Preliminary Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 01:37 AM EDT

Deposition ID : D_1000258613

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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

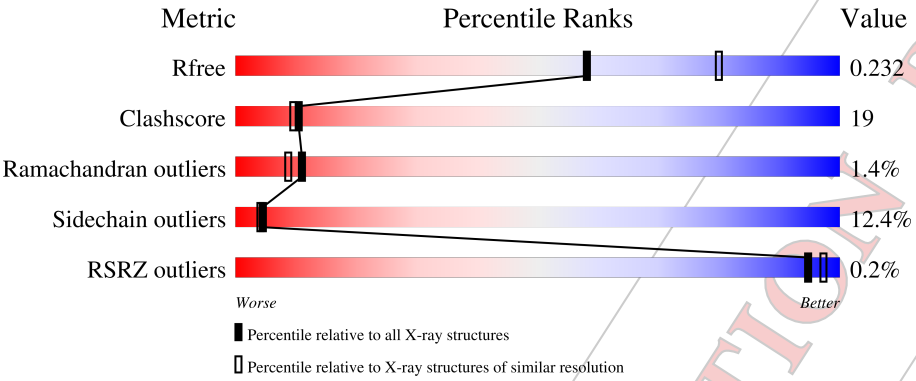
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	306	60% 33% 6%
1	B	306	60% 36%
1	C	306	63% 33%
1	D	306	% 54% 39% 6%
2	W	16	25% 25% 12% 38%

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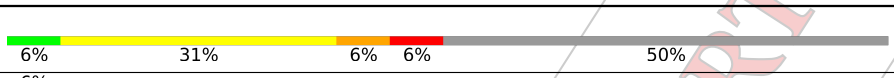
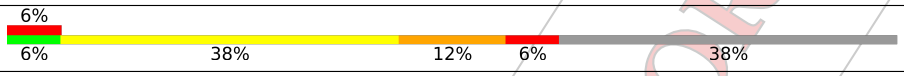
Mol	Chain	Length	Quality of chain
2	X	16	
2	Y	16	
2	Z	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTY	Z	1	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9819 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2340	1481	398	439	22			
1	B	304	Total	C	N	O	S	0	0	0
			2347	1485	399	441	22			
1	C	304	Total	C	N	O	S	0	0	0
			2347	1485	399	441	22			
1	D	303	Total	C	N	O	S	0	0	0
			2340	1481	398	439	22			

- Molecule 2 is a protein called ACE-DTY-LEU-GLN-TYR-ALA-VAL-LEU-ARG-HIS-LYS-ARG-ARG-GLU-SEC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	8	Total	C	N	O	0	0	0
			65	44	8	13			
2	Y	10	Total	C	N	O	0	1	0
			94	61	17	16			
2	Z	13	Total	C	N	O	0	1	0
			122	80	23	19			
2	W	10	Total	C	N	O	0	0	0
			89	57	17	15			

- Molecule 3 is a ligand with the chemical component id SEW but there is no existing wwPDB Chemical Component Dictionary definition for SEW. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	N	O	Se	0	0
			7	3	2	1	1		
3	Y	1	Total	C	N	O	Se	0	0
			7	3	2	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Z	1	Total	C	N	O	Se	0	0
			7	3	2	1	1		
3	W	1	Total	C	N	O	Se	0	0
			7	3	2	1	1		

- Molecule 4 is water.

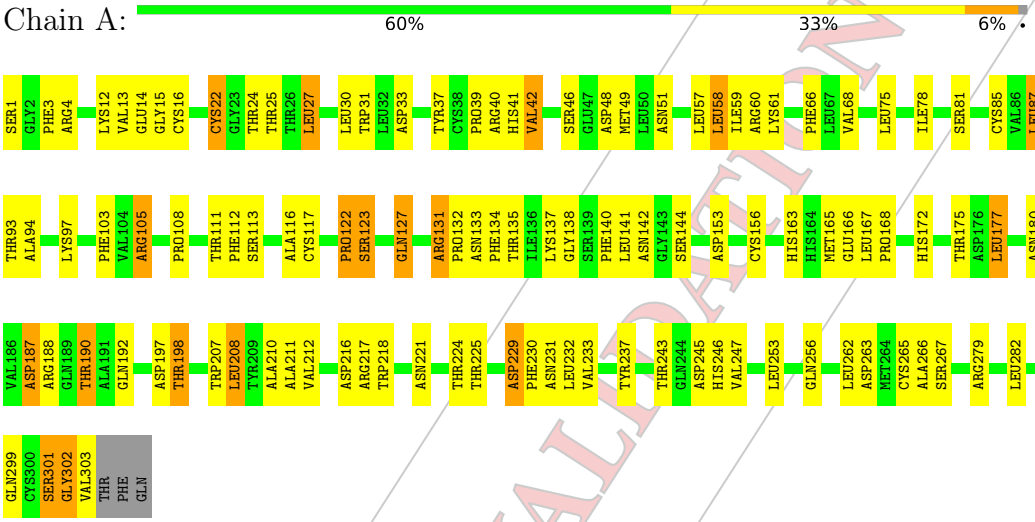
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	47	Total	O	0	0
			47	47		

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.

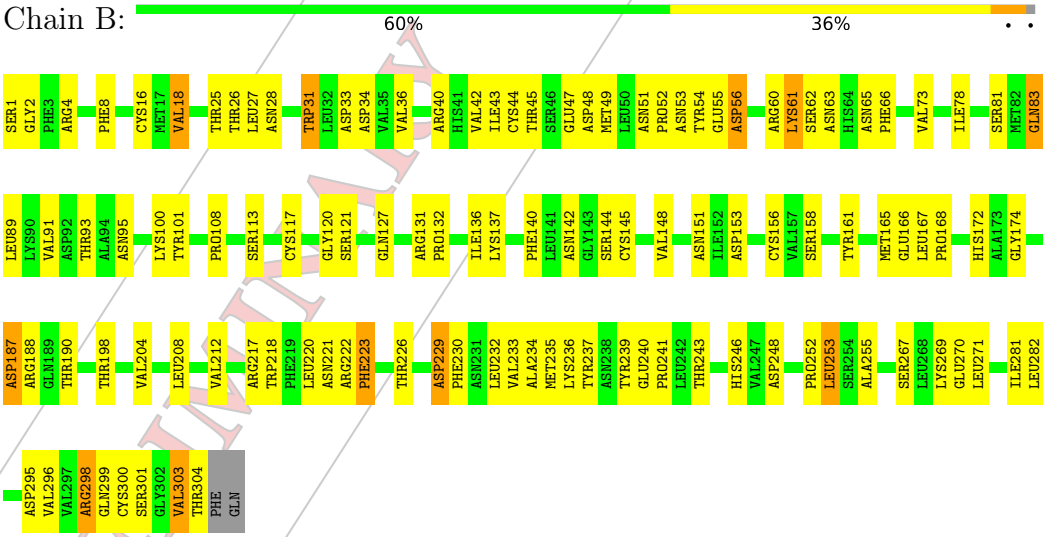
• Molecule 1: 3C-like proteinase

Chain A:



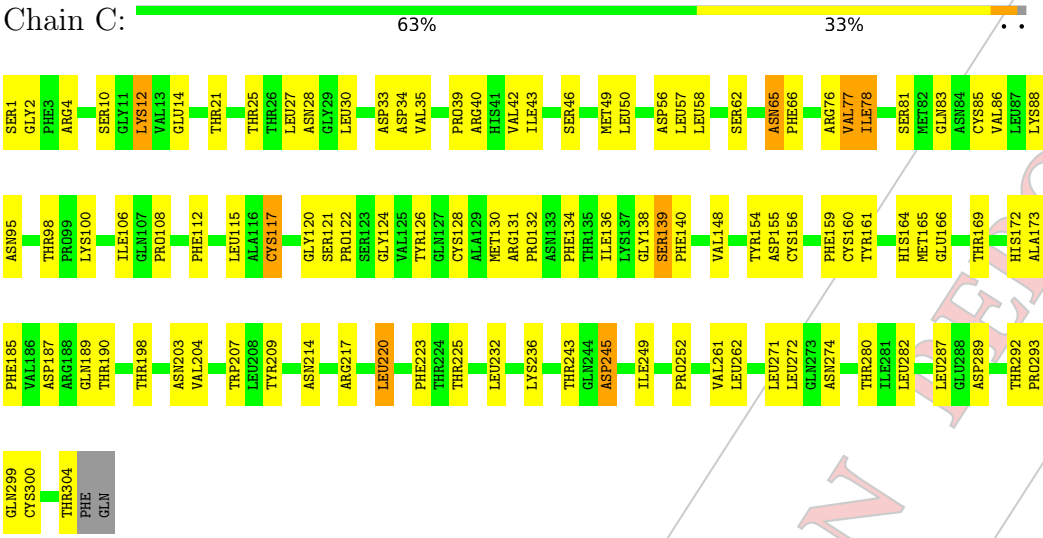
• Molecule 1: 3C-like proteinase

Chain B:



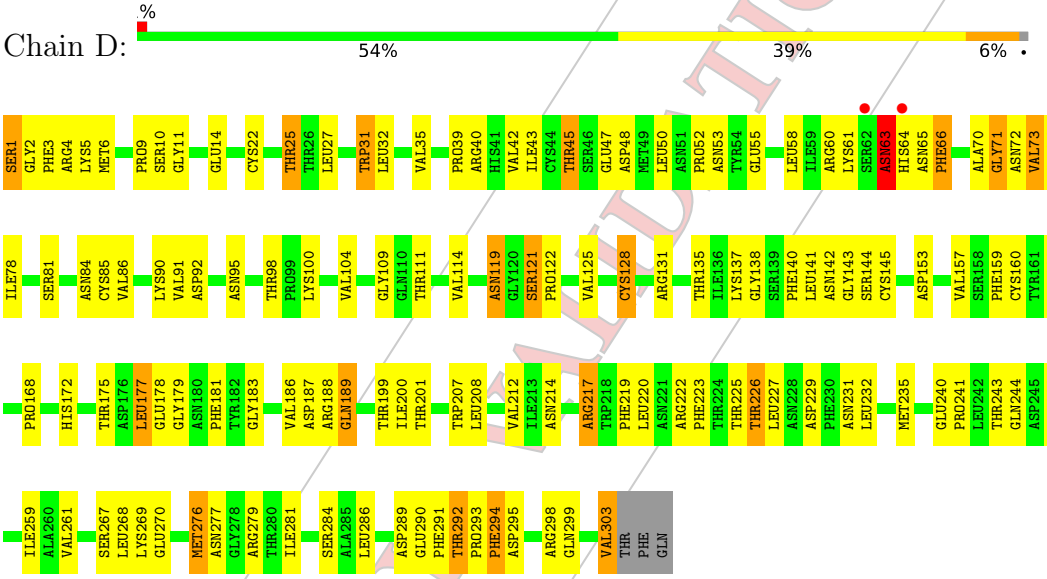
• Molecule 1: 3C-like proteinase

Chain C:



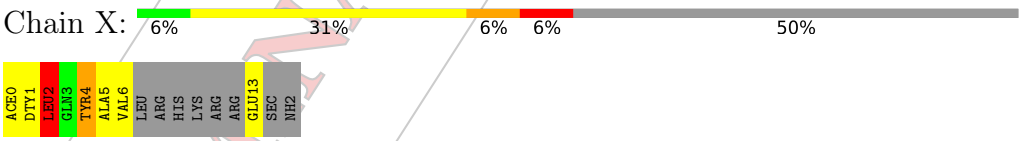
• Molecule 1: 3C-like proteinase

Chain D:



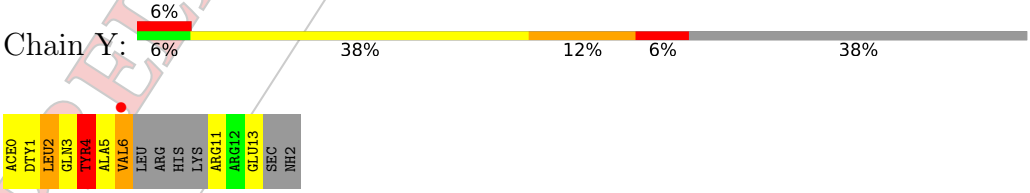
• Molecule 2: ACE-DTY-LEU-GLN-TYR-ALA-VAL-LEU-ARG-HIS-LYS-ARG-ARG-GLU-SEC

Chain X:



• Molecule 2: ACE-DTY-LEU-GLN-TYR-ALA-VAL-LEU-ARG-HIS-LYS-ARG-ARG-GLU-SEC

Chain Y:

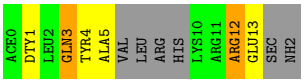


• Molecule 2: ACE-DTY-LEU-GLN-TYR-ALA-VAL-LEU-ARG-HIS-LYS-ARG-ARG-GLU-SEC

Chain Z:

• Molecule 2: ACE-DTY-LEU-GLN-TYR-ALA-VAL-LEU-ARG-HIS-LYS-ARG-ARG-GLU-SEC

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.36Å 201.73Å 60.54Å 90.00° 113.49° 90.00°	Depositor
Resolution (Å)	33.62 – 2.35 33.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.62-2.35) 99.6 (33.62-2.35)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.171 , 0.231 0.173 , 0.232	Depositor DCC
R_{free} test set	2306 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	1.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 19.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.508 for H, K, L 0.492 for -H, -K, H+L	Depositor
Outliers	2 of 44016 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9819	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% 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

Bond lengths and bond angles in the following residue types are not validated in this section: DTY, ACE, SEW

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	0.70	0/2392	0.90	0/3251
1	B	0.68	0/2399	0.90	0/3261
1	C	0.71	0/2399	0.93	0/3261
1	D	0.71	0/2392	0.93	0/3251
2	W	0.74	0/73	1.24	0/93
2	X	0.67	0/49	1.04	0/64
2	Y	0.75	0/77	1.26	1/99 (1.0%)
2	Z	0.70	0/107	1.22	0/140
All	All	0.70	0/9888	0.93	1/13420 (0.0%)

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	D	0	1
2	W	0	2
2	Z	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	4	TYR	CB-CA-C	5.79	121.97	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	183	GLY	Peptide
2	W	12	ARG	Peptide
2	W	3	GLN	Peptide
2	Z	7	LEU	Peptide
2	Z	8	ARG	Peptide

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	2340	0	2290	87	0
1	B	2347	0	2297	89	0
1	C	2347	0	2297	83	0
1	D	2340	0	2290	102	0
2	W	89	0	88	9	0
2	X	65	0	57	9	0
2	Y	94	0	93	11	0
2	Z	122	0	125	17	0
3	W	7	0	0	1	0
3	X	7	0	0	0	0
3	Y	7	0	0	0	0
3	Z	7	0	0	0	0
4	E	47	0	0	7	0
All	All	9819	0	9537	358	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 19.

