



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:28 PM GMT

PDB ID : 4IH4  
Title : Crystal structure of Arabidopsis DWARF14 orthologue, AtD14  
Authors : Zhou, X.E.; Zhao, L.-H.; Wu, Z.-S.; Yi, W.; Li, S.; Li, Y.; Xu, Y.; Xu, T.-H.; Liu, Y.; Chen, R.-Z.; Kovach, A.; Kang, Y.; Hou, L.; He, Y.; Zhang, C.; Melcher, K.; Xu, H.E.  
Deposited on : 2012-12-18  
Resolution : 3.50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

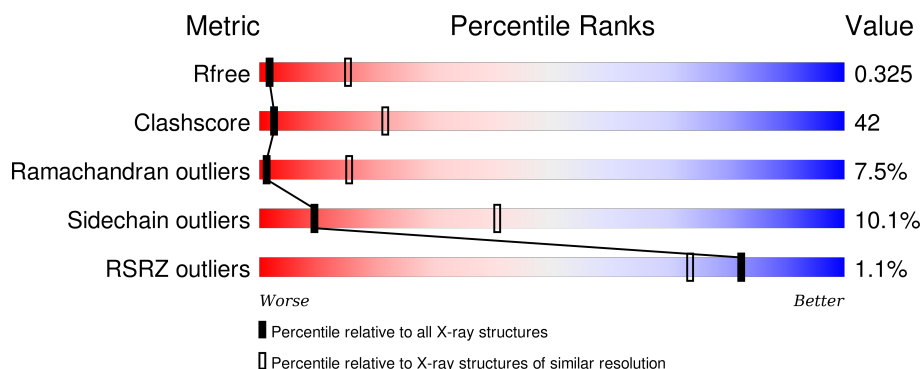
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	267	<div> <div>32%</div> <div>54%</div> <div>11%</div> <div>..</div> </div>
1	B	267	<div> <div>33%</div> <div>55%</div> <div>10%</div> <div>.</div> </div>
1	C	267	<div> <div>31%</div> <div>57%</div> <div>9%</div> <div>..</div> </div>
1	D	267	<div> <div>30%</div> <div>57%</div> <div>10%</div> <div>.</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8160 atoms, of which 0 are hydrogens and 0 are deuteriums.

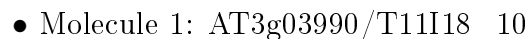
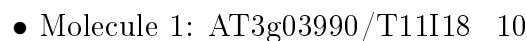
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

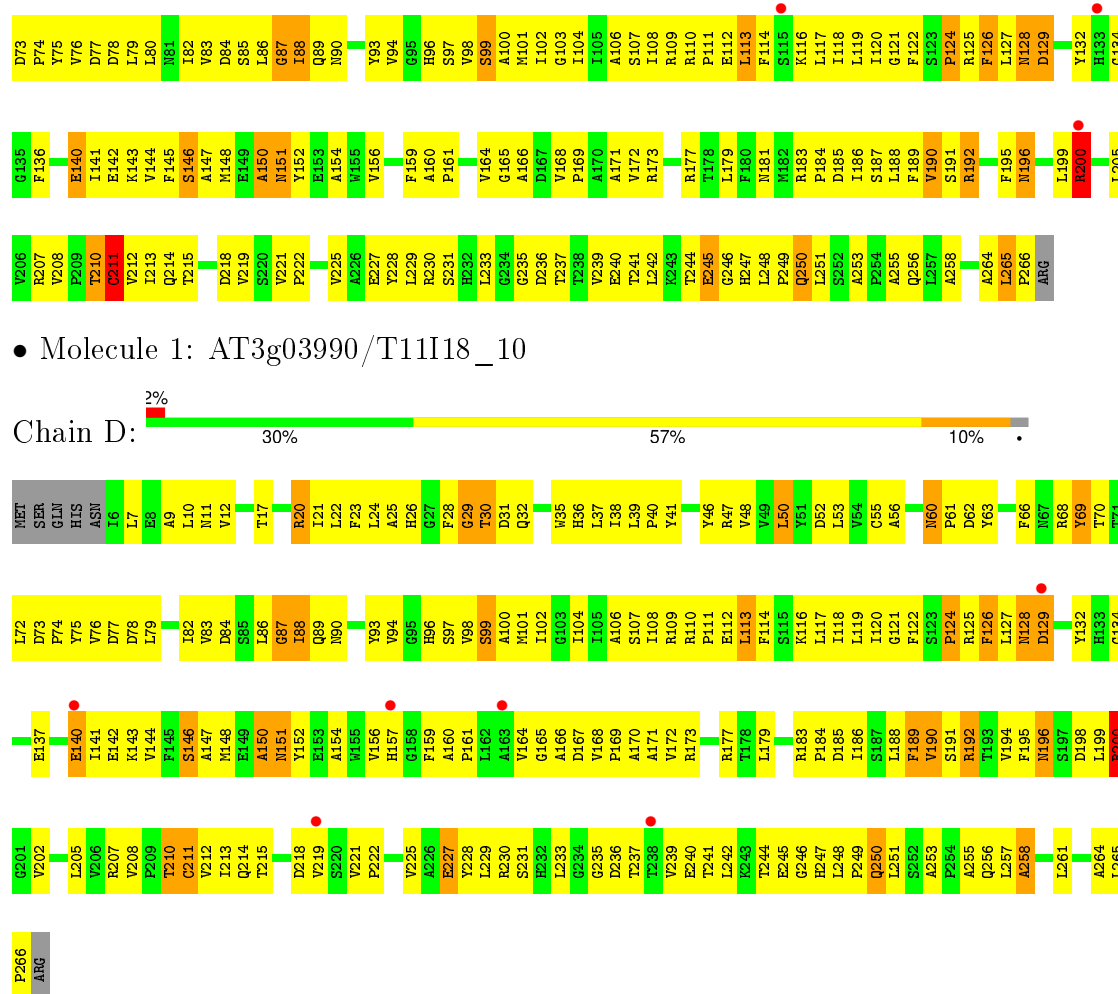
- Molecule 1 is a protein called AT3g03990/T11I18\_10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total 2040	C 1312	N 346	O 376	S 6	0	0	0
1	B	261	Total 2040	C 1312	N 346	O 376	S 6	0	0	0
1	C	261	Total 2040	C 1312	N 346	O 376	S 6	0	0	0
1	D	261	Total 2040	C 1312	N 346	O 376	S 6	0	0	0



- Molecule 1: AT3g03990/T11I18 10





• Molecule 1: AT3g03990/T11I18\_10

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.86Å 44.63Å 160.97Å 90.00° 121.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 29.58 – 3.48	Depositor EDS
% Data completeness (in resolution range)	64.3 (30.00-3.50) 66.5 (29.58-3.48)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.47Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.279 , 0.336 0.295 , 0.325	Depositor DCC
$R_{free}$ test set	818 reflections (7.72%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , -15.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 12471 reflections	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	8160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/2089	0.65	0/2847
1	B	0.53	1/2089 (0.0%)	0.66	0/2847
1	C	0.50	0/2089	0.65	0/2847
1	D	0.50	0/2089	0.66	0/2847
All	All	0.51	1/8356 (0.0%)	0.66	0/11388

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	CYS	CB-SG	-6.20	1.71	1.82

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	2040	0	2014	175	0
1	B	2040	0	2014	177	0
1	C	2040	0	2014	168	0
1	D	2040	0	2014	182	0
All	All	8160	0	8056	681	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 42.

