



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:03 pm BST

PDB ID : 1LUL  
Title : DB58, A LEGUME LECTIN FROM DOLICHOS BIFLORUS  
Authors : Hamelryck, T.W.; Bouckaert, J.; Dao-Thi, M.H.; Wyns, L.; Etzler, M.; Loris, R.  
Deposited on : 1998-06-30  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

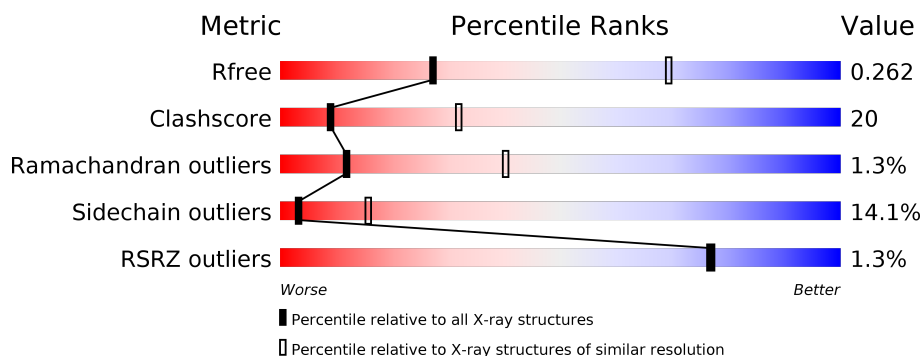
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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  $\leq 5\%$ . 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	253	<div> <div>2%</div> <div>56% 30% 10%</div> </div>
1	B	253	<div> <div>%</div> <div>55% 36% 6%</div> </div>
1	C	253	<div> <div>2%</div> <div>57% 35% 5%</div> </div>
1	D	253	<div> <div></div> <div>56% 30% 10%</div> </div>
1	E	253	<div> <div>2%</div> <div>58% 34% 5%</div> </div>
1	F	253	<div> <div>%</div> <div>56% 30% 10%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10515 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 LECTIN DB58.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	0	0	0
			1685	1067	275	343			
1	B	246	Total	C	N	O	0	0	0
			1816	1150	294	372			
1	C	246	Total	C	N	O	0	0	0
			1816	1150	294	372			
1	D	228	Total	C	N	O	0	0	0
			1685	1067	275	343			
1	E	246	Total	C	N	O	0	0	0
			1816	1150	294	372			
1	F	228	Total	C	N	O	0	0	0
			1685	1067	275	343			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

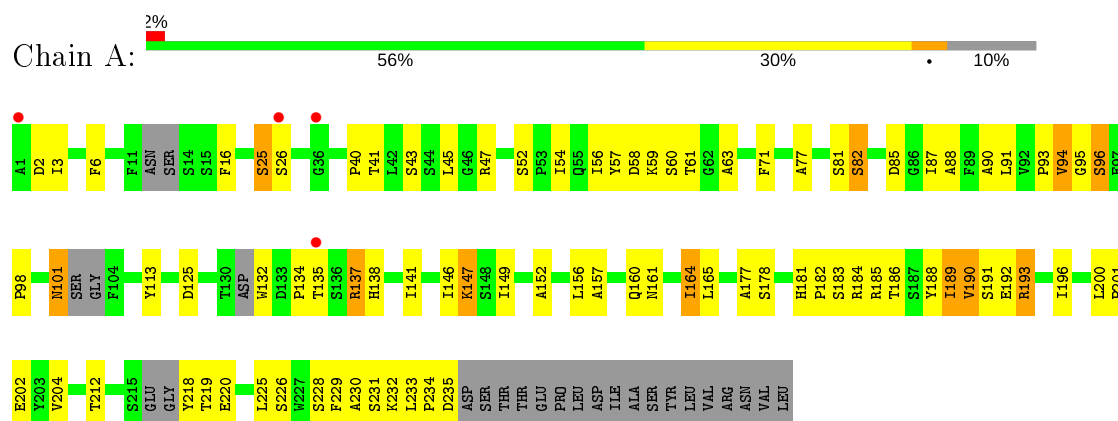
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

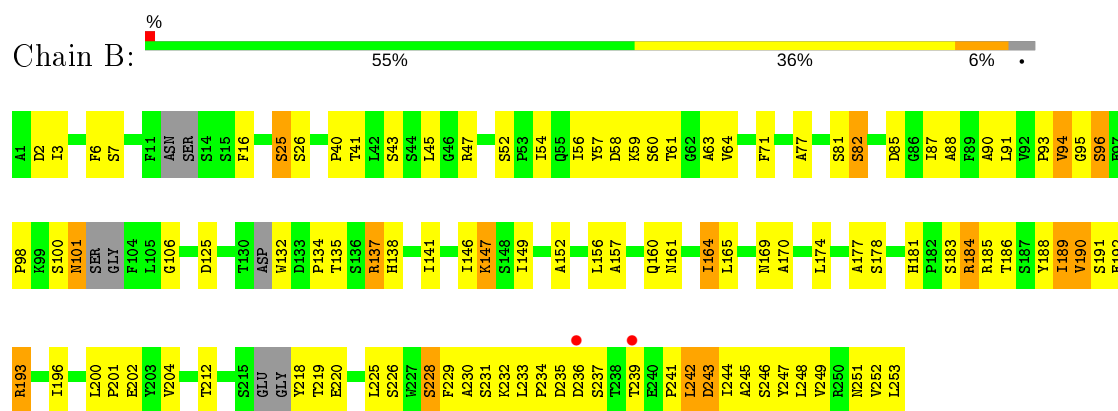
### 3 Residue-property plots

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.

