2.03	0.58
1:E:62:ALA:O	1:H:167:PRO:HG3	2.04	0.58
1:E:144:GLN:HE21	1:E:195:VAL:HG11	1.67	0.58
1:D:189:ARG:HG3	1:D:189:ARG:HH11	1.69	0.57
1:B:260:PHE:HB2	1:B:262:GLN:HE21	1.69	0.57
1:G:237:HIS:HB3	1:G:240:ILE:HD13	1.86	0.57
1:B:134:THR:HG21	1:B:189:ARG:HH22	1.69	0.57
1:F:162:GLU:HG2	1:F:178:THR:O	2.05	0.57
1:B:207:ARG:O	1:B:211:LEU:HD23	2.04	0.57
1:G:144:GLN:HE21	1:G:195:VAL:HG21	1.67	0.57
1:H:226:MET:CE	1:H:279:ILE:HG22	2.35	0.57
1:C:224:GLN:HG2	3:C:1322:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ALA:N	1:E:87:GLU:OE2	2.33	0.57
1:C:15:LEU:HD23	1:C:16:GLY:O	2.04	0.57
1:E:144:GLN:NE2	1:E:195:VAL:HG11	2.20	0.57
1:E:226:MET:HE3	1:E:281:ALA:HB3	1.86	0.57
1:F:147:VAL:HG23	1:F:294:ILE:HD13	1.87	0.57
1:E:162:GLU:CB	1:E:178:THR:HA	2.35	0.56
1:F:62:ALA:O	1:G:167:PRO:HG3	2.05	0.56
1:F:220:LEU:H	1:F:224:GLN:NE2	2.03	0.56
1:B:143:GLU:HG2	1:B:144:GLN:N	2.21	0.56
1:G:251:HIS:HD2	3:G:1413:HOH:O	1.88	0.56
1:E:127:ARG:HB3	1:F:154:THR:HB	1.87	0.56
1:H:162:GLU:HB3	1:H:178:THR:HA	1.87	0.56
1:E:292:HIS:HD2	1:E:294:ILE:H	1.52	0.56
1:D:27:LEU:HD23	1:D:28:VAL:N	2.21	0.56
1:F:115:TRP:CZ2	1:F:127:ARG:HD3	2.40	0.56
1:A:226:MET:CE	1:A:279:ILE:HG22	2.36	0.56
1:E:188:ALA:HB1	1:E:243:ILE:HD11	1.88	0.56
1:B:167:PRO:HG3	1:C:62:ALA:O	2.05	0.56
1:E:251:HIS:CE1	1:H:22:LYS:NZ	2.74	0.56
1:B:22:LYS:HZ3	1:C:251:HIS:HE1	1.54	0.56
1:B:188:ALA:HB2	1:B:245:MET:HG2	1.88	0.56
1:D:162:GLU:HG3	1:D:220:LEU:HD23	1.88	0.56
1:A:127:ARG:NH2	3:A:1308:HOH:O	2.40	0.55
1:D:237:HIS:HB3	1:D:239:GLU:OE2	2.06	0.55
1:C:242:GLU:HB3	1:C:284:GLN:HB3	1.88	0.55
1:H:226:MET:HE2	1:H:279:ILE:HG22	1.88	0.55
1:H:162:GLU:CB	1:H:178:THR:HA	2.37	0.55
1:C:189:ARG:HG3	1:C:189:ARG:HH11	1.70	0.54
1:H:21:GLY:HA3	1:H:46:SER:O	2.07	0.54
1:E:190:TRP:HB3	1:E:243:ILE:HD13	1.90	0.54
1:E:22:LYS:HZ3	1:H:251:HIS:HE1	1.56	0.54
1:E:189:ARG:HG3	1:E:189:ARG:NH1	2.22	0.54
1:D:31:THR:HB	1:D:38:GLU:HB2	1.90	0.54
1:E:193:ASN:ND2	1:E:194:THR:HG22	2.23	0.54
1:G:72:ASN:HB3	1:H:260:PHE:CZ	2.43	0.54
1:B:21:GLY:HA3	1:B:46:SER:O	2.08	0.54
1:F:194:THR:OG1	1:F:196:GLU:HG2	2.08	0.54
1:G:19:GLN:HE21	1:G:47:GLN:NE2	2.06	0.54
1:C:21:GLY:HA3	1:C:46:SER:O	2.08	0.53
1:A:251:HIS:CE1	1:D:22:LYS:HZ2	2.26	0.53
1:F:292:HIS:CD2	1:F:294:ILE:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:ARG:HG3	1:H:189:ARG:NH1	2.20	0.53
1:A:22:LYS:NZ	1:D:251:HIS:CE1	2.76	0.53
1:H:226:MET:HE3	1:H:281:ALA:HB3	1.90	0.53
1:A:21:GLY:HA3	1:A:46:SER:O	2.08	0.53
1:A:162:GLU:HB3	1:A:178:THR:HA	1.91	0.53
1:B:22:LYS:NZ	1:C:251:HIS:HE1	2.07	0.53
