Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:38 PM GMT

PDB ID	:	1XZO
Title	:	Identification of a disulfide switch in BsSco, a member of the Sco family of cytochrome c oxidase assembly proteins
Authors	:	Ye, Q.; Imriskova-Sosova, I.; Hill, B.C.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2004-11-12
Resolution	:	1.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

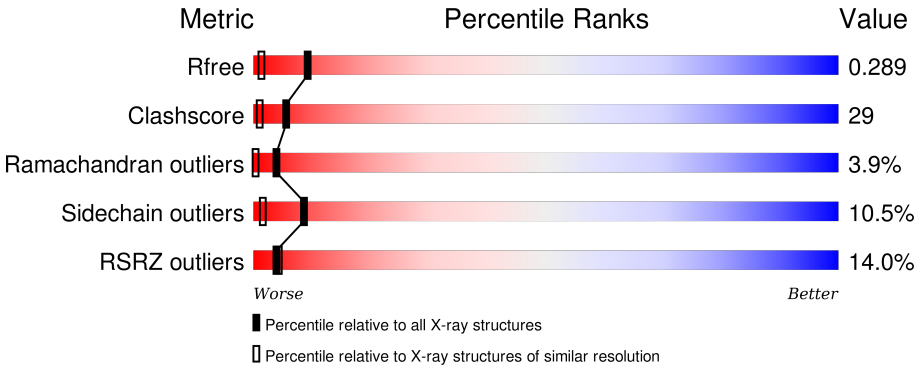
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 <=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	174	13% 60% 30% 8% ••
1	B	174	14% 61% 24% 10% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3128 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 Hypothetical protein ypmQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1366	872	217	273	4			
1	B	171	Total	C	N	O	S	0	0	0
			1355	864	216	271	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLY	CLONING ARTIFACT	UNP P54178
A	66	GLU	GLY	CONFLICT	UNP P54178
B	2	SER	GLY	CLONING ARTIFACT	UNP P54178
B	66	GLU	GLY	CONFLICT	UNP P54178

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cd	0	0
			1	1		
2	A	4	Total	Cd	0	0
			4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total	Ca	0	0
			6	6		
3	A	8	Total	Ca	0	0
			8	8		

- Molecule 4 is water.

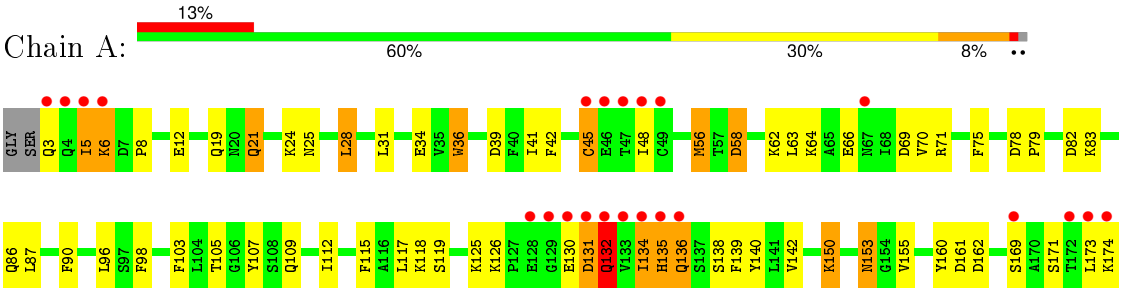
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	183	Total O 183 183	0	0
4	B	205	Total O 205 205	0	0

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.