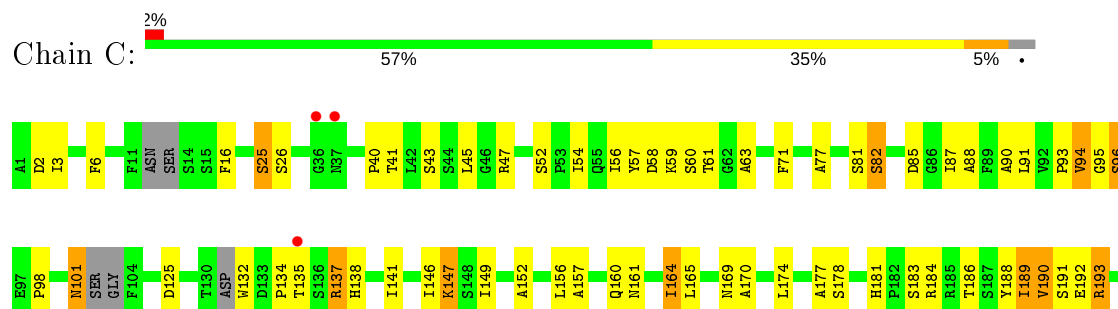
#### • Molecule 1: LECTIN DB58

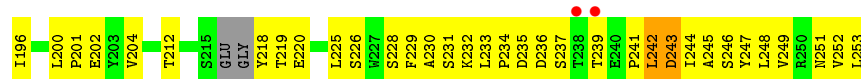


#### • Molecule 1: LECTIN DB58

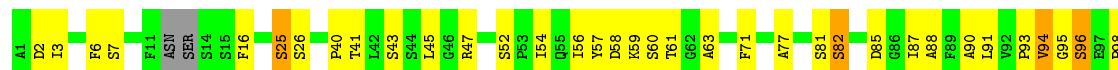


#### • Molecule 1: LECTIN DB58

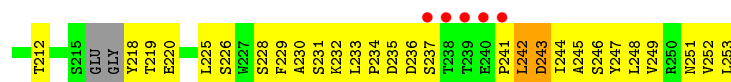
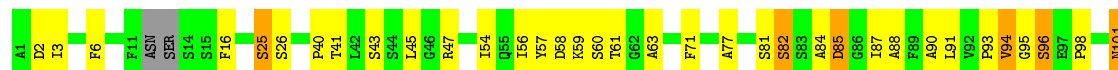




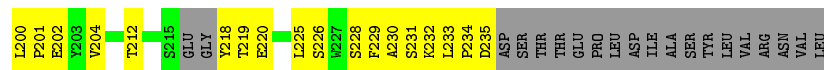
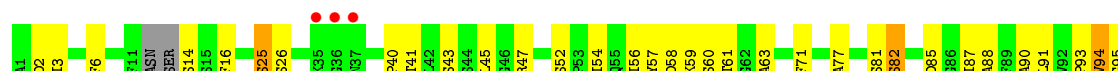
• Molecule 1: LECTIN DB58



• Molecule 1: LECTIN DB58



• Molecule 1: LECTIN DB58



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.39Å 130.95Å 138.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	80.7 (20.00-3.30) 80.7 (19.98-3.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.11 (at 3.29Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.226 , 0.266 0.225 , 0.262	Depositor DCC
$R_{free}$ test set	1797 reflections (7.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 97.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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

### 5.1 Standard geometry

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

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	0.54	0/1719	0.76	0/2344
1	B	0.55	0/1852	0.77	0/2528
1	C	0.55	0/1852	0.77	0/2528
1	D	0.53	0/1719	0.76	0/2344
1	E	0.55	0/1852	0.77	0/2528
1	F	0.54	0/1719	0.76	0/2344
All	All	0.54	0/10713	0.76	0/14616

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

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	1685	0	1591	67	0
1	B	1816	0	1716	95	0
1	C	1816	0	1716	83	0
1	D	1685	0	1591	66	0
1	E	1816	0	1716	73	0
1	F	1685	0	1591	73	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	10515	0	9921	412	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 20.