All (358) 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:165:MET:HE3	2:Z:1:DTY:HE1	1.28	1.12
1:D:247:VAL:HG13	1:D:261:VAL:HG11	1.43	0.98
2:Z:6:VAL:HG11	2:Z:9:HIS:CE1	2.05	0.91
1:A:1:SER:OG	1:B:166:GLU:OE2	1.89	0.90
1:B:165:MET:HE3	2:Z:1:DTY:CE1	2.04	0.88
1:A:165:MET:HA	2:Y:2:LEU:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLN:O	1:C:86:VAL:HG12	1.81	0.81
1:A:33:ASP:O	1:A:94:ALA:HA	1.81	0.80
1:B:4:ARG:H	1:B:299:GLN:HE22	1.31	0.79
1:C:232:LEU:O	1:C:236:LYS:HG2	1.83	0.78
1:B:62:SER:H	1:B:65:ASN:ND2	1.82	0.77
1:B:26:THR:O	1:B:27:LEU:HD23	1.84	0.77
1:A:123:SER:OG	1:B:303:VAL:N	2.20	0.74
1:A:140:PHE:HD1	1:A:144:SER:HG	1.36	0.74
1:A:229:ASP:HB2	4:E:40:HOH:O	1.87	0.74
1:D:145:CYS:SG	2:W:3:GLN:N	2.61	0.74
1:A:27:LEU:HG	1:A:42:VAL:HG13	1.71	0.72
1:B:217:ARG:HA	1:B:220:LEU:HD13	1.72	0.72
1:D:269:LYS:NZ	4:E:50:HOH:O	2.16	0.72
1:A:1:SER:N	1:B:140:PHE:O	2.22	0.71
2:X:1:DTY:O	2:X:2:LEU:HB2	1.90	0.71
1:A:166:GLU:O	2:Y:1:DTY:N	2.24	0.71
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.73	0.70
1:A:3:PHE:O	1:A:4:ARG:HG2	1.92	0.69
1:C:27:LEU:HD22	1:C:42:VAL:HB	1.71	0.69
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.74	0.69
1:A:27:LEU:HD21	1:A:42:VAL:HG22	1.73	0.69
1:C:140:PHE:HB2	1:C:172:HIS:NE2	2.06	0.69
1:D:109:GLY:HA2	1:D:200:ILE:HD13	1.74	0.69
1:B:221:ASN:HB3	1:B:223:PHE:CZ	2.28	0.68
1:D:284:SER:OG	1:D:286:LEU:O	2.07	0.68
2:Z:1:DTY:C	2:Z:1:DTY:HD1	2.24	0.68
1:C:40:ARG:HD3	1:C:85:CYS:HA	1.77	0.67
1:D:247:VAL:CG1	1:D:261:VAL:HG11	2.23	0.67
1:D:268:LEU:HD12	1:D:268:LEU:O	1.95	0.67
1:D:212:VAL:HG11	1:D:259:ILE:HD12	1.75	0.67
1:D:4:ARG:H	1:D:299:GLN:HE22	1.40	0.66
1:B:83:GLN:O	1:B:86:VAL:HG12	1.96	0.66
2:Y:1:DTY:O	2:Y:2:LEU:HG	1.94	0.66
1:B:45:THR:HG1	1:B:48:ASP:CG	1.99	0.66
1:C:245:ASP:O	1:C:249:ILE:HG13	1.96	0.66
1:C:40:ARG:O	1:C:43:ILE:HG12	1.96	0.65
1:D:217:ARG:HB3	1:D:220:LEU:HD12	1.77	0.65
1:C:117:CYS:SG	1:C:121:SER:C	2.74	0.65
1:D:52:PRO:HD3	1:D:188:ARG:HG3	1.79	0.65
1:D:10:SER:O	1:D:14:GLU:HG3	1.97	0.65
1:C:126:TYR:HE1	1:C:128:CYS:HG	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ILE:O	1:D:63:ASN:ND2	2.30	0.64
1:C:4:ARG:H	1:C:299:GLN:HE22	1.46	0.64
1:C:130:MET:SD	1:C:134:PHE:HA	2.38	0.64
1:C:165:MET:CG	1:C:173:ALA:HB3	2.28	0.63
1:A:140:PHE:O	1:B:1:SER:N	2.24	0.63
1:C:166:GLU:OE2	1:D:1:SER:HB3	1.99	0.63
1:D:219:PHE:O	1:D:267:SER:HB2	1.98	0.62
1:B:292:THR:HG22	1:B:295:ASP:CG	2.19	0.62
1:A:140:PHE:HB2	1:A:172:HIS:CE1	2.35	0.62
1:C:112:PHE:HZ	1:C:136:ILE:HG12	1.65	0.62
1:A:301:SER:O	1:A:301:SER:OG	2.18	0.62
1:D:31:TRP:CH2	1:D:95:ASN:HA	2.34	0.61
1:D:145:CYS:SG	2:W:3:GLN:CA	2.88	0.61
1:B:267:SER:O	1:B:271:LEU:HD13	2.00	0.61
1:C:100:LYS:HG3	1:C:156:CYS:HA	1.81	0.61
1:B:44:CYS:HB3	1:B:49:MET:HG3	1.84	0.60
1:B:45:THR:OG1	1:B:48:ASP:CG	2.39	0.60
1:C:117:CYS:SG	1:C:121:SER:O	2.59	0.60
1:A:140:PHE:HD1	1:A:144:SER:OG	1.85	0.60
1:D:70:ALA:HB3	1:D:73:VAL:HG23	1.82	0.60
1:C:189:GLN:NE2	2:X:6:VAL:HG21	2.16	0.60
1:C:33:ASP:OD2	1:C:34:ASP:OD1	2.21	0.59
1:A:40:ARG:CD	1:A:85:CYS:HA	2.32	0.59
1:B:108:PRO:HB3	1:B:132:PRO:HA	1.84	0.59
1:B:217:ARG:HG3	1:B:220:LEU:HD22	1.85	0.59
1:D:52:PRO:CD	1:D:188:ARG:HG3	2.33	0.58
1:C:136:ILE:HD13	1:C:161:TYR:CE1	2.39	0.58
1:D:207:TRP:CH2	1:D:281:ILE:HB	2.38	0.58
1:C:28:ASN:HD22	1:C:120:GLY:H	1.52	0.58
1:D:226:THR:OG1	1:D:229:ASP:N	2.33	0.58
1:A:22:CYS:HG	1:A:66:PHE:HD1	1.52	0.58
1:C:214:ASN:HB2	1:C:282:LEU:HD21	1.86	0.58
1:B:53:ASN:HD22	1:B:56:ASP:HB2	1.69	0.57
2:Z:1:DTY:C	2:Z:1:DTY:CD1	2.83	0.57
1:A:243:THR:O	1:A:247:VAL:HG23	2.03	0.57
2:Z:7:LEU:HG	4:E:42:HOH:O	2.03	0.57
1:A:133:ASN:OD1	1:A:135:THR:OG1	2.22	0.57
1:D:207:TRP:HZ2	1:D:281:ILE:O	1.87	0.57
1:A:208:LEU:O	1:A:212:VAL:HG23	2.05	0.57
1:B:217:ARG:O	1:B:220:LEU:HB2	2.04	0.57
2:X:2:LEU:O	2:X:6:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TRP:O	1:A:210:ALA:HB3	2.05	0.57
1:C:2:GLY:HA3	1:D:138:GLY:O	2.05	0.56
1:C:95:ASN:HB3	1:C:98:THR:OG1	2.05	0.56
1:D:45:THR:O	1:D:48:ASP:N	2.39	0.56
1:B:62:SER:H	1:B:65:ASN:HD22	1.48	0.56
1:A:138:GLY:H	1:A:172:HIS:HD2	1.53	0.56
1:D:70:ALA:O	1:D:71:GLY:C	2.43	0.56
1:A:57:LEU:O	1:A:60:ARG:HB2	2.05	0.56
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.88	0.55
1:B:28:ASN:ND2	1:B:120:GLY:H	2.04	0.55
1:B:27:LEU:CD2	2:Z:4:TYR:HA	2.36	0.55
1:C:4:ARG:NH1	1:D:128:CYS:SG	2.74	0.55
1:B:226:THR:OG1	1:B:229:ASP:HB3	2.07	0.55
1:B:240:GLU:HG3	1:B:241:PRO:HD2	1.87	0.55
1:B:31:TRP:HB2	1:B:36:VAL:HG22	1.87	0.55
1:D:50:LEU:O	1:D:188:ARG:HG2	2.07	0.55
1:C:293:PRO:O	1:C:297:VAL:HG23	2.07	0.55
1:B:27:LEU:HG	1:B:42:VAL:HG23	1.88	0.54
1:D:159:PHE:HB3	1:D:177:LEU:HD13	1.89	0.54
1:B:168:PRO:HD3	2:Z:1:DTY:HE2	1.89	0.54
1:D:104:VAL:O	1:D:160:CYS:HA	2.08	0.54
1:D:141:LEU:HB3	2:W:13:GLU:OE2	2.07	0.54
1:D:163:HIS:HE1	1:D:172:HIS:HB3	1.72	0.54
1:D:40:ARG:HG2	1:D:187:ASP:OD2	2.08	0.54
1:B:16:CYS:SG	1:B:95:ASN:ND2	2.81	0.54
1:D:208:LEU:O	1:D:212:VAL:HG23	2.07	0.54
2:Y:3:GLN:O	2:Y:4:TYR:HB2	2.08	0.54
1:A:117:CYS:HA	1:A:122:PRO:HA	1.89	0.54
1:B:234:ALA:O	1:B:239:TYR:HB2	2.08	0.54
1:D:27:LEU:HD21	1:D:42:VAL:HB	1.89	0.54
1:B:45:THR:OG1	1:B:48:ASP:OD2	2.25	0.53
1:A:229:ASP:OD1	1:A:229:ASP:C	2.47	0.53
1:C:78:ILE:HD11	1:C:92:ASP:OD2	2.09	0.53
1:B:298:ARG:HA	1:B:303:VAL:HG23	1.89	0.53
1:C:140:PHE:HD2	1:C:172:HIS:CD2	2.27	0.53
1:B:25:THR:HB	1:B:42:VAL:O	2.09	0.53
1:B:140:PHE:HB2	1:B:172:HIS:CE1	2.44	0.53
1:D:145:CYS:SG	2:W:3:GLN:HB2	2.49	0.53
1:C:65:ASN:H	1:C:65:ASN:HD22	1.54	0.53
1:A:108:PRO:HD3	1:A:134:PHE:HE1	1.74	0.52
1:A:165:MET:CA	2:Y:2:LEU:HA	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PRO:O	1:B:255:ALA:HB3	2.09	0.52
1:C:4:ARG:NH2	1:D:137:LYS:O	2.42	0.52
1:C:165:MET:HG2	1:C:173:ALA:HB3	1.91	0.52
1:D:276:MET:HE1	1:D:281:ILE:HG13	1.90	0.52
1:D:212:VAL:HG11	1:D:259:ILE:CD1	2.39	0.52
1:A:218:TRP:CE2	1:A:279:ARG:HD3	2.46	0.51
1:C:138:GLY:O	1:D:2:GLY:HA3	2.10	0.51
1:C:117:CYS:HG	1:C:121:SER:C	2.10	0.51
1:C:217:ARG:O	1:C:220:LEU:HB2	2.11	0.51
1:B:40:ARG:O	1:B:43:ILE:HG12	2.10	0.51
1:B:165:MET:CE	2:Z:1:DTY:HE1	2.21	0.51
1:A:166:GLU:OE1	1:B:1:SER:N	2.36	0.51
1:B:91:VAL:HG23	1:B:93:THR:O	2.11	0.51
1:B:187:ASP:OD1	1:B:187:ASP:N	2.44	0.51
1:A:103:PHE:CE1	1:A:177:LEU:HD22	2.46	0.51
1:C:28:ASN:ND2	1:C:120:GLY:H	2.07	0.51
1:A:132:PRO:HG2	1:A:198:THR:O	2.11	0.51
1:A:31:TRP:CZ2	1:A:93:THR:HG23	2.45	0.51
1:B:140:PHE:HD2	1:B:172:HIS:CG	2.29	0.51
1:D:3:PHE:HE2	1:D:291:PHE:CD2	2.28	0.50
1:D:163:HIS:CE1	1:D:172:HIS:HB3	2.46	0.50
1:B:142:ASN:OD1	2:Z:3:GLN:HA	2.12	0.50
1:C:10:SER:O	1:C:14:GLU:HG3	2.11	0.50
1:C:140:PHE:HB2	1:C:172:HIS:CD2	2.46	0.50
1:C:184:PRO:HD2	1:C:185:PHE:CE2	2.46	0.50
1:C:245:ASP:N	1:C:245:ASP:OD1	2.43	0.50
1:D:131:ARG:NH1	1:D:289:ASP:OD2	2.44	0.50
1:D:70:ALA:O	1:D:72:ASN:N	2.45	0.50
1:D:298:ARG:HB2	1:D:303:VAL:HG11	1.93	0.50
1:B:60:ARG:HH21	1:B:61:LYS:HE2	1.76	0.50
1:B:204:VAL:HG13	1:B:287:LEU:HD22	1.92	0.50
1:B:83:GLN:HB3	1:B:86:VAL:HG12	1.94	0.50
1:C:140:PHE:O	1:D:1:SER:N	2.44	0.50
1:A:233:VAL:O	1:A:237:TYR:HD2	1.95	0.50
1:D:131:ARG:HB2	1:D:135:THR:O	2.12	0.50
1:C:249:ILE:O	1:C:252:PRO:HD2	2.12	0.50
1:B:243:THR:HG23	1:B:246:HIS:CE1	2.46	0.49
1:A:166:GLU:HB3	2:Y:0:ACE:H2	1.93	0.49
1:A:243:THR:HG23	1:A:245:ASP:H	1.77	0.49
1:B:243:THR:O	1:B:246:HIS:HB2	2.12	0.49
1:D:66:PHE:CD1	1:D:77:VAL:HG11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:HA	1:A:192:GLN:OE1	2.13	0.49
2:Z:9:HIS:C	2:Z:10:LYS:HD2	2.33	0.49
1:A:211:ALA:HA	1:A:282:LEU:HD21	1.95	0.49
1:A:301:SER:O	1:A:303:VAL:HG23	2.12	0.49
1:B:300:CYS:SG	1:B:300:CYS:O	2.70	0.49
1:A:78:ILE:CG1	1:A:90:LYS:HG3	2.43	0.49
1:B:166:GLU:HB2	2:Z:3:GLN:NE2	2.27	0.49
1:B:113:SER:OG	1:B:127:GLN:OE1	2.13	0.48
1:C:4:ARG:CZ	1:D:137:LYS:O	2.61	0.48
1:C:166:GLU:HB3	2:X:0:ACE:H2	1.95	0.48
1:A:4:ARG:N	1:A:299:GLN:HE22	2.10	0.48
1:B:63:ASN:ND2	1:B:78:ILE:O	2.47	0.48
1:C:140:PHE:HD2	1:C:172:HIS:CG	2.31	0.48
1:D:40:ARG:HD3	1:D:85:CYS:HA	1.95	0.48
1:D:143:GLY:N	2:W:3:GLN:O	2.30	0.48
1:B:18:VAL:HG21	1:B:36:VAL:HG13	1.95	0.48
1:B:208:LEU:O	1:B:212:VAL:HG23	2.13	0.48
1:D:225:THR:HG21	1:D:269:LYS:HD3	1.96	0.48
1:A:41:HIS:HB2	1:A:49:MET:SD	2.54	0.48
1:A:132:PRO:HD2	1:A:197:ASP:OD1	2.14	0.48
1:A:230:PHE:CD1	1:A:265:CYS:HB3	2.48	0.48
