Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:42 PM GMT

PDB ID	:	1YDW
Title	:	X-RAY STRUCTURE OF GENE PRODUCT FROM ARABIDOPSIS THALIANA AT4G09670
Authors	:	Wesenberg, G.E.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Allard, S.T.M.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2004-12-26
Resolution	:	2.49 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:

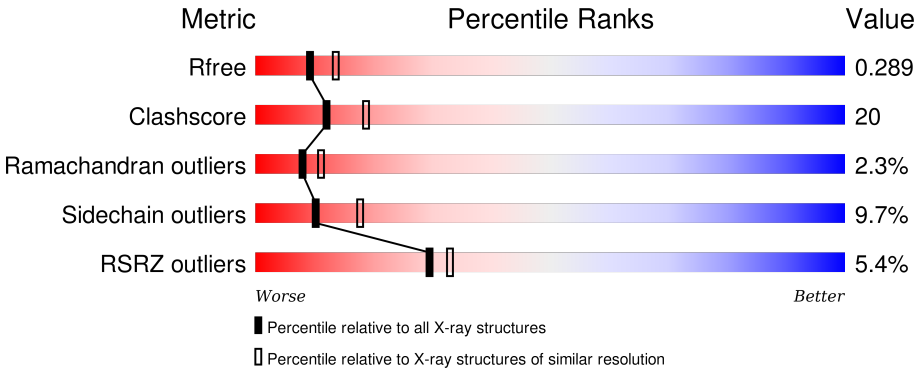
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.49 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	362	6% 60% 28% 5% • 5%
1	B	362	4% 70% 22% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5463 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 AX110P-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	MET	CLONING ARTIFACT	UNP Q9SZ83
A	12	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	106	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	126	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	130	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	249	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	310	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	1	SER	MET	CLONING ARTIFACT	UNP Q9SZ83
B	12	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	106	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	126	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	130	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	249	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	310	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83

- Molecule 2 is water.

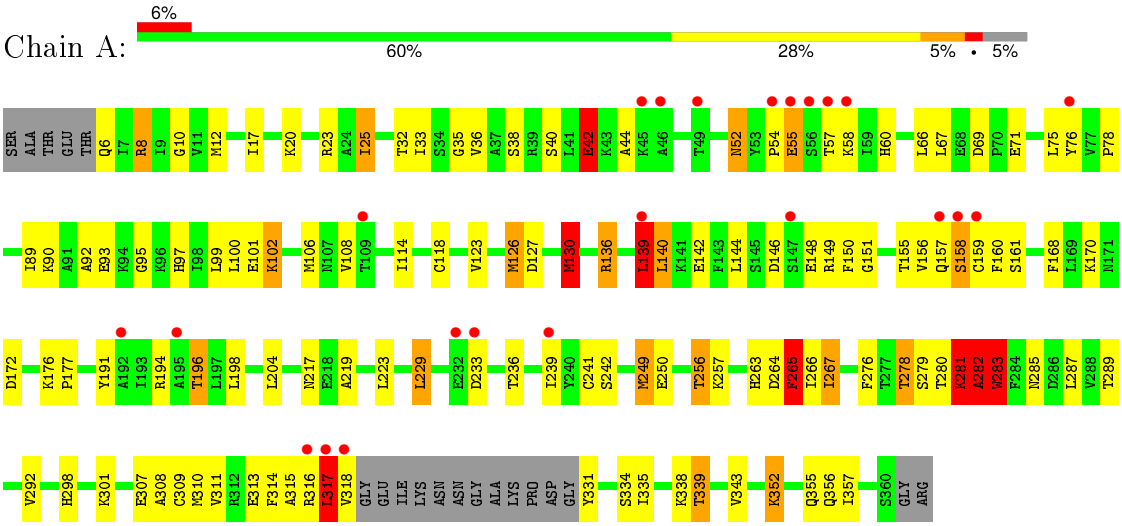
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	60	Total	O	0	0
			60	60		
2	B	63	Total	O	0	0
			63	63		

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.

