



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:46 am GMT

PDB ID : 2R3Y  
Title : Crystal structure of the DegS protease in complex with the YWF activating peptide  
Authors : Clausen, T.; Hasselblatt, H.  
Deposited on : 2007-08-30  
Resolution : 2.50 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  
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

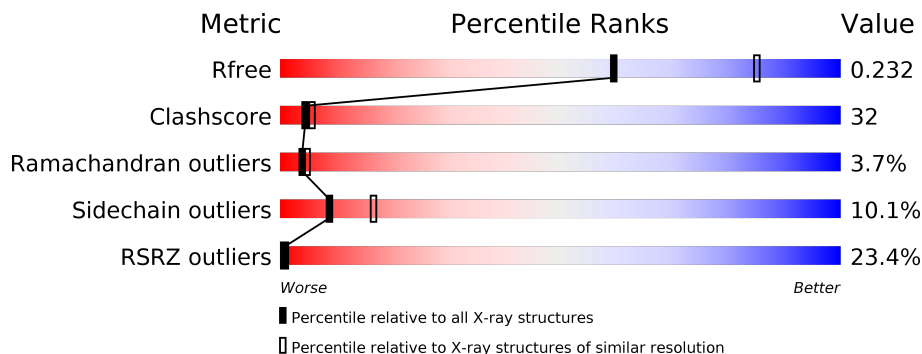
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	314	<div> <div>20%</div> <div>53%</div> <div>26%</div> <div>10%</div> <div>11%</div> </div>
1	B	314	<div> <div>20%</div> <div>49%</div> <div>32%</div> <div>6%</div> <div>13%</div> </div>
1	C	314	<div> <div>20%</div> <div>51%</div> <div>32%</div> <div>•</div> <div>12%</div> </div>
2	D	10	<div> <div>40%</div> <div>10%</div> <div>20%</div> <div>10%</div> <div>60%</div> </div>
2	E	10	<div> <div>30%</div> <div>40%</div> <div>60%</div> </div>
2	F	10	<div> <div>40%</div> <div>10%</div> <div>20%</div> <div>10%</div> <div>60%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6446 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 Protease degS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2080	1302	372	401	5			
1	B	274	Total	C	N	O	S	0	0	0
			2033	1277	361	390	5			
1	C	275	Total	C	N	O	S	0	0	0
			2041	1281	363	392	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	INITIATING METHIONINE	UNP P0AEE3
B	42	MET	-	INITIATING METHIONINE	UNP P0AEE3
C	42	MET	-	INITIATING METHIONINE	UNP P0AEE3

- Molecule 2 is a protein called Synthetic peptide YWF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			45	34	5	6			
2	E	4	Total	C	N	O	0	0	0
			45	34	5	6			
2	F	4	Total	C	N	O	0	0	0
			45	34	5	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	45	Total	O	0	0
			45	45		

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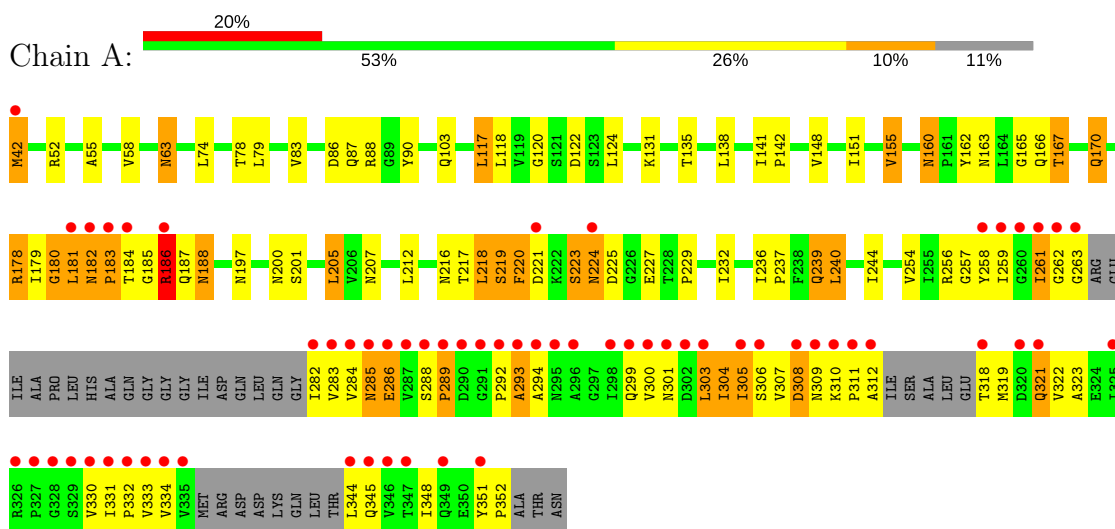
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	41	Total	O	0	0
			41	41		

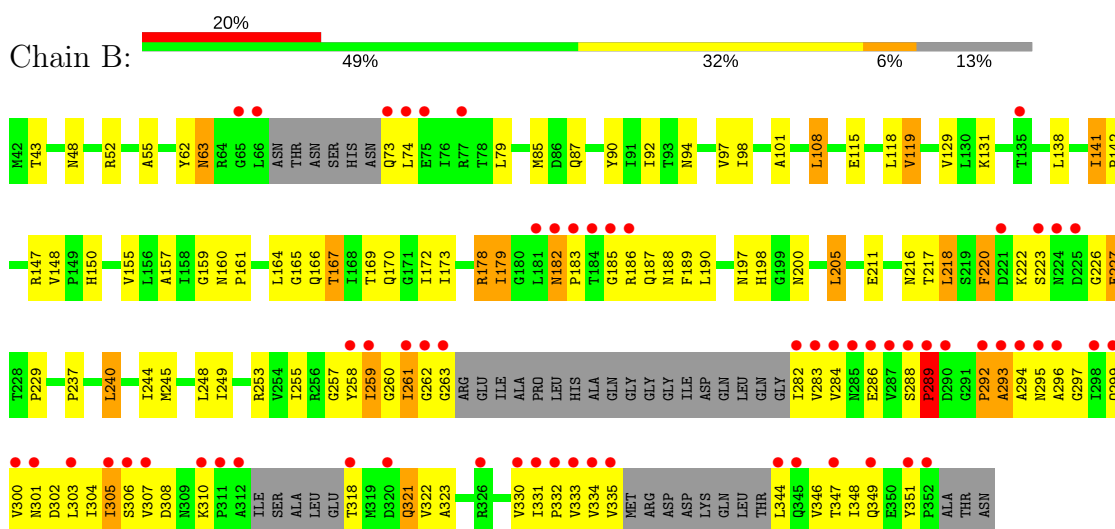
### 3 Residue-property plots

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: Protease degS

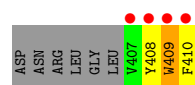


#### • Molecule 1: Protease degS



#### • Molecule 1: Protease degS





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.80Å 142.70Å 41.10Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 14.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (15.00-2.50) 95.0 (14.92-2.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.234 0.204 , 0.232	Depositor DCC
$R_{free}$ test set	1923 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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](#)

