



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 03:37 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

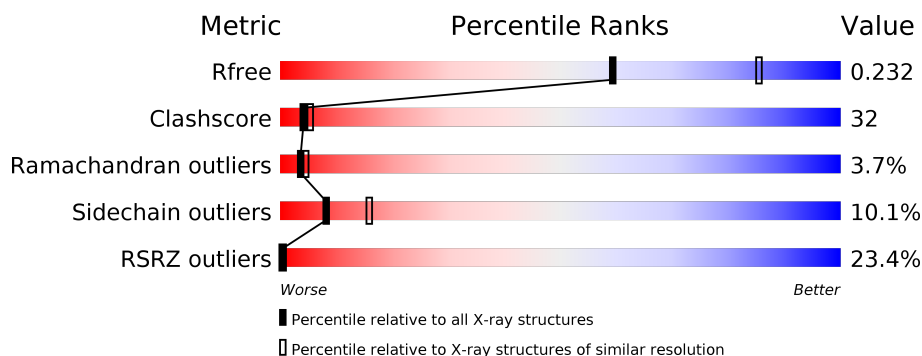
1 Overall quality at a glance

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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (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 ≥ 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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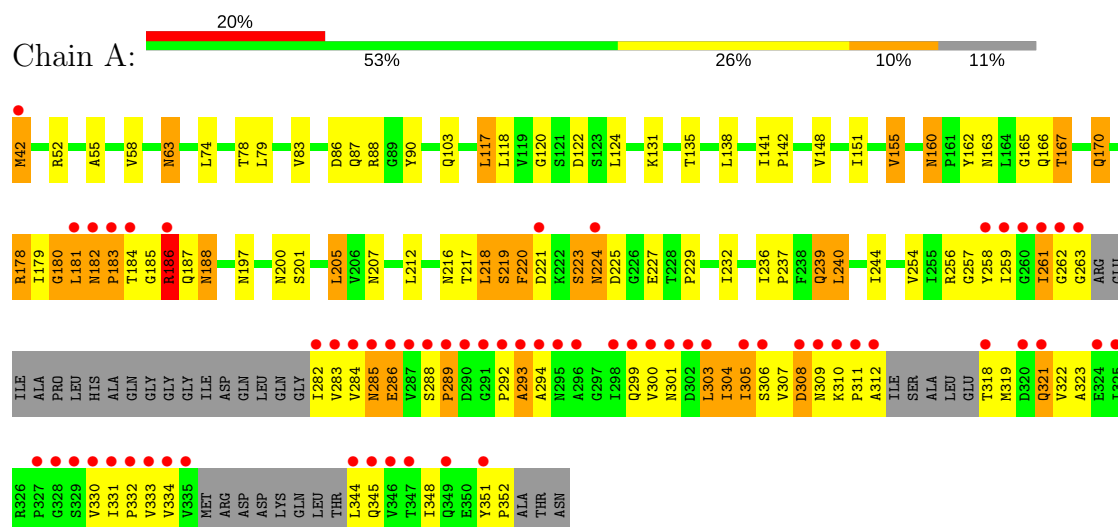
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	41	Total	O	0	0
			41	41		

