



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:01 am GMT

PDB ID : 2V4I  
Title : STRUCTURE OF A NOVEL N-ACYL-ENZYME INTERMEDIATE OF AN  
N-TERMINAL NUCLEOPHILE (NTN) HYDROLASE, OAT2  
Authors : Iqbal, A.; Clifton, I.J.; Schofield, C.J.  
Deposited on : 2008-09-22  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

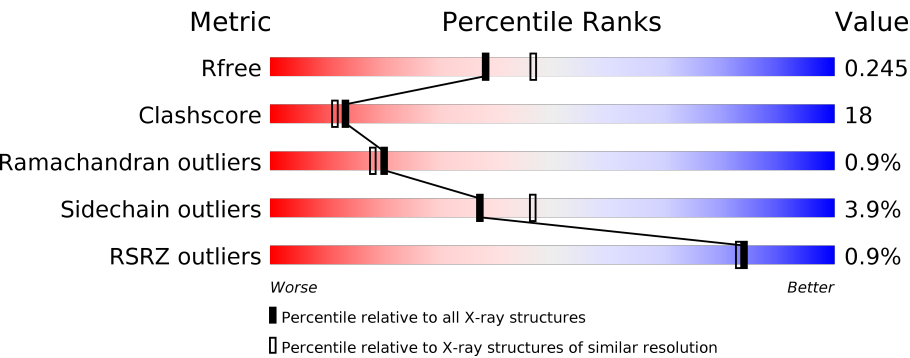
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	173	<div><div>%</div><div><div></div><div>62%</div><div>36%</div><div></div></div><div></div></div>
1	C	173	<div><div></div><div>65%</div><div>33%</div><div></div></div> <div></div>
1	E	173	<div><div>3%</div><div></div><div>63%</div><div>35%</div><div></div></div> <div></div>
1	G	173	<div><div>4%</div><div></div><div>65%</div><div>32%</div><div></div></div> <div></div>
2	B	213	<div><div></div><div>68%</div><div>26%</div><div>5%</div></div> <div></div>
2	D	213	<div><div></div><div>71%</div><div>23%</div><div>5%</div></div> <div></div>

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Mol	Chain	Length	Quality of chain
2	F	213	 69% 25% • 5%
2	H	213	 69% 25% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AYA	F	181	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11153 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 GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1215	758	221	230	6			
1	C	173	Total	C	N	O	S	0	0	0
			1215	758	221	230	6			
1	E	173	Total	C	N	O	S	0	0	0
			1215	758	221	230	6			
1	G	173	Total	C	N	O	S	0	0	0
			1215	758	221	230	6			

- Molecule 2 is a protein called GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1498	933	261	299	5			
2	D	203	Total	C	N	O	S	0	0	0
			1498	933	261	299	5			
2	F	203	Total	C	N	O	S	0	0	0
			1498	933	261	299	5			
2	H	203	Total	C	N	O	S	0	0	0
			1498	933	261	299	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	AYA	THR	ENGINEERED MUTATION	UNP Q53940
D	181	AYA	THR	ENGINEERED MUTATION	UNP Q53940
F	181	AYA	THR	ENGINEERED MUTATION	UNP Q53940
H	181	AYA	THR	ENGINEERED MUTATION	UNP Q53940

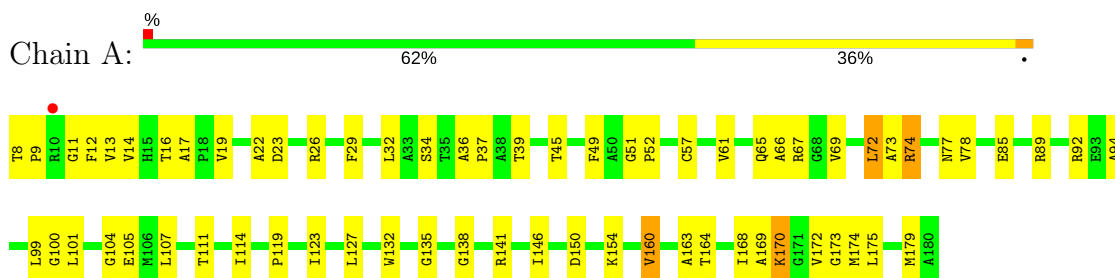
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	56	Total 56	O 56	0	0
3	C	35	Total 35	O 35	0	0
3	D	46	Total 46	O 46	0	0
3	E	23	Total 23	O 23	0	0
3	F	40	Total 40	O 40	0	0
3	G	21	Total 21	O 21	0	0
3	H	33	Total 33	O 33	0	0

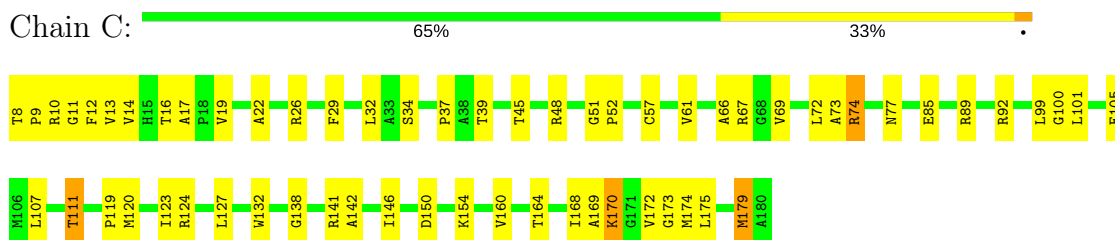
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

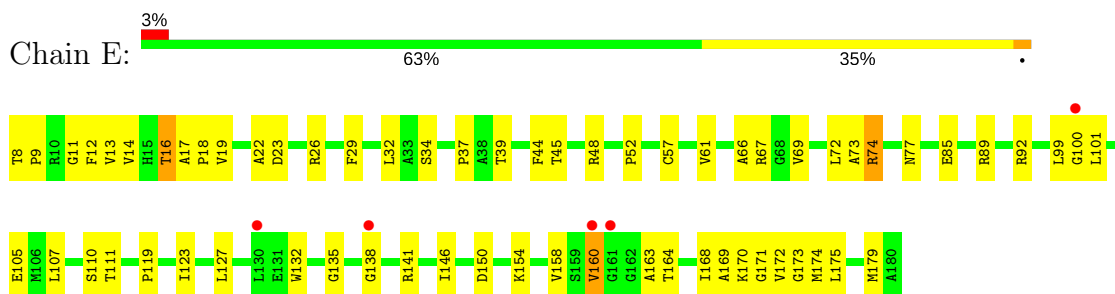
- Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN



