Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:18 am GMT

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
http://wwpdb.org/validation/2016/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:

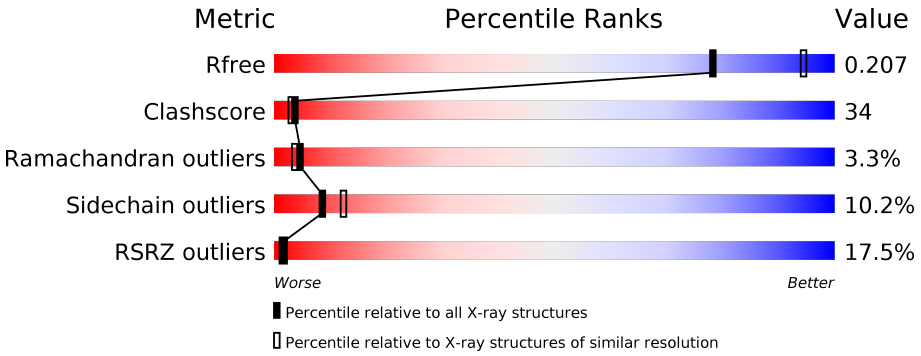
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 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 <=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	17% 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.

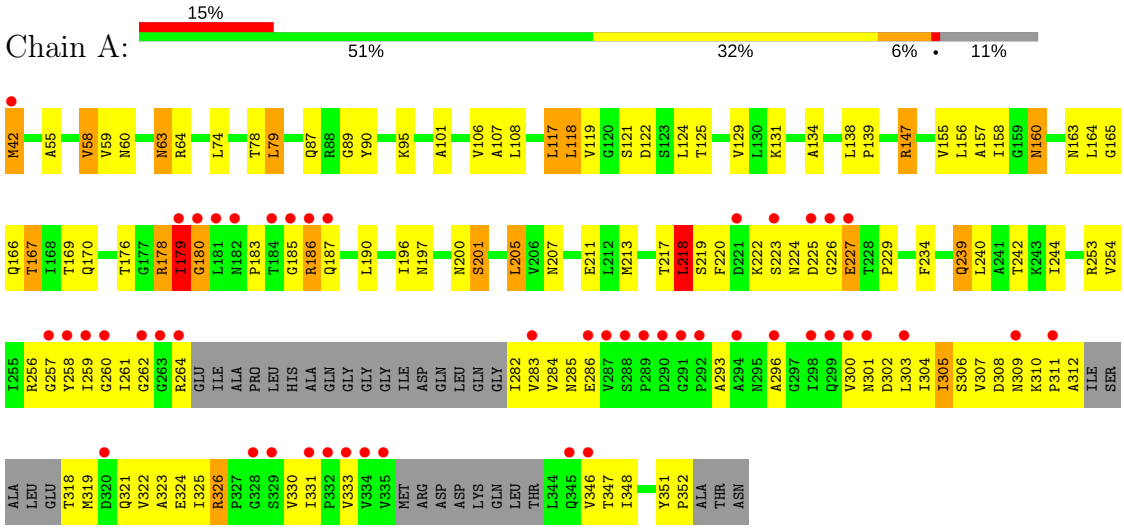
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	56	Total	O	0	0
			56	56		
3	C	66	Total	O	0	0
			66	66		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

