Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 01:33 PM EDT

PDB ID	:	3QO6
Title	:	Crystal structure analysis of the plant protease Deg1
Authors	:	Clausen, T.
Deposited on	:	2011-02-09
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

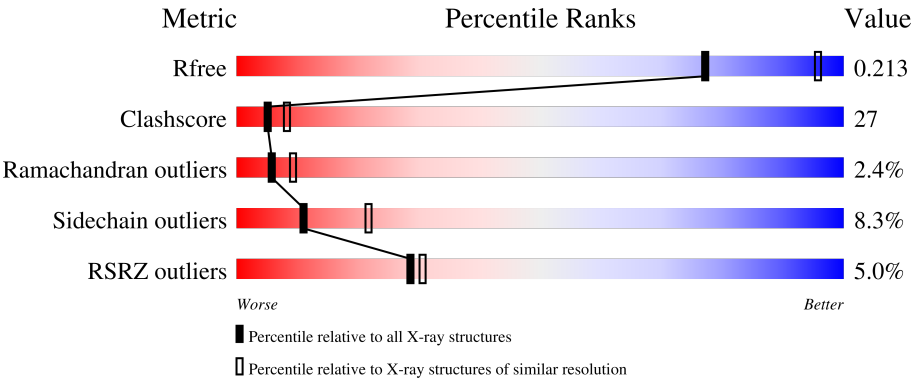
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	348	6% 49% 39% 6% 6%
1	B	348	3% 52% 37% 5% 6%
1	C	348	5% 62% 28% · 6%
2	D	7	100%
3	E	4	100%

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Mol	Chain	Length	Quality of chain
3	H	4	75% 25%
3	I	4	100%
4	F	5	100%
5	G	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7566 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 Do-like 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2420	1524	422	473	1			
1	B	328	Total	C	N	O	S	0	0	0
			2437	1533	424	479	1			
1	C	328	Total	C	N	O	S	0	0	0
			2433	1531	424	477	1			

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	0	0	0
			35	21	7	7			

- Molecule 3 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			20	12	4	4			
3	H	4	Total	C	N	O	0	0	0
			21	12	4	5			
3	I	4	Total	C	N	O	0	0	0
			21	12	4	5			

- Molecule 4 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 5 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			16	9	3	4			

- Molecule 6 is water.

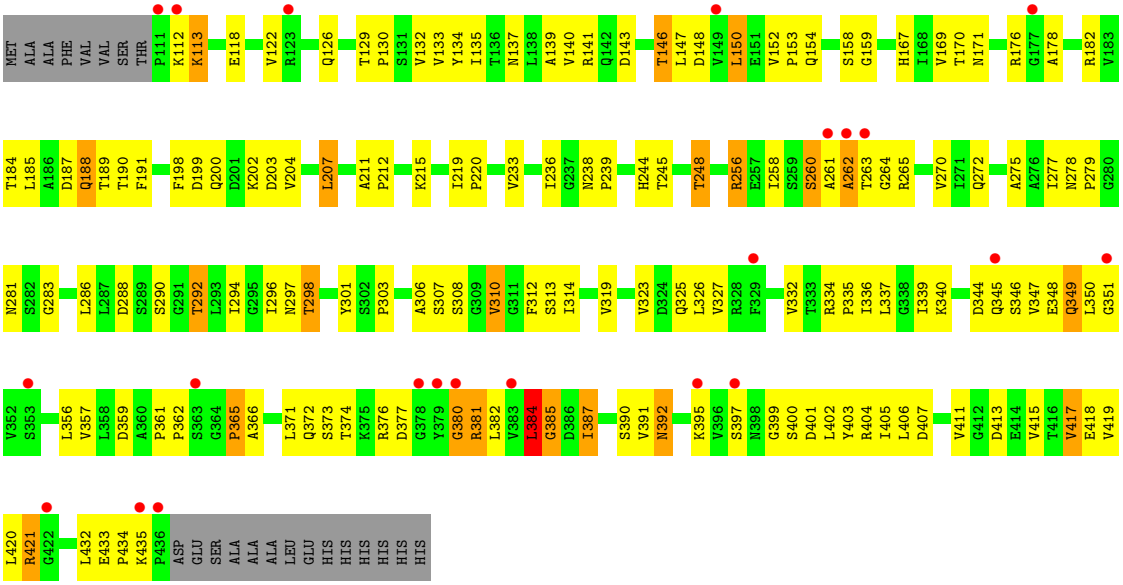
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	44	Total	O	0	0
			44	44		
6	C	48	Total	O	0	0
			48	48		
6	D	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

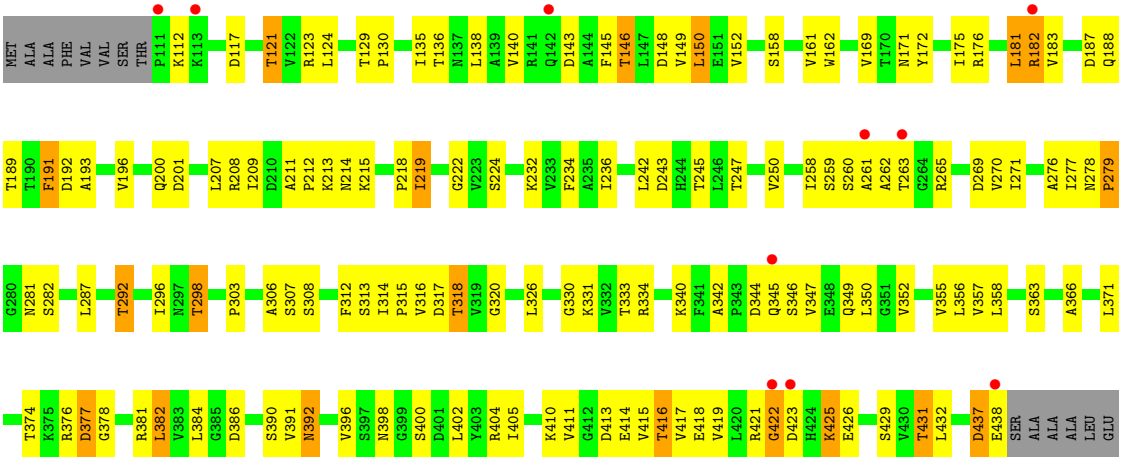
• Molecule 1: Protease Do-like 1, chloroplastic