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	0/2106	0.72	1/2865 (0.0%)
1	B	0.35	0/2057	0.67	1/2796 (0.0%)
1	C	0.37	0/2065	0.67	0/2807
2	D	0.53	0/48	0.41	0/64
2	E	0.53	0/48	0.40	0/64
2	F	0.53	0/48	0.40	0/64
All	All	0.38	0/6372	0.68	2/8660 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	GLU	N-CA-C	-5.22	96.90	111.00
1	A	223	SER	N-CA-C	-5.02	97.46	111.00

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	2080	0	2118	145	0
1	B	2033	0	2080	126	0
1	C	2041	0	2086	141	0
2	D	45	0	36	9	0
2	E	45	0	36	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	45	0	36	9	0
3	A	71	0	0	7	0
3	B	45	0	0	2	0
3	C	41	0	0	4	0
All	All	6446	0	6392	401	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 32.

All (401) 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:A:305:ILE:HA	1:A:312:ALA:HB2	1.41	1.03
1:B:305:ILE:HG12	1:B:306:SER:H	1.24	1.02
1:C:223:SER:HB3	1:C:227:GLU:O	1.60	1.00
1:B:300:VAL:HG13	1:B:301:ASN:H	1.32	0.94
1:A:305:ILE:HG12	1:A:306:SER:H	1.34	0.92
1:C:300:VAL:HG13	1:C:301:ASN:H	1.31	0.91
1:A:300:VAL:HG13	1:A:301:ASN:H	1.34	0.90
1:A:141:ILE:HD13	1:A:212:LEU:HD13	1.52	0.90
1:C:63:ASN:C	1:C:63:ASN:HD22	1.76	0.89
1:C:65:GLY:HA3	1:C:77:ARG:HD2	1.53	0.89
1:B:257:GLY:H	1:B:323:ALA:HA	1.40	0.87
1:A:257:GLY:H	1:A:323:ALA:HA	1.40	0.86
1:B:141:ILE:HD13	1:B:142:PRO:HD2	1.59	0.85
1:B:147:ARG:HD2	1:B:211:GLU:OE2	1.75	0.85
1:C:197:ASN:H	1:C:200:ASN:HD22	1.20	0.84
1:B:330:VAL:HG22	1:B:347:THR:HG22	1.60	0.83
1:B:63:ASN:HD22	1:B:63:ASN:C	1.82	0.83
1:B:307:VAL:HG12	1:B:331:ILE:HD11	1.62	0.79
1:C:303:LEU:H	1:C:303:LEU:HD23	1.47	0.79
1:B:305:ILE:HG12	1:B:306:SER:N	1.98	0.79
1:A:155:VAL:HG13	1:A:205:LEU:HD21	1.64	0.79
1:A:182:ASN:H	1:A:183:PRO:HD2	1.47	0.78
1:C:64:ARG:HD3	1:C:105:ILE:HD13	1.65	0.77
1:B:187:GLN:HG3	1:B:188:ASN:H	1.48	0.77
1:C:348:ILE:HD12	1:C:348:ILE:H	1.49	0.77
1:C:239:GLN:HB2	3:C:358:HOH:O	1.84	0.77
1:A:220:PHE:HD1	1:A:229:PRO:HG2	1.50	0.77
1:A:258:TYR:HB2	1:A:351:TYR:HA	1.67	0.77
1:A:141:ILE:CD1	1:A:212:LEU:HD13	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:C	1:A:63:ASN:HD22	1.88	0.76
1:C:178:ARG:O	1:C:188:ASN:HA	1.86	0.75
1:B:305:ILE:HD13	1:B:305:ILE:H	1.51	0.75
1:C:63:ASN:ND2	1:C:77:ARG:HD3	2.02	0.74
1:C:308:ASP:HB2	1:C:331:ILE:HG13	1.68	0.74
1:B:197:ASN:H	1:B:200:ASN:HD22	1.33	0.74
1:A:308:ASP:HB2	1:A:331:ILE:HD11	1.69	0.74
1:A:305:ILE:HD13	1:A:305:ILE:H	1.54	0.72
1:B:286:GLU:HB3	1:B:288:SER:O	1.90	0.71
1:A:310:LYS:HG3	1:A:311:PRO:HD2	1.72	0.71
1:C:293:ALA:HB2	1:C:349:GLN:OE1	1.89	0.71
1:C:296:ALA:HB3	1:C:346:VAL:HG13	1.73	0.71
1:A:257:GLY:N	1:A:323:ALA:HA	2.06	0.70
1:A:155:VAL:CG1	1:A:205:LEU:HD21	2.21	0.70
1:C:186:ARG:HB2	2:F:409:TRP:HE1	1.57	0.70
1:B:263:GLY:HA2	2:E:407:VAL:HA	1.74	0.69
1:A:160:ASN:ND2	1:A:165:GLY:H	1.90	0.69
1:A:167:THR:HG22	1:B:178:ARG:NH2	2.08	0.69
1:B:283:VAL:HG12	1:B:284:VAL:H	1.58	0.69
1:A:155:VAL:HG13	1:A:205:LEU:CD2	2.22	0.68
1:C:63:ASN:HD21	1:C:77:ARG:HD3	1.58	0.68
1:A:308:ASP:HB2	1:A:331:ILE:CD1	2.24	0.68
1:B:257:GLY:N	1:B:323:ALA:HA	2.08	0.68
1:C:177:GLY:HA2	1:C:188:ASN:HB2	1.76	0.68
1:B:161:PRO:HD2	1:B:167:THR:HG23	1.74	0.68
1:C:197:ASN:H	1:C:200:ASN:ND2	1.92	0.68
1:C:298:ILE:HG23	1:C:333:VAL:HG21	1.77	0.67
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.59	0.67
1:A:300:VAL:HG22	1:A:301:ASN:ND2	2.09	0.67
1:B:155:VAL:HB	1:B:205:LEU:HD22	1.76	0.67
1:C:334:VAL:HG12	1:C:335:VAL:HG23	1.77	0.67
1:C:305:ILE:N	1:C:305:ILE:HD13	2.09	0.67
1:A:160:ASN:HD21	1:A:165:GLY:H	1.39	0.67
1:A:167:THR:HG22	1:B:178:ARG:HH21	1.60	0.67
1:B:141:ILE:HD13	1:B:142:PRO:CD	2.24	0.66
1:A:257:GLY:H	1:A:323:ALA:CA	2.08	0.66
1:B:293:ALA:HB2	1:B:349:GLN:OE1	1.94	0.66
1:C:307:VAL:HG12	1:C:331:ILE:HD11	1.78	0.66
1:A:300:VAL:HG13	1:A:301:ASN:N	2.10	0.66
1:B:303:LEU:H	1:B:303:LEU:HD23	1.61	0.66
1:C:296:ALA:HB1	1:C:346:VAL:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG12	1:B:284:VAL:N	2.12	0.65
1:B:288:SER:O	1:B:289:PRO:O	2.14	0.65
1:C:286:GLU:HB3	1:C:288:SER:O	1.96	0.65
1:C:304:ILE:HG13	1:C:334:VAL:O	1.97	0.65
1:A:303:LEU:H	1:A:303:LEU:HD23	1.61	0.65
1:A:178:ARG:NH2	1:C:167:THR:HG22	2.11	0.65
1:A:184:THR:HG23	1:A:186:ARG:HD3	1.77	0.65
1:A:223:SER:O	1:A:225:ASP:N	2.30	0.65
1:A:185:GLY:O	1:A:187:GLN:N	2.31	0.64
1:A:307:VAL:HG13	1:A:333:VAL:HG12	1.77	0.64
1:B:308:ASP:HB2	1:B:331:ILE:CD1	2.27	0.64
1:C:98:ILE:HD11	1:C:128:ALA:HB1	1.79	0.64
1:B:223:SER:HB3	1:B:227:GLU:OE2	1.98	0.64
1:B:262:GLY:O	1:B:286:GLU:HG2	1.98	0.64
1:C:147:ARG:HD2	1:C:211:GLU:OE2	1.98	0.63
1:B:197:ASN:H	1:B:200:ASN:ND2	1.96	0.63
1:B:63:ASN:HD21	1:B:101:ALA:HA	1.64	0.63
1:A:263:GLY:C	2:D:408:TYR:H	2.01	0.62
