Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 11:35 AM EDT

PDB ID	:	1SOT
Title	:	Crystal Structure of the DegS stress sensor
Authors	:	Wilken, C.; Kitzing, K.; Kurzbauer, R.; Ehrmann, M.; Clausen, T.
Deposited on	:	2004-03-15
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

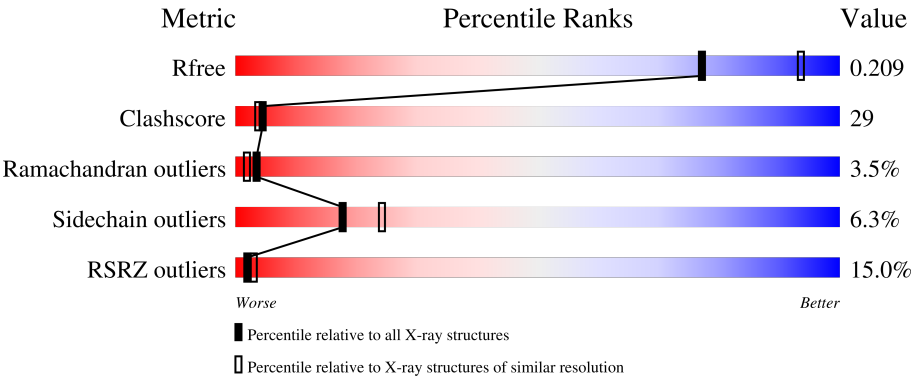
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	320	11% 52% 32% • 12%
1	B	320	13% 53% 35% • • 8%
1	C	320	15% 56% 27% • • 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6617 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	283	Total	C	N	O	Se	0	0	0
			2066	1294	370	397	5			
1	B	294	Total	C	N	O	Se	91	0	0
			2175	1363	394	412	6			
1	C	281	Total	C	N	O	Se	91	0	0
			2046	1280	366	395	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MSE	-	modified residue	UNP P31137
A	85	MSE	MET	modified residue	UNP P31137
A	213	MSE	MET	modified residue	UNP P31137
A	245	MSE	MET	modified residue	UNP P31137
A	319	MSE	MET	modified residue	UNP P31137
A	336	MSE	MET	modified residue	UNP P31137
A	356	HIS	-	expression tag	UNP P31137
A	357	HIS	-	expression tag	UNP P31137
A	358	HIS	-	expression tag	UNP P31137
A	359	HIS	-	expression tag	UNP P31137
A	360	HIS	-	expression tag	UNP P31137
A	361	HIS	-	expression tag	UNP P31137
B	42	MSE	-	modified residue	UNP P31137
B	85	MSE	MET	modified residue	UNP P31137
B	213	MSE	MET	modified residue	UNP P31137
B	245	MSE	MET	modified residue	UNP P31137
B	319	MSE	MET	modified residue	UNP P31137
B	336	MSE	MET	modified residue	UNP P31137
B	356	HIS	-	expression tag	UNP P31137
B	357	HIS	-	expression tag	UNP P31137
B	358	HIS	-	expression tag	UNP P31137
B	359	HIS	-	expression tag	UNP P31137
B	360	HIS	-	expression tag	UNP P31137

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Chain	Residue	Modelled	Actual	Comment	Reference
B	361	HIS	-	expression tag	UNP P31137
C	42	MSE	-	modified residue	UNP P31137
C	85	MSE	MET	modified residue	UNP P31137
C	213	MSE	MET	modified residue	UNP P31137
C	245	MSE	MET	modified residue	UNP P31137
C	319	MSE	MET	modified residue	UNP P31137
C	336	MSE	MET	modified residue	UNP P31137
C	356	HIS	-	expression tag	UNP P31137
C	357	HIS	-	expression tag	UNP P31137
C	358	HIS	-	expression tag	UNP P31137
C	359	HIS	-	expression tag	UNP P31137
C	360	HIS	-	expression tag	UNP P31137
C	361	HIS	-	expression tag	UNP P31137

- Molecule 2 is water.

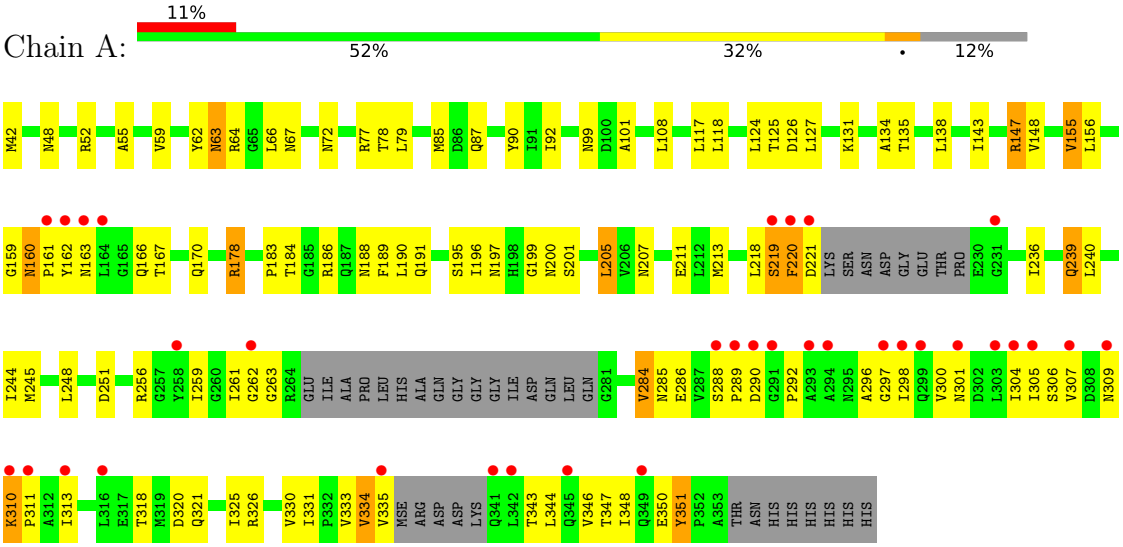
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	139	Total O 139 139	0	0
2	B	98	Total O 98 98	0	0
2	C	93	Total O 93 93	0	0

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.