1:C:189:GLN:HE22	2:X:6:VAL:HG21	1.77	0.48
1:B:166:GLU:OE1	1:B:172:HIS:HE1	1.97	0.48
1:C:190:THR:O	2:X:1:DTY:CD1	2.62	0.47
1:D:231:ASN:O	1:D:235:MET:HG3	2.14	0.47
1:C:34:ASP:O	1:C:91:VAL:HG22	2.15	0.47
1:A:31:TRP:HZ2	1:A:93:THR:HG23	1.78	0.47
1:A:131:ARG:HD2	1:A:131:ARG:HA	1.61	0.47
1:A:138:GLY:O	1:B:2:GLY:HA3	2.15	0.47
1:A:141:LEU:HB3	2:Y:13:GLU:OE1	2.14	0.47
1:A:37:TYR:CD2	1:A:88:LYS:HG2	2.50	0.47
1:A:123:SER:OG	1:B:304:THR:N	2.43	0.47
1:B:298:ARG:HA	1:B:303:VAL:CG2	2.45	0.47
1:C:165:MET:HG3	1:C:173:ALA:HB3	1.97	0.47
1:A:39:PRO:HB2	1:A:41:HIS:CD2	2.50	0.47
1:B:8:PHE:HE2	1:B:151:ASN:HD22	1.61	0.47
1:D:168:PRO:HG3	2:W:1:DTY:HE1	1.96	0.47
1:A:4:ARG:NH2	1:B:137:LYS:O	2.48	0.47
1:A:13:VAL:O	1:A:15:GLY:N	2.48	0.46
1:A:108:PRO:HB3	1:A:132:PRO:HA	1.97	0.46
1:C:66:PHE:HB2	1:C:77:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASN:OD1	1:D:55:GLU:HB2	2.16	0.46
1:B:230:PHE:HA	1:B:269:LYS:HE3	1.96	0.46
1:C:126:TYR:HE1	1:C:128:CYS:SG	2.38	0.46
1:A:113:SER:OG	1:A:127:GLN:NE2	2.49	0.46
1:B:144:SER:O	1:B:145:CYS:C	2.53	0.46
1:D:27:LEU:HG	1:D:42:VAL:HG23	1.96	0.46
1:D:32:LEU:HD11	1:D:159:PHE:CE2	2.50	0.46
1:D:119:ASN:OD1	1:D:119:ASN:N	2.48	0.46
1:D:157:VAL:HG13	1:D:157:VAL:O	2.15	0.46
1:C:207:TRP:HZ3	1:C:287:LEU:HD23	1.80	0.46
1:C:140:PHE:CD2	1:C:172:HIS:CD2	3.04	0.46
1:C:148:VAL:HA	1:C:161:TYR:O	2.15	0.46
2:X:1:DTY:O	2:X:2:LEU:CB	2.61	0.46
2:Z:7:LEU:HG	2:Z:8:ARG:H	1.80	0.46
1:A:13:VAL:C	1:A:15:GLY:N	2.68	0.46
1:B:165:MET:HE2	1:B:167:LEU:HD23	1.97	0.46
1:C:39:PRO:HB3	1:C:164:HIS:CD2	2.51	0.46
1:C:106:ILE:HG23	1:C:160:CYS:HB2	1.98	0.46
1:B:131:ARG:NH2	1:B:198:THR:O	2.48	0.46
1:D:145:CYS:SG	2:W:3:GLN:C	2.94	0.46
1:D:45:THR:HG22	1:D:48:ASP:H	1.81	0.46
2:Z:6:VAL:HG11	2:Z:9:HIS:NE2	2.30	0.46
1:C:27:LEU:HD23	1:C:39:PRO:HD2	1.98	0.45
1:D:31:TRP:CE3	1:D:75:LEU:HD21	2.52	0.45
1:D:175:THR:HG22	1:D:181:PHE:HA	1.98	0.45
1:D:40:ARG:HB3	1:D:85:CYS:O	2.17	0.45
1:B:236:LYS:HA	1:B:236:LYS:HD3	1.66	0.45
1:C:62:SER:H	1:C:65:ASN:ND2	2.15	0.45
1:D:114:VAL:O	1:D:125:VAL:HG23	2.16	0.45
1:A:16:CYS:O	1:A:30:LEU:HA	2.16	0.45
1:A:224:THR:OG1	1:A:225:THR:N	2.50	0.45
1:C:139:SER:CB	1:D:299:GLN:HE21	2.28	0.45
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.16	0.45
1:A:122:PRO:O	1:B:304:THR:OG1	2.34	0.45
1:C:271:LEU:HD13	1:C:287:LEU:HD21	1.99	0.45
1:D:3:PHE:HE2	1:D:291:PHE:CE2	2.35	0.45
1:A:190:THR:O	1:A:192:GLN:HG3	2.16	0.45
1:C:115:LEU:HD21	1:C:122:PRO:HB3	1.99	0.45
1:C:207:TRP:CZ3	1:C:287:LEU:HD23	2.52	0.45
1:D:225:THR:HG22	1:D:229:ASP:OD2	2.16	0.45
2:W:4:TYR:HA	2:W:5:ALA:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:SER:OG	1:D:14:GLU:OE2	2.35	0.45
1:B:304:THR:OG1	4:E:51:HOH:O	2.18	0.45
1:C:203:ASN:OD1	1:C:292:THR:HA	2.17	0.45
1:D:60:ARG:HG2	1:D:61:LYS:H	1.82	0.45
1:A:25:THR:HB	1:A:42:VAL:O	2.17	0.44
1:B:40:ARG:CZ	1:B:54:TYR:CD2	3.00	0.44
1:D:45:THR:H	1:D:48:ASP:HB2	1.80	0.44
1:D:292:THR:HG22	1:D:295:ASP:H	1.82	0.44
1:B:233:VAL:O	1:B:237:TYR:HD1	2.00	0.44
1:C:1:SER:N	1:D:140:PHE:O	2.50	0.44
1:B:40:ARG:HG3	1:B:54:TYR:CE1	2.52	0.44
1:B:204:VAL:CG1	1:B:287:LEU:HD22	2.47	0.44
1:C:112:PHE:CE2	1:C:128:CYS:HB2	2.53	0.44
1:A:58:LEU:HD11	1:A:87:LEU:HD11	2.00	0.44
1:B:117:CYS:HA	1:B:121:SER:O	2.18	0.44
1:B:60:ARG:NH2	1:B:61:LYS:HE2	2.33	0.44
1:C:108:PRO:HG3	1:C:134:PHE:CE1	2.52	0.44
1:D:35:VAL:HG22	1:D:90:LYS:HD2	2.00	0.44
1:D:76:ARG:HB2	1:D:92:ASP:CG	2.37	0.44
1:D:111:THR:HG21	1:D:290:GLU:O	2.17	0.44
1:D:189:GLN:HG2	2:W:1:DTY:HD2	1.99	0.44
1:A:302:GLY:O	1:A:303:VAL:HB	2.17	0.43
1:B:27:LEU:HD12	1:B:42:VAL:HB	1.99	0.43
1:B:218:TRP:CZ2	1:B:281:ILE:HD11	2.53	0.43
1:A:112:PHE:O	1:A:127:GLN:HG3	2.16	0.43
1:A:122:PRO:O	1:A:122:PRO:CD	2.65	0.43
1:C:189:GLN:NE2	2:X:1:DTY:O	2.39	0.43
1:D:84:ASN:ND2	1:D:178:GLU:O	2.41	0.43
1:D:122:PRO:O	1:D:122:PRO:HG2	2.18	0.43
1:A:221:ASN:HD21	1:A:267:SER:HA	1.83	0.43
1:C:14:GLU:OE1	1:D:11:GLY:N	2.50	0.43
1:D:86:VAL:HG22	1:D:179:GLY:HA3	2.00	0.43
1:D:165:MET:CE	1:D:186:VAL:O	2.66	0.43
1:D:254:SER:OG	1:D:259:ILE:O	2.32	0.43
1:C:12:LYS:HD2	1:C:12:LYS:N	2.34	0.43
1:A:37:TYR:HE2	1:A:88:LYS:CD	2.31	0.43
1:A:132:PRO:HB2	1:A:198:THR:HG23	2.00	0.43
1:A:175:THR:HG22	1:A:181:PHE:HA	2.00	0.43
2:Z:7:LEU:HD12	2:Z:7:LEU:C	2.39	0.43
1:B:148:VAL:HA	1:B:161:TYR:O	2.19	0.43
1:C:65:ASN:ND2	1:C:65:ASN:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.54	0.43
1:C:35:VAL:HG21	1:C:88:LYS:HD2	2.01	0.43
1:C:124:GLY:HA3	1:D:6:MET:CG	2.49	0.43
1:C:131:ARG:HA	1:C:131:ARG:HD2	1.84	0.43
1:C:159:PHE:HB3	1:C:177:LEU:HD13	2.01	0.43
1:D:293:PRO:HG2	4:E:48:HOH:O	2.19	0.43
1:A:51:ASN:H	1:A:188:ARG:HE	1.65	0.43
1:B:66:PHE:HB3	1:B:89:LEU:HD21	2.01	0.43
1:C:115:LEU:HD11	1:C:122:PRO:HB3	2.01	0.43
1:C:304:THR:O	1:D:121:SER:HB2	2.19	0.43
1:D:32:LEU:HA	1:D:98:THR:OG1	2.19	0.43
1:D:22:CYS:SG	1:D:63:ASN:HB3	2.58	0.43
1:B:230:PHE:CD1	1:B:230:PHE:C	2.91	0.42
2:Z:8:ARG:N	4:E:42:HOH:O	2.45	0.42
1:A:142:ASN:ND2	2:Y:6[A]:VAL:O	2.51	0.42
1:C:30:LEU:CD2	1:C:177:LEU:HD21	2.50	0.42
1:D:240:GLU:HG3	1:D:241:PRO:HD2	2.00	0.42
1:B:253:LEU:HD21	1:B:296:VAL:HB	2.00	0.42
1:A:78:ILE:HG13	1:A:90:LYS:HG3	2.02	0.42
1:A:105:ARG:NH1	1:A:180:ASN:O	2.52	0.42
1:A:263:ASP:O	1:A:266:ALA:HB3	2.18	0.42
1:B:100:LYS:HG3	1:B:156:CYS:HA	2.02	0.42
1:D:45:THR:CG2	1:D:47:GLU:HB2	2.50	0.42
1:B:40:ARG:NH2	1:B:85:CYS:SG	2.92	0.42
1:A:111:THR:HG23	1:A:292:THR:HG23	2.01	0.42
1:B:188:ARG:HG2	1:B:190:THR:HG23	2.02	0.42
1:A:116:ALA:O	1:A:122:PRO:HA	2.20	0.42
1:B:83:GLN:HB3	1:B:86:VAL:CG1	2.50	0.42
1:C:139:SER:OG	1:D:299:GLN:NE2	2.37	0.42
1:D:225:THR:CG2	1:D:229:ASP:OD2	2.67	0.42
1:A:163:HIS:NE2	2:Y:3:GLN:HG3	2.35	0.42
1:D:3:PHE:CE2	1:D:291:PHE:CE2	3.08	0.42
1:D:292:THR:HG23	1:D:294:PHE:H	1.85	0.41
1:C:122:PRO:HB2	1:D:9:PRO:HG3	2.01	0.41
1:C:292:THR:O	1:C:296:VAL:HG23	2.20	0.41
1:A:243:THR:H	1:A:246:HIS:HB2	1.86	0.41
1:C:204:VAL:CG2	1:C:289:ASP:HB3	2.49	0.41
2:X:4:TYR:HA	2:X:5:ALA:HA	1.65	0.41
1:C:209:TYR:OH	1:C:261:VAL:HA	2.21	0.41
1:A:90:LYS:HD3	1:A:90:LYS:HA	1.89	0.41
1:C:140:PHE:HB2	1:C:172:HIS:HE2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:THR:O	1:D:246:HIS:HB2	2.21	0.41
1:B:161:TYR:CE1	1:B:174:GLY:HA3	2.56	0.41
1:A:243:THR:HG23	1:A:245:ASP:N	2.36	0.41
1:C:207:TRP:HZ3	1:C:287:LEU:CD2	2.34	0.41
2:Y:4:TYR:CD2	2:Y:5:ALA:HB2	2.55	0.41
3:W:14:SEW:NB	3:W:14:SEW:SE	3.03	0.41
1:A:37:TYR:HE2	1:A:88:LYS:HD2	1.85	0.41
1:D:25:THR:HB	1:D:42:VAL:O	2.20	0.41
1:D:227:LEU:HD23	1:D:227:LEU:C	2.41	0.41
1:D:276:MET:HE2	1:D:279:ARG:O	2.20	0.41
2:Y:4:TYR:HA	2:Y:5:ALA:HA	1.50	0.40
1:A:68:VAL:HB	1:A:75:LEU:HB2	2.04	0.40
1:C:21:THR:HA	1:C:25:THR:O	2.22	0.40
1:A:287:LEU:HD13	1:A:287:LEU:HA	1.93	0.40
1:B:44:CYS:SG	1:B:52:PRO:HB3	2.62	0.40
1:B:232:LEU:O	1:B:235:MET:HG2	2.21	0.40
1:A:253:LEU:HD22	1:A:253:LEU:N	2.36	0.40
1:B:63:ASN:ND2	1:B:78:ILE:C	2.74	0.40
1:D:39:PRO:HD3	1:D:162:MET:SD	2.62	0.40
1:D:64:HIS:O	1:D:65:ASN:HB3	2.21	0.40
1:D:225:THR:HG21	1:D:269:LYS:CD	2.51	0.40
1:A:24:THR:HG22	1:A:24:THR:O	2.20	0.40
1:A:40:ARG:HH21	1:A:187:ASP:HB2	1.87	0.40
2:Z:6:VAL:HG12	4:E:42:HOH:O	2.20	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	301/306 (98%)	280 (93%)	16 (5%)	5 (2%)	9 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	302/306 (99%)	284 (94%)	16 (5%)	2 (1%)	22	23
1	C	302/306 (99%)	286 (95%)	14 (5%)	2 (1%)	22	23
1	D	301/306 (98%)	280 (93%)	19 (6%)	2 (1%)	22	23
2	W	5/16 (31%)	2 (40%)	3 (60%)	0	100	100
2	X	4/16 (25%)	2 (50%)	0	2 (50%)	0	0
2	Y	5/16 (31%)	2 (40%)	1 (20%)	2 (40%)	0	0
2	Z	10/16 (62%)	5 (50%)	3 (30%)	2 (20%)	0	0
All	All	1230/1288 (96%)	1141 (93%)	72 (6%)	17 (1%)	11	9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	D	71	GLY
2	Y	4	TYR
1	A	14	GLU
1	A	302	GLY
1	C	77	VAL
1	D	63	ASN
2	Z	7	LEU
1	A	187	ASP
1	B	33	ASP
2	X	2	LEU
2	Y	2	LEU
2	X	4	TYR
2	Z	6	VAL
1	C	154	TYR
1	B	184	PRO
1	A	184	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/263 (99%)	228 (88%)	32 (12%)	4	4
1	B	261/263 (99%)	233 (89%)	28 (11%)	6	6
1	C	261/263 (99%)	231 (88%)	30 (12%)	5	5
1	D	260/263 (99%)	223 (86%)	37 (14%)	3	3
2	W	7/11 (64%)	6 (86%)	1 (14%)	3	3
2	X	5/11 (46%)	3 (60%)	2 (40%)	0	0
2	Y	8/11 (73%)	5 (62%)	3 (38%)	0	0
2	Z	11/11 (100%)	10 (91%)	1 (9%)	9	8
All	All	1073/1096 (98%)	939 (88%)	134 (12%)	4	4