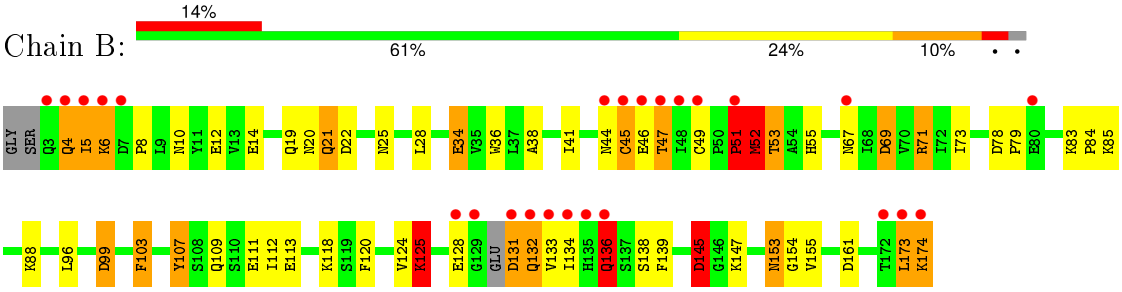
- Molecule 1: Hypothetical protein ypmQ

Chain A:



- Molecule 1: Hypothetical protein ypmQ

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	68.03Å 68.03Å 191.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.20 – 1.70 37.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.20-1.70) 94.6 (37.18-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.238 , 0.289 0.248 , 0.289	Depositor DCC
R_{free} test set	2771 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 71.0	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 54325 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3128	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, CD

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	1.52	17/1395 (1.2%)	1.43	10/1890 (0.5%)
1	B	1.49	10/1383 (0.7%)	1.32	14/1870 (0.7%)
All	All	1.50	27/2778 (1.0%)	1.38	24/3760 (0.6%)

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	0	1
1	B	0	1
All	All	0	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	GLU	CD-OE2	14.06	1.41	1.25
1	A	56	MET	SD-CE	-10.21	1.20	1.77
1	B	55	HIS	C-O	-9.82	1.04	1.23
1	B	12	GLU	CD-OE2	9.69	1.36	1.25
1	A	36	TRP	CB-CG	-9.01	1.34	1.50
1	A	36	TRP	CE3-CZ3	-8.61	1.23	1.38
1	A	58	ASP	CB-CG	7.89	1.68	1.51
1	A	160	TYR	CD1-CE1	-7.49	1.28	1.39
1	A	36	TRP	CG-CD2	-6.76	1.32	1.43
1	A	98	PHE	CD2-CE2	-6.74	1.25	1.39
1	A	160	TYR	CD2-CE2	-6.74	1.29	1.39
1	A	56	MET	CG-SD	-6.64	1.63	1.81
1	A	58	ASP	CG-OD2	6.59	1.40	1.25
1	B	34	GLU	CG-CD	6.35	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	PHE	CE1-CZ	6.32	1.49	1.37
1	B	145	ASP	CB-CG	6.24	1.64	1.51
1	A	36	TRP	CZ3-CH2	-6.14	1.30	1.40
1	B	34	GLU	CB-CG	5.75	1.63	1.52
1	B	111	GLU	CD-OE1	-5.43	1.19	1.25
1	B	36	TRP	CE3-CZ3	-5.39	1.29	1.38
1	A	90	PHE	CD1-CE1	5.39	1.50	1.39
1	A	119	SER	CB-OG	5.33	1.49	1.42
1	A	75	PHE	CB-CG	-5.26	1.42	1.51
1	B	107	TYR	CE1-CZ	-5.16	1.31	1.38
1	A	58	ASP	CA-CB	5.16	1.65	1.53
1	B	103	PHE	CD2-CE2	5.13	1.49	1.39
1	A	115	PHE	CD2-CE2	-5.06	1.29	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ASP	CB-CG-OD2	23.35	139.31	118.30
1	A	58	ASP	CB-CG-OD1	-11.02	108.38	118.30
1	A	56	MET	CG-SD-CE	10.66	117.25	100.20
1	B	145	ASP	CB-CG-OD2	8.60	126.04	118.30
1	A	78	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	125	LYS	CD-CE-NZ	7.41	128.74	111.70
1	B	55	HIS	CA-C-O	7.29	135.41	120.10
1	B	99	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	58	ASP	CB-CA-C	6.91	124.22	110.40
1	B	131	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	139	PHE	CB-CG-CD1	6.09	125.06	120.80
1	B	22	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	69	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	131	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	58	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	B	55	HIS	CA-C-N	-5.78	104.49	117.20
1	B	145	ASP	OD1-CG-OD2	-5.70	112.46	123.30
1	B	161	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	173	LEU	N-CA-C	5.30	125.32	111.00
1	A	162	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	28	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	139	PHE	CB-CG-CD1	5.24	124.47	120.80
1	B	120	PHE	CB-CG-CD2	5.20	124.44	120.80
1	A	69	ASP	CB-CG-OD2	5.07	122.87	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLN	Peptide
1	B	51	PRO	Peptide