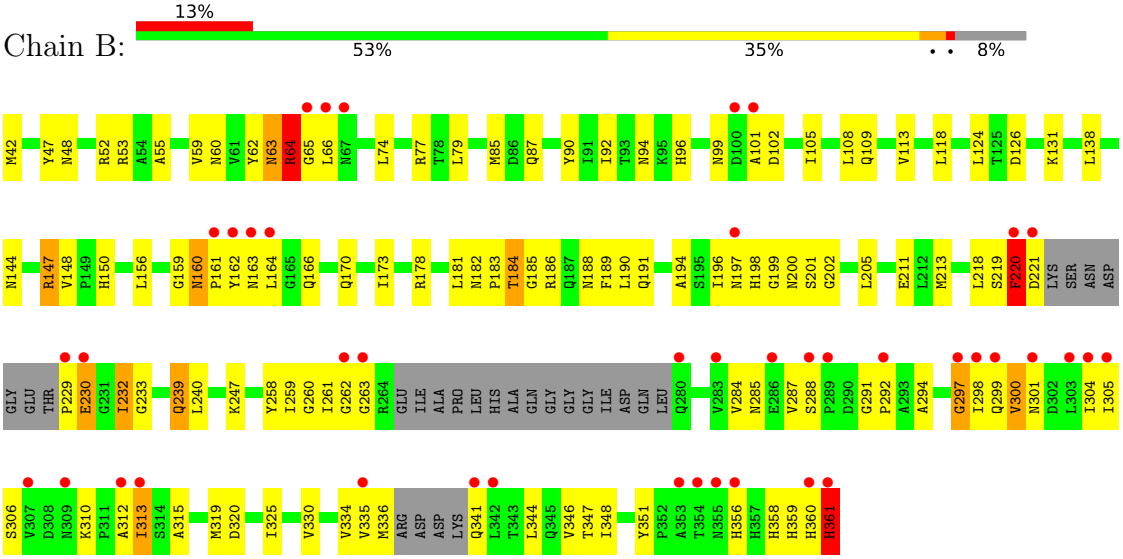
• Molecule 1: Protease degS

Chain A:



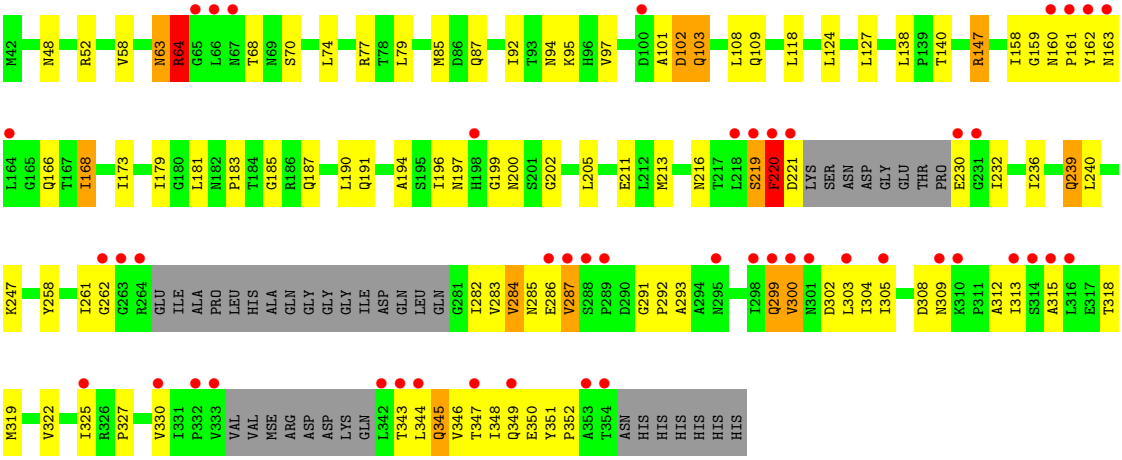
• Molecule 1: Protease degS

Chain B:



• Molecule 1: Protease degS

Chain C:


M42 N48 R52 V58 N63 R64 G65 L66 N67 T68 N69 S70 L74 R77 T78 L79 M85 D86 Q87 I92 T93 N94 K95 H96 V97 D100 A101 D102 Q103 L108 Q109 L118 L124 L127 L138 P139 T140 R147 I158 G159 N160 P161 Y162 N163
L164 G165 Q166 T167 I168 I173 I179 G180 L181 N182 P183 T184 G185 R186 Q187 L190 Q191 A194 S195 I196 N197 H198 G199 N200 S201 G202 L205 E211 L212 M213 N216 T217 L218 S219 F220 D221 LYS SER ASN ASP GLY GLU THR PRO E230 G231 I232 I236 Q239 L240
K247 Y258 I261 G262 G263 R264 GLU ILE ALA PRO LEU HIS ALA GLN GLY GLY GLY ILE ASP GLN LEU GLN G281 I282 V283 V284 N285 E286 V287 S288 P289 D290 G291 P292 A293 A294 N295 I298 Q299 V300 N301 D302 L303 I304 I305 D308 N309 K310 P311 A312 I313 S314 A315 L316 E317 T318
M319 V322 I325 R326 P327 V330 I331 P332 V333 VAL VAL MSE ARG ASP ASP LYS GLN L342 T343 L344 Q345 V346 T347 I348 Q349 E350 Y351 P352 A353 T354 ASN HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	207.68Å 143.06Å 41.53Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 93.7 (15.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.248 0.208 , 0.209	Depositor DCC
R_{free} test set	4132 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 75.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6617	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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	0.66	0/2087	0.78	0/2835
1	B	0.67	3/2202 (0.1%)	0.80	3/2988 (0.1%)
1	C	0.57	2/2067 (0.1%)	1.35	8/2808 (0.3%)
All	All	0.64	5/6356 (0.1%)	1.01	11/8631 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	ARG	C-N	-17.66	0.93	1.34
1	C	77	ARG	C-N	-9.72	1.11	1.34
1	B	361	HIS	C-OXT	6.91	1.36	1.23
1	B	64	ARG	C-N	-5.81	1.22	1.33
1	C	64	ARG	C-N	-5.17	1.23	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	ARG	O-C-N	-55.67	28.57	123.20
1	C	64	ARG	CA-C-N	-9.94	96.33	116.20
1	B	77	ARG	C-N-CA	7.86	141.34	121.70
1	B	77	ARG	O-C-N	-7.61	110.52	122.70
1	C	77	ARG	O-C-N	-7.36	110.93	122.70
1	C	77	ARG	C-N-CA	6.16	137.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	THR	CA-C-N	5.97	130.33	117.20
1	B	194	ALA	N-CA-C	-5.59	95.90	111.00
1	C	70	SER	C-N-CA	5.44	135.31	121.70
1	C	70	SER	N-CA-C	5.21	125.06	111.00
1	C	70	SER	CA-C-N	-5.15	105.86	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	64	ARG	Mainchain
1	C	64	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2066	0	2071	120	0
1	B	2175	0	2182	141	1
1	C	2046	0	2040	95	0
2	A	139	0	0	13	0
2	B	98	0	0	5	0
2	C	93	0	0	5	0
All	All	6617	0	6293	349	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 29.