Chain A:



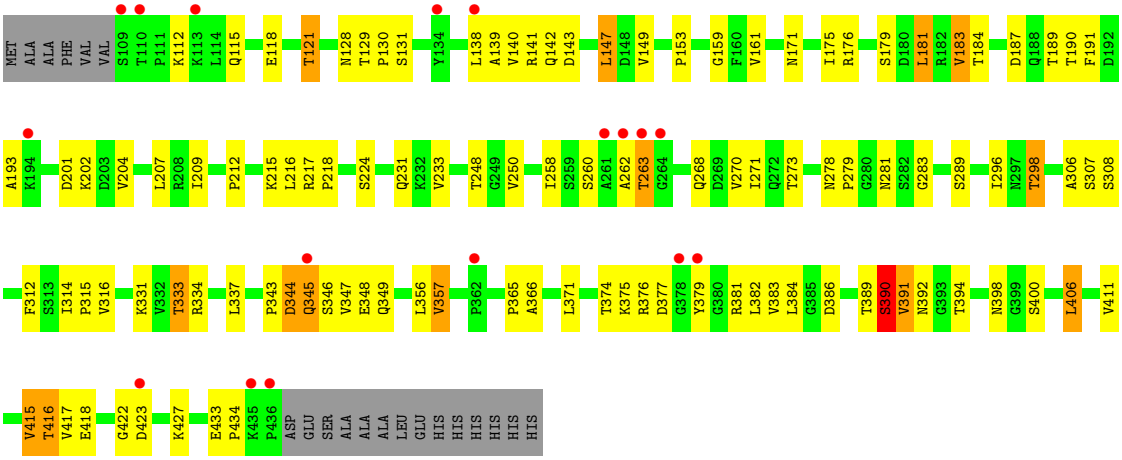
• Molecule 1: Protease Do-like 1, chloroplastic

Chain B:



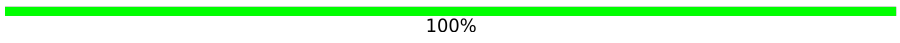
• Molecule 1: Protease Do-like 1, chloroplastic

Chain C:



• Molecule 2: peptide

Chain D:



There are no outlier residues recorded for this chain.

• Molecule 3: peptide

Chain E:

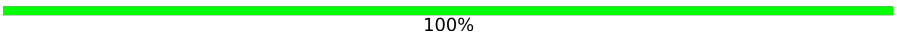
There are no outlier residues recorded for this chain.

• Molecule 3: peptide

Chain H:

• Molecule 3: peptide

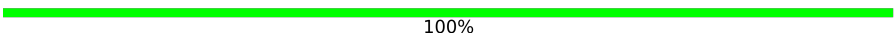
Chain I:



There are no outlier residues recorded for this chain.

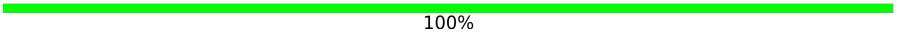
• Molecule 4: peptide

Chain F:



There are no outlier residues recorded for this chain.

• Molecule 5: peptide

Chain G: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.14Å 126.14Å 328.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 14.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.50) 98.2 (14.96-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.268 0.208 , 0.213	Depositor DCC
R_{free} test set	2689 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7566	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.53	0/2459	0.78	1/3345 (0.0%)
1	B	0.56	0/2476	0.81	0/3368
1	C	0.57	0/2472	0.80	2/3364 (0.1%)
All	All	0.55	0/7407	0.80	3/10077 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	181	LEU	CA-CB-CG	6.14	129.41	115.30
1	C	382	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	264	GLY	N-CA-C	5.55	126.97	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2420	0	2470	158	0
1	B	2437	0	2480	155	1
1	C	2433	0	2481	103	0
2	D	35	0	9	0	0
3	E	20	0	6	0	0
3	H	21	0	6	1	0
3	I	21	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	25	0	7	0	0
5	G	16	0	5	0	0
6	A	44	0	0	3	0
6	B	44	0	0	4	0
6	C	48	0	0	6	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
All	All	7566	0	7470	401	1

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 27.