All (412) 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:185:ARG:CZ	1:F:14:SER:O	2.05	1.05
1:C:233:LEU:HD12	1:C:234:PRO:HD2	1.38	1.04
1:F:233:LEU:HD12	1:F:234:PRO:HD2	1.39	1.04
1:E:233:LEU:HD12	1:E:234:PRO:HD2	1.40	1.03
1:D:233:LEU:HD12	1:D:234:PRO:HD2	1.39	1.02
1:B:233:LEU:HD12	1:B:234:PRO:HD2	1.39	1.01
1:B:247:TYR:O	1:B:251:ASN:HB2	1.61	1.01
1:B:185:ARG:NE	1:F:14:SER:O	1.93	1.00
1:D:212:THR:HB	1:D:219:THR:HG22	1.43	1.00
1:A:212:THR:HB	1:A:219:THR:HG22	1.43	1.00
1:E:247:TYR:O	1:E:251:ASN:HB2	1.61	0.99
1:F:212:THR:HB	1:F:219:THR:HG22	1.43	0.99
1:B:212:THR:HB	1:B:219:THR:HG22	1.44	0.99
1:A:233:LEU:HD12	1:A:234:PRO:HD2	1.38	0.98
1:E:212:THR:HB	1:E:219:THR:HG22	1.44	0.98
1:C:247:TYR:O	1:C:251:ASN:HB2	1.62	0.98
1:C:212:THR:HB	1:C:219:THR:HG22	1.43	0.96
1:E:189:ILE:HG13	1:F:189:ILE:HG13	1.49	0.94
1:A:113:TYR:CB	1:F:94:VAL:HG21	1.98	0.94
1:A:113:TYR:HB3	1:F:94:VAL:HG21	1.47	0.93
1:B:185:ARG:HE	1:F:14:SER:CB	1.85	0.90
1:B:185:ARG:CD	1:F:14:SER:O	2.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:OE2	1:D:185:ARG:NH1	2.08	0.86
1:C:189:ILE:HG13	1:D:189:ILE:HG13	1.56	0.86
1:F:94:VAL:HG23	1:F:95:GLY:H	1.42	0.84
1:C:94:VAL:HG23	1:C:95:GLY:H	1.41	0.84
1:B:94:VAL:HG23	1:B:95:GLY:H	1.41	0.84
1:B:185:ARG:NE	1:F:14:SER:CB	2.41	0.84
1:B:185:ARG:HD3	1:F:14:SER:O	1.78	0.84
1:A:94:VAL:HG23	1:A:95:GLY:H	1.42	0.83
1:E:94:VAL:HG23	1:E:95:GLY:H	1.43	0.83
1:D:94:VAL:HG23	1:D:95:GLY:H	1.43	0.83
1:E:189:ILE:HG13	1:F:189:ILE:CG1	2.11	0.81
1:E:189:ILE:CG1	1:F:189:ILE:HG13	2.11	0.81
1:A:189:ILE:HG13	1:B:189:ILE:HG13	1.61	0.80
1:B:248:LEU:O	1:B:252:VAL:N	2.17	0.77
1:A:185:ARG:NH1	1:B:192:GLU:OE2	2.17	0.77
1:B:185:ARG:HG3	1:F:14:SER:CB	2.15	0.77
1:C:248:LEU:O	1:C:252:VAL:N	2.18	0.76
1:E:248:LEU:O	1:E:252:VAL:N	2.18	0.76
1:C:189:ILE:CG1	1:D:189:ILE:HG13	2.15	0.76
1:C:189:ILE:HG13	1:D:189:ILE:CG1	2.17	0.75
1:B:242:LEU:CD2	1:B:243:ASP:H	2.01	0.74
1:A:52:SER:HB2	1:D:52:SER:HB2	1.68	0.74
1:C:242:LEU:CD2	1:C:243:ASP:H	2.01	0.74
1:E:242:LEU:CD2	1:E:243:ASP:H	2.00	0.74
1:A:132:TRP:HB2	1:A:147:LYS:HG2	1.70	0.73
1:B:132:TRP:HB2	1:B:147:LYS:HG2	1.70	0.73
1:D:132:TRP:HB2	1:D:147:LYS:HG2	1.70	0.72
1:C:132:TRP:HB2	1:C:147:LYS:HG2	1.70	0.72
1:E:242:LEU:HD22	1:E:243:ASP:H	1.55	0.72
1:F:132:TRP:HB2	1:F:147:LYS:HG2	1.70	0.71
1:E:132:TRP:HB2	1:E:147:LYS:HG2	1.70	0.71
1:C:242:LEU:HD22	1:C:243:ASP:H	1.55	0.71
1:B:242:LEU:HD22	1:B:243:ASP:H	1.55	0.71
1:B:52:SER:HB2	1:C:52:SER:HB2	1.73	0.70
1:E:249:VAL:HA	1:E:253:LEU:HB2	1.74	0.69
1:E:157:ALA:HB1	1:E:160:GLN:HG3	1.74	0.69
1:C:157:ALA:HB1	1:C:160:GLN:HG3	1.74	0.69
1:B:185:ARG:CG	1:F:14:SER:CB	2.71	0.69
1:A:157:ALA:HB1	1:A:160:GLN:HG3	1.74	0.69
1:A:113:TYR:HB2	1:F:94:VAL:HG21	1.75	0.68
1:B:157:ALA:HB1	1:B:160:GLN:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HA	1:B:253:LEU:HB2	1.74	0.68
1:A:189:ILE:HG13	1:B:189:ILE:CG1	2.24	0.67
1:C:249:VAL:HA	1:C:253:LEU:HB2	1.74	0.67
1:F:157:ALA:HB1	1:F:160:GLN:HG3	1.75	0.67
1:D:157:ALA:HB1	1:D:160:GLN:HG3	1.76	0.67
1:C:233:LEU:HD12	1:C:234:PRO:CD	2.22	0.67
1:D:233:LEU:HD12	1:D:234:PRO:CD	2.22	0.66
1:A:189:ILE:CG1	1:B:189:ILE:HG13	2.26	0.66
1:D:212:THR:CB	1:D:219:THR:HG22	2.23	0.66
1:B:212:THR:CB	1:B:219:THR:HG22	2.24	0.65
1:A:94:VAL:HG23	1:A:95:GLY:N	2.12	0.65
1:C:212:THR:CB	1:C:219:THR:HG22	2.24	0.65
1:E:94:VAL:HG23	1:E:95:GLY:N	2.12	0.65
1:F:94:VAL:HG23	1:F:95:GLY:N	2.11	0.65
1:E:233:LEU:HD12	1:E:234:PRO:CD	2.24	0.64
1:D:94:VAL:HG23	1:D:95:GLY:N	2.12	0.64
1:E:212:THR:CB	1:E:219:THR:HG22	2.24	0.64
1:B:248:LEU:CD2	1:B:252:VAL:HG21	2.27	0.64
1:C:248:LEU:CD2	1:C:252:VAL:HG21	2.28	0.64
1:C:94:VAL:HG23	1:C:95:GLY:N	2.11	0.64
1:E:185:ARG:NH1	1:F:192:GLU:OE2	2.30	0.64
1:A:25:SER:O	1:A:26:SER:HB2	1.98	0.64
1:E:25:SER:O	1:E:26:SER:HB2	1.98	0.64
1:C:25:SER:O	1:C:26:SER:HB2	1.98	0.64
1:F:212:THR:CB	1:F:219:THR:HG22	2.24	0.63
1:A:185:ARG:HD2	1:B:192:GLU:OE2	1.97	0.63
1:E:248:LEU:CD2	1:E:252:VAL:HG21	2.28	0.63
1:F:25:SER:O	1:F:26:SER:HB2	1.98	0.63
1:B:94:VAL:HG23	1:B:95:GLY:N	2.11	0.63
1:B:25:SER:O	1:B:26:SER:HB2	1.97	0.63
1:D:25:SER:O	1:D:26:SER:HB2	1.97	0.63
1:B:185:ARG:NH1	1:F:14:SER:O	2.32	0.63
1:C:192:GLU:OE2	1:D:185:ARG:HD2	1.99	0.62
1:A:233:LEU:HD12	1:A:234:PRO:CD	2.22	0.62
1:D:91:LEU:HD12	1:D:91:LEU:N	2.15	0.62
1:F:77:ALA:HB2	1:F:220:GLU:HB3	1.82	0.62
1:C:91:LEU:HD12	1:C:91:LEU:N	2.15	0.62
1:C:77:ALA:HB2	1:C:220:GLU:HB3	1.82	0.62
1:A:77:ALA:HB2	1:A:220:GLU:HB3	1.82	0.61
1:A:93:PRO:O	1:A:96:SER:HB2	2.00	0.61
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:LEU:HD12	1:E:91:LEU:N	2.15	0.61
1:A:91:LEU:HD12	1:A:91:LEU:N	2.15	0.61
1:B:137:ARG:HH11	1:B:137:ARG:HG2	1.65	0.61
1:B:91:LEU:HD12	1:B:91:LEU:N	2.15	0.61
1:E:77:ALA:HB2	1:E:220:GLU:HB3	1.83	0.61
1:F:137:ARG:HH11	1:F:137:ARG:HG2	1.66	0.61
1:F:91:LEU:HD12	1:F:91:LEU:N	2.15	0.61
1:A:212:THR:CB	1:A:219:THR:HG22	2.23	0.60
1:F:233:LEU:HD12	1:F:234:PRO:CD	2.23	0.60
1:C:93:PRO:O	1:C:96:SER:HB2	2.01	0.60
1:D:77:ALA:HB2	1:D:220:GLU:HB3	1.83	0.60
1:E:93:PRO:O	1:E:96:SER:HB2	2.01	0.60
1:F:93:PRO:O	1:F:96:SER:HB2	2.01	0.60
1:B:93:PRO:O	1:B:96:SER:HB2	2.01	0.60
1:E:137:ARG:HH11	1:E:137:ARG:HG2	1.65	0.60
1:A:125:ASP:HB3	1:A:138:HIS:CE1	2.37	0.60
1:B:77:ALA:HB2	1:B:220:GLU:HB3	1.82	0.60
1:C:137:ARG:HH11	1:C:137:ARG:HG2	1.67	0.60
1:D:93:PRO:O	1:D:96:SER:HB2	2.01	0.60
1:C:125:ASP:HB3	1:C:138:HIS:CE1	2.37	0.60
1:D:137:ARG:HG2	1:D:137:ARG:HH11	1.66	0.59
1:B:233:LEU:HD12	1:B:234:PRO:CD	2.23	0.59
1:F:125:ASP:HB3	1:F:138:HIS:CE1	2.37	0.59
1:A:41:THR:C	1:A:219:THR:HG21	2.23	0.59
1:E:125:ASP:HB3	1:E:138:HIS:CE1	2.37	0.59
1:E:41:THR:C	1:E:219:THR:HG21	2.23	0.58
1:F:41:THR:C	1:F:219:THR:HG21	2.24	0.58
1:C:41:THR:C	1:C:219:THR:HG21	2.23	0.58
1:B:41:THR:C	1:B:219:THR:HG21	2.24	0.58
1:D:41:THR:C	1:D:219:THR:HG21	2.23	0.58
1:E:71:PHE:CZ	1:E:164:ILE:HG12	2.39	0.58
1:C:193:ARG:H	1:D:185:ARG:HD2	1.68	0.58
1:D:125:ASP:HB3	1:D:138:HIS:CE1	2.38	0.58
1:A:71:PHE:CZ	1:A:164:ILE:HG12	2.39	0.58
1:B:125:ASP:HB3	1:B:138:HIS:CE1	2.39	0.57
1:B:71:PHE:CZ	1:B:164:ILE:HG12	2.39	0.57
1:C:71:PHE:CZ	1:C:164:ILE:HG12	2.39	0.57
1:D:71:PHE:CZ	1:D:164:ILE:HG12	2.39	0.57