All (349) 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:B:65:GLY:HA2	1:B:102:ASP:OD2	1.36	1.22
1:C:330:VAL:HG22	1:C:347:THR:HG22	1.23	1.11
1:C:185:GLY:HA2	1:C:221:ASP:HB2	1.17	1.10
1:B:184:THR:HG21	1:B:188:ASN:HB2	1.33	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD11	1:B:247:LYS:HE3	1.41	1.03
1:B:65:GLY:CA	1:B:102:ASP:OD2	2.08	1.01
1:A:161:PRO:HB3	1:A:199:GLY:HA3	1.47	0.97
1:A:330:VAL:HG22	1:A:347:THR:HG22	1.47	0.94
1:C:63:ASN:HD21	1:C:101:ALA:HA	1.32	0.93
1:B:305:ILE:HD12	1:B:334:VAL:HG12	1.51	0.93
1:B:356:HIS:ND1	1:B:361:HIS:CE1	2.38	0.92
1:A:239:GLN:H	1:A:239:GLN:HE21	1.07	0.91
1:B:184:THR:HG21	1:B:188:ASN:HD22	1.34	0.91
1:B:239:GLN:HE21	1:B:239:GLN:H	1.15	0.89
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.34	0.88
1:B:173:ILE:HD11	1:B:213:MSE:HE3	1.53	0.87
1:B:184:THR:CG2	1:B:188:ASN:HD22	1.86	0.87
1:C:63:ASN:ND2	1:C:101:ALA:HA	1.88	0.87
1:C:239:GLN:H	1:C:239:GLN:HE21	1.15	0.86
1:C:161:PRO:HB2	1:C:163:ASN:OD1	1.77	0.84
1:C:185:GLY:HA2	1:C:221:ASP:CB	2.04	0.84
1:A:263:GLY:HA2	1:A:285:ASN:HB2	1.61	0.82
1:B:356:HIS:CG	1:B:361:HIS:HE1	1.98	0.82
1:C:63:ASN:C	1:C:63:ASN:HD22	1.81	0.81
1:B:184:THR:HG21	1:B:188:ASN:CB	2.09	0.81
1:B:330:VAL:HG22	1:B:347:THR:HG22	1.63	0.81
1:C:181:LEU:HD21	1:C:247:LYS:HE3	1.62	0.81
1:C:127:LEU:HD21	1:C:236:ILE:HD13	1.63	0.79
1:B:305:ILE:HD11	1:B:336:MSE:HG2	1.65	0.78
1:B:184:THR:CG2	1:B:188:ASN:HB2	2.14	0.78
1:B:356:HIS:ND1	1:B:361:HIS:HE1	1.81	0.78
1:B:325:ILE:HG21	1:B:348:ILE:HD12	1.66	0.77
1:A:135:THR:HG23	2:A:375:HOH:O	1.85	0.76
1:B:87:GLN:HE22	1:B:138:LEU:H	1.30	0.76
1:B:184:THR:HG21	1:B:188:ASN:ND2	1.99	0.76
1:C:161:PRO:HB3	1:C:199:GLY:HA3	1.68	0.76
1:C:173:ILE:HD11	1:C:213:MSE:HE3	1.67	0.75
1:A:117:LEU:HD23	2:A:421:HOH:O	1.87	0.75
1:B:124:LEU:HD21	1:B:183:PRO:HB3	1.68	0.75
1:A:306:SER:OG	1:A:334:VAL:HG23	1.87	0.74
1:A:213:MSE:SE	2:A:442:HOH:O	2.53	0.74
1:A:160:ASN:ND2	1:A:166:GLN:HG3	2.04	0.73
1:A:134:ALA:HB2	1:A:138:LEU:HD11	1.71	0.73
1:B:359:HIS:HD1	1:B:361:HIS:CD2	2.06	0.73
1:B:356:HIS:HD1	1:B:361:HIS:CE1	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:SER:N	1:A:289:PRO:HD3	2.04	0.72
1:B:105:ILE:HD11	1:B:113:VAL:CG1	2.20	0.72
1:A:42:MSE:HE1	1:B:53:ARG:HH12	1.54	0.72
1:B:173:ILE:CD1	1:B:213:MSE:HE3	2.19	0.72
1:A:207:ASN:HB3	1:A:213:MSE:HE2	1.70	0.72
1:A:42:MSE:HE1	1:B:53:ARG:HH22	1.55	0.71
1:C:161:PRO:HG3	2:C:412:HOH:O	1.91	0.70
1:B:305:ILE:CD1	1:B:336:MSE:HE3	2.22	0.70
1:A:62:TYR:HD2	1:A:79:LEU:HD11	1.56	0.69
1:B:359:HIS:ND1	1:B:361:HIS:NE2	2.32	0.69
1:A:161:PRO:HB2	1:A:163:ASN:OD1	1.92	0.69
1:C:87:GLN:HE22	1:C:138:LEU:H	1.41	0.69
1:B:63:ASN:HD21	1:B:101:ALA:HA	1.58	0.68
1:A:305:ILE:HB	1:A:334:VAL:HG11	1.73	0.68
1:B:62:TYR:HB2	1:B:105:ILE:HG23	1.75	0.67
1:A:160:ASN:N	1:A:160:ASN:HD22	1.91	0.67
1:A:334:VAL:HG12	1:A:335:VAL:N	2.09	0.67
1:B:124:LEU:HD21	1:B:183:PRO:HA	1.77	0.67
1:B:124:LEU:HD21	1:B:183:PRO:CB	2.24	0.67
1:C:185:GLY:CA	1:C:221:ASP:HB2	2.11	0.66
1:B:178:ARG:HH11	1:B:178:ARG:HB3	1.60	0.66
1:A:55:ALA:HB1	1:A:166:GLN:HE22	1.60	0.66
1:A:87:GLN:HE21	1:A:138:LEU:H	1.44	0.66
1:C:299:GLN:HB3	1:C:302:ASP:OD1	1.96	0.66
1:A:63:ASN:C	1:A:63:ASN:HD22	1.97	0.65
1:B:189:PHE:HE1	1:B:220:PHE:CD2	2.15	0.65
1:C:124:LEU:HD13	1:C:183:PRO:HB3	1.79	0.65
1:A:79:LEU:HD23	1:A:162:TYR:CB	2.27	0.65
1:B:62:TYR:HB2	1:B:105:ILE:CG2	2.27	0.65
1:B:55:ALA:HB1	1:B:166:GLN:NE2	2.12	0.65
1:B:356:HIS:CG	1:B:361:HIS:CE1	2.83	0.64
1:B:261:ILE:HG22	1:B:263:GLY:H	1.62	0.64
1:B:356:HIS:HB3	1:B:361:HIS:CE1	2.32	0.64
1:C:258:TYR:HB3	1:C:349:GLN:O	1.98	0.64
1:A:304:ILE:HD13	1:A:335:VAL:C	2.19	0.63
1:A:77:ARG:CZ	2:A:384:HOH:O	2.46	0.63
1:A:259:ILE:HA	1:A:292:PRO:CG	2.28	0.63
1:B:305:ILE:HD11	1:B:336:MSE:HE3	1.79	0.63
1:A:155:VAL:HG13	1:A:205:LEU:CD2	2.29	0.62
1:C:308:ASP:O	1:C:309:ASN:CB	2.45	0.62
1:B:258:TYR:CZ	1:B:260:GLY:HA2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HD2	1:A:211:GLU:OE2	2.00	0.62
1:B:262:GLY:O	1:B:285:ASN:HB2	2.00	0.62
1:C:63:ASN:ND2	1:C:63:ASN:C	2.53	0.62
1:B:124:LEU:HD21	1:B:183:PRO:CA	2.30	0.62
1:A:127:LEU:HD21	1:A:236:ILE:HD13	1.81	0.61
1:C:327:PRO:HB3	1:C:350:GLU:H	1.65	0.61
1:B:124:LEU:CD2	1:B:183:PRO:HB3	2.31	0.61
1:A:125:THR:HG21	1:A:244:ILE:CD1	2.31	0.61
1:A:259:ILE:HA	1:A:292:PRO:HG3	1.81	0.61
1:A:300:VAL:HG22	1:A:300:VAL:O	2.01	0.61
1:C:161:PRO:HB3	1:C:199:GLY:CA	2.30	0.60
1:A:207:ASN:HD22	1:A:213:MSE:HE2	1.64	0.60
1:A:289:PRO:O	1:A:290:ASP:HB3	2.00	0.60
1:A:124:LEU:HD13	1:A:183:PRO:HB3	1.82	0.60
1:C:102:ASP:C	1:C:102:ASP:OD2	2.39	0.60
1:B:197:ASN:CG	1:B:198:HIS:H	2.04	0.59
1:A:155:VAL:HG13	1:A:205:LEU:HD22	1.82	0.59
1:B:359:HIS:O	1:B:360:HIS:HB3	2.02	0.59
1:C:158:ILE:HG12	1:C:168:ILE:HD13	1.84	0.59
1:B:190:LEU:C	1:B:190:LEU:HD23	2.22	0.59
1:C:351:TYR:CG	1:C:352:PRO:HD2	2.38	0.59
1:C:173:ILE:CD1	1:C:213:MSE:HE3	2.33	0.59
1:A:55:ALA:HB1	1:A:166:GLN:NE2	2.17	0.58
1:B:63:ASN:HD22	1:B:64:ARG:N	2.01	0.58
1:B:126:ASP:HB2	1:B:220:PHE:CZ	2.38	0.58
1:C:159:GLY:HA3	1:C:200:ASN:HA	1.85	0.58
1:B:94:ASN:OD1	1:B:202:GLY:N	2.37	0.58
1:B:126:ASP:HB2	1:B:220:PHE:CE2	2.38	0.58
1:C:160:ASN:ND2	1:C:166:GLN:HG3	2.17	0.58