1:C:15:LEU:HD21	1:C:18:ASN:HD22	1.72	0.53
1:B:31:THR:HB	1:B:38:GLU:HB2	1.92	0.52
1:C:15:LEU:HD23	1:C:15:LEU:C	2.29	0.52
1:C:83:ALA:HB3	1:C:87:GLU:OE2	2.08	0.52
1:G:220:LEU:H	1:G:224:GLN:HE21	1.51	0.52
1:B:22:LYS:NZ	1:C:251:HIS:CE1	2.78	0.52
1:H:279:ILE:N	1:H:279:ILE:HD12	2.24	0.52
1:E:251:HIS:HE1	1:H:22:LYS:NZ	2.07	0.52
1:G:189:ARG:HG3	1:G:189:ARG:HH11	1.74	0.52
1:A:260:PHE:HB2	1:A:262:GLN:HE21	1.75	0.52
1:B:162:GLU:CB	1:B:178:THR:HA	2.35	0.52
1:F:239:GLU:CD	1:F:239:GLU:H	2.13	0.52
1:G:154:THR:HB	1:H:127:ARG:HB3	1.92	0.52
1:B:134:THR:HG21	1:B:189:ARG:NH2	2.24	0.52
1:F:184:THR:HA	1:F:250:LYS:HG3	1.90	0.52
1:B:49:ARG:HH12	1:B:138:GLU:CD	2.12	0.52
1:C:87:GLU:HB2	3:C:1315:HOH:O	2.09	0.52
1:F:21:GLY:HA3	1:F:46:SER:O	2.10	0.52
1:F:242:GLU:HB3	1:F:284:GLN:HB3	1.91	0.51
1:E:86:GLU:OE1	1:E:86:GLU:N	2.44	0.51
1:D:114:PHE:O	1:D:127:ARG:HD2	2.10	0.50
1:A:279:ILE:N	1:A:279:ILE:HD12	2.26	0.50
1:G:31:THR:HB	1:G:38:GLU:HB2	1.91	0.50
1:E:202:VAL:O	1:E:206:VAL:HG23	2.12	0.50
1:E:244:LYS:HE2	1:E:282:THR:OG1	2.11	0.50
1:B:62:ALA:O	1:C:167:PRO:HG3	2.12	0.50
1:E:251:HIS:HE1	1:H:22:LYS:HZ3	1.60	0.50
1:C:76:ALA:HB1	1:D:262:GLN:HE22	1.76	0.50
1:G:114:PHE:O	1:G:127:ARG:HD2	2.11	0.50
1:A:49:ARG:HH12	1:A:138:GLU:CD	2.15	0.49
1:B:193:ASN:C	1:B:193:ASN:ND2	2.65	0.49
1:B:157:LYS:HE3	1:B:159:THR:O	2.12	0.49
1:E:167:PRO:HG3	1:H:62:ALA:O	2.12	0.49
1:B:164:HIS:HB3	1:B:176:GLU:HB3	1.93	0.49
1:B:230:GLY:HA3	1:B:283:ILE:HG13	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:ILE:N	1:E:283:ILE:HD12	2.27	0.49
1:G:19:GLN:HE21	1:G:47:GLN:HE22	1.58	0.49
1:A:162:GLU:CB	1:A:178:THR:HA	2.42	0.49
1:C:170:LYS:HE3	1:C:171:TYR:CZ	2.47	0.49
1:A:231:ARG:HG3	1:D:13:VAL:HG21	1.94	0.49
1:F:279:ILE:N	1:F:279:ILE:HD12	2.28	0.49
1:A:205:SER:OG	1:A:237:HIS:HE1	1.96	0.49
1:B:63:HIS:HB3	1:B:102:TRP:CD1	2.48	0.49
1:H:125:PHE:CD1	1:H:125:PHE:N	2.81	0.49
1:A:226:MET:HB2	1:A:247:LEU:HD12	1.94	0.49
1:A:258:GLN:N	1:A:259:PRO:CD	2.76	0.49
1:G:127:ARG:HG2	1:G:127:ARG:HH11	1.77	0.49
1:D:226:MET:CE	1:D:279:ILE:HG22	2.43	0.48
1:D:285:ARG:HG3	1:D:285:ARG:HH11	1.78	0.48
1:E:164:HIS:HB3	1:E:176:GLU:HB3	1.94	0.48
1:B:113:PHE:HB3	1:B:127:ARG:CZ	2.43	0.48
1:F:127:ARG:HB3	1:F:127:ARG:NH1	2.29	0.48
1:G:258:GLN:N	1:G:259:PRO:CD	2.76	0.48
1:A:170:LYS:HE3	1:A:171:TYR:CE2	2.49	0.48
1:B:251:HIS:CE1	1:C:22:LYS:NZ	2.82	0.48
1:C:15:LEU:HD12	1:C:56:HIS:HB2	1.95	0.48
1:A:226:MET:HE2	1:A:279:ILE:HG22	1.95	0.48
1:D:279:ILE:N	1:D:279:ILE:HD12	2.29	0.48
1:F:156:LEU:C	1:F:156:LEU:HD23	2.34	0.48