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	22	CYS
1	A	27	LEU
1	A	42	VAL
1	A	46	SER
1	A	48	ASP
1	A	58	LEU
1	A	59	ILE
1	A	81	SER
1	A	87	LEU
1	A	97	LYS
1	A	105	ARG
1	A	122	PRO
1	A	123	SER
1	A	127	GLN
1	A	131	ARG
1	A	137	LYS
1	A	153	ASP
1	A	156	CYS
1	A	177	LEU
1	A	190	THR
1	A	198	THR
1	A	208	LEU
1	A	216	ASP
1	A	217	ARG
1	A	229	ASP
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	232	LEU
1	A	256	GLN
1	A	262	LEU
1	A	287	LEU
1	A	301	SER
1	B	18	VAL
1	B	31	TRP
1	B	34	ASP
1	B	47	GLU
1	B	51	ASN
1	B	55	GLU
1	B	56	ASP
1	B	61	LYS
1	B	73	VAL
1	B	81	SER
1	B	83	GLN
1	B	101	TYR
1	B	136	ILE
1	B	153	ASP
1	B	158	SER
1	B	181	PHE
1	B	187	ASP
1	B	222	ARG
1	B	223	PHE
1	B	229	ASP
1	B	248	ASP
1	B	253	LEU
1	B	270	GLU
1	B	282	LEU
1	B	292	THR
1	B	298	ARG
1	B	301	SER
1	B	303	VAL
1	C	12	LYS
1	C	46	SER
1	C	49	MET
1	C	50	LEU
1	C	56	ASP
1	C	57	LEU
1	C	58	LEU
1	C	65	ASN
1	C	76	ARG