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:339:ILE:HD11	1:A:357:VAL:HG13	1.32	1.09
1:A:135:ILE:HD12	1:A:170:THR:HG21	1.39	1.02
1:B:175:ILE:HD12	1:B:181:LEU:HD22	1.39	1.01
1:C:374:THR:HG23	1:C:384:LEU:HA	1.42	1.00
1:B:391:VAL:HG11	1:B:405:ILE:HG21	1.43	0.97
1:C:398:ASN:HD21	1:C:400:SER:HB3	1.27	0.95
1:B:222:GLY:HA3	1:B:292:THR:CG2	1.98	0.94
1:A:339:ILE:CD1	1:A:357:VAL:HG13	1.97	0.93
1:A:265:ARG:HG3	1:A:265:ARG:HH11	1.35	0.89
1:C:278:ASN:H	1:C:281:ASN:HD22	1.20	0.87
1:B:224:SER:HB3	1:B:316:VAL:HG12	1.57	0.86
1:C:139:ALA:HA	1:C:179:SER:HB3	1.58	0.86
1:B:298:THR:HG21	1:B:314:ILE:HG12	1.59	0.83
1:B:278:ASN:H	1:B:281:ASN:HD22	1.27	0.82
1:A:158:SER:HB3	1:A:238:ASN:ND2	1.96	0.81
1:C:375:LYS:HD2	1:C:376:ARG:H	1.44	0.81
1:A:278:ASN:H	1:A:281:ASN:HD22	1.28	0.81
1:A:262:ALA:O	1:A:263:THR:HG23	1.81	0.80
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.46	0.79
1:A:143:ASP:O	1:A:147:LEU:HA	1.83	0.78
1:A:260:SER:HB2	1:A:265:ARG:O	1.83	0.78
1:B:392:ASN:HD21	1:B:415:VAL:HG22	1.48	0.78
1:A:400:SER:O	1:A:404:ARG:HB2	1.84	0.77
1:A:376:ARG:HD2	1:A:380:GLY:O	1.83	0.77
1:B:334:ARG:HG2	1:B:334:ARG:HH11	1.50	0.77
1:A:405:ILE:HG23	1:A:406:LEU:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:THR:HG21	1:C:112:LYS:NZ	2.00	0.76
1:A:256:ARG:NH1	1:A:272:GLN:OE1	2.20	0.74
1:A:349:GLN:H	1:A:349:GLN:NE2	1.85	0.74
1:A:202:LYS:O	1:A:204:VAL:HG23	1.88	0.74
1:B:222:GLY:HA3	1:B:292:THR:HG23	1.69	0.73
1:C:176:ARG:HG2	1:C:176:ARG:HH11	1.53	0.73
1:A:265:ARG:HG3	1:A:265:ARG:NH1	2.01	0.73
1:C:344:ASP:OD2	1:C:398:ASN:HB2	1.90	0.72
1:B:315:PRO:HG2	1:B:318:THR:HG23	1.71	0.72
1:C:381:ARG:HG3	1:C:381:ARG:HH11	1.53	0.72
1:B:172:TYR:HE2	1:B:200:GLN:HE21	1.36	0.72
1:B:356:LEU:HD22	1:B:358:LEU:HD23	1.71	0.72
6:A:459:HOH:O	1:C:231:GLN:HG2	1.87	0.72
1:B:189:THR:HG21	1:B:215:LYS:NZ	2.05	0.71
1:B:187:ASP:OD2	1:B:215:LYS:HE3	1.91	0.71
1:B:402:LEU:O	1:B:405:ILE:HG22	1.89	0.71
1:B:344:ASP:OD1	1:B:398:ASN:HB2	1.90	0.71
1:B:146:THR:HG22	1:B:148:ASP:H	1.55	0.71
1:B:189:THR:HG21	1:B:215:LYS:HZ2	1.53	0.71
1:B:260:SER:C	1:B:262:ALA:H	1.93	0.71
1:A:401:ASP:O	1:A:405:ILE:HG22	1.90	0.71
1:A:339:ILE:HD12	1:A:340:LYS:H	1.54	0.70
1:A:351:GLY:HA2	6:A:464:HOH:O	1.91	0.70
1:C:298:THR:HG21	1:C:314:ILE:HD12	1.74	0.70
1:B:349:GLN:C	1:B:350:LEU:HD22	2.11	0.70
1:A:297:ASN:HA	1:A:313:SER:HB3	1.73	0.70
1:C:331:LYS:HE2	1:C:333:THR:HG23	1.71	0.70
1:A:135:ILE:CD1	1:A:170:THR:HG21	2.18	0.69
1:A:345:GLN:HA	1:A:348:GLU:OE1	1.92	0.69
1:A:323:VAL:O	1:A:327:VAL:HG23	1.92	0.69
1:B:146:THR:CG2	1:B:148:ASP:H	2.05	0.69
1:C:398:ASN:ND2	1:C:400:SER:HB3	2.06	0.69
1:A:139:ALA:HB2	1:A:154:GLN:OE1	1.94	0.68
1:C:224:SER:HB3	1:C:316:VAL:HG12	1.76	0.68
1:B:222:GLY:CA	1:B:292:THR:HG23	2.24	0.68
1:A:298:THR:HG21	1:A:314:ILE:HD12	1.75	0.67
1:B:392:ASN:HB3	1:B:416:THR:HG23	1.77	0.67
1:B:392:ASN:ND2	1:B:415:VAL:HG22	2.10	0.67
1:B:278:ASN:ND2	1:B:307:SER:H	1.93	0.66
1:A:392:ASN:ND2	1:A:415:VAL:HG13	2.09	0.66
1:B:260:SER:O	1:B:262:ALA:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLY:HA3	1:B:292:THR:HG21	1.77	0.66
1:B:172:TYR:CE2	1:B:200:GLN:HG2	2.31	0.66
1:B:278:ASN:H	1:B:281:ASN:ND2	1.95	0.65
1:C:391:VAL:HG13	1:C:415:VAL:HG13	1.78	0.65
1:C:381:ARG:HG3	1:C:381:ARG:NH1	2.09	0.65
1:A:349:GLN:H	1:A:349:GLN:CD	1.98	0.65
1:C:187:ASP:OD2	1:C:189:THR:HG23	1.97	0.65
1:A:143:ASP:HB3	1:A:146:THR:HG22	1.78	0.64
1:A:191:PHE:CE2	1:A:211:ALA:HB2	2.32	0.64
1:A:308:SER:CB	1:B:306:ALA:HB1	2.27	0.64
1:B:392:ASN:ND2	1:B:415:VAL:HG13	2.13	0.64
