



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:48 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 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/ValidationPDFNotes.html>

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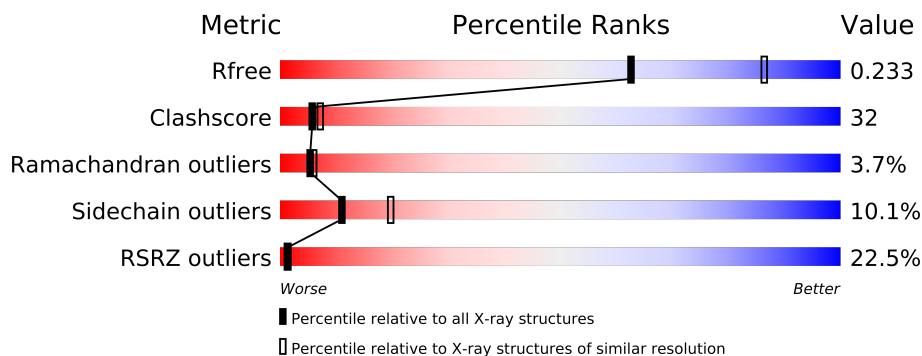
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	
2	D	10	
2	E	10	
2	F	10	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6446 atoms, of which 0 are hydrogen and 0 are deuterium.

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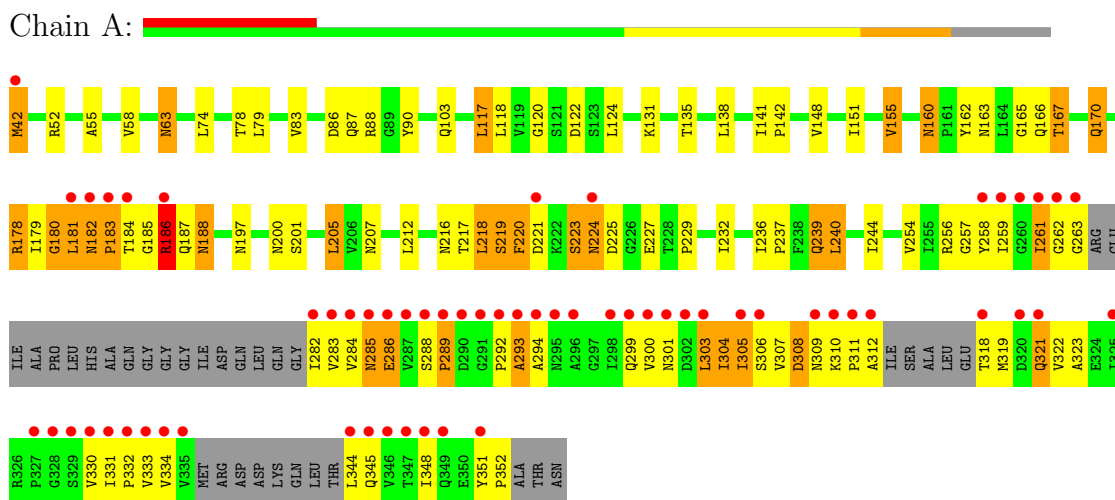
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	41	Total	O	0	0
			41	41		

