Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 09:45 AM JST

PDB ID	:	6LII
Title	:	A quinone oxidoreductase
Authors	:	Hakoshima, T.; Kim, S.-Y.; Mori, T.
Deposited on	:	2019-12-11
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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

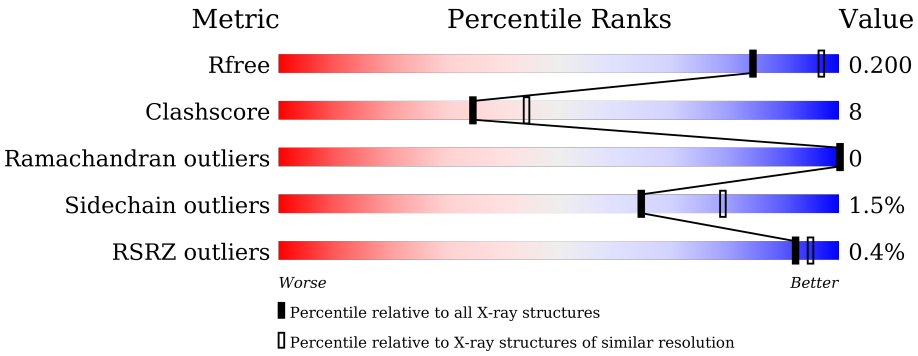
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	353	82% 14%
1	B	353	% 77% 19%
1	C	353	% 81% 16%
1	D	353	79% 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10545 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 Synaptic vesicle membrane protein VAT-1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2609	1671	449	471	18			
1	B	340	Total	C	N	O	S	0	0	0
			2552	1629	441	465	17			
1	C	345	Total	C	N	O	S	0	0	0
			2582	1658	443	463	18			
1	D	342	Total	C	N	O	S	0	0	0
			2577	1650	442	468	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLY	-	expression tag	UNP Q99536
A	42	PRO	-	expression tag	UNP Q99536
B	41	GLY	-	expression tag	UNP Q99536
B	42	PRO	-	expression tag	UNP Q99536
C	41	GLY	-	expression tag	UNP Q99536
C	42	PRO	-	expression tag	UNP Q99536
D	41	GLY	-	expression tag	UNP Q99536
D	42	PRO	-	expression tag	UNP Q99536

- Molecule 2 is water.

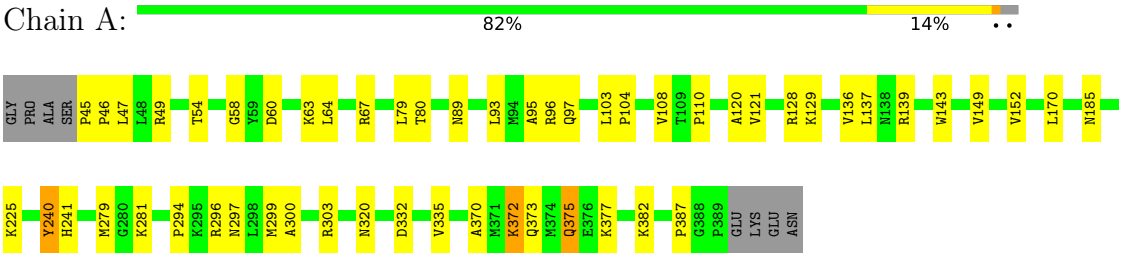
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	53	Total	O	0	0
			53	53		
2	C	58	Total	O	0	0
			58	58		
2	D	58	Total	O	0	0
			58	58		

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.

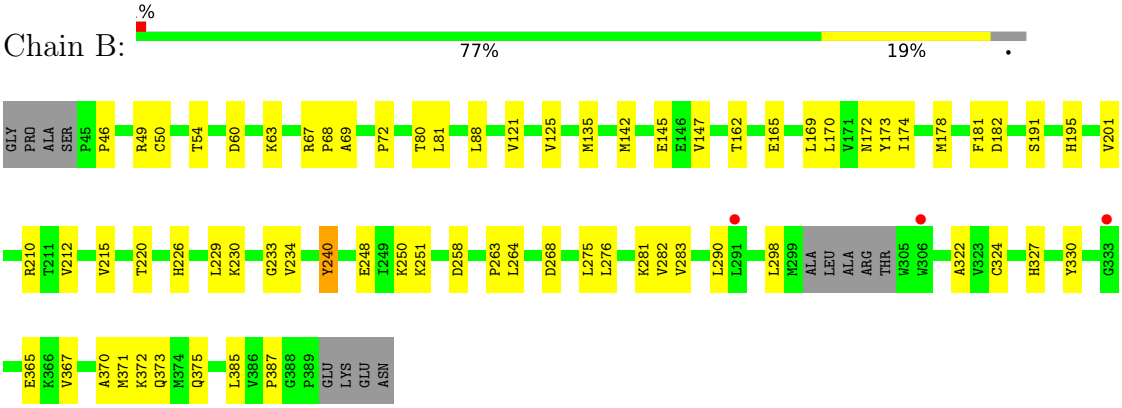
• Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog

Chain A:



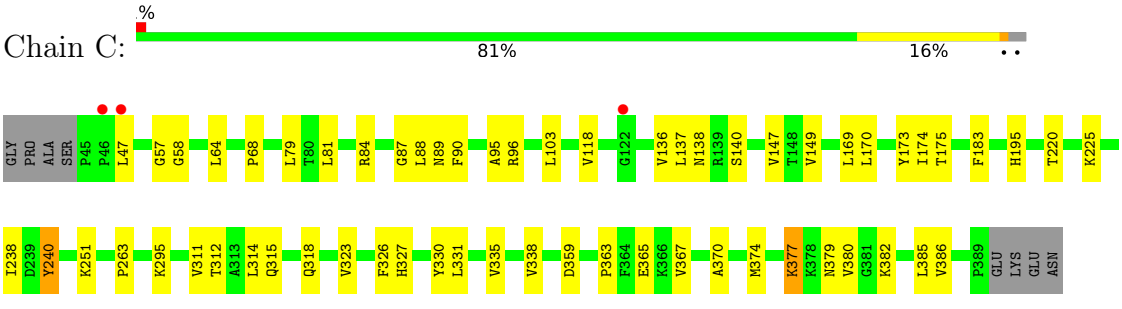
• Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog

Chain B:



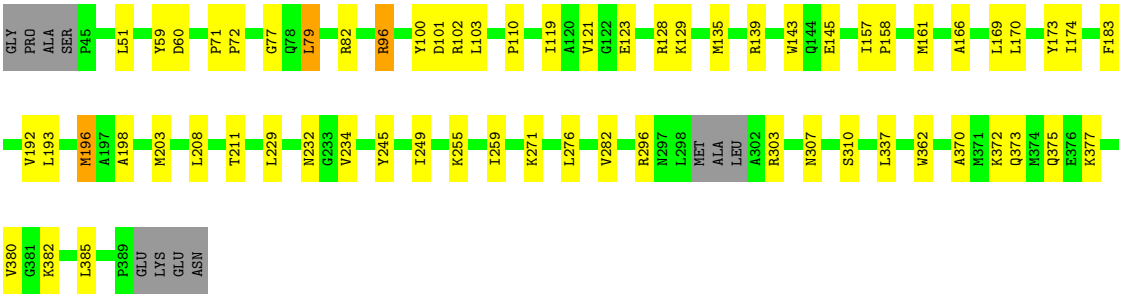
• Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog

Chain C:



• Molecule 1: Synaptic vesicle membrane protein VAT-1 homolog

Chain D:


GLY PRO ALA SER P45
L51
Y59 D60
P71 P72
G77 Q78 L79
R82
R96
Y100 D101 R102 L103
P110
I119 A120 V121 G122 E123
R128 K129
M135
R139
W143 Q144 E145
I157 P158
M161
A166
L169 L170
Y173 I174
F183
V192 L193
M196 A197 A198
M203
L208
T211
L229
N232 G233 V234
Y245
I249
K255
I259
K271
L276
V282
R296 N297 L298 MET ALA LEU A302
R303
N307
S310
L337
W362
A370 M371 K372 Q373 M374 Q375 E376 K377
V380 G381 K382
L385
P389 GLU LYS GLU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.35Å 69.35Å 581.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.68 – 2.30 48.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.68-2.30) 99.2 (48.68-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.180 , 0.203 0.180 , 0.200	Depositor DCC
R_{free} test set	3734 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.469 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10545	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	0.37	0/2667	0.47	0/3625
1	B	0.29	0/2605	0.46	0/3538
1	C	0.50	0/2640	0.53	0/3592
1	D	0.31	0/2634	0.45	0/3582
All	All	0.37	0/10546	0.48	0/14337

There are no bond length outliers.