1:B:181:LEU:HD11	1:B:247:LYS:CE	2.26	0.58
1:C:247:LYS:HD3	2:C:433:HOH:O	2.04	0.58
1:C:325:ILE:CD1	1:C:348:ILE:HG13	2.33	0.58
1:A:79:LEU:HD23	1:A:162:TYR:HB3	1.84	0.58
1:B:184:THR:CG2	1:B:188:ASN:ND2	2.62	0.57
1:C:299:GLN:HG3	1:C:300:VAL:N	2.20	0.57
1:A:236:ILE:HD12	1:A:236:ILE:N	2.20	0.57
1:C:299:GLN:HG3	1:C:300:VAL:H	1.70	0.57
1:B:178:ARG:HB3	1:B:178:ARG:NH1	2.19	0.57
1:B:304:ILE:HD12	1:B:304:ILE:N	2.19	0.57
1:C:291:GLY:C	1:C:293:ALA:H	2.08	0.57
1:B:85:MSE:HG3	1:B:92:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG13	1:C:293:ALA:HB3	1.86	0.56
1:A:239:GLN:H	1:A:239:GLN:NE2	1.91	0.56
1:B:161:PRO:HB2	1:B:163:ASN:OD1	2.05	0.56
1:B:359:HIS:ND1	1:B:361:HIS:CD2	2.74	0.56
1:C:124:LEU:HD13	1:C:183:PRO:CB	2.35	0.56
1:A:42:MSE:HE1	1:B:53:ARG:NH1	2.21	0.56
1:B:297:GLY:HA3	1:B:344:LEU:HD13	1.87	0.56
1:B:306:SER:HA	1:B:312:ALA:HB2	1.86	0.56
1:C:284:VAL:HG12	1:C:285:ASN:N	2.20	0.56
1:A:296:ALA:CB	1:A:346:VAL:HG22	2.36	0.56
1:C:239:GLN:H	1:C:239:GLN:NE2	1.95	0.56
1:C:287:VAL:HG12	1:C:287:VAL:O	2.07	0.56
1:A:48:ASN:OD1	1:A:52:ARG:HD3	2.06	0.55
1:B:163:ASN:O	1:B:164:LEU:HD22	2.07	0.55
1:B:190:LEU:HD23	1:B:191:GLN:N	2.21	0.55
1:C:161:PRO:HD3	1:C:199:GLY:O	2.07	0.55
1:A:305:ILE:HB	1:A:334:VAL:CG1	2.37	0.55
1:C:344:LEU:O	1:C:345:GLN:C	2.45	0.55
1:A:42:MSE:HE1	1:B:53:ARG:NH2	2.21	0.55
1:C:127:LEU:CD2	1:C:236:ILE:HD13	2.34	0.54
1:B:160:ASN:ND2	1:B:166:GLN:HB2	2.23	0.54
1:B:66:LEU:N	1:B:102:ASP:OD2	2.40	0.54
1:C:239:GLN:HE21	1:C:239:GLN:N	1.96	0.54
1:B:160:ASN:HD21	1:B:166:GLN:HB2	1.71	0.54
1:B:161:PRO:HB3	1:B:199:GLY:HA2	1.90	0.54
1:A:189:PHE:HE1	1:A:220:PHE:CD2	2.26	0.54
1:C:330:VAL:HG22	1:C:347:THR:CG2	2.17	0.53
1:B:79:LEU:CD2	1:B:162:TYR:HB3	2.39	0.53
1:B:109:GLN:HG2	2:B:459:HOH:O	2.07	0.53
1:B:315:ALA:O	1:B:319:MSE:HG2	2.09	0.53
1:C:147:ARG:CD	1:C:211:GLU:OE2	2.57	0.53
1:B:313:ILE:N	1:B:313:ILE:HD12	2.24	0.53
1:C:160:ASN:N	1:C:160:ASN:HD22	2.06	0.53
1:A:159:GLY:C	1:A:160:ASN:HD22	2.12	0.52
1:A:288:SER:N	1:A:289:PRO:CD	2.71	0.52
1:B:325:ILE:CG2	1:B:348:ILE:HD12	2.39	0.52
1:C:64:ARG:CZ	1:C:103:GLN:OE1	2.57	0.52
1:B:346:VAL:HA	2:B:420:HOH:O	2.08	0.52
1:B:304:ILE:HD12	1:B:304:ILE:H	1.75	0.52
1:B:191:GLN:NE2	1:B:232:ILE:HD11	2.24	0.52
1:A:160:ASN:HA	1:A:166:GLN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:NE	2:A:384:HOH:O	2.42	0.52
1:A:318:THR:HA	1:A:321:GLN:OE1	2.10	0.52
1:A:261:ILE:HG22	1:A:262:GLY:N	2.24	0.52
1:B:191:GLN:HE21	1:B:232:ILE:CD1	2.21	0.51
1:B:63:ASN:ND2	1:B:101:ALA:HA	2.25	0.51
1:B:90:TYR:CE2	1:B:131:LYS:HD3	2.46	0.51
1:B:63:ASN:ND2	1:B:63:ASN:C	2.64	0.51
1:B:191:GLN:NE2	1:B:232:ILE:CD1	2.73	0.51
1:A:306:SER:H	1:A:334:VAL:CG2	2.23	0.51
1:A:196:ILE:HA	1:A:200:ASN:HD22	1.76	0.51
1:B:181:LEU:CD1	1:B:247:LYS:HE3	2.28	0.51
1:B:356:HIS:CB	1:B:361:HIS:CE1	2.94	0.51
1:C:147:ARG:HD3	1:C:211:GLU:OE2	2.10	0.51
1:C:303:LEU:HD11	1:C:305:ILE:HD11	1.93	0.51
1:B:213:MSE:HE1	2:B:365:HOH:O	2.11	0.51
1:B:259:ILE:C	1:B:292:PRO:HG2	2.31	0.51
1:C:346:VAL:HG12	1:C:347:THR:N	2.25	0.51
1:B:361:HIS:OXT	1:B:361:HIS:ND1	2.36	0.50
1:C:230:GLU:O	1:C:230:GLU:HG2	2.11	0.50
1:A:350:GLU:O	1:A:351:TYR:C	2.49	0.50
1:A:63:ASN:HD22	1:A:64:ARG:N	2.08	0.50
1:A:236:ILE:HD12	1:A:236:ILE:H	1.76	0.50
1:A:305:ILE:HB	1:A:334:VAL:CB	2.42	0.50
1:B:336:MSE:HE2	1:B:341:GLN:CB	2.42	0.50
1:B:287:VAL:HG12	1:B:287:VAL:O	2.12	0.49
1:C:258:TYR:HB2	1:C:351:TYR:HA	1.94	0.49
1:A:59:VAL:HG12	1:A:108:LEU:HD22	1.94	0.49
1:B:63:ASN:HD22	1:B:63:ASN:C	2.14	0.49
1:A:66:LEU:O	1:A:72:ASN:HA	2.13	0.49
1:B:105:ILE:HD11	1:B:113:VAL:HG11	1.95	0.49
1:C:79:LEU:CD2	1:C:162:TYR:HB3	2.43	0.49
1:A:284:VAL:HG12	1:A:284:VAL:O	2.12	0.49
1:A:309:ASN:O	1:A:310:LYS:HD3	2.12	0.49
1:A:297:GLY:HA3	1:A:344:LEU:CB	2.43	0.49
1:B:220:PHE:O	1:B:221:ASP:CB	2.61	0.49
1:B:288:SER:O	1:B:294:ALA:HB2	2.13	0.49
1:B:305:ILE:HD12	1:B:334:VAL:CG1	2.35	0.49
1:B:159:GLY:HA3	1:B:200:ASN:HA	1.95	0.48
1:A:190:LEU:HD23	1:A:191:GLN:N	2.28	0.48
1:A:63:ASN:CG	1:A:101:ALA:HB2	2.33	0.48
1:A:148:VAL:HG12	2:A:399:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD23	1:A:190:LEU:C	2.34	0.48
1:C:63:ASN:HD22	1:C:64:ARG:N	2.10	0.48
1:C:194:ALA:O	1:C:196:ILE:HG12	2.14	0.48
1:A:248:LEU:O	1:A:251:ASP:O	2.32	0.48
1:B:147:ARG:HD3	1:B:211:GLU:OE2	2.13	0.48
1:A:159:GLY:HA3	1:A:200:ASN:HA	1.96	0.48
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.78	0.48
1:C:94:ASN:HB2	1:C:97:VAL:HG23	1.94	0.48
1:C:190:LEU:C	1:C:190:LEU:HD23	2.34	0.48
1:A:62:TYR:CD2	1:A:79:LEU:HD11	2.43	0.48
1:C:219:SER:O	1:C:220:PHE:HB2	2.13	0.47
1:B:182:ASN:HB3	1:B:320:ASP:OD1	2.14	0.47
1:C:282:ILE:O	1:C:303:LEU:HA	2.14	0.47
1:A:160:ASN:ND2	1:A:160:ASN:N	2.62	0.47
1:B:161:PRO:HB3	1:B:199:GLY:CA	2.44	0.47
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.15	0.47
1:A:135:THR:CG2	2:A:375:HOH:O	2.54	0.47
1:C:299:GLN:CG	1:C:300:VAL:H	2.27	0.47
1:A:156:LEU:CD2	1:A:170:GLN:HB3	2.45	0.47
1:C:261:ILE:HG23	1:C:284:VAL:HG13	1.97	0.47
1:B:96:HIS:HA	1:B:99:ASN:HD22	1.81	0.46
1:A:124:LEU:HD13	1:A:183:PRO:CB	2.46	0.46
1:A:134:ALA:HB2	1:A:138:LEU:CD1	2.43	0.46
1:B:55:ALA:HB1	1:B:166:GLN:HE22	1.78	0.46
1:A:42:MSE:CE	1:B:53:ARG:HH12	2.25	0.46