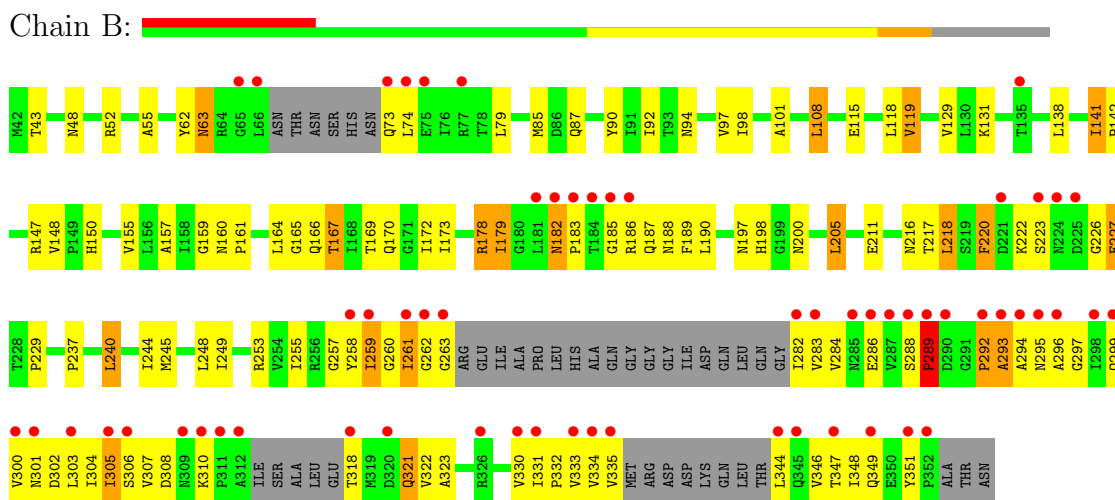
### 3 Residue-property plots

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

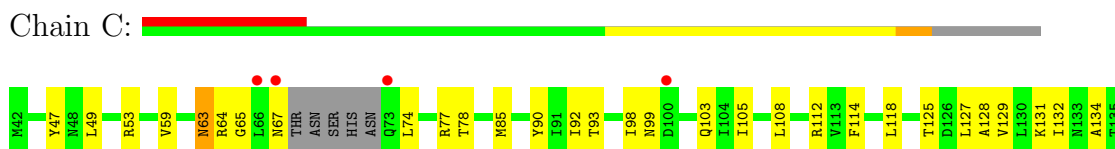
#### • Molecule 1: Protease degS

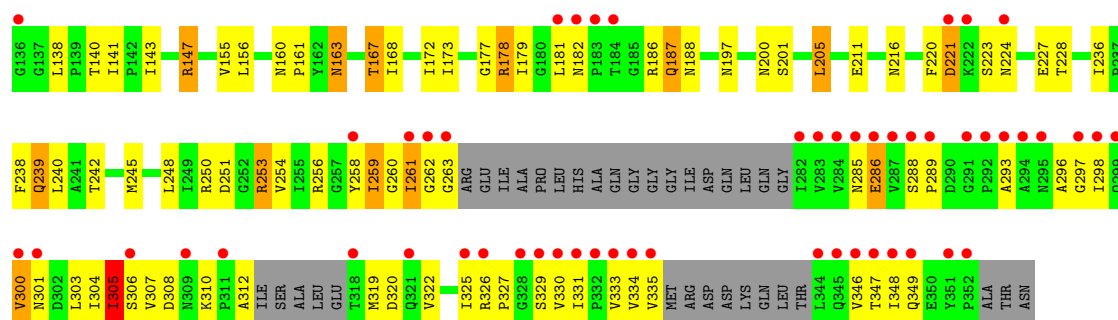


#### • Molecule 1: Protease degS



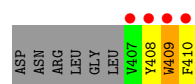
#### • Molecule 1: Protease degS





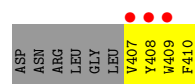
- Molecule 2: Synthetic peptide YWF

Chain D:



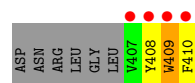
- Molecule 2: Synthetic peptide YWF

Chain E:



- Molecule 2: Synthetic peptide YWF

Chain F:



## 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 , 0.233	Depositor DCC
$R_{free}$ test set	1923 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.5	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38774 reflections	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.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	45	0	36	9	0
2	E	45	0	36	4	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (401) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:C:348:ILE:HD12	1:C:348:ILE:H	1.49	0.77
1:B:187:GLN:HG3	1:B:188:ASN:H	1.48	0.77
1:C:239:GLN:HB2	3:C:358:HOH:O	1.84	0.77
1:A:258:TYR:HB2	1:A:351:TYR:HA	1.67	0.77
1:A:220:PHE:HD1	1:A:229:PRO:HG2	1.50	0.77
1:A:141:ILE:CD1	1:A:212:LEU:HD13	2.16	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(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: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:A:308:ASP:HB2	1:A:331:ILE:CD1	2.24	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:300:VAL:HG22	1:A:301:ASN:ND2	2.09	0.67
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.59	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:C:296:ALA:HB1	1:C:346:VAL:HA	1.76	0.66
1:B:303:LEU:HD23	1:B:303:LEU:H	1.61	0.66
1:B:288:SER:O	1:B:289:PRO:O	2.14	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:283:VAL:HG12	1:B:284:VAL:N	2.12	0.65
1:C:304:ILE:HG13	1:C:334:VAL:O	1.97	0.65
1:C:286:GLU:HB3	1:C:288:SER:O	1.96	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:B:308:ASP:HB2	1:B:331:ILE:CD1	2.27	0.64
1:A:307:VAL:HG13	1:A:333:VAL:HG12	1.77	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:63:ASN:HD21	1:B:101:ALA:HA	1.64	0.63
1:B:197:ASN:H	1:B:200:ASN:ND2	1.96	0.63
1:A:263:GLY:C	2:D:408:TYR:H	2.01	0.62
1:B:305:ILE:N	1:B:305:ILE:HD13	2.13	0.62
1:B:205:LEU:HG	1:B:216:ASN:HD21	1.64	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: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:A:261:ILE:HD13	1:A:261:ILE:H	1.65	0.62
1:C:250:ARG:HG2	1:C:250:ARG:HH11	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: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:87:GLN:HE21	1:A:138:LEU:H	1.49	0.61
1:C:53:ARG:HG2	1:C:53:ARG:HH11	1.66	0.60
1:A:217:THR:O	1:A:218:LEU:HD13	2.01	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
1:A:322:VAL:HG21	2:D:410:PHE:HD2	1.67	0.60
1:C:155:VAL:HG11	1:C:173:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:SER:C	1:A:221:ASP:H	2.04	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:259:ILE:O	1:B:293:ALA:HB3	2.02	0.59
1:B:55:ALA:HB1	1:B:166:GLN:NE2	2.18	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:C:262:GLY:C	1:C:286:GLU:HG2	2.23	0.59
1:B:261:ILE:HD13	1:B:261:ILE:N	2.18	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:C:346:VAL:HG12	1:C:347:THR:N	2.17	0.59
1:B:87:GLN:HE22	1:B:138:LEU:H	1.50	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:C:65:GLY:CA	1:C:77:ARG:HD2	2.28	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: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:94:ASN:HB2	1:B:97:VAL:HG23	1.86	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: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:348:ILE:HD12	1:A:348:ILE:N	2.21	0.56
1:C:262:GLY:O	1:C:286:GLU:HG2	2.06	0.56