There are no bond angle outliers.

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	2609	0	2659	37	0
1	B	2552	0	2591	49	0
1	C	2582	0	2624	45	0
1	D	2577	0	2610	43	0
2	A	56	0	0	1	0
2	B	53	0	0	0	0
2	C	58	0	0	1	0
2	D	58	0	0	7	0
All	All	10545	0	10484	172	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 8.

All (172) 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:121:VAL:CG1	1:B:125:VAL:HB	1.93	0.97
1:B:121:VAL:HG11	1:B:125:VAL:CG1	1.94	0.97
1:A:240:TYR:HE2	1:A:241:HIS:CE1	1.95	0.84
1:D:196:MET:CE	1:D:377:LYS:HE3	2.07	0.84
1:B:121:VAL:CG1	1:B:125:VAL:CB	2.57	0.82
1:B:121:VAL:HG12	1:B:125:VAL:HB	1.63	0.80
1:C:58:GLY:HA3	1:C:295:LYS:HD3	1.64	0.79
1:D:196:MET:HE2	1:D:377:LYS:HE3	1.67	0.75
1:B:121:VAL:HG11	1:B:125:VAL:CB	2.17	0.74
1:B:121:VAL:CG1	1:B:125:VAL:CG1	2.65	0.74
1:B:121:VAL:HG11	1:B:125:VAL:HB	1.70	0.73
1:C:331:LEU:HD23	1:C:331:LEU:O	1.90	0.71
1:B:121:VAL:CG1	1:B:125:VAL:HG11	2.21	0.69
1:D:79:LEU:C	1:D:79:LEU:HD12	2.12	0.69
1:A:46:PRO:C	1:A:47:LEU:HD12	2.12	0.69
1:B:121:VAL:HG11	1:B:125:VAL:HG11	1.72	0.69
1:C:377:LYS:HD2	1:C:379:ASN:HD21	1.58	0.68
1:D:196:MET:HE3	1:D:377:LYS:HE3	1.77	0.66
1:B:195:HIS:HB2	1:B:263:PRO:HD2	1.78	0.65
1:D:121:VAL:HG11	1:D:129:LYS:HA	1.80	0.63
1:C:195:HIS:HB2	1:C:263:PRO:HD2	1.80	0.63
1:C:57:GLY:O	1:C:96:ARG:NH1	2.34	0.61
1:D:82:ARG:HG2	1:D:119:ILE:HG13	1.83	0.61
1:C:175:THR:HG22	1:C:326:PHE:HE2	1.66	0.60
1:A:294:PRO:HB3	1:A:375:GLN:NE2	2.17	0.59
1:C:88:LEU:HD22	1:C:374:MET:HG3	1.85	0.59
1:D:135:MET:HG3	1:D:157:ILE:HG12	1.85	0.59
1:A:139:ARG:HE	1:A:332:ASP:HB2	1.68	0.58
1:C:318:GLN:NE2	1:D:101:ASP:OD1	2.36	0.58
1:C:377:LYS:HD2	1:C:379:ASN:ND2	2.17	0.58
1:C:138:ASN:ND2	1:C:140:SER:O	2.37	0.58
1:A:93:LEU:HD13	1:A:375:GLN:HG2	1.86	0.57
1:A:97:GLN:NE2	1:A:296:ARG:O	2.38	0.57
1:B:230:LYS:NZ	1:B:234:VAL:O	2.38	0.57
1:D:129:LYS:NZ	2:D:401:HOH:O	2.38	0.57
1:A:49:ARG:HB3	1:A:64:LEU:HD11	1.87	0.56
1:C:377:LYS:NZ	1:C:379:ASN:HD21	2.03	0.56
1:C:79:LEU:HD21	1:C:118:VAL:HG22	1.86	0.56
1:A:45:PRO:O	1:A:47:LEU:HD13	2.06	0.56
1:B:46:PRO:O	1:B:69:ALA:CB	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:O	1:D:174:ILE:HB	2.06	0.56
1:B:72:PRO:HB3	1:B:80:THR:HG21	1.88	0.55
1:A:225:LYS:NZ	1:A:377:LYS:O	2.31	0.55
1:C:136:VAL:HG21	1:C:149:VAL:HG11	1.90	0.54
1:D:77:GLY:N	1:D:123:GLU:O	2.31	0.54