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	1366	0	1281	70	1
1	B	1355	0	1251	81	0
2	A	4	0	0	2	0
2	B	1	0	0	1	0
3	A	8	0	0	1	0
3	B	6	0	0	1	0
4	A	183	0	0	23	0
4	B	205	0	0	40	3
All	All	3128	0	2532	153	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 29.

All (153) 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:73:ILE:CG1	4:B:1204:HOH:O	1.71	1.31
1:B:73:ILE:HG22	4:B:1165:HOH:O	1.16	1.30
1:A:56:MET:CE	1:A:56:MET:SD	1.20	1.29
1:A:36:TRP:CZ2	4:A:1188:HOH:O	1.69	1.25
1:B:118:LYS:HE2	4:B:1192:HOH:O	1.38	1.24
1:B:118:LYS:HB2	4:B:1201:HOH:O	1.34	1.23
1:B:34:GLU:OE2	4:B:1206:HOH:O	1.52	1.23
1:A:36:TRP:HZ2	4:A:1188:HOH:O	1.01	1.22
1:A:56:MET:SD	1:A:56:MET:HE3	1.78	1.17
3:A:1008:CA:CA	4:A:1187:HOH:O	1.24	1.15
1:B:52:MET:SD	4:B:1140:HOH:O	2.03	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1000:CD:CD	4:B:1203:HOH:O	1.15	1.14
1:A:56:MET:SD	1:A:56:MET:HE2	1.78	1.14
1:A:82:ASP:O	1:A:105:THR:HG21	1.42	1.13
1:A:56:MET:SD	1:A:56:MET:HE1	1.78	1.12
1:B:147:LYS:CB	4:B:1209:HOH:O	1.97	1.11
1:B:34:GLU:CD	4:B:1206:HOH:O	1.81	1.11
1:B:125:LYS:CE	4:B:1210:HOH:O	1.98	1.10
3:B:1006:CA:CA	4:B:1153:HOH:O	1.27	1.08
2:A:1001:CD:CD	4:A:1186:HOH:O	1.19	1.07
1:A:39:ASP:HA	4:A:1108:HOH:O	1.56	1.03
1:B:153:ASN:HD21	1:B:155:VAL:HG12	1.20	1.02
2:A:1002:CD:CD	4:B:1208:HOH:O	1.28	1.00
1:B:153:ASN:HD21	1:B:155:VAL:CG1	1.75	0.98
1:A:56:MET:CG	1:A:56:MET:CE	2.43	0.96
1:B:125:LYS:HE2	4:B:1210:HOH:O	1.59	0.95
1:A:64:LYS:HB3	4:A:1050:HOH:O	1.68	0.94
1:A:31:LEU:HD22	1:A:34:GLU:OE2	1.66	0.94
1:A:87:LEU:HD11	1:A:105:THR:HG23	1.52	0.92
1:B:153:ASN:ND2	1:B:155:VAL:HG12	1.85	0.91
1:A:34:GLU:OE2	1:A:36:TRP:HB3	1.72	0.88
1:B:125:LYS:HE3	4:B:1210:HOH:O	1.65	0.86
1:B:41:ILE:CG1	4:B:1212:HOH:O	2.23	0.86
1:A:28:LEU:HD13	1:A:28:LEU:O	1.84	0.77
1:B:145:ASP:HB3	4:B:1142:HOH:O	1.83	0.77
1:A:41:ILE:CG1	4:A:1131:HOH:O	2.32	0.76
1:A:6:LYS:HE2	1:A:150:LYS:NZ	2.00	0.76
1:A:83:LYS:HB2	1:A:86:GLN:NE2	2.02	0.74
1:B:34:GLU:OE1	4:B:1206:HOH:O	1.90	0.74
1:A:83:LYS:HB2	1:A:86:GLN:HE22	1.52	0.74
1:A:28:LEU:HD13	1:A:28:LEU:C	2.08	0.74
1:B:113:GLU:OE1	1:B:125:LYS:NZ	2.20	0.73
1:A:118:LYS:NZ	4:A:1083:HOH:O	2.17	0.73
1:A:36:TRP:HZ3	4:A:1019:HOH:O	1.73	0.72
1:A:19:GLN:OE1	4:A:1165:HOH:O	2.07	0.72
1:A:171:SER:OG	4:A:1190:HOH:O	2.09	0.70
1:A:42:PHE:HE2	1:A:45:CYS:HG	1.40	0.69