All (681) 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:B:128:ASN:HB3	1:B:134:GLY:H	1.21	1.01
1:C:128:ASN:HB3	1:C:134:GLY:H	1.24	0.99
1:D:128:ASN:HB3	1:D:134:GLY:H	1.23	0.99
1:A:128:ASN:HB3	1:A:134:GLY:H	1.23	0.98
1:A:104:ILE:HD11	1:A:119:LEU:HD11	1.49	0.95
1:C:233:LEU:HD13	1:C:237:THR:HG21	1.48	0.93
1:D:104:ILE:HD11	1:D:119:LEU:HD11	1.49	0.92
1:B:233:LEU:HD13	1:B:237:THR:HG21	1.48	0.92
1:C:104:ILE:HD11	1:C:119:LEU:HD11	1.50	0.91
1:D:233:LEU:HD13	1:D:237:THR:HG21	1.53	0.90
1:A:85:SER:HB3	1:B:157:HIS:NE2	1.89	0.87
1:A:218:ASP:OD1	1:A:247:HIS:ND1	2.07	0.87
1:C:218:ASP:OD1	1:C:247:HIS:ND1	2.05	0.86
1:C:86:LEU:HD23	1:D:169:PRO:HB3	1.55	0.86
1:B:60:ASN:HD22	1:B:61:PRO:HD2	1.38	0.86
1:D:110:ARG:HD2	1:D:113:LEU:HD22	1.57	0.86
1:A:233:LEU:HD13	1:A:237:THR:HG21	1.56	0.85
1:B:104:ILE:HD11	1:B:119:LEU:HD11	1.57	0.84
1:C:214:GLN:HB3	1:C:241:THR:HG22	1.60	0.82
1:C:164:VAL:HG21	1:C:172:VAL:HA	1.61	0.82
1:A:164:VAL:HG21	1:A:172:VAL:HA	1.60	0.82
1:A:110:ARG:HD2	1:A:113:LEU:HD22	1.62	0.82
1:B:121:GLY:H	1:B:213:ILE:HG22	1.45	0.82
1:D:99:SER:HA	1:D:102:ILE:HD12	1.61	0.82
1:B:164:VAL:HG21	1:B:172:VAL:HA	1.61	0.81
1:C:22:LEU:HD12	1:C:23:PHE:H	1.44	0.81
1:B:110:ARG:HD2	1:B:113:LEU:HD22	1.60	0.81
1:D:218:ASP:OD1	1:D:247:HIS:ND1	2.14	0.81
1:B:205:LEU:HD11	1:D:202:VAL:HG21	1.61	0.81
1:A:22:LEU:HD12	1:A:23:PHE:H	1.45	0.81
1:C:121:GLY:H	1:C:213:ILE:HG22	1.47	0.79
1:C:129:ASP:HB2	1:C:132:TYR:HB3	1.62	0.79
1:A:214:GLN:HB3	1:A:241:THR:HG22	1.64	0.79
1:B:218:ASP:OD1	1:B:247:HIS:ND1	2.15	0.79
1:B:99:SER:HA	1:B:102:ILE:HD12	1.63	0.79
1:A:60:ASN:HD22	1:A:61:PRO:HD2	1.45	0.79
1:D:32:GLN:HB2	1:D:50:LEU:HD12	1.63	0.78
1:C:60:ASN:HD22	1:C:61:PRO:HD2	1.47	0.78
1:B:214:GLN:HB3	1:B:241:THR:HG22	1.65	0.78
1:A:124:PRO:HG2	1:A:125:ARG:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASN:HD22	1:D:61:PRO:HD2	1.48	0.78
1:C:32:GLN:HB2	1:C:50:LEU:HD12	1.66	0.78
1:D:121:GLY:H	1:D:213:ILE:HG22	1.48	0.78
1:B:32:GLN:HB2	1:B:50:LEU:HD12	1.65	0.78
1:A:121:GLY:H	1:A:213:ILE:HG22	1.49	0.77
1:B:129:ASP:HB2	1:B:132:TYR:HB3	1.67	0.76
1:B:7:LEU:O	1:B:12:VAL:HG22	1.86	0.76
1:D:214:GLN:HB3	1:D:241:THR:HG22	1.67	0.76
1:B:60:ASN:HD22	1:B:61:PRO:CD	1.99	0.76
1:B:205:LEU:HD11	1:D:202:VAL:CG2	2.15	0.76
1:B:124:PRO:HG2	1:B:125:ARG:H	1.52	0.75
1:C:212:VAL:HB	1:C:239:VAL:HG13	1.67	0.75
1:D:164:VAL:HG21	1:D:172:VAL:HA	1.67	0.74
1:B:98:VAL:HA	1:B:101:MET:HE2	1.68	0.74
1:B:212:VAL:HB	1:B:239:VAL:HG13	1.70	0.74
1:C:110:ARG:HD2	1:C:113:LEU:HD22	1.70	0.74
1:C:210:THR:HB	1:C:237:THR:HG23	1.70	0.73
1:D:7:LEU:O	1:D:12:VAL:HG22	1.88	0.73
1:C:124:PRO:HG2	1:C:125:ARG:H	1.54	0.73
1:C:99:SER:HA	1:C:102:ILE:HD12	1.70	0.73
1:C:218:ASP:CG	1:C:247:HIS:HD1	1.92	0.73
1:D:129:ASP:HB2	1:D:132:TYR:HB3	1.69	0.72
1:A:32:GLN:HB2	1:A:50:LEU:HD12	1.71	0.72
1:C:141:ILE:HD12	1:C:142:GLU:N	2.04	0.72
1:D:124:PRO:HG2	1:D:125:ARG:H	1.55	0.72
1:D:60:ASN:HD22	1:D:61:PRO:CD	2.03	0.72
1:A:129:ASP:HB2	1:A:132:TYR:HB3	1.70	0.72
1:D:22:LEU:HD12	1:D:23:PHE:H	1.54	0.72
1:C:108:ILE:O	1:C:111:PRO:HD3	1.90	0.72
1:A:85:SER:HB3	1:B:157:HIS:CE1	2.24	0.71
1:D:25:ALA:HB1	1:D:99:SER:OG	1.90	0.71
1:A:212:VAL:HB	1:A:239:VAL:HG13	1.73	0.71
1:B:22:LEU:HD12	1:B:23:PHE:H	1.56	0.70
1:B:119:LEU:HD13	1:B:122:PHE:CD2	2.27	0.70
1:B:112:GLU:HG2	1:B:113:LEU:H	1.55	0.70
1:B:109:ARG:O	1:B:110:ARG:HG2	1.91	0.70
1:D:119:LEU:HD13	1:D:122:PHE:CD2	2.27	0.70
1:B:210:THR:HB	1:B:237:THR:HG23	1.73	0.70
1:D:218:ASP:CG	1:D:247:HIS:HD1	1.95	0.69
1:B:192:ARG:O	1:B:196:ASN:HB2	1.93	0.69
1:D:210:THR:HB	1:D:237:THR:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:HB1	1:A:99:SER:OG	1.92	0.69
1:A:60:ASN:HD22	1:A:61:PRO:CD	2.06	0.68
1:C:112:GLU:HG2	1:C:113:LEU:H	1.58	0.68
1:A:7:LEU:O	1:A:12:VAL:HG22	1.93	0.68
1:C:185:ASP:O	1:C:188:LEU:HB3	1.92	0.68
1:A:99:SER:HA	1:A:102:ILE:HD12	1.74	0.68
1:C:85:SER:HB3	1:D:157:HIS:NE2	2.09	0.68
1:B:108:ILE:O	1:B:111:PRO:HD3	1.94	0.68
1:D:108:ILE:O	1:D:111:PRO:HD3	1.93	0.68
1:C:25:ALA:HB1	1:C:99:SER:OG	1.94	0.68
1:C:7:LEU:O	1:C:12:VAL:HG22	1.93	0.68
1:A:98:VAL:HA	1:A:101:MET:HE1	1.74	0.67
1:A:218:ASP:CG	1:A:247:HIS:HD1	1.97	0.67
1:A:117:LEU:HD23	1:A:208:VAL:HG11	1.75	0.67
1:C:124:PRO:HD3	1:C:229:LEU:HD21	1.76	0.67
1:C:192:ARG:O	1:C:196:ASN:HB2	1.94	0.67
1:B:185:ASP:O	1:B:188:LEU:HB3	1.95	0.67
1:D:98:VAL:HA	1:D:101:MET:HE2	1.75	0.66
1:A:185:ASP:O	1:A:188:LEU:HB3	1.95	0.66
1:A:141:ILE:HD12	1:A:142:GLU:N	2.09	0.66
1:C:119:LEU:HD13	1:C:122:PHE:CD2	2.31	0.66
1:B:218:ASP:CG	1:B:247:HIS:HD1	1.98	0.66
1:D:212:VAL:HB	1:D:239:VAL:HG13	1.78	0.66
1:A:210:THR:HB	1:A:237:THR:HG23	1.78	0.65
1:D:117:LEU:HD23	1:D:208:VAL:HG11	1.79	0.65
1:C:60:ASN:HD22	1:C:61:PRO:CD	2.09	0.65
1:B:125:ARG:HB3	1:B:132:TYR:CE2	2.31	0.65
1:B:141:ILE:HD12	1:B:142:GLU:N	2.12	0.65
1:A:119:LEU:HD13	1:A:122:PHE:CD2	2.32	0.64
1:D:21:ILE:HD13	1:D:90:ASN:O	1.96	0.64
1:C:233:LEU:CD1	1:C:237:THR:HG21	2.27	0.64
1:B:124:PRO:HD3	1:B:229:LEU:HD21	1.79	0.64
1:D:141:ILE:HD12	1:D:142:GLU:N	2.12	0.64
1:C:14:VAL:HG11	1:D:170:ALA:HB2	1.79	0.63
1:A:112:GLU:HG2	1:A:113:LEU:H	1.62	0.63
1:D:112:GLU:HG2	1:D:113:LEU:H	1.64	0.63
1:C:20:ARG:HB3	1:C:46:TYR:HD2	1.63	0.63
1:C:24:LEU:HD23	1:C:94:VAL:HB	1.80	0.63
1:D:192:ARG:O	1:D:196:ASN:HB2	1.99	0.62
1:B:98:VAL:HA	1:B:101:MET:CE	2.28	0.62
1:C:96:HIS:CE1	1:C:97:SER:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ALA:HB1	1:B:119:LEU:HD22	1.82	0.62
1:D:185:ASP:O	1:D:188:LEU:HB3	1.99	0.62
1:A:124:PRO:HD3	1:A:229:LEU:HD21	1.81	0.62
1:B:101:MET:O	1:B:104:ILE:N	2.33	0.62
1:D:124:PRO:HD3	1:D:229:LEU:HD21	1.81	0.62
1:D:253:ALA:HB1	1:D:256:GLN:HE21	1.64	0.62
1:A:26:HIS:O	1:A:99:SER:HB2	2.01	0.61
1:B:116:LYS:O	1:B:118:ILE:HD12	1.99	0.61
1:D:101:MET:O	1:D:104:ILE:N	2.33	0.61
1:D:76:VAL:HG22	1:D:102:ILE:HG23	1.82	0.61
1:B:112:GLU:HG2	1:B:113:LEU:N	2.16	0.61
1:D:125:ARG:HB3	1:D:132:TYR:CE2	2.35	0.61
1:C:88:ILE:HA	1:D:167:ASP:OD2	2.01	0.61
1:D:247:HIS:HD2	1:D:248:LEU:HD11	1.65	0.61
1:B:25:ALA:HB1	1:B:99:SER:OG	2.01	0.60
1:A:20:ARG:HB3	1:A:46:TYR:HD2	1.65	0.60
1:B:84:ASP:O	1:B:87:GLY:N	2.31	0.60
1:D:17:THR:HA	1:D:47:ARG:NE	2.16	0.60
1:B:109:ARG:NH1	1:D:207:ARG:HH22	2.00	0.60
1:C:21:ILE:HD13	1:C:90:ASN:O	2.01	0.60
1:C:125:ARG:HB3	1:C:132:TYR:CE2	2.37	0.60
1:C:22:LEU:HD12	1:C:23:PHE:N	2.16	0.60
1:C:222:PRO:HB2	1:C:225:VAL:HG23	1.84	0.60
1:A:125:ARG:HB3	1:A:132:TYR:CE2	2.37	0.60
1:A:69:TYR:HB3	1:A:75:TYR:CE1	2.37	0.59
1:A:116:LYS:O	1:A:118:ILE:HD12	2.01	0.59
1:A:76:VAL:HG22	1:A:102:ILE:HG23	1.83	0.59
1:A:109:ARG:O	1:A:110:ARG:HG2	2.02	0.59
1:C:76:VAL:HG22	1:C:102:ILE:HG23	1.84	0.59
1:D:98:VAL:HA	1:D:101:MET:CE	2.32	0.59
1:C:101:MET:O	1:C:104:ILE:N	2.36	0.59
1:D:109:ARG:O	1:D:110:ARG:HG2	2.02	0.59
1:A:46:TYR:OH	1:A:266:PRO:HD3	2.02	0.59
1:A:35:TRP:O	1:A:38:ILE:HG22	2.03	0.58
1:A:17:THR:HA	1:A:47:ARG:NE	2.18	0.58
1:B:35:TRP:O	1:B:38:ILE:HG22	2.04	0.58
1:C:247:HIS:HD2	1:C:248:LEU:HD11	1.68	0.58
1:B:69:TYR:HB3	1:B:75:TYR:CE1	2.38	0.58
1:B:222:PRO:HB2	1:B:225:VAL:HG23	1.84	0.58
1:D:128:ASN:HB3	1:D:134:GLY:N	2.07	0.58
1:B:148:MET:HE3	1:B:188:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:O	1:A:196:ASN:HB2	2.04	0.58
1:A:50:LEU:HG	1:A:50:LEU:O	2.04	0.57
1:B:21:ILE:HD13	1:B:90:ASN:O	2.04	0.57
1:B:233:LEU:CD1	1:B:237:THR:HG21	2.28	0.57
1:B:76:VAL:HG22	1:B:102:ILE:HG23	1.85	0.57