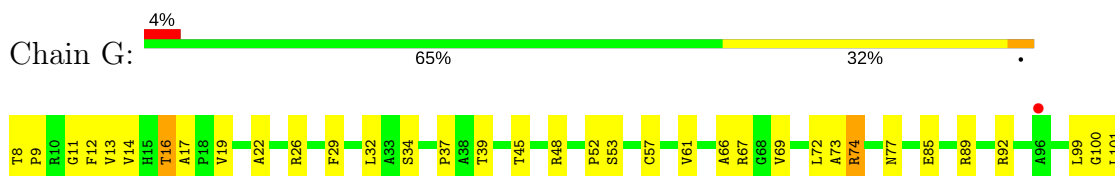
- Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN

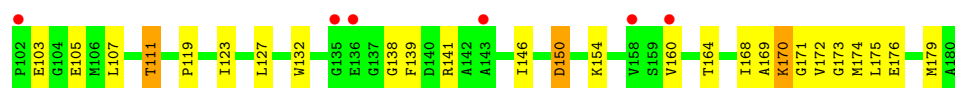


- Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN



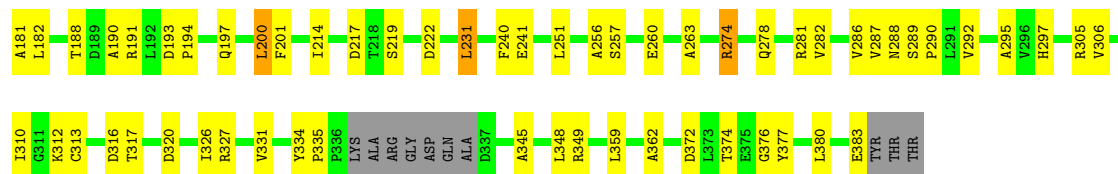
- Molecule 1: GLUTAMATE N-ACETYLTRANSFERASE 2 ALPHA CHAIN





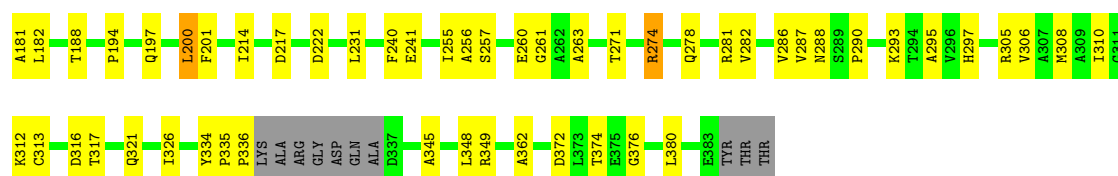
• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain B: 68% 26% • 5%



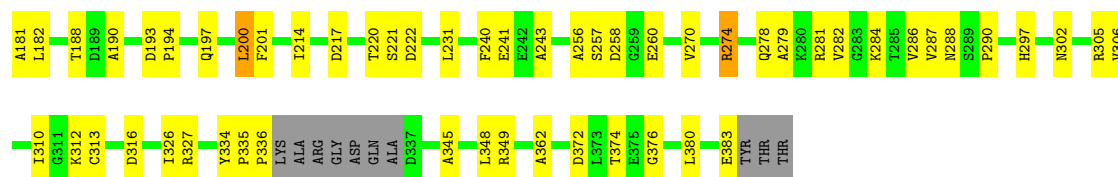
• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain D: 71% 23% • 5%



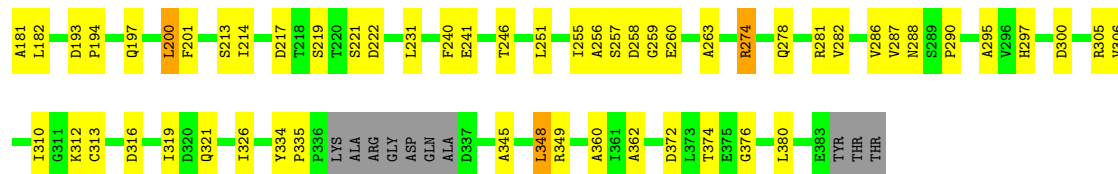
• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain F: 69% 25% • 5%



• Molecule 2: GLUTAMATE N-ACETYLTRANSFERASE 2 BETA CHAIN

Chain H: 69% 25% • 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.45Å 180.16Å 60.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.20 29.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.70-2.20) 99.6 (29.70-2.20)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.214 , 0.247 0.214 , 0.245	Depositor DCC
$R_{free}$ test set	4006 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.763	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.418 for -h,-k,l	Xtriage
Reported twinning fraction	0.471 for H,-K,-L	Depositor
Outliers	0 of 79803 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.40	0/1233	0.53	0/1681
1	C	0.38	0/1233	0.55	0/1681
1	E	0.39	0/1233	0.54	0/1681
1	G	0.38	0/1233	0.54	0/1681
2	B	0.36	0/1509	0.55	0/2052
2	D	0.38	0/1509	0.55	0/2052
2	F	0.37	0/1509	0.55	0/2052
2	H	0.39	0/1509	0.55	0/2052
All	All	0.38	0/10968	0.55	0/14932

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	1215	0	1196	68	1
1	C	1215	0	1196	63	0
1	E	1215	0	1196	69	0
1	G	1215	0	1196	63	1
2	B	1498	0	1450	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1498	0	1450	46	0
2	F	1498	0	1450	52	0
2	H	1498	0	1450	51	0
3	A	47	0	0	6	0
3	B	56	0	0	8	0
3	C	35	0	0	4	0
3	D	46	0	0	5	0
3	E	23	0	0	1	0
3	F	40	0	0	7	0
3	G	21	0	0	3	0
3	H	33	0	0	4	0
All	All	11153	0	10584	387	1

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 18.