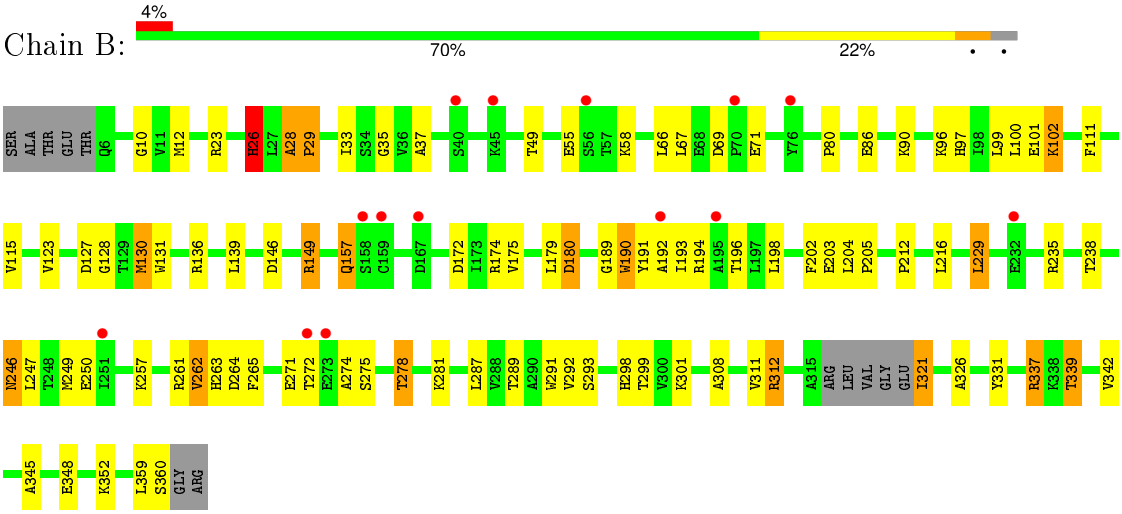
- Molecule 1: AX110P-like protein

Chain A:



- Molecule 1: AX110P-like protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.20Å 107.66Å 129.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.06 – 2.49 29.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (31.06-2.49) 98.4 (29.73-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.60 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.218 , 0.283 0.228 , 0.289	Depositor DCC
R_{free} test set	1472 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 28862 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5463	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.72% 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

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	3/2698 (0.1%)	1.00	5/3656 (0.1%)
1	B	0.99	0/2743	0.96	4/3716 (0.1%)
All	All	0.98	3/5441 (0.1%)	0.98	9/7372 (0.1%)

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	3
1	B	0	1
All	All	1	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	MSE	SE-CE	-6.14	1.59	1.95
1	A	309	CYS	CB-SG	-5.42	1.73	1.81
1	A	159	CYS	CB-SG	-5.23	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	LEU	CB-CG-CD1	-8.32	96.85	111.00
1	A	282	ALA	N-CA-C	-7.62	90.42	111.00
1	A	317	LEU	CA-CB-CG	7.43	132.39	115.30
1	B	235	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	235	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	283	TRP	N-CA-C	6.18	127.69	111.00
1	B	337	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	264	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	126	MSE	CG-SE-CE	5.01	109.92	98.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	283	TRP	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	MSE	Peptide
1	A	282	ALA	Peptide
1	A	317	LEU	Peptide
1	B	26	HIS	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	2648	0	2642	139	0
1	B	2692	0	2680	76	0
2	A	60	0	0	12	0
2	B	63	0	0	19	0
All	All	5463	0	5322	212	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 20.