1:D:50:LEU:O	1:D:50:LEU:HG	2.03	0.57
1:B:117:LEU:HD23	1:B:208:VAL:HG11	1.87	0.57
1:A:84:ASP:O	1:A:87:GLY:N	2.32	0.57
1:C:98:VAL:HA	1:C:101:MET:CE	2.34	0.57
1:D:125:ARG:HG2	1:D:127:LEU:O	2.04	0.57
1:C:17:THR:HA	1:C:47:ARG:NE	2.19	0.57
1:B:253:ALA:HB1	1:B:256:GLN:HE21	1.68	0.57
1:A:85:SER:HB3	1:B:157:HIS:CD2	2.39	0.57
1:C:35:TRP:O	1:C:38:ILE:HG22	2.04	0.57
1:D:126:PHE:HB3	1:D:195:PHE:CD1	2.40	0.57
1:A:98:VAL:HA	1:A:101:MET:CE	2.35	0.57
1:B:26:HIS:O	1:B:99:SER:HB2	2.04	0.56
1:B:89:GLN:O	1:B:113:LEU:HA	2.05	0.56
1:A:183:ARG:O	1:A:186:ILE:HB	2.05	0.56
1:C:26:HIS:O	1:C:99:SER:HB2	2.06	0.56
1:B:39:LEU:N	1:B:40:PRO:HD2	2.20	0.56
1:C:20:ARG:HB3	1:C:46:TYR:CD2	2.41	0.56
1:B:20:ARG:HB3	1:B:46:TYR:HD2	1.70	0.56
1:C:116:LYS:O	1:C:118:ILE:HD12	2.05	0.56
1:A:108:ILE:O	1:A:111:PRO:HD3	2.05	0.56
1:A:126:PHE:HB3	1:A:195:PHE:CD1	2.40	0.56
1:C:69:TYR:HB3	1:C:75:TYR:CE1	2.40	0.56
1:C:117:LEU:HD23	1:C:208:VAL:HG11	1.87	0.55
1:D:210:THR:HG22	1:D:211:CYS:H	1.71	0.55
1:B:183:ARG:O	1:B:186:ILE:HB	2.06	0.55
1:B:24:LEU:HD23	1:B:94:VAL:HB	1.88	0.55
1:C:46:TYR:OH	1:C:266:PRO:HD3	2.06	0.55
1:C:98:VAL:HA	1:C:101:MET:HE2	1.88	0.55
1:B:110:ARG:C	1:B:112:GLU:H	2.09	0.55
1:B:184:PRO:O	1:B:185:ASP:C	2.45	0.55
1:D:60:ASN:ND2	1:D:62:ASP:H	2.05	0.55
1:B:125:ARG:HG2	1:B:127:LEU:O	2.06	0.55
1:C:112:GLU:HG2	1:C:113:LEU:N	2.20	0.55
1:C:109:ARG:O	1:C:110:ARG:HG2	2.06	0.55
1:D:69:TYR:HB3	1:D:75:TYR:CE1	2.42	0.55
1:A:39:LEU:N	1:A:40:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:PRO:HB2	1:D:225:VAL:HG23	1.87	0.55
1:B:50:LEU:HD23	1:B:50:LEU:N	2.22	0.55
1:A:210:THR:HG22	1:A:211:CYS:H	1.71	0.55
1:C:85:SER:HB3	1:D:157:HIS:CE1	2.42	0.54
1:D:184:PRO:O	1:D:185:ASP:C	2.46	0.54
1:B:126:PHE:HB3	1:B:195:PHE:CD1	2.42	0.54
1:D:247:HIS:HD2	1:D:248:LEU:CD1	2.20	0.54
1:C:72:LEU:O	1:C:76:VAL:HG23	2.08	0.54
1:D:117:LEU:HB3	1:D:210:THR:HG23	1.90	0.54
1:A:101:MET:O	1:A:104:ILE:N	2.41	0.54
1:A:247:HIS:HD2	1:A:248:LEU:HD11	1.72	0.54
1:A:50:LEU:HD23	1:A:50:LEU:N	2.22	0.54
1:D:38:ILE:HD11	1:D:258:ALA:N	2.23	0.54
1:C:210:THR:HG22	1:C:211:CYS:H	1.72	0.54
1:D:100:ALA:HB1	1:D:119:LEU:HD22	1.88	0.54
1:B:46:TYR:OH	1:B:266:PRO:HD3	2.08	0.54
1:A:21:ILE:HD13	1:A:90:ASN:O	2.07	0.54
1:D:46:TYR:OH	1:D:266:PRO:HD3	2.08	0.54
1:C:100:ALA:HB1	1:C:119:LEU:HD22	1.90	0.54
1:D:112:GLU:HG2	1:D:113:LEU:HD13	1.89	0.54
1:D:244:THR:HB	1:D:256:GLN:OE1	2.08	0.54
1:C:205:LEU:O	1:C:207:ARG:HD2	2.08	0.54
1:B:228:TYR:O	1:B:231:SER:HB2	2.08	0.53
1:A:36:HIS:O	1:A:38:ILE:N	2.41	0.53
1:C:151:ASN:HB3	1:C:154:ALA:HB3	1.89	0.53
1:D:114:PHE:HB3	1:D:117:LEU:CD2	2.39	0.53
1:A:22:LEU:HD12	1:A:23:PHE:N	2.18	0.53
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.73	0.53
1:D:50:LEU:HD23	1:D:50:LEU:N	2.22	0.53
1:A:20:ARG:HB3	1:A:46:TYR:CD2	2.43	0.53
1:D:183:ARG:O	1:D:186:ILE:HB	2.08	0.53
1:C:93:TYR:HB2	1:C:114:PHE:HE1	1.74	0.53
1:A:72:LEU:O	1:A:76:VAL:HG23	2.09	0.53
1:A:186:ILE:O	1:A:190:VAL:HG23	2.07	0.53
1:A:110:ARG:C	1:A:112:GLU:H	2.12	0.53
1:C:183:ARG:O	1:C:186:ILE:HB	2.09	0.53
1:D:60:ASN:HD22	1:D:61:PRO:N	2.07	0.53
1:B:128:ASN:HB3	1:B:134:GLY:N	2.06	0.53
1:D:228:TYR:O	1:D:231:SER:HB2	2.09	0.53
1:C:126:PHE:HB3	1:C:195:PHE:CD1	2.43	0.53
1:A:36:HIS:C	1:A:38:ILE:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:O	1:C:190:VAL:HG23	2.08	0.53
1:B:124:PRO:HG2	1:B:132:TYR:OH	2.08	0.53
1:B:38:ILE:HD11	1:B:258:ALA:N	2.24	0.53
1:A:240:GLU:HG3	1:A:241:THR:N	2.24	0.53
1:D:24:LEU:HD23	1:D:94:VAL:HB	1.91	0.53
1:B:17:THR:HA	1:B:47:ARG:NE	2.24	0.53
1:D:10:LEU:HB3	1:D:52:ASP:O	2.09	0.53
1:B:96:HIS:CE1	1:B:97:SER:HB2	2.44	0.53
1:A:222:PRO:HB2	1:A:225:VAL:HG23	1.90	0.52
1:B:60:ASN:ND2	1:B:61:PRO:HD2	2.16	0.52
1:D:112:GLU:HG2	1:D:113:LEU:N	2.24	0.52
1:C:169:PRO:HA	1:C:172:VAL:CG1	2.39	0.52
1:A:143:LYS:O	1:A:146:SER:HB3	2.09	0.52
1:B:205:LEU:O	1:B:207:ARG:HD2	2.08	0.52
1:A:200:ARG:HH11	1:A:200:ARG:HG2	1.74	0.52
1:B:207:ARG:CZ	1:D:73:ASP:OD1	2.57	0.52
1:D:20:ARG:HB3	1:D:46:TYR:HD2	1.75	0.52
1:C:210:THR:HB	1:C:237:THR:CG2	2.39	0.52
1:D:110:ARG:C	1:D:112:GLU:H	2.12	0.52
1:B:120:ILE:HG23	1:B:213:ILE:HG21	1.91	0.52
1:C:17:THR:HG22	1:C:47:ARG:NH2	2.25	0.52
1:A:147:ALA:O	1:A:150:ALA:HB3	2.10	0.52
1:B:207:ARG:NH2	1:D:73:ASP:OD1	2.43	0.52
1:D:22:LEU:HD23	1:D:48:VAL:HG22	1.92	0.52
1:D:186:ILE:O	1:D:190:VAL:HG23	2.10	0.52
1:C:140:GLU:O	1:C:144:VAL:HG23	2.10	0.52
1:A:117:LEU:HB3	1:A:210:THR:HG23	1.90	0.52
1:B:247:HIS:HD2	1:B:248:LEU:CD1	2.23	0.52
1:B:22:LEU:HD23	1:B:48:VAL:HG22	1.92	0.52
1:D:26:HIS:O	1:D:99:SER:HB2	2.10	0.52
1:B:219:VAL:HG22	1:B:219:VAL:O	2.10	0.52
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.74	0.51
1:D:116:LYS:O	1:D:118:ILE:HD12	2.10	0.51
1:D:205:LEU:O	1:D:207:ARG:HD2	2.09	0.51
1:D:39:LEU:N	1:D:40:PRO:HD2	2.25	0.51
1:D:35:TRP:O	1:D:38:ILE:HG22	2.10	0.51
1:A:205:LEU:O	1:A:207:ARG:HD2	2.09	0.51
1:C:93:TYR:CE2	1:C:103:GLY:HA3	2.45	0.51
1:C:79:LEU:O	1:C:83:VAL:HG23	2.09	0.51
1:C:248:LEU:N	1:C:248:LEU:HD12	2.26	0.51
1:D:240:GLU:HG3	1:D:241:THR:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:PHE:HB3	1:D:195:PHE:HD1	1.75	0.51
1:C:152:TYR:O	1:C:156:VAL:HG23	2.10	0.51
1:D:73:ASP:N	1:D:74:PRO:HD2	2.26	0.51
1:C:169:PRO:HA	1:C:172:VAL:HG12	1.92	0.51
1:D:96:HIS:CE1	1:D:97:SER:HB2	2.45	0.51
1:C:169:PRO:O	1:C:173:ARG:HB2	2.10	0.51
1:C:110:ARG:C	1:C:112:GLU:H	2.12	0.51
1:D:190:VAL:O	1:D:194:VAL:HG23	2.11	0.51
1:D:84:ASP:O	1:D:87:GLY:N	2.36	0.51
1:A:125:ARG:HG2	1:A:127:LEU:O	2.10	0.51
1:B:210:THR:HG22	1:B:211:CYS:H	1.76	0.51
1:B:117:LEU:HB3	1:B:210:THR:HG23	1.92	0.51
1:A:112:GLU:HG2	1:A:113:LEU:N	2.25	0.51
1:C:242:LEU:HB3	1:C:244:THR:HG22	1.93	0.51
1:C:128:ASN:HB3	1:C:134:GLY:N	2.09	0.51
1:C:228:TYR:O	1:C:231:SER:HB2	2.11	0.51
1:B:20:ARG:HB3	1:B:46:TYR:CD2	2.45	0.51
1:B:169:PRO:O	1:B:173:ARG:HB2	2.11	0.50
1:D:23:PHE:O	1:D:24:LEU:HD23	2.11	0.50
1:C:143:LYS:O	1:C:146:SER:HB3	2.10	0.50
1:A:39:LEU:CD1	1:A:48:VAL:HG11	2.41	0.50
1:C:50:LEU:HG	1:C:50:LEU:O	2.11	0.50
1:A:128:ASN:HB3	1:A:134:GLY:N	2.07	0.50
1:B:79:LEU:O	1:B:83:VAL:HG23	2.11	0.50
1:A:233:LEU:CD1	1:A:237:THR:HG21	2.33	0.50
1:D:230:ARG:HG3	1:D:230:ARG:HH11	1.75	0.50
1:C:38:ILE:HD11	1:C:258:ALA:N	2.27	0.50
1:B:79:LEU:HD11	1:B:93:TYR:CE1	2.45	0.50
1:A:38:ILE:HG12	1:A:38:ILE:O	2.11	0.50
1:A:248:LEU:HD12	1:A:248:LEU:N	2.27	0.50
1:C:21:ILE:N	1:C:21:ILE:HD12	2.27	0.50
1:D:219:VAL:HG22	1:D:219:VAL:O	2.12	0.50
1:B:74:PRO:O	1:B:77:ASP:HB2	2.12	0.50
1:B:147:ALA:O	1:B:150:ALA:HB3	2.11	0.50
1:D:248:LEU:N	1:D:248:LEU:HD12	2.27	0.50
1:B:82:ILE:O	1:B:86:LEU:HD13	2.12	0.50
1:D:110:ARG:CD	1:D:113:LEU:HD22	2.36	0.49
1:B:50:LEU:HG	1:B:50:LEU:O	2.11	0.49
1:C:112:GLU:HG2	1:C:113:LEU:HD13	1.94	0.49
1:D:242:LEU:HB3	1:D:244:THR:HG22	1.94	0.49
1:C:126:PHE:HE2	1:C:221:VAL:HG22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:O	1:A:113:LEU:HA	2.12	0.49
1:B:112:GLU:HG2	1:B:113:LEU:HD13	1.94	0.49
1:B:198:ASP:OD1	1:B:200:ARG:HD3	2.11	0.49
1:A:230:ARG:HH11	1:A:230:ARG:HG3	1.76	0.49
1:A:253:ALA:HB1	1:A:256:GLN:HE21	1.76	0.49
1:A:100:ALA:HB1	1:A:119:LEU:HD22	1.95	0.49
1:D:168:VAL:HG12	1:D:171:ALA:H	1.76	0.49
1:A:242:LEU:HB3	1:A:244:THR:HG22	1.94	0.49
1:B:38:ILE:O	1:B:38:ILE:HG12	2.12	0.49
1:D:198:ASP:OD1	1:D:200:ARG:HD3	2.13	0.49
1:C:100:ALA:O	1:C:104:ILE:HG12	2.12	0.49
1:C:22:LEU:HD23	1:C:48:VAL:HG22	1.95	0.49
1:A:124:PRO:HG2	1:A:125:ARG:N	2.24	0.49
