Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 06:57 AM EST

PDB ID	:	1SOZ
Title	:	Crystal Structure of DegS protease in complex with an activating peptide
Authors	:	Wilken, C.; Kitzing, K.; Kurzbauer, R.; Ehrmann, M.; Clausen, T.
Deposited on	:	2004-03-16
Resolution	:	2.40 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:

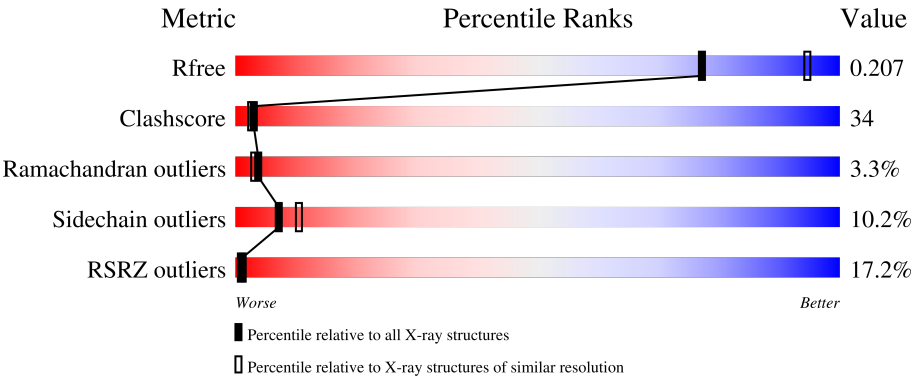
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	314	15% 51% 32% 6% • 11%
1	B	314	16% 51% 34% • 11%
1	C	314	12% 46% 27% 8% 18%
2	D	10	30% 40% 60%
2	E	10	20% 10% 30% 60%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6264 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	281	Total	C	N	O	S	8	0	0
			2034	1271	367	391	5			
1	B	281	Total	C	N	O	S	8	0	0
			2043	1277	366	395	5			
1	C	257	Total	C	N	O	S	8	0	0
			1883	1171	342	365	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	initiating methionine	UNP P31137
B	42	MET	-	initiating methionine	UNP P31137
C	42	MET	-	initiating methionine	UNP P31137

- Molecule 2 is a protein called activating peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			40	28	5	7			
2	E	4	Total	C	N	O	0	0	0
			40	28	5	7			

- Molecule 3 is water.

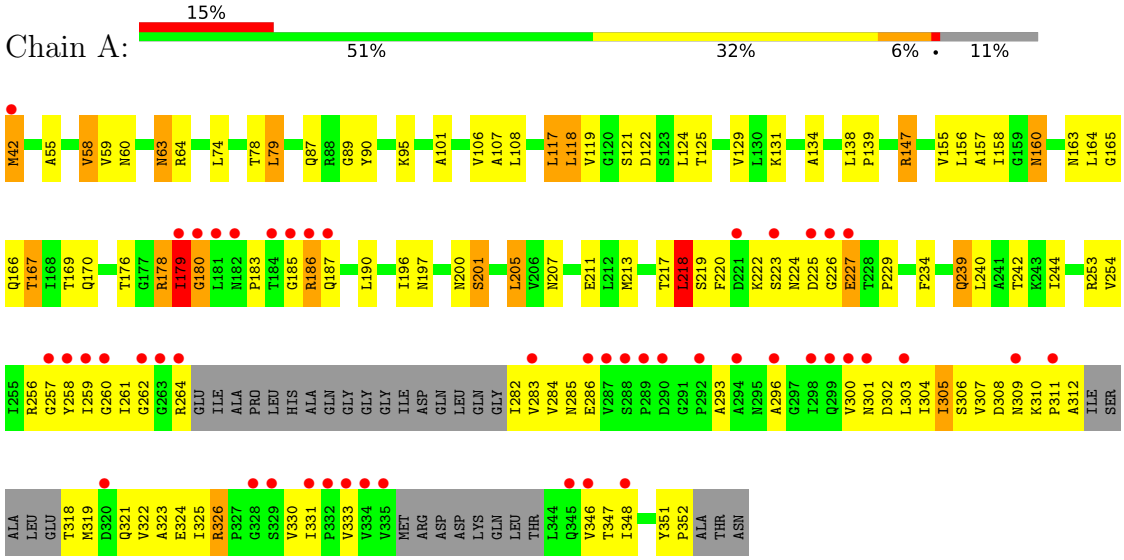
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	56	Total	O	0	0
			56	56		
3	C	66	Total	O	0	0
			66	66		

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.

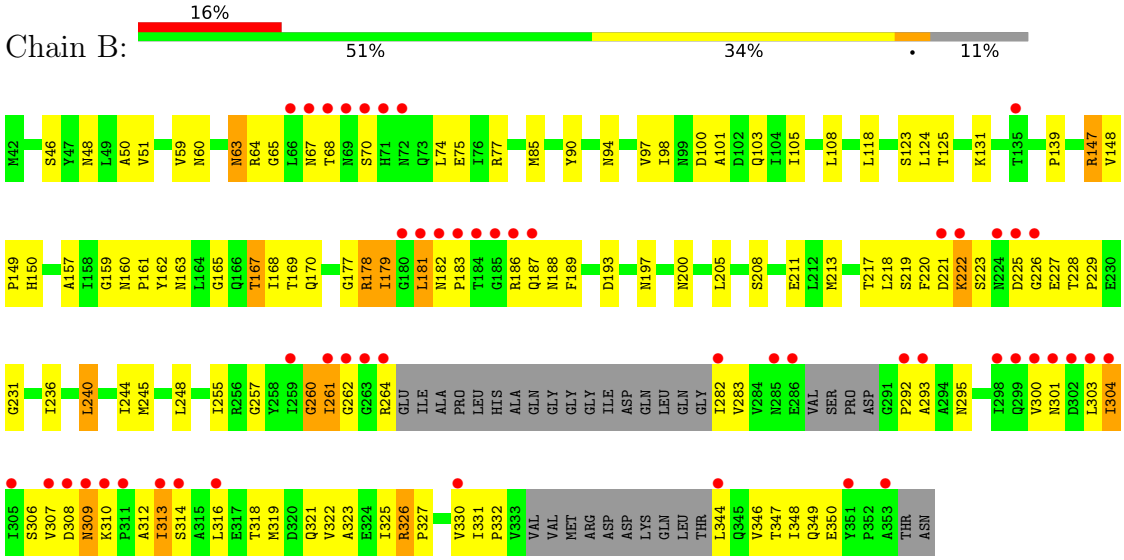
• Molecule 1: Protease degS

Chain A:

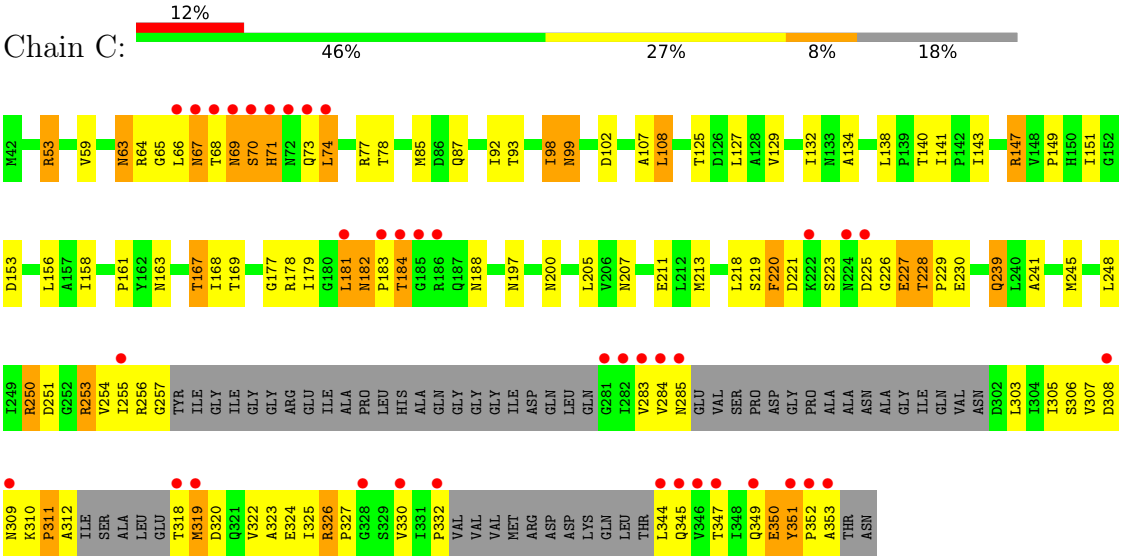


• Molecule 1: Protease degS

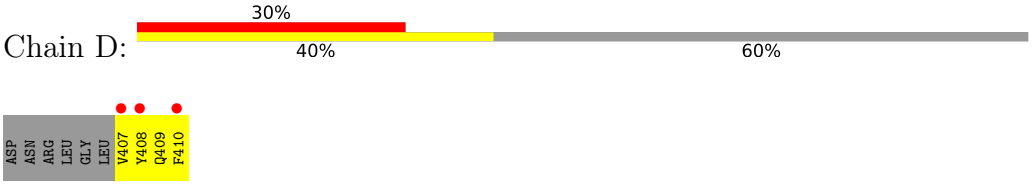
Chain B:



• Molecule 1: Protease degS



• Molecule 2: activating peptide



• Molecule 2: activating peptide

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	205.98Å 142.71Å 41.17Å 90.00° 89.24° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.40) 91.0 (14.94-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.272 0.226 , 0.207	Depositor DCC
R_{free} test set	2135 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.55	0/2060	0.82	1/2805 (0.0%)
1	B	0.49	0/2067	0.77	0/2811
1	C	0.49	0/1905	0.77	0/2589
2	D	0.53	0/41	0.46	0/53
2	E	0.60	0/41	0.33	0/53
All	All	0.51	0/6114	0.78	1/8311 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	LEU	CA-CB-CG	5.72	128.45	115.30

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	2034	0	2013	163	0
1	B	2043	0	2033	135	0
1	C	1883	0	1865	127	0
2	D	40	0	34	9	0
2	E	40	0	34	9	0
3	A	102	0	0	6	0
3	B	56	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	66	0	0	3	0
All	All	6264	0	5979	410	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 34.