All (212) 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:176:LYS:HE3	2:A:391:HOH:O	1.04	1.18
1:A:281:LYS:HB2	2:A:364:HOH:O	1.42	1.18
1:A:317:LEU:HD13	1:A:318:VAL:H	1.07	1.16
1:A:157:GLN:HA	2:A:421:HOH:O	1.44	1.16
1:A:139:LEU:N	1:A:139:LEU:HD12	1.47	1.09
1:B:198:LEU:HB3	2:B:422:HOH:O	1.49	1.08
1:A:139:LEU:CD1	1:A:139:LEU:H	1.67	1.07
1:A:264:ASP:O	1:A:265:PHE:HB3	1.34	1.06
1:B:28:ALA:CB	1:B:29:PRO:HA	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:HD12	2:B:424:HOH:O	1.61	1.00
1:A:264:ASP:O	1:A:265:PHE:CB	2.07	0.99
1:A:93:GLU:HB2	2:A:397:HOH:O	1.62	0.99
1:A:285:ASN:HD21	1:A:289:THR:HG22	1.27	0.99
1:B:28:ALA:HB3	1:B:29:PRO:HA	1.44	0.98
1:B:337:ARG:HD3	2:B:365:HOH:O	1.64	0.97
1:A:285:ASN:HD21	1:A:289:THR:CG2	1.79	0.94
1:A:102:LYS:NZ	2:A:412:HOH:O	2.01	0.92
1:A:139:LEU:CD1	1:A:139:LEU:N	2.29	0.92
1:B:203:GLU:HB3	2:B:408:HOH:O	1.71	0.91
1:B:146:ASP:OD2	1:B:149:ARG:HG3	1.72	0.88
1:A:280:THR:O	1:A:281:LYS:O	1.91	0.88
1:A:317:LEU:HD13	1:A:318:VAL:N	1.89	0.87
1:B:198:LEU:HD12	1:B:202:PHE:HE1	1.38	0.87
1:A:108:VAL:HG12	2:A:390:HOH:O	1.75	0.87
1:A:256:THR:HG22	1:A:257:LYS:CG	2.08	0.84
1:A:97:HIS:CE1	1:A:123:VAL:HG12	2.14	0.83
1:A:285:ASN:ND2	1:A:289:THR:HG22	1.94	0.83
1:A:281:LYS:HD2	1:A:281:LYS:C	1.99	0.82
1:B:247:LEU:HD11	1:B:249:MSE:HE3	1.60	0.81
1:B:194:ARG:HE	1:B:339:THR:HG21	1.45	0.80
1:A:256:THR:HG22	1:A:257:LYS:HG2	1.61	0.80
1:A:139:LEU:H	1:A:139:LEU:HD12	0.74	0.79
1:B:26:HIS:CA	2:B:371:HOH:O	2.30	0.79
1:B:28:ALA:CB	1:B:29:PRO:CA	2.57	0.79
1:B:308:ALA:O	1:B:312:ARG:HB2	1.83	0.79
1:A:317:LEU:CD1	1:A:318:VAL:H	1.92	0.78
1:B:250:GLU:OE1	1:B:263:HIS:ND1	2.11	0.78
1:A:139:LEU:O	1:A:139:LEU:HD13	1.83	0.78
1:B:198:LEU:HD12	1:B:202:PHE:CE1	2.18	0.78
1:A:8:ARG:HH11	1:A:8:ARG:HG3	1.49	0.77
1:A:140:LEU:HD23	1:A:140:LEU:C	2.05	0.76
1:B:198:LEU:CD1	1:B:202:PHE:HE1	1.99	0.76
1:B:102:LYS:HE2	1:B:191:TYR:CE2	2.21	0.75
1:B:130:MSE:HG3	2:B:399:HOH:O	1.85	0.75
1:A:194:ARG:HH21	1:A:339:THR:HG21	1.52	0.75
1:A:204:LEU:CD2	1:A:338:LYS:HG2	2.17	0.74
1:A:76:TYR:CE2	1:A:78:PRO:HG3	2.23	0.73
1:A:102:LYS:HE3	1:A:191:TYR:OH	1.89	0.73
1:B:28:ALA:HB1	1:B:29:PRO:HA	1.71	0.73
1:A:256:THR:CG2	1:A:257:LYS:HG2	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:MSE:HE3	1:A:66:LEU:HD23	1.70	0.72
1:A:287:LEU:HD23	2:B:413:HOH:O	1.90	0.71
1:A:204:LEU:HD21	1:A:338:LYS:HG2	1.72	0.71
