



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2017 – 02:57 PM EDT

PDB ID : 3GVZ
Title : Crystal structure of the protein CV2077 from *Chromobacterium violaceum*.
Northeast Structural Genomics Consortium Target CvR62
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Fang, F.; Xiao, R.; Cunningham, K.; Maglaqui, M.; Owens, L.; Chen, C.X.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : unknown
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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

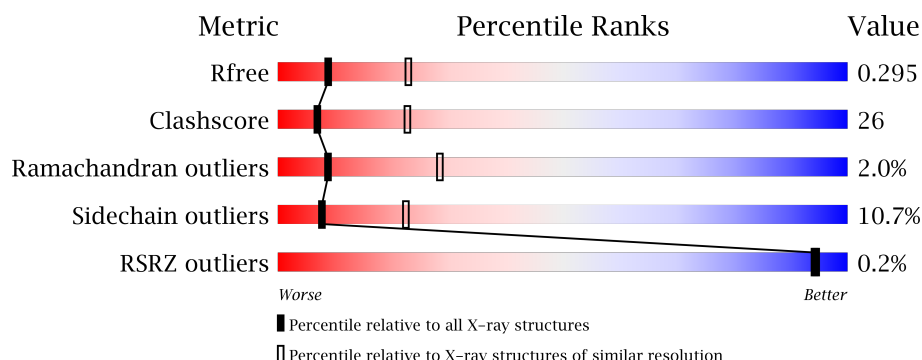
1 Overall quality at a glance ⓘ

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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	299	
1	B	299	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4082 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 Uncharacterized protein CV2077.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	Se	0	0	0
			1970	1230	374	363	1	2			
1	B	256	Total	C	N	O	S	Se	0	0	0
			1970	1230	374	363	1	2			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	LYS	-	EXPRESSION TAG	UNP Q7NWB3
A	288	LEU	-	EXPRESSION TAG	UNP Q7NWB3
A	289	ALA	-	EXPRESSION TAG	UNP Q7NWB3
A	290	ALA	-	EXPRESSION TAG	UNP Q7NWB3
A	291	ALA	-	EXPRESSION TAG	UNP Q7NWB3
A	292	LEU	-	EXPRESSION TAG	UNP Q7NWB3
A	293	GLU	-	EXPRESSION TAG	UNP Q7NWB3
A	294	HIS	-	EXPRESSION TAG	UNP Q7NWB3
A	295	HIS	-	EXPRESSION TAG	UNP Q7NWB3
A	296	HIS	-	EXPRESSION TAG	UNP Q7NWB3
A	297	HIS	-	EXPRESSION TAG	UNP Q7NWB3
A	298	HIS	-	EXPRESSION TAG	UNP Q7NWB3
A	299	HIS	-	EXPRESSION TAG	UNP Q7NWB3
B	287	LYS	-	EXPRESSION TAG	UNP Q7NWB3
B	288	LEU	-	EXPRESSION TAG	UNP Q7NWB3
B	289	ALA	-	EXPRESSION TAG	UNP Q7NWB3
B	290	ALA	-	EXPRESSION TAG	UNP Q7NWB3
B	291	ALA	-	EXPRESSION TAG	UNP Q7NWB3
B	292	LEU	-	EXPRESSION TAG	UNP Q7NWB3
B	293	GLU	-	EXPRESSION TAG	UNP Q7NWB3
B	294	HIS	-	EXPRESSION TAG	UNP Q7NWB3
B	295	HIS	-	EXPRESSION TAG	UNP Q7NWB3
B	296	HIS	-	EXPRESSION TAG	UNP Q7NWB3
B	297	HIS	-	EXPRESSION TAG	UNP Q7NWB3
B	298	HIS	-	EXPRESSION TAG	UNP Q7NWB3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	299	HIS	-	EXPRESSION TAG	UNP Q7NWB3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	65	Total O 65 65	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.10Å 87.05Å 115.12Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.62 – 2.80 29.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	76.4 (19.62-2.80) 85.4 (29.38-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.56 (at 2.80Å)	Xtriage
Refinement program	REFMAC, CNS 1.2	Depositor
R, R_{free}	0.259 , 0.290 0.266 , 0.295	Depositor DCC
R_{free} test set	1530 reflections (9.48%)	DCC
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.943	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -7.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	4082	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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, 0.333 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	0.39	0/2012	0.62	0/2726
1	B	0.39	0/2012	0.62	0/2726
All	All	0.39	0/4024	0.62	0/5452

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	1970	0	1942	103	0
1	B	1970	0	1942	97	0
2	A	77	0	0	6	0
2	B	65	0	0	5	0
All	All	4082	0	3884	200	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 26.