All (410) 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:59:VAL:HG11	1:A:106:VAL:HG13	1.10	1.06
1:B:186:ARG:HA	1:B:186:ARG:CZ	1.87	1.03
1:A:258:TYR:HB2	1:A:351:TYR:HA	1.42	0.98
1:B:186:ARG:NH1	1:B:187:GLN:H	1.64	0.95
1:C:63:ASN:C	1:C:63:ASN:HD22	1.68	0.95
1:A:178:ARG:HG3	1:A:179:ILE:H	1.29	0.94
1:B:300:VAL:HG13	1:B:301:ASN:H	1.32	0.93
1:A:264:ARG:HA	2:D:407:VAL:HA	1.50	0.93
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.36	0.90
1:A:257:GLY:N	1:A:323:ALA:HA	1.86	0.90
1:A:178:ARG:NH2	1:C:167:THR:HG22	1.86	0.90
1:C:250:ARG:HG3	1:C:251:ASP:N	1.85	0.89
1:A:59:VAL:HG13	1:A:107:ALA:O	1.72	0.89
1:B:147:ARG:HD2	1:B:211:GLU:OE2	1.73	0.89
1:C:177:GLY:HA2	1:C:188:ASN:HB2	1.54	0.88
1:C:66:LEU:HD23	1:C:73:GLN:HB3	1.54	0.87
1:A:59:VAL:HG11	1:A:106:VAL:CG1	2.02	0.86
1:B:161:PRO:HD2	1:B:167:THR:HG23	1.57	0.85
1:C:197:ASN:H	1:C:200:ASN:HD22	1.23	0.85
1:B:313:ILE:HG23	1:B:314:SER:H	1.41	0.83
1:A:207:ASN:HB3	1:A:213:MET:HE2	1.61	0.83
1:A:310:LYS:HG2	1:A:311:PRO:HD2	1.61	0.83
1:C:66:LEU:HD23	1:C:73:GLN:CB	2.09	0.82
1:B:160:ASN:HD21	1:B:165:GLY:H	1.27	0.81
1:B:177:GLY:HA2	1:B:188:ASN:OD1	1.80	0.81
1:A:321:GLN:O	1:A:325:ILE:HG12	1.80	0.79
1:C:181:LEU:HD21	1:C:218:LEU:HB2	1.64	0.79
1:B:183:PRO:HA	1:B:186:ARG:HE	1.48	0.79
1:A:348:ILE:HD12	1:A:348:ILE:H	1.49	0.76
1:A:262:GLY:HA2	2:D:409:GLN:HA	1.69	0.75
1:B:308:ASP:HB2	1:B:331:ILE:HD11	1.66	0.75
1:A:160:ASN:ND2	1:A:165:GLY:H	1.83	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:HB2	1:A:331:ILE:HD11	1.69	0.75
1:A:160:ASN:HD21	1:A:165:GLY:H	1.33	0.75
1:A:197:ASN:H	1:A:200:ASN:HD22	1.35	0.74
1:C:63:ASN:C	1:C:63:ASN:ND2	2.40	0.74
1:B:186:ARG:HH11	1:B:187:GLN:H	1.34	0.74
1:C:134:ALA:HA	3:C:367:HOH:O	1.85	0.73
1:C:325:ILE:O	1:C:326:ARG:HB2	1.86	0.73
1:B:264:ARG:HA	2:E:407:VAL:HG23	1.70	0.73
1:B:319:MET:HG3	2:E:410:PHE:HB2	1.68	0.73
1:B:262:GLY:HA2	2:E:409:GLN:HA	1.68	0.73
1:B:283:VAL:HA	1:B:303:LEU:HA	1.69	0.73
1:A:207:ASN:HD22	1:A:213:MET:CE	2.02	0.73
1:A:319:MET:HB3	2:D:410:PHE:CE2	2.23	0.73
1:B:327:PRO:HA	1:B:348:ILE:HG22	1.69	0.73
1:A:258:TYR:CB	1:A:351:TYR:HA	2.19	0.72
1:A:167:THR:HG22	1:B:178:ARG:NH2	2.05	0.72
1:B:186:ARG:NH1	1:B:187:GLN:N	2.38	0.71
1:C:327:PRO:HB3	1:C:349:GLN:HA	1.71	0.71
1:B:63:ASN:C	1:B:63:ASN:HD22	1.92	0.71
1:A:258:TYR:HB2	1:A:351:TYR:CA	2.20	0.71
1:C:147:ARG:HD2	1:C:211:GLU:OE2	1.91	0.71
1:B:319:MET:HG3	2:E:410:PHE:CB	2.21	0.71
1:C:330:VAL:HG22	1:C:347:THR:OG1	1.90	0.71
1:A:178:ARG:HH21	1:C:167:THR:HG22	1.56	0.70
1:A:325:ILE:O	1:A:326:ARG:HB3	1.92	0.70
1:A:351:TYR:CD2	1:A:352:PRO:HD2	2.27	0.70
1:B:186:ARG:HA	1:B:186:ARG:NE	2.06	0.70
1:C:197:ASN:H	1:C:200:ASN:ND2	1.89	0.70
1:B:125:THR:HG22	1:B:187:GLN:NE2	2.07	0.70
1:B:197:ASN:H	1:B:200:ASN:HD22	1.40	0.70
1:C:225:ASP:OD1	1:C:226:GLY:N	2.26	0.69
1:C:350:GLU:C	1:C:352:PRO:HD3	2.13	0.69
1:C:179:ILE:HD12	1:C:179:ILE:H	1.57	0.69
1:A:124:LEU:HD12	1:A:256:ARG:CZ	2.23	0.69
1:A:283:VAL:HG22	1:A:303:LEU:CB	2.23	0.68
1:B:330:VAL:HA	1:B:347:THR:HG22	1.76	0.68
1:C:257:GLY:H	1:C:323:ALA:HA	1.58	0.68
1:B:300:VAL:HG22	1:B:301:ASN:ND2	2.10	0.67
1:A:261:ILE:HG13	2:D:410:PHE:HB2	1.75	0.67
1:C:161:PRO:HD2	1:C:167:THR:HG23	1.76	0.67
1:B:260:GLY:O	1:B:261:ILE:HG23	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:VAL:HG11	1:C:256:ARG:NH1	2.10	0.67
1:A:167:THR:HG22	1:B:178:ARG:HH21	1.60	0.67
1:C:179:ILE:HD12	1:C:179:ILE:N	2.09	0.66
1:C:318:THR:C	1:C:320:ASP:H	1.97	0.66
1:A:42:MET:SD	1:A:42:MET:N	2.69	0.66
1:A:63:ASN:C	1:A:63:ASN:HD22	1.98	0.66
1:C:227:GLU:O	1:C:227:GLU:HG2	1.95	0.65
1:B:292:PRO:HA	1:B:295:ASN:ND2	2.12	0.65
1:B:189:PHE:HE1	1:B:217:THR:HG21	1.61	0.65
1:C:349:GLN:HG2	1:C:350:GLU:H	1.61	0.65
1:A:90:TYR:CE2	1:A:131:LYS:HD3	2.31	0.65
1:A:207:ASN:HD22	1:A:213:MET:HE1	1.61	0.65
1:A:254:VAL:HG12	3:A:396:HOH:O	1.95	0.65
1:B:125:THR:HG22	1:B:187:GLN:HE21	1.62	0.65
1:B:218:LEU:HG	1:B:219:SER:H	1.61	0.65
1:B:326:ARG:HG3	1:B:327:PRO:HD2	1.79	0.65
1:C:257:GLY:N	1:C:323:ALA:HA	2.11	0.65
1:A:119:VAL:HG13	1:A:129:VAL:O	1.97	0.65
1:B:183:PRO:HB3	1:B:186:ARG:HD2	1.78	0.65
1:C:53:ARG:HG2	1:C:53:ARG:HH11	1.62	0.65
1:B:319:MET:CE	2:E:410:PHE:HB3	2.27	0.64
1:A:283:VAL:HA	1:A:303:LEU:HA	1.78	0.64
1:B:165:GLY:C	1:C:178:ARG:NH2	2.51	0.64
1:A:125:THR:HG21	1:A:244:ILE:CD1	2.27	0.64
1:B:319:MET:HE3	2:E:410:PHE:HB3	1.79	0.64
1:A:87:GLN:HE21	1:A:138:LEU:H	1.44	0.64
1:B:179:ILE:O	1:B:179:ILE:HG22	1.96	0.64
1:B:218:LEU:HG	1:B:219:SER:N	2.13	0.64
1:A:59:VAL:HG12	1:A:60:ASN:N	2.13	0.64
1:C:284:VAL:C	1:C:285:ASN:HD22	2.02	0.64