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)
2:H:349:ARG:HB2	3:H:2024:HOH:O	1.70	0.90
1:C:173:GLY:HA3	2:D:260:GLU:OE2	1.72	0.89
2:D:271:THR:HG23	3:D:2016:HOH:O	1.71	0.89
2:H:181:AYA:HM1	2:H:221:SER:HB2	1.57	0.85
1:G:19:VAL:HG11	1:G:123:ILE:HG12	1.60	0.83
1:E:173:GLY:HA3	2:F:260:GLU:OE2	1.80	0.82
1:C:19:VAL:HG11	1:C:123:ILE:HG12	1.63	0.81
2:H:181:AYA:CM	2:H:221:SER:HB2	2.10	0.81
2:B:312:LYS:O	3:B:2039:HOH:O	1.98	0.80
1:G:22:ALA:HB3	1:G:74:ARG:NH1	1.97	0.80
1:C:22:ALA:HB3	1:C:74:ARG:NH1	1.97	0.80
1:C:10:ARG:NH2	3:C:2003:HOH:O	2.15	0.79
1:E:179:MET:CE	2:F:222:ASP:HB3	2.14	0.78
1:E:19:VAL:HG11	1:E:123:ILE:HG12	1.65	0.77
1:C:51:GLY:HA2	3:C:2016:HOH:O	1.86	0.76
1:C:8:THR:HG21	3:C:2001:HOH:O	1.85	0.76
1:A:22:ALA:HB3	1:A:74:ARG:NH1	2.01	0.75
1:A:19:VAL:HG11	1:A:123:ILE:HG12	1.68	0.74
1:E:110:SER:HB2	3:E:2010:HOH:O	1.87	0.74
2:H:246:THR:HG23	3:H:2009:HOH:O	1.87	0.74
1:E:22:ALA:HB3	1:E:74:ARG:NH1	2.02	0.74
1:A:146:ILE:HD13	1:A:168:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:PRO:HA	1:G:67:ARG:HD2	1.70	0.73
1:E:146:ILE:HD13	1:E:168:ILE:HD12	1.71	0.72
1:G:146:ILE:HD13	1:G:168:ILE:HD12	1.70	0.72
1:A:173:GLY:HA3	2:B:260:GLU:OE2	1.89	0.72
1:C:146:ILE:HD13	1:C:168:ILE:HD12	1.70	0.71
2:H:376:GLY:O	2:H:380:LEU:HG	1.90	0.71
2:D:376:GLY:O	2:D:380:LEU:HG	1.91	0.70
1:G:173:GLY:HA3	2:H:260:GLU:OE2	1.92	0.70
1:A:37:PRO:HA	1:A:67:ARG:HD2	1.73	0.70
1:E:37:PRO:HA	1:E:67:ARG:HD2	1.73	0.70
1:G:19:VAL:CG1	1:G:123:ILE:HG12	2.21	0.69
1:A:119:PRO:O	1:A:123:ILE:HG13	1.93	0.69
1:C:172:VAL:O	2:D:260:GLU:HG3	1.92	0.69
2:F:284:LYS:HB3	3:F:2020:HOH:O	1.92	0.69
1:G:9:PRO:HB2	1:G:12:PHE:HD2	1.58	0.69
1:E:19:VAL:CG1	1:E:123:ILE:HG12	2.23	0.69
2:F:376:GLY:O	2:F:380:LEU:HG	1.93	0.68
1:A:179:MET:CE	2:B:222:ASP:HB3	2.23	0.68
2:B:376:GLY:O	2:B:380:LEU:HG	1.94	0.68
1:C:37:PRO:HA	1:C:67:ARG:HD2	1.74	0.68
1:E:119:PRO:O	1:E:123:ILE:HG13	1.94	0.68
1:C:179:MET:CE	2:D:222:ASP:HB3	2.23	0.68
2:B:377:TYR:HB2	3:B:2025:HOH:O	1.93	0.68
1:G:179:MET:HE3	2:H:182:LEU:HD12	1.77	0.67
2:B:181:AYA:CM	2:B:181:AYA:HB3	2.24	0.67
1:C:9:PRO:HB2	1:C:12:PHE:HD2	1.59	0.67
2:B:191:ARG:HG3	3:B:2020:HOH:O	1.94	0.66
1:E:9:PRO:HB2	1:E:12:PHE:HD2	1.60	0.66
1:C:179:MET:HE3	2:D:222:ASP:HB3	1.77	0.66
1:G:175:LEU:HD23	2:H:214:ILE:HG12	1.76	0.66
1:A:19:VAL:CG1	1:A:123:ILE:HG12	2.26	0.66
1:C:19:VAL:CG1	1:C:123:ILE:HG12	2.24	0.66
1:E:172:VAL:O	2:F:260:GLU:HG3	1.96	0.65
1:G:179:MET:CE	2:H:222:ASP:HB3	2.26	0.65
1:E:179:MET:HE3	2:F:222:ASP:HB3	1.76	0.65
1:E:11:GLY:O	1:E:34:SER:HA	1.97	0.65
1:G:11:GLY:O	1:G:34:SER:HA	1.96	0.65
1:E:174:MET:O	2:F:181:AYA:HB3	1.97	0.64
1:G:154:LYS:HA	3:G:2019:HOH:O	1.97	0.64
1:G:119:PRO:O	1:G:123:ILE:HG13	1.98	0.64
1:E:175:LEU:HD23	2:F:214:ILE:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLY:O	1:C:34:SER:HA	1.97	0.64
1:A:9:PRO:HB2	1:A:12:PHE:HD2	1.63	0.64
1:G:9:PRO:HB2	1:G:12:PHE:CD2	2.32	0.64
2:D:335:PRO:HG3	3:D:2035:HOH:O	1.97	0.64
1:E:45:THR:HA	3:F:2009:HOH:O	1.96	0.63
2:D:297:HIS:ND1	2:D:374:THR:HG22	2.13	0.63
2:H:181:AYA:HM1	2:H:221:SER:CB	2.29	0.63
1:C:9:PRO:HB2	1:C:12:PHE:CD2	2.34	0.62
1:A:179:MET:HE3	2:B:182:LEU:HD12	1.81	0.62
1:A:11:GLY:O	1:A:34:SER:HA	2.00	0.62
1:C:48:ARG:NH2	1:E:23:ASP:O	2.28	0.62
2:F:181:AYA:HM3	2:F:221:SER:HB2	1.81	0.62
2:B:181:AYA:HM3	2:B:181:AYA:HB3	1.82	0.62
2:F:214:ILE:HD11	2:F:256:ALA:HA	1.82	0.62
2:H:297:HIS:ND1	2:H:374:THR:HG22	2.14	0.62
1:A:172:VAL:O	2:B:260:GLU:HG3	1.99	0.62
1:E:179:MET:HE3	2:F:182:LEU:HD12	1.81	0.62
1:E:9:PRO:HB2	1:E:12:PHE:CD2	2.34	0.62
1:C:175:LEU:HD23	2:D:214:ILE:HG12	1.81	0.61
1:C:119:PRO:O	1:C:123:ILE:HG13	2.00	0.61
1:E:179:MET:HE2	2:F:222:ASP:HB3	1.81	0.61
1:G:179:MET:CE	2:H:182:LEU:HD12	2.30	0.61
1:E:160:VAL:HG11	2:F:240:PHE:HA	1.83	0.61
1:E:14:VAL:HG11	1:E:138:GLY:O	2.01	0.61
1:A:14:VAL:HG11	1:A:138:GLY:O	2.01	0.60
2:D:345:ALA:O	2:D:349:ARG:HG3	2.01	0.60
1:G:14:VAL:HG11	1:G:138:GLY:O	2.01	0.60
2:B:214:ILE:HD11	2:B:256:ALA:HA	1.84	0.60
1:G:103:GLU:HB2	3:G:2010:HOH:O	2.00	0.60
2:B:297:HIS:ND1	2:B:374:THR:HG22	2.15	0.60
2:H:345:ALA:O	2:H:349:ARG:HG3	2.02	0.59
1:A:179:MET:HE3	2:B:222:ASP:HB3	1.83	0.59
1:A:9:PRO:HB2	1:A:12:PHE:CD2	2.37	0.59