All (200) 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:80:ILE:H	1:B:80:ILE:HD12	1.21	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:H	1:A:80:ILE:HD12	1.23	1.00
1:A:175:ASN:HD22	1:A:196:ARG:HH22	1.10	0.96
1:B:175:ASN:HD22	1:B:196:ARG:HH22	1.09	0.92
1:A:94:ALA:HB3	1:A:141:PHE:HB2	1.56	0.85
1:B:94:ALA:HB3	1:B:141:PHE:HB2	1.56	0.84
1:B:166:GLN:NE2	1:B:168:SER:H	1.78	0.82
1:A:33:GLY:HA3	1:A:168:SER:HA	1.64	0.80
1:A:166:GLN:NE2	1:A:168:SER:H	1.81	0.78
1:A:276:PHE:O	1:A:279:GLN:HG2	1.84	0.78
1:B:80:ILE:HD12	1:B:80:ILE:N	1.98	0.78
1:B:276:PHE:O	1:B:279:GLN:HG2	1.83	0.77
1:B:33:GLY:HA3	1:B:168:SER:HA	1.67	0.77
1:A:80:ILE:N	1:A:80:ILE:HD12	1.99	0.74
1:B:258:LEU:HD12	1:B:285:LEU:HD22	1.70	0.74
1:A:258:LEU:HD12	1:A:285:LEU:HD22	1.71	0.73
1:B:175:ASN:ND2	1:B:196:ARG:HH22	1.85	0.73
1:A:175:ASN:ND2	1:A:196:ARG:HH22	1.87	0.73
1:B:46:ARG:NE	1:B:81:LYS:HG3	2.07	0.69
1:B:144:LEU:HD22	1:B:151:MSE:HE2	1.74	0.68
1:A:46:ARG:NE	1:A:81:LYS:HG3	2.07	0.67
1:A:144:LEU:HD22	1:A:151:MSE:HE2	1.77	0.66
1:A:126:VAL:HG11	1:A:151:MSE:HE1	1.77	0.65
1:B:126:VAL:HG11	1:B:151:MSE:HE1	1.78	0.65
1:B:98:SER:HB3	1:B:187:GLN:HB2	1.78	0.65
1:B:166:GLN:HE22	1:B:168:SER:H	1.41	0.64
1:B:62:GLU:H	1:B:62:GLU:CD	2.00	0.64
1:A:140:VAL:HG22	1:A:141:PHE:N	2.13	0.64
1:A:166:GLN:HE22	1:A:168:SER:H	1.44	0.64
1:A:98:SER:HB3	1:A:187:GLN:HB2	1.80	0.64
1:B:99:LEU:HD23	1:B:99:LEU:H	1.63	0.64
1:A:99:LEU:H	1:A:99:LEU:HD23	1.62	0.64
1:A:96:ALA:O	1:A:104:ARG:HD2	1.99	0.63
1:A:115:ARG:HH21	1:A:133:LEU:HD12	1.64	0.63
1:A:200:ILE:HD12	1:A:201:ARG:N	2.14	0.62
1:B:200:ILE:HD12	1:B:201:ARG:N	2.13	0.62
1:B:140:VAL:HG22	1:B:141:PHE:N	2.14	0.62
1:A:62:GLU:CD	1:A:62:GLU:H	2.02	0.61
1:B:96:ALA:O	1:B:104:ARG:HD2	2.00	0.61
1:A:70:LEU:HD11	2:A:366:HOH:O	2.00	0.61
1:B:28:LEU:CD2	1:B:44:LYS:HG2	2.30	0.61
1:B:115:ARG:HH21	1:B:133:LEU:HD12	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD23	1:B:252:PRO:HB3	1.83	0.60
1:A:28:LEU:CD2	1:A:44:LYS:HG2	2.31	0.60
1:B:96:ALA:HA	1:B:141:PHE:CE1	2.36	0.60