1:A:186:ARG:CZ	1:A:186:ARG:HA	2.28	0.63
1:B:63:ASN:HD21	1:B:101:ALA:HA	1.63	0.63
1:B:313:ILE:HG23	1:B:314:SER:N	2.11	0.63
1:B:330:VAL:HG22	1:B:347:THR:HG22	1.81	0.63
1:B:189:PHE:CE1	1:B:217:THR:HG21	2.33	0.63
1:A:179:ILE:O	1:A:180:GLY:O	2.17	0.62
1:B:331:ILE:HG22	1:B:346:VAL:O	1.99	0.62
1:C:149:PRO:HG3	1:C:213:MET:SD	2.39	0.62
1:C:65:GLY:HA3	1:C:77:ARG:HD2	1.80	0.62
1:A:125:THR:HG23	1:A:187:GLN:HG3	1.80	0.62
1:A:222:LYS:HG2	1:A:223:SER:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PRO:HG3	1:B:200:ASN:HD21	1.63	0.62
1:C:223:SER:HB2	1:C:227:GLU:OE1	2.00	0.62
1:A:225:ASP:CG	1:A:226:GLY:N	2.52	0.61
1:C:59:VAL:HG12	1:C:108:LEU:HD22	1.82	0.61
1:B:161:PRO:HG3	1:B:200:ASN:ND2	2.15	0.61
1:A:225:ASP:CG	1:A:226:GLY:H	2.03	0.61
1:A:257:GLY:H	1:A:323:ALA:HA	1.63	0.61
1:A:306:SER:HB2	1:A:310:LYS:O	2.01	0.61
1:A:283:VAL:HG13	1:A:302:ASP:C	2.20	0.61
1:C:327:PRO:CB	1:C:349:GLN:HA	2.29	0.61
1:B:300:VAL:HG13	1:B:301:ASN:N	2.11	0.61
1:C:283:VAL:HA	1:C:303:LEU:HA	1.83	0.60
1:A:117:LEU:HD22	1:A:118:LEU:N	2.17	0.60
1:A:217:THR:O	1:A:218:LEU:HB2	2.01	0.60
1:A:261:ILE:HG23	1:A:293:ALA:CB	2.31	0.60
1:A:178:ARG:CG	1:A:179:ILE:H	2.06	0.60
1:B:264:ARG:HA	2:E:407:VAL:CG2	2.30	0.59
1:C:239:GLN:HB2	3:C:373:HOH:O	2.01	0.59
1:A:122:ASP:OD1	1:A:254:VAL:HG11	2.02	0.59
1:C:253:ARG:HG2	1:C:254:VAL:N	2.16	0.59
1:A:239:GLN:HA	1:A:239:GLN:NE2	2.12	0.59
1:B:306:SER:HB2	1:B:310:LYS:N	2.17	0.59
1:A:178:ARG:HG3	1:A:179:ILE:N	2.08	0.59
1:A:201:SER:HB2	3:A:364:HOH:O	2.01	0.59
1:C:306:SER:HA	1:C:312:ALA:HB2	1.84	0.59
1:B:325:ILE:HD13	1:B:331:ILE:HD12	1.85	0.58
1:A:197:ASN:H	1:A:200:ASN:ND2	1.99	0.58
1:A:218:LEU:HD12	1:A:219:SER:H	1.68	0.58
1:A:310:LYS:HG2	1:A:311:PRO:CD	2.32	0.58
1:C:66:LEU:CD2	1:C:73:GLN:HB3	2.32	0.58
1:B:94:ASN:HB2	1:B:97:VAL:HG23	1.86	0.58
1:B:261:ILE:HG13	2:E:410:PHE:OXT	2.04	0.57
1:A:170:GLN:HE22	1:B:170:GLN:HE22	1.50	0.57
1:C:59:VAL:CG1	1:C:108:LEU:HD22	2.33	0.57
1:A:156:LEU:HD23	1:A:170:GLN:HB3	1.84	0.57
1:B:160:ASN:ND2	1:B:165:GLY:H	2.00	0.57
1:C:351:TYR:N	1:C:352:PRO:HD3	2.19	0.57
1:A:222:LYS:HG2	1:A:223:SER:N	2.19	0.57
1:A:183:PRO:HB2	1:A:186:ARG:HE	1.69	0.57
1:B:149:PRO:HG3	1:B:213:MET:SD	2.45	0.57
1:C:327:PRO:HG2	1:C:350:GLU:OE2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:HG3	1:B:187:GLN:N	2.20	0.56
1:A:283:VAL:HG13	1:A:303:LEU:HA	1.88	0.56
1:B:231:GLY:N	1:C:230:GLU:OE1	2.37	0.56
1:C:59:VAL:HB	1:C:107:ALA:O	2.06	0.56
1:C:132:ILE:O	1:C:132:ILE:HG13	2.06	0.56
1:A:178:ARG:HH22	1:C:167:THR:HG22	1.67	0.56
1:B:160:ASN:HD21	1:B:165:GLY:N	2.00	0.56
1:C:66:LEU:HD23	1:C:73:GLN:HB2	1.88	0.56
1:B:63:ASN:ND2	1:B:101:ALA:HA	2.21	0.55
1:B:309:ASN:CG	1:B:309:ASN:O	2.44	0.55
1:C:67:ASN:OD1	1:C:69:ASN:HB2	2.06	0.55
1:B:51:VAL:HG22	1:B:168:ILE:HD13	1.88	0.55
1:A:283:VAL:HG13	1:A:303:LEU:N	2.22	0.55
1:C:310:LYS:HG3	1:C:311:PRO:HD2	1.87	0.55
1:A:257:GLY:CA	1:A:323:ALA:HA	2.36	0.55
1:A:117:LEU:HD22	1:A:118:LEU:H	1.71	0.55
1:B:165:GLY:C	1:C:178:ARG:HH22	2.08	0.55
1:B:63:ASN:C	1:B:63:ASN:ND2	2.60	0.54
1:C:181:LEU:O	1:C:181:LEU:HD12	2.07	0.54
1:B:257:GLY:H	1:B:323:ALA:HA	1.71	0.54
1:A:220:PHE:CD1	1:A:229:PRO:HG3	2.43	0.54
1:C:349:GLN:HG2	1:C:350:GLU:N	2.23	0.54
1:A:259:ILE:O	1:A:293:ALA:HB2	2.06	0.54
1:C:178:ARG:HG3	1:C:178:ARG:HH11	1.71	0.54
1:A:64:ARG:HH21	1:A:74:LEU:HD13	1.73	0.54
1:A:325:ILE:O	1:A:325:ILE:HG22	2.08	0.54
1:B:197:ASN:H	1:B:200:ASN:ND2	2.05	0.54
1:A:319:MET:HA	1:A:322:VAL:CG2	2.38	0.53
1:A:331:ILE:HG22	1:A:346:VAL:O	2.08	0.53
1:A:348:ILE:HD12	1:A:348:ILE:N	2.21	0.53
1:B:51:VAL:HG13	1:B:168:ILE:CD1	2.38	0.53
1:A:59:VAL:CG1	1:A:60:ASN:N	2.72	0.53
1:B:182:ASN:N	1:B:183:PRO:CD	2.72	0.53
1:B:159:GLY:C	1:B:161:PRO:HD3	2.29	0.53
1:C:318:THR:C	1:C:320:ASP:N	2.60	0.53
1:A:305:ILE:O	1:A:312:ALA:HB3	2.09	0.52
1:C:129:VAL:HG23	1:C:248:LEU:HD12	1.91	0.52
1:A:87:GLN:NE2	1:A:138:LEU:H	2.06	0.52
1:A:108:LEU:N	1:A:108:LEU:HD23	2.23	0.52
1:A:118:LEU:HD12	3:A:456:HOH:O	2.10	0.52
1:A:260:GLY:O	1:A:293:ALA:HB3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLY:O	1:C:178:ARG:NH2	2.43	0.52
1:B:257:GLY:N	1:B:323:ALA:HA	2.25	0.52
1:C:141:ILE:HG23	1:C:141:ILE:O	2.10	0.52
1:A:318:THR:O	1:A:318:THR:HG22	2.10	0.52
1:A:156:LEU:CD2	1:A:170:GLN:HB3	2.40	0.51
1:B:326:ARG:HG3	1:B:327:PRO:CD	2.40	0.51
1:B:124:LEU:O	1:B:124:LEU:HD23	2.10	0.51
1:A:147:ARG:HD2	1:A:211:GLU:OE2	2.10	0.51
1:B:257:GLY:O	1:B:322:VAL:HG12	2.10	0.51
1:C:127:LEU:HD11	1:C:241:ALA:HA	1.92	0.51
1:C:85:MET:HG3	1:C:245:MET:SD	2.50	0.51
1:A:224:ASN:CG	1:A:225:ASP:N	2.64	0.51