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Mol	Chain	Res	Type
1	C	78	ILE
1	C	81	SER
1	C	92	ASP
1	C	117	CYS
1	C	132	PRO
1	C	139	SER
1	C	155	ASP
1	C	169	THR
1	C	187	ASP
1	C	198	THR
1	C	220	LEU
1	C	223	PHE
1	C	225	THR
1	C	243	THR
1	C	245	ASP
1	C	262	LEU
1	C	272	LEU
1	C	274	ASN
1	C	280	THR
1	C	298	ARG
1	C	300	CYS
1	D	1	SER
1	D	5	LYS
1	D	25	THR
1	D	31	TRP
1	D	45	THR
1	D	58	LEU
1	D	63	ASN
1	D	66	PHE
1	D	73	VAL
1	D	74	GLN
1	D	78	ILE
1	D	81	SER
1	D	91	VAL
1	D	100	LYS
1	D	119	ASN
1	D	121	SER
1	D	128	CYS
1	D	142	ASN
1	D	144	SER
1	D	153	ASP
1	D	177	LEU

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Mol	Chain	Res	Type
1	D	189	GLN
1	D	199	THR
1	D	201	THR
1	D	214	ASN
1	D	217	ARG
1	D	222	ARG
1	D	223	PHE
1	D	226	THR
1	D	232	LEU
1	D	244	GLN
1	D	270	GLU
1	D	276	MET
1	D	277	ASN
1	D	292	THR
1	D	294	PHE
1	D	303	VAL
2	X	2	LEU
2	X	13	GLU
2	Y	6[A]	VAL
2	Y	6[B]	VAL
2	Y	11	ARG
2	Z	10	LYS
2	W	12	ARG