1:B:205:LEU:HG	1:B:216:ASN:HD21	1.64	0.62
1:B:305:ILE:N	1:B:305:ILE:HD13	2.13	0.62
1:C:186:ARG:H	2:F:409:TRP:HZ2	1.48	0.62
1:A:306:SER:HA	1:A:310:LYS:O	1.99	0.62
1:B:63:ASN:ND2	1:B:63:ASN:C	2.53	0.62
1:A:261:ILE:HD13	1:A:261:ILE:H	1.65	0.62
1:A:305:ILE:HD13	1:A:305:ILE:N	2.13	0.62
1:C:305:ILE:HG12	1:C:306:SER:H	1.65	0.62
1:C:250:ARG:HH11	1:C:250:ARG:HG2	1.64	0.61
1:A:318:THR:O	1:A:321:GLN:HB2	2.01	0.61
1:B:305:ILE:CG1	1:B:306:SER:H	2.07	0.61
1:A:118:LEU:C	1:A:118:LEU:HD23	2.19	0.61
1:A:254:VAL:HG12	3:A:385:HOH:O	2.00	0.61
1:C:305:ILE:HA	1:C:312:ALA:HB3	1.83	0.61
1:A:87:GLN:HE21	1:A:138:LEU:H	1.49	0.61
1:B:257:GLY:H	1:B:323:ALA:CA	2.13	0.61
1:C:259:ILE:HG22	1:C:260:GLY:N	2.16	0.61
1:A:217:THR:O	1:A:218:LEU:HD13	2.01	0.60
1:C:53:ARG:HG2	1:C:53:ARG:HH11	1.66	0.60
1:B:222:LYS:HG3	1:B:227:GLU:O	2.00	0.60
1:C:155:VAL:HB	1:C:205:LEU:CD2	2.31	0.60
1:C:64:ARG:HH21	1:C:74:LEU:HB3	1.66	0.60
1:B:178:ARG:O	1:B:189:PHE:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:C	1:A:221:ASP:H	2.04	0.60
1:C:155:VAL:HG11	1:C:173:ILE:HD11	1.83	0.60
1:A:322:VAL:HG21	2:D:410:PHE:HD2	1.67	0.60
1:C:181:LEU:HD23	1:C:182:ASN:H	1.66	0.59
1:C:329:SER:O	1:C:347:THR:HA	2.02	0.59
1:A:304:ILE:HG13	1:A:334:VAL:O	2.03	0.59
1:C:300:VAL:HG22	1:C:301:ASN:ND2	2.18	0.59
1:B:55:ALA:HB1	1:B:166:GLN:NE2	2.18	0.59
1:B:259:ILE:O	1:B:293:ALA:HB3	2.02	0.59
1:C:63:ASN:C	1:C:63:ASN:ND2	2.50	0.59
1:A:182:ASN:N	1:A:183:PRO:HD2	2.17	0.59
1:B:261:ILE:HD13	1:B:261:ILE:N	2.18	0.59
1:C:262:GLY:C	1:C:286:GLU:HG2	2.23	0.59
1:B:296:ALA:HB3	1:B:346:VAL:HG13	1.85	0.59
1:A:305:ILE:HG12	1:A:306:SER:N	2.11	0.59
1:B:87:GLN:HE22	1:B:138:LEU:H	1.50	0.59
1:C:346:VAL:HG12	1:C:347:THR:N	2.17	0.59
1:A:197:ASN:H	1:A:200:ASN:HD22	1.52	0.58
1:B:129:VAL:HG23	1:B:248:LEU:HD12	1.86	0.58
1:A:261:ILE:HD13	1:A:261:ILE:N	2.19	0.58
1:A:220:PHE:CD1	1:A:229:PRO:HG2	2.34	0.58
1:A:307:VAL:HG12	1:A:331:ILE:CD1	2.33	0.58
1:C:65:GLY:CA	1:C:77:ARG:HD2	2.28	0.58
1:B:240:LEU:O	1:B:240:LEU:HD22	2.04	0.58
1:B:292:PRO:O	1:B:294:ALA:N	2.36	0.58
1:B:304:ILE:HG12	1:B:305:ILE:N	2.19	0.57
1:B:296:ALA:CB	1:B:346:VAL:HG13	2.34	0.57
1:B:348:ILE:HD12	1:B:348:ILE:N	2.18	0.57
1:B:94:ASN:HB2	1:B:97:VAL:HG23	1.86	0.57
1:C:261:ILE:N	1:C:261:ILE:HD13	2.19	0.57
1:A:305:ILE:HD11	1:A:334:VAL:HG12	1.85	0.57
1:C:300:VAL:HG13	1:C:301:ASN:N	2.10	0.57
1:A:223:SER:HB2	1:A:229:PRO:HD3	1.87	0.57
1:C:178:ARG:HG3	1:C:178:ARG:HH11	1.69	0.57
1:A:282:ILE:HG22	1:A:283:VAL:N	2.19	0.57
1:B:160:ASN:ND2	1:B:165:GLY:H	2.03	0.57
1:A:184:THR:CG2	1:A:186:ARG:HD3	2.35	0.57
1:C:179:ILE:HG22	1:C:179:ILE:O	2.04	0.57
1:A:257:GLY:O	1:A:322:VAL:HG12	2.05	0.56
1:B:262:GLY:HA2	2:E:408:TYR:O	2.05	0.56
1:C:205:LEU:HG	1:C:216:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HA	3:A:368:HOH:O	2.05	0.56
1:A:286:GLU:HB3	1:A:288:SER:O	2.06	0.56
1:A:319:MET:HA	2:D:410:PHE:CZ	2.40	0.56
1:A:348:ILE:N	1:A:348:ILE:HD12	2.21	0.56
1:B:296:ALA:HB3	1:B:346:VAL:HG22	1.86	0.56
1:C:262:GLY:O	1:C:286:GLU:HG2	2.06	0.56
1:C:147:ARG:CD	1:C:211:GLU:OE2	2.54	0.55
1:B:304:ILE:HG12	1:B:305:ILE:H	1.70	0.55
1:A:259:ILE:HG13	1:A:322:VAL:HG13	1.88	0.55
1:B:308:ASP:HB2	1:B:331:ILE:HD11	1.88	0.55
1:C:103:GLN:CD	1:C:105:ILE:HD11	2.27	0.55
1:C:155:VAL:HB	1:C:205:LEU:HD22	1.87	0.55
1:C:307:VAL:HG13	1:C:333:VAL:HG12	1.88	0.55
1:C:296:ALA:CB	1:C:346:VAL:HG13	2.37	0.54
1:C:263:GLY:N	2:F:408:TYR:HB2	2.23	0.54
1:A:303:LEU:O	1:A:304:ILE:HB	2.07	0.54
1:B:300:VAL:HG13	1:B:301:ASN:N	2.12	0.54
1:C:348:ILE:N	1:C:348:ILE:HD12	2.19	0.54
1:C:160:ASN:HD21	1:C:163:ASN:HD22	1.56	0.54
1:B:334:VAL:HG12	1:B:335:VAL:HG23	1.89	0.53
1:A:283:VAL:HG12	1:A:284:VAL:N	2.24	0.53
1:A:118:LEU:HD23	1:A:120:GLY:N	2.24	0.53
1:A:322:VAL:HG21	2:D:410:PHE:CD2	2.43	0.53
1:B:260:GLY:O	1:B:261:ILE:HG23	2.09	0.53
1:B:318:THR:HG22	2:E:410:PHE:HE2	1.73	0.53
1:A:188:ASN:HD22	1:A:188:ASN:N	2.07	0.53
1:B:260:GLY:H	1:B:261:ILE:HD13	1.72	0.53
1:B:150:HIS:HD2	3:B:360:HOH:O	1.91	0.53
1:C:305:ILE:O	1:C:312:ALA:HB2	2.09	0.53
1:B:164:LEU:HD21	1:C:220:PHE:CE2	2.44	0.53
1:A:83:VAL:CG1	1:A:141:ILE:HD12	2.39	0.52
1:C:223:SER:CB	1:C:227:GLU:O	2.47	0.52
1:C:259:ILE:O	1:C:293:ALA:HB3	2.09	0.52
1:C:296:ALA:CB	1:C:346:VAL:HA	2.38	0.52
1:A:117:LEU:HD22	1:A:118:LEU:N	2.24	0.52
1:C:308:ASP:HB2	1:C:331:ILE:CG1	2.38	0.52
1:C:178:ARG:HG3	1:C:178:ARG:NH1	2.24	0.52
1:A:282:ILE:HG22	1:A:283:VAL:H	1.75	0.52
1:A:307:VAL:HG12	1:A:331:ILE:HD11	1.90	0.52
1:B:170:GLN:HG2	1:C:172:ILE:HG23	1.90	0.52
1:B:159:GLY:C	1:B:161:PRO:HD3	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ILE:HG22	1:B:283:VAL:N	2.25	0.52
1:B:79:LEU:N	1:B:79:LEU:HD22	2.25	0.52
1:B:173:ILE:HG23	1:B:190:LEU:HD21	1.92	0.51