1:A:239:GLN:HE21	1:A:239:GLN:CA	2.12	0.51
1:B:304:ILE:HD13	1:B:307:VAL:HG22	1.93	0.51
1:A:187:GLN:HA	1:A:187:GLN:OE1	2.11	0.51
1:B:330:VAL:CA	1:B:347:THR:HG22	2.40	0.51
1:A:207:ASN:HD22	1:A:213:MET:HE2	1.74	0.51
1:A:283:VAL:HG22	1:A:303:LEU:HA	1.93	0.51
1:B:51:VAL:HG13	1:B:168:ILE:HD11	1.92	0.51
1:C:67:ASN:CG	1:C:68:THR:N	2.64	0.51
1:C:250:ARG:HG3	1:C:251:ASP:H	1.70	0.51
1:C:181:LEU:HD21	1:C:218:LEU:CB	2.37	0.50
1:C:332:PRO:HA	1:C:344:LEU:O	2.11	0.50
2:D:408:TYR:O	2:D:409:GLN:HG3	2.10	0.50
1:A:186:ARG:HA	1:A:186:ARG:NE	2.27	0.50
1:B:228:THR:HG21	1:C:228:THR:HG21	1.93	0.50
1:C:257:GLY:H	1:C:323:ALA:CA	2.23	0.50
1:A:284:VAL:HG23	1:A:302:ASP:O	2.11	0.50
1:C:327:PRO:HB3	1:C:349:GLN:HG3	1.93	0.50
1:A:306:SER:HB2	1:A:310:LYS:C	2.32	0.50
1:C:66:LEU:N	1:C:102:ASP:OD2	2.45	0.50
1:A:160:ASN:HD21	1:A:165:GLY:N	2.07	0.50
2:D:407:VAL:O	2:D:408:TYR:HB3	2.12	0.50
2:D:408:TYR:C	2:D:409:GLN:HG3	2.33	0.49
1:A:259:ILE:HG22	1:A:293:ALA:HB2	1.94	0.49
1:A:156:LEU:HD23	1:A:170:GLN:CB	2.42	0.49
1:A:304:ILE:HD11	1:A:307:VAL:HG22	1.93	0.49
1:B:292:PRO:HA	1:B:295:ASN:HD22	1.75	0.49
1:A:259:ILE:HG22	1:A:293:ALA:CB	2.42	0.49
1:B:293:ALA:HB1	1:B:346:VAL:HG11	1.95	0.49
1:A:183:PRO:CB	1:A:186:ARG:NE	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:HB3	1:A:346:VAL:HG22	1.95	0.49
1:B:46:SER:HB2	1:C:153:ASP:OD1	2.12	0.49
1:B:330:VAL:HG22	1:B:347:THR:CG2	2.42	0.48
1:C:248:LEU:CD2	1:C:253:ARG:HA	2.43	0.48
1:B:220:PHE:O	1:B:229:PRO:HG2	2.14	0.48
1:A:283:VAL:HG13	1:A:303:LEU:CA	2.43	0.48
1:A:307:VAL:HG12	1:A:331:ILE:HD11	1.96	0.48
1:C:66:LEU:HG	1:C:102:ASP:OD2	2.13	0.48
1:A:319:MET:HB3	2:D:410:PHE:CZ	2.49	0.48
1:A:222:LYS:HZ1	1:A:225:ASP:HA	1.78	0.48
1:C:223:SER:HB3	1:C:229:PRO:HD3	1.96	0.48
1:A:183:PRO:HB3	1:A:186:ARG:NE	2.29	0.48
1:B:139:PRO:O	1:B:139:PRO:HG2	2.13	0.48
1:A:79:LEU:O	1:A:79:LEU:HD12	2.13	0.48
1:B:161:PRO:CD	1:B:167:THR:HG23	2.37	0.48
1:B:292:PRO:HB2	1:B:349:GLN:OE1	2.13	0.48
1:C:63:ASN:HD22	1:C:64:ARG:N	2.11	0.48
1:B:186:ARG:NE	1:B:186:ARG:CA	2.75	0.47
1:B:77:ARG:HH12	1:B:100:ASP:HB3	1.80	0.47
1:C:257:GLY:CA	1:C:323:ALA:HA	2.44	0.47
1:B:168:ILE:HD12	1:C:151:ILE:CG2	2.45	0.47
1:A:224:ASN:CG	1:A:225:ASP:H	2.16	0.47
1:B:50:ALA:HB2	1:B:208:SER:O	2.15	0.47
1:A:58:VAL:CG1	1:A:158:ILE:HG21	2.45	0.47
1:B:85:MET:HG3	1:B:245:MET:SD	2.54	0.47
1:A:258:TYR:CG	1:A:352:PRO:HD3	2.49	0.47
1:B:313:ILE:CG2	1:B:314:SER:H	2.22	0.47
1:C:251:ASP:C	1:C:253:ARG:H	2.18	0.47
1:C:310:LYS:CG	1:C:311:PRO:HD2	2.44	0.47
1:A:253:ARG:HD3	3:A:402:HOH:O	2.14	0.47
1:C:53:ARG:HG2	1:C:53:ARG:NH1	2.28	0.47
1:C:92:ILE:HG22	1:C:93:THR:N	2.29	0.47
1:B:240:LEU:HD22	1:B:244:ILE:HG12	1.96	0.47
1:B:331:ILE:N	1:B:346:VAL:O	2.37	0.47
1:A:283:VAL:HG22	1:A:303:LEU:CA	2.45	0.46
1:A:324:GLU:O	1:A:324:GLU:HG3	2.15	0.46
1:B:60:ASN:ND2	1:B:160:ASN:OD1	2.49	0.46
1:C:285:ASN:HD22	1:C:285:ASN:N	2.12	0.46
1:C:307:VAL:O	1:C:309:ASN:N	2.49	0.46
1:A:186:ARG:O	1:A:187:GLN:HG2	2.16	0.46
1:A:259:ILE:C	1:A:293:ALA:HB2	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:TYR:CE2	1:B:131:LYS:HD3	2.50	0.46
1:C:310:LYS:CD	1:C:311:PRO:HD2	2.46	0.46
1:A:222:LYS:NZ	1:A:227:GLU:O	2.40	0.46
1:A:224:ASN:ND2	1:A:225:ASP:H	2.14	0.46
1:B:162:TYR:CE1	1:C:229:PRO:HB3	2.51	0.46
1:A:124:LEU:CD2	1:A:185:GLY:HA3	2.46	0.46
1:A:348:ILE:H	1:A:348:ILE:CD1	2.22	0.46
1:B:319:MET:HG3	2:E:410:PHE:HB3	1.95	0.46
1:C:310:LYS:HD3	1:C:311:PRO:CD	2.45	0.46
1:A:169:THR:HG22	1:B:193:ASP:HB3	1.98	0.46
1:A:222:LYS:HE2	1:A:222:LYS:HB3	1.67	0.46
1:C:178:ARG:HH11	1:C:178:ARG:CG	2.29	0.46
1:C:182:ASN:C	1:C:184:THR:H	2.19	0.46
1:A:89:GLY:O	1:A:131:LYS:HA	2.16	0.45
1:A:326:ARG:O	1:A:326:ARG:HG3	2.16	0.45
1:B:150:HIS:HD2	3:B:363:HOH:O	2.00	0.45
1:B:304:ILE:HG23	1:B:304:ILE:O	2.16	0.45
1:C:63:ASN:HD21	1:C:77:ARG:HD3	1.80	0.45
1:C:306:SER:HA	1:C:312:ALA:CB	2.46	0.45
1:C:248:LEU:HD21	1:C:254:VAL:HG23	1.99	0.45
1:A:222:LYS:HE3	1:A:224:ASN:C	2.37	0.45
1:B:178:ARG:O	1:B:179:ILE:HB	2.17	0.45
1:A:160:ASN:ND2	1:A:165:GLY:N	2.59	0.45
1:A:58:VAL:HG13	1:A:158:ILE:HG21	1.98	0.45
1:A:220:PHE:HB2	1:A:234:PHE:HE1	1.81	0.45
1:A:261:ILE:HG23	1:A:293:ALA:HB3	1.98	0.45
1:B:183:PRO:CA	1:B:186:ARG:HE	2.25	0.45
1:B:307:VAL:O	1:B:308:ASP:HB3	2.16	0.45
1:A:285:ASN:HB3	1:A:286:GLU:H	1.57	0.45
1:C:156:LEU:HA	1:C:169:THR:O	2.17	0.45
1:C:141:ILE:O	1:C:141:ILE:CG2	2.65	0.44
1:C:310:LYS:HD3	1:C:311:PRO:HD2	1.97	0.44
1:B:325:ILE:CG2	1:B:348:ILE:HG12	2.47	0.44
1:C:251:ASP:CG	1:C:255:ILE:HD12	2.38	0.44
1:C:309:ASN:O	1:C:310:LYS:HE2	2.17	0.44
