



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:54 PM GMT

PDB ID : 1Z1I
Title : Crystal structure of native SARS CLpro
Authors : Liang, P.H.; Wang, A.H.
Deposited on : 2005-03-04
Resolution : 2.80 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

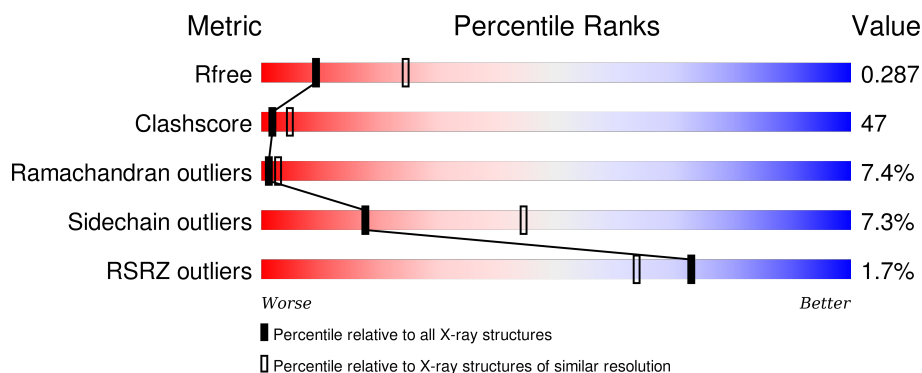
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	 2% 35% 51% 9% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2472 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	301	Total	C	N	O	S	0	0	0
			2332	1474	399	437	22			

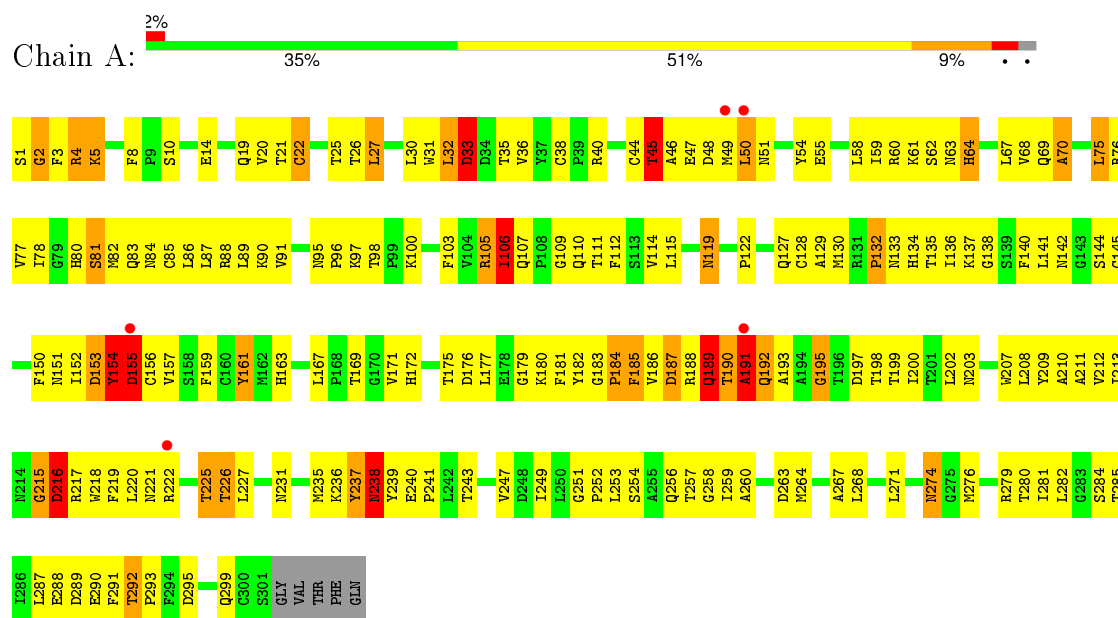
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	140	Total	O	0	0
			140	140		