1:B:296:ALA:HB3	1:B:346:VAL:HG22	1.86	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:C:223:SER:CB	1:C:227:GLU:O	2.47	0.52
1:A:83:VAL:CG1	1:A:141:ILE:HD12	2.39	0.52
1:C:296:ALA:CB	1:C:346:VAL:HA	2.38	0.52
1:C:259:ILE:O	1:C:293:ALA:HB3	2.09	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
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:260:GLY:HA3	1:B:294:ALA:HB2	1.92	0.51
1:B:173:ILE:HG23	1:B:190:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:CD2	1:B:303:LEU:H	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:C:303:LEU:O	1:C:335:VAL:HG12	2.10	0.50
1:C:177:GLY:HA2	1:C:188:ASN:HD22	1.76	0.50
1:B:55:ALA:HB1	1:B:166:GLN:HE22	1.75	0.50
1:C:250:ARG:HG2	1:C:250:ARG:NH1	2.27	0.50
1:A:330:VAL:CG1	1:A:345:GLN:HB3	2.42	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:305:ILE:CA	1:A:312:ALA:HB2	2.28	0.49
1:A:185:GLY:HA2	2:D:409:TRP:HH2	1.77	0.49
1:C:258:TYR:HD1	2:F:410:PHE:OXT	1.94	0.49
1:A:292:PRO:O	1:A:294:ALA:N	2.45	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:261:ILE:HD13	1:C:261:ILE:H	1.76	0.49
1:C:143:ILE:HD11	3:C:387:HOH:O	2.12	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:C:298:ILE:HG23	1:C:333:VAL:CG2	2.42	0.49
1:B:165:GLY:C	1:C:178:ARG:NH2	2.66	0.49
1:A:303:LEU:H	1:A:303:LEU:CD2	2.26	0.49
1:A:300:VAL:CG1	1:A:301:ASN:H	2.17	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:305:ILE:HA	1:C:312:ALA:CB	2.42	0.48
1:A:333:VAL:O	1:A:344:LEU:HB3	2.13	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:B:119:VAL:HG13	1:B:129:VAL:O	2.14	0.48
1:A:88:ARG:O	1:A:131:LYS:NZ	2.47	0.48
1:B:245:MET:HG2	1:B:249:ILE:HD13	1.94	0.48
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.72	0.47
1:A:148:VAL:HG12	3:A:416:HOH:O	2.14	0.47
1:C:223:SER:HB2	1:C:227:GLU:CD	2.34	0.47
1:C:300:VAL:C	1:C:301:ASN:HD22	2.18	0.47
1:A:300:VAL:C	1:A:301:ASN:HD22	2.18	0.47
1:A:179:ILE:HG12	3:A:417:HOH:O	2.14	0.47
1:A:319:MET:SD	2:D:409:TRP:HD1	2.38	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:C:92:ILE:HG22	1:C:93:THR:N	2.30	0.47
1:B:253:ARG:CZ	1:B:255:ILE:HD11	2.44	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:C:155:VAL:HG11	1:C:173:ILE:CD1	2.45	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:307:VAL:O	1:A:308:ASP:HB3	2.15	0.47
1:A:254:VAL:HG13	1:A:254:VAL:O	2.14	0.47
1:C:129:VAL:HG23	1:C:248:LEU:HD12	1.96	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:B:303:LEU:HD23	1:B:303:LEU:N	2.30	0.47
1:A:348:ILE:HD12	1:A:348:ILE:H	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:284:VAL:HB	1:B:302:ASP:O	2.15	0.46
1:B:108:LEU:HD23	1:B:108:LEU:N	2.30	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:304:ILE:HG12	1:C:305:ILE:N	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:59:VAL:CG1	1:C:108:LEU:HD22	2.46	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: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: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:258:TYR:HB2	1:B:351:TYR:HA	1.98	0.45
1:C:259:ILE:HG13	1:C:322:VAL:HG11	1.99	0.45
1:A:207:ASN:HB2	3:A:358:HOH:O	2.16	0.45
1:B:305:ILE:N	1:B:305:ILE:CD1	2.79	0.45
2:D:408:TYR:HB3	2:D:410:PHE:CE1	2.52	0.45
1:B:170:GLN:HG2	1:C:172:ILE:CG2	2.46	0.45
1:B:321:GLN:N	1:B:321:GLN:OE1	2.50	0.45
1:C:259:ILE:HG13	1:C:322:VAL:CG1	2.46	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:A:124:LEU:HD12	1:A:256:ARG:CZ	2.47	0.45