1:B:260:GLY:HA3	1:B:294:ALA:HB2	1.92	0.51
1:A:122:ASP:OD1	1:A:254:VAL:HG11	2.10	0.51
1:B:198:HIS:HB2	3:C:395:HOH:O	2.09	0.51
1:B:157:ALA:HB3	1:B:169:THR:OG1	2.10	0.51
1:C:254:VAL:HG11	1:C:256:ARG:CZ	2.40	0.51
1:A:87:GLN:NE2	1:A:138:LEU:H	2.08	0.51
1:C:161:PRO:HD2	1:C:167:THR:HG23	1.93	0.51
1:B:303:LEU:H	1:B:303:LEU:CD2	2.23	0.51
1:B:160:ASN:HD21	1:B:165:GLY:H	1.58	0.50
1:C:125:THR:HA	1:C:187:GLN:HE21	1.75	0.50
1:A:74:LEU:HD13	1:A:103:GLN:OE1	2.10	0.50
1:B:55:ALA:HB1	1:B:166:GLN:HE22	1.75	0.50
1:C:177:GLY:HA2	1:C:188:ASN:HD22	1.76	0.50
1:C:303:LEU:O	1:C:335:VAL:HG12	2.10	0.50
1:A:330:VAL:CG1	1:A:345:GLN:HB3	2.42	0.50
1:C:250:ARG:HG2	1:C:250:ARG:NH1	2.27	0.50
1:A:184:THR:HG23	1:A:186:ARG:HH11	1.77	0.50
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.77	0.50
1:B:332:PRO:HA	1:B:344:LEU:O	2.12	0.50
1:C:238:PHE:CZ	1:C:239:GLN:NE2	2.79	0.50
1:B:260:GLY:C	1:B:261:ILE:HD13	2.33	0.50
1:B:73:GLN:HG2	1:B:74:LEU:N	2.27	0.50
1:A:283:VAL:HA	1:A:303:LEU:HA	1.94	0.49
1:A:292:PRO:O	1:A:294:ALA:N	2.45	0.49
1:A:305:ILE:CA	1:A:312:ALA:HB2	2.28	0.49
1:C:258:TYR:HD1	2:F:410:PHE:OXT	1.94	0.49
1:A:185:GLY:HA2	2:D:409:TRP:HH2	1.77	0.49
1:A:259:ILE:HG13	1:A:322:VAL:CG1	2.41	0.49
1:B:308:ASP:HB2	1:B:331:ILE:HG13	1.94	0.49
1:C:296:ALA:HB3	1:C:346:VAL:HG22	1.94	0.49
1:A:90:TYR:CE2	1:A:131:LYS:HD2	2.47	0.49
1:C:143:ILE:HD11	3:C:387:HOH:O	2.12	0.49
1:C:261:ILE:HD13	1:C:261:ILE:H	1.76	0.49
1:C:307:VAL:HG12	1:C:331:ILE:CD1	2.41	0.49
1:A:178:ARG:HH21	1:C:167:THR:HG22	1.74	0.49
1:C:53:ARG:HG2	1:C:53:ARG:NH1	2.28	0.49
1:B:165:GLY:C	1:C:178:ARG:NH2	2.66	0.49
1:C:298:ILE:HG23	1:C:333:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:CG1	1:A:301:ASN:H	2.17	0.49
1:A:303:LEU:H	1:A:303:LEU:CD2	2.26	0.49
1:B:63:ASN:ND2	1:B:101:ALA:HA	2.27	0.49
1:C:90:TYR:CE2	1:C:131:LYS:HD2	2.47	0.49
1:A:223:SER:HB3	1:A:227:GLU:O	2.12	0.48
1:A:333:VAL:O	1:A:344:LEU:HB3	2.13	0.48
1:C:305:ILE:HA	1:C:312:ALA:CB	2.42	0.48
1:C:186:ARG:CB	2:F:409:TRP:HE1	2.24	0.48
1:A:258:TYR:HD1	2:D:410:PHE:OXT	1.97	0.48
1:C:98:ILE:HD11	1:C:128:ALA:CB	2.43	0.48
1:A:86:ASP:OD2	1:A:88:ARG:HB2	2.14	0.48
1:B:90:TYR:CE2	1:B:131:LYS:HD3	2.49	0.48
1:A:88:ARG:O	1:A:131:LYS:NZ	2.47	0.48
1:B:119:VAL:HG13	1:B:129:VAL:O	2.14	0.48
1:B:245:MET:HG2	1:B:249:ILE:HD13	1.94	0.48
1:A:148:VAL:HG12	3:A:416:HOH:O	2.14	0.47
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.72	0.47
1:C:223:SER:HB2	1:C:227:GLU:CD	2.34	0.47
1:A:300:VAL:C	1:A:301:ASN:HD22	2.18	0.47
1:C:300:VAL:C	1:C:301:ASN:HD22	2.18	0.47
1:A:179:ILE:HG12	3:A:417:HOH:O	2.14	0.47
1:A:205:LEU:HG	1:A:216:ASN:HD21	1.79	0.47
1:A:220:PHE:HB2	1:A:232:ILE:HG22	1.96	0.47
1:A:319:MET:SD	2:D:409:TRP:HD1	2.38	0.47
1:B:253:ARG:CZ	1:B:255:ILE:HD11	2.44	0.47
1:C:92:ILE:HG22	1:C:93:THR:N	2.30	0.47
1:C:155:VAL:HG11	1:C:173:ILE:CD1	2.45	0.47
1:A:258:TYR:CD2	1:A:352:PRO:HD3	2.50	0.47
1:B:147:ARG:CD	1:B:211:GLU:OE2	2.57	0.47
1:B:333:VAL:O	1:B:344:LEU:HD22	2.14	0.47
1:C:348:ILE:CD1	1:C:348:ILE:H	2.22	0.47
1:A:254:VAL:HG13	1:A:254:VAL:O	2.14	0.47
1:A:307:VAL:O	1:A:308:ASP:HB3	2.15	0.47
1:C:129:VAL:HG23	1:C:248:LEU:HD12	1.96	0.47
1:B:303:LEU:HD23	1:B:303:LEU:N	2.30	0.47
1:C:306:SER:HA	1:C:310:LYS:O	2.14	0.47
1:C:186:ARG:HG3	1:C:319:MET:HG2	1.96	0.47
1:A:348:ILE:H	1:A:348:ILE:HD12	1.79	0.46
1:C:112:ARG:HB3	1:C:114:PHE:CE1	2.50	0.46
1:A:182:ASN:H	1:A:183:PRO:CD	2.21	0.46
1:B:108:LEU:HD23	1:B:108:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:VAL:HB	1:B:302:ASP:O	2.15	0.46
1:B:240:LEU:O	1:B:244:ILE:HG12	2.15	0.46
1:C:134:ALA:CB	1:C:138:LEU:HD21	2.45	0.46
1:A:292:PRO:C	1:A:294:ALA:H	2.19	0.46
1:A:179:ILE:HG23	1:A:184:THR:O	2.15	0.46
1:C:59:VAL:CG1	1:C:108:LEU:HD22	2.46	0.46
1:C:304:ILE:HG12	1:C:305:ILE:N	2.31	0.46
1:C:49:LEU:HB3	3:C:364:HOH:O	2.16	0.46
1:A:63:ASN:C	1:A:63:ASN:ND2	2.62	0.45
1:B:220:PHE:O	1:B:229:PRO:HG2	2.16	0.45
1:A:219:SER:C	1:A:221:ASP:N	2.69	0.45
1:A:79:LEU:C	1:A:79:LEU:HD12	2.36	0.45
1:B:306:SER:HA	1:B:310:LYS:O	2.16	0.45
1:B:94:ASN:OD1	1:B:217:THR:HA	2.16	0.45
1:B:258:TYR:HB2	1:B:351:TYR:HA	1.98	0.45
1:A:207:ASN:HB2	3:A:358:HOH:O	2.16	0.45
1:C:259:ILE:HG13	1:C:322:VAL:HG11	1.99	0.45
1:B:305:ILE:N	1:B:305:ILE:CD1	2.79	0.45
1:B:321:GLN:N	1:B:321:GLN:OE1	2.50	0.45
1:B:170:GLN:HG2	1:C:172:ILE:CG2	2.46	0.45
2:D:408:TYR:HB3	2:D:410:PHE:CE1	2.52	0.45
1:A:124:LEU:HD12	1:A:256:ARG:CZ	2.47	0.45
1:A:188:ASN:O	1:A:188:ASN:ND2	2.49	0.45
1:A:240:LEU:HD22	1:A:244:ILE:HG12	1.99	0.45
1:C:259:ILE:HG13	1:C:322:VAL:CG1	2.46	0.45
1:A:117:LEU:HD22	1:A:118:LEU:H	1.82	0.45
1:C:134:ALA:HB3	1:C:138:LEU:HD21	1.98	0.45
1:C:186:ARG:HD3	1:C:320:ASP:OD1	2.17	0.45