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 errors 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.19 Å 45.06 Å 53.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 24.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 97.5 (24.85-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.31 Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.241 , 0.288 0.245 , 0.287	Depositor DCC
R_{free} test set	695 reflections (11.59%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 11956 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2472	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.97	12/2384 (0.5%)	1.06	27/3239 (0.8%)

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	A	1	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ALA	C-O	19.04	1.59	1.23
1	A	154	TYR	C-N	16.72	1.72	1.34
1	A	50	LEU	C-N	15.30	1.69	1.34
1	A	216	ASP	C-N	14.84	1.68	1.34
1	A	238	ASN	C-N	13.28	1.64	1.34
1	A	106	ILE	C-N	12.45	1.62	1.34
1	A	44	CYS	C-N	10.71	1.58	1.34
1	A	33	ASP	CA-CB	-6.73	1.39	1.53
1	A	191	ALA	C-N	-5.94	1.20	1.34
1	A	153	ASP	C-N	5.91	1.47	1.34
1	A	155	ASP	C-N	-5.57	1.21	1.34
1	A	190	THR	C-N	-5.23	1.22	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASN	CA-CB-CG	13.90	143.97	113.40
1	A	33	ASP	N-CA-CB	-12.55	88.00	110.60
1	A	33	ASP	CB-CA-C	11.15	132.71	110.40
1	A	238	ASN	CA-C-N	-10.54	94.01	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	TYR	CA-CB-CG	10.36	133.09	113.40
1	A	105	ARG	O-C-N	10.16	138.96	122.70
1	A	33	ASP	CA-CB-CG	9.89	135.16	113.40
1	A	106	ILE	CA-CB-CG2	9.48	129.86	110.90
1	A	154	TYR	N-CA-CB	9.32	127.37	110.60
1	A	191	ALA	O-C-N	-8.52	109.07	122.70
1	A	190	THR	O-C-N	8.33	136.03	122.70
1	A	105	ARG	CA-C-N	-7.83	99.98	117.20
1	A	154	TYR	O-C-N	-7.49	110.71	122.70
1	A	44	CYS	O-C-N	7.05	133.98	122.70
1	A	237	TYR	O-C-N	-6.81	111.80	122.70
1	A	154	TYR	C-N-CA	-6.71	104.93	121.70
1	A	190	THR	CA-C-N	-6.54	102.80	117.20
1	A	191	ALA	C-N-CA	6.46	137.86	121.70
1	A	238	ASN	O-C-N	6.39	132.92	122.70
1	A	106	ILE	CB-CG1-CD1	6.29	131.52	113.90
1	A	105	ARG	C-N-CA	-6.23	106.14	121.70
1	A	238	ASN	C-N-CA	-6.02	106.66	121.70
1	A	44	CYS	CA-C-N	-5.62	104.84	117.20
1	A	32	LEU	O-C-N	-5.40	114.06	122.70
1	A	45	THR	N-CA-C	-5.31	96.65	111.00
1	A	153	ASP	O-C-N	-5.19	114.40	122.70
1	A	215	GLY	O-C-N	5.01	130.72	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	106	ILE	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ALA	Mainchain
1	A	238	ASN	Mainchain
1	A	32	LEU	Mainchain
1	A	45	THR	Mainchain

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	2332	0	2284	219	2
2	A	140	0	0	14	2
All	All	2472	0	2284	219	3

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 47.