1:B:51:PRO:O	1:B:53:THR:N	2.23	0.69
1:A:153:ASN:HD22	1:A:155:VAL:H	1.42	0.68
1:B:52:MET:CE	1:B:155:VAL:HA	2.24	0.68
1:A:6:LYS:HE2	1:A:150:LYS:HZ2	1.58	0.68
1:A:138:SER:OG	1:A:140:TYR:CZ	2.46	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:VAL:O	1:B:125:LYS:HD2	1.94	0.67
1:B:69:ASP:OD2	4:B:1206:HOH:O	2.13	0.66
1:A:64:LYS:HE2	4:A:1037:HOH:O	1.95	0.65
1:A:36:TRP:HB2	1:A:71:ARG:O	1.97	0.65
1:B:52:MET:HE3	1:B:155:VAL:HA	1.80	0.63
1:B:153:ASN:HD22	1:B:155:VAL:H	1.46	0.63
1:B:88:LYS:NZ	4:B:1174:HOH:O	2.06	0.62
1:A:6:LYS:O	1:A:8:PRO:HD3	1.99	0.62
1:B:19:GLN:NE2	4:B:1067:HOH:O	2.32	0.62
1:A:96:LEU:HD12	1:A:96:LEU:C	2.20	0.62
1:A:5:ILE:HD13	1:A:6:LYS:N	2.16	0.61
1:A:34:GLU:OE2	1:A:34:GLU:CG	2.48	0.61
1:A:21:GLN:H	1:A:21:GLN:NE2	2.00	0.60
1:A:5:ILE:HD13	1:A:5:ILE:C	2.23	0.59
1:B:125:LYS:HE3	4:B:1194:HOH:O	2.03	0.59
1:B:67:ASN:O	1:B:67:ASN:ND2	2.35	0.59
1:B:88:LYS:CE	4:B:1174:HOH:O	2.50	0.58
1:A:153:ASN:ND2	1:A:155:VAL:H	2.00	0.58
1:A:19:GLN:HE22	1:B:25:ASN:HD21	1.52	0.58
1:B:153:ASN:ND2	1:B:155:VAL:H	2.02	0.57
1:B:4:GLN:O	1:B:5:ILE:HB	2.04	0.57
1:B:53:THR:HB	4:B:1024:HOH:O	2.04	0.57
1:B:153:ASN:HD21	1:B:155:VAL:HG13	1.67	0.56
1:A:63:LEU:HD13	1:A:70:VAL:HG11	1.85	0.56
1:A:64:LYS:CB	4:A:1050:HOH:O	2.40	0.56
1:B:21:GLN:H	1:B:21:GLN:NE2	2.04	0.56
1:A:28:LEU:CD1	1:A:28:LEU:C	2.73	0.56
1:B:125:LYS:HD3	4:B:1054:HOH:O	2.06	0.55
1:B:113:GLU:CD	1:B:125:LYS:NZ	2.61	0.54
1:A:36:TRP:CH2	1:A:142:VAL:HG11	2.43	0.53
1:A:21:GLN:NE2	1:A:103:PHE:H	2.07	0.53
1:B:174:LYS:NZ	4:B:1151:HOH:O	2.01	0.53
1:B:173:LEU:CA	4:B:1156:HOH:O	2.56	0.53
1:A:19:GLN:NE2	1:B:25:ASN:HD21	2.06	0.52
1:A:136:GLN:HB3	4:A:1099:HOH:O	2.08	0.52
1:A:86:GLN:NE2	1:A:86:GLN:H	2.08	0.52
1:A:36:TRP:NE1	4:A:1188:HOH:O	2.38	0.52
1:B:5:ILE:CG1	4:B:1143:HOH:O	2.58	0.52
1:B:46:GLU:O	1:B:47:THR:HB	2.10	0.52
1:B:6:LYS:O	1:B:8:PRO:HD3	2.11	0.52
1:A:6:LYS:HE2	1:A:150:LYS:HZ1	1.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:CD	4:A:1141:HOH:O	2.58	0.51
1:A:138:SER:OG	1:A:140:TYR:CE2	2.64	0.51
1:A:64:LYS:HG2	4:A:1037:HOH:O	2.10	0.51
1:A:19:GLN:HG2	4:A:1181:HOH:O	2.11	0.50
1:B:174:LYS:HB2	4:B:1074:HOH:O	2.11	0.50
1:B:113:GLU:OE2	1:B:125:LYS:NZ	2.43	0.50
1:A:5:ILE:HD11	1:A:150:LYS:HD2	1.94	0.50
1:B:133:VAL:HG23	4:B:1159:HOH:O	2.10	0.49
1:B:96:LEU:C	1:B:96:LEU:HD12	2.32	0.49