1:A:55:ALA:HB1	1:A:166:GLN:NE2	2.32	0.44
1:C:330:VAL:HG11	1:C:345:GLN:HG3	1.98	0.44
1:C:250:ARG:HG3	1:C:251:ASP:CG	2.38	0.44
1:A:155:VAL:HG12	1:A:156:LEU:N	2.31	0.44
1:C:66:LEU:HA	1:C:73:GLN:HA	1.99	0.44
1:C:98:ILE:C	1:C:98:ILE:HD12	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ILE:HG23	1:A:304:ILE:O	2.18	0.44
1:A:325:ILE:O	1:A:325:ILE:CG2	2.65	0.44
1:A:63:ASN:ND2	1:A:101:ALA:HB2	2.33	0.44
1:C:140:THR:HG22	1:C:141:ILE:N	2.33	0.44
1:A:63:ASN:C	1:A:63:ASN:ND2	2.70	0.43
1:A:134:ALA:HB3	3:A:424:HOH:O	2.18	0.43
1:A:217:THR:O	1:A:217:THR:HG22	2.17	0.43
1:B:178:ARG:HG3	1:B:179:ILE:H	1.82	0.43
1:A:95:LYS:HD2	1:A:121:SER:HB2	1.99	0.43
1:A:178:ARG:O	1:A:179:ILE:HB	2.19	0.43
1:A:282:ILE:O	1:A:304:ILE:HG22	2.18	0.43
1:A:164:LEU:HD23	1:B:181:LEU:HD11	2.01	0.43
1:A:60:ASN:N	1:A:60:ASN:HD22	2.16	0.43
1:A:222:LYS:HE3	1:A:224:ASN:O	2.18	0.43
1:A:330:VAL:HA	1:A:347:THR:HG22	2.01	0.43
1:B:64:ARG:HA	1:B:75:GLU:O	2.18	0.43
1:B:326:ARG:HA	1:B:327:PRO:HD3	1.90	0.43
1:A:217:THR:O	1:A:218:LEU:CB	2.62	0.43
1:A:304:ILE:HD11	1:A:307:VAL:CG2	2.49	0.43
1:B:68:THR:CB	1:B:75:GLU:HG2	2.49	0.43
1:A:261:ILE:HG23	1:A:293:ALA:HB1	1.99	0.43
1:C:352:PRO:O	1:C:353:ALA:HB3	2.18	0.43
1:A:333:VAL:HG13	1:A:333:VAL:O	2.19	0.42
1:B:282:ILE:O	1:B:303:LEU:HA	2.19	0.42
1:A:196:ILE:HD13	1:A:196:ILE:HA	1.75	0.42
1:A:306:SER:HA	1:A:312:ALA:CB	2.49	0.42
1:B:189:PHE:CE1	1:B:236:ILE:HD13	2.54	0.42
1:B:255:ILE:HG23	1:B:350:GLU:HG3	2.01	0.42
1:C:322:VAL:HG13	1:C:323:ALA:N	2.34	0.42
1:A:257:GLY:HA3	1:A:323:ALA:HA	2.01	0.42
1:B:103:GLN:OE1	1:B:105:ILE:HD11	2.19	0.42
1:B:178:ARG:HG3	1:B:179:ILE:N	2.34	0.42
1:B:307:VAL:HG21	1:B:318:THR:CG2	2.50	0.42
1:C:248:LEU:HD23	1:C:253:ARG:HA	2.02	0.42
1:A:226:GLY:C	1:A:227:GLU:HG3	2.39	0.42
1:B:157:ALA:HB3	1:B:169:THR:OG1	2.20	0.42
1:C:63:ASN:ND2	1:C:77:ARG:HD3	2.34	0.42
1:A:321:GLN:O	1:A:325:ILE:N	2.52	0.42
1:B:220:PHE:HD2	1:B:229:PRO:HG3	1.83	0.42
1:B:98:ILE:C	1:B:98:ILE:HD12	2.39	0.42
1:C:69:ASN:O	1:C:70:SER:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:ND2	1:A:101:ALA:CB	2.83	0.42
1:C:305:ILE:O	1:C:312:ALA:HB3	2.20	0.42
1:A:58:VAL:HG11	1:A:158:ILE:CG2	2.50	0.41
1:A:139:PRO:HD3	3:A:398:HOH:O	2.19	0.41
1:A:157:ALA:HB1	1:A:196:ILE:HD11	2.02	0.41
1:A:176:THR:HG22	1:A:190:LEU:CD1	2.49	0.41
1:C:349:GLN:CG	1:C:350:GLU:H	2.32	0.41
1:A:258:TYR:CD1	1:A:352:PRO:HD3	2.54	0.41
1:B:157:ALA:O	1:B:168:ILE:HA	2.20	0.41
1:B:165:GLY:CA	1:C:178:ARG:NH2	2.83	0.41
1:B:331:ILE:HG21	1:B:348:ILE:HD11	2.02	0.41
1:C:183:PRO:O	1:C:184:THR:CB	2.69	0.41
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.78	0.41
1:B:332:PRO:HA	1:B:344:LEU:O	2.20	0.41
1:B:240:LEU:HD22	1:B:240:LEU:O	2.20	0.41
1:C:158:ILE:HG12	1:C:168:ILE:HD12	2.01	0.41
1:C:161:PRO:CD	1:C:167:THR:HG23	2.47	0.41
1:A:178:ARG:HH21	1:C:167:THR:CG2	2.27	0.41
1:B:257:GLY:H	1:B:323:ALA:CA	2.32	0.41
1:C:134:ALA:CB	1:C:138:LEU:HD21	2.50	0.41
1:C:207:ASN:HB2	3:C:368:HOH:O	2.20	0.41
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.86	0.41
1:A:319:MET:HA	1:A:322:VAL:HG23	2.02	0.41
1:B:257:GLY:CA	1:B:323:ALA:HA	2.50	0.41
1:B:312:ALA:O	1:B:314:SER:N	2.53	0.41
1:C:319:MET:CE	1:C:322:VAL:HG11	2.51	0.41
1:C:324:GLU:HG3	1:C:324:GLU:O	2.21	0.41
1:C:92:ILE:CG2	1:C:93:THR:N	2.83	0.41
1:C:219:SER:O	1:C:220:PHE:C	2.59	0.41
1:C:325:ILE:O	1:C:326:ARG:CB	2.61	0.41
1:A:63:ASN:HD22	1:A:64:ARG:N	2.18	0.40
1:A:122:ASP:OD1	1:A:254:VAL:CG1	2.68	0.40
1:C:98:ILE:HD12	1:C:99:ASN:N	2.36	0.40
1:C:250:ARG:HD2	1:C:251:ASP:OD1	2.21	0.40
1:A:58:VAL:CG1	1:A:158:ILE:CG2	2.99	0.40
1:B:65:GLY:O	1:B:74:LEU:HA	2.21	0.40
1:B:161:PRO:HD2	1:B:167:THR:CG2	2.41	0.40
1:B:221:ASP:O	1:B:222:LYS:C	2.60	0.40
1:C:70:SER:O	1:C:71:HIS:HB2	2.21	0.40
1:C:327:PRO:CA	1:C:349:GLN:HA	2.51	0.40
1:B:48:ASN:O	1:B:51:VAL:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HD12	1:C:151:ILE:HG21	2.03	0.40
1:C:125:THR:OG1	1:C:127:LEU:HB2	2.21	0.40
1:B:59:VAL:HG12	3:B:377:HOH:O	2.22	0.40
1:B:182:ASN:N	1:B:183:PRO:HD3	2.37	0.40
1:C:327:PRO:HA	1:C:349:GLN:HA	2.03	0.40
1:B:159:GLY:O	1:B:161:PRO:HD3	2.22	0.40
1:B:160:ASN:ND2	1:B:165:GLY:N	2.65	0.40
1:C:74:LEU:H	1:C:74:LEU:HD12	1.85	0.40
2:D:408:TYR:HB2	2:D:410:PHE:HE1	1.86	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	273/314 (87%)	234 (86%)	32 (12%)	7 (3%)	5 5
1	B	273/314 (87%)	235 (86%)	28 (10%)	10 (4%)	3 2
1	C	247/314 (79%)	215 (87%)	23 (9%)	9 (4%)	3 3
2	D	2/10 (20%)	1 (50%)	1 (50%)	0	100 100
2	E	2/10 (20%)	2 (100%)	0	0	100 100
All	All	797/962 (83%)	687 (86%)	84 (10%)	26 (3%)	4 3