1:C:377:ASP:C	1:C:379:TYR:H	2.00	0.64
1:B:143:ASP:CG	1:B:146:THR:HB	2.19	0.63
1:A:356:LEU:HD12	1:A:357:VAL:N	2.12	0.63
1:B:421:ARG:HG2	1:B:422:GLY:H	1.62	0.63
6:B:458:HOH:O	1:C:121:THR:HG21	1.99	0.63
1:A:256:ARG:NH2	1:B:243:ASP:O	2.32	0.63
1:C:278:ASN:H	1:C:281:ASN:ND2	1.95	0.63
1:A:303:PRO:HD2	1:B:306:ALA:HB2	1.80	0.62
1:B:391:VAL:HG11	1:B:405:ILE:CG2	2.25	0.62
1:A:112:LYS:O	1:A:113:LYS:HB3	1.99	0.62
1:B:419:VAL:HG22	1:B:426:GLU:HB2	1.82	0.62
1:A:399:GLY:O	1:A:403:TYR:HB2	2.00	0.61
1:B:392:ASN:HB3	1:B:416:THR:CG2	2.30	0.61
1:A:137:ASN:ND2	1:A:178:ALA:HB2	2.15	0.61
1:B:222:GLY:CA	1:B:292:THR:CG2	2.76	0.61
1:C:191:PHE:HB2	1:C:209:ILE:HD12	1.81	0.61
1:C:258:ILE:HG13	1:C:258:ILE:O	2.00	0.61
1:A:392:ASN:CG	1:A:415:VAL:HG13	2.20	0.61
1:A:278:ASN:H	1:A:281:ASN:ND2	1.98	0.61
1:C:391:VAL:HG12	1:C:392:ASN:N	2.16	0.61
1:B:350:LEU:HB2	1:B:352:VAL:HG23	1.83	0.60
1:A:159:GLY:CA	1:A:170:THR:HG22	2.30	0.60
1:B:334:ARG:HG2	1:B:334:ARG:NH1	2.08	0.60
1:C:139:ALA:HA	1:C:179:SER:CB	2.32	0.60
1:B:172:TYR:CZ	1:B:176:ARG:HG2	2.37	0.59
1:A:270:VAL:CG1	1:A:312:PHE:HB3	2.32	0.59
1:A:345:GLN:HG3	1:A:348:GLU:OE1	2.02	0.59
1:A:146:THR:HG23	1:A:148:ASP:CG	2.23	0.59
1:B:129:THR:HG22	1:B:130:PRO:HD3	1.84	0.59
1:B:182:ARG:HH11	1:B:182:ARG:CG	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:HB3	1:A:238:ASN:HD22	1.67	0.59
1:C:184:THR:HG23	1:C:190:THR:HG22	1.85	0.59
1:B:331:LYS:HE3	1:B:437:ASP:OD2	2.03	0.58
1:A:275:ALA:O	1:A:277:ILE:HG12	2.03	0.58
1:A:308:SER:HB3	1:B:306:ALA:HB1	1.83	0.58
1:A:395:LYS:HG3	1:A:395:LYS:O	2.02	0.58
1:A:159:GLY:HA3	1:A:170:THR:CG2	2.34	0.58
1:B:129:THR:CG2	1:B:130:PRO:HD3	2.32	0.58
1:B:270:VAL:HG11	1:B:312:PHE:HB3	1.85	0.58
1:C:374:THR:CG2	1:C:384:LEU:HA	2.28	0.58
1:A:411:VAL:HG11	1:A:434:PRO:HD3	1.86	0.58
1:B:161:VAL:HG12	1:B:218:PRO:HA	1.84	0.58
1:C:296:ILE:O	1:C:298:THR:HG22	2.04	0.58
1:A:278:ASN:ND2	1:A:307:SER:H	2.02	0.57
1:A:387:ILE:HG12	1:A:387:ILE:O	2.05	0.57
1:A:405:ILE:HG23	1:A:406:LEU:N	2.20	0.57
1:C:129:THR:N	1:C:130:PRO:HD2	2.20	0.57
1:B:187:ASP:O	1:B:188:GLN:HB2	2.05	0.57
1:B:377:ASP:HB2	1:B:381:ARG:HB2	1.86	0.57
1:B:398:ASN:HD21	1:B:400:SER:HB3	1.69	0.57
1:A:187:ASP:OD1	1:A:215:LYS:HE3	2.05	0.56
1:A:158:SER:O	1:A:170:THR:HG22	2.05	0.56
1:B:350:LEU:HD22	1:B:350:LEU:N	2.20	0.56
1:B:175:ILE:HD12	1:B:181:LEU:CD2	2.26	0.56
1:B:342:ALA:HB2	1:B:358:LEU:HD21	1.86	0.56
1:C:159:GLY:HA2	1:C:283:GLY:O	2.06	0.55
1:A:143:ASP:CB	1:A:146:THR:HG22	2.37	0.55
1:A:211:ALA:HB1	1:A:212:PRO:HD2	1.86	0.55
1:A:129:THR:N	1:A:130:PRO:CD	2.69	0.55
1:B:183:VAL:CG2	1:B:209:ILE:HG21	2.36	0.55
1:C:128:ASN:C	1:C:130:PRO:HD2	2.26	0.55
1:C:260:SER:C	1:C:262:ALA:H	2.10	0.55
1:C:278:ASN:ND2	1:C:307:SER:H	2.05	0.55
1:A:239:PRO:HB3	1:A:281:ASN:ND2	2.22	0.55
1:A:411:VAL:CG1	1:A:434:PRO:HD3	2.37	0.54
1:B:278:ASN:HD21	1:B:307:SER:H	1.55	0.54
1:C:383:VAL:HA	6:C:461:HOH:O	2.08	0.54
1:A:187:ASP:O	1:A:188:GLN:HB2	2.06	0.54
1:B:270:VAL:CG1	1:B:312:PHE:HB3	2.37	0.54
1:A:187:ASP:OD2	1:A:189:THR:HG23	2.07	0.54
1:B:320:GLY:HA3	6:B:8:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:O	1:B:423:ASP:N	2.39	0.54
1:A:296:ILE:HG13	1:A:319:VAL:HG21	1.90	0.54
1:A:339:ILE:HD12	1:A:340:LYS:N	2.22	0.54
1:B:129:THR:N	1:B:130:PRO:CD	2.71	0.54
1:B:143:ASP:HB3	1:B:146:THR:HG22	1.88	0.54
1:B:306:ALA:HB3	6:B:44:HOH:O	2.08	0.54
1:B:121:THR:HB	1:B:234:PHE:HE1	1.72	0.53
1:C:202:LYS:O	1:C:204:VAL:HG23	2.08	0.53
1:A:377:ASP:OD1	1:A:381:ARG:HG3	2.08	0.53
1:A:306:ALA:HB1	1:C:308:SER:OG	2.07	0.53
1:B:232:LYS:HG3	1:C:118:GLU:HB3	1.90	0.53