1:A:32:ALA:HB2	1:A:150:LEU:HD21	1.83	0.59
1:A:215:PHE:HA	1:A:218:LEU:HD12	1.84	0.59
1:B:32:ALA:HB2	1:B:150:LEU:HD21	1.85	0.59
1:B:285:LEU:HD23	1:B:286:PRO:HA	1.84	0.59
1:B:215:PHE:HA	1:B:218:LEU:HD12	1.83	0.59
1:A:96:ALA:HA	1:A:141:PHE:CE1	2.38	0.58
1:A:33:GLY:C	1:A:35:ALA:H	2.06	0.58
1:B:166:GLN:HE21	1:B:169:GLY:N	2.00	0.58
1:A:246:LEU:HD23	1:A:252:PRO:HB3	1.85	0.57
1:B:33:GLY:C	1:B:35:ALA:H	2.07	0.57
1:A:285:LEU:HD23	1:A:286:PRO:HA	1.85	0.57
1:A:166:GLN:HE21	1:A:169:GLY:N	2.02	0.56
1:B:80:ILE:CD1	1:B:80:ILE:H	2.01	0.56
1:A:80:ILE:H	1:A:80:ILE:CD1	2.02	0.56
1:A:44:LYS:HB2	1:A:92:VAL:HG11	1.88	0.55
1:A:60:HIS:HE1	1:A:279:GLN:O	1.90	0.55
1:B:166:GLN:OE1	1:B:166:GLN:HA	2.06	0.54
1:B:240:ALA:HA	1:B:257:THR:O	2.07	0.54
1:A:240:ALA:HA	1:A:257:THR:O	2.07	0.54
1:B:200:ILE:O	1:B:204:LEU:HB2	2.07	0.54
1:B:44:LYS:HB2	1:B:92:VAL:HG11	1.88	0.54
1:A:166:GLN:OE1	1:A:166:GLN:HA	2.07	0.54
1:A:172:ALA:HB1	1:A:200:ILE:HD13	1.90	0.54
1:A:46:ARG:HH21	1:A:81:LYS:HE3	1.72	0.54
1:B:246:LEU:CD2	1:B:252:PRO:HB3	2.38	0.54
1:B:103:LEU:HD22	1:B:157:GLN:HE22	1.74	0.53
1:B:26:CYS:N	1:B:175:ASN:HD21	2.06	0.53
1:B:166:GLN:NE2	1:B:168:SER:N	2.54	0.53
1:B:172:ALA:HB1	1:B:200:ILE:HD13	1.90	0.53
1:A:223:HIS:O	1:A:229:SER:HB3	2.08	0.53
1:B:258:LEU:HD12	1:B:285:LEU:HD13	1.91	0.53
1:B:191:PRO:HD2	2:B:353:HOH:O	2.09	0.53
1:A:103:LEU:HD22	1:A:157:GLN:HE22	1.74	0.53
1:A:46:ARG:HE	1:A:81:LYS:HG3	1.73	0.53
1:B:46:ARG:HE	1:B:81:LYS:HG3	1.73	0.53
1:B:60:HIS:HE1	1:B:279:GLN:O	1.92	0.53
1:A:26:CYS:N	1:A:175:ASN:HD21	2.06	0.52
1:B:28:LEU:HD11	1:B:94:ALA:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD22	1:B:151:MSE:CE	2.40	0.52
1:A:56:LEU:HB3	1:A:285:LEU:HB2	1.92	0.52
1:B:56:LEU:HB3	1:B:285:LEU:HB2	1.92	0.52
1:B:46:ARG:HH21	1:B:81:LYS:HE3	1.75	0.52
1:A:87:LYS:HE3	2:A:319:HOH:O	2.10	0.51
1:B:140:VAL:HG22	1:B:141:PHE:H	1.74	0.51
1:B:223:HIS:O	1:B:229:SER:HB3	2.10	0.51
1:A:32:ALA:HB2	1:A:150:LEU:CD2	2.40	0.51
1:A:140:VAL:HG22	1:A:141:PHE:H	1.74	0.51
1:A:60:HIS:HD2	1:A:66:ALA:HB2	1.74	0.51