1:A:249:MSE:SE	1:A:266:ILE:O	2.58	0.71
1:A:156:VAL:O	2:A:421:HOH:O	2.08	0.71
1:A:126:MSE:HE3	1:A:310:MSE:CG	2.21	0.71
1:B:26:HIS:C	2:B:371:HOH:O	2.27	0.70
1:A:126:MSE:HE3	1:A:310:MSE:HG3	1.72	0.70
1:A:194:ARG:HE	1:A:339:THR:HG21	1.56	0.70
1:B:26:HIS:ND1	1:B:28:ALA:HB2	2.06	0.69
1:A:314:PHE:C	1:A:316:ARG:H	1.95	0.69
1:B:360:SER:C	2:B:421:HOH:O	2.31	0.69
1:A:8:ARG:NH1	1:A:8:ARG:HG3	2.07	0.68
1:A:317:LEU:O	1:A:318:VAL:HG22	1.95	0.66
1:B:146:ASP:CG	1:B:149:ARG:HG3	2.14	0.66
1:A:249:MSE:CE	1:A:264:ASP:HA	2.26	0.66
1:B:28:ALA:HB1	1:B:29:PRO:CA	2.23	0.65
1:A:256:THR:HG22	1:A:257:LYS:HG3	1.77	0.65
1:A:23:ARG:HH21	1:B:289:THR:HG21	1.62	0.65
1:A:314:PHE:O	1:A:316:ARG:N	2.29	0.64
1:A:100:LEU:O	1:A:127:ASP:HA	1.97	0.64
1:B:194:ARG:HH21	1:B:339:THR:HG21	1.62	0.64
1:B:97:HIS:HA	1:B:123:VAL:HB	1.80	0.63
1:B:194:ARG:NE	1:B:339:THR:HG21	2.13	0.63
1:A:316:ARG:O	1:A:317:LEU:HB3	1.96	0.63
1:B:348:GLU:OE2	1:B:352:LYS:NZ	2.32	0.62
1:A:194:ARG:HH21	1:A:339:THR:CG2	2.12	0.62
1:A:146:ASP:OD2	1:A:149:ARG:HD3	1.99	0.62
1:B:100:LEU:O	1:B:127:ASP:HA	2.00	0.60
1:B:174:ARG:NE	2:B:420:HOH:O	2.33	0.60
1:B:26:HIS:ND1	1:B:28:ALA:CB	2.64	0.60
1:A:32:THR:HA	2:A:414:HOH:O	2.02	0.60
1:B:192:ALA:O	1:B:196:THR:HG23	2.02	0.60
1:B:102:LYS:HE2	1:B:191:TYR:CZ	2.37	0.59
1:A:151:GLY:HA3	1:A:257:LYS:HG3	1.83	0.59
1:A:335:ILE:O	1:A:339:THR:HG22	2.03	0.58
1:B:345:ALA:HB2	1:B:359:LEU:HD21	1.84	0.58
1:A:331:TYR:O	1:A:334:SER:HB3	2.04	0.58
1:B:136:ARG:HD3	1:B:274:ALA:HB1	1.85	0.58
1:B:10:GLY:HA2	1:B:35:GLY:O	2.03	0.58
1:A:313:GLU:O	1:A:316:ARG:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HD2	1:A:282:ALA:N	2.19	0.57
1:B:102:LYS:C	1:B:102:LYS:HD2	2.24	0.57
1:B:28:ALA:HB3	1:B:29:PRO:CA	2.25	0.57
1:B:146:ASP:OD2	1:B:149:ARG:CG	2.49	0.57
1:B:257:LYS:HD2	1:B:281:LYS:HE2	1.85	0.57
1:A:250:GLU:OE2	1:B:261:ARG:HD2	2.05	0.57
1:A:281:LYS:O	1:A:281:LYS:HD2	2.04	0.57
1:A:136:ARG:NH2	1:A:265:PHE:HA	2.20	0.57
1:B:26:HIS:HB3	2:B:371:HOH:O	2.05	0.55
1:A:204:LEU:HD22	1:A:338:LYS:HG2	1.87	0.55
1:B:174:ARG:CZ	2:B:420:HOH:O	2.54	0.55
1:A:278:THR:HB	1:A:298:HIS:NE2	2.22	0.55
1:A:256:THR:HG21	1:A:257:LYS:HZ3	1.70	0.55
1:A:10:GLY:HA2	1:A:35:GLY:O	2.07	0.54
1:B:194:ARG:NH2	1:B:339:THR:HG21	2.23	0.54
1:A:40:SER:OG	1:A:42:GLU:HB2	2.07	0.54
1:A:285:ASN:HD21	1:A:289:THR:HG23	1.71	0.54
1:A:194:ARG:NH2	1:A:339:THR:HG21	2.21	0.53