1:H:170:LYS:HE3	1:H:171:TYR:CZ	2.49	0.48
1:D:125:PHE:CD1	1:D:125:PHE:N	2.82	0.48
1:E:292:HIS:CD2	1:E:294:ILE:H	2.31	0.48
1:F:106:GLY:HA3	1:F:108:TRP:CH2	2.49	0.48
1:G:156:LEU:HD23	1:G:156:LEU:C	2.35	0.48
1:C:193:ASN:ND2	1:C:194:THR:HG22	2.29	0.47
1:C:222:LEU:HD13	1:C:279:ILE:HB	1.96	0.47
1:D:127:ARG:HG2	1:D:127:ARG:HH11	1.79	0.47
1:C:258:GLN:N	1:C:259:PRO:CD	2.78	0.47
1:D:21:GLY:HA3	1:D:46:SER:O	2.14	0.47
1:E:27:LEU:HD13	1:E:27:LEU:C	2.35	0.47
1:H:147:VAL:HG23	1:H:294:ILE:HD13	1.96	0.47
1:A:226:MET:HE3	1:A:281:ALA:HB3	1.96	0.47
1:B:258:GLN:N	1:B:259:PRO:CD	2.77	0.47
1:D:242:GLU:HB3	1:D:284:GLN:HB3	1.96	0.47
1:E:49:ARG:HH12	1:E:138:GLU:CD	2.17	0.47
1:G:158:SER:HA	1:G:181:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:HIS:HB2	1:G:240:ILE:HD13	1.96	0.47
1:H:49:ARG:HH12	1:H:138:GLU:CD	2.18	0.47
1:C:49:ARG:HH12	1:C:138:GLU:CD	2.17	0.47
1:E:193:ASN:HD22	1:E:194:THR:HG22	1.79	0.47
1:G:83:ALA:HB3	1:G:87:GLU:OE2	2.15	0.47
1:C:123:HIS:CG	1:D:159:THR:HG22	2.50	0.47
1:F:283:ILE:N	1:F:283:ILE:HD12	2.30	0.47
1:G:127:ARG:HG2	1:G:127:ARG:NH1	2.30	0.47
1:F:193:ASN:C	1:F:193:ASN:HD22	2.18	0.47
1:B:279:ILE:HD12	1:B:279:ILE:N	2.29	0.47
1:D:292:HIS:CD2	1:D:294:ILE:H	2.27	0.47
1:E:83:ALA:HB3	1:E:87:GLU:OE2	2.15	0.47
1:A:22:LYS:HZ2	1:D:251:HIS:CE1	2.29	0.46
1:B:226:MET:HE3	1:B:281:ALA:HB3	1.97	0.46
1:D:226:MET:HE2	1:D:279:ILE:HG22	1.96	0.46
1:E:156:LEU:HD23	1:E:156:LEU:C	2.35	0.46
1:D:156:LEU:C	1:D:156:LEU:HD23	2.35	0.46
1:E:70:GLN:O	1:E:74:VAL:HG23	2.14	0.46
1:F:53:GLU:O	1:F:57:THR:HG23	2.16	0.46
1:G:184:THR:HA	1:G:250:LYS:HG3	1.97	0.46
1:H:164:HIS:HB3	1:H:176:GLU:HB3	1.97	0.46
1:B:212:LYS:O	1:B:216:GLU:HG3	2.16	0.46
1:E:139:ILE:HG12	1:E:144:GLN:HB3	1.96	0.46
1:F:125:PHE:CD1	1:F:125:PHE:N	2.84	0.46
1:G:205:SER:OG	1:G:237:HIS:HE1	1.96	0.46
1:D:162:GLU:HB3	1:D:178:THR:CA	2.42	0.46
1:A:23:ALA:HA	1:A:45:THR:HG23	1.98	0.46
1:B:224:GLN:HG2	3:C:1335:HOH:O	2.14	0.46
1:G:19:GLN:NE2	1:G:47:GLN:NE2	2.64	0.46
1:A:156:LEU:C	1:A:156:LEU:HD23	2.36	0.46
1:F:220:LEU:H	1:F:224:GLN:HE21	1.63	0.46
1:G:90:LEU:O	1:G:94:LYS:HG3	2.14	0.46
1:E:251:HIS:CE1	1:H:22:LYS:HZ3	2.34	0.46
1:A:193:ASN:ND2	1:A:194:THR:HG22	2.32	0.45
1:F:51:ASP:O	1:F:63:HIS:HD2	1.99	0.45
1:A:127:ARG:HB2	1:B:154:THR:HB	1.98	0.45
1:B:162:GLU:HB3	1:B:178:THR:CA	2.42	0.45
1:F:212:LYS:O	1:F:216:GLU:HG3	2.16	0.45
1:E:155:VAL:HG23	1:E:214:PHE:CZ	2.52	0.45
1:G:193:ASN:C	1:G:193:ASN:HD22	2.20	0.45
1:A:193:ASN:HD22	1:A:194:THR:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASN:HD22	1:B:194:THR:HG22	1.79	0.45