1:A:304:ILE:HG22	1:A:305:ILE:N	2.30	0.46
1:C:322:VAL:O	1:C:325:ILE:HG12	2.15	0.46
1:A:78:THR:HG23	2:A:393:HOH:O	2.16	0.46
1:B:156:LEU:CD2	1:B:170:GLN:HB3	2.45	0.46
1:A:155:VAL:HG13	1:A:205:LEU:HD21	1.98	0.46
1:A:284:VAL:CG2	1:A:304:ILE:HG12	2.46	0.46
1:B:148:VAL:HG22	1:B:150:HIS:CE1	2.51	0.46
1:B:160:ASN:ND2	1:B:166:GLN:CB	2.79	0.46
1:C:160:ASN:ND2	1:C:160:ASN:N	2.64	0.46
1:C:330:VAL:CG2	1:C:347:THR:HG22	2.17	0.46
1:A:261:ILE:CG2	1:A:262:GLY:N	2.79	0.45
1:B:48:ASN:OD1	1:B:52:ARG:NH1	2.42	0.45
1:C:230:GLU:O	1:C:230:GLU:CG	2.64	0.45
1:B:356:HIS:CB	1:B:361:HIS:HE1	2.28	0.45
1:A:67:ASN:O	1:A:67:ASN:CG	2.55	0.45
1:A:126:ASP:HB2	1:A:220:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:OD1	1:C:52:ARG:NH1	2.40	0.45
1:C:219:SER:O	1:C:220:PHE:CB	2.64	0.45
1:B:184:THR:HG21	1:B:188:ASN:CG	2.37	0.45
1:A:59:VAL:CG1	1:A:108:LEU:HD22	2.47	0.45
1:A:199:GLY:C	2:A:397:HOH:O	2.55	0.45
1:A:161:PRO:HD3	1:A:199:GLY:O	2.17	0.45
1:B:305:ILE:CD1	1:B:336:MSE:HG2	2.42	0.45
1:C:181:LEU:CD2	1:C:247:LYS:HE3	2.39	0.45
1:C:287:VAL:CG1	1:C:293:ALA:HB3	2.47	0.45
1:B:191:GLN:HE21	1:B:232:ILE:HD11	1.82	0.45
1:C:109:GLN:NE2	1:C:160:ASN:OD1	2.50	0.45
1:C:159:GLY:C	1:C:160:ASN:HD22	2.20	0.45
1:B:305:ILE:HD11	1:B:336:MSE:CE	2.47	0.45
1:B:306:SER:HB2	1:B:310:LYS:O	2.17	0.45
1:C:262:GLY:O	1:C:285:ASN:HB3	2.17	0.45
1:A:48:ASN:O	1:A:52:ARG:HG3	2.17	0.44
1:C:161:PRO:CG	2:C:412:HOH:O	2.60	0.44
1:A:126:ASP:HB2	1:A:220:PHE:CE2	2.52	0.44
1:B:213:MSE:CE	2:B:365:HOH:O	2.64	0.44
1:C:303:LEU:O	1:C:304:ILE:HD13	2.17	0.44
1:B:60:ASN:OD1	1:B:160:ASN:O	2.35	0.44
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.31	0.44
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.84	0.44
1:A:331:ILE:HG12	1:A:348:ILE:HD11	1.98	0.44
1:B:183:PRO:HG3	1:B:351:TYR:CZ	2.52	0.44
1:A:85:MSE:HE1	1:A:143:ILE:HD11	1.99	0.44
1:A:220:PHE:O	1:A:221:ASP:CB	2.65	0.44
1:C:330:VAL:HA	1:C:346:VAL:O	2.18	0.44
1:A:124:LEU:HD12	1:A:256:ARG:CZ	2.48	0.43
1:A:307:VAL:HG21	1:A:321:GLN:OE1	2.17	0.43
1:C:85:MSE:HG3	1:C:92:ILE:HG13	1.99	0.43
1:B:197:ASN:ND2	1:B:198:HIS:H	2.16	0.43
1:C:282:ILE:CD1	1:C:312:ALA:HB1	2.48	0.43
1:B:258:TYR:OH	1:B:260:GLY:HA2	2.18	0.43
1:C:94:ASN:OD1	1:C:202:GLY:N	2.50	0.43
1:A:63:ASN:C	1:A:63:ASN:ND2	2.69	0.43
1:B:163:ASN:ND2	1:B:164:LEU:HD23	2.34	0.43
1:C:79:LEU:HD23	1:C:162:TYR:HB3	1.99	0.43
1:A:197:ASN:ND2	1:B:230:GLU:HG3	2.34	0.43
1:C:58:VAL:O	1:C:160:ASN:OD1	2.35	0.43
1:A:321:GLN:N	2:A:470:HOH:O	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:O	1:B:292:PRO:HG2	2.18	0.43
1:A:284:VAL:HG23	1:A:304:ILE:HG12	2.00	0.43
1:C:291:GLY:O	1:C:293:ALA:N	2.52	0.43
1:B:182:ASN:OD1	1:B:183:PRO:HD2	2.19	0.43
1:B:184:THR:HG23	1:B:188:ASN:HD22	1.78	0.43
1:B:300:VAL:HG13	1:B:301:ASN:N	2.34	0.43
1:A:90:TYR:CE2	1:A:131:LYS:HD3	2.53	0.42
1:A:296:ALA:HB3	1:A:346:VAL:HG22	2.01	0.42
1:B:47:TYR:HB3	1:B:156:LEU:HD11	2.01	0.42
1:B:197:ASN:CG	1:B:198:HIS:N	2.70	0.42
1:C:179:ILE:HG21	1:C:239:GLN:HB2	2.00	0.42
1:C:291:GLY:C	1:C:293:ALA:N	2.73	0.42
1:B:196:ILE:HG12	1:B:233:GLY:HA3	2.01	0.42
1:C:213:MSE:CE	2:C:365:HOH:O	2.67	0.42
1:A:245:MSE:SE	2:A:478:HOH:O	2.87	0.42
1:B:291:GLY:H	1:B:294:ALA:HB3	1.83	0.42
1:A:195:SER:O	1:A:200:ASN:ND2	2.53	0.42
1:B:147:ARG:CD	1:B:211:GLU:OE2	2.67	0.42
1:B:299:GLN:HA	1:B:299:GLN:OE1	2.19	0.42
1:B:313:ILE:HD12	1:B:313:ILE:H	1.83	0.42
1:C:284:VAL:CG1	1:C:285:ASN:N	2.83	0.42
1:A:85:MSE:HG3	1:A:92:ILE:HG13	2.01	0.42
1:B:220:PHE:O	1:B:221:ASP:HB3	2.20	0.42
1:A:79:LEU:HD23	1:A:162:TYR:HB2	1.99	0.42
1:A:167:THR:HG22	2:B:433:HOH:O	2.20	0.42
1:A:259:ILE:HA	1:A:292:PRO:HG2	2.00	0.42
1:A:184:THR:OG1	1:A:188:ASN:ND2	2.48	0.41
1:B:239:GLN:H	1:B:239:GLN:NE2	1.98	0.41
1:A:320:ASP:HB2	2:A:470:HOH:O	2.19	0.41
1:C:196:ILE:HA	1:C:200:ASN:HD22	1.85	0.41
1:C:284:VAL:HG23	1:C:302:ASP:O	2.20	0.41
1:B:185:GLY:HA2	1:B:358:HIS:CE1	2.55	0.41
1:C:147:ARG:HD2	1:C:211:GLU:OE2	2.20	0.41
1:A:186:ARG:CB	1:A:221:ASP:HB2	2.50	0.41
1:C:190:LEU:HD23	1:C:191:GLN:N	2.35	0.41
1:A:321:GLN:O	1:A:325:ILE:HG12	2.21	0.41
1:B:284:VAL:HB	1:B:300:VAL:O	2.20	0.41
1:A:42:MSE:CE	1:B:53:ARG:HH22	2.30	0.41
1:B:184:THR:HG22	1:B:185:GLY:O	2.21	0.41
1:B:220:PHE:HE1	1:B:358:HIS:CD2	2.39	0.41
1:C:179:ILE:CG2	1:C:239:GLN:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:VAL:HG23	1:C:283:VAL:O	2.20	0.41
1:C:315:ALA:O	1:C:319:MSE:HG2	2.21	0.41
1:A:62:TYR:HD2	1:A:79:LEU:CD1	2.30	0.41
1:A:304:ILE:HD12	1:A:333:VAL:CG1	2.51	0.41
1:B:42:MSE:HA	1:B:42:MSE:HE2	2.02	0.41
1:B:229:PRO:HA	1:B:232:ILE:HG23	2.02	0.41
1:C:95:LYS:HE3	2:C:407:HOH:O	2.21	0.41
1:B:335:VAL:HG12	1:B:336:MSE:N	2.36	0.40
1:C:196:ILE:HD12	1:C:216:ASN:HB3	2.03	0.40
1:A:99:ASN:ND2	2:A:481:HOH:O	2.46	0.40
1:A:290:ASP:CG	1:A:290:ASP:O	2.59	0.40
1:A:330:VAL:CG2	1:A:347:THR:HG22	2.35	0.40
1:B:105:ILE:HD11	1:B:113:VAL:HG13	1.98	0.40
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.91	0.40
1:C:325:ILE:HD12	1:C:348:ILE:HG13	2.03	0.40
1:C:318:THR:O	1:C:322:VAL:HG23	2.22	0.40
1:B:59:VAL:HG11	1:B:108:LEU:HD22	2.03	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:144:ASN:ND2	1:B:361:HIS:NE2[1_554]	2.17	0.03