1:D:212:VAL:HG11	1:D:229:LEU:HD12	1.93	0.49
1:B:160:ALA:N	1:B:161:PRO:HD2	2.28	0.49
1:C:125:ARG:HG2	1:C:127:LEU:O	2.12	0.49
1:B:240:GLU:HG3	1:B:241:THR:N	2.27	0.49
1:B:55:CYS:O	1:B:186:ILE:HG21	2.13	0.49
1:C:184:PRO:O	1:C:185:ASP:C	2.49	0.49
1:B:126:PHE:HB3	1:B:195:PHE:HD1	1.77	0.49
1:C:55:CYS:O	1:C:186:ILE:HG21	2.13	0.49
1:B:125:ARG:HD3	1:B:129:ASP:OD1	2.13	0.49
1:C:235:GLY:O	1:C:237:THR:N	2.46	0.49
1:A:32:GLN:HG2	1:A:52:ASP:OD1	2.13	0.49
1:A:240:GLU:HG3	1:A:241:THR:H	1.78	0.48
1:A:10:LEU:HB3	1:A:52:ASP:O	2.12	0.48
1:D:148:MET:HE3	1:D:188:LEU:HD12	1.95	0.48
1:C:39:LEU:N	1:C:40:PRO:HD2	2.28	0.48
1:A:140:GLU:O	1:A:144:VAL:HG23	2.12	0.48
1:C:212:VAL:HG11	1:C:229:LEU:HD12	1.95	0.48
1:D:21:ILE:HD12	1:D:21:ILE:N	2.28	0.48
1:C:219:VAL:HG22	1:C:219:VAL:O	2.13	0.48
1:B:60:ASN:HD22	1:B:61:PRO:N	2.11	0.48
1:A:148:MET:HE3	1:A:188:LEU:HD12	1.94	0.48
1:A:160:ALA:N	1:A:161:PRO:HD2	2.27	0.48
1:B:72:LEU:O	1:B:76:VAL:HG23	2.14	0.48
1:B:55:CYS:HB2	1:B:190:VAL:HG21	1.95	0.48
1:C:253:ALA:HB1	1:C:256:GLN:HE21	1.78	0.48
1:D:143:LYS:O	1:D:146:SER:HB3	2.14	0.48
1:A:126:PHE:HB3	1:A:195:PHE:HD1	1.79	0.48
1:D:249:PRO:O	1:D:251:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:TYR:CE2	1:B:103:GLY:HA3	2.48	0.48
1:D:151:ASN:HB3	1:D:154:ALA:HB3	1.94	0.48
1:C:247:HIS:HB3	1:C:248:LEU:HD12	1.95	0.48
1:D:169:PRO:O	1:D:173:ARG:HB2	2.13	0.48
1:C:128:ASN:ND2	1:C:136:PHE:N	2.62	0.48
1:B:36:HIS:C	1:B:38:ILE:H	2.17	0.48
1:B:200:ARG:HG2	1:B:200:ARG:HH11	1.78	0.48
1:A:24:LEU:HD23	1:A:94:VAL:HB	1.96	0.48
1:D:210:THR:HB	1:D:237:THR:CG2	2.43	0.47
1:B:242:LEU:HB3	1:B:244:THR:HG22	1.95	0.47
1:B:186:ILE:O	1:B:190:VAL:HG23	2.14	0.47
1:D:86:LEU:O	1:D:87:GLY:O	2.32	0.47
1:C:244:THR:HB	1:C:256:GLN:OE1	2.14	0.47
1:B:140:GLU:O	1:B:144:VAL:HG23	2.14	0.47
1:D:233:LEU:CD1	1:D:237:THR:HG21	2.35	0.47
1:A:235:GLY:O	1:A:237:THR:N	2.48	0.47
1:B:110:ARG:C	1:B:112:GLU:N	2.67	0.47
1:A:228:TYR:O	1:A:231:SER:HB2	2.14	0.47
1:A:184:PRO:O	1:A:185:ASP:C	2.50	0.47
1:A:244:THR:HB	1:A:256:GLN:NE2	2.30	0.47
1:D:200:ARG:HH11	1:D:200:ARG:HG2	1.79	0.47
1:B:175:PHE:CZ	1:B:179:LEU:HD23	2.49	0.47
1:C:120:ILE:HG23	1:C:213:ILE:HG21	1.96	0.47
1:D:110:ARG:C	1:D:112:GLU:N	2.67	0.47
1:C:240:GLU:HG3	1:C:241:THR:N	2.29	0.47
1:D:22:LEU:HD12	1:D:23:PHE:N	2.26	0.47
1:A:198:ASP:OD1	1:A:200:ARG:HD3	2.15	0.47
1:B:60:ASN:ND2	1:B:62:ASP:H	2.12	0.47
1:A:114:PHE:HB3	1:A:117:LEU:CD2	2.44	0.47
1:D:25:ALA:CB	1:D:99:SER:OG	2.62	0.47
1:D:74:PRO:O	1:D:77:ASP:HB2	2.14	0.47
1:D:60:ASN:ND2	1:D:61:PRO:HD2	2.25	0.47
1:C:14:VAL:CG1	1:D:170:ALA:HB2	2.43	0.47
1:D:38:ILE:HG12	1:D:38:ILE:O	2.15	0.47
1:D:160:ALA:N	1:D:161:PRO:HD2	2.29	0.47
1:D:110:ARG:HD3	1:D:112:GLU:OE1	2.15	0.47
1:B:148:MET:CE	1:B:188:LEU:HD12	2.44	0.47
1:D:36:HIS:C	1:D:38:ILE:H	2.18	0.47
1:D:169:PRO:HA	1:D:172:VAL:HG12	1.97	0.47
1:B:244:THR:HB	1:B:256:GLN:OE1	2.14	0.47
1:D:126:PHE:HE2	1:D:221:VAL:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PHE:O	1:D:160:ALA:C	2.54	0.47
1:A:151:ASN:HB3	1:A:154:ALA:HB3	1.95	0.47
1:B:152:TYR:O	1:B:156:VAL:HG23	2.15	0.47
1:A:219:VAL:HG22	1:A:219:VAL:O	2.15	0.47
1:A:93:TYR:HB2	1:A:114:PHE:HE1	1.80	0.46
1:B:169:PRO:HA	1:B:172:VAL:HG12	1.97	0.46
1:B:212:VAL:HG11	1:B:229:LEU:HD12	1.97	0.46
1:C:110:ARG:HD3	1:C:112:GLU:OE1	2.15	0.46
1:A:128:ASN:ND2	1:A:136:PHE:N	2.63	0.46
1:D:235:GLY:O	1:D:237:THR:N	2.48	0.46
1:D:72:LEU:O	1:D:76:VAL:HG23	2.15	0.46
1:B:248:LEU:HD12	1:B:248:LEU:N	2.30	0.46
1:D:120:ILE:HG23	1:D:213:ILE:HG21	1.96	0.46
1:D:147:ALA:O	1:D:150:ALA:HB3	2.16	0.46
1:A:79:LEU:HD11	1:A:93:TYR:CE1	2.50	0.46
1:B:247:HIS:HD2	1:B:248:LEU:HD11	1.79	0.46
1:C:50:LEU:N	1:C:50:LEU:HD23	2.30	0.46
1:B:39:LEU:CD1	1:B:48:VAL:HG11	2.45	0.46
1:A:47:ARG:NH1	1:B:168:VAL:HG13	2.30	0.46
1:B:159:PHE:O	1:B:160:ALA:C	2.54	0.46
1:B:38:ILE:HD11	1:B:258:ALA:CA	2.44	0.46
1:B:70:THR:OG1	1:B:71:THR:HG23	2.16	0.46
1:B:114:PHE:HB3	1:B:117:LEU:CD2	2.46	0.46
1:A:110:ARG:CD	1:A:113:LEU:HD22	2.40	0.46
1:B:112:GLU:CG	1:B:113:LEU:HD13	2.46	0.46
1:A:21:ILE:HD12	1:A:21:ILE:N	2.30	0.46
1:A:159:PHE:O	1:A:160:ALA:C	2.53	0.46
1:C:10:LEU:HB3	1:C:52:ASP:O	2.15	0.46
1:D:38:ILE:HD11	1:D:258:ALA:CA	2.46	0.46
1:C:77:ASP:O	1:C:78:ASP:C	2.54	0.46
1:A:96:HIS:CE1	1:A:97:SER:HB2	2.51	0.46
1:C:110:ARG:C	1:C:112:GLU:N	2.69	0.46
1:B:53:LEU:HD13	1:B:53:LEU:HA	1.81	0.46
1:A:93:TYR:CE2	1:A:103:GLY:HA3	2.50	0.46
1:A:244:THR:HB	1:A:256:GLN:OE1	2.15	0.46
1:C:147:ALA:O	1:C:150:ALA:HB3	2.15	0.46
1:B:31:ASP:C	1:B:31:ASP:OD2	2.53	0.46
1:A:74:PRO:O	1:A:77:ASP:HB2	2.16	0.46
1:A:77:ASP:O	1:A:78:ASP:C	2.53	0.46
1:B:230:ARG:HB2	1:B:239:VAL:HG21	1.98	0.46
1:D:140:GLU:O	1:D:144:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HA	1:A:47:ARG:HE	1.81	0.46
1:D:20:ARG:HB3	1:D:46:TYR:CD2	2.51	0.46
1:C:169:PRO:C	1:C:172:VAL:HG12	2.36	0.46
1:A:169:PRO:O	1:A:173:ARG:HB2	2.16	0.46
1:A:110:ARG:C	1:A:112:GLU:N	2.69	0.46
1:D:55:CYS:HB2	1:D:190:VAL:HG21	1.98	0.46
1:C:160:ALA:N	1:C:161:PRO:HD2	2.30	0.46
1:B:10:LEU:HB3	1:B:52:ASP:O	2.15	0.45
1:B:74:PRO:O	1:B:77:ASP:N	2.49	0.45
1:A:86:LEU:HD23	1:B:169:PRO:HB3	1.99	0.45
1:C:112:GLU:CG	1:C:113:LEU:HD13	2.46	0.45
1:A:190:VAL:O	1:A:194:VAL:HG23	2.16	0.45
1:B:235:GLY:O	1:B:237:THR:N	2.49	0.45
1:A:83:VAL:O	1:A:88:ILE:HG13	2.16	0.45
1:C:169:PRO:CA	1:C:172:VAL:HG12	2.47	0.45
1:A:228:TYR:HE2	1:A:232:HIS:CE1	2.34	0.45
1:C:77:ASP:O	1:C:80:LEU:N	2.49	0.45
1:A:73:ASP:N	1:A:74:PRO:HD2	2.31	0.45
1:D:29:GLY:O	1:D:30:THR:O	2.34	0.45
1:A:38:ILE:HD11	1:A:258:ALA:N	2.32	0.45
1:C:36:HIS:C	1:C:38:ILE:H	2.20	0.45
1:C:84:ASP:O	1:C:87:GLY:N	2.37	0.45
1:C:82:ILE:O	1:C:86:LEU:HD13	2.17	0.45
1:D:112:GLU:CG	1:D:113:LEU:HD13	2.47	0.45
1:D:31:ASP:C	1:D:31:ASP:OD2	2.53	0.45
1:B:110:ARG:HD3	1:B:112:GLU:OE1	2.16	0.45
1:C:47:ARG:NH1	1:D:168:VAL:HG13	2.32	0.45
1:C:38:ILE:O	1:C:38:ILE:HG12	2.17	0.45
1:C:200:ARG:HG2	1:C:200:ARG:HH11	1.82	0.45
1:C:68:ARG:O	1:C:70:THR:HG23	2.16	0.45
1:C:114:PHE:HB3	1:C:117:LEU:CD2	2.46	0.45
1:C:117:LEU:HB3	1:C:210:THR:HG23	1.97	0.45
1:D:93:TYR:HB2	1:D:114:PHE:HE1	1.81	0.45
1:B:22:LEU:HD12	1:B:23:PHE:N	2.28	0.45
1:D:36:HIS:O	1:D:38:ILE:N	2.50	0.45
1:C:31:ASP:OD2	1:C:31:ASP:C	2.55	0.45
1:C:76:VAL:HG13	1:C:106:ALA:HB2	1.98	0.45
1:B:21:ILE:N	1:B:21:ILE:HD12	2.31	0.45
1:C:126:PHE:HB3	1:C:195:PHE:HD1	1.82	0.45
1:C:97:SER:O	1:C:100:ALA:HB3	2.17	0.45
1:A:112:GLU:HG2	1:A:113:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:TYR:HB2	1:B:114:PHE:HE1	1.82	0.44
1:A:200:ARG:NH1	1:A:200:ARG:HG2	2.32	0.44
1:B:39:LEU:H	1:B:40:PRO:HD2	1.82	0.44
1:B:83:VAL:O	1:B:88:ILE:HG13	2.16	0.44
1:B:23:PHE:O	1:B:24:LEU:HD23	2.16	0.44
1:C:79:LEU:C	1:C:79:LEU:HD23	2.37	0.44
1:D:89:GLN:O	1:D:113:LEU:HA	2.17	0.44
1:C:244:THR:HB	1:C:256:GLN:NE2	2.32	0.44
1:B:249:PRO:O	1:B:251:LEU:N	2.50	0.44
1:A:265:LEU:HD12	1:A:265:LEU:O	2.17	0.44
1:C:93:TYR:HB2	1:C:114:PHE:CE1	2.50	0.44
1:A:79:LEU:O	1:A:83:VAL:HG23	2.17	0.44
1:A:250:GLN:HA	1:A:257:LEU:HD23	1.99	0.44
1:C:89:GLN:O	1:C:113:LEU:HA	2.18	0.44
1:D:55:CYS:O	1:D:186:ILE:HG21	2.17	0.44
1:D:249:PRO:C	1:D:251:LEU:N	2.71	0.44
1:C:120:ILE:HG21	1:C:250:GLN:HE22	1.83	0.44
1:A:120:ILE:HG23	1:A:213:ILE:HG21	1.99	0.44
1:A:25:ALA:CB	1:A:99:SER:OG	2.64	0.44
1:B:36:HIS:O	1:B:38:ILE:N	2.51	0.44
1:D:68:ARG:O	1:D:70:THR:HG23	2.16	0.44
1:D:83:VAL:O	1:D:88:ILE:HG13	2.16	0.44
1:B:28:PHE:O	1:B:30:THR:N	2.51	0.44