1:B:14:GLU:OE1	1:B:118:LYS:NZ	2.42	0.49
1:A:34:GLU:OE2	1:A:71:ARG:HB2	2.13	0.49
1:B:78:ASP:OD2	4:B:1103:HOH:O	2.19	0.49
1:B:153:ASN:C	1:B:153:ASN:HD22	2.17	0.48
1:A:125:LYS:HG3	1:A:126:LYS:N	2.28	0.48
1:B:21:GLN:NE2	1:B:103:PHE:H	2.13	0.47
1:B:174:LYS:CE	4:B:1151:HOH:O	2.57	0.47
1:B:125:LYS:NZ	4:B:1189:HOH:O	2.48	0.47
1:A:31:LEU:CD2	1:A:34:GLU:OE2	2.52	0.47
1:B:5:ILE:HG23	1:B:5:ILE:O	2.15	0.47
1:B:85:LYS:NZ	4:B:1137:HOH:O	2.44	0.47
1:B:14:GLU:OE1	1:B:118:LYS:HE3	2.15	0.47
1:B:125:LYS:HG3	4:B:1189:HOH:O	2.15	0.47
1:B:73:ILE:C	4:B:1165:HOH:O	2.53	0.46
1:A:117:LEU:HD23	4:A:1168:HOH:O	2.14	0.46
1:A:12:GLU:N	1:A:12:GLU:OE1	2.48	0.46
1:A:36:TRP:CE2	4:A:1188:HOH:O	2.23	0.46
1:B:153:ASN:ND2	1:B:155:VAL:CG1	2.56	0.45
1:B:52:MET:CE	1:B:155:VAL:HB	2.47	0.45
1:B:124:VAL:O	1:B:125:LYS:CD	2.65	0.44
1:B:52:MET:CE	1:B:155:VAL:CA	2.95	0.44
1:A:64:LYS:CA	4:A:1050:HOH:O	2.66	0.44
1:B:99:ASP:OD1	4:B:1152:HOH:O	2.21	0.44
1:B:136:GLN:O	1:B:136:GLN:HG3	2.18	0.44
1:A:5:ILE:HD11	1:A:150:LYS:CD	2.46	0.44
1:A:42:PHE:HE2	1:A:45:CYS:SG	2.38	0.44
1:B:145:ASP:CA	4:B:1142:HOH:O	2.66	0.43
1:B:20:ASN:HA	1:B:103:PHE:O	2.18	0.43
1:B:125:LYS:HA	1:B:125:LYS:HD2	1.70	0.43
1:B:6:LYS:HG3	4:B:1114:HOH:O	2.19	0.43
1:A:135:HIS:N	4:A:1178:HOH:O	2.52	0.43
1:B:45:CYS:HB3	1:B:49:CYS:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD11	4:A:1039:HOH:O	2.18	0.42
1:A:25:ASN:HD21	1:B:19:GLN:HE22	1.67	0.42
1:A:107:TYR:CE1	1:A:112:ILE:HB	2.55	0.42
1:B:107:TYR:CD1	1:B:112:ILE:HB	2.55	0.42
1:B:10:ASN:HB3	1:B:147:LYS:HE2	2.02	0.41
1:A:58:ASP:O	1:A:62:LYS:HG3	2.20	0.41
1:B:53:THR:HG23	4:B:1019:HOH:O	2.19	0.41
1:A:134:ILE:O	1:A:135:HIS:HB2	2.20	0.41
1:B:83:LYS:HB3	1:B:84:PRO:CD	2.50	0.41
1:A:6:LYS:O	1:A:8:PRO:CD	2.67	0.41
1:B:38:ALA:HA	1:B:73:ILE:O	2.20	0.41
1:B:153:ASN:HD22	1:B:154:GLY:N	2.19	0.41
1:B:71:ARG:HH11	1:B:71:ARG:HD3	1.78	0.41
1:B:14:GLU:OE1	1:B:118:LYS:CE	2.69	0.41
1:B:52:MET:HE2	1:B:155:VAL:HB	2.02	0.41
1:A:66:GLU:CG	1:A:66:GLU:O	2.68	0.41
1:B:79:PRO:HD2	1:B:109:GLN:HE22	1.87	0.40
1:A:79:PRO:HD2	1:A:109:GLN:NE2	2.36	0.40
1:B:88:LYS:HE2	4:B:1174:HOH:O	2.17	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)
4:B:1037:HOH:O	4:B:1037:HOH:O[4_555]	1.28	0.92
4:B:1040:HOH:O	4:B:1040:HOH:O[4_555]	1.64	0.56
1:A:161:ASP:OD2	4:B:1203:HOH:O[1_455]	2.13	0.07