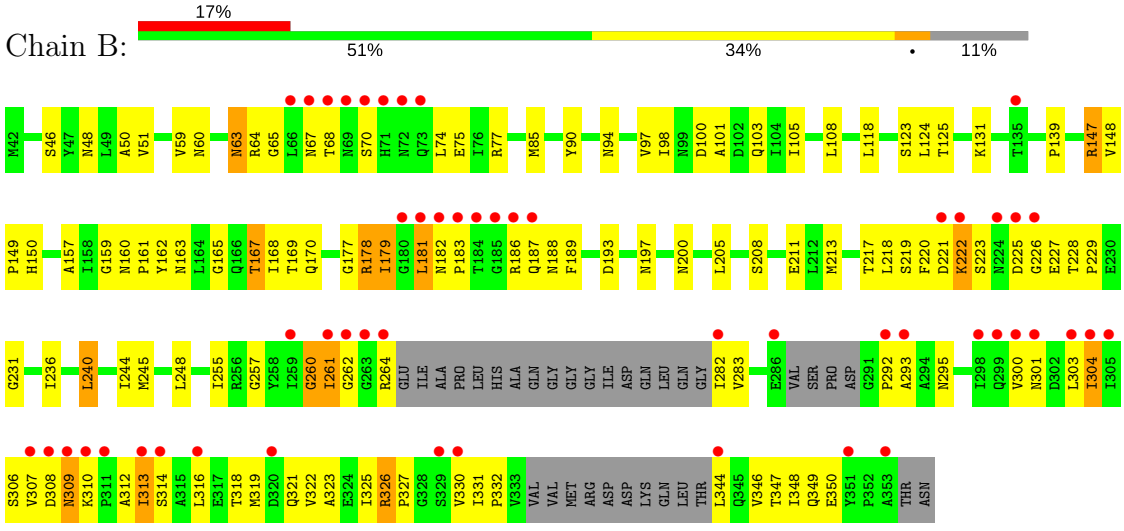
• Molecule 1: Protease degS

Chain A:



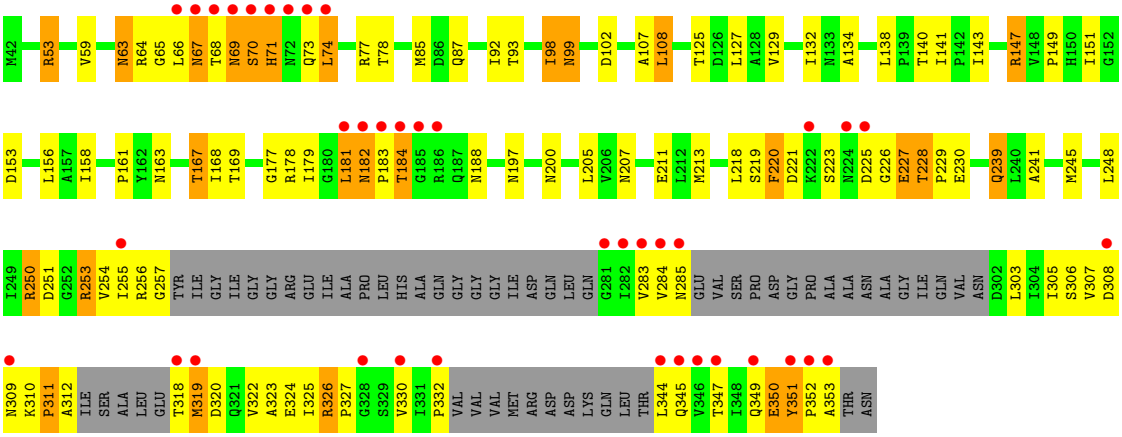
• Molecule 1: Protease degS

Chain B:

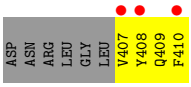


• Molecule 1: Protease degS

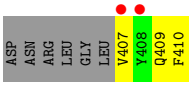
Chain C:



• 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%)	DCC
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

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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:HA	1:A:239:GLN:HE21	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:H	1:A:348:ILE:HD12	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

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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:HD22	1:B:63:ASN:C	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:H	1:C:179:ILE:HD12	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

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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:N	1:C:179:ILE:HD12	2.09	0.66
1:C:318:THR:C	1:C:320:ASP:H	1.97	0.66
1:A:42:MET:N	1:A:42:MET:SD	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:313:ILE:HG23	1:B:314:SER:N	2.11	0.63
1:B:63:ASN:HD21	1:B:101:ALA:HA	1.63	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

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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

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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:B:160:ASN:HD21	1:B:165:GLY:N	2.00	0.56
1:A:178:ARG:HH22	1:C:167:THR:HG22	1.67	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:O	1:B:309:ASN:CG	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:ND2	1:B:63:ASN:C	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:325:ILE:O	1:A:325:ILE:HG22	2.08	0.54
1:A:64:ARG:HH21	1:A:74:LEU:HD13	1.73	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:N	1:A:348:ILE:HD12	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:108:LEU:HD23	1:A:108:LEU:N	2.23	0.52
1:A:87:GLN:NE2	1:A:138:LEU:H	2.06	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

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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:O	1:C:141:ILE:HG23	2.10	0.52
1:A:318:THR:HG22	1:A:318:THR:O	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:CA	1:A:239:GLN:HE21	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:250:ARG:HG3	1:C:251:ASP:H	1.70	0.51
1:C:67:ASN:CG	1:C:68:THR:N	2.64	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

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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:C:310:LYS:CG	1:C:311:PRO:HD2	2.44	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: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:HG3	1:A:324:GLU:O	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