1:C:260:SER:HG	1:C:263:THR:HG22	1.74	0.53
1:B:191:PHE:N	1:B:191:PHE:CD2	2.75	0.53
1:B:390:SER:OG	1:B:418:GLU:HB3	2.09	0.53
1:A:176:ARG:HG2	1:A:176:ARG:HH11	1.74	0.52
1:C:422:GLY:O	1:C:423:ASP:HB2	2.08	0.52
1:B:333:THR:HG22	1:B:411:VAL:HG21	1.91	0.52
1:C:375:LYS:HD2	1:C:376:ARG:N	2.20	0.52
1:A:158:SER:O	1:A:170:THR:CG2	2.58	0.52
1:A:392:ASN:ND2	1:A:415:VAL:HG22	2.25	0.52
1:C:176:ARG:NH2	6:C:34:HOH:O	2.41	0.52
1:C:375:LYS:O	1:C:383:VAL:N	2.40	0.52
1:B:292:THR:HG21	1:C:112:LYS:HZ2	1.75	0.52
1:C:142:GLN:HE21	1:C:147:LEU:CA	2.22	0.52
1:A:390:SER:HB3	1:A:418:GLU:HB3	1.91	0.52
1:A:167:HIS:HA	1:A:207:LEU:O	2.09	0.52
1:C:377:ASP:OD2	1:C:379:TYR:HB3	2.09	0.51
1:A:359:ASP:O	1:A:361:PRO:HD3	2.09	0.51
1:A:248:THR:HG22	6:C:458:HOH:O	2.09	0.51
1:A:392:ASN:HB3	1:A:415:VAL:HG13	1.91	0.51
1:B:345:GLN:C	1:B:347:VAL:H	2.14	0.51
1:A:141:ARG:HB2	1:A:150:LEU:CD1	2.41	0.51
1:B:292:THR:HG21	1:C:112:LYS:HZ3	1.71	0.51
1:B:219:ILE:HD12	1:B:219:ILE:O	2.11	0.51
1:A:374:THR:HA	1:A:385:GLY:H	1.76	0.50
1:B:260:SER:C	1:B:262:ALA:N	2.63	0.50
1:C:344:ASP:O	1:C:346:SER:N	2.37	0.50
1:B:124:LEU:C	1:B:124:LEU:HD23	2.31	0.50
1:B:344:ASP:O	1:B:347:VAL:HG12	2.12	0.50
1:C:344:ASP:C	1:C:346:SER:H	2.13	0.50
1:C:201:ASP:HB2	1:C:334:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ASN:HD21	1:C:400:SER:CB	2.10	0.50
1:A:258:ILE:O	1:A:258:ILE:HD12	2.11	0.50
1:C:138:LEU:CD2	1:C:153:PRO:HD3	2.41	0.50
1:A:391:VAL:HG12	1:A:415:VAL:HG11	1.92	0.50
1:B:181:LEU:HD12	1:B:193:ALA:HB3	1.92	0.50
1:A:336:ILE:HG21	1:A:435:LYS:HB3	1.94	0.50
1:A:122:VAL:O	1:A:126:GLN:HB2	2.12	0.49
1:A:171:ASN:HA	1:A:203:ASP:O	2.12	0.49
1:B:149:VAL:CG1	1:B:150:LEU:N	2.75	0.49
1:B:308:SER:OG	1:C:306:ALA:HB1	2.11	0.49
1:A:325:GLN:HG3	1:A:332:VAL:HG23	1.94	0.49
1:B:138:LEU:N	1:B:138:LEU:HD12	2.27	0.49
1:B:191:PHE:N	1:B:191:PHE:HD2	2.10	0.49
1:A:260:SER:C	1:A:262:ALA:H	2.16	0.49
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.77	0.49
1:B:340:LYS:HA	3:H:2:UNK:O	2.12	0.49
1:C:260:SER:OG	1:C:263:THR:HG22	2.13	0.49
1:A:270:VAL:HG11	1:A:312:PHE:HB3	1.94	0.49
1:B:271:ILE:O	1:B:312:PHE:HA	2.12	0.49
1:B:392:ASN:CB	1:B:416:THR:HG23	2.41	0.49
1:A:391:VAL:CG1	1:A:415:VAL:HG11	2.43	0.49
1:C:270:VAL:HA	1:C:315:PRO:HD3	1.95	0.49
1:A:339:ILE:HG12	1:A:357:VAL:HG22	1.95	0.49
1:A:159:GLY:HA3	1:A:170:THR:HG22	1.93	0.48
1:B:376:ARG:O	1:B:378:GLY:N	2.46	0.48
1:C:212:PRO:HG2	1:C:215:LYS:HD2	1.95	0.48
1:A:337:LEU:HB2	1:A:406:LEU:HD21	1.94	0.48
1:C:381:ARG:HH11	1:C:381:ARG:CG	2.23	0.48
1:C:171:ASN:ND2	1:C:298:THR:HB	2.29	0.48
1:C:391:VAL:O	1:C:416:THR:O	2.32	0.48
1:B:191:PHE:CE1	1:B:211:ALA:HB2	2.48	0.48
1:A:202:LYS:HG2	1:A:334:ARG:HH22	1.77	0.48
1:A:349:GLN:NE2	1:A:349:GLN:N	2.58	0.48
1:A:420:LEU:HD12	1:A:421:ARG:N	2.29	0.48
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.78	0.48
1:B:391:VAL:HG13	1:B:391:VAL:O	2.13	0.48
1:B:183:VAL:HG21	1:B:209:ILE:HG21	1.96	0.48
1:C:176:ARG:HG2	1:C:176:ARG:NH1	2.24	0.48
1:C:260:SER:C	1:C:262:ALA:N	2.67	0.48
1:A:132:VAL:HG21	1:A:236:ILE:HG21	1.96	0.48
1:A:392:ASN:CB	1:A:415:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:THR:HB	1:B:234:PHE:CE1	2.49	0.47
1:B:421:ARG:CG	1:B:422:GLY:H	2.25	0.47
1:A:399:GLY:C	1:A:401:ASP:N	2.63	0.47
1:B:234:PHE:N	1:B:234:PHE:CD2	2.82	0.47
1:C:183:VAL:HG13	1:C:193:ALA:HB2	1.96	0.47
1:C:260:SER:HB2	6:C:23:HOH:O	2.15	0.47
1:B:146:THR:CG2	1:B:148:ASP:HB2	2.43	0.47
1:B:376:ARG:HE	1:B:382:LEU:CD1	2.28	0.47
1:C:202:LYS:O	1:C:314:ILE:HD13	2.13	0.47
1:A:159:GLY:HA2	1:A:283:GLY:O	2.14	0.47