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	170/174 (98%)	158 (93%)	7 (4%)	5 (3%)	6 1
1	B	167/174 (96%)	155 (93%)	4 (2%)	8 (5%)	3 0
All	All	337/348 (97%)	313 (93%)	11 (3%)	13 (4%)	4 0

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	48	ILE
1	A	131	ASP
1	A	132	GLN
1	B	5	ILE
1	B	52	MET
1	B	134	ILE
1	A	135	HIS
1	B	47	THR
1	B	51	PRO
1	B	136	GLN
1	B	4	GLN
1	B	132	GLN

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	145/158 (92%)	131 (90%)	14 (10%)	10 2
1	B	140/158 (89%)	124 (89%)	16 (11%)	7 1
All	All	285/316 (90%)	255 (90%)	30 (10%)	8 1

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	ILE
1	A	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	28	LEU
1	A	45	CYS
1	A	130	GLU
1	A	132	GLN
1	A	134	ILE
1	A	136	GLN
1	A	150	LYS
1	A	153	ASN
1	A	169	SER
1	A	173	LEU
1	A	174	LYS
1	B	6	LYS
1	B	21	GLN
1	B	44	ASN
1	B	45	CYS
1	B	52	MET
1	B	53	THR
1	B	71	ARG
1	B	125	LYS
1	B	128	GLU
1	B	131	ASP
1	B	132	GLN
1	B	136	GLN
1	B	138	SER
1	B	145	ASP
1	B	153	ASN
1	B	174	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	10	ASN
1	A	21	GLN
1	A	25	ASN
1	A	81	ASN
1	A	86	GLN
1	A	109	GLN
1	A	136	GLN
1	A	153	ASN
1	B	21	GLN
1	B	25	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	81	ASN
1	B	109	GLN
1	B	136	GLN
1	B	153	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 19 are monoatomic - 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