1:B:226:MET:CE	1:B:279:ILE:HG22	2.47	0.45
1:E:118:ILE:O	1:E:121:HIS:HB2	2.17	0.45
1:E:267:GLU:HG2	1:F:30:VAL:O	2.17	0.45
1:E:164:HIS:CB	1:E:176:GLU:HB3	2.47	0.45
1:F:13:VAL:HG21	1:G:231:ARG:HG3	1.98	0.45
1:H:193:ASN:HD21	1:H:239:GLU:HA	1.81	0.45
1:B:64:VAL:O	1:C:167:PRO:HD2	2.17	0.45
1:F:115:TRP:CZ3	1:F:127:ARG:HG2	2.52	0.45
1:G:296:SER:O	1:G:297:ASN:C	2.55	0.45
1:D:162:GLU:CB	1:D:178:THR:HA	2.41	0.45
1:A:154:THR:HB	1:B:127:ARG:HB3	1.98	0.44
1:A:205:SER:OG	1:A:237:HIS:CE1	2.70	0.44
1:C:283:ILE:N	1:C:283:ILE:HD12	2.32	0.44
1:F:22:LYS:HZ2	1:G:251:HIS:CE1	2.36	0.44
1:H:89:LEU:HD22	1:H:108:TRP:HB3	1.98	0.44
1:D:153:LEU:HD21	1:D:211:LEU:HD11	1.99	0.44
1:E:251:HIS:CE1	1:H:22:LYS:HZ2	2.36	0.44
1:G:279:ILE:HD12	1:G:279:ILE:N	2.32	0.44
1:A:158:SER:HA	1:A:181:ILE:HG12	2.00	0.44
1:A:169:ASP:HB2	3:A:1383:HOH:O	2.18	0.44
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.83	0.44
1:B:153:LEU:HD21	1:B:211:LEU:HD21	1.98	0.44
1:F:193:ASN:HD21	1:F:239:GLU:HA	1.83	0.44
1:F:292:HIS:CD2	1:F:293:PRO:HD2	2.52	0.44
1:F:17:GLN:HG3	3:F:1443:HOH:O	2.17	0.44
1:G:226:MET:HE3	1:G:281:ALA:HB3	1.99	0.44
1:A:239:GLU:CD	1:A:239:GLU:H	2.21	0.44
1:D:258:GLN:NE2	1:D:258:GLN:HA	2.33	0.44
1:F:251:HIS:CE1	1:G:22:LYS:HZ2	2.36	0.44
1:D:184:THR:HA	1:D:250:LYS:HG3	2.00	0.43
1:D:237:HIS:HA	1:D:238:PRO:HD3	1.89	0.43
1:G:36:ARG:HH22	1:G:120:ASP:CG	2.21	0.43
1:H:71:LYS:HE2	1:H:71:LYS:HB3	1.90	0.43
1:G:125:PHE:CD1	1:G:125:PHE:N	2.87	0.43
1:H:112:GLN:HB3	1:H:133:ARG:HB3	2.00	0.43
1:A:251:HIS:CE1	1:D:22:LYS:NZ	2.86	0.43
1:E:22:LYS:HZ3	1:H:251:HIS:CE1	2.36	0.43
1:H:226:MET:HE2	1:H:279:ILE:CG2	2.48	0.43
1:A:244:LYS:HE2	1:A:282:THR:OG1	2.19	0.43
1:C:162:GLU:HB3	1:C:178:THR:CA	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:THR:OG1	1:C:196:GLU:HG2	2.19	0.43
1:E:19:GLN:NE2	1:E:47:GLN:NE2	2.66	0.43
1:E:64:VAL:O	1:H:167:PRO:HD2	2.18	0.43
1:E:162:GLU:HB3	1:E:178:THR:CA	2.47	0.43
1:E:279:ILE:HD12	1:E:279:ILE:N	2.34	0.43
1:B:251:HIS:HE1	1:C:22:LYS:NZ	2.17	0.43
1:B:22:LYS:HZ3	1:C:251:HIS:CE1	2.32	0.43
1:F:162:GLU:HG2	1:F:178:THR:C	2.39	0.43
1:B:224:GLN:HE21	1:B:224:GLN:HB3	1.71	0.42
1:E:258:GLN:N	1:E:259:PRO:CD	2.82	0.42
1:F:24:GLU:HB3	1:G:274:ARG:HD2	2.01	0.42
1:G:90:LEU:HB3	1:G:94:LYS:HE3	2.00	0.42
1:H:83:ALA:N	1:H:87:GLU:OE2	2.52	0.42
1:H:258:GLN:N	1:H:259:PRO:CD	2.82	0.42
1:A:182:LEU:HD11	1:A:222:LEU:HG	2.00	0.42
1:C:154:THR:HB	1:D:127:ARG:HB3	1.99	0.42
1:D:33:ASN:OD1	1:D:34:THR:HG23	2.18	0.42
1:E:205:SER:OG	1:E:237:HIS:HE1	2.02	0.42
