Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:04 PM GMT

PDB ID	:	1RZV
Title	:	Crystal structure of the glycogen synthase from Agrobacterium tumefaciens (non-complexed form)
Authors	:	Buschiazzo, A.; Guerin, M.E.; Ugalde, J.E.; Ugalde, R.A.; Shepard, W.; Alzari, P.M.
Deposited on	:	2003-12-29
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
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:

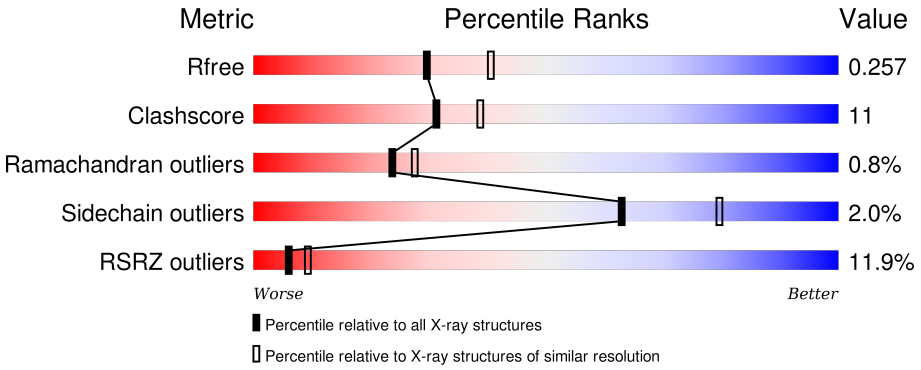
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	485	9% 78% 19%
1	B	485	14% 77% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7651 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 Glycogen synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	Se	0	0	0
			3622	2314	624	669	5	10			
1	B	477	Total	C	N	O	S	Se	0	0	0
			3622	2314	624	669	5	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	133	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	143	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	148	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	188	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	228	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	309	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	362	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	450	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	455	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
A	481	HIS	-	EXPRESSION TAG	UNP P0A3F3
A	482	HIS	-	EXPRESSION TAG	UNP P0A3F3
A	483	HIS	-	EXPRESSION TAG	UNP P0A3F3
A	484	HIS	-	EXPRESSION TAG	UNP P0A3F3
A	485	HIS	-	EXPRESSION TAG	UNP P0A3F3
B	1	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	133	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	143	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	148	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	188	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	228	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	309	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	362	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	450	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3
B	455	MSE	MET	MODIFIED RESIDUE	UNP P0A3F3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	HIS	-	EXPRESSION TAG	UNP P0A3F3
B	482	HIS	-	EXPRESSION TAG	UNP P0A3F3
B	483	HIS	-	EXPRESSION TAG	UNP P0A3F3
B	484	HIS	-	EXPRESSION TAG	UNP P0A3F3
B	485	HIS	-	EXPRESSION TAG	UNP P0A3F3

- Molecule 2 is water.

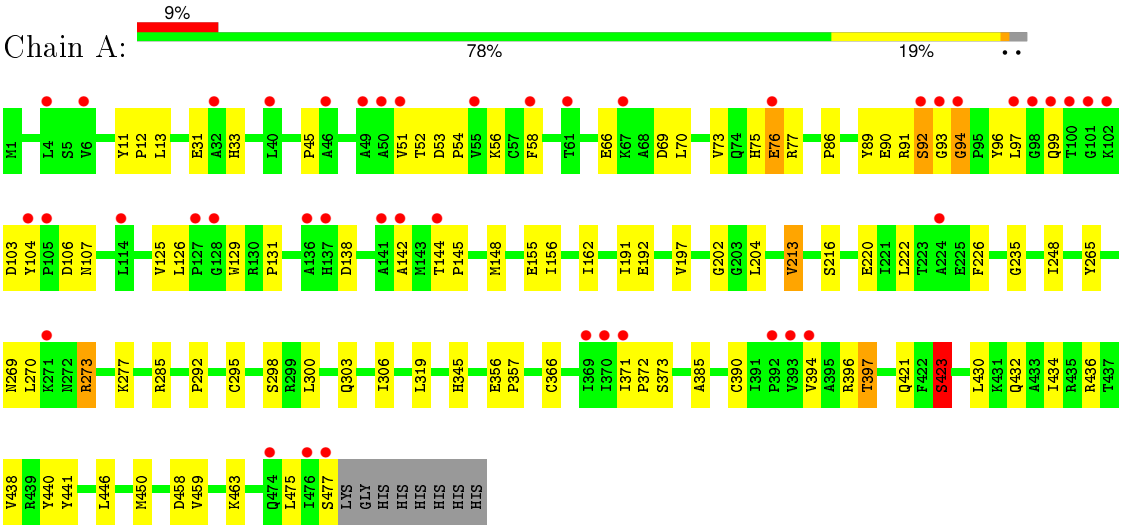
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	245	Total O 245 245	0	0
2	B	162	Total O 162 162	0	0