2:F:345:ALA:O	2:F:349:ARG:HG3	2.02	0.59
2:B:278:GLN:HB2	3:B:2032:HOH:O	2.03	0.59
1:C:132:TRP:HD1	3:C:2025:HOH:O	1.85	0.59
2:D:214:ILE:HD11	2:D:256:ALA:HA	1.85	0.59
2:B:345:ALA:O	2:B:349:ARG:HG3	2.03	0.58
2:D:293:LYS:HE2	3:D:2008:HOH:O	2.02	0.58
2:F:258:ASP:HB2	3:F:2012:HOH:O	2.03	0.58
2:F:327:ARG:NH1	3:F:2032:HOH:O	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:MET:HE3	2:H:222:ASP:HB3	1.84	0.58
2:F:297:HIS:ND1	2:F:374:THR:HG22	2.18	0.58
1:A:111:THR:HG21	1:A:170:LYS:HE2	1.85	0.57
2:B:316:ASP:O	1:C:48:ARG:HD2	2.02	0.57
1:G:45:THR:HB	2:H:222:ASP:HB2	1.86	0.57
1:A:175:LEU:HD23	2:B:214:ILE:HG12	1.85	0.57
1:E:111:THR:HG21	1:E:170:LYS:HE2	1.85	0.57
2:B:312:LYS:HD3	2:D:217:ASP:HA	1.86	0.57
1:C:179:MET:HE3	2:D:182:LEU:HD12	1.86	0.57
2:D:274:ARG:HA	2:D:362:ALA:HB3	1.87	0.57
2:H:214:ILE:HD11	2:H:256:ALA:HA	1.86	0.57
1:E:179:MET:HE2	2:F:222:ASP:C	2.25	0.57
2:B:274:ARG:HA	2:B:362:ALA:HB3	1.87	0.56
2:F:274:ARG:HA	2:F:362:ALA:HB3	1.87	0.56
1:G:16:THR:HG21	1:G:141:ARG:HG3	1.86	0.56
2:D:288:ASN:O	2:D:290:PRO:HD3	2.04	0.56
1:E:179:MET:CE	2:F:182:LEU:HD12	2.35	0.56
2:D:278:GLN:O	2:D:282:VAL:HG23	2.04	0.56
2:H:278:GLN:O	2:H:282:VAL:HG23	2.05	0.56
1:C:39:THR:HG21	2:D:194:PRO:HG3	1.87	0.56
1:C:14:VAL:HG11	1:C:138:GLY:O	2.06	0.55
2:B:200:LEU:HD23	2:B:201:PHE:N	2.21	0.55
1:E:16:THR:HG21	1:E:141:ARG:HG3	1.88	0.55
1:G:111:THR:HG21	1:G:170:LYS:HE2	1.87	0.55
1:A:26:ARG:HB3	1:A:74:ARG:NH2	2.21	0.55
1:G:22:ALA:HB3	1:G:74:ARG:HH12	1.69	0.55
1:A:179:MET:CE	2:B:182:LEU:HD12	2.37	0.55
1:E:66:ALA:HA	1:E:105:GLU:HA	1.88	0.54
2:F:200:LEU:HD23	2:F:201:PHE:N	2.22	0.54
1:A:66:ALA:HA	1:A:105:GLU:HA	1.88	0.54
2:B:200:LEU:HD11	2:B:240:PHE:HD2	1.72	0.54
2:H:360:ALA:HA	3:H:2027:HOH:O	2.08	0.54
1:C:66:ALA:HA	1:C:105:GLU:HA	1.88	0.54
1:C:9:PRO:HG3	1:C:164:THR:HG22	1.90	0.54
1:G:66:ALA:HA	1:G:105:GLU:HA	1.88	0.54
1:A:39:THR:HG21	2:B:194:PRO:HG3	1.89	0.54
2:B:288:ASN:O	2:B:290:PRO:HD3	2.08	0.54
1:C:22:ALA:HB3	1:C:74:ARG:HH12	1.71	0.53
2:F:200:LEU:HD11	2:F:240:PHE:HD2	1.73	0.53
1:C:179:MET:CE	2:D:182:LEU:HD12	2.37	0.53
1:A:9:PRO:HG3	1:A:164:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA2	3:A:2016:HOH:O	2.09	0.53
1:E:9:PRO:HG3	1:E:164:THR:HG22	1.90	0.53
1:C:72:LEU:N	1:C:72:LEU:HD12	2.24	0.53
2:H:274:ARG:HA	2:H:362:ALA:HB3	1.91	0.53
1:A:179:MET:HE2	2:B:222:ASP:HB3	1.91	0.53
1:E:154:LYS:HE3	3:F:2012:HOH:O	2.08	0.53
1:A:146:ILE:CD1	1:A:168:ILE:HD12	2.39	0.52
1:C:164:THR:O	2:D:188:THR:HA	2.09	0.52
1:E:174:MET:O	2:F:181:AYA:CB	2.57	0.52
2:F:217:ASP:HA	2:H:312:LYS:HD3	1.91	0.52
1:G:26:ARG:HB3	1:G:74:ARG:NH2	2.24	0.52
2:H:288:ASN:O	2:H:290:PRO:HD3	2.09	0.52
3:B:2004:HOH:O	1:E:23:ASP:CB	2.56	0.52
2:H:200:LEU:HD23	2:H:201:PHE:N	2.25	0.52
1:E:57:CYS:O	1:E:61:VAL:HG13	2.10	0.52
1:G:99:LEU:HD22	1:G:132:TRP:CD1	2.45	0.52
1:G:13:VAL:O	1:G:32:LEU:HD12	2.09	0.52
1:A:16:THR:HG21	1:A:141:ARG:HG3	1.91	0.52
1:G:150:ASP:HB3	1:G:154:LYS:NZ	2.25	0.52
1:E:13:VAL:O	1:E:32:LEU:HD12	2.10	0.52
1:E:163:ALA:CB	2:F:190:ALA:HB2	2.39	0.52
2:F:288:ASN:O	2:F:290:PRO:HD3	2.10	0.52
2:D:200:LEU:HD23	2:D:201:PHE:N	2.26	0.51
1:G:9:PRO:HG3	1:G:164:THR:HG22	1.92	0.51
2:H:200:LEU:HD11	2:H:240:PHE:HD2	1.75	0.51
1:G:67:ARG:CZ	1:G:101:LEU:HD21	2.41	0.51
1:E:99:LEU:HD22	1:E:132:TRP:CD1	2.46	0.51
1:E:26:ARG:HB3	1:E:74:ARG:NH2	2.26	0.51
1:C:16:THR:HG21	1:C:141:ARG:HG3	1.91	0.51
1:G:154:LYS:HB2	1:G:169:ALA:O	2.11	0.51
1:A:65:GLN:HG3	3:A:2028:HOH:O	2.10	0.51
1:C:111:THR:HG21	1:C:170:LYS:HE2	1.91	0.51
1:E:67:ARG:CZ	1:E:101:LEU:HD21	2.41	0.51
2:B:278:GLN:HA	2:B:281:ARG:NH1	2.25	0.51
2:B:217:ASP:HA	2:D:312:LYS:HD3	1.93	0.51
2:B:320:ASP:HA	3:B:2045:HOH:O	2.11	0.51
2:B:278:GLN:O	2:B:282:VAL:HG23	2.11	0.50
1:C:174:MET:HB3	2:D:181:AYA:HB3	1.92	0.50
1:E:69:VAL:HA	1:E:107:LEU:O	2.11	0.50
2:D:297:HIS:HB2	2:D:372:ASP:HB2	1.94	0.50
1:C:123:ILE:O	1:C:127:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ARG:HB3	1:C:74:ARG:NH2	2.27	0.50
1:A:22:ALA:HB3	1:A:74:ARG:HH12	1.76	0.50
1:E:146:ILE:CD1	1:E:168:ILE:HD12	2.42	0.50
1:C:13:VAL:O	1:C:32:LEU:HD12	2.11	0.50
1:C:69:VAL:HA	1:C:107:LEU:O	2.11	0.50
2:D:313:CYS:HB3	2:D:316:ASP:OD1	2.11	0.50