1:A:372:GLN:CD	1:A:421:ARG:NH1	2.68	0.47
1:A:411:VAL:HG13	1:A:433:GLU:HA	1.97	0.47
1:C:392:ASN:HD21	1:C:415:VAL:HA	1.79	0.47
1:C:418:GLU:HG3	1:C:427:LYS:HG2	1.97	0.47
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.14	0.47
1:A:344:ASP:O	1:A:347:VAL:HG12	2.15	0.47
1:A:359:ASP:HA	1:A:373:SER:HB3	1.97	0.47
1:C:131:SER:HG	1:C:217:ARG:HG2	1.79	0.47
1:B:260:SER:CB	1:B:265:ARG:O	2.63	0.47
1:A:371:LEU:CD1	1:A:419:VAL:HG11	2.45	0.47
1:B:222:GLY:N	1:B:292:THR:HG23	2.30	0.47
1:A:141:ARG:HB2	1:A:150:LEU:HD11	1.97	0.46
1:B:181:LEU:CD1	1:B:193:ALA:HB3	2.46	0.46
1:C:176:ARG:HH11	1:C:176:ARG:CG	2.24	0.46
1:A:334:ARG:O	1:A:434:PRO:HA	2.15	0.46
1:B:145:PHE:CD1	1:B:145:PHE:N	2.83	0.46
1:B:258:ILE:HG12	1:B:270:VAL:HG21	1.97	0.46
1:C:398:ASN:ND2	1:C:400:SER:H	2.13	0.46
1:B:278:ASN:N	1:B:281:ASN:HD22	2.05	0.46
1:B:298:THR:CG2	1:B:314:ILE:HG12	2.39	0.46
1:B:392:ASN:HD22	1:B:415:VAL:HA	1.80	0.46
1:C:391:VAL:HG13	1:C:415:VAL:CG1	2.42	0.46
1:B:247:THR:HG21	1:B:276:ALA:HB3	1.98	0.46
1:A:134:TYR:HB3	1:A:184:THR:HB	1.97	0.46
1:B:398:ASN:HD22	1:B:400:SER:N	2.13	0.46
1:A:292:THR:HG21	1:B:112:LYS:NZ	2.30	0.46
1:B:350:LEU:N	1:B:350:LEU:CD2	2.79	0.46
1:C:356:LEU:HD21	1:C:384:LEU:HB2	1.98	0.46
1:B:175:ILE:CD1	1:B:181:LEU:HD22	2.29	0.45
1:A:152:VAL:HG22	1:A:153:PRO:HD2	1.98	0.45
1:A:391:VAL:HG22	1:A:417:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:OD1	1:B:189:THR:HG23	2.16	0.45
1:B:419:VAL:CG2	1:B:426:GLU:HB2	2.45	0.45
1:C:433:GLU:HB3	1:C:434:PRO:HD2	1.98	0.45
1:A:301:TYR:HB2	1:A:310:VAL:HG22	1.97	0.45
1:A:372:GLN:CD	1:A:421:ARG:HH11	2.19	0.45
1:A:112:LYS:HE3	6:C:467:HOH:O	2.16	0.45
1:B:425:LYS:O	1:B:426:GLU:HG2	2.16	0.45
1:C:357:VAL:HG12	1:C:386:ASP:O	2.16	0.45
1:B:398:ASN:HD22	1:B:400:SER:H	1.65	0.45
1:A:198:PHE:HA	1:A:326:LEU:HD11	1.98	0.45
1:A:290:SER:HB2	1:A:292:THR:HG23	1.99	0.45
1:B:140:VAL:HG13	1:B:149:VAL:CG1	2.46	0.45
1:C:366:ALA:HB1	1:C:371:LEU:HD22	1.98	0.45
1:A:366:ALA:O	1:A:371:LEU:HD23	2.16	0.45
1:B:212:PRO:O	1:B:214:ASN:N	2.50	0.45
1:B:287:LEU:HA	1:B:292:THR:O	2.17	0.45
1:B:392:ASN:N	1:B:416:THR:O	2.34	0.45
1:B:296:ILE:O	1:B:298:THR:HG22	2.17	0.44
1:B:377:ASP:CB	1:B:381:ARG:HB2	2.46	0.44
1:C:118:GLU:HA	1:C:121:THR:HG23	1.99	0.44
1:A:404:ARG:O	1:A:407:ASP:HB3	2.16	0.44
1:A:132:VAL:HG12	1:A:133:VAL:N	2.32	0.44
1:A:239:PRO:HD2	1:A:245:THR:HB	1.99	0.44
1:B:326:LEU:O	1:B:330:GLY:HA2	2.17	0.44
1:A:140:VAL:O	1:A:141:ARG:HD2	2.17	0.44
1:A:190:THR:C	1:A:191:PHE:CD1	2.91	0.44
1:A:376:ARG:HE	1:A:382:LEU:HD23	1.82	0.44
1:A:401:ASP:O	1:A:402:LEU:C	2.55	0.44
1:B:432:LEU:HD12	1:B:432:LEU:H	1.83	0.44
1:C:357:VAL:CG1	1:C:386:ASP:O	2.66	0.44
1:A:345:GLN:HA	1:A:348:GLU:CD	2.37	0.44
1:A:347:VAL:O	1:A:347:VAL:HG22	2.16	0.44
1:B:437:ASP:O	1:B:438:GLU:HG2	2.17	0.44
1:C:337:LEU:C	1:C:365:PRO:HG2	2.38	0.44
1:A:132:VAL:HG21	1:A:236:ILE:CG2	2.48	0.44
1:A:141:ARG:CG	1:A:152:VAL:HG12	2.47	0.44
1:A:219:ILE:HG13	1:A:220:PRO:HD2	2.00	0.44
1:B:135:ILE:HG12	1:B:183:VAL:HG12	1.99	0.44
1:B:138:LEU:N	1:B:138:LEU:CD1	2.81	0.44
1:B:172:TYR:CD2	1:B:200:GLN:HG2	2.53	0.44
1:C:129:THR:N	1:C:130:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASP:CG	1:B:265:ARG:HD3	2.38	0.43
1:B:391:VAL:HG23	1:B:417:VAL:HG12	2.00	0.43
1:A:203:ASP:OD1	1:A:262:ALA:HB2	2.18	0.43
1:A:376:ARG:HE	1:A:382:LEU:CD2	2.29	0.43
1:B:182:ARG:CG	1:B:182:ARG:NH1	2.77	0.43
1:B:386:ASP:HB3	1:B:419:VAL:HB	2.00	0.43
1:B:316:VAL:HG13	1:B:317:ASP:N	2.33	0.43
1:B:150:LEU:N	1:B:150:LEU:HD12	2.33	0.43
1:B:366:ALA:HB1	1:B:371:LEU:HD22	2.00	0.43