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	275/320 (86%)	244 (89%)	22 (8%)	9 (3%)	4	2
1	B	286/320 (89%)	253 (88%)	25 (9%)	8 (3%)	5	3
1	C	273/320 (85%)	228 (84%)	33 (12%)	12 (4%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	834/960 (87%)	725 (87%)	80 (10%)	29 (4%)	3 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	A	313	ILE
1	A	334	VAL
1	B	219	SER
1	B	300	VAL
1	C	220	PHE
1	C	343	THR
1	A	343	THR
1	B	186	ARG
1	B	298	ILE
1	C	313	ILE
1	C	345	GLN
1	B	220	PHE
1	C	299	GLN
1	A	301	ASN
1	B	74	LEU
1	C	103	GLN
1	A	351	TYR
1	C	74	LEU
1	C	219	SER
1	C	287	VAL
1	C	292	PRO
1	A	311	PRO
1	C	300	VAL
1	A	298	ILE
1	B	313	ILE
1	A	284	VAL
1	B	297	GLY
1	C	284	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	217/253 (86%)	203 (94%)	14 (6%)	17 23
1	B	232/253 (92%)	219 (94%)	13 (6%)	21 29
1	C	214/253 (85%)	199 (93%)	15 (7%)	15 19
All	All	663/759 (87%)	621 (94%)	42 (6%)	18 24