1:B:48:ASN:O	1:B:52:ARG:HG3	2.17	0.45
1:C:251:ASP:C	1:C:253:ARG:H	2.20	0.44
1:C:331:ILE:O	1:C:331:ILE:HG23	2.17	0.44
1:A:165:GLY:O	1:B:178:ARG:NH2	2.50	0.44
1:B:308:ASP:HB2	1:B:331:ILE:CG1	2.47	0.44
1:A:303:LEU:HG	1:A:304:ILE:N	2.32	0.44
1:A:307:VAL:O	1:A:308:ASP:CB	2.65	0.44
1:A:83:VAL:HG11	1:A:141:ILE:HD12	2.00	0.44
1:C:236:ILE:CG2	1:C:240:LEU:HD12	2.47	0.44
1:A:239:GLN:HA	1:A:239:GLN:NE2	2.29	0.44
1:C:263:GLY:CA	2:F:408:TYR:HB2	2.48	0.44
1:C:47:TYR:HB3	1:C:156:LEU:HD11	1.99	0.44
1:C:263:GLY:H	2:F:408:TYR:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:CG1	1:C:306:SER:H	2.31	0.44
1:B:217:THR:HG23	1:B:218:LEU:N	2.32	0.44
1:C:303:LEU:HD23	1:C:303:LEU:N	2.24	0.44
1:C:305:ILE:HD13	1:C:305:ILE:H	1.82	0.44
1:C:253:ARG:HG2	1:C:254:VAL:N	2.33	0.44
1:A:151:ILE:HG21	1:C:168:ILE:HD13	2.00	0.43
1:A:284:VAL:O	1:A:285:ASN:HB3	2.18	0.43
1:B:161:PRO:HG3	1:B:200:ASN:ND2	2.33	0.43
1:B:62:TYR:CE2	1:B:79:LEU:HD12	2.53	0.43
1:C:346:VAL:CG1	1:C:347:THR:N	2.81	0.43
1:A:42:MET:N	1:A:42:MET:SD	2.92	0.43
1:A:141:ILE:HA	1:A:142:PRO:HD3	1.89	0.43
1:B:253:ARG:CZ	1:B:255:ILE:CD1	2.96	0.43
1:B:292:PRO:O	1:B:295:ASN:ND2	2.51	0.43
1:A:319:MET:SD	2:D:409:TRP:CD1	3.12	0.43
1:C:132:ILE:O	1:C:132:ILE:HG13	2.19	0.43
1:A:182:ASN:N	1:A:183:PRO:CD	2.80	0.43
1:A:220:PHE:O	1:A:220:PHE:CD1	2.72	0.43
1:B:187:GLN:HG3	1:B:188:ASN:N	2.24	0.43
1:A:305:ILE:HD11	1:A:334:VAL:CG1	2.47	0.43
1:C:325:ILE:HD13	1:C:331:ILE:HD12	2.01	0.43
1:B:220:PHE:HD2	1:B:229:PRO:HG3	1.83	0.43
1:B:85:MET:HG3	1:B:245:MET:SD	2.59	0.43
1:A:55:ALA:HB1	1:A:166:GLN:NE2	2.34	0.42
1:A:170:GLN:HG2	1:B:172:ILE:HG23	2.01	0.42
1:C:319:MET:HE1	2:F:410:PHE:HA	2.01	0.42
1:C:326:ARG:HA	1:C:327:PRO:HD3	1.88	0.42
1:B:240:LEU:HD22	1:B:244:ILE:HG12	2.00	0.42
1:A:83:VAL:HG13	1:A:141:ILE:HD12	2.02	0.42
1:B:189:PHE:CE1	1:B:217:THR:HG21	2.54	0.42
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.88	0.42
1:B:304:ILE:HG13	1:B:334:VAL:O	2.19	0.42
1:B:307:VAL:HG12	1:B:331:ILE:CD1	2.41	0.42
1:B:85:MET:SD	1:B:92:ILE:HD12	2.60	0.42
1:C:141:ILE:O	1:C:141:ILE:HG23	2.18	0.42
1:A:118:LEU:C	1:A:118:LEU:CD2	2.88	0.42
1:A:262:GLY:C	1:A:286:GLU:HG2	2.40	0.42
1:B:188:ASN:ND2	1:B:237:PRO:HG2	2.35	0.42
1:B:283:VAL:CG1	1:B:284:VAL:H	2.29	0.42
1:B:300:VAL:CG1	1:B:301:ASN:H	2.14	0.42
1:A:259:ILE:O	1:A:293:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HA	1:C:127:LEU:HD23	1.93	0.42
1:C:333:VAL:CG2	1:C:346:VAL:HG23	2.49	0.42
1:C:322:VAL:HG21	2:F:410:PHE:HD2	1.84	0.42
1:A:219:SER:O	1:A:221:ASP:N	2.49	0.42
1:A:307:VAL:HG12	1:A:331:ILE:HD13	2.01	0.42
1:A:258:TYR:CB	1:A:351:TYR:HA	2.42	0.42
1:B:348:ILE:HD12	1:B:348:ILE:H	1.85	0.42
1:B:165:GLY:CA	1:C:178:ARG:NH2	2.83	0.41
1:A:87:GLN:HG3	3:A:415:HOH:O	2.20	0.41
1:B:257:GLY:HA3	1:B:322:VAL:O	2.21	0.41
1:C:300:VAL:CG1	1:C:301:ASN:H	2.14	0.41
1:C:331:ILE:HB	1:C:348:ILE:HD11	2.01	0.41
1:A:331:ILE:CG2	1:A:348:ILE:HD11	2.51	0.41
1:C:248:LEU:CD2	1:C:253:ARG:HA	2.49	0.41
1:C:59:VAL:HG12	1:C:108:LEU:HD22	2.02	0.41
1:A:223:SER:C	1:A:225:ASP:H	2.23	0.41
1:C:98:ILE:HD12	1:C:118:LEU:HD13	2.02	0.41
1:C:330:VAL:HA	1:C:346:VAL:O	2.20	0.41
1:A:179:ILE:O	1:A:181:LEU:N	2.53	0.41
1:C:168:ILE:HD12	1:C:168:ILE:N	2.35	0.41
1:A:184:THR:O	1:A:185:GLY:C	2.58	0.41
1:C:160:ASN:HD21	1:C:163:ASN:ND2	2.17	0.41
1:B:98:ILE:C	1:B:98:ILE:HD12	2.41	0.41
1:A:188:ASN:N	1:A:188:ASN:ND2	2.68	0.41
1:A:257:GLY:CA	1:A:323:ALA:HA	2.51	0.41
1:A:331:ILE:HG13	1:A:332:PRO:HD2	2.03	0.41
1:B:182:ASN:HA	1:B:183:PRO:HD3	1.95	0.41
1:B:292:PRO:C	1:B:294:ALA:H	2.24	0.41
1:C:85:MET:HG3	1:C:245:MET:SD	2.61	0.41
1:A:309:ASN:O	1:A:310:LYS:HE2	2.20	0.41
1:C:305:ILE:HG12	1:C:306:SER:N	2.34	0.41
1:B:282:ILE:HG22	1:B:283:VAL:H	1.85	0.41
1:B:300:VAL:HG22	1:B:301:ASN:N	2.36	0.41
1:C:333:VAL:O	1:C:333:VAL:HG23	2.21	0.41
1:C:74:LEU:HA	1:C:74:LEU:HD12	1.86	0.41
1:A:236:ILE:HA	1:A:237:PRO:HD3	1.90	0.40
1:A:201:SER:HB2	3:A:406:HOH:O	2.21	0.40
1:C:248:LEU:HD21	1:C:254:VAL:HG23	2.04	0.40
1:C:300:VAL:HG22	1:C:301:ASN:N	2.35	0.40
1:A:180:GLY:O	1:A:181:LEU:O	2.39	0.40
1:B:179:ILE:HD12	3:B:380:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HG12	2:E:410:PHE:HB2	2.04	0.40
1:C:105:ILE:N	1:C:105:ILE:HD12	2.37	0.40
1:C:92:ILE:CG2	1:C:93:THR:N	2.85	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	272/314 (87%)	238 (88%)	19 (7%)	15 (6%)	2	2
1	B	264/314 (84%)	237 (90%)	19 (7%)	8 (3%)	5	7
1	C	265/314 (84%)	242 (91%)	16 (6%)	7 (3%)	6	9
2	D	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
2	E	2/10 (20%)	2 (100%)	0	0	100	100
2	F	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
All	All	807/972 (83%)	721 (89%)	56 (7%)	30 (4%)	4	5