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	41	HIS
1	A	65	ASN
1	A	80	HIS
1	A	127	GLN
1	A	172	HIS
1	A	221	ASN
1	A	228	ASN
1	A	231	ASN
1	A	299	GLN
1	B	19	GLN
1	B	28	ASN
1	B	41	HIS
1	B	51	ASN
1	B	53	ASN
1	B	65	ASN

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Mol	Chain	Res	Type
1	B	80	HIS
1	B	119	ASN
1	B	172	HIS
1	B	203	ASN
1	B	214	ASN
1	B	221	ASN
1	B	299	GLN
1	C	28	ASN
1	C	63	ASN
1	C	65	ASN
1	C	74	GLN
1	C	119	ASN
1	C	214	ASN
1	C	256	GLN
1	C	274	ASN
1	C	299	GLN
1	D	41	HIS
1	D	164	HIS
1	D	180	ASN
1	D	214	ASN
1	D	299	GLN
2	Z	3	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	303/306 (99%)	-0.53	0 100 100	21, 39, 56, 79	0
1	B	304/306 (99%)	-0.53	0 100 100	23, 38, 56, 79	0
1	C	304/306 (99%)	-0.67	0 100 100	21, 32, 45, 78	0
1	D	303/306 (99%)	-0.57	2 (0%) 87 92	21, 34, 56, 107	0
2	W	8/16 (50%)	-0.46	0 100 100	29, 45, 50, 52	0
2	X	6/16 (37%)	-0.34	0 100 100	32, 39, 40, 40	0
2	Y	8/16 (50%)	0.18	1 (12%) 3 6	34, 44, 53, 53	0
2	Z	11/16 (68%)	-0.37	0 100 100	28, 38, 63, 76	0
All	All	1247/1288 (96%)	-0.57	3 (0%) 95 97	21, 36, 56, 107	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	SER	2.5
2	Y	6[A]	VAL	2.2
1	D	64	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTY	Y	1	12/?	0.92	0.15	53,60,64,70	0
2	DTY	Z	1	12/?	0.93	0.14	36,44,47,50	0
2	DTY	W	1	12/?	0.96	0.11	31,37,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTY	X	1	12/?	0.97	0.11	30,34,37,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SEW	X	14	7/?	0.97	0.11	32,37,50,56	0
3	SEW	Z	14	7/?	0.97	0.07	42,49,58,71	0
3	SEW	Y	14	7/?	0.99	0.08	37,42,51,61	0
3	SEW	W	14	7/?	0.99	0.09	43,52,66,71	0

6.5 Other polymers (i)

There are no such residues in this entry.