All (219) 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:50:LEU:C	1:A:51:ASN:N	1.69	1.46
1:A:216:ASP:C	1:A:217:ARG:N	1.68	1.45
1:A:154:TYR:C	1:A:155:ASP:N	1.72	1.42
1:A:64:HIS:CD2	2:A:655:HOH:O	1.96	1.14
1:A:154:TYR:O	1:A:155:ASP:HB2	1.50	1.11
1:A:154:TYR:O	1:A:155:ASP:CB	2.01	1.07
1:A:191:ALA:O	1:A:192:GLN:HG3	1.61	0.99
1:A:77:VAL:HA	1:A:91:VAL:HG12	1.49	0.92
1:A:253:LEU:HD12	1:A:253:LEU:H	1.33	0.92
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.50	0.92
1:A:21:THR:HB	1:A:67:LEU:HB3	1.53	0.90
1:A:105:ARG:NH2	1:A:182:TYR:HA	1.86	0.90
1:A:49:MET:SD	1:A:189:GLN:HG2	2.20	0.82
1:A:190:THR:O	2:A:593:HOH:O	1.97	0.81
1:A:70:ALA:HB2	1:A:75:LEU:HD11	1.62	0.81
1:A:190:THR:O	1:A:191:ALA:O	1.99	0.79
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.65	0.78
1:A:154:TYR:C	1:A:155:ASP:CA	2.53	0.77
1:A:64:HIS:CB	2:A:655:HOH:O	2.33	0.77
1:A:75:LEU:HD12	1:A:75:LEU:H	1.50	0.76
1:A:198:THR:HG22	1:A:199:THR:H	1.47	0.76
1:A:191:ALA:O	1:A:192:GLN:CG	2.32	0.76
1:A:86:LEU:HG	1:A:179:GLY:HA2	1.66	0.76
1:A:64:HIS:CG	2:A:655:HOH:O	2.24	0.76
1:A:268:LEU:HA	1:A:271:LEU:HD12	1.66	0.76
1:A:152:ILE:HG22	1:A:153:ASP:N	2.00	0.76
1:A:105:ARG:HH22	1:A:182:TYR:HA	1.50	0.74
1:A:152:ILE:HG22	1:A:153:ASP:H	1.52	0.73
1:A:137:LYS:HE3	1:A:171:VAL:HG12	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HG22	1:A:154:TYR:H	1.53	0.73
1:A:64:HIS:HB3	2:A:655:HOH:O	1.88	0.73
1:A:186:VAL:H	1:A:192:GLN:NE2	1.88	0.71
1:A:161:TYR:HA	1:A:175:THR:O	1.91	0.71
1:A:115:LEU:HD11	1:A:122:PRO:HB2	1.73	0.71
1:A:154:TYR:C	1:A:155:ASP:CB	2.59	0.70
1:A:64:HIS:HD2	2:A:655:HOH:O	1.51	0.70
1:A:140:PHE:HB3	1:A:144:SER:OG	1.90	0.70
1:A:260:ALA:O	1:A:263:ASP:HB2	1.90	0.70
1:A:288:GLU:HG2	1:A:291:PHE:HD2	1.57	0.70
1:A:154:TYR:O	1:A:155:ASP:CG	2.30	0.70
1:A:175:THR:HG22	1:A:181:PHE:HA	1.74	0.70
1:A:70:ALA:CB	1:A:75:LEU:HD11	2.23	0.68
1:A:5:LYS:H	1:A:5:LYS:HZ2	1.38	0.68
1:A:40:ARG:CD	1:A:85:CYS:HA	2.23	0.68
1:A:202:LEU:HD23	2:A:661:HOH:O	1.93	0.68
1:A:237:TYR:O	1:A:239:TYR:HD1	1.76	0.67
1:A:50:LEU:CB	1:A:51:ASN:N	2.57	0.67
1:A:100:LYS:HB3	1:A:155:ASP:O	1.95	0.67
1:A:105:ARG:O	1:A:106:ILE:O	2.11	0.67
1:A:207:TRP:CZ3	1:A:287:LEU:HA	2.28	0.67
1:A:78:ILE:HG12	1:A:90:LYS:O	1.94	0.67
1:A:235:MET:HE3	1:A:241:PRO:HB3	1.77	0.67
1:A:30:LEU:HD23	1:A:177:LEU:HD21	1.76	0.67
1:A:258:GLY:C	1:A:259:ILE:HD12	2.15	0.67