1:A:28:LEU:HD11	1:A:94:ALA:HB2	1.93	0.51
1:A:258:LEU:HD12	1:A:285:LEU:HD13	1.91	0.51
1:B:60:HIS:HD2	1:B:66:ALA:HB2	1.75	0.51
1:A:132:LYS:HE2	1:A:136:GLN:NE2	2.26	0.50
1:A:197:LEU:O	1:A:201:ARG:HB2	2.11	0.50
1:A:200:ILE:O	1:A:204:LEU:HB2	2.10	0.50
1:A:199:ARG:NE	1:A:203:LEU:HD11	2.25	0.50
1:A:246:LEU:CD2	1:A:252:PRO:HB3	2.41	0.50
1:B:129:ALA:O	1:B:133:LEU:HB2	2.11	0.50
1:A:179:ASP:OD2	1:A:182:LEU:HG	2.11	0.50
1:B:92:VAL:HG23	1:B:143:LEU:HB3	1.93	0.50
1:B:32:ALA:HB2	1:B:150:LEU:CD2	2.42	0.50
1:B:112:VAL:HG23	1:B:115:ARG:CZ	2.42	0.50
1:B:132:LYS:HE2	1:B:136:GLN:NE2	2.27	0.50
1:A:162:ARG:HB3	1:A:182:LEU:HD11	1.93	0.49
1:B:98:SER:HA	1:B:188:THR:O	2.12	0.49
1:A:129:ALA:O	1:A:133:LEU:HB2	2.12	0.49
1:A:144:LEU:HD22	1:A:151:MSE:CE	2.42	0.49
1:A:33:GLY:O	1:A:35:ALA:N	2.46	0.49
1:B:197:LEU:O	1:B:201:ARG:HB2	2.12	0.48
1:A:199:ARG:CZ	1:A:223:HIS:HD2	2.26	0.48
1:B:199:ARG:NE	1:B:203:LEU:HD11	2.29	0.48
1:A:166:GLN:NE2	1:A:168:SER:N	2.56	0.48
1:A:92:VAL:HG23	1:A:143:LEU:HB3	1.94	0.48
1:B:179:ASP:OD2	1:B:182:LEU:HG	2.13	0.48
1:B:54:GLN:NE2	1:B:239:LEU:HB3	2.29	0.47
1:A:191:PRO:HD2	2:A:353:HOH:O	2.14	0.47
1:A:54:GLN:NE2	1:A:239:LEU:HB3	2.29	0.47
1:B:162:ARG:HB3	1:B:182:LEU:HD11	1.95	0.47
1:A:98:SER:HA	1:A:188:THR:O	2.14	0.47
1:B:33:GLY:C	1:B:35:ALA:N	2.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:O	1:A:104:ARG:HD3	2.14	0.47
1:B:132:LYS:HE2	1:B:136:GLN:HE21	1.79	0.47
1:B:199:ARG:CZ	1:B:223:HIS:HD2	2.27	0.47
1:B:256:LEU:HD23	1:B:285:LEU:CD1	2.44	0.47
1:A:196:ARG:O	1:A:200:ILE:HG13	2.15	0.47
1:B:33:GLY:O	1:B:35:ALA:N	2.47	0.47
1:B:99:LEU:O	1:B:104:ARG:HD3	2.14	0.47
1:A:256:LEU:HD23	1:A:285:LEU:CD1	2.44	0.47
1:B:200:ILE:H	1:B:200:ILE:HG13	1.58	0.47
1:B:52:HIS:HB2	1:B:74:ASN:OD1	2.15	0.47
1:A:132:LYS:HE2	1:A:136:GLN:HE21	1.79	0.46
1:A:33:GLY:C	1:A:35:ALA:N	2.68	0.46
1:A:52:HIS:HB2	1:A:74:ASN:OD1	2.14	0.46
1:A:97:SER:HA	1:A:104:ARG:NH2	2.30	0.46
1:B:201:ARG:HG3	2:B:300:HOH:O	2.14	0.46
1:B:196:ARG:O	1:B:200:ILE:HG13	2.16	0.46
1:A:139:PRO:O	1:A:140:VAL:HB	2.16	0.46