1:A:2:ASP:HA	1:D:7:SER:O	2.04	0.57
1:D:164:ILE:HD12	1:D:165:LEU:N	2.20	0.57
1:F:71:PHE:CZ	1:F:164:ILE:HG12	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LYS:HD2	1:F:202:GLU:CD	2.26	0.56
1:C:59:LYS:HD2	1:C:202:GLU:CD	2.26	0.56
1:C:253:LEU:O	1:D:232:LYS:NZ	2.39	0.56
1:B:184:ARG:C	1:F:14:SER:CB	2.74	0.56
1:A:59:LYS:HD2	1:A:202:GLU:CD	2.26	0.56
1:B:248:LEU:HD23	1:B:252:VAL:CG2	2.36	0.56
1:A:41:THR:O	1:A:219:THR:HG21	2.06	0.56
1:A:164:ILE:HD12	1:A:165:LEU:N	2.21	0.56
1:D:59:LYS:HD2	1:D:202:GLU:CD	2.26	0.56
1:B:164:ILE:HD12	1:B:165:LEU:N	2.21	0.56
1:F:164:ILE:HD12	1:F:165:LEU:N	2.20	0.55
1:B:244:ILE:O	1:B:245:ALA:C	2.45	0.55
1:A:3:ILE:O	1:D:6:PHE:HA	2.06	0.55
1:C:244:ILE:O	1:C:245:ALA:C	2.44	0.55
1:D:41:THR:O	1:D:219:THR:HG21	2.06	0.55
1:B:169:ASN:OD1	1:B:241:PRO:HG3	2.06	0.55
1:B:41:THR:O	1:B:219:THR:HG21	2.07	0.55
1:E:164:ILE:HD12	1:E:165:LEU:N	2.22	0.55
1:E:59:LYS:HD2	1:E:202:GLU:CD	2.26	0.55
1:B:59:LYS:HD2	1:B:202:GLU:CD	2.25	0.55
1:F:41:THR:O	1:F:219:THR:HG21	2.07	0.55
1:C:164:ILE:HD12	1:C:165:LEU:N	2.21	0.55
1:C:248:LEU:HD23	1:C:252:VAL:CG2	2.37	0.55
1:E:248:LEU:HD23	1:E:252:VAL:CG2	2.37	0.54
1:E:244:ILE:O	1:E:245:ALA:C	2.44	0.54
1:E:41:THR:O	1:E:219:THR:HG21	2.06	0.54
1:C:41:THR:O	1:C:219:THR:HG21	2.07	0.54
1:C:169:ASN:OD1	1:C:241:PRO:HG3	2.08	0.53
1:C:170:ALA:HB1	1:C:239:THR:HG21	1.91	0.53
1:C:200:LEU:HB3	1:C:201:PRO:CD	2.40	0.52
1:E:200:LEU:HB3	1:E:201:PRO:CD	2.40	0.52
1:F:178:SER:HA	1:F:188:TYR:O	2.10	0.52
1:A:200:LEU:HB3	1:A:201:PRO:CD	2.40	0.51
1:C:178:SER:HA	1:C:188:TYR:O	2.10	0.51
1:A:82:SER:O	1:A:218:TYR:HA	2.10	0.51
1:A:161:ASN:O	1:A:181:HIS:HD2	1.94	0.51
1:B:82:SER:O	1:B:218:TYR:HA	2.11	0.51
1:B:248:LEU:CD2	1:B:252:VAL:CG2	2.89	0.51
1:E:169:ASN:OD1	1:E:241:PRO:HG3	2.10	0.51
1:E:178:SER:HA	1:E:188:TYR:O	2.11	0.51
1:A:178:SER:HA	1:A:188:TYR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:SER:HA	1:D:188:TYR:O	2.11	0.51
1:D:200:LEU:HB3	1:D:201:PRO:CD	2.41	0.51
1:F:82:SER:O	1:F:218:TYR:HA	2.11	0.51
1:B:178:SER:HA	1:B:188:TYR:O	2.11	0.51
1:C:82:SER:O	1:C:218:TYR:HA	2.11	0.51
1:B:137:ARG:HD3	1:B:156:LEU:HB3	1.93	0.51
1:E:82:SER:O	1:E:218:TYR:HA	2.11	0.50
1:C:248:LEU:CD2	1:C:252:VAL:CG2	2.90	0.50
1:F:82:SER:HA	1:F:218:TYR:CE1	2.47	0.50
1:D:161:ASN:O	1:D:181:HIS:HD2	1.94	0.50
1:E:161:ASN:O	1:E:181:HIS:HD2	1.94	0.50
1:A:56:ILE:HD13	1:A:56:ILE:N	2.27	0.50
1:B:185:ARG:CD	1:F:14:SER:CB	2.90	0.50
1:D:71:PHE:HB2	1:D:226:SER:O	2.12	0.50
1:D:82:SER:O	1:D:218:TYR:HA	2.12	0.50
1:E:248:LEU:CD2	1:E:252:VAL:CG2	2.90	0.50
1:F:200:LEU:HB3	1:F:201:PRO:CD	2.41	0.50
1:B:82:SER:HA	1:B:218:TYR:CE1	2.47	0.50
1:B:200:LEU:HB3	1:B:201:PRO:CD	2.41	0.49
1:E:178:SER:HB3	1:E:189:ILE:HG23	1.93	0.49
1:E:71:PHE:HB2	1:E:226:SER:O	2.12	0.49
1:A:137:ARG:HD3	1:A:156:LEU:HB3	1.94	0.49
1:C:178:SER:HB3	1:C:189:ILE:HG23	1.93	0.49
1:D:178:SER:HB3	1:D:189:ILE:HG23	1.94	0.49
1:D:82:SER:HA	1:D:218:TYR:CE1	2.47	0.49
1:D:63:ALA:HB1	1:D:234:PRO:HG2	1.94	0.49
1:F:161:ASN:O	1:F:181:HIS:HD2	1.94	0.49
1:B:178:SER:HB3	1:B:189:ILE:HG23	1.94	0.49
1:C:63:ALA:HB1	1:C:234:PRO:HG2	1.95	0.49
1:F:71:PHE:HB2	1:F:226:SER:O	2.12	0.49
1:B:161:ASN:O	1:B:181:HIS:HD2	1.94	0.49
1:C:82:SER:HA	1:C:218:TYR:CE1	2.47	0.49
1:A:178:SER:HB3	1:A:189:ILE:HG23	1.93	0.49
1:A:82:SER:HA	1:A:218:TYR:CE1	2.47	0.49
1:B:63:ALA:HB1	1:B:234:PRO:HG2	1.94	0.49
1:C:161:ASN:O	1:C:181:HIS:HD2	1.95	0.49
1:F:137:ARG:HD3	1:F:156:LEU:HB3	1.94	0.49
1:A:71:PHE:HB2	1:A:226:SER:O	2.13	0.49
1:C:247:TYR:CD1	1:C:247:TYR:C	2.86	0.49
1:D:137:ARG:HD3	1:D:156:LEU:HB3	1.95	0.49
1:B:247:TYR:C	1:B:247:TYR:CD1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:PHE:HB2	1:C:226:SER:O	2.12	0.49
1:E:137:ARG:HD3	1:E:156:LEU:HB3	1.94	0.49
1:E:82:SER:HA	1:E:218:TYR:CE1	2.47	0.49
1:D:90:ALA:C	1:D:91:LEU:HD12	2.34	0.48
1:C:137:ARG:HD3	1:C:156:LEU:HB3	1.94	0.48
1:B:248:LEU:HD23	1:B:252:VAL:HG21	1.94	0.48
1:C:56:ILE:N	1:C:56:ILE:HD13	2.29	0.48
1:E:63:ALA:HB1	1:E:234:PRO:HG2	1.94	0.48
1:A:182:PRO:HA	1:B:174:LEU:HD22	1.96	0.48
1:D:56:ILE:HD13	1:D:56:ILE:N	2.28	0.48
1:E:90:ALA:C	1:E:91:LEU:HD12	2.34	0.48
1:F:178:SER:HB3	1:F:189:ILE:HG23	1.95	0.48
1:F:63:ALA:HB1	1:F:234:PRO:HG2	1.95	0.48
1:B:71:PHE:HB2	1:B:226:SER:O	2.13	0.48
1:C:90:ALA:C	1:C:91:LEU:HD12	2.34	0.48
1:B:56:ILE:HD13	1:B:56:ILE:N	2.29	0.48
1:F:101:ASN:HD22	1:F:101:ASN:C	2.18	0.48
1:E:247:TYR:C	1:E:247:TYR:CD1	2.86	0.48
1:F:90:ALA:C	1:F:91:LEU:HD12	2.35	0.47
1:A:63:ALA:HB1	1:A:234:PRO:HG2	1.94	0.47
1:F:56:ILE:N	1:F:56:ILE:HD13	2.28	0.47
1:C:101:ASN:C	1:C:101:ASN:HD22	2.18	0.47
1:E:56:ILE:N	1:E:56:ILE:HD13	2.28	0.47
1:A:90:ALA:C	1:A:91:LEU:HD12	2.34	0.47
1:B:170:ALA:HB1	1:B:239:THR:HG21	1.96	0.47
1:B:90:ALA:C	1:B:91:LEU:HD12	2.35	0.47
1:D:101:ASN:HD22	1:D:101:ASN:C	2.17	0.47
1:E:248:LEU:HD23	1:E:252:VAL:HG21	1.95	0.47
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.28	0.47
1:C:177:ALA:O	1:C:189:ILE:HA	2.15	0.47
1:D:177:ALA:O	1:D:189:ILE:HA	2.15	0.47
1:B:134:PRO:HD2	1:B:138:HIS:CE1	2.49	0.47
1:C:248:LEU:HD23	1:C:252:VAL:HG21	1.95	0.47
1:A:134:PRO:HD2	1:A:138:HIS:CE1	2.50	0.47
1:A:57:TYR:O	1:A:202:GLU:HG2	2.15	0.47
1:D:134:PRO:HD2	1:D:138:HIS:CE1	2.50	0.47
1:A:101:ASN:C	1:A:101:ASN:HD22	2.19	0.47
1:C:134:PRO:HD2	1:C:138:HIS:CE1	2.50	0.47
1:B:101:ASN:HD22	1:B:101:ASN:C	2.17	0.46
1:B:57:TYR:O	1:B:202:GLU:HG2	2.15	0.46
1:E:137:ARG:CG	1:E:137:ARG:HH11	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ALA:O	1:E:189:ILE:HA	2.16	0.46
1:B:7:SER:N	1:C:3:ILE:O	2.42	0.46
1:E:101:ASN:C	1:E:101:ASN:HD22	2.18	0.46
1:A:177:ALA:O	1:A:189:ILE:HA	2.15	0.46
1:A:193:ARG:HH22	1:F:52:SER:HB2	1.80	0.46
1:E:134:PRO:HD2	1:E:138:HIS:CE1	2.50	0.46
1:B:87:ILE:HG12	1:B:88:ALA:N	2.31	0.46
1:C:57:TYR:O	1:C:202:GLU:HG2	2.15	0.46
1:D:137:ARG:HH11	1:D:137:ARG:CG	2.29	0.46
1:E:181:HIS:HB2	1:E:186:THR:OG1	2.16	0.46
1:E:57:TYR:O	1:E:202:GLU:HG2	2.15	0.46
1:B:177:ALA:O	1:B:189:ILE:HA	2.15	0.46
1:F:47:ARG:CZ	1:F:98:PRO:HA	2.45	0.46
1:A:47:ARG:CZ	1:A:98:PRO:HA	2.46	0.45
1:A:165:LEU:HD22	1:B:244:ILE:HG21	1.98	0.45
1:D:181:HIS:HB2	1:D:186:THR:OG1	2.16	0.45