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	118	LEU
1	A	147	ARG
1	A	155	VAL
1	A	160	ASN
1	A	178	ARG
1	A	201	SER
1	A	205	LEU
1	A	219	SER
1	A	220	PHE
1	A	239	GLN
1	A	240	LEU
1	A	286	GLU
1	A	310	LYS
1	B	63	ASN
1	B	118	LEU
1	B	147	ARG
1	B	160	ASN
1	B	184	THR
1	B	201	SER
1	B	205	LEU
1	B	220	PHE
1	B	230	GLU
1	B	232	ILE
1	B	239	GLN
1	B	240	LEU
1	B	361	HIS
1	C	63	ASN
1	C	102	ASP
1	C	108	LEU
1	C	118	LEU
1	C	140	THR

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Mol	Chain	Res	Type
1	C	147	ARG
1	C	168	ILE
1	C	187	GLN
1	C	197	ASN
1	C	205	LEU
1	C	220	PHE
1	C	232	ILE
1	C	239	GLN
1	C	240	LEU
1	C	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	73	GLN
1	A	87	GLN
1	A	109	GLN
1	A	133	ASN
1	A	160	ASN
1	A	166	GLN
1	A	170	GLN
1	A	182	ASN
1	A	188	ASN
1	A	216	ASN
1	A	239	GLN
1	A	299	GLN
1	A	309	ASN
1	A	345	GLN
1	B	60	ASN
1	B	63	ASN
1	B	87	GLN
1	B	109	GLN
1	B	150	HIS
1	B	160	ASN
1	B	166	GLN
1	B	170	GLN
1	B	188	ASN
1	B	191	GLN
1	B	197	ASN
1	B	239	GLN
1	C	63	ASN