1:C:168:VAL:HG12	1:C:171:ALA:H	1.82	0.44
1:B:110:ARG:CD	1:B:113:LEU:HD22	2.41	0.44
1:A:124:PRO:CG	1:A:125:ARG:H	2.24	0.44
1:D:82:ILE:O	1:D:86:LEU:HD13	2.18	0.44
1:B:57:GLY:HA3	1:B:181:ASN:HB3	1.99	0.44
1:D:215:THR:HG21	1:D:246:GLY:O	2.18	0.44
1:B:109:ARG:NH1	1:D:207:ARG:NH2	2.66	0.44
1:B:54:VAL:HG13	1:B:55:CYS:N	2.33	0.44
1:A:36:HIS:C	1:A:38:ILE:N	2.71	0.44
1:D:77:ASP:O	1:D:78:ASP:C	2.54	0.44
1:A:39:LEU:O	1:A:40:PRO:C	2.56	0.44
1:A:60:ASN:ND2	1:A:62:ASP:H	2.16	0.44
1:D:124:PRO:CG	1:D:125:ARG:H	2.28	0.44
1:D:79:LEU:O	1:D:83:VAL:HG23	2.17	0.44
1:A:169:PRO:HA	1:A:172:VAL:HG12	2.00	0.43
1:C:36:HIS:O	1:C:38:ILE:N	2.51	0.43
1:C:125:ARG:HD3	1:C:129:ASP:OD1	2.19	0.43
1:A:124:PRO:HG2	1:A:132:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:HG21	1:B:246:GLY:O	2.18	0.43
1:D:104:ILE:HG13	1:D:122:PHE:CZ	2.53	0.43
1:C:141:ILE:CD1	1:C:142:GLU:N	2.80	0.43
1:A:116:LYS:HE2	1:A:264:ALA:HB1	2.01	0.43
1:D:17:THR:HA	1:D:47:ARG:HE	1.84	0.43
1:C:249:PRO:O	1:C:251:LEU:N	2.51	0.43
1:A:68:ARG:O	1:A:70:THR:HG23	2.18	0.43
1:C:83:VAL:O	1:C:88:ILE:HG13	2.18	0.43
1:D:124:PRO:HG2	1:D:132:TYR:OH	2.18	0.43
1:B:168:VAL:HG12	1:B:171:ALA:H	1.83	0.43
1:B:38:ILE:HD11	1:B:258:ALA:HA	2.00	0.43
1:B:257:LEU:HG	1:B:261:LEU:HD12	2.00	0.43
1:C:73:ASP:N	1:C:74:PRO:HD2	2.33	0.43
1:A:100:ALA:O	1:A:104:ILE:HG12	2.19	0.43
1:A:148:MET:CE	1:A:188:LEU:HD12	2.49	0.43
1:B:257:LEU:O	1:B:258:ALA:C	2.57	0.43
1:D:53:LEU:HA	1:D:53:LEU:HD13	1.84	0.43
1:A:169:PRO:C	1:A:172:VAL:HG12	2.39	0.43
1:A:22:LEU:HD23	1:A:48:VAL:HG22	2.00	0.43
1:A:210:THR:HB	1:A:237:THR:CG2	2.46	0.42
1:C:159:PHE:O	1:C:160:ALA:C	2.57	0.42
1:B:240:GLU:HG3	1:B:241:THR:H	1.84	0.42
1:A:121:GLY:H	1:A:213:ILE:CG2	2.26	0.42
1:A:55:CYS:O	1:A:186:ILE:HG21	2.18	0.42
1:B:175:PHE:O	1:B:179:LEU:HB2	2.19	0.42
1:B:79:LEU:C	1:B:79:LEU:HD23	2.39	0.42
1:D:121:GLY:H	1:D:213:ILE:CG2	2.26	0.42
1:A:32:GLN:HG2	1:A:52:ASP:OD2	2.19	0.42
1:D:148:MET:CE	1:D:188:LEU:HD12	2.49	0.42
1:D:17:THR:HG22	1:D:47:ARG:NH2	2.34	0.42
1:C:145:PHE:HZ	1:C:192:ARG:HA	1.84	0.42
1:C:145:PHE:CZ	1:C:192:ARG:HA	2.54	0.42
1:C:57:GLY:HA3	1:C:181:ASN:HB3	2.01	0.42
1:C:86:LEU:O	1:D:172:VAL:HG11	2.20	0.42
1:B:124:PRO:CG	1:B:125:ARG:H	2.26	0.42
1:B:249:PRO:C	1:B:251:LEU:N	2.72	0.42
1:A:39:LEU:H	1:A:40:PRO:HD2	1.84	0.42
1:C:124:PRO:CG	1:C:125:ARG:H	2.29	0.42
1:A:35:TRP:O	1:A:36:HIS:C	2.56	0.42
1:C:41:TYR:CD1	1:C:258:ALA:HB1	2.55	0.42
1:A:29:GLY:O	1:A:30:THR:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:SER:O	1:C:191:SER:OG	2.37	0.42
1:B:151:ASN:HB3	1:B:154:ALA:HB3	2.00	0.42
1:D:117:LEU:CB	1:D:210:THR:HG23	2.50	0.42
1:A:82:ILE:O	1:A:86:LEU:HD13	2.19	0.42
1:D:247:HIS:CD2	1:D:248:LEU:CD1	3.02	0.42
1:A:120:ILE:HG21	1:A:250:GLN:HE22	1.84	0.42
1:C:35:TRP:O	1:C:36:HIS:C	2.58	0.42
1:D:66:PHE:HD1	1:D:189:PHE:CD2	2.37	0.42
1:C:79:LEU:HD11	1:C:93:TYR:CE1	2.55	0.42
1:C:230:ARG:HB2	1:C:239:VAL:HG21	2.01	0.42
1:C:116:LYS:HE2	1:C:264:ALA:HB1	2.02	0.42
1:A:151:ASN:OD1	1:A:154:ALA:HB2	2.20	0.42
1:A:168:VAL:HG12	1:A:171:ALA:H	1.85	0.42
1:A:128:ASN:HD21	1:A:136:PHE:C	2.22	0.42
1:B:120:ILE:O	1:B:121:GLY:C	2.56	0.42
1:B:121:GLY:H	1:B:213:ILE:CG2	2.22	0.42
1:D:227:GLU:OE1	1:D:230:ARG:HB3	2.19	0.42
1:A:152:TYR:O	1:A:156:VAL:HG23	2.19	0.42
1:A:117:LEU:CB	1:A:210:THR:HG23	2.49	0.42
1:A:112:GLU:CG	1:A:113:LEU:HD13	2.50	0.42
1:B:169:PRO:HA	1:B:172:VAL:CG1	2.50	0.42
1:A:125:ARG:HD2	1:A:198:ASP:CG	2.40	0.42
1:A:17:THR:HG22	1:A:47:ARG:NH2	2.35	0.42
1:D:38:ILE:HD11	1:D:258:ALA:HA	2.02	0.42
1:B:77:ASP:O	1:B:78:ASP:C	2.57	0.42
1:B:28:PHE:CG	1:B:29:GLY:N	2.88	0.42
1:B:189:PHE:O	1:B:191:SER:N	2.53	0.42
1:D:240:GLU:HG3	1:D:241:THR:H	1.84	0.41
1:D:230:ARG:HB2	1:D:239:VAL:HG21	2.02	0.41
1:A:26:HIS:N	1:A:35:TRP:HE1	2.18	0.41
1:A:189:PHE:O	1:A:191:SER:N	2.53	0.41
1:B:172:VAL:HG22	1:B:172:VAL:O	2.20	0.41
1:C:28:PHE:CG	1:C:29:GLY:N	2.87	0.41
1:A:169:PRO:HA	1:A:172:VAL:CG1	2.50	0.41
1:C:39:LEU:CD1	1:C:48:VAL:HG11	2.51	0.41
1:B:109:ARG:CZ	1:D:207:ARG:HH22	2.33	0.41
1:B:32:GLN:HG2	1:B:52:ASP:OD1	2.20	0.41
1:B:145:PHE:HZ	1:B:192:ARG:HA	1.85	0.41
1:B:73:ASP:N	1:B:74:PRO:HD2	2.35	0.41
1:B:68:ARG:O	1:B:70:THR:HG23	2.20	0.41
1:C:74:PRO:O	1:C:77:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:TYR:O	1:D:156:VAL:HG23	2.20	0.41
1:A:110:ARG:HD3	1:A:112:GLU:OE1	2.20	0.41
1:D:76:VAL:HG13	1:D:106:ALA:HB2	2.02	0.41
1:D:144:VAL:O	1:D:148:MET:HB2	2.20	0.41
1:D:28:PHE:O	1:D:30:THR:N	2.54	0.41
1:C:100:ALA:HB1	1:C:122:PHE:HB2	2.03	0.41
1:C:119:LEU:HB3	1:C:122:PHE:HB2	2.03	0.41
1:D:169:PRO:HA	1:D:172:VAL:CG1	2.51	0.41
1:C:32:GLN:HG2	1:C:52:ASP:OD1	2.21	0.41
1:B:86:LEU:O	1:B:87:GLY:O	2.39	0.41
1:C:28:PHE:O	1:C:30:THR:N	2.53	0.41
1:A:97:SER:O	1:A:100:ALA:HB3	2.21	0.41
1:A:145:PHE:HZ	1:A:192:ARG:HA	1.85	0.41
1:C:256:GLN:HG2	1:C:256:GLN:H	1.65	0.41
1:A:57:GLY:C	1:A:59:VAL:H	2.23	0.41
1:C:53:LEU:HD13	1:C:53:LEU:HA	1.81	0.41
1:C:104:ILE:HG13	1:C:122:PHE:CZ	2.55	0.41
1:C:39:LEU:O	1:C:40:PRO:C	2.57	0.41
1:A:60:ASN:HD22	1:A:61:PRO:N	2.19	0.41
1:A:35:TRP:O	1:A:38:ILE:N	2.48	0.41
1:A:147:ALA:HA	1:A:150:ALA:HB3	2.02	0.41
1:B:73:ASP:O	1:B:74:PRO:C	2.57	0.41
1:D:151:ASN:OD1	1:D:154:ALA:HB2	2.21	0.41
1:C:249:PRO:C	1:C:251:LEU:N	2.72	0.41
1:D:9:ALA:HA	1:D:63:TYR:CE1	2.56	0.41
1:A:102:ILE:HG13	1:A:102:ILE:H	1.71	0.41
1:C:55:CYS:HB2	1:C:190:VAL:HG21	2.01	0.41
1:D:189:PHE:O	1:D:191:SER:N	2.53	0.41
1:A:37:LEU:HD13	1:A:37:LEU:HA	1.89	0.41
1:B:117:LEU:CB	1:B:210:THR:HG23	2.50	0.41
1:A:86:LEU:O	1:A:87:GLY:O	2.38	0.41
1:A:257:LEU:HG	1:A:261:LEU:HD12	2.02	0.41
1:D:39:LEU:CD1	1:D:48:VAL:HG11	2.50	0.41
1:C:148:MET:HE3	1:C:188:LEU:HD12	2.01	0.41
1:A:54:VAL:HG11	1:A:69:TYR:CE1	2.55	0.41
1:B:265:LEU:HA	1:B:266:PRO:HA	1.92	0.41
1:D:66:PHE:HD1	1:D:189:PHE:HD2	1.67	0.41
1:C:215:THR:HG21	1:C:246:GLY:O	2.19	0.41
1:C:42:PHE:HE2	1:C:265:LEU:HD11	1.85	0.41
1:A:249:PRO:C	1:A:251:LEU:N	2.72	0.41
1:D:26:HIS:CD2	1:D:31:ASP:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HG23	1:B:207:ARG:HH11	1.86	0.41
1:D:137:GLU:H	1:D:140:GLU:HB2	1.85	0.41
1:D:244:THR:HB	1:D:256:GLN:NE2	2.36	0.41
1:D:244:THR:HB	1:D:256:GLN:CD	2.42	0.41
1:A:156:VAL:HG22	1:A:179:LEU:HD12	2.03	0.41
1:A:175:PHE:CZ	1:A:179:LEU:HD23	2.56	0.41
1:A:66:PHE:HD1	1:A:189:PHE:CD2	2.39	0.41
1:D:114:PHE:HB3	1:D:117:LEU:HD21	2.03	0.40
1:D:172:VAL:HG22	1:D:172:VAL:O	2.20	0.40
1:B:55:CYS:CB	1:B:190:VAL:HG21	2.51	0.40
1:B:21:ILE:HA	1:B:47:ARG:HB2	2.02	0.40
1:A:225:VAL:C	1:A:227:GLU:N	2.75	0.40
1:B:229:LEU:C	1:B:231:SER:N	2.74	0.40
1:D:116:LYS:HE2	1:D:264:ALA:HB1	2.04	0.40
1:D:79:LEU:C	1:D:79:LEU:HD23	2.42	0.40
1:C:121:GLY:H	1:C:213:ILE:CG2	2.25	0.40
1:D:41:TYR:CD1	1:D:258:ALA:HB1	2.56	0.40
1:C:245:GLU:CD	1:C:246:GLY:H	2.25	0.40
1:A:229:LEU:C	1:A:231:SER:N	2.74	0.40
1:B:35:TRP:O	1:B:38:ILE:N	2.52	0.40
1:C:47:ARG:HH11	1:D:168:VAL:HG13	1.85	0.40
1:D:86:LEU:O	1:D:87:GLY:C	2.59	0.40
1:A:249:PRO:O	1:A:251:LEU:N	2.55	0.40
1:D:257:LEU:HG	1:D:261:LEU:HD12	2.03	0.40
1:B:10:LEU:CD2	1:B:54:VAL:HA	2.52	0.40
1:B:126:PHE:HA	1:B:126:PHE:HD2	1.78	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	259/267 (97%)	187 (72%)	52 (20%)	20 (8%)	1	14
1	B	259/267 (97%)	187 (72%)	53 (20%)	19 (7%)	1	16
1	C	259/267 (97%)	189 (73%)	52 (20%)	18 (7%)	1	18
1	D	259/267 (97%)	189 (73%)	49 (19%)	21 (8%)	1	13
All	All	1036/1068 (97%)	752 (73%)	206 (20%)	78 (8%)	1	15