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.

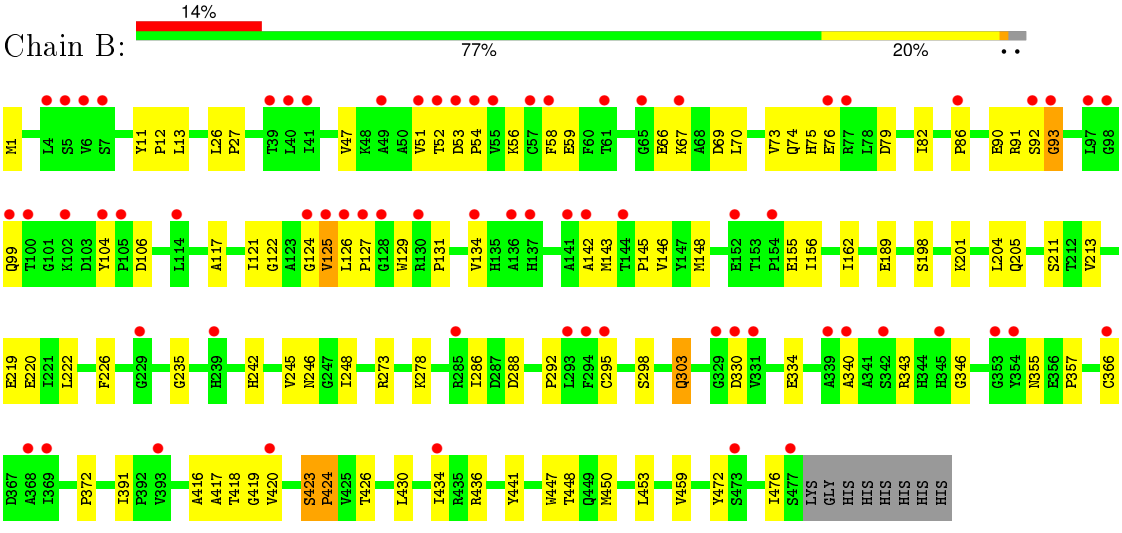
- Molecule 1: Glycogen synthase 1

Chain A:



- Molecule 1: Glycogen synthase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.27Å 87.29Å 88.49Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	29.97 – 2.30 29.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.97-2.30) 98.1 (29.97-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.240 0.221 , 0.257	Depositor DCC
R_{free} test set	2255 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 88890 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7651	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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, 0.375 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	0.45	0/3697	0.70	2/5018 (0.0%)
1	B	0.44	0/3697	0.72	5/5018 (0.1%)
All	All	0.44	0/7394	0.71	7/10036 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	423	SER	O-C-N	-10.07	101.96	121.10
1	B	423	SER	C-N-CD	-7.93	103.16	120.60
1	B	423	SER	CA-C-N	7.05	136.85	117.10
1	A	423	SER	C-N-CD	-6.28	106.80	120.60
1	A	213	VAL	N-CA-C	5.92	127.00	111.00
1	B	213	VAL	N-CA-C	5.09	124.73	111.00
1	B	424	PRO	CA-N-CD	-5.06	104.42	111.50

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	3622	0	3614	68	0
1	B	3622	0	3614	89	0
2	A	245	0	0	3	0
2	B	162	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7651	0	7228	156	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 11.