1:C:186:ARG:HD3	1:C:320:ASP:OD1	2.17	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:B:48:ASN:O	1:B:52:ARG:HG3	2.17	0.45
1:C:331:ILE:HG23	1:C:331:ILE:O	2.17	0.44
1:C:251:ASP:C	1:C:253:ARG:H	2.20	0.44
1:B:308:ASP:HB2	1:B:331:ILE:CG1	2.47	0.44
1:A:165:GLY:O	1:B:178:ARG:NH2	2.50	0.44
1:A:303:LEU:HG	1:A:304:ILE:N	2.32	0.44
1:A:83:VAL:HG11	1:A:141:ILE:HD12	2.00	0.44
1:A:307:VAL:O	1:A:308:ASP:CB	2.65	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:305:ILE:CG1	1:C:306:SER:H	2.31	0.44
1:C:263:GLY:H	2:F:408:TYR:HB2	1.82	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:B:217:THR:HG23	1:B:218:LEU:N	2.32	0.44
1:C:253:ARG:HG2	1:C:254:VAL:N	2.33	0.44
1:A:284:VAL:O	1:A:285:ASN:HB3	2.18	0.43
1:C:346:VAL:CG1	1:C:347:THR:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:151:ILE:HG21	1:C:168:ILE:HD13	2.00	0.43
1:A:42:MET:SD	1:A:42:MET:N	2.92	0.43
1:A:141:ILE:HA	1:A:142:PRO:HD3	1.89	0.43
1:A:319:MET:SD	2:D:409:TRP:CD1	3.12	0.43
1:B:292:PRO:O	1:B:295:ASN:ND2	2.51	0.43
1:B:253:ARG:CZ	1:B:255:ILE:CD1	2.96	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:B:187:GLN:HG3	1:B:188:ASN:N	2.24	0.43
1:A:220:PHE:O	1:A:220:PHE:CD1	2.72	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:85:MET:HG3	1:B:245:MET:SD	2.59	0.43
1:B:220:PHE:HD2	1:B:229:PRO:HG3	1.83	0.43
1:C:319:MET:HE1	2:F:410:PHE:HA	2.01	0.42
1:A:170:GLN:HG2	1:B:172:ILE:HG23	2.01	0.42
1:A:55:ALA:HB1	1:A:166:GLN:NE2	2.34	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:B:300:VAL:CG1	1:B:301:ASN:H	2.14	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: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:A:259:ILE:O	1:A:293:ALA:HB3	2.19	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:C:127:LEU:HA	1:C:127:LEU:HD23	1.93	0.42
1:A:258:TYR:CB	1:A:351:TYR:HA	2.42	0.42
1:A:307:VAL:HG12	1:A:331:ILE:HD13	2.01	0.42
1:A:219:SER:O	1:A:221:ASP:N	2.49	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:87:GLN:HG3	3:A:415:HOH:O	2.20	0.41
1:C:300:VAL:CG1	1:C:301:ASN:H	2.14	0.41
1:B:257:GLY:HA3	1:B:322:VAL:O	2.21	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:C:330:VAL:HA	1:C:346:VAL:O	2.20	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: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:309:ASN:O	1:A:310:LYS:HE2	2.20	0.41
1:A:257:GLY:CA	1:A:323:ALA:HA	2.51	0.41
1:C:305:ILE:HG12	1:C:306:SER:N	2.34	0.41
1:A:331:ILE:HG13	1:A:332:PRO:HD2	2.03	0.41
1:B:292:PRO:C	1:B:294:ALA:H	2.24	0.41
1:A:188:ASN:N	1:A:188:ASN:ND2	2.68	0.41
1:C:85:MET:HG3	1:C:245:MET:SD	2.61	0.41
1:B:182:ASN:HA	1:B:183:PRO:HD3	1.95	0.41
1:B:300:VAL:HG22	1:B:301:ASN:N	2.36	0.41
1:C:74:LEU:HA	1:C:74:LEU:HD12	1.86	0.41
1:C:333:VAL:O	1:C:333:VAL:HG23	2.21	0.41
1:B:282:ILE:HG22	1:B:283:VAL:H	1.85	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:300:VAL:HG22	1:C:301:ASN:N	2.35	0.40
1:C:248:LEU:HD21	1:C:254:VAL:HG23	2.04	0.40
1:A:180:GLY:O	1:A:181:LEU:O	2.39	0.40
1:C:105:ILE:N	1:C:105:ILE:HD12	2.37	0.40
1:B:261:ILE:HG12	2:E:410:PHE:HB2	2.04	0.40
1:C:92:ILE:CG2	1:C:93:THR:N	2.85	0.40
1:B:179:ILE:HD12	3:B:380:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	3	2
1	B	264/314 (84%)	237 (90%)	19 (7%)	8 (3%)	7	9
1	C	265/314 (84%)	242 (91%)	16 (6%)	7 (3%)	8	11
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%)	5	6