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	GLY
1	B	261	ILE
1	B	313	ILE
1	C	71	HIS
1	C	220	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	ASP
1	C	326	ARG
1	C	350	GLU
1	A	179	ILE
1	A	305	ILE
1	B	67	ASN
1	B	70	SER
1	B	223	SER
1	C	70	SER
1	C	184	THR
1	C	308	ASP
1	A	218	LEU
1	B	179	ILE
1	B	226	GLY
1	B	304	ILE
1	A	301	ASN
1	B	222	LYS
1	C	311	PRO
1	A	326	ARG
1	B	260	GLY
1	A	300	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	210/253 (83%)	188 (90%)	22 (10%)	7 9
1	B	211/253 (83%)	193 (92%)	18 (8%)	10 16
1	C	198/253 (78%)	174 (88%)	24 (12%)	5 6
2	D	4/9 (44%)	4 (100%)	0	100 100
2	E	4/9 (44%)	4 (100%)	0	100 100
All	All	627/777 (81%)	563 (90%)	64 (10%)	7 10

All (64) 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	79	LEU
1	A	117	LEU
1	A	118	LEU
1	A	147	ARG
1	A	160	ASN
1	A	163	ASN
1	A	167	THR
1	A	178	ARG
1	A	179	ILE
1	A	186	ARG
1	A	201	SER
1	A	205	LEU
1	A	218	LEU
1	A	227	GLU
1	A	239	GLN
1	A	240	LEU
1	A	242	THR
1	A	309	ASN
1	B	63	ASN
1	B	108	LEU
1	B	118	LEU
1	B	123	SER
1	B	147	ARG
1	B	148	VAL
1	B	163	ASN
1	B	167	THR
1	B	178	ARG
1	B	181	LEU
1	B	205	LEU
1	B	225	ASP
1	B	227	GLU
1	B	240	LEU
1	B	309	ASN
1	B	316	LEU
1	B	321	GLN
1	B	326	ARG
1	C	53	ARG
1	C	63	ASN
1	C	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	69	ASN
1	C	74	LEU
1	C	78	THR
1	C	87	GLN
1	C	98	ILE
1	C	99	ASN
1	C	108	LEU
1	C	143	ILE
1	C	147	ARG
1	C	163	ASN
1	C	167	THR
1	C	181	LEU
1	C	182	ASN
1	C	205	LEU
1	C	227	GLU
1	C	228	THR
1	C	239	GLN
1	C	250	ARG
1	C	253	ARG
1	C	319	MET
1	C	351	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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	170	GLN
1	A	200	ASN
1	A	239	GLN
1	A	285	ASN
1	B	60	ASN
1	B	63	ASN
1	B	73	GLN
1	B	99	ASN
1	B	160	ASN
1	B	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	166	GLN
1	B	182	ASN
1	B	200	ASN
1	B	216	ASN
1	B	285	ASN
1	B	295	ASN
1	B	301	ASN
1	B	309	ASN
1	C	63	ASN
1	C	73	GLN
1	C	87	GLN
1	C	109	GLN
1	C	163	ASN
1	C	166	GLN
1	C	200	ASN
1	C	216	ASN
1	C	239	GLN
1	C	285	ASN
1	C	309	ASN
1	C	345	GLN