1:B:142:MET:HE1	1:B:147:VAL:HG21	1.89	0.54
1:A:281:LYS:NZ	2:A:404:HOH:O	2.40	0.54
1:A:96:ARG:NH2	1:A:375:GLN:OE1	2.40	0.53
1:B:250:LYS:HE2	1:B:275:LEU:HD23	1.89	0.53
1:A:89:ASN:OD1	1:A:382:LYS:NZ	2.41	0.53
1:D:276:LEU:HD11	1:D:282:VAL:HG12	1.91	0.53
1:C:64:LEU:HD22	1:C:365:GLU:HG3	1.92	0.52
1:C:174:ILE:HD13	1:C:338:VAL:HG13	1.92	0.52
1:C:195:HIS:HA	1:C:220:THR:OG1	2.10	0.52
1:C:377:LYS:CD	1:C:379:ASN:HD21	2.22	0.52
1:A:300:ALA:HB3	1:A:303:ARG:HG2	1.91	0.52
1:B:367:VAL:HG23	1:B:385:LEU:HD21	1.91	0.52
1:C:47:LEU:HB2	1:C:68:PRO:HA	1.92	0.52
1:B:49:ARG:NH2	1:B:365:GLU:OE2	2.43	0.52
1:B:46:PRO:O	1:B:69:ALA:HB3	2.10	0.51
1:D:196:MET:SD	1:D:196:MET:N	2.83	0.51
1:C:367:VAL:HG23	1:C:385:LEU:HD11	1.92	0.51
1:D:102:ARG:HH21	1:D:139:ARG:HH21	1.57	0.51
1:C:89:ASN:ND2	2:C:405:HOH:O	2.43	0.51
1:A:60:ASP:N	1:A:60:ASP:OD1	2.39	0.51
1:B:121:VAL:HG11	1:B:125:VAL:HG12	1.90	0.50
1:A:79:LEU:HD23	1:A:121:VAL:HA	1.93	0.50
1:A:240:TYR:CE2	1:A:241:HIS:CE1	2.87	0.50
1:C:87:GLY:HA3	1:C:382:LYS:HZ1	1.77	0.50
1:D:100:TYR:CZ	1:D:102:ARG:HB2	2.46	0.50
1:A:121:VAL:HG21	1:A:129:LYS:HA	1.93	0.50
1:B:210:ARG:HD3	1:B:233:GLY:HA3	1.93	0.50
1:B:135:MET:HB3	1:B:170:LEU:HD11	1.94	0.49
1:D:59:TYR:CZ	1:D:372:LYS:HG2	2.48	0.49
1:D:79:LEU:HD12	1:D:79:LEU:O	2.12	0.49
1:D:208:LEU:O	1:D:211:THR:HG22	2.13	0.49
1:A:139:ARG:NE	1:A:332:ASP:HB2	2.27	0.49
1:B:54:THR:OG1	1:B:63:LYS:NZ	2.46	0.49
1:B:88:LEU:HD11	1:B:371:MET:HG2	1.93	0.49
1:C:327:HIS:HB3	1:C:330:TYR:HD1	1.78	0.49
1:C:225:LYS:HG2	1:C:380:VAL:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LEU:HG	1:B:298:LEU:HD22	1.94	0.48
1:D:307:ASN:ND2	2:D:405:HOH:O	2.46	0.48
1:A:152:VAL:HG22	1:A:335:VAL:HG11	1.95	0.48
1:D:192:VAL:HG22	1:D:259:ILE:HB	1.94	0.48
1:C:367:VAL:O	1:C:370:ALA:HB3	2.14	0.48
1:A:294:PRO:HB3	1:A:375:GLN:HE22	1.78	0.47
1:C:137:LEU:HB2	1:C:170:LEU:HD13	1.95	0.47
1:C:225:LYS:NZ	1:C:377:LYS:O	2.47	0.47
1:B:67:ARG:CG	1:B:68:PRO:HD2	2.45	0.47
1:B:68:PRO:O	1:B:69:ALA:C	2.53	0.47
1:B:283:VAL:HG13	1:B:324:CYS:HB2	1.97	0.47
1:C:251:LYS:HB2	1:C:251:LYS:HE2	1.81	0.47
1:C:377:LYS:HD2	1:C:377:LYS:HA	1.57	0.47
1:A:136:VAL:HG21	1:A:149:VAL:HG21	1.96	0.47
1:A:49:ARG:CZ	1:A:387:PRO:O	2.63	0.47
1:B:248:GLU:HA	1:B:251:LYS:HZ3	1.79	0.47
1:C:87:GLY:HA3	1:C:382:LYS:NZ	2.30	0.47
1:A:370:ALA:O	1:A:373:GLN:HB3	2.15	0.46