1:C:244:ILE:HA	1:C:247:TYR:HB3	1.98	0.45
1:E:149:ILE:HG13	1:E:192:GLU:HG2	1.98	0.45
1:F:134:PRO:HD2	1:F:138:HIS:CE1	2.50	0.45
1:F:181:HIS:HB2	1:F:186:THR:OG1	2.17	0.45
1:F:177:ALA:O	1:F:189:ILE:HA	2.15	0.45
1:C:47:ARG:CZ	1:C:98:PRO:HA	2.47	0.45
1:A:149:ILE:HG13	1:A:192:GLU:HG2	1.99	0.45
1:D:47:ARG:CZ	1:D:98:PRO:HA	2.46	0.45
1:B:181:HIS:HB2	1:B:186:THR:OG1	2.16	0.45
1:B:149:ILE:HG13	1:B:192:GLU:HG2	1.99	0.45
1:C:181:HIS:HB2	1:C:186:THR:OG1	2.16	0.45
1:C:192:GLU:OE2	1:D:185:ARG:CZ	2.65	0.45
1:E:47:ARG:CZ	1:E:98:PRO:HA	2.46	0.45
1:F:57:TYR:O	1:F:202:GLU:HG2	2.16	0.45
1:A:45:LEU:HD23	1:A:45:LEU:C	2.37	0.45
1:B:244:ILE:HA	1:B:247:TYR:HB3	1.98	0.45
1:C:149:ILE:HG13	1:C:192:GLU:HG2	1.99	0.45
1:A:181:HIS:HB2	1:A:186:THR:OG1	2.16	0.45
1:A:87:ILE:HG12	1:A:88:ALA:N	2.32	0.45
1:B:77:ALA:HB2	1:B:220:GLU:CB	2.47	0.45
1:C:45:LEU:C	1:C:45:LEU:HD23	2.38	0.45
1:D:57:TYR:O	1:D:202:GLU:HG2	2.15	0.45
1:B:47:ARG:CZ	1:B:98:PRO:HA	2.47	0.45
1:E:87:ILE:HG12	1:E:88:ALA:N	2.31	0.45
1:E:244:ILE:HA	1:E:247:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:HG12	1:C:88:ALA:N	2.32	0.44
1:F:77:ALA:HB2	1:F:220:GLU:CB	2.47	0.44
1:C:77:ALA:HB2	1:C:220:GLU:CB	2.47	0.44
1:F:45:LEU:C	1:F:45:LEU:HD23	2.37	0.44
1:D:101:ASN:C	1:D:101:ASN:ND2	2.71	0.44
1:C:174:LEU:HD22	1:D:182:PRO:HA	1.99	0.44
1:F:87:ILE:HG12	1:F:88:ALA:N	2.31	0.44
1:B:248:LEU:O	1:B:249:VAL:C	2.56	0.44
1:D:149:ILE:HG13	1:D:192:GLU:HG2	1.99	0.44
1:D:45:LEU:C	1:D:45:LEU:HD23	2.37	0.44
1:D:152:ALA:HB2	1:D:190:VAL:HG13	2.00	0.44
1:E:45:LEU:HD23	1:E:45:LEU:C	2.38	0.44
1:E:248:LEU:O	1:E:249:VAL:C	2.55	0.44
1:F:149:ILE:HG13	1:F:192:GLU:HG2	1.99	0.44
1:A:146:ILE:HG13	1:A:146:ILE:O	2.18	0.44
1:B:45:LEU:C	1:B:45:LEU:HD23	2.38	0.44
1:D:141:ILE:HD12	1:D:192:GLU:HB2	2.00	0.44
1:E:141:ILE:HD12	1:E:192:GLU:HB2	2.00	0.44
1:F:101:ASN:C	1:F:101:ASN:ND2	2.71	0.44
1:D:56:ILE:HD11	1:D:204:VAL:HG22	2.00	0.44
1:D:77:ALA:HB2	1:D:220:GLU:CB	2.48	0.44
1:B:101:ASN:ND2	1:B:101:ASN:C	2.71	0.44
1:F:111:ASP:OD1	1:F:111:ASP:N	2.47	0.44
1:D:146:ILE:O	1:D:146:ILE:HG13	2.18	0.43
1:C:101:ASN:C	1:C:101:ASN:ND2	2.71	0.43
1:D:2:ASP:C	1:D:3:ILE:HD12	2.39	0.43
1:A:141:ILE:HD12	1:A:192:GLU:HB2	2.00	0.43
1:A:77:ALA:HB2	1:A:220:GLU:CB	2.47	0.43
1:D:87:ILE:HG12	1:D:88:ALA:N	2.32	0.43
1:E:2:ASP:C	1:E:3:ILE:HD12	2.38	0.43
1:C:146:ILE:HG13	1:C:146:ILE:O	2.18	0.43
1:F:146:ILE:O	1:F:146:ILE:HG13	2.18	0.43
1:F:152:ALA:HB2	1:F:190:VAL:HG13	2.00	0.43
1:C:248:LEU:O	1:C:249:VAL:C	2.56	0.43
1:E:101:ASN:C	1:E:101:ASN:ND2	2.72	0.43
1:E:16:PHE:N	1:E:16:PHE:CD1	2.87	0.43
1:A:2:ASP:C	1:A:3:ILE:HD12	2.39	0.43
1:C:152:ALA:HB2	1:C:190:VAL:HG13	2.00	0.43
1:C:141:ILE:HD12	1:C:192:GLU:HB2	2.00	0.43
1:A:101:ASN:ND2	1:A:101:ASN:C	2.72	0.43
1:B:152:ALA:HB2	1:B:190:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:HB2	1:A:190:VAL:HG13	2.00	0.43
1:B:141:ILE:HD12	1:B:192:GLU:HB2	2.00	0.43
1:C:16:PHE:N	1:C:16:PHE:CD1	2.87	0.43
1:E:146:ILE:O	1:E:146:ILE:HG13	2.19	0.43
1:C:6:PHE:CD1	1:C:6:PHE:C	2.92	0.43
1:C:200:LEU:HB3	1:C:201:PRO:HD2	2.00	0.42
1:E:58:ASP:HB3	1:E:61:THR:OG1	2.19	0.42
1:F:16:PHE:CD1	1:F:16:PHE:N	2.87	0.42
1:B:146:ILE:HG13	1:B:146:ILE:O	2.18	0.42
1:B:228:SER:HB3	1:B:247:TYR:OH	2.20	0.42
1:E:152:ALA:HB2	1:E:190:VAL:HG13	2.00	0.42
1:F:200:LEU:HB3	1:F:201:PRO:HD2	2.02	0.42
1:A:52:SER:HB2	1:D:52:SER:CB	2.43	0.42
1:B:2:ASP:C	1:B:3:ILE:HD12	2.40	0.42
1:D:229:PHE:CD1	1:D:230:ALA:N	2.87	0.42
1:E:200:LEU:HB3	1:E:201:PRO:HD2	2.01	0.42
1:F:141:ILE:HD12	1:F:192:GLU:HB2	2.01	0.42
1:F:56:ILE:HD11	1:F:204:VAL:HG22	2.00	0.42
1:A:58:ASP:HB3	1:A:61:THR:OG1	2.20	0.42
1:B:52:SER:CB	1:C:52:SER:HB2	2.45	0.42
1:D:200:LEU:HB3	1:D:201:PRO:HD2	2.02	0.42
1:F:2:ASP:C	1:F:3:ILE:HD12	2.39	0.42
1:B:16:PHE:CD1	1:B:16:PHE:N	2.87	0.42
1:C:2:ASP:C	1:C:3:ILE:HD12	2.39	0.42
1:B:58:ASP:HB3	1:B:61:THR:OG1	2.19	0.42
1:C:170:ALA:CB	1:C:239:THR:HG21	2.50	0.42
1:D:16:PHE:N	1:D:16:PHE:CD1	2.87	0.42
1:C:56:ILE:HD11	1:C:204:VAL:HG22	2.02	0.42
1:F:58:ASP:HB3	1:F:61:THR:OG1	2.20	0.42
1:A:16:PHE:CD1	1:A:16:PHE:N	2.87	0.42
1:A:200:LEU:HB3	1:A:201:PRO:HD2	2.01	0.42
1:B:200:LEU:HB3	1:B:201:PRO:HD2	2.01	0.42
1:B:248:LEU:HD22	1:B:252:VAL:HG21	2.02	0.42
1:F:229:PHE:CD1	1:F:230:ALA:N	2.88	0.42
1:A:56:ILE:HD11	1:A:204:VAL:HG22	2.02	0.41
1:C:58:ASP:HB3	1:C:61:THR:OG1	2.20	0.41
1:A:229:PHE:CD1	1:A:230:ALA:N	2.88	0.41
1:B:229:PHE:CD1	1:B:230:ALA:N	2.88	0.41
1:B:52:SER:HB2	1:C:52:SER:CB	2.48	0.41
1:C:229:PHE:CD1	1:C:230:ALA:N	2.88	0.41
1:A:185:ARG:HD2	1:B:193:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ASP:OD1	1:D:111:ASP:N	2.48	0.41
1:E:229:PHE:CD1	1:E:230:ALA:N	2.88	0.41
1:E:56:ILE:HD11	1:E:204:VAL:HG22	2.02	0.41
1:E:6:PHE:CD1	1:E:6:PHE:C	2.94	0.41
1:B:64:VAL:O	1:B:239:THR:HG22	2.21	0.41
1:B:6:PHE:C	1:B:6:PHE:CD1	2.94	0.41
1:B:56:ILE:HD11	1:B:204:VAL:HG22	2.02	0.41
1:C:164:ILE:HA	1:C:178:SER:O	2.21	0.41
1:D:58:ASP:HB3	1:D:61:THR:OG1	2.20	0.41
1:C:248:LEU:HD23	1:C:252:VAL:HG23	2.03	0.41
1:E:192:GLU:OE2	1:F:185:ARG:NH1	2.54	0.40
1:E:84:ALA:HA	1:E:85:ASP:HA	1.83	0.40
1:C:137:ARG:HH11	1:C:137:ARG:CG	2.30	0.40
1:E:248:LEU:HD23	1:E:252:VAL:HG23	2.04	0.40
1:E:77:ALA:HB2	1:E:220:GLU:CB	2.48	0.40
1:F:6:PHE:C	1:F:6:PHE:CD1	2.94	0.40
1:A:6:PHE:CD1	1:A:6:PHE:C	2.94	0.40
1:B:248:LEU:HD23	1:B:252:VAL:HG23	2.02	0.40
1:D:6:PHE:C	1:D:6:PHE:CD1	2.95	0.40
1:B:100:SER:O	1:B:106:GLY:HA2	2.22	0.40
1:F:184:ARG:HB2	1:F:186:THR:HG23	2.04	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	218/253 (86%)	203 (93%)	12 (6%)	3 (1%)	11	38
1	B	236/253 (93%)	215 (91%)	18 (8%)	3 (1%)	12	40
1	C	236/253 (93%)	216 (92%)	17 (7%)	3 (1%)	12	40
1	D	218/253 (86%)	203 (93%)	12 (6%)	3 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	236/253 (93%)	216 (92%)	17 (7%)	3 (1%)	12	40
1	F	218/253 (86%)	203 (93%)	12 (6%)	3 (1%)	11	38
All	All	1362/1518 (90%)	1256 (92%)	88 (6%)	18 (1%)	12	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	B	94	VAL
1	C	94	VAL
1	D	94	VAL
1	E	94	VAL
1	F	94	VAL
1	A	40	PRO
1	B	40	PRO
1	C	40	PRO
1	D	40	PRO
1	E	40	PRO
1	F	40	PRO
1	A	96	SER
1	E	96	SER
1	F	96	SER
1	B	96	SER
1	C	96	SER
1	D	96	SER