1:A:67:ARG:CZ	1:A:101:LEU:HD21	2.42	0.50
1:C:67:ARG:CZ	1:C:101:LEU:HD21	2.42	0.50
1:G:72:LEU:HD12	1:G:72:LEU:H	1.77	0.49
1:C:72:LEU:HD12	1:C:72:LEU:H	1.78	0.49
2:H:313:CYS:HB3	2:H:316:ASP:OD1	2.11	0.49
1:G:174:MET:HG2	2:H:219:SER:HB3	1.94	0.49
2:D:200:LEU:HD11	2:D:240:PHE:HD2	1.77	0.49
1:C:45:THR:HB	2:D:222:ASP:HB2	1.94	0.49
1:G:169:ALA:HB2	2:H:251:LEU:HD13	1.94	0.49
1:G:179:MET:HE2	2:H:222:ASP:HB3	1.93	0.49
2:D:282:VAL:O	2:D:286:VAL:HG23	2.13	0.49
1:E:22:ALA:HB3	1:E:74:ARG:HH12	1.78	0.49
1:E:72:LEU:N	1:E:72:LEU:HD12	2.28	0.49
1:G:72:LEU:N	1:G:72:LEU:HD12	2.28	0.49
1:A:85:GLU:O	1:A:89:ARG:HG3	2.13	0.49
1:E:123:ILE:O	1:E:127:LEU:HG	2.12	0.49
1:A:123:ILE:O	1:A:127:LEU:HG	2.12	0.49
1:A:13:VAL:O	1:A:32:LEU:HD12	2.14	0.48
2:B:313:CYS:HB3	2:B:316:ASP:OD1	2.13	0.48
1:C:73:ALA:O	1:C:74:ARG:HD3	2.13	0.48
1:G:172:VAL:O	2:H:260:GLU:HG3	2.12	0.48
2:D:326:ILE:HB	2:D:334:TYR:HB3	1.95	0.48
1:A:72:LEU:N	1:A:72:LEU:HD12	2.28	0.48
2:B:334:TYR:HA	2:B:335:PRO:C	2.33	0.48
2:F:282:VAL:O	2:F:286:VAL:HG23	2.13	0.48
1:G:19:VAL:HG12	1:G:19:VAL:O	2.13	0.48
1:A:99:LEU:HD22	1:A:132:TRP:CD1	2.49	0.48
1:C:154:LYS:HB2	1:C:169:ALA:O	2.14	0.48
1:G:8:THR:HB	1:G:164:THR:HG21	1.96	0.48
1:C:99:LEU:HD22	1:C:132:TRP:CD1	2.49	0.48
1:E:164:THR:O	2:F:188:THR:HA	2.13	0.48
1:E:48:ARG:HD3	2:H:319:ILE:O	2.13	0.48
1:G:69:VAL:HA	1:G:107:LEU:O	2.13	0.48
1:A:73:ALA:O	1:A:74:ARG:HD3	2.14	0.48
1:G:37:PRO:HA	1:G:67:ARG:CD	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:HE2	2:D:222:ASP:HB3	1.96	0.47
1:E:48:ARG:O	2:H:321:GLN:HB3	2.14	0.47
1:A:69:VAL:HA	1:A:107:LEU:O	2.14	0.47
1:A:150:ASP:HB3	1:A:154:LYS:NZ	2.29	0.47
1:E:119:PRO:HD2	1:E:123:ILE:HD11	1.96	0.47
2:F:278:GLN:O	2:F:282:VAL:HG23	2.13	0.47
2:H:278:GLN:HA	2:H:281:ARG:NH1	2.29	0.47
1:A:45:THR:HB	2:B:222:ASP:HB2	1.95	0.47
1:E:85:GLU:O	1:E:89:ARG:HG3	2.14	0.47
1:E:8:THR:HB	1:E:164:THR:HG21	1.97	0.47
1:G:123:ILE:O	1:G:127:LEU:HG	2.14	0.47
2:H:326:ILE:HB	2:H:334:TYR:HB3	1.96	0.47
1:A:57:CYS:O	1:A:61:VAL:HG13	2.14	0.47
1:C:175:LEU:HD21	2:D:255:ILE:HG21	1.97	0.47
1:E:72:LEU:H	1:E:72:LEU:HD12	1.79	0.47
1:A:8:THR:HB	1:A:164:THR:HG21	1.97	0.47
1:A:160:VAL:HG11	2:B:240:PHE:HA	1.96	0.47
1:C:150:ASP:HB3	1:C:154:LYS:NZ	2.30	0.47
2:F:334:TYR:HA	2:F:335:PRO:C	2.34	0.47
1:G:39:THR:HG21	2:H:194:PRO:HG3	1.96	0.47
1:G:172:VAL:HB	2:H:259:GLY:HA2	1.96	0.47
1:C:8:THR:HB	1:C:164:THR:HG21	1.97	0.46
1:E:170:LYS:C	1:E:170:LYS:HD3	2.34	0.46
2:F:278:GLN:HA	2:F:281:ARG:NH1	2.29	0.46
1:G:172:VAL:HG12	2:H:255:ILE:O	2.14	0.46
2:B:197:GLN:O	2:B:200:LEU:HD22	2.16	0.46
1:A:11:GLY:HA3	2:B:231:LEU:HD12	1.98	0.46
1:A:26:ARG:HD3	3:A:2002:HOH:O	2.15	0.46
1:A:119:PRO:HD2	1:A:123:ILE:HD11	1.98	0.46
1:A:72:LEU:HD12	1:A:72:LEU:H	1.81	0.46
1:A:12:PHE:CE2	2:B:188:THR:O	2.69	0.46
2:B:317:THR:HA	1:C:48:ARG:CZ	2.46	0.46
2:D:297:HIS:CE1	2:D:374:THR:HG22	2.50	0.46
3:B:2018:HOH:O	2:D:308:MET:HG2	2.15	0.45
1:A:52:PRO:HD2	1:A:77:ASN:O	2.17	0.45
2:F:326:ILE:HB	2:F:334:TYR:HB3	1.98	0.45
1:C:142:ALA:O	1:C:146:ILE:HG23	2.17	0.45
1:E:19:VAL:O	1:E:19:VAL:HG12	2.17	0.45
1:G:53:SER:HB2	3:G:2005:HOH:O	2.17	0.45
2:H:297:HIS:HB2	2:H:372:ASP:HB2	1.98	0.45
1:C:85:GLU:O	1:C:89:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:LYS:HE3	2:F:181:AYA:O	2.15	0.45
2:B:297:HIS:HB2	2:B:372:ASP:HB2	1.98	0.45
1:C:170:LYS:HD3	1:C:170:LYS:C	2.37	0.45
1:E:154:LYS:HB2	1:E:169:ALA:O	2.16	0.45
2:F:200:LEU:HD12	2:F:241:GLU:HB2	1.98	0.45
2:F:313:CYS:HB3	2:F:316:ASP:OD1	2.17	0.45
2:H:334:TYR:HA	2:H:335:PRO:C	2.37	0.45
2:D:306:VAL:O	2:D:310:ILE:HG13	2.17	0.45
1:A:12:PHE:HE2	2:B:188:THR:O	2.00	0.45
1:A:174:MET:HG2	2:B:219:SER:HB3	1.99	0.45
1:E:73:ALA:O	1:E:74:ARG:HD3	2.17	0.45
1:G:175:LEU:HD21	2:H:255:ILE:HG21	1.97	0.45
2:F:297:HIS:HB2	2:F:372:ASP:HB2	1.99	0.45
1:A:94:ALA:N	3:A:2020:HOH:O	2.51	0.44
1:C:19:VAL:O	1:C:19:VAL:HG12	2.17	0.44
1:E:17:ALA:HA	1:E:18:PRO:HD3	1.83	0.44
1:C:8:THR:N	1:C:9:PRO:CD	2.80	0.44
2:D:278:GLN:HA	2:D:281:ARG:NH1	2.32	0.44
2:F:284:LYS:C	3:F:2020:HOH:O	2.55	0.44
2:H:197:GLN:O	2:H:200:LEU:HD22	2.18	0.44
2:H:306:VAL:O	2:H:310:ILE:HG13	2.18	0.44
2:B:326:ILE:HB	2:B:334:TYR:HB3	2.00	0.44
2:H:281:ARG:NH2	3:H:2015:HOH:O	2.49	0.44