1:A:256:THR:CG2	1:A:257:LYS:NZ	2.72	0.53
1:A:8:ARG:CG	1:A:8:ARG:HH11	2.21	0.53
1:A:67:LEU:HD13	1:A:90:LYS:O	2.08	0.52
1:A:20:LYS:NZ	1:A:130:MSE:SE	2.93	0.52
1:A:281:LYS:CD	1:A:281:LYS:C	2.73	0.52
1:B:348:GLU:HG2	1:B:348:GLU:O	2.09	0.52
1:A:126:MSE:CE	1:A:310:MSE:CG	2.87	0.52
1:A:266:ILE:O	1:A:267:ILE:HB	2.10	0.52
1:A:126:MSE:CE	1:A:310:MSE:HG2	2.40	0.52
1:B:194:ARG:HH21	1:B:339:THR:CG2	2.23	0.52
1:B:80:PRO:HB3	1:B:179:LEU:HB3	1.91	0.51
1:A:139:LEU:O	1:A:140:LEU:HB2	2.10	0.51
1:B:12:MSE:HE3	1:B:66:LEU:HD23	1.92	0.51
1:A:157:GLN:HG3	2:A:421:HOH:O	2.10	0.51
1:A:97:HIS:ND1	1:A:123:VAL:HG12	2.26	0.51
1:A:20:LYS:HZ1	1:A:130:MSE:SE	2.43	0.51
1:A:157:GLN:CA	2:A:421:HOH:O	2.25	0.51
1:A:89:ILE:O	1:A:93:GLU:HG3	2.09	0.51
1:A:139:LEU:C	1:A:139:LEU:HD13	2.28	0.51
1:A:136:ARG:HA	1:A:139:LEU:HD11	1.93	0.50
1:B:26:HIS:HA	1:B:28:ALA:HB2	1.92	0.50
1:B:58:LYS:HD2	1:B:69:ASP:OD2	2.11	0.50
1:A:314:PHE:C	1:A:316:ARG:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:NE	1:A:339:THR:HG21	2.26	0.49
1:A:249:MSE:HE2	1:B:291:TRP:HZ2	1.77	0.49
1:A:146:ASP:CG	1:A:149:ARG:HB2	2.33	0.49
1:B:23:ARG:HD3	2:B:413:HOH:O	2.12	0.49
1:A:92:ALA:O	1:A:95:GLY:N	2.43	0.49
1:A:155:THR:HA	1:A:236:THR:O	2.13	0.49
1:A:307:GLU:HA	1:A:310:MSE:HE2	1.94	0.48
1:A:256:THR:CG2	1:A:257:LYS:HZ3	2.26	0.48
1:A:158:SER:O	1:A:239:ILE:HA	2.13	0.48
1:A:60:HIS:HE1	1:A:69:ASP:HB2	1.78	0.48
1:A:12:MSE:CE	1:A:66:LEU:HD23	2.41	0.48
1:B:174:ARG:CD	2:B:420:HOH:O	2.62	0.48
1:B:172:ASP:O	1:B:175:VAL:HG22	2.13	0.48
1:A:233:ASP:N	1:A:233:ASP:OD1	2.44	0.48
1:B:331:TYR:C	1:B:331:TYR:CD2	2.86	0.48
1:A:356:GLN:O	1:A:357:ILE:HD13	2.14	0.47
1:B:278:THR:HG22	1:B:298:HIS:NE2	2.29	0.47
1:A:266:ILE:O	1:A:267:ILE:CB	2.61	0.47
1:A:352:LYS:O	1:A:355:GLN:HG3	2.14	0.47
1:A:6:GLN:HG3	2:A:418:HOH:O	2.14	0.47
1:A:67:LEU:CD2	1:A:75:LEU:HD11	2.45	0.47
1:A:140:LEU:HD23	1:A:140:LEU:O	2.14	0.47
1:A:144:LEU:HD23	1:A:150:PHE:CZ	2.50	0.47
1:A:307:GLU:HG2	1:A:308:ALA:N	2.30	0.46
1:A:160:PHE:O	1:A:241:CYS:HA	2.16	0.46
1:A:177:PRO:HG3	1:A:219:ALA:HB1	1.97	0.46
1:A:54:PRO:HD2	1:A:57:THR:OG1	2.14	0.46
1:B:67:LEU:O	1:B:96:LYS:HE2	2.16	0.46
1:B:58:LYS:CE	1:B:71:GLU:OE2	2.64	0.45
1:B:111:PHE:O	1:B:115:VAL:HG23	2.16	0.45
1:A:196:THR:HG21	1:A:229:LEU:HD11	1.99	0.45
1:A:52:ASN:CG	1:A:52:ASN:O	2.54	0.45
1:A:281:LYS:O	1:A:282:ALA:HB2	2.16	0.45
1:A:168:PHE:C	1:A:168:PHE:CD2	2.90	0.45