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	LEU
1	A	183	PRO
1	A	186	ARG
1	A	224	ASN
1	A	289	PRO
1	A	293	ALA
1	A	299	GLN
1	A	304	ILE
1	B	289	PRO

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Mol	Chain	Res	Type
1	B	293	ALA
1	C	221	ASP
1	C	259	ILE
1	C	300	VAL
1	A	180	GLY
1	A	308	ASP
1	B	297	GLY
1	A	162	TYR
1	A	285	ASN
1	B	226	GLY
1	B	292	PRO
1	B	299	GLN
1	C	285	ASN
1	C	297	GLY
1	B	185	GLY
1	A	220	PHE
1	A	303	LEU
1	A	182	ASN
1	C	289	PRO
1	C	305	ILE
1	B	259	ILE

### 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	227/253 (90%)	203 (89%)	24 (11%)	8	15
1	B	221/253 (87%)	200 (90%)	21 (10%)	10	19
1	C	222/253 (88%)	201 (90%)	21 (10%)	10	19
2	D	4/9 (44%)	3 (75%)	1 (25%)	1	1
2	E	4/9 (44%)	3 (75%)	1 (25%)	1	1
2	F	4/9 (44%)	3 (75%)	1 (25%)	1	1
All	All	682/786 (87%)	613 (90%)	69 (10%)	9	17