1:A:274:ASN:HD22	1:A:274:ASN:N	1.91	0.66
1:A:152:ILE:CD1	1:A:157:VAL:HG22	2.25	0.66
1:A:45:THR:C	1:A:47:GLU:H	1.98	0.66
1:A:100:LYS:HE3	1:A:156:CYS:SG	2.35	0.66
1:A:159:PHE:HB3	1:A:177:LEU:HD13	1.76	0.66
1:A:217:ARG:NH1	2:A:644:HOH:O	2.15	0.66
1:A:260:ALA:HB3	1:A:263:ASP:OD2	1.96	0.66
1:A:154:TYR:O	1:A:155:ASP:OD2	2.15	0.65
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.61	0.65
1:A:197:ASP:O	1:A:238:ASN:ND2	2.30	0.65
1:A:19:GLN:HB3	1:A:69:GLN:HB3	1.78	0.65
1:A:237:TYR:O	1:A:238:ASN:C	2.33	0.64
1:A:249:ILE:O	1:A:252:PRO:HD2	1.98	0.64
1:A:191:ALA:O	1:A:192:GLN:CB	2.45	0.64
1:A:63:ASN:HD22	1:A:63:ASN:N	1.96	0.63
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PHE:HE1	1:A:114:VAL:HG23	1.64	0.62
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.34	0.62
1:A:112:PHE:CE1	1:A:114:VAL:HG23	2.34	0.62
1:A:50:LEU:CA	1:A:51:ASN:N	2.61	0.62
1:A:280:THR:HB	1:A:284:SER:O	2.00	0.61
1:A:213:ILE:CD1	1:A:256:GLN:HE22	2.12	0.61
1:A:45:THR:C	1:A:47:GLU:N	2.52	0.61
1:A:276:MET:HE2	1:A:279:ARG:O	2.01	0.61
1:A:199:THR:HG23	1:A:289:ASP:OD2	2.01	0.61
1:A:154:TYR:C	1:A:155:ASP:CG	2.59	0.61
1:A:5:LYS:HB2	1:A:5:LYS:HZ3	1.66	0.60
1:A:130:MET:CE	1:A:136:ILE:HD11	2.31	0.60
1:A:213:ILE:HD13	1:A:256:GLN:HE22	1.65	0.60
1:A:135:THR:C	1:A:136:ILE:HD12	2.22	0.60
1:A:253:LEU:HD12	1:A:253:LEU:N	2.13	0.60
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.66	0.60
1:A:75:LEU:N	1:A:75:LEU:HD12	2.17	0.59
1:A:1:SER:O	1:A:2:GLY:O	2.21	0.59
1:A:10:SER:O	1:A:14:GLU:HG3	2.03	0.58
1:A:190:THR:C	1:A:191:ALA:O	2.41	0.58
1:A:58:LEU:O	1:A:60:ARG:N	2.37	0.58
1:A:107:GLN:H	1:A:110:GLN:NE2	2.02	0.57
1:A:30:LEU:HD23	1:A:177:LEU:CD2	2.35	0.57
1:A:40:ARG:HG2	1:A:85:CYS:O	2.04	0.57
1:A:208:LEU:HG	1:A:219:PHE:CE1	2.40	0.57
1:A:50:LEU:HB3	1:A:51:ASN:H	1.69	0.57
1:A:151:ASN:O	1:A:152:ILE:HD13	2.05	0.56
1:A:152:ILE:CG2	1:A:153:ASP:H	2.18	0.56
1:A:5:LYS:NZ	1:A:5:LYS:H	2.04	0.56
1:A:198:THR:HG22	1:A:199:THR:N	2.19	0.56
1:A:50:LEU:CB	1:A:51:ASN:H	2.19	0.56
1:A:40:ARG:HA	1:A:87:LEU:HB2	1.88	0.55
1:A:175:THR:HB	1:A:180:LYS:O	2.06	0.55
1:A:186:VAL:HG23	1:A:188:ARG:HB2	1.88	0.55
1:A:100:LYS:CG	1:A:155:ASP:O	2.55	0.55
1:A:251:GLY:O	1:A:254:SER:HB3	2.07	0.55
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.72	0.55
1:A:288:GLU:HG2	1:A:291:PHE:CD2	2.38	0.54
1:A:88:ARG:C	1:A:89:LEU:HD23	2.27	0.54