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	172/174 (98%)	1.04	23 (13%)	4	5	17, 26, 60, 77	0
1	B	171/174 (98%)	1.13	25 (14%)	3	4	17, 27, 64, 76	0
All	All	343/348 (98%)	1.09	48 (13%)	4	4	17, 27, 64, 77	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	16.7
1	B	134	ILE	11.3
1	A	129	GLY	10.8
1	A	173	LEU	10.8
1	A	133	VAL	10.7
1	B	47	THR	10.4
1	B	129	GLY	10.2
1	A	134	ILE	9.9
1	B	3	GLN	9.8
1	B	135	HIS	9.6
1	B	173	LEU	9.3
1	B	48	ILE	8.9
1	A	47	THR	7.7
1	A	132	GLN	7.5
1	B	4	GLN	7.4
1	A	48	ILE	7.3
1	B	133	VAL	6.8
1	A	131	ASP	6.8
1	A	135	HIS	6.1
1	A	130	GLU	6.0
1	A	45	CYS	6.0
1	B	132	GLN	5.8
1	B	45	CYS	5.7
1	B	131	ASP	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	174	LYS	5.4
1	B	46	GLU	5.3
1	B	174	LYS	5.0
1	A	46	GLU	4.9
1	B	128	GLU	4.7
1	A	128	GLU	4.6
1	A	172	THR	4.4
1	A	6	LYS	4.3
1	A	49	CYS	4.3
1	A	3	GLN	4.0
1	B	6	LYS	4.0
1	B	51	PRO	3.9
1	A	67	ASN	3.9
1	B	172	THR	3.8
1	A	5	ILE	3.8
1	A	4	GLN	3.8
1	B	136	GLN	3.4
1	B	49	CYS	3.3
1	A	169	SER	3.1
1	A	136	GLN	2.7
1	B	7	ASP	2.4
1	B	80	GLU	2.1
1	B	67	ASN	2.1
1	B	44	ASN	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	CA	A	1005	1/1	0.97	0.09	-1.00	18,18,18,18	0
3	CA	A	1010	1/1	0.93	0.06	-2.64	38,38,38,38	0
3	CA	A	1016	1/1	0.98	0.06	-4.05	25,25,25,25	0
3	CA	B	1012	1/1	0.98	0.05	-4.78	24,24,24,24	0
2	CD	B	1000	1/1	0.99	0.04	-	29,29,29,29	0
2	CD	A	1002	1/1	0.99	0.03	-	36,36,36,36	0
3	CA	A	1013	1/1	0.94	0.07	-	39,39,39,39	0
3	CA	A	1014	1/1	0.99	0.04	-	34,34,34,34	0
2	CD	A	1003	1/1	0.99	0.03	-	41,41,41,41	0
3	CA	B	1006	1/1	0.95	0.04	-	27,27,27,27	0
3	CA	A	1015	1/1	0.93	0.07	-	33,33,33,33	0
3	CA	B	1018	1/1	0.96	0.16	-	28,28,28,28	0
3	CA	A	1009	1/1	0.88	0.07	-	32,32,32,32	0
3	CA	B	1011	1/1	0.97	0.08	-	34,34,34,34	0
3	CA	B	1017	1/1	0.97	0.05	-	34,34,34,34	0
3	CA	B	1007	1/1	0.96	0.16	-	32,32,32,32	0
2	CD	A	1004	1/1	0.96	0.05	-	48,48,48,48	0
3	CA	A	1008	1/1	0.96	0.05	-	34,34,34,34	0
2	CD	A	1001	1/1	0.98	0.04	-	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.