1:G:160:GLY:HA3	3:H:1445:HOH:O	2.19	0.42
1:D:239:GLU:H	1:D:239:GLU:CD	2.23	0.42
1:D:258:GLN:N	1:D:259:PRO:CD	2.81	0.42
1:D:278:LEU:C	1:D:279:ILE:HD12	2.39	0.42
1:E:193:ASN:C	1:E:193:ASN:ND2	2.70	0.42
1:F:158:SER:HA	1:F:181:ILE:HG12	2.02	0.42
1:F:278:LEU:C	1:F:279:ILE:HD12	2.39	0.42
1:H:127:ARG:HH11	1:H:127:ARG:HG2	1.84	0.42
1:B:224:GLN:CG	3:C:1335:HOH:O	2.68	0.42
1:D:27:LEU:CD2	1:D:28:VAL:N	2.82	0.42
1:D:101:ASP:HB2	3:D:1451:HOH:O	2.20	0.42
1:A:43:ASN:O	1:A:110:ALA:HA	2.19	0.42
1:H:162:GLU:HB3	1:H:178:THR:CA	2.49	0.42
1:H:226:MET:HE3	1:H:281:ALA:CB	2.50	0.42
1:H:230:GLY:HA3	1:H:283:ILE:HG13	2.02	0.42
1:E:149:GLY:HA2	1:E:190:TRP:CZ3	2.55	0.42
1:F:258:GLN:N	1:F:259:PRO:CD	2.83	0.42
1:E:158:SER:OG	1:F:123:HIS:HB2	2.19	0.41
1:F:24:GLU:HA	1:F:43:ASN:ND2	2.35	0.41
1:G:91:ARG:HG3	3:G:1422:HOH:O	2.19	0.41
1:B:87:GLU:HB2	3:B:1361:HOH:O	2.19	0.41
1:C:125:PHE:CD1	1:C:125:PHE:N	2.88	0.41
1:C:189:ARG:HG3	1:C:189:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:SER:OG	1:H:237:HIS:HE1	2.03	0.41
1:B:54:ALA:HB1	1:B:60:ASP:HB3	2.02	0.41
1:G:224:GLN:HE21	1:G:224:GLN:HB3	1.65	0.41
1:B:24:GLU:HA	1:B:43:ASN:ND2	2.36	0.41
1:E:184:THR:HA	1:E:250:LYS:HG3	2.02	0.41
1:E:243:ILE:HG23	1:E:243:ILE:O	2.20	0.41
1:H:97:THR:HG21	1:H:139:ILE:HG21	2.02	0.41
1:B:15:LEU:CD2	1:B:18:ASN:HD22	2.32	0.41
1:G:278:LEU:C	1:G:279:ILE:HD12	2.40	0.41
1:G:292:HIS:CD2	1:G:293:PRO:HD2	2.55	0.41
1:C:193:ASN:HD22	1:C:194:THR:N	2.19	0.41
1:F:220:LEU:HB2	1:F:224:GLN:NE2	2.35	0.41
1:A:251:HIS:HE1	1:D:22:LYS:NZ	2.14	0.41
1:B:17:GLN:HG3	3:B:1386:HOH:O	2.19	0.41
1:E:97:THR:HG21	1:E:139:ILE:HG21	2.02	0.41
1:E:220:LEU:H	1:E:224:GLN:NE2	2.19	0.41
1:G:116:ASP:OD2	1:G:128:ASN:HB2	2.21	0.41
1:H:239:GLU:CD	1:H:239:GLU:H	2.24	0.41
1:H:279:ILE:N	1:H:279:ILE:CD1	2.83	0.41
1:A:118:ILE:O	1:A:121:HIS:HB2	2.21	0.41
1:D:205:SER:OG	1:D:237:HIS:CE1	2.74	0.41
1:E:114:PHE:O	1:E:127:ARG:HD2	2.21	0.41
1:E:154:THR:O	1:F:126:SER:HA	2.21	0.41
1:E:292:HIS:CD2	1:E:294:ILE:HG22	2.56	0.41
1:F:167:PRO:HD3	1:G:62:ALA:O	2.21	0.41
1:G:248:PRO:HA	1:G:277:GLY:O	2.20	0.41
1:A:154:THR:CG2	1:A:250:LYS:HZ2	2.26	0.41
1:B:61:ASN:HA	1:B:64:VAL:HG23	2.02	0.40
1:E:188:ALA:O	1:E:189:ARG:HG3	2.21	0.40
1:G:82:PHE:CD1	1:G:82:PHE:N	2.90	0.40
1:A:125:PHE:CD1	1:A:125:PHE:N	2.88	0.40
1:D:224:GLN:HE21	1:D:224:GLN:HB3	1.66	0.40
1:G:205:SER:OG	1:G:237:HIS:CE1	2.73	0.40
1:H:14:VAL:HG12	1:H:15:LEU:N	2.36	0.40
1:E:278:LEU:C	1:E:279:ILE:HD12	2.41	0.40
1:G:240:ILE:HD12	1:G:240:ILE:N	2.36	0.40
1:H:189:ARG:NH1	1:H:189:ARG:CG	2.85	0.40