1:A:274:ASN:ND2	1:A:274:ASN:N	2.55	0.54
1:A:112:PHE:HE1	1:A:114:VAL:CG2	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD23	1:A:264:MET:SD	2.48	0.54
1:A:58:LEU:HD11	1:A:80:HIS:HD2	1.72	0.54
1:A:63:ASN:N	1:A:63:ASN:ND2	2.55	0.53
1:A:50:LEU:HB3	1:A:51:ASN:N	2.22	0.53
1:A:58:LEU:O	1:A:61:LYS:N	2.41	0.53
1:A:213:ILE:HG12	1:A:257:THR:HG22	1.90	0.53
1:A:106:ILE:CD1	1:A:130:MET:HB2	2.39	0.53
1:A:46:ALA:HB2	2:A:654:HOH:O	2.08	0.53
1:A:215:GLY:O	1:A:216:ASP:C	2.46	0.53
1:A:83:GLN:O	1:A:84:ASN:HB2	2.09	0.53
1:A:106:ILE:HD11	1:A:130:MET:HB2	1.90	0.52
1:A:188:ARG:C	1:A:190:THR:H	2.13	0.52
1:A:207:TRP:O	1:A:210:ALA:HB3	2.09	0.52
1:A:45:THR:OG1	1:A:47:GLU:HG3	2.09	0.52
1:A:106:ILE:HD11	1:A:130:MET:CE	2.41	0.51
1:A:27:LEU:HD12	1:A:27:LEU:O	2.10	0.51
1:A:154:TYR:O	1:A:155:ASP:CA	2.55	0.51
1:A:33:ASP:H	1:A:98:THR:HG21	1.76	0.51
1:A:217:ARG:HB2	1:A:220:LEU:HD12	1.93	0.50
1:A:218:TRP:CE2	1:A:279:ARG:HB3	2.45	0.50
1:A:215:GLY:HA3	2:A:640:HOH:O	2.12	0.50
1:A:5:LYS:NZ	1:A:5:LYS:HB2	2.27	0.49
1:A:152:ILE:HD12	1:A:157:VAL:HG22	1.93	0.49
1:A:115:LEU:HD11	1:A:122:PRO:CB	2.42	0.49
1:A:138:GLY:HA3	1:A:140:PHE:HE1	1.78	0.49
1:A:236:LYS:NZ	1:A:236:LYS:HB3	2.27	0.49
1:A:21:THR:HG22	1:A:22:CYS:N	2.27	0.49
1:A:77:VAL:HG13	1:A:77:VAL:O	2.13	0.49
1:A:105:ARG:C	1:A:106:ILE:O	2.51	0.49
1:A:119:ASN:HD22	1:A:119:ASN:N	2.10	0.49
1:A:35:THR:HG22	1:A:36:VAL:N	2.28	0.48
1:A:132:PRO:C	1:A:134:HIS:H	2.15	0.48
1:A:40:ARG:NE	1:A:85:CYS:HA	2.27	0.48
1:A:127:GLN:HG3	1:A:128:CYS:N	2.27	0.48
1:A:152:ILE:HG22	1:A:154:TYR:N	2.24	0.48
1:A:100:LYS:CB	1:A:155:ASP:O	2.62	0.48
1:A:58:LEU:C	1:A:60:ARG:N	2.67	0.47
1:A:235:MET:CE	1:A:241:PRO:HB3	2.43	0.47
1:A:88:ARG:O	1:A:89:LEU:HD23	2.13	0.47
1:A:63:ASN:ND2	1:A:63:ASN:H	2.11	0.47
1:A:111:THR:HG22	1:A:129:ALA:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:CD2	1:A:150:PHE:N	2.83	0.47
1:A:200:ILE:HG21	1:A:203:ASN:ND2	2.30	0.47
1:A:81:SER:OG	1:A:82:MET:N	2.47	0.47
1:A:207:TRP:CD2	1:A:288:GLU:HB3	2.50	0.46
1:A:107:GLN:N	1:A:110:GLN:NE2	2.62	0.46
1:A:240:GLU:CD	1:A:241:PRO:HD2	2.36	0.46
1:A:186:VAL:C	1:A:188:ARG:H	2.19	0.45
1:A:276:MET:CE	1:A:281:ILE:HG13	2.47	0.45
1:A:138:GLY:HA3	1:A:140:PHE:CE1	2.51	0.45
1:A:191:ALA:O	1:A:192:GLN:HB2	2.15	0.45
1:A:107:GLN:H	1:A:110:GLN:HE21	1.64	0.45
1:A:8:PHE:CD1	1:A:152:ILE:HB	2.52	0.45