1:A:55:GLU:CD	1:A:55:GLU:N	2.70	0.45
1:A:106:MSE:HB3	1:A:106:MSE:HE3	1.93	0.45
1:A:38:SER:HB3	1:A:44:ALA:HB2	1.98	0.45
1:A:140:LEU:CD2	1:A:140:LEU:C	2.80	0.45
1:A:12:MSE:HB2	1:A:12:MSE:HE3	1.67	0.45
1:B:131:TRP:N	2:B:396:HOH:O	2.48	0.45
1:B:205:PRO:HG3	1:B:229:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:CD	1:A:263:HIS:HD1	2.21	0.44
1:A:339:THR:O	1:A:343:VAL:HG23	2.17	0.44
1:B:157:GLN:HG3	1:B:238:THR:OG1	2.18	0.44
1:B:86:GLU:HG3	1:B:90:LYS:HD2	2.00	0.44
1:B:278:THR:CG2	1:B:298:HIS:NE2	2.81	0.44
1:A:276:PHE:N	1:A:276:PHE:CD2	2.85	0.43
1:A:118:CYS:O	1:A:123:VAL:N	2.48	0.43
1:B:26:HIS:HB2	2:B:424:HOH:O	2.18	0.43
1:B:246:ASN:O	1:B:247:LEU:C	2.57	0.43
1:A:76:TYR:CZ	1:A:78:PRO:HG3	2.54	0.43
1:A:126:MSE:CE	1:A:310:MSE:HG3	2.46	0.43
1:A:217:ASN:HB3	1:A:223:LEU:HD11	2.00	0.43
1:B:37:ALA:HB2	1:B:66:LEU:HB2	2.00	0.43
1:A:17:ILE:HG13	1:A:17:ILE:O	2.18	0.43
1:B:212:PRO:HD2	2:B:390:HOH:O	2.19	0.42
1:A:161:SER:HB2	1:A:242:SER:HB3	2.01	0.42
1:A:289:THR:HG21	2:B:392:HOH:O	2.19	0.42
1:B:136:ARG:O	1:B:139:LEU:HB2	2.19	0.42
1:A:25:ILE:HA	1:A:311:VAL:HG11	2.00	0.42
1:A:114:ILE:O	1:A:114:ILE:HG22	2.19	0.42
1:B:262:VAL:HG22	1:B:265:PHE:HB3	2.02	0.42
1:A:292:VAL:HG23	2:A:409:HOH:O	2.18	0.42
1:A:283:TRP:O	1:A:292:VAL:HG22	2.20	0.42
1:B:149:ARG:HD2	2:B:406:HOH:O	2.20	0.41
1:A:317:LEU:HD22	1:A:318:VAL:C	2.41	0.41
1:A:256:THR:HG23	1:A:257:LYS:HG2	2.01	0.41
1:A:69:ASP:C	1:A:69:ASP:OD1	2.58	0.41
1:B:321:ILE:HA	1:B:326:ALA:H	1.84	0.41
1:B:193:ILE:HG21	1:B:342:VAL:HB	2.02	0.41
1:A:102:LYS:CE	1:A:191:TYR:OH	2.64	0.41
1:B:80:PRO:HA	1:B:180:ASP:OD1	2.21	0.41
1:A:256:THR:HG23	1:A:257:LYS:HZ2	1.86	0.41
1:A:249:MSE:HE3	1:A:264:ASP:C	2.41	0.41
1:A:52:ASN:ND2	1:A:52:ASN:O	2.54	0.41
1:B:189:GLY:O	1:B:190:TRP:C	2.59	0.41
1:A:101:GLU:HA	1:A:101:GLU:OE2	2.21	0.40
1:A:140:LEU:H	1:A:142:GLU:H	1.69	0.40
1:A:250:GLU:OE1	1:A:263:HIS:ND1	2.44	0.40
1:A:60:HIS:CE1	1:A:69:ASP:HB2	2.55	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	339/362 (94%)	296 (87%)	31 (9%)	12 (4%)	4 5
1	B	346/362 (96%)	330 (95%)	12 (4%)	4 (1%)	16 27
All	All	685/724 (95%)	626 (91%)	43 (6%)	16 (2%)	8 11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	265	PHE
1	A	281	LYS
1	A	283	TRP
1	A	315	ALA
1	A	317	LEU
1	B	28	ALA
1	A	282	ALA
1	B	246	ASN
1	B	128	GLY
1	B	190	TRP
1	A	42	GLU
1	A	136	ARG
1	A	198	LEU
1	A	25	ILE
1	A	267	ILE