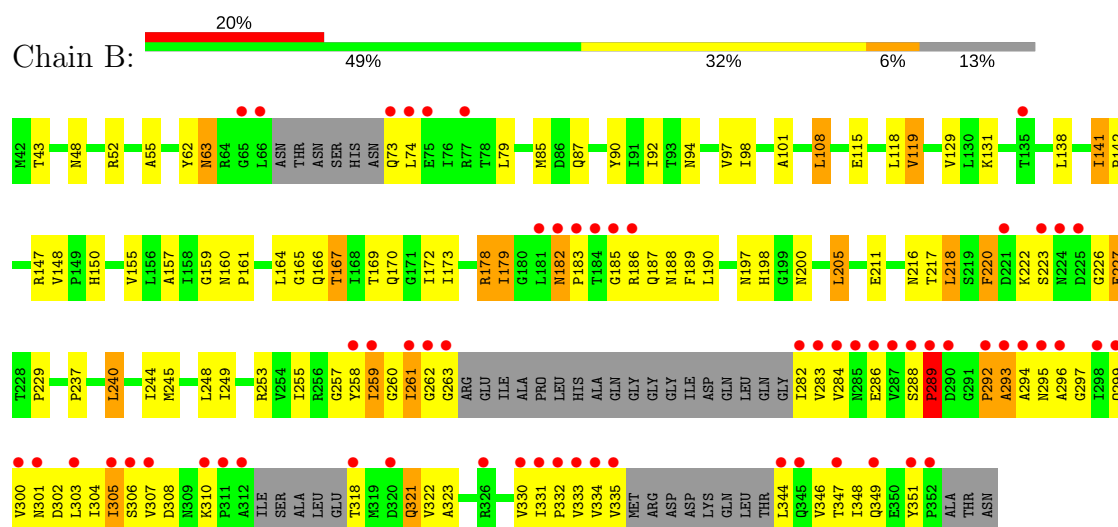
3 Residue-property plots

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

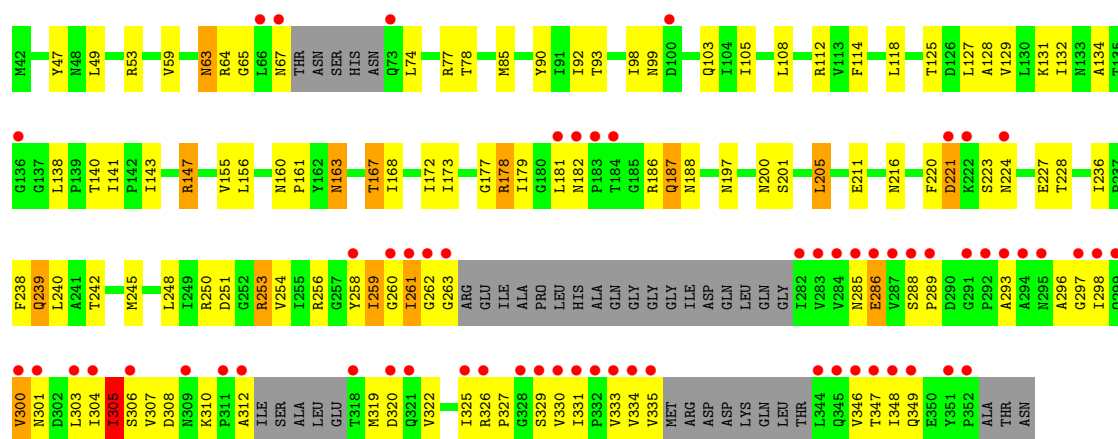


• Molecule 1: Protease degS



• Molecule 1: Protease degS





• Molecule 2: Synthetic peptide YWF



• Molecule 2: Synthetic peptide YWF



• Molecule 2: Synthetic peptide YWF



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	4

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%)	7	14
1	B	221/253 (87%)	200 (90%)	21 (10%)	9	18
1	C	222/253 (88%)	201 (90%)	21 (10%)	9	18
2	D	4/9 (44%)	3 (75%)	1 (25%)	0	1
2	E	4/9 (44%)	3 (75%)	1 (25%)	0	1
2	F	4/9 (44%)	3 (75%)	1 (25%)	0	1
All	All	682/786 (87%)	613 (90%)	69 (10%)	8	16