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Mol	Chain	Res	Type
1	C	87	GLN
1	C	96	HIS
1	C	109	GLN
1	C	160	ASN
1	C	166	GLN
1	C	170	GLN
1	C	216	ASN
1	C	239	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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	77:ARG	C	78:THR	N	1.11
1	B	77:ARG	C	78:THR	N	0.93

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	278/320 (86%)	0.33	34 (12%)	4	6	14, 44, 139, 145	0
1	B	277/320 (86%)	0.60	42 (15%)	2	3	24, 54, 124, 143	0
1	C	265/320 (82%)	0.68	47 (17%)	1	1	24, 54, 142, 149	0
All	All	820/960 (85%)	0.53	123 (15%)	2	3	14, 51, 137, 149	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	19.7
1	C	66	LEU	13.2
1	C	220	PHE	11.3
1	B	67	ASN	11.1
1	C	162	TYR	10.8
1	A	220	PHE	10.2
1	A	221	ASP	9.0
1	C	67	ASN	8.8
1	B	220	PHE	8.4
1	B	162	TYR	8.1
1	A	162	TYR	7.8
1	B	229	PRO	7.8
1	B	221	ASP	7.6
1	C	309	ASN	7.4
1	B	360	HIS	7.1
1	A	342	LEU	7.1
1	C	221	ASP	6.4
1	B	280	GLN	6.2
1	C	288	SER	5.7
1	A	293	ALA	5.5
1	C	342	LEU	5.4
1	C	343	THR	5.1
1	A	310	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	305	ILE	4.7
1	C	354	THR	4.6
1	A	305	ILE	4.5
1	A	313	ILE	4.5
1	C	344	LEU	4.5
1	B	297	GLY	4.4
1	C	231	GLY	4.4
1	C	219	SER	4.4
1	A	291	GLY	4.4
1	C	160	ASN	4.4
1	B	289	PRO	4.3
1	B	298	ILE	4.2
1	A	297	GLY	4.2
1	B	65	GLY	4.1
1	C	349	GLN	4.1
1	B	304	ILE	4.1
1	C	353	ALA	3.9
1	B	262	GLY	3.9
1	B	341	GLN	3.9
1	C	287	VAL	3.9
1	C	330	VAL	3.9
1	C	347	THR	3.8
1	A	219	SER	3.8
1	B	283	VAL	3.8
1	B	354	THR	3.7
1	B	263	GLY	3.7
1	B	163	ASN	3.7
1	B	305	ILE	3.6
1	A	304	ILE	3.6
1	C	286	GLU	3.6
1	C	303	LEU	3.5
1	C	316	LEU	3.5
1	A	303	LEU	3.5
1	B	299	GLN	3.5
1	C	264	ARG	3.5
1	C	65	GLY	3.4
1	C	295	ASN	3.4
1	B	288	SER	3.3
1	C	314	SER	3.3
1	C	263	GLY	3.2
1	A	309	ASN	3.2
1	C	299	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	307	VAL	3.1
1	B	342	LEU	3.0
1	B	161	PRO	3.0
1	B	101	ALA	3.0
1	A	316	LEU	3.0
1	C	289	PRO	3.0
1	C	300	VAL	2.9
1	A	161	PRO	2.9
1	A	163	ASN	2.9
1	B	309	ASN	2.8
1	A	341	GLN	2.8
1	A	294	ALA	2.8
1	C	161	PRO	2.8
1	C	325	ILE	2.8
1	B	312	ALA	2.7
1	C	230	GLU	2.8
1	C	332	PRO	2.7
1	C	218	LEU	2.7
1	B	301	ASN	2.7
1	B	355	ASN	2.7
1	A	290	ASP	2.7
1	A	288	SER	2.7
1	B	286	GLU	2.6
1	C	298	ILE	2.6
1	B	335	VAL	2.6
1	B	164	LEU	2.6
1	B	197	ASN	2.6
1	A	164	LEU	2.6
1	A	299	GLN	2.5
1	C	198	HIS	2.5
1	A	349	GLN	2.5
1	C	100	ASP	2.5
1	C	313	ILE	2.5
1	C	164	LEU	2.5
1	B	356	HIS	2.4
1	C	163	ASN	2.4
1	C	301	ASN	2.4
1	C	262	GLY	2.4
1	C	333	VAL	2.4
1	A	335	VAL	2.4
1	A	298	ILE	2.3
1	B	303	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	345	GLN	2.3
1	A	311	PRO	2.3
1	B	313	ILE	2.3
1	B	353	ALA	2.3
1	A	301	ASN	2.3
1	C	310	LYS	2.2
1	A	258	TYR	2.2
1	A	231	GLY	2.2
1	A	289	PRO	2.2
1	A	262	GLY	2.1
1	B	361	HIS	2.1
1	B	292	PRO	2.1
1	B	307	VAL	2.1
1	B	230	GLU	2.0
1	B	100	ASP	2.0
1	C	315	ALA	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.