1:A:243:ILE:HG23	1:A:243:ILE:O	2.21	0.40
1:E:22:LYS:NZ	1:H:251:HIS:CE1	2.90	0.40
1:E:151:GLU:OE2	1:E:189:ARG:NH2	2.53	0.40
1:F:61:ASN:O	1:G:166:PHE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:PRO:HA	1:F:277:GLY:O	2.21	0.40
1:B:127:ARG:HH11	1:B:127:ARG:HG2	1.87	0.40
1:G:33:ASN:N	3:G:1453:HOH:O	2.53	0.40
1:H:292:HIS:CD2	1:H:293:PRO:HD2	2.57	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	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
1	B	285/302 (94%)	274 (96%)	10 (4%)	1 (0%)	34	35
1	C	285/302 (94%)	275 (96%)	9 (3%)	1 (0%)	34	35
1	D	285/302 (94%)	281 (99%)	4 (1%)	0	100	100
1	E	285/302 (94%)	277 (97%)	8 (3%)	0	100	100
1	F	285/302 (94%)	277 (97%)	8 (3%)	0	100	100
1	G	285/302 (94%)	275 (96%)	10 (4%)	0	100	100
1	H	285/302 (94%)	275 (96%)	10 (4%)	0	100	100
All	All	2280/2416 (94%)	2213 (97%)	65 (3%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	291	ASP
1	C	221	ALA

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	237/250 (95%)	232 (98%)	5 (2%)	53	60
1	B	237/250 (95%)	231 (98%)	6 (2%)	47	54
1	C	237/250 (95%)	227 (96%)	10 (4%)	30	32
1	D	237/250 (95%)	228 (96%)	9 (4%)	33	36
1	E	237/250 (95%)	230 (97%)	7 (3%)	41	47
1	F	238/250 (95%)	233 (98%)	5 (2%)	53	60
1	G	237/250 (95%)	232 (98%)	5 (2%)	53	60
1	H	237/250 (95%)	233 (98%)	4 (2%)	60	68
All	All	1897/2000 (95%)	1846 (97%)	51 (3%)	44	51

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

Mol	Chain	Res	Type
1	A	15	LEU
1	A	87	GLU
1	A	193	ASN
1	A	222	LEU
1	A	224	GLN
1	B	15	LEU
1	B	33	ASN
1	B	43	ASN
1	B	193	ASN
1	B	196	GLU
1	B	222	LEU
1	C	33	ASN
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

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Mol	Chain	Res	Type
1	C	270	TYR
1	C	284	GLN
1	D	27	LEU
1	D	101	ASP
1	D	125	PHE
1	D	193	ASN
1	D	211	LEU
1	D	222	LEU
1	D	224	GLN
1	D	270	TYR
1	D	284	GLN
1	E	15	LEU
1	E	33	ASN
1	E	63	HIS
1	E	193	ASN
1	E	222	LEU
1	E	224	GLN
1	E	270	TYR
1	F	101	ASP
1	F	125	PHE
1	F	193	ASN
1	F	211	LEU
1	F	222	LEU
1	G	15	LEU
1	G	125	PHE
1	G	193	ASN
1	G	211	LEU
1	G	222	LEU
1	H	125	PHE
1	H	193	ASN
1	H	211	LEU
1	H	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	43	ASN
1	A	63	HIS
1	A	111	GLN
1	A	193	ASN
1	A	237	HIS

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Mol	Chain	Res	Type
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	111	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	292	HIS
1	C	18	ASN
1	C	43	ASN
1	C	111	GLN
1	C	193	ASN
1	C	237	HIS
1	C	251	HIS
1	C	258	GLN
1	C	292	HIS