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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:224:ASN:ND2	1:A:225:ASP:H	2.14	0.46
1:A:222:LYS:NZ	1:A:227:GLU:O	2.40	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:CD1	1:A:348:ILE:H	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:326:ARG:HG3	1:A:326:ARG:O	2.16	0.45
1:A:89:GLY:O	1:A:131:LYS:HA	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:CG2	1:C:141:ILE:O	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:HD12	1:C:98:ILE:C	2.38	0.44

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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:CG2	1:A:325:ILE:O	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: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:A:63:ASN:C	1:A:63:ASN:ND2	2.70	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: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:A:60:ASN:N	1:A:60:ASN:HD22	2.16	0.43
1:B:326:ARG:HA	1:B:327:PRO:HD3	1.90	0.43
1:B:64:ARG:HA	1:B:75:GLU:O	2.18	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:O	1:A:333:VAL:HG13	2.19	0.42
1:B:282:ILE:O	1:B:303:LEU:HA	2.19	0.42
1:A:196:ILE:HA	1:A:196:ILE:HD13	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

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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:139:PRO:HD3	3:A:398:HOH:O	2.19	0.41
1:A:58:VAL:HG11	1:A:158:ILE:CG2	2.50	0.41
1:A:176:THR:HG22	1:A:190:LEU:CD1	2.49	0.41
1:A:157:ALA:HB1	1:A:196:ILE:HD11	2.02	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:331:ILE:HG21	1:B:348:ILE:HD11	2.02	0.41
1:B:165:GLY:CA	1:C:178:ARG:NH2	2.83	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:O	1:B:240:LEU:HD22	2.20	0.41
1:C:161:PRO:CD	1:C:167:THR:HG23	2.47	0.41
1:C:158:ILE:HG12	1:C:168:ILE:HD12	2.01	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:B:312:ALA:O	1:B:314:SER:N	2.53	0.41
1:B:257:GLY:CA	1:B:323:ALA:HA	2.50	0.41
1:C:319:MET:CE	1:C:322:VAL:HG11	2.51	0.41
1:C:324:GLU:O	1:C:324:GLU:HG3	2.21	0.41
1:A:319:MET:HA	1:A:322:VAL:HG23	2.02	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:C:92:ILE:CG2	1:C:93:THR:N	2.83	0.41
1:A:122:ASP:OD1	1:A:254:VAL:CG1	2.68	0.40
1:A:63:ASN:HD22	1:A:64:ARG:N	2.18	0.40
1:C:250:ARG:HD2	1:C:251:ASP:OD1	2.21	0.40
1:C:98:ILE:HD12	1:C:99:ASN:N	2.36	0.40
1:A:58:VAL:CG1	1:A:158:ILE:CG2	2.99	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:B:65:GLY:O	1:B:74:LEU:HA	2.21	0.40
1:C:327:PRO:CA	1:C:349:GLN:HA	2.51	0.40
1:C:70:SER:O	1:C:71:HIS:HB2	2.21	0.40
1:B:168:ILE:HD12	1:C:151:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:O	1:B:51:VAL:HB	2.21	0.40
1:C:125:THR:OG1	1:C:127:LEU:HB2	2.21	0.40
1:B:182:ASN:N	1:B:183:PRO:HD3	2.37	0.40
1:B:59:VAL:HG12	3:B:377:HOH:O	2.22	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%)	6 6
1	B	273/314 (87%)	235 (86%)	28 (10%)	10 (4%)	4 3
1	C	247/314 (79%)	215 (87%)	23 (9%)	9 (4%)	4 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 4

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

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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%)	8 11
1	B	211/253 (83%)	193 (92%)	18 (8%)	12 19
1	C	198/253 (78%)	174 (88%)	24 (12%)	6 7
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%)	8 12

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

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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