1:A:137:LYS:CE	1:A:171:VAL:HG12	2.44	0.45
1:A:225:THR:HG23	1:A:226:THR:N	2.31	0.45
1:A:30:LEU:CD2	1:A:177:LEU:HD21	2.44	0.45
1:A:213:ILE:CD1	1:A:256:GLN:NE2	2.79	0.45
1:A:209:TYR:CE1	1:A:264:MET:HG2	2.52	0.45
1:A:35:THR:HA	1:A:89:LEU:O	2.17	0.44
1:A:62:SER:HB2	1:A:64:HIS:NE2	2.32	0.44
1:A:26:THR:O	1:A:26:THR:HG23	2.17	0.44
1:A:253:LEU:H	1:A:253:LEU:CD1	2.13	0.44
1:A:100:LYS:HG2	1:A:155:ASP:O	2.18	0.43
1:A:105:ARG:HG3	1:A:176:ASP:OD2	2.19	0.43
1:A:276:MET:HE3	1:A:281:ILE:HG13	2.00	0.43
1:A:107:GLN:N	1:A:110:GLN:HE21	2.16	0.43
1:A:76:ARG:NH1	1:A:76:ARG:HG3	2.33	0.43
1:A:50:LEU:C	1:A:51:ASN:HD22	2.22	0.43
1:A:45:THR:CG2	2:A:629:HOH:O	2.66	0.43
1:A:185:PHE:HA	1:A:192:GLN:HE21	1.82	0.43
1:A:203:ASN:OD1	1:A:292:THR:HA	2.18	0.43
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.19	0.43
1:A:213:ILE:HD13	1:A:256:GLN:NE2	2.30	0.43
1:A:193:ALA:CB	2:A:637:HOH:O	2.66	0.43
1:A:202:LEU:HD21	1:A:293:PRO:HG2	2.01	0.43
1:A:140:PHE:N	1:A:140:PHE:CD1	2.86	0.42
1:A:27:LEU:HB2	1:A:145:CYS:O	2.18	0.42
1:A:183:GLY:O	1:A:184:PRO:O	2.37	0.42
1:A:154:TYR:C	1:A:155:ASP:OD2	2.55	0.42
1:A:280:THR:CG2	1:A:285:THR:HG22	2.50	0.42
1:A:221:ASN:ND2	1:A:267:ALA:HA	2.35	0.42
1:A:103:PHE:CE2	1:A:177:LEU:HD22	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:O	1:A:55:GLU:C	2.58	0.42
1:A:62:SER:HB2	1:A:64:HIS:CE1	2.54	0.42
1:A:207:TRP:HZ3	1:A:287:LEU:HA	1.79	0.42
1:A:40:ARG:HD3	1:A:85:CYS:CA	2.43	0.42
1:A:208:LEU:O	1:A:212:VAL:HG23	2.20	0.42
1:A:68:VAL:HG12	1:A:75:LEU:HD13	2.02	0.42
1:A:225:THR:CG2	1:A:226:THR:N	2.83	0.42
1:A:243:THR:O	1:A:247:VAL:HG23	2.20	0.41
1:A:141:LEU:H	1:A:144:SER:HB3	1.85	0.41
1:A:259:ILE:N	1:A:259:ILE:HD12	2.35	0.41
1:A:19:GLN:HG2	1:A:20:VAL:N	2.35	0.41
1:A:95:ASN:HA	1:A:96:PRO:HD2	1.91	0.41
1:A:167:LEU:C	1:A:169:THR:N	2.74	0.41
1:A:186:VAL:O	1:A:188:ARG:N	2.47	0.41
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.56	0.41
1:A:227:LEU:O	1:A:231:ASN:ND2	2.53	0.41
1:A:21:THR:CG2	1:A:22:CYS:N	2.84	0.41
1:A:130:MET:HE1	1:A:136:ILE:HD11	2.03	0.41
1:A:211:ALA:HA	1:A:282:LEU:HG	2.02	0.41
1:A:106:ILE:HD11	1:A:130:MET:HE3	2.03	0.41
1:A:58:LEU:C	1:A:60:ARG:H	2.24	0.40
1:A:195:GLY:HA2	2:A:631:HOH:O	2.21	0.40
1:A:3:PHE:HE1	1:A:299:GLN:HB2	1.86	0.40
1:A:50:LEU:O	1:A:190:THR:CG2	2.70	0.40
1:A:45:THR:HG21	2:A:629:HOH:O	2.22	0.40
1:A:97:LYS:O	1:A:98:THR:C	2.59	0.40