1	D	43	ASN
1	D	63	HIS
1	D	111	GLN
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	144	GLN
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	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	251	HIS
1	F	262	GLN
1	F	292	HIS
1	G	33	ASN
1	G	43	ASN
1	G	47	GLN
1	G	111	GLN
1	G	119	ASN
1	G	144	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	292	HIS
1	H	33	ASN
1	H	40	GLN
1	H	43	ASN
1	H	47	GLN
1	H	111	GLN
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 monosaccharides 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	C	1304	-	9,12,12	2.00	2 (22%)	4,17,17	7.64	3 (75%)
2	AZA	F	1307	-	9,12,12	2.16	2 (22%)	4,17,17	7.39	3 (75%)
2	AZA	H	1306	-	9,12,12	2.07	2 (22%)	4,17,17	7.57	3 (75%)
2	AZA	B	1303	-	9,12,12	2.02	2 (22%)	4,17,17	7.53	3 (75%)
2	AZA	E	1305	-	9,12,12	2.06	2 (22%)	4,17,17	7.51	3 (75%)
2	AZA	D	1302	-	9,12,12	2.02	2 (22%)	4,17,17	7.72	3 (75%)
2	AZA	G	1308	-	9,12,12	1.96	2 (22%)	4,17,17	7.68	3 (75%)
2	AZA	A	1301	-	9,12,12	2.06	2 (22%)	4,17,17	7.44	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	C	1304	-	-	-	0/2/2/2
2	AZA	F	1307	-	-	-	0/2/2/2
2	AZA	H	1306	-	-	-	0/2/2/2
2	AZA	B	1303	-	-	-	0/2/2/2
2	AZA	E	1305	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AZA	D	1302	-	-	-	0/2/2/2
2	AZA	G	1308	-	-	-	0/2/2/2
2	AZA	A	1301	-	-	-	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1307	AZA	C6-N1	4.64	1.41	1.33
2	A	1301	AZA	C6-N1	4.52	1.40	1.33
2	E	1305	AZA	C6-N1	4.35	1.40	1.33
2	H	1306	AZA	C6-N1	4.32	1.40	1.33
2	C	1304	AZA	C6-N1	4.06	1.40	1.33
2	B	1303	AZA	C6-N1	3.98	1.40	1.33
2	D	1302	AZA	C6-N1	3.98	1.40	1.33
2	D	1302	AZA	C5-C6	3.94	1.48	1.41
2	H	1306	AZA	C5-C6	3.92	1.48	1.41
2	B	1303	AZA	C5-C6	3.87	1.48	1.41
2	G	1308	AZA	C6-N1	3.86	1.39	1.33
2	G	1308	AZA	C5-C6	3.82	1.47	1.41
2	F	1307	AZA	C5-C6	3.74	1.47	1.41
2	E	1305	AZA	C5-C6	3.69	1.47	1.41
2	C	1304	AZA	C5-C6	3.64	1.47	1.41
2	A	1301	AZA	C5-C6	3.60	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1308	AZA	C2-N1-C6	12.83	125.97	115.14
2	D	1302	AZA	C2-N1-C6	12.78	125.93	115.14
2	C	1304	AZA	C2-N1-C6	12.63	125.80	115.14
2	H	1306	AZA	C2-N1-C6	12.46	125.66	115.14
2	E	1305	AZA	C2-N1-C6	12.44	125.65	115.14
2	A	1301	AZA	C2-N1-C6	12.40	125.61	115.14
2	B	1303	AZA	C2-N1-C6	12.35	125.57	115.14
2	F	1307	AZA	C2-N1-C6	12.10	125.36	115.14
2	D	1302	AZA	C5-C6-N1	-8.11	112.33	123.43
2	H	1306	AZA	C5-C6-N1	-8.07	112.39	123.43
2	B	1303	AZA	C5-C6-N1	-8.07	112.39	123.43
2	C	1304	AZA	C5-C6-N1	-8.04	112.44	123.43
2	F	1307	AZA	C5-C6-N1	-7.97	112.54	123.43