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	30	THR
1	A	37	LEU
1	A	150	ALA
1	B	11	ASN
1	B	30	THR
1	B	150	ALA
1	C	11	ASN
1	C	30	THR
1	C	150	ALA
1	C	236	ASP
1	D	11	ASN
1	D	30	THR
1	D	150	ALA
1	A	56	ALA
1	A	87	GLY
1	A	124	PRO
1	A	146	SER
1	A	236	ASP
1	B	37	LEU
1	B	87	GLY
1	B	124	PRO
1	B	236	ASP
1	C	29	GLY
1	C	37	LEU
1	C	87	GLY
1	C	124	PRO
1	D	37	LEU
1	D	56	ALA
1	D	87	GLY
1	D	124	PRO
1	D	236	ASP
1	A	200	ARG

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Mol	Chain	Res	Type
1	B	29	GLY
1	B	107	SER
1	B	146	SER
1	B	166	ALA
1	B	200	ARG
1	C	56	ALA
1	D	107	SER
1	D	146	SER
1	D	166	ALA
1	A	29	GLY
1	A	107	SER
1	A	113	LEU
1	A	166	ALA
1	A	211	CYS
1	A	258	ALA
1	B	113	LEU
1	B	255	ALA
1	B	258	ALA
1	C	107	SER
1	C	113	LEU
1	C	146	SER
1	C	200	ARG
1	C	255	ALA
1	D	29	GLY
1	D	113	LEU
1	D	200	ARG
1	A	69	TYR
1	A	190	VAL
1	B	56	ALA
1	B	211	CYS
1	C	166	ALA
1	C	211	CYS
1	D	211	CYS
1	D	250	GLN
1	D	255	ALA
1	D	258	ALA
1	D	69	TYR
1	D	190	VAL
1	B	190	VAL
1	C	165	GLY
1	A	38	ILE
1	B	38	ILE