1:B:191:SER:N	1:B:258:ASP:OD1	2.47	0.46
1:D:362:TRP:HB2	1:D:385:LEU:CD2	2.45	0.46
1:B:226:HIS:O	1:B:229:LEU:HB2	2.16	0.46
1:B:264:LEU:HD13	1:B:268:ASP:OD2	2.15	0.46
1:B:121:VAL:HG13	1:B:125:VAL:HG11	1.95	0.46
1:D:60:ASP:OD1	1:D:60:ASP:N	2.48	0.46
1:D:96:ARG:NH1	1:D:375:GLN:OE1	2.38	0.46
1:A:80:THR:HB	1:A:120:ALA:HB3	1.98	0.46
1:C:90:PHE:HZ	1:C:377:LYS:HD3	1.79	0.46
1:D:193:LEU:HD13	1:D:249:ILE:HD11	1.97	0.46
1:D:198:ALA:HB1	1:D:380:VAL:HG13	1.97	0.46
1:B:220:THR:HB	1:B:240:TYR:CD2	2.51	0.46
1:C:147:VAL:HG12	1:C:149:VAL:HG13	1.98	0.46
1:D:158:PRO:HG2	1:D:161:MET:HB3	1.98	0.46
1:C:312:THR:HG23	1:C:315:GLN:H	1.81	0.45
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.78	0.45
1:B:67:ARG:HG2	1:B:68:PRO:HD2	1.99	0.45
1:C:311:VAL:HG21	1:C:323:VAL:HG21	1.97	0.45
1:C:359:ASP:N	1:C:382:LYS:O	2.35	0.45
1:D:100:TYR:HD2	1:D:103:LEU:HB2	1.81	0.45
1:D:203:MET:HA	1:D:232:ASN:HD21	1.82	0.45
1:A:47:LEU:HD12	1:A:47:LEU:N	2.31	0.44
1:B:60:ASP:OD1	1:B:60:ASP:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PRO:O	1:A:47:LEU:CD1	2.65	0.44
1:B:281:LYS:HG3	1:B:322:ALA:HB3	1.99	0.44
1:D:51:LEU:HD12	1:D:143:TRP:HB3	1.98	0.44
1:D:245:TYR:OH	1:D:271:LYS:HD3	2.17	0.44
1:B:212:VAL:HB	1:B:215:VAL:HG21	2.00	0.44
1:C:84:ARG:O	1:C:386:VAL:HG12	2.17	0.44
1:D:135:MET:HG2	1:D:166:ALA:HB1	2.00	0.44
1:D:337:LEU:HA	2:D:429:HOH:O	2.18	0.44
1:B:290:LEU:HD21	1:B:298:LEU:HD13	2.00	0.44
1:C:95:ALA:HB1	1:C:103:LEU:HD22	2.00	0.44
1:C:169:LEU:O	1:C:173:TYR:HB2	2.18	0.44
1:C:220:THR:HB	1:C:240:TYR:CD2	2.53	0.43
1:A:297:ASN:ND2	1:A:299:MET:SD	2.81	0.43
1:D:51:LEU:O	1:D:110:PRO:HD2	2.19	0.43
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.93	0.43
1:D:370:ALA:O	1:D:373:GLN:HB3	2.17	0.43
1:A:54:THR:OG1	1:A:63:LYS:NZ	2.52	0.43
1:B:370:ALA:O	1:B:373:GLN:HB3	2.18	0.43
1:D:82:ARG:HA	1:D:145:GLU:O	2.18	0.43
1:B:178:MET:O	1:B:182:ASP:HB2	2.19	0.43
1:C:79:LEU:HD22	1:C:81:LEU:HD23	2.01	0.43
1:A:110:PRO:HG2	1:A:143:TRP:CE3	2.53	0.43
1:B:327:HIS:HB3	1:B:330:TYR:HD2	1.84	0.42
1:A:95:ALA:HB1	1:A:103:LEU:HD22	2.01	0.42
1:B:170:LEU:O	1:B:174:ILE:HB	2.19	0.42
1:B:372:LYS:HA	1:B:375:GLN:HB2	2.01	0.42
1:B:145:GLU:HG2	1:B:387:PRO:HB2	2.01	0.42
1:B:172:ASN:HA	1:B:201:VAL:HG22	2.01	0.42
1:D:382:LYS:NZ	2:D:407:HOH:O	2.47	0.42
1:A:79:LEU:HD11	1:A:128:ARG:HG3	2.01	0.42