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	MET
1	A	58	VAL
1	A	63	ASN
1	A	78	THR
1	A	117	LEU
1	A	155	VAL
1	A	160	ASN
1	A	163	ASN
1	A	167	THR
1	A	170	GLN
1	A	178	ARG
1	A	186	ARG
1	A	188	ASN
1	A	205	LEU
1	A	218	LEU
1	A	219	SER
1	A	224	ASN
1	A	239	GLN
1	A	240	LEU
1	A	261	ILE
1	A	286	GLU
1	A	289	PRO
1	A	305	ILE
1	A	321	GLN
1	B	43	THR
1	B	63	ASN
1	B	108	LEU
1	B	118	LEU
1	B	119	VAL
1	B	141	ILE
1	B	148	VAL
1	B	167	THR
1	B	178	ARG
1	B	179	ILE
1	B	182	ASN
1	B	186	ARG
1	B	205	LEU
1	B	218	LEU
1	B	220	PHE
1	B	227	GLU
1	B	240	LEU
1	B	261	ILE

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Mol	Chain	Res	Type
1	B	289	PRO
1	B	305	ILE
1	B	321	GLN
1	C	63	ASN
1	C	67	ASN
1	C	78	THR
1	C	99	ASN
1	C	140	THR
1	C	147	ARG
1	C	163	ASN
1	C	167	THR
1	C	178	ARG
1	C	187	GLN
1	C	201	SER
1	C	205	LEU
1	C	221	ASP
1	C	224	ASN
1	C	228	THR
1	C	239	GLN
1	C	242	THR
1	C	253	ARG
1	C	261	ILE
1	C	286	GLU
1	C	305	ILE
2	D	409	TRP
2	E	409	TRP
2	F	409	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	ASN
1	A	73	GLN
1	A	87	GLN
1	A	160	ASN
1	A	163	ASN
1	A	166	GLN
1	A	187	GLN
1	A	188	ASN
1	A	200	ASN
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	224	ASN
1	A	239	GLN
1	A	295	ASN
1	A	301	ASN
1	B	63	ASN
1	B	73	GLN
1	B	87	GLN
1	B	150	HIS
1	B	160	ASN
1	B	163	ASN
1	B	166	GLN
1	B	170	GLN
1	B	191	GLN
1	B	200	ASN
1	B	216	ASN
1	B	301	ASN
1	C	63	ASN
1	C	67	ASN
1	C	87	GLN
1	C	109	GLN
1	C	163	ASN
1	C	166	GLN
1	C	170	GLN
1	C	187	GLN
1	C	200	ASN
1	C	216	ASN
1	C	239	GLN
1	C	295	ASN
1	C	301	ASN

### 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

### 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	280/314 (89%)	0.96	62 (22%)  	18, 40, 163, 166	0
1	B	274/314 (87%)	1.05	62 (22%)  	22, 51, 163, 166	0
1	C	275/314 (87%)	1.21	62 (22%)  	24, 52, 160, 167	0
2	D	4/10 (40%)	6.25	4 (100%)  	156, 157, 159, 161	0
2	E	4/10 (40%)	5.25	3 (75%)  	152, 156, 157, 159	0
2	F	4/10 (40%)	8.35	4 (100%)  	160, 160, 161, 163	0
All	All	841/972 (86%)	1.15	197 (23%)  	18, 49, 163, 167	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	GLY	16.7
2	F	407	VAL	14.2
1	A	344	LEU	12.4
1	B	286	GLU	12.4
1	C	334	VAL	11.1
1	C	289	PRO	10.9
1	C	287	VAL	10.8
1	C	263	GLY	10.3
1	A	260	GLY	10.1
2	E	409	TRP	9.8
1	B	300	VAL	9.6
1	B	335	VAL	9.6
1	C	344	LEU	9.4
1	B	288	SER	8.8
1	A	333	VAL	8.8
1	A	289	PRO	8.7
1	C	282	ILE	8.5
2	D	409	TRP	8.4
1	B	290	ASP	8.2