Some 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

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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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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%)	2	1	37, 59, 190, 200	0
1	B	280/314 (89%)	0.83	52 (18%)	1	1	40, 73, 191, 200	0
1	C	256/314 (81%)	0.50	39 (15%)	2	2	43, 71, 186, 196	0
2	D	4/10 (40%)	3.84	3 (75%)	0	0	156, 159, 161, 166	0
2	E	4/10 (40%)	3.62	2 (50%)	0	0	148, 158, 159, 159	0
All	All	824/962 (85%)	0.71	144 (17%)	2	1	37, 69, 190, 200	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	ASN	11.2
1	A	288	SER	11.1
1	A	301	ASN	10.9
1	B	185	GLY	10.0
1	B	301	ASN	9.5
1	C	181	LEU	9.1
1	A	289	PRO	8.9
1	A	298	ILE	8.4
1	B	70	SER	8.4
1	A	181	LEU	8.2
1	A	287	VAL	8.2
2	E	407	VAL	8.2
1	A	180	GLY	8.1
2	D	408	TYR	7.8
1	A	299	GLN	7.6
1	B	71	HIS	7.4
1	B	292	PRO	7.3
1	B	300	VAL	7.1
1	B	68	THR	7.1
1	A	329	SER	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	264	ARG	6.7
1	C	309	ASN	6.4
1	C	73	GLN	6.3
1	B	299	GLN	6.2
1	A	264	ARG	6.0
1	C	183	PRO	5.9
1	C	332	PRO	5.9
1	A	259	ILE	5.5
1	C	74	LEU	5.5
1	B	303	LEU	5.4
1	C	353	ALA	5.4
1	C	351	TYR	5.4
1	A	187	GLN	5.4
1	B	180	GLY	5.4
1	B	67	ASN	5.3
1	B	184	THR	5.2
1	C	184	THR	5.2
1	B	308	ASP	5.0
1	B	305	ILE	4.8
1	A	184	THR	4.8
1	A	258	TYR	4.8
1	C	344	LEU	4.8
1	B	224	ASN	4.7
1	A	286	GLU	4.7
2	E	408	TYR	4.6
1	A	223	SER	4.6
1	B	263	GLY	4.5
1	A	300	VAL	4.5
1	A	262	GLY	4.5
1	B	298	ILE	4.4
1	C	71	HIS	4.3
1	B	69	ASN	4.2
1	B	262	GLY	4.2
1	B	351	TYR	4.1
1	B	186	ARG	4.1
1	C	319	MET	4.0
1	B	221	ASP	4.0
1	B	316	LEU	4.0
1	A	333	VAL	4.0
1	B	181	LEU	3.9
1	B	183	PRO	3.9
1	A	225	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	260	GLY	3.8
1	B	314	SER	3.7
1	A	334	VAL	3.7
1	C	318	THR	3.7
1	A	263	GLY	3.7
1	C	346	VAL	3.7
1	B	66	LEU	3.6
1	A	226	GLY	3.6
1	C	66	LEU	3.6
1	C	345	GLN	3.5
1	A	182	ASN	3.5
1	A	346	VAL	3.5
1	A	303	LEU	3.4
1	B	310	LYS	3.4
1	A	294	ALA	3.4
1	A	42	MET	3.4
1	C	224	ASN	3.4
1	C	283	VAL	3.4
1	C	330	VAL	3.3
1	C	281	GLY	3.3
1	C	70	SER	3.3
1	B	313	ILE	3.3
2	D	407	VAL	3.3
1	B	344	LEU	3.3
1	A	292	PRO	3.2
1	C	186	ARG	3.2
1	B	286	GLU	3.2
1	C	285	ASN	3.2
1	A	186	ARG	3.2
1	C	284	VAL	3.2
1	B	259	ILE	3.1
1	A	332	PRO	3.1
1	B	353	ALA	3.1
1	C	308	ASP	3.1
1	B	282	ILE	3.1
1	B	222	LYS	3.1
1	A	185	GLY	3.1
1	C	69	ASN	3.1
1	A	179	ILE	3.0
2	D	410	PHE	3.0
1	B	330	VAL	3.0
1	A	320	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	68	THR	3.0
1	C	185	GLY	2.9
1	A	227	GLU	2.9
1	B	135	THR	2.9
1	A	345	GLN	2.9
1	B	307	VAL	2.9
1	A	309	ASN	2.8
1	B	309	ASN	2.8
1	C	328	GLY	2.7
1	C	282	ILE	2.7
1	B	311	PRO	2.7
1	C	255	ILE	2.6
1	B	225	ASP	2.6
1	C	352	PRO	2.5
1	A	335	VAL	2.5
1	C	72	ASN	2.5
1	B	329	SER	2.4
1	A	290	ASP	2.4
1	B	261	ILE	2.4
1	A	221	ASP	2.4
1	B	182	ASN	2.3
1	A	296	ALA	2.3
1	B	226	GLY	2.3
1	B	293	ALA	2.3
1	A	328	GLY	2.2
1	B	187	GLN	2.2
1	B	320	ASP	2.2
1	B	304	ILE	2.2
1	A	311	PRO	2.2
1	A	257	GLY	2.2
1	A	331	ILE	2.1
1	C	222	LYS	2.1
1	A	283	VAL	2.1
1	C	349	GLN	2.1
1	A	291	GLY	2.1
1	C	67	ASN	2.1
1	B	73	GLN	2.1
1	C	225	ASP	2.0
1	C	182	ASN	2.0
1	C	347	THR	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.