1:D:196:MET:HG3	1:D:377:LYS:HD2	2.01	0.42
1:C:335:VAL:HG12	1:C:335:VAL:O	2.19	0.42
1:D:128:ARG:NH2	2:D:406:HOH:O	2.47	0.42
1:A:137:LEU:HB2	1:A:170:LEU:HD13	2.02	0.41
1:D:229:LEU:HB3	1:D:234:VAL:HG21	2.02	0.41
1:B:162:THR:HG23	1:B:165:GLU:H	1.86	0.41
1:B:276:LEU:HD11	1:B:282:VAL:HG12	2.02	0.41
1:C:365:GLU:H	1:C:365:GLU:CD	2.23	0.41
1:A:185:ASN:ND2	1:B:181:PHE:O	2.54	0.41
1:D:169:LEU:O	1:D:173:TYR:HB2	2.21	0.41
1:A:58:GLY:HA2	1:A:294:PRO:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HA	1:A:375:GLN:HB2	2.03	0.41
1:C:377:LYS:HZ3	1:C:379:ASN:HD21	1.67	0.41
1:A:104:PRO:HB2	1:A:108:VAL:HG21	2.03	0.40
1:C:363:PRO:HA	1:C:386:VAL:HG23	2.03	0.40
1:A:279:MET:N	1:A:320:ASN:O	2.52	0.40
1:B:169:LEU:O	1:B:173:TYR:HB2	2.21	0.40
1:C:220:THR:HA	1:C:238:ILE:O	2.21	0.40
1:D:255:LYS:NZ	2:D:408:HOH:O	2.48	0.40
1:D:296:ARG:HA	2:D:452:HOH:O	2.22	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	343/353 (97%)	338 (98%)	5 (2%)	0	100	100
1	B	336/353 (95%)	330 (98%)	6 (2%)	0	100	100
1	C	343/353 (97%)	334 (97%)	9 (3%)	0	100	100
1	D	338/353 (96%)	331 (98%)	7 (2%)	0	100	100
All	All	1360/1412 (96%)	1333 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	278/284 (98%)	274 (99%)	4 (1%)	67	81
1	B	271/284 (95%)	268 (99%)	3 (1%)	73	86
1	C	271/284 (95%)	268 (99%)	3 (1%)	73	86
1	D	273/284 (96%)	267 (98%)	6 (2%)	52	69
All	All	1093/1136 (96%)	1077 (98%)	16 (2%)	65	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	240	TYR
1	A	372	LYS
1	A	375	GLN
1	B	50	CYS
1	B	81	LEU
1	B	240	TYR
1	C	183	PHE
1	C	240	TYR
1	C	377	LYS
1	D	79	LEU
1	D	96	ARG
1	D	183	PHE
1	D	196	MET
1	D	303	ARG
1	D	310	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	GLN
1	B	232	ASN
1	C	89	ASN
1	C	153	GLN
1	C	172	ASN
1	C	274	ASN
1	C	379	ASN
1	D	232	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	345/353 (97%)	-0.37	0 100 100	24, 39, 55, 90	0
1	B	340/353 (96%)	-0.26	3 (0%) 84 88	26, 46, 75, 117	0
1	C	345/353 (97%)	-0.29	3 (0%) 84 88	26, 41, 65, 146	0
1	D	342/353 (96%)	-0.32	0 100 100	30, 44, 66, 95	0
All	All	1372/1412 (97%)	-0.31	6 (0%) 92 95	24, 43, 67, 146	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	GLY	5.0
1	C	46	PRO	4.0
1	C	47	LEU	2.4
1	C	122	GLY	2.3
1	B	291	LEU	2.3
1	B	306	TRP	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.