### 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	181/216 (84%)	157 (87%)	24 (13%)	4	17
1	B	196/216 (91%)	167 (85%)	29 (15%)	3	13
1	C	196/216 (91%)	167 (85%)	29 (15%)	3	13
1	D	181/216 (84%)	157 (87%)	24 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	196/216 (91%)	167 (85%)	29 (15%)	3	13
1	F	181/216 (84%)	157 (87%)	24 (13%)	4	17
All	All	1131/1296 (87%)	972 (86%)	159 (14%)	3	16

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	43	SER
1	A	54	ILE
1	A	60	SER
1	A	81	SER
1	A	82	SER
1	A	85	ASP
1	A	101	ASN
1	A	135	THR
1	A	137	ARG
1	A	147	LYS
1	A	164	ILE
1	A	183	SER
1	A	184	ARG
1	A	189	ILE
1	A	190	VAL
1	A	191	SER
1	A	193	ARG
1	A	196	ILE
1	A	225	LEU
1	A	228	SER
1	A	231	SER
1	A	232	LYS
1	A	235	ASP
1	B	25	SER
1	B	43	SER
1	B	54	ILE
1	B	60	SER
1	B	81	SER
1	B	82	SER
1	B	85	ASP
1	B	101	ASN
1	B	135	THR
1	B	137	ARG