All (3) 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:A:154:TYR:OH	2:A:536:HOH:O[2_655]	1.96	0.24
1:A:285:THR:OG1	1:A:285:THR:OG1[2_655]	1.99	0.21
2:A:652:HOH:O	2:A:652:HOH:O[2_655]	2.19	0.01

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	299/306 (98%)	228 (76%)	49 (16%)	22 (7%)	1 3

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLY
1	A	33	ASP
1	A	106	ILE
1	A	154	TYR
1	A	184	PRO
1	A	191	ALA
1	A	192	GLN
1	A	216	ASP
1	A	238	ASN
1	A	59	ILE
1	A	70	ALA
1	A	142	ASN
1	A	155	ASP
1	A	195	GLY
1	A	64	HIS
1	A	81	SER
1	A	133	ASN
1	A	161	TYR
1	A	187	ASP
1	A	185	PHE
1	A	189	GLN
1	A	132	PRO

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	259/263 (98%)	240 (93%)	19 (7%)	17	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	LYS
1	A	22	CYS
1	A	25	THR
1	A	27	LEU
1	A	38	CYS
1	A	48	ASP
1	A	75	LEU
1	A	119	ASN
1	A	187	ASP
1	A	189	GLN
1	A	222	ARG
1	A	225	THR
1	A	226	THR
1	A	238	ASN
1	A	274	ASN
1	A	290	GLU
1	A	292	THR
1	A	295	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	51	ASN
1	A	63	ASN
1	A	74	GLN
1	A	110	GLN
1	A	119	ASN
1	A	172	HIS
1	A	192	GLN
1	A	214	ASN
1	A	238	ASN
1	A	256	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	273	GLN
1	A	274	ASN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	301/306 (98%)	-0.14	5 (1%) 73 63	21, 55, 77, 88	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	MET	4.6
1	A	155	ASP	3.3
1	A	50	LEU	3.0
1	A	222	ARG	2.5
1	A	191	ALA	2.1

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.