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Mol	Chain	Res	Type
1	C	190	VAL
1	A	165	GLY
1	D	165	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	220/226 (97%)	197 (90%)	23 (10%)	8	38
1	B	220/226 (97%)	199 (90%)	21 (10%)	11	43
1	C	220/226 (97%)	197 (90%)	23 (10%)	8	38
1	D	220/226 (97%)	198 (90%)	22 (10%)	9	41
All	All	880/904 (97%)	791 (90%)	89 (10%)	9	40

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	44	GLN
1	A	50	LEU
1	A	60	ASN
1	A	99	SER
1	A	126	PHE
1	A	128	ASN
1	A	129	ASP
1	A	140	GLU
1	A	151	ASN
1	A	177	ARG
1	A	179	LEU
1	A	189	PHE
1	A	192	ARG
1	A	196	ASN
1	A	199	LEU
1	A	200	ARG
1	A	210	THR

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Mol	Chain	Res	Type
1	A	211	CYS
1	A	227	GLU
1	A	245	GLU
1	A	250	GLN
1	A	265	LEU
1	B	20	ARG
1	B	50	LEU
1	B	60	ASN
1	B	99	SER
1	B	126	PHE
1	B	128	ASN
1	B	129	ASP
1	B	140	GLU
1	B	151	ASN
1	B	177	ARG
1	B	179	LEU
1	B	189	PHE
1	B	192	ARG
1	B	196	ASN
1	B	199	LEU
1	B	200	ARG
1	B	210	THR
1	B	227	GLU
1	B	245	GLU
1	B	250	GLN
1	B	265	LEU
1	C	20	ARG
1	C	50	LEU
1	C	60	ASN
1	C	88	ILE
1	C	99	SER
1	C	126	PHE
1	C	128	ASN
1	C	129	ASP
1	C	140	GLU
1	C	151	ASN
1	C	177	ARG
1	C	179	LEU
1	C	189	PHE
1	C	192	ARG
1	C	196	ASN
1	C	199	LEU