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
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

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Mol	Chain	Res	Type
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%)	10	18
1	B	221/253 (87%)	200 (90%)	21 (10%)	12	22
1	C	222/253 (88%)	201 (90%)	21 (10%)	12	22
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%)	11	20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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%)	0.86	61 (21%) 1 1	18, 40, 163, 166	0
1	B	274/314 (87%)	0.96	60 (21%) 1 1	22, 51, 163, 166	0
1	C	275/314 (87%)	1.09	57 (20%) 1 1	24, 52, 160, 167	0
2	D	4/10 (40%)	6.51	4 (100%) 0 0	156, 157, 159, 161	0
2	E	4/10 (40%)	4.86	3 (75%) 0 0	152, 156, 157, 159	0
2	F	4/10 (40%)	8.16	4 (100%) 0 0	160, 160, 161, 163	0
All	All	841/972 (86%)	1.05	189 (22%) 1 1	18, 49, 163, 167	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	GLY	14.2
2	F	407	VAL	11.8
1	A	344	LEU	11.6
1	B	286	GLU	11.4
1	C	287	VAL	10.7
1	C	344	LEU	10.5
2	D	409	TRP	10.3
1	C	334	VAL	10.2
1	C	289	PRO	10.0
2	E	409	TRP	9.5
1	B	300	VAL	9.3
2	F	409	TRP	9.0
1	B	288	SER	8.5
1	C	181	LEU	8.4
1	A	289	PRO	8.3
1	C	309	ASN	7.9
1	B	335	VAL	7.8
1	B	299	GLN	7.7
1	C	288	SER	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	290	ASP	7.5
1	C	263	GLY	7.5
1	A	260	GLY	7.5
1	C	184	THR	7.5
1	A	333	VAL	7.2
1	A	287	VAL	7.1
1	A	311	PRO	6.9
1	B	66	LEU	6.9
1	C	299	GLN	6.9
1	C	335	VAL	6.8
1	C	295	ASN	6.7
1	A	312	ALA	6.6
2	D	408	TYR	6.4
1	C	283	VAL	6.3
1	C	282	ILE	6.3
1	C	294	ALA	6.2
1	B	305	ILE	6.2
1	B	186	ARG	6.2
1	C	333	VAL	6.1
2	F	410	PHE	6.1
1	B	287	VAL	6.1
2	D	407	VAL	6.1
1	A	299	GLN	6.1
1	A	305	ILE	6.0
1	C	330	VAL	6.0
1	B	289	PRO	5.9
1	C	349	GLN	5.9
2	F	408	TYR	5.8
1	A	292	PRO	5.8
2	E	408	TYR	5.7
1	A	347	THR	5.7
1	A	258	TYR	5.7
1	B	224	ASN	5.7
1	C	328	GLY	5.6
1	A	300	VAL	5.5
1	A	261	ILE	5.5
1	B	292	PRO	5.5
1	C	286	GLU	5.4
1	C	291	GLY	5.4
1	C	318	THR	5.4
1	C	292	PRO	5.4
1	A	294	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	5.3
1	A	335	VAL	5.3
1	A	334	VAL	5.2
1	A	349	GLN	5.2
1	B	301	ASN	5.1
1	C	300	VAL	5.1
1	A	318	THR	5.1