1:A:140:VAL:CG2	1:A:141:PHE:N	2.78	0.46
1:B:140:VAL:CG2	1:B:141:PHE:N	2.79	0.46
1:B:91:VAL:HG22	1:B:92:VAL:N	2.31	0.45
1:B:97:SER:HA	1:B:104:ARG:NH2	2.31	0.45
1:A:91:VAL:HG22	1:A:92:VAL:N	2.31	0.45
1:A:34:THR:HA	2:A:305:HOH:O	2.16	0.45
1:A:144:LEU:HD13	1:A:151:MSE:HE2	1.98	0.45
1:A:251:PRO:HA	1:A:252:PRO:HD3	1.89	0.44
1:B:200:ILE:HG23	1:B:230:LEU:HD21	1.99	0.44
1:B:139:PRO:O	1:B:140:VAL:HB	2.18	0.44
1:A:254:LEU:HD12	1:A:255:GLN:N	2.32	0.44
1:A:252:PRO:HD2	1:A:272:LEU:O	2.18	0.43
1:A:149:GLY:C	1:A:150:LEU:HD23	2.38	0.43
1:B:97:SER:HA	1:B:104:ARG:HH21	1.84	0.43
1:B:252:PRO:HD2	1:B:272:LEU:O	2.18	0.43
1:A:97:SER:HA	1:A:104:ARG:HH21	1.83	0.43
1:A:255:GLN:HA	1:A:268:GLY:O	2.19	0.43
1:A:65:TYR:CE2	1:A:87:LYS:HE3	2.53	0.43
1:B:91:VAL:HG12	1:B:117:LEU:HD11	2.02	0.42
1:B:166:GLN:NE2	1:B:168:SER:C	2.73	0.42
1:B:217:ARG:NE	2:B:355:HOH:O	2.52	0.42
1:B:256:LEU:HD23	1:B:285:LEU:HD13	2.01	0.42
1:A:200:ILE:HG13	1:A:200:ILE:H	1.60	0.42
1:A:35:ALA:O	1:A:210:HIS:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ARG:HG2	2:B:321:HOH:O	2.20	0.42
1:B:283:THR:HG22	1:B:285:LEU:H	1.84	0.42
1:B:44:LYS:HG3	1:B:92:VAL:HB	2.00	0.42
1:A:71:TYR:CE1	1:A:80:ILE:HG13	2.55	0.42
1:B:254:LEU:HD12	1:B:255:GLN:N	2.34	0.42
1:B:28:LEU:HD22	1:B:44:LYS:HG2	2.01	0.42
1:B:71:TYR:CE1	1:B:80:ILE:HG13	2.55	0.42
1:A:44:LYS:HG3	1:A:92:VAL:HB	2.01	0.42
1:B:161:TYR:CE2	1:B:163:LEU:HD13	2.54	0.42
1:B:99:LEU:N	1:B:99:LEU:HD23	2.33	0.42
1:A:283:THR:HG22	1:A:285:LEU:H	1.85	0.42
1:B:130:ALA:C	1:B:132:LYS:H	2.23	0.42
1:A:200:ILE:HG23	1:A:230:LEU:HD21	2.01	0.42
1:A:166:GLN:NE2	1:A:168:SER:C	2.73	0.42
1:A:220:ARG:HB3	2:A:375:HOH:O	2.20	0.42
1:A:130:ALA:C	1:A:132:LYS:H	2.23	0.41
1:A:256:LEU:HD23	1:A:285:LEU:HD13	2.02	0.41
1:A:161:TYR:CE2	1:A:163:LEU:HD13	2.54	0.41
1:A:140:VAL:CG2	1:A:141:PHE:H	2.33	0.41
1:A:144:LEU:HD13	1:A:151:MSE:CE	2.51	0.41
1:A:99:LEU:N	1:A:99:LEU:HD23	2.33	0.41
1:A:137:ALA:HB3	1:A:155:ILE:HD13	2.02	0.41
1:B:255:GLN:HA	1:B:268:GLY:O	2.20	0.41
1:B:241:GLY:O	1:B:256:LEU:HD12	2.21	0.41