2	G	1308	AZA	C5-C6-N1	-7.90	112.63	123.43
2	E	1305	AZA	C5-C6-N1	-7.86	112.69	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1301	AZA	C5-C6-N1	-7.73	112.86	123.43
2	C	1304	AZA	N9-N8-N7	3.12	115.30	111.25
2	D	1302	AZA	N9-N8-N7	3.09	115.26	111.25
2	E	1305	AZA	N9-N8-N7	3.03	115.18	111.25
2	G	1308	AZA	N9-N8-N7	3.02	115.16	111.25
2	B	1303	AZA	N9-N8-N7	3.01	115.16	111.25
2	H	1306	AZA	N9-N8-N7	2.99	115.13	111.25
2	F	1307	AZA	N9-N8-N7	2.88	114.98	111.25
2	A	1301	AZA	N9-N8-N7	2.87	114.97	111.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1304	AZA	1	0
2	F	1307	AZA	1	0
2	H	1306	AZA	1	0
2	B	1303	AZA	1	0
2	E	1305	AZA	1	0
2	D	1302	AZA	1	0
2	G	1308	AZA	1	0
2	A	1301	AZA	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	287/302 (95%)	-0.42	4 (1%)	75	76	17, 24, 34, 52	0
1	B	287/302 (95%)	-0.24	9 (3%)	49	49	18, 30, 47, 60	0
1	C	287/302 (95%)	-0.28	3 (1%)	82	83	18, 30, 41, 52	0
1	D	287/302 (95%)	-0.32	3 (1%)	82	83	17, 25, 40, 51	0
1	E	287/302 (95%)	-0.21	12 (4%)	36	35	19, 29, 44, 62	0
1	F	287/302 (95%)	-0.35	7 (2%)	59	60	17, 26, 39, 52	0
1	G	287/302 (95%)	-0.28	5 (1%)	70	71	19, 26, 43, 57	0
1	H	287/302 (95%)	-0.29	3 (1%)	82	83	16, 26, 38, 51	0
All	All	2296/2416 (95%)	-0.30	46 (2%)	65	66	16, 27, 41, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	THR	4.1
1	F	11	THR	4.1
1	G	11	THR	3.7
1	G	33	ASN	3.5
1	B	33	ASN	3.2
1	H	11	THR	3.2
1	C	33	ASN	3.1
1	F	297	ASN	3.0
1	F	33	ASN	2.9
1	E	142	SER	2.9
1	E	291	ASP	2.9
1	E	297	ASN	2.8
1	E	148	ALA	2.7
1	E	33	ASN	2.7
1	D	143	GLU	2.6
1	A	101	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	196	GLU	2.6
1	A	33	ASN	2.6
1	B	64	VAL	2.6
1	F	12	LYS	2.6
1	G	297	ASN	2.6
1	B	296	SER	2.5
1	F	34	THR	2.5
1	B	288	SER	2.5
1	A	119	ASN	2.5
1	F	291	ASP	2.5
1	D	291	ASP	2.4
1	E	141	GLY	2.4
1	H	101	ASP	2.4
1	E	190	TRP	2.4
1	E	287	GLY	2.3
1	G	291	ASP	2.3
1	E	189	ARG	2.3
1	C	101	ASP	2.3
1	E	296	SER	2.3
1	B	290	ALA	2.3
1	D	11	THR	2.3
1	H	296	SER	2.3
1	B	101	ASP	2.2
1	E	101	ASP	2.1
1	B	297	ASN	2.1
1	B	291	ASP	2.1
1	E	143	GLU	2.1
1	G	35	ALA	2.1
1	B	287	GLY	2.1
1	C	296	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AZA	B	1303	11/11	0.96	0.15	34,36,37,38	0
2	AZA	E	1305	11/11	0.96	0.11	28,29,30,30	0
2	AZA	F	1307	11/11	0.96	0.14	22,23,24,25	0
2	AZA	A	1301	11/11	0.97	0.12	20,22,25,25	0
2	AZA	D	1302	11/11	0.97	0.15	22,23,25,26	0
2	AZA	C	1304	11/11	0.98	0.15	36,37,38,38	0
2	AZA	G	1308	11/11	0.98	0.13	19,19,21,21	0
2	AZA	H	1306	11/11	0.98	0.14	23,26,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.