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Mol	Chain	Res	Type
1	B	147	LYS
1	B	164	ILE
1	B	183	SER
1	B	184	ARG
1	B	189	ILE
1	B	190	VAL
1	B	191	SER
1	B	193	ARG
1	B	196	ILE
1	B	225	LEU
1	B	228	SER
1	B	231	SER
1	B	232	LYS
1	B	235	ASP
1	B	236	ASP
1	B	237	SER
1	B	242	LEU
1	B	243	ASP
1	B	246	SER
1	C	25	SER
1	C	43	SER
1	C	54	ILE
1	C	60	SER
1	C	81	SER
1	C	82	SER
1	C	85	ASP
1	C	101	ASN
1	C	135	THR
1	C	137	ARG
1	C	147	LYS
1	C	164	ILE
1	C	183	SER
1	C	184	ARG
1	C	189	ILE
1	C	190	VAL
1	C	191	SER
1	C	193	ARG
1	C	196	ILE
1	C	225	LEU
1	C	228	SER
1	C	231	SER
1	C	232	LYS

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Mol	Chain	Res	Type
1	C	235	ASP
1	C	236	ASP
1	C	237	SER
1	C	242	LEU
1	C	243	ASP
1	C	246	SER
1	D	25	SER
1	D	43	SER
1	D	54	ILE
1	D	60	SER
1	D	81	SER
1	D	82	SER
1	D	85	ASP
1	D	101	ASN
1	D	135	THR
1	D	137	ARG
1	D	147	LYS
1	D	164	ILE
1	D	183	SER
1	D	184	ARG
1	D	189	ILE
1	D	190	VAL
1	D	191	SER
1	D	193	ARG
1	D	196	ILE
1	D	225	LEU
1	D	228	SER
1	D	231	SER
1	D	232	LYS
1	D	235	ASP
1	E	25	SER
1	E	43	SER
1	E	54	ILE
1	E	60	SER
1	E	81	SER
1	E	82	SER
1	E	85	ASP
1	E	101	ASN
1	E	135	THR
1	E	137	ARG
1	E	147	LYS
1	E	164	ILE