1	B	311	PRO	5.1
1	C	284	VAL	4.9
1	A	301	ASN	4.9
1	B	184	THR	4.9
1	A	288	SER	4.8
1	A	293	ALA	4.8
1	B	298	ILE	4.7
1	C	182	ASN	4.7
1	A	286	GLU	4.7
1	B	334	VAL	4.7
1	B	283	VAL	4.7
1	C	183	PRO	4.6
1	C	285	ASN	4.6
1	A	290	ASP	4.6
1	A	181	LEU	4.6
1	C	261	ILE	4.5
1	C	347	THR	4.5
1	A	259	ILE	4.4
1	B	183	PRO	4.3
1	B	285	ASN	4.3
1	A	330	VAL	4.3
1	B	345	GLN	4.2
1	B	221	ASP	4.2
1	B	65	GLY	4.2
1	B	73	GLN	4.1
1	B	333	VAL	4.1
1	C	258	TYR	4.1
1	B	344	LEU	4.0
1	A	182	ASN	4.0
1	C	224	ASN	4.0
1	B	293	ALA	4.0
1	C	66	LEU	3.9
1	B	294	ALA	3.9
1	A	285	ASN	3.9
1	A	183	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	349	GLN	3.9
1	C	329	SER	3.9
1	A	303	LEU	3.9
1	C	298	ILE	3.8
1	B	303	LEU	3.8
1	B	347	THR	3.8
1	A	282	ILE	3.7
1	C	311	PRO	3.7
1	A	309	ASN	3.7
1	B	75	GLU	3.7
1	A	351	TYR	3.7
1	C	326	ARG	3.7
1	B	318	THR	3.7
1	B	77	ARG	3.7
1	B	262	GLY	3.7
1	B	351	TYR	3.7
1	C	346	VAL	3.6
1	A	262	GLY	3.6
1	C	345	GLN	3.6
1	A	186	ARG	3.6
1	C	262	GLY	3.6
1	A	329	SER	3.6
1	C	297	GLY	3.5
1	B	223	SER	3.5
1	B	282	ILE	3.5
1	A	296	ALA	3.5
1	A	345	GLN	3.5
1	B	331	ILE	3.4
2	D	410	PHE	3.3
1	C	351	TYR	3.3
1	C	321	GLN	3.3
1	B	182	ASN	3.2
1	A	331	ILE	3.2
1	A	310	LYS	3.2
1	C	293	ALA	3.2
1	A	332	PRO	3.2
1	A	346	VAL	3.1
1	C	67	ASN	3.1
1	A	291	GLY	3.1
1	B	306	SER	3.0
1	B	295	ASN	3.0
1	B	310	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	295	ASN	2.9
2	E	407	VAL	2.9
1	B	225	ASP	2.9
1	B	320	ASP	2.9
1	B	259	ILE	2.9
1	A	325	ILE	2.9
1	B	261	ILE	2.9
1	B	330	VAL	2.9
1	C	301	ASN	2.8
1	B	181	LEU	2.8
1	A	306	SER	2.8
1	C	306	SER	2.8
1	A	302	ASP	2.8
1	A	224	ASN	2.8
1	C	222	LYS	2.7
1	C	331	ILE	2.7
1	A	42	MET	2.6
1	C	136	GLY	2.6
1	A	327	PRO	2.6
1	C	352	PRO	2.6
1	A	283	VAL	2.6
1	C	221	ASP	2.6
1	A	284	VAL	2.6
1	B	74	LEU	2.4
1	C	73	GLN	2.4
1	B	352	PRO	2.4
1	A	321	GLN	2.4
1	C	332	PRO	2.4
1	C	325	ILE	2.4
1	B	258	TYR	2.4
1	A	263	GLY	2.3
1	B	312	ALA	2.3
1	A	184	THR	2.3
1	B	135	THR	2.3
1	A	328	GLY	2.3
1	B	309	ASN	2.3
1	B	296	ALA	2.3
1	B	185	GLY	2.2
1	C	100	ASP	2.2
1	A	221	ASP	2.2
1	A	320	ASP	2.2
1	B	326	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	348	ILE	2.1
1	A	348	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.