1:A:36:ALA:CB	2:B:231:LEU:HD21	2.48	0.44
2:D:334:TYR:HA	2:D:335:PRO:C	2.38	0.44
1:G:57:CYS:O	1:G:61:VAL:HG13	2.18	0.44
1:A:170:LYS:HD3	1:A:170:LYS:C	2.37	0.44
1:E:8:THR:N	1:E:9:PRO:CD	2.79	0.44
1:C:179:MET:HE2	2:D:222:ASP:C	2.38	0.44
2:F:302:ASN:OD1	2:F:305:ARG:HG3	2.17	0.44
2:D:197:GLN:O	2:D:200:LEU:HD22	2.18	0.44
2:D:288:ASN:ND2	3:D:2024:HOH:O	2.51	0.44
1:E:39:THR:HG21	2:F:194:PRO:HG3	2.00	0.44
1:E:52:PRO:HD2	1:E:77:ASN:O	2.18	0.43
1:A:19:VAL:HG12	1:A:19:VAL:O	2.19	0.43
1:C:146:ILE:CD1	1:C:168:ILE:HD12	2.42	0.43
2:H:282:VAL:O	2:H:286:VAL:HG23	2.18	0.43
2:B:297:HIS:CE1	2:B:374:THR:HG22	2.52	0.43
2:F:197:GLN:O	2:F:200:LEU:HD22	2.19	0.43
2:D:317:THR:HG23	3:D:2030:HOH:O	2.18	0.43
1:G:85:GLU:O	1:G:89:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:THR:HG21	2:F:220:THR:C	2.38	0.43
1:A:8:THR:N	1:A:9:PRO:CD	2.81	0.43
2:B:282:VAL:O	2:B:286:VAL:HG23	2.17	0.43
1:E:158:VAL:HG11	2:F:243:ALA:HB1	2.01	0.43
1:A:174:MET:HG2	2:B:219:SER:CB	2.49	0.43
1:C:174:MET:O	1:C:174:MET:HG2	2.19	0.43
1:G:171:GLY:O	2:H:255:ILE:HG23	2.18	0.43
2:D:200:LEU:HD12	2:D:241:GLU:HB2	2.01	0.43
1:E:150:ASP:HB3	1:E:154:LYS:NZ	2.34	0.43
1:A:163:ALA:CB	2:B:190:ALA:HB2	2.49	0.43
1:E:17:ALA:O	1:E:29:PHE:HB3	2.19	0.43
1:G:146:ILE:CD1	1:G:168:ILE:HD12	2.43	0.43
1:G:176:GLU:HB2	2:H:213:SER:OG	2.18	0.43
2:B:193:ASP:OD1	2:B:194:PRO:HD2	2.19	0.42
1:C:52:PRO:HD2	1:C:77:ASN:O	2.19	0.42
2:B:306:VAL:O	2:B:310:ILE:HG13	2.19	0.42
2:F:383:GLU:CB	3:F:2039:HOH:O	2.66	0.42
1:G:73:ALA:O	1:G:74:ARG:HD3	2.19	0.42
2:H:295:ALA:HB2	2:H:305:ARG:HH11	1.83	0.42
1:G:170:LYS:HD3	1:G:170:LYS:C	2.40	0.42
2:B:383:GLU:C	3:B:2055:HOH:O	2.58	0.42
1:G:8:THR:N	1:G:9:PRO:CD	2.82	0.42
1:G:17:ALA:O	1:G:29:PHE:HB3	2.19	0.42
1:A:169:ALA:HB2	2:B:251:LEU:HD13	2.01	0.42
1:A:26:ARG:NE	1:A:74:ARG:HH21	2.18	0.41
2:B:200:LEU:HD12	2:B:241:GLU:HB2	2.01	0.41
2:F:193:ASP:OD1	2:F:194:PRO:HD2	2.20	0.41
1:A:78:VAL:HB	1:A:114:ILE:HG23	2.02	0.41
1:A:179:MET:HE2	2:B:222:ASP:C	2.41	0.41
1:G:99:LEU:HB3	1:G:132:TRP:CE2	2.55	0.41
2:H:297:HIS:CE1	2:H:374:THR:HG22	2.54	0.41
1:C:120:MET:O	1:C:124:ARG:HD2	2.20	0.41
2:D:335:PRO:HA	2:D:336:PRO:HD3	1.86	0.41
1:E:45:THR:HB	2:F:222:ASP:HB2	2.02	0.41
1:A:17:ALA:O	1:A:29:PHE:HB3	2.21	0.41
1:G:37:PRO:CA	1:G:67:ARG:HD2	2.46	0.41
1:A:111:THR:OG1	1:A:170:LYS:CE	2.69	0.41
1:A:26:ARG:HB3	1:A:74:ARG:HH22	1.85	0.41
1:A:49:PHE:CE2	2:D:321:GLN:HB2	2.55	0.41
1:C:17:ALA:O	1:C:29:PHE:HB3	2.20	0.41
1:C:37:PRO:HA	1:C:67:ARG:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:THR:OG1	1:E:170:LYS:CE	2.69	0.41
1:E:99:LEU:HB3	1:E:132:TRP:CE2	2.56	0.41
1:G:119:PRO:HD2	1:G:123:ILE:HD11	2.03	0.41
2:H:200:LEU:HD12	2:H:241:GLU:HB2	2.02	0.41
1:A:26:ARG:CD	3:A:2002:HOH:O	2.67	0.41
2:B:289:SER:OG	2:B:292:VAL:HG23	2.20	0.41
1:A:104:GLY:HA3	3:A:2027:HOH:O	2.21	0.41
2:B:295:ALA:HB2	2:B:305:ARG:HH11	1.86	0.41
2:F:306:VAL:O	2:F:310:ILE:HG13	2.21	0.41
1:C:111:THR:OG1	1:C:170:LYS:CE	2.69	0.41
1:E:170:LYS:HG2	1:E:171:GLY:N	2.36	0.41
1:C:119:PRO:HD2	1:C:123:ILE:HD11	2.03	0.41
1:C:57:CYS:O	1:C:61:VAL:HG13	2.20	0.41
2:B:327:ARG:HB2	2:B:331:VAL:O	2.20	0.41
1:G:172:VAL:HG11	2:H:258:ASP:HB3	2.03	0.41
1:A:37:PRO:HA	1:A:67:ARG:CD	2.45	0.40
1:E:8:THR:C	1:E:164:THR:HG21	2.41	0.40
1:G:9:PRO:HD2	1:G:139:PHE:HE2	1.86	0.40
1:A:99:LEU:O	1:A:132:TRP:NE1	2.43	0.40
2:B:200:LEU:C	2:B:200:LEU:HD23	2.42	0.40
2:B:282:VAL:HG21	2:B:359:LEU:HD11	2.02	0.40
1:E:174:MET:O	1:E:174:MET:HG2	2.22	0.40
1:E:44:PHE:CE2	1:E:57:CYS:HB3	2.56	0.40
2:F:181:AYA:HM3	2:F:221:SER:CB	2.49	0.40
2:F:200:LEU:C	2:F:200:LEU:HD23	2.42	0.40
2:F:270:VAL:HG11	2:F:279:ALA:HA	2.03	0.40
2:H:193:ASP:OD1	2:H:194:PRO:HD2	2.22	0.40
2:H:300:ASP:C	2:H:348:LEU:HD22	2.42	0.40
1:C:173:GLY:O	2:D:181:AYA:CB	2.69	0.40
2:D:295:ALA:HB2	2:D:305:ARG:HH11	1.86	0.40
2:F:335:PRO:HA	2:F:336:PRO:HD3	1.87	0.40
2:F:297:HIS:CE1	2:F:374:THR:HG22	2.55	0.40
1:G:26:ARG:CZ	1:G:74:ARG:HE	2.34	0.40
2:F:312:LYS:HD3	2:H:217:ASP:HA	2.04	0.40
2:D:261:GLY:O	2:D:374:THR:OG1	2.26	0.40
1:G:174:MET:HG2	1:G:174:MET:O	2.22	0.40
1:G:52:PRO:HD2	1:G:77:ASN:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:O	1:G:48:ARG:NH2[1_455]	2.19	0.01