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	286/293 (98%)	258 (90%)	28 (10%)	10	17
1	B	290/293 (99%)	262 (90%)	28 (10%)	10	18
All	All	576/586 (98%)	520 (90%)	56 (10%)	10	18

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	33	ILE
1	A	36	VAL
1	A	42	GLU
1	A	52	ASN
1	A	55	GLU
1	A	58	LYS
1	A	71	GLU
1	A	99	LEU
1	A	102	LYS
1	A	130	MSE
1	A	139	LEU
1	A	148	GLU
1	A	158	SER
1	A	170	LYS
1	A	172	ASP
1	A	196	THR
1	A	229	LEU
1	A	256	THR
1	A	265	PHE
1	A	278	THR
1	A	279	SER
1	A	281	LYS
1	A	283	TRP
1	A	301	LYS
1	A	317	LEU
1	A	339	THR
1	A	352	LYS
1	B	26	HIS
1	B	29	PRO
1	B	49	THR
1	B	55	GLU
1	B	99	LEU
1	B	101	GLU
1	B	102	LYS

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Mol	Chain	Res	Type
1	B	130	MSE
1	B	149	ARG
1	B	157	GLN
1	B	180	ASP
1	B	204	LEU
1	B	216	LEU
1	B	229	LEU
1	B	262	VAL
1	B	271	GLU
1	B	272	THR
1	B	275	SER
1	B	278	THR
1	B	287	LEU
1	B	292	VAL
1	B	293	SER
1	B	299	THR
1	B	301	LYS
1	B	311	VAL
1	B	312	ARG
1	B	321	ILE
1	B	339	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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	337/362 (93%)	0.33	23 (6%)	20	22	13, 33, 53, 81	0
1	B	344/362 (95%)	0.17	14 (4%)	41	45	14, 31, 46, 54	0
All	All	681/724 (94%)	0.25	37 (5%)	29	33	13, 32, 51, 81	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	PRO	4.0
1	A	56	SER	3.8
1	A	57	THR	3.3
1	A	55	GLU	3.3
1	A	317	LEU	3.2
1	B	40	SER	3.2
1	A	46	ALA	3.1
1	A	49	THR	3.0
1	A	58	LYS	3.0
1	A	318	VAL	2.9
1	B	232	GLU	2.9
1	A	192	ALA	2.9
1	A	316	ARG	2.9
1	B	56	SER	2.8
1	A	195	ALA	2.7
1	B	192	ALA	2.6
1	B	158	SER	2.5
1	A	158	SER	2.5
1	A	45	LYS	2.5
1	A	233	ASP	2.4
1	B	272	THR	2.4
1	B	45	LYS	2.4
1	A	147	SER	2.4
1	A	109	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.3
1	B	167	ASP	2.3
1	B	159	CYS	2.2
1	A	157	GLN	2.2
1	A	232	GLU	2.1
1	B	273	GLU	2.1
1	A	159	CYS	2.1
1	A	76	TYR	2.1
1	B	76	TYR	2.1
1	A	239	ILE	2.1
1	B	251	ILE	2.0
1	B	70	PRO	2.0
1	B	195	ALA	2.0

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.