1:A:256:ARG:HG2	1:B:242:LEU:HD22	2.00	0.43
1:A:298:THR:HG21	1:A:314:ILE:CD1	2.45	0.43
1:B:303:PRO:CG	1:C:306:ALA:HB2	2.47	0.43
1:A:219:ILE:O	1:A:219:ILE:HG23	2.17	0.43
1:A:356:LEU:HD11	1:A:374:THR:OG1	2.19	0.43
1:B:183:VAL:HG22	1:B:209:ILE:HG21	2.00	0.43
1:B:296:ILE:O	1:B:313:SER:HA	2.18	0.43
1:C:161:VAL:HG12	1:C:218:PRO:HA	2.01	0.43
1:C:343:PRO:O	1:C:346:SER:HB3	2.19	0.43
1:C:389:THR:O	1:C:390:SER:HB3	2.17	0.43
1:A:132:VAL:HB	1:A:244:HIS:CE1	2.54	0.43
1:A:349:GLN:HG2	1:A:350:LEU:HD22	2.01	0.43
1:C:176:ARG:NH1	1:C:176:ARG:CG	2.78	0.43
1:A:303:PRO:CD	1:B:306:ALA:HB2	2.45	0.43
1:A:377:ASP:CG	1:A:381:ARG:HG3	2.39	0.43
1:A:211:ALA:HB1	1:A:212:PRO:CD	2.49	0.43
1:B:391:VAL:O	1:B:392:ASN:C	2.57	0.43
1:B:425:LYS:HA	1:B:425:LYS:HD2	1.79	0.43
1:C:175:ILE:HG21	1:C:207:LEU:HD11	2.00	0.43
1:B:398:ASN:ND2	1:B:400:SER:HB3	2.33	0.42
1:B:143:ASP:CB	1:B:146:THR:HG22	2.48	0.42
1:C:149:VAL:HG13	1:C:149:VAL:O	2.19	0.42
1:C:406:LEU:HD12	1:C:406:LEU:HA	1.88	0.42
1:A:159:GLY:HA2	1:A:170:THR:HG22	2.01	0.42
1:A:372:GLN:OE1	1:A:421:ARG:NH1	2.52	0.42
1:B:162:TRP:HB2	1:B:169:VAL:HG23	2.00	0.42
1:A:288:ASP:HB3	1:A:294:ILE:HG21	2.01	0.42
1:C:171:ASN:OD1	1:C:298:THR:HB	2.19	0.42
1:C:270:VAL:HG11	1:C:312:PHE:HB3	2.01	0.42
1:A:278:ASN:O	1:A:279:PRO:C	2.57	0.42
1:B:171:ASN:ND2	1:B:298:THR:HB	2.35	0.42
1:B:236:ILE:HA	1:B:245:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LEU:HD21	1:B:374:THR:OG1	2.19	0.42
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.84	0.42
1:C:375:LYS:CD	1:C:376:ARG:H	2.22	0.42
1:A:187:ASP:OD2	1:A:187:ASP:C	2.58	0.42
1:A:191:PHE:CE2	1:A:211:ALA:CB	3.02	0.42
1:B:260:SER:HB2	1:B:265:ARG:O	2.20	0.42
1:B:276:ALA:O	1:B:277:ILE:HD13	2.19	0.42
1:C:391:VAL:HG12	1:C:392:ASN:H	1.84	0.42
1:C:394:THR:HA	6:C:70:HOH:O	2.19	0.42
1:A:296:ILE:O	1:A:298:THR:CG2	2.68	0.42
1:C:140:VAL:O	1:C:141:ARG:NH1	2.41	0.42
1:A:336:ILE:HG12	1:A:433:GLU:O	2.20	0.41
1:C:296:ILE:O	1:C:298:THR:CG2	2.66	0.41
1:B:196:VAL:CG2	1:B:208:ARG:HB2	2.49	0.41
1:B:278:ASN:HB3	1:B:279:PRO:HD2	2.02	0.41
1:B:146:THR:HG23	1:B:148:ASP:H	1.82	0.41
1:B:355:VAL:HG23	1:B:396:VAL:CG1	2.51	0.41
1:A:335:PRO:HB2	1:A:432:LEU:HD13	2.02	0.41
1:C:271:ILE:O	1:C:312:PHE:HA	2.21	0.41
1:A:233:VAL:HB	1:A:286:LEU:HD11	2.03	0.41
1:B:405:ILE:HD12	1:B:405:ILE:HA	1.81	0.41
1:C:187:ASP:CG	1:C:189:THR:HG23	2.41	0.41
1:A:141:ARG:HG3	1:A:152:VAL:CG1	2.50	0.41
1:A:202:LYS:CG	1:A:334:ARG:HH22	2.33	0.41
1:C:187:ASP:OD2	1:C:189:THR:CG2	2.66	0.41
1:A:169:VAL:O	1:A:170:THR:HG23	2.21	0.41
1:C:142:GLN:NE2	1:C:147:LEU:HB3	2.35	0.41
1:C:143:ASP:O	1:C:147:LEU:HA	2.21	0.41
1:C:189:THR:HG1	1:C:191:PHE:HE1	1.66	0.41
1:A:118:GLU:OE1	1:C:289:SER:OG	2.33	0.41
1:A:278:ASN:HB3	1:A:279:PRO:HD2	2.03	0.41
1:A:346:SER:C	1:A:349:GLN:NE2	2.74	0.41
1:B:414:GLU:HG3	1:B:431:THR:HG23	2.03	0.41
1:B:315:PRO:HG2	1:B:318:THR:CG2	2.46	0.41
1:C:347:VAL:C	1:C:349:GLN:N	2.74	0.41
1:A:199:ASP:OD1	1:A:199:ASP:C	2.58	0.41
1:A:339:ILE:HD13	1:A:357:VAL:HG13	1.93	0.40
1:C:115:GLN:HB2	1:C:118:GLU:HG2	2.03	0.40
1:C:345:GLN:NE2	1:C:348:GLU:OE2	2.54	0.40
1:A:349:GLN:HB3	6:A:33:HOH:O	2.21	0.40
1:A:182:ARG:HG2	1:A:182:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:HG3	1:B:413:ASP:OD1	2.21	0.40
1:C:233:VAL:HG21	1:C:273:THR:OG1	2.20	0.40
1:C:377:ASP:C	1:C:379:TYR:N	2.69	0.40
1:A:141:ARG:HG2	1:A:152:VAL:HG12	2.03	0.40
1:B:381:ARG:NH1	6:B:465:HOH:O	2.55	0.40
1:A:384:LEU:O	1:A:385:GLY:O	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:NH2	1:B:123:ARG:NH2[8_555]	1.47	0.73