## 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	171/173 (99%)	159 (93%)	10 (6%)	2 (1%)	15	12
1	C	171/173 (99%)	155 (91%)	15 (9%)	1 (1%)	28	29
1	E	171/173 (99%)	158 (92%)	11 (6%)	2 (1%)	15	12
1	G	171/173 (99%)	155 (91%)	15 (9%)	1 (1%)	28	29
2	B	199/213 (93%)	188 (94%)	9 (4%)	2 (1%)	18	16
2	D	199/213 (93%)	187 (94%)	10 (5%)	2 (1%)	18	16
2	F	199/213 (93%)	185 (93%)	13 (6%)	1 (0%)	32	34
2	H	199/213 (93%)	188 (94%)	9 (4%)	2 (1%)	18	16
All	All	1480/1544 (96%)	1375 (93%)	92 (6%)	13 (1%)	20	18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	231	LEU
1	E	100	GLY
2	F	231	LEU
1	G	100	GLY
2	D	231	LEU
2	H	263	ALA
2	B	263	ALA
1	C	100	GLY
1	A	100	GLY
2	D	263	ALA
2	H	231	LEU
1	A	135	GLY

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Mol	Chain	Res	Type
1	E	135	GLY

### 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	116/128 (91%)	111 (96%)	5 (4%)	33	41
1	C	116/128 (91%)	110 (95%)	6 (5%)	27	32
1	E	116/128 (91%)	112 (97%)	4 (3%)	42	53
1	G	116/128 (91%)	109 (94%)	7 (6%)	22	25
2	B	150/165 (91%)	145 (97%)	5 (3%)	43	54
2	D	150/165 (91%)	145 (97%)	5 (3%)	43	54
2	F	150/165 (91%)	145 (97%)	5 (3%)	43	54
2	H	150/165 (91%)	145 (97%)	5 (3%)	43	54
All	All	1064/1172 (91%)	1022 (96%)	42 (4%)	37	46