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Mol	Chain	Res	Type	RSRZ
1	C	288	SER	8.1
1	B	299	GLN	8.1
1	A	287	VAL	8.0
1	C	181	LEU	7.7
2	F	409	TRP	7.5
1	A	311	PRO	7.5
1	C	299	GLN	7.5
1	C	286	GLU	7.4
1	C	184	THR	7.4
2	D	408	TYR	7.3
1	C	328	GLY	7.2
1	C	309	ASN	7.2
1	B	287	VAL	7.0
1	C	295	ASN	6.9
1	A	299	GLN	6.9
2	D	407	VAL	6.8
1	A	294	ALA	6.8
1	C	330	VAL	6.6
1	B	289	PRO	6.6
1	C	291	GLY	6.5
1	B	66	LEU	6.5
2	E	408	TYR	6.4
1	B	305	ILE	6.4
1	C	333	VAL	6.3
1	C	294	ALA	6.3
1	A	312	ALA	6.3
1	B	292	PRO	6.2
1	C	300	VAL	6.2
1	C	283	VAL	6.2
1	B	298	ILE	6.2
1	C	318	THR	6.2
1	A	258	TYR	6.2
1	C	335	VAL	6.1
2	F	410	PHE	6.0
1	B	224	ASN	6.0
1	C	292	PRO	5.9
1	A	305	ILE	5.9
1	B	186	ARG	5.9
1	A	300	VAL	5.8
1	A	301	ASN	5.8
1	B	184	THR	5.7
2	F	408	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	5.6
1	A	288	SER	5.6
1	C	285	ASN	5.5
1	C	284	VAL	5.5
1	A	286	GLU	5.5
1	B	311	PRO	5.4
1	C	182	ASN	5.3
1	C	183	PRO	5.3
1	A	290	ASP	5.3
1	C	349	GLN	5.2
1	A	349	GLN	5.1
1	A	298	ILE	5.1
1	A	292	PRO	5.1
1	B	183	PRO	5.0
1	A	347	THR	5.0
1	B	221	ASP	4.9
1	A	318	THR	4.8
1	A	259	ILE	4.8
1	A	293	ALA	4.8
1	A	303	LEU	4.8
1	B	283	VAL	4.8
1	A	261	ILE	4.7
1	C	261	ILE	4.7
1	A	181	LEU	4.7
1	A	335	VAL	4.7
1	B	301	ASN	4.6
1	A	329	SER	4.6
1	C	347	THR	4.6
1	A	334	VAL	4.5
1	A	186	ARG	4.5
1	B	293	ALA	4.4
1	A	309	ASN	4.4
1	B	344	LEU	4.4
1	A	345	GLN	4.4
1	C	311	PRO	4.4
1	A	296	ALA	4.4
1	C	298	ILE	4.3
1	A	182	ASN	4.3
1	B	73	GLN	4.3
1	B	294	ALA	4.3
1	C	346	VAL	4.3
1	B	285	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	329	SER	4.2
1	A	284	VAL	4.2
1	C	297	GLY	4.2
1	A	291	GLY	4.2
1	B	65	GLY	4.2
1	B	320	ASP	4.1
1	A	285	ASN	4.1
1	B	262	GLY	4.1
1	B	345	GLN	4.1
1	B	303	LEU	4.0
1	C	306	SER	4.0
1	B	318	THR	4.0
1	B	333	VAL	4.0
1	B	351	TYR	4.0
1	C	351	TYR	3.9
1	A	183	PRO	3.9
1	A	330	VAL	3.9
1	C	224	ASN	3.9
1	C	301	ASN	3.8
1	B	259	ILE	3.8
1	A	282	ILE	3.7
1	B	331	ILE	3.7
1	B	77	ARG	3.7
1	B	223	SER	3.6
1	B	182	ASN	3.6
1	C	345	GLN	3.6
1	C	258	TYR	3.6
1	B	75	GLU	3.5
1	C	326	ARG	3.5
1	B	282	ILE	3.5
1	A	351	TYR	3.4
1	A	332	PRO	3.4
1	A	310	LYS	3.4
1	B	347	THR	3.4
2	E	407	VAL	3.4
1	C	293	ALA	3.3
1	A	262	GLY	3.3
1	C	321	GLN	3.3
1	A	346	VAL	3.3
1	B	295	ASN	3.3
1	B	284	VAL	3.3
1	A	325	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	328	GLY	3.2
1	A	42	MET	3.2
1	C	222	LYS	3.2
1	C	262	GLY	3.2
1	C	332	PRO	3.2
1	B	225	ASP	3.2
1	C	66	LEU	3.1
1	A	224	ASN	3.1
1	C	136	GLY	3.1
1	B	349	GLN	3.1
1	A	295	ASN	3.1
1	A	331	ILE	3.0
1	B	310	LYS	3.0
1	C	73	GLN	3.0
1	B	261	ILE	2.9
1	A	263	GLY	2.9
1	B	185	GLY	2.9
1	C	67	ASN	2.8
1	A	302	ASP	2.8
1	B	330	VAL	2.8
1	A	306	SER	2.8
1	A	327	PRO	2.7
1	B	326	ARG	2.7
1	C	221	ASP	2.7
1	C	331	ILE	2.7
1	A	320	ASP	2.7
1	B	306	SER	2.6
1	C	348	ILE	2.6
1	A	283	VAL	2.6
1	B	135	THR	2.6
1	B	181	LEU	2.6
1	B	258	TYR	2.5
1	B	296	ALA	2.5
1	B	74	LEU	2.5
1	B	312	ALA	2.5
1	B	332	PRO	2.5
1	C	325	ILE	2.5
1	C	303	LEU	2.4
2	D	410	PHE	2.4
1	B	352	PRO	2.4
1	C	312	ALA	2.4
1	A	321	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	352	PRO	2.4
1	C	320	ASP	2.4
1	A	184	THR	2.4
1	C	260	GLY	2.3
1	C	100	ASP	2.3
1	B	307	VAL	2.2
1	A	221	ASP	2.2
1	C	304	ILE	2.1
1	A	326	ARG	2.1
1	A	308	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.