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	324/348 (93%)	287 (89%)	26 (8%)	11 (3%)	3 5
1	B	326/348 (94%)	300 (92%)	19 (6%)	7 (2%)	7 11
1	C	326/348 (94%)	300 (92%)	21 (6%)	5 (2%)	10 18
All	All	976/1044 (94%)	887 (91%)	66 (7%)	23 (2%)	6 9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	PRO
1	A	384	LEU
1	B	377	ASP
1	B	422	GLY
1	C	263	THR
1	A	260	SER

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Mol	Chain	Res	Type
1	A	413	ASP
1	B	213	LYS
1	B	261	ALA
1	B	346	SER
1	B	392	ASN
1	C	147	LEU
1	C	345	GLN
1	A	385	GLY
1	A	113	LYS
1	A	261	ALA
1	A	380	GLY
1	A	392	ASN
1	A	262	ALA
1	A	397	SER
1	B	263	THR
1	C	390	SER
1	C	391	VAL

5.3.2 Protein sidechains (i)

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	269/286 (94%)	250 (93%)	19 (7%)	14 28
1	B	271/286 (95%)	241 (89%)	30 (11%)	6 11
1	C	271/286 (95%)	253 (93%)	18 (7%)	16 32
All	All	811/858 (94%)	744 (92%)	67 (8%)	11 22

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	THR
1	A	150	LEU
1	A	185	LEU
1	A	188	GLN
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	248	THR
1	A	256	ARG
1	A	292	THR
1	A	298	THR
1	A	310	VAL
1	A	349	GLN
1	A	362	PRO
1	A	365	PRO
1	A	381	ARG
1	A	384	LEU
1	A	387	ILE
1	A	417	VAL
1	A	421	ARG
1	B	117	ASP
1	B	121	THR
1	B	136	THR
1	B	146	THR
1	B	150	LEU
1	B	152	VAL
1	B	158	SER
1	B	181	LEU
1	B	182	ARG
1	B	191	PHE
1	B	192	ASP
1	B	207	LEU
1	B	219	ILE
1	B	250	VAL
1	B	259	SER
1	B	269	ASP
1	B	279	PRO
1	B	282	SER
1	B	292	THR
1	B	298	THR
1	B	318	THR
1	B	357	VAL
1	B	363	SER
1	B	382	LEU
1	B	384	LEU
1	B	416	THR
1	B	425	LYS
1	B	429	SER

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Mol	Chain	Res	Type
1	B	431	THR
1	B	437	ASP
1	C	121	THR
1	C	181	LEU
1	C	183	VAL
1	C	216	LEU
1	C	248	THR
1	C	250	VAL
1	C	268	GLN
1	C	279	PRO
1	C	298	THR
1	C	333	THR
1	C	344	ASP
1	C	357	VAL
1	C	390	SER
1	C	406	LEU
1	C	411	VAL
1	C	415	VAL
1	C	416	THR
1	C	417	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	278	ASN
1	A	281	ASN
1	A	349	GLN
1	A	372	GLN
1	B	142	GLN
1	B	154	GLN
1	B	278	ASN
1	B	281	ASN
1	B	392	ASN
1	B	398	ASN
1	C	142	GLN
1	C	154	GLN
1	C	278	ASN
1	C	281	ASN
1	C	345	GLN
1	C	372	GLN
1	C	392	ASN

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Mol	Chain	Res	Type
1	C	398	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 monosaccharides 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^{th} 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	326/348 (93%)	0.15	22 (6%)	17	18	49, 88, 135, 151	0
1	B	328/348 (94%)	-0.07	10 (3%)	50	53	47, 78, 116, 136	2 (0%)
1	C	328/348 (94%)	-0.00	17 (5%)	27	29	50, 79, 121, 144	1 (0%)
2	D	0/7	-	-			-	-
3	E	0/4	-	-			-	-
3	H	0/4	-	-			-	-
3	I	0/4	-	-			-	-
4	F	0/5	-	-			-	-
5	G	0/3	-	-			-	-
All	All	982/1071 (91%)	0.02	49 (4%)	28	30	47, 81, 127, 151	3 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	345	GLN	6.5
1	A	262	ALA	6.5
1	A	379	TYR	5.6
1	C	379	TYR	4.6
1	C	109	SER	4.4
1	C	263	THR	4.2
1	B	422	GLY	4.1
1	A	111	PRO	4.1
1	A	378	GLY	4.0
1	A	112	LYS	3.9
1	C	378	GLY	3.8
1	A	261	ALA	3.8
1	A	395	LYS	3.6
1	C	261	ALA	3.5
1	C	362	PRO	3.3
1	A	397	SER	3.0
1	B	423	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	142	GLN	3.0
1	A	263	THR	2.9
1	C	436	PRO	2.9
1	B	261	ALA	2.7
1	C	110	THR	2.7
1	A	149	VAL	2.7
1	C	423	ASP	2.7
1	A	329	PHE	2.6
1	A	380	GLY	2.6
1	A	123	ARG	2.6
1	A	435	LYS	2.6
1	A	383	VAL	2.5
1	A	422	GLY	2.5
1	C	264	GLY	2.5
1	C	435	LYS	2.4
1	C	262	ALA	2.4
1	A	345	GLN	2.4
1	B	345	GLN	2.3
1	A	363	SER	2.3
1	A	353	SER	2.3
1	B	438	GLU	2.3
1	A	351	GLY	2.3
1	B	111	PRO	2.3
1	B	113	LYS	2.3
1	A	177	GLY	2.3
1	B	182	ARG	2.2
1	A	436	PRO	2.2
1	C	113	LYS	2.1
1	C	194	LYS	2.1
1	B	263	THR	2.1
1	C	134	TYR	2.1
1	C	138	LEU	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 monosaccharides 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.