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	74	ARG
1	A	92	ARG
1	A	160	VAL
1	A	170	LYS
2	B	200	LEU
2	B	257	SER
2	B	274	ARG
2	B	287	VAL
2	B	348	LEU
1	C	74	ARG
1	C	92	ARG
1	C	111	THR
1	C	160	VAL

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Mol	Chain	Res	Type
1	C	170	LYS
1	C	179	MET
2	D	200	LEU
2	D	257	SER
2	D	274	ARG
2	D	287	VAL
2	D	348	LEU
1	E	16	THR
1	E	74	ARG
1	E	92	ARG
1	E	160	VAL
2	F	200	LEU
2	F	257	SER
2	F	274	ARG
2	F	287	VAL
2	F	348	LEU
1	G	16	THR
1	G	74	ARG
1	G	92	ARG
1	G	111	THR
1	G	150	ASP
1	G	160	VAL
1	G	170	LYS
2	H	200	LEU
2	H	257	SER
2	H	274	ARG
2	H	287	VAL
2	H	348	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	AYA	B	181	2	7,7,8	1.89	1 (14%)	6,8,10	1.57	2 (33%)
2	AYA	D	181	2	7,7,8	0.90	0	6,8,10	2.57	3 (50%)
2	AYA	F	181	2	7,7,8	1.39	1 (14%)	6,8,10	2.71	3 (50%)
2	AYA	H	181	2	7,7,8	1.28	1 (14%)	6,8,10	1.85	3 (50%)

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	AYA	B	181	2	-	0/4/6/8	0/0/0/0
2	AYA	D	181	2	-	0/4/6/8	0/0/0/0
2	AYA	F	181	2	-	0/4/6/8	0/0/0/0
2	AYA	H	181	2	-	1/4/6/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	181	AYA	CA-C	2.79	1.53	1.50
2	H	181	AYA	CA-C	3.04	1.54	1.50
2	B	181	AYA	CA-C	4.33	1.55	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	181	AYA	OT-CT-N	-3.95	114.31	121.92
2	D	181	AYA	OT-CT-N	-3.82	114.56	121.92
2	D	181	AYA	CA-N-CT	-3.07	116.93	121.49
2	H	181	AYA	CA-N-CT	-2.08	118.40	121.49
2	H	181	AYA	OT-CT-N	-2.08	117.92	121.92
2	B	181	AYA	OT-CT-N	-2.04	118.00	121.92
2	B	181	AYA	CM-CT-N	2.49	120.60	116.11
2	H	181	AYA	C-CA-N	2.94	116.49	110.64
2	F	181	AYA	C-CA-N	3.12	116.84	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	181	AYA	CM-CT-N	3.27	122.02	116.11
2	F	181	AYA	CM-CT-N	4.10	123.52	116.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	181	AYA	CM-CT-N-CA

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	181	AYA	2	0
2	D	181	AYA	2	0
2	F	181	AYA	5	0
2	H	181	AYA	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	173/173 (100%)	-0.24	1 (0%) 89 88	15, 34, 48, 64	0
1	C	173/173 (100%)	-0.23	0 100 100	17, 35, 48, 62	0
1	E	173/173 (100%)	-0.03	5 (2%) 52 50	17, 37, 50, 65	0
1	G	173/173 (100%)	0.09	7 (4%) 39 37	18, 37, 50, 67	0
2	B	202/213 (94%)	-0.39	0 100 100	16, 28, 47, 61	0
2	D	202/213 (94%)	-0.41	0 100 100	16, 29, 47, 61	0
2	F	202/213 (94%)	-0.30	0 100 100	17, 30, 50, 63	0
2	H	202/213 (94%)	-0.30	0 100 100	17, 30, 49, 63	0
All	All	1500/1544 (97%)	-0.24	13 (0%) 84 83	15, 32, 50, 67	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	160	VAL	4.6
1	G	102	PRO	4.0
1	E	161	GLY	3.8
1	E	130	LEU	3.3
1	E	160	VAL	3.2
1	G	96	ALA	2.8
1	E	100	GLY	2.7
1	E	138	GLY	2.7
1	G	136	GLU	2.6
1	G	135	GLY	2.6
1	A	10	ARG	2.3
1	G	158	VAL	2.2
1	G	143	ALA	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AYA	H	181	8/9	0.97	0.16	-	11,18,34,38	0
2	AYA	F	181	8/9	0.95	0.13	-	8,19,23,25	0
2	AYA	D	181	8/9	0.96	0.14	-	11,17,25,25	0
2	AYA	B	181	8/9	0.84	0.18	-	5,21,34,44	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.