1:A:91:VAL:HG12	1:A:117:LEU:HD11	2.02	0.41
1:B:251:PRO:HA	1:B:252:PRO:HD3	1.89	0.41
1:B:34:THR:HA	2:B:305:HOH:O	2.21	0.41
1:A:103:LEU:HB3	2:A:369:HOH:O	2.20	0.41
1:A:49:LYS:HD3	1:A:51:ASP:OD2	2.21	0.41
1:B:65:TYR:CE2	1:B:87:LYS:HE3	2.56	0.41
1:B:144:LEU:HD13	1:B:151:MSE:HE2	2.03	0.41
1:B:35:ALA:O	1:B:210:HIS:N	2.54	0.41
1:A:115:ARG:HE	1:A:133:LEU:CD1	2.34	0.40
1:A:126:VAL:CG1	1:A:151:MSE:HE1	2.48	0.40
1:A:28:LEU:HD22	1:A:44:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	252/299 (84%)	225 (89%)	22 (9%)	5 (2%)	9	28
1	B	252/299 (84%)	225 (89%)	22 (9%)	5 (2%)	9	28
All	All	504/598 (84%)	450 (89%)	44 (9%)	10 (2%)	9	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	73	ASP
1	A	157	GLN
1	B	34	THR
1	B	73	ASP
1	B	157	GLN
1	A	112	VAL
1	B	112	VAL
1	A	140	VAL
1	B	140	VAL

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	197/224 (88%)	176 (89%)	21 (11%)	8	22
1	B	197/224 (88%)	176 (89%)	21 (11%)	8	22
All	All	394/448 (88%)	352 (89%)	42 (11%)	8	22

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	62	GLU
1	A	80	ILE
1	A	97	SER
1	A	113	LEU
1	A	117	LEU
1	A	118	ARG
1	A	132	LYS
1	A	138	ARG
1	A	146	ASP
1	A	150	LEU
1	A	157	GLN
1	A	166	GLN
1	A	168	SER
1	A	180	THR
1	A	201	ARG
1	A	236	GLU
1	A	266	ARG
1	A	270	TYR
1	A	284	LEU
1	A	285	LEU
1	B	54	GLN
1	B	62	GLU
1	B	80	ILE
1	B	97	SER
1	B	113	LEU
1	B	117	LEU
1	B	118	ARG
1	B	132	LYS
1	B	138	ARG
1	B	146	ASP
1	B	150	LEU
1	B	157	GLN
1	B	166	GLN
1	B	168	SER
1	B	180	THR
1	B	201	ARG
1	B	236	GLU
1	B	266	ARG
1	B	270	TYR
1	B	284	LEU
1	B	285	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	152	GLN
1	A	166	GLN
1	A	167	GLN
1	A	175	ASN
1	B	60	HIS
1	B	136	GLN
1	B	166	GLN
1	B	167	GLN
1	B	175	ASN
1	B	210	HIS
1	B	237	HIS

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	254/299 (84%)	-0.18	1 (0%) 92 90	1, 5, 17, 30	0
1	B	254/299 (84%)	-0.19	0 100 100	1, 5, 17, 31	0
All	All	508/598 (84%)	-0.19	1 (0%) 94 94	1, 5, 17, 31	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	ARG	2.2

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.