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Mol	Chain	Res	Type
1	E	183	SER
1	E	184	ARG
1	E	189	ILE
1	E	190	VAL
1	E	191	SER
1	E	193	ARG
1	E	196	ILE
1	E	225	LEU
1	E	228	SER
1	E	231	SER
1	E	232	LYS
1	E	235	ASP
1	E	236	ASP
1	E	237	SER
1	E	242	LEU
1	E	243	ASP
1	E	246	SER
1	F	25	SER
1	F	43	SER
1	F	54	ILE
1	F	60	SER
1	F	81	SER
1	F	82	SER
1	F	85	ASP
1	F	101	ASN
1	F	135	THR
1	F	137	ARG
1	F	147	LYS
1	F	164	ILE
1	F	183	SER
1	F	184	ARG
1	F	189	ILE
1	F	190	VAL
1	F	191	SER
1	F	193	ARG
1	F	196	ILE
1	F	225	LEU
1	F	228	SER
1	F	231	SER
1	F	232	LYS
1	F	235	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	101	ASN
1	A	115	ASN
1	A	161	ASN
1	A	181	HIS
1	A	222	HIS
1	B	55	GLN
1	B	101	ASN
1	B	115	ASN
1	B	161	ASN
1	B	181	HIS
1	B	222	HIS
1	C	55	GLN
1	C	101	ASN
1	C	115	ASN
1	C	161	ASN
1	C	181	HIS
1	C	222	HIS
1	D	55	GLN
1	D	101	ASN
1	D	115	ASN
1	D	161	ASN
1	D	181	HIS
1	D	222	HIS
1	E	55	GLN
1	E	101	ASN
1	E	115	ASN
1	E	161	ASN
1	E	181	HIS
1	E	222	HIS
1	F	55	GLN
1	F	101	ASN
1	F	115	ASN
1	F	161	ASN
1	F	181	HIS
1	F	222	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	228/253 (90%)	-0.38	4 (1%) 68 67	25, 49, 77, 99	0
1	B	246/253 (97%)	-0.36	2 (0%) 86 86	25, 50, 86, 100	0
1	C	246/253 (97%)	-0.29	5 (2%) 65 64	24, 51, 86, 100	0
1	D	228/253 (90%)	-0.40	0 100 100	25, 49, 77, 99	0
1	E	246/253 (97%)	-0.40	5 (2%) 65 64	24, 50, 87, 100	0
1	F	228/253 (90%)	-0.39	3 (1%) 77 77	23, 50, 78, 98	0
All	All	1422/1518 (93%)	-0.37	19 (1%) 77 77	23, 50, 83, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	240	GLU	3.2
1	C	36	GLY	3.0
1	C	239	THR	3.0
1	A	135	THR	3.0
1	F	37	ASN	2.9
1	A	1	ALA	2.8
1	E	238	THR	2.8
1	B	239	THR	2.7
1	B	236	ASP	2.6
1	E	241	PRO	2.5
1	C	135	THR	2.4
1	E	237	SER	2.3
1	A	26	SER	2.2
1	C	238	THR	2.2
1	C	37	ASN	2.1
1	A	36	GLY	2.1
1	E	239	THR	2.0
1	F	36	GLY	2.0
1	F	35	LYS	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 carbohydrates 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	302	1/1	0.92	0.10	45,45,45,45	0
2	MN	F	301	1/1	0.93	0.06	61,61,61,61	0
3	CA	C	302	1/1	0.94	0.07	45,45,45,45	0
2	MN	D	301	1/1	0.95	0.09	49,49,49,49	0
2	MN	A	301	1/1	0.96	0.11	56,56,56,56	0
3	CA	A	302	1/1	0.96	0.08	50,50,50,50	0
3	CA	D	302	1/1	0.96	0.11	50,50,50,50	0
3	CA	F	302	1/1	0.96	0.05	56,56,56,56	0
2	MN	B	301	1/1	0.97	0.08	49,49,49,49	0
2	MN	C	301	1/1	0.97	0.06	57,57,57,57	0
2	MN	E	301	1/1	0.97	0.10	49,49,49,49	0
3	CA	E	302	1/1	0.97	0.11	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.