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, 95th 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 ²)	Q<0.9
1	A	280/314 (89%)	0.95	62 (22%) 0 0	18, 40, 163, 166	0
1	B	274/314 (87%)	1.05	62 (22%) 0 0	22, 51, 163, 166	0
1	C	275/314 (87%)	1.20	62 (22%) 0 0	24, 52, 160, 167	0
2	D	4/10 (40%)	6.31	4 (100%) 0 0	156, 157, 159, 161	0
2	E	4/10 (40%)	5.29	3 (75%) 0 0	152, 156, 157, 159	0
2	F	4/10 (40%)	8.25	4 (100%) 0 0	160, 160, 161, 163	0
All	All	841/972 (86%)	1.14	197 (23%) 0 0	18, 49, 163, 167	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	GLY	16.6
2	F	407	VAL	14.1
1	A	344	LEU	12.6
1	B	286	GLU	12.3
1	C	334	VAL	10.8
1	C	289	PRO	10.8
1	C	287	VAL	10.8
1	C	263	GLY	10.3
2	E	409	TRP	9.9
1	A	260	GLY	9.7
1	B	335	VAL	9.6
1	B	300	VAL	9.6
1	C	344	LEU	9.5
1	B	288	SER	8.9
1	A	289	PRO	8.7
1	A	333	VAL	8.7
1	C	282	ILE	8.6
2	D	409	TRP	8.4
1	B	290	ASP	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	299	GLN	8.1
1	C	288	SER	8.1
1	A	287	VAL	8.0
1	C	181	LEU	7.7
1	C	184	THR	7.5
2	D	408	TYR	7.5
2	F	409	TRP	7.4
1	C	299	GLN	7.4
1	A	311	PRO	7.4
1	C	309	ASN	7.2
1	C	286	GLU	7.2
1	C	328	GLY	7.2
1	B	287	VAL	7.0
2	D	407	VAL	6.9
1	C	295	ASN	6.9
1	A	299	GLN	6.8
1	A	294	ALA	6.7
1	C	330	VAL	6.6
1	B	66	LEU	6.6
1	B	289	PRO	6.6
1	C	291	GLY	6.5
2	E	408	TYR	6.5
1	A	312	ALA	6.5
1	B	305	ILE	6.4
1	B	292	PRO	6.4
1	B	298	ILE	6.3
1	C	300	VAL	6.2
1	C	283	VAL	6.2
1	C	294	ALA	6.2
1	C	318	THR	6.1
1	A	258	TYR	6.1
1	C	333	VAL	6.1
1	B	224	ASN	6.0
2	F	410	PHE	6.0
1	C	292	PRO	6.0
1	A	305	ILE	5.9
1	A	301	ASN	5.9
1	A	300	VAL	5.9
1	C	335	VAL	5.9
1	B	186	ARG	5.8
1	B	184	THR	5.7
1	A	288	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	5.6
1	C	285	ASN	5.6
2	F	408	TYR	5.5
1	C	284	VAL	5.5
1	B	311	PRO	5.4
1	A	286	GLU	5.4
1	A	290	ASP	5.4
1	C	183	PRO	5.3
1	C	182	ASN	5.3
1	C	349	GLN	5.1
1	A	349	GLN	5.1
1	A	298	ILE	5.1
1	A	292	PRO	5.0
1	A	347	THR	5.0
1	B	183	PRO	5.0
1	B	221	ASP	5.0
1	A	293	ALA	4.9
1	B	283	VAL	4.9
1	A	318	THR	4.8
1	A	335	VAL	4.8
1	A	303	LEU	4.7
1	A	181	LEU	4.7
1	B	301	ASN	4.7
1	C	261	ILE	4.6
1	A	259	ILE	4.6
1	A	261	ILE	4.6
1	A	329	SER	4.5
1	A	334	VAL	4.5
1	C	347	THR	4.5
1	B	344	LEU	4.5
1	A	309	ASN	4.4
1	B	293	ALA	4.4
1	A	186	ARG	4.4
1	C	311	PRO	4.4
1	C	298	ILE	4.3
1	A	345	GLN	4.3
1	B	285	ASN	4.3
1	C	329	SER	4.3
1	A	182	ASN	4.3
1	B	73	GLN	4.2
1	A	296	ALA	4.2
1	C	346	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	65	GLY	4.2
1	C	297	GLY	4.2
1	A	285	ASN	4.2
1	B	294	ALA	4.2
1	A	284	VAL	4.1
1	B	320	ASP	4.1
1	B	262	GLY	4.1
1	A	291	GLY	4.1
1	B	303	LEU	4.1
1	B	345	GLN	4.0
1	B	333	VAL	4.0
1	B	351	TYR	4.0
1	C	306	SER	4.0
1	B	318	THR	3.9
1	A	330	VAL	3.9
1	C	351	TYR	3.9
1	A	183	PRO	3.9
1	C	224	ASN	3.8
1	C	301	ASN	3.8
1	B	259	ILE	3.7
1	A	282	ILE	3.6
1	B	331	ILE	3.6
1	B	77	ARG	3.6
1	C	345	GLN	3.6
1	B	223	SER	3.6
1	B	182	ASN	3.6
1	C	258	TYR	3.6
1	B	347	THR	3.5
1	B	75	GLU	3.4
1	C	326	ARG	3.4
1	B	282	ILE	3.4
1	C	293	ALA	3.4
1	A	351	TYR	3.4
1	B	284	VAL	3.4
1	A	325	ILE	3.4
2	E	407	VAL	3.4
1	A	310	LYS	3.3
1	C	321	GLN	3.3
1	B	295	ASN	3.3
1	A	332	PRO	3.2
1	A	346	VAL	3.2
1	A	42	MET	3.2

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

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Mol	Chain	Res	Type	RSRZ
1	C	352	PRO	2.4
1	A	184	THR	2.4
1	C	100	ASP	2.3
1	C	320	ASP	2.3
1	B	307	VAL	2.2
1	C	260	GLY	2.2
1	C	304	ILE	2.2
1	A	221	ASP	2.1
1	A	308	ASP	2.0
1	A	324	GLU	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.