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	280/314 (89%)	0.71	48 (17%) 1 1	37, 59, 190, 200	0
1	B	280/314 (89%)	0.82	51 (18%) 1 1	40, 73, 191, 200	0
1	C	256/314 (81%)	0.48	38 (14%) 2 2	43, 71, 186, 196	0
2	D	4/10 (40%)	3.83	3 (75%) 0 0	156, 159, 161, 166	0
2	E	4/10 (40%)	3.39	2 (50%) 0 0	148, 158, 159, 159	0
All	All	824/962 (85%)	0.70	142 (17%) 1 1	37, 69, 190, 200	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ASN	11.4
1	B	72	ASN	11.3
1	A	288	SER	10.3
1	B	185	GLY	9.7
1	B	301	ASN	8.8
1	A	287	VAL	8.6
1	A	289	PRO	8.6
1	C	181	LEU	8.6
1	A	298	ILE	8.3
2	D	408	TYR	8.1
1	A	180	GLY	8.1
1	A	181	LEU	8.0
1	A	299	GLN	7.9
1	B	70	SER	7.9
2	E	407	VAL	7.7
1	B	292	PRO	7.5
1	B	68	THR	7.3
1	B	71	HIS	7.1
1	B	300	VAL	7.0
1	B	299	GLN	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	264	ARG	6.6
1	C	73	GLN	6.6
1	C	309	ASN	6.1
1	C	183	PRO	6.0
1	A	264	ARG	5.8
1	C	332	PRO	5.8
1	A	329	SER	5.8
1	B	180	GLY	5.8
1	B	303	LEU	5.7
1	C	353	ALA	5.5
1	A	259	ILE	5.4
1	C	184	THR	5.4
1	C	74	LEU	5.3
1	A	187	GLN	5.2
1	B	184	THR	5.2
1	A	184	THR	5.2
1	C	351	TYR	5.1
1	B	308	ASP	5.1
1	C	344	LEU	5.0
1	A	262	GLY	5.0
1	B	67	ASN	4.8
1	A	258	TYR	4.8
1	B	224	ASN	4.8
1	A	223	SER	4.7
1	B	263	GLY	4.7
1	B	305	ILE	4.6
1	A	300	VAL	4.6
1	B	69	ASN	4.6
1	A	286	GLU	4.5
2	E	408	TYR	4.3
1	B	262	GLY	4.3
1	C	71	HIS	4.2
1	A	294	ALA	4.2
1	A	263	GLY	4.2
1	B	316	LEU	4.1
1	B	181	LEU	4.1
1	B	183	PRO	4.1
1	B	221	ASP	4.1
1	B	298	ILE	4.0
1	A	334	VAL	4.0
1	A	333	VAL	4.0
1	B	186	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	GLY	3.9
1	B	351	TYR	3.8
1	A	225	ASP	3.8
1	C	66	LEU	3.7
1	C	319	MET	3.7
1	B	344	LEU	3.6
1	B	66	LEU	3.6
1	A	226	GLY	3.6
1	C	346	VAL	3.6
1	A	42	MET	3.5
1	C	283	VAL	3.5
1	A	186	ARG	3.5
1	C	69	ASN	3.4
1	B	310	LYS	3.4
1	B	314	SER	3.4
1	C	318	THR	3.4
1	B	286	GLU	3.4
1	A	303	LEU	3.4
1	A	346	VAL	3.4
1	A	292	PRO	3.3
1	C	186	ARG	3.3
1	A	182	ASN	3.2
1	C	284	VAL	3.2
1	B	282	ILE	3.2
1	C	70	SER	3.1
1	A	185	GLY	3.1
1	C	345	GLN	3.1
1	B	222	LYS	3.1
1	C	285	ASN	3.1
1	A	179	ILE	3.0
1	B	259	ILE	3.0
1	C	330	VAL	3.0
1	C	224	ASN	3.0
2	D	407	VAL	3.0
1	A	332	PRO	2.9
1	C	255	ILE	2.9
1	C	282	ILE	2.9
1	B	307	VAL	2.9
1	A	320	ASP	2.9
2	D	410	PHE	2.9
1	B	309	ASN	2.8
1	B	330	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	68	THR	2.8
1	C	308	ASP	2.8
1	A	290	ASP	2.8
1	A	309	ASN	2.8
1	A	345	GLN	2.7
1	C	185	GLY	2.7
1	B	353	ALA	2.6
1	B	313	ILE	2.6
1	B	311	PRO	2.6
1	C	281	GLY	2.6
1	B	135	THR	2.5
1	C	352	PRO	2.5
1	B	304	ILE	2.5
1	A	227	GLU	2.5
1	B	225	ASP	2.5
1	C	347	THR	2.5
1	C	72	ASN	2.5
1	A	311	PRO	2.4
1	A	221	ASP	2.3
1	A	335	VAL	2.3
1	C	328	GLY	2.3
1	B	187	GLN	2.2
1	C	225	ASP	2.2
1	B	293	ALA	2.2
1	B	261	ILE	2.2
1	A	283	VAL	2.2
1	A	328	GLY	2.2
1	B	226	GLY	2.2
1	A	348	ILE	2.2
1	B	182	ASN	2.2
1	B	285	ASN	2.1
1	C	67	ASN	2.1
1	C	222	LYS	2.1
1	A	257	GLY	2.1
1	B	302	ASP	2.1
1	A	296	ALA	2.1
1	A	331	ILE	2.1
1	C	349	GLN	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.