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Mol	Chain	Res	Type
1	C	200	ARG
1	C	210	THR
1	C	211	CYS
1	C	227	GLU
1	C	245	GLU
1	C	250	GLN
1	C	265	LEU
1	D	20	ARG
1	D	50	LEU
1	D	60	ASN
1	D	88	ILE
1	D	99	SER
1	D	126	PHE
1	D	128	ASN
1	D	129	ASP
1	D	140	GLU
1	D	151	ASN
1	D	177	ARG
1	D	179	LEU
1	D	189	PHE
1	D	192	ARG
1	D	196	ASN
1	D	199	LEU
1	D	200	ARG
1	D	210	THR
1	D	227	GLU
1	D	245	GLU
1	D	250	GLN
1	D	265	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	60	ASN
1	A	128	ASN
1	A	151	ASN
1	A	214	GLN
1	A	250	GLN
1	A	256	GLN
1	A	259	GLN
1	B	44	GLN

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Mol	Chain	Res	Type
1	B	60	ASN
1	B	128	ASN
1	B	151	ASN
1	B	214	GLN
1	B	250	GLN
1	B	256	GLN
1	B	259	GLN
1	C	44	GLN
1	C	60	ASN
1	C	128	ASN
1	C	151	ASN
1	C	214	GLN
1	C	250	GLN
1	C	256	GLN
1	C	259	GLN
1	D	44	GLN
1	D	60	ASN
1	D	81	ASN
1	D	128	ASN
1	D	151	ASN
1	D	214	GLN
1	D	250	GLN
1	D	256	GLN
1	D	259	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 [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, 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	261/267 (97%)	-0.20	1 (0%) 93 90	2, 27, 56, 68	0
1	B	261/267 (97%)	-0.07	1 (0%) 93 90	3, 34, 60, 67	0
1	C	261/267 (97%)	0.02	3 (1%) 82 73	5, 44, 71, 80	0
1	D	261/267 (97%)	0.04	6 (2%) 64 54	2, 41, 67, 83	0
All	All	1044/1068 (97%)	-0.05	11 (1%) 82 73	2, 36, 63, 83	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	HIS	4.1
1	D	129	ASP	3.4
1	C	200	ARG	2.8
1	D	219	VAL	2.7
1	A	234	GLY	2.6
1	B	126	PHE	2.4
1	D	140	GLU	2.3
1	D	238	THR	2.3
1	C	115	SER	2.3
1	D	157	HIS	2.1
1	D	163	ALA	2.1

### 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 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.