All (156) 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:148:MSE:HE1	1:A:156:ILE:HG12	1.30	1.07
1:B:54:PRO:HA	1:B:73:VAL:HG12	1.44	0.98
1:A:54:PRO:HA	1:A:73:VAL:CG1	1.96	0.95
1:A:54:PRO:HA	1:A:73:VAL:HG12	1.49	0.92
1:B:70:LEU:CD2	1:B:126:LEU:HD11	2.05	0.86
1:B:122:GLY:HA3	1:B:148:MSE:HE1	1.58	0.85
1:B:1:MSE:CE	1:B:472:TYR:HB3	2.10	0.82
1:B:1:MSE:HE3	1:B:476:ILE:CD1	2.10	0.81
1:B:1:MSE:HE3	1:B:476:ILE:HD12	1.60	0.81
1:A:373:SER:O	1:A:397:THR:HG21	1.82	0.79
1:A:51:VAL:HG11	1:A:73:VAL:HG11	1.64	0.78
1:B:1:MSE:CE	1:B:476:ILE:HD12	2.14	0.76
1:B:292:PRO:HG3	1:B:441:TYR:CD2	2.21	0.76
1:A:75:HIS:O	1:A:76:GLU:C	2.25	0.74
1:B:1:MSE:HE2	1:B:472:TYR:HB3	1.69	0.74
1:B:70:LEU:HD23	1:B:126:LEU:HD11	1.72	0.72
1:B:142:ALA:O	1:B:145:PRO:HD2	1.91	0.71
1:B:122:GLY:HA3	1:B:148:MSE:CE	2.21	0.70
1:A:356:GLU:HB3	1:A:357:PRO:HD3	1.74	0.69
1:B:148:MSE:HG2	1:B:155:GLU:HB2	1.73	0.69
1:B:340:ALA:HA	1:B:343:ARG:NH1	2.08	0.69
1:B:58:PHE:HB2	1:B:126:LEU:HD21	1.76	0.68
1:B:1:MSE:HE1	1:B:472:TYR:HB3	1.77	0.65
1:B:51:VAL:CG1	1:B:73:VAL:HG21	2.27	0.65
1:B:54:PRO:HG3	1:B:73:VAL:HG11	1.80	0.64
1:B:476:ILE:O	1:B:476:ILE:HG22	1.99	0.63
1:B:54:PRO:HA	1:B:73:VAL:CG1	2.24	0.63
1:A:142:ALA:O	1:A:145:PRO:HD2	1.99	0.63
1:B:70:LEU:HD21	1:B:126:LEU:HD11	1.79	0.62
1:B:58:PHE:CZ	1:B:125:VAL:HG22	2.34	0.62
1:B:148:MSE:HG2	1:B:155:GLU:CB	2.29	0.62
1:A:148:MSE:HE1	1:A:156:ILE:H	1.66	0.61
1:B:476:ILE:O	1:B:476:ILE:CG2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TRP:CZ3	1:A:131:PRO:HG3	2.35	0.60
1:A:148:MSE:HE2	1:A:155:GLU:HA	1.84	0.60
1:A:58:PHE:CZ	1:A:125:VAL:HG22	2.38	0.59
1:B:129:TRP:CZ3	1:B:131:PRO:HG3	2.37	0.59
1:A:75:HIS:O	1:A:76:GLU:O	2.21	0.59
1:B:51:VAL:HG11	1:B:73:VAL:HG21	1.84	0.58
1:B:416:ALA:HA	1:B:453:LEU:HD21	1.85	0.58
1:A:396:ARG:HH11	1:A:423:SER:HB2	1.68	0.57
1:A:103:ASP:HB3	1:A:107:ASN:ND2	2.20	0.56
1:B:129:TRP:CH2	1:B:131:PRO:HG3	2.40	0.56
1:B:91:ARG:NH2	1:B:106:ASP:OD2	2.31	0.55
1:A:148:MSE:CE	1:A:156:ILE:H	2.19	0.55
1:B:124:GLY:O	1:B:126:LEU:N	2.40	0.55
1:A:51:VAL:HG12	1:A:52:THR:N	2.22	0.55
1:B:355:ASN:OD1	1:B:357:PRO:HG2	2.06	0.55
1:A:104:TYR:C	1:A:106:ASP:H	2.09	0.55
1:B:248:ILE:HG13	1:B:459:VAL:O	2.06	0.55
1:A:51:VAL:CG1	1:A:73:VAL:HG11	2.37	0.54
1:A:148:MSE:CE	1:A:156:ILE:HG12	2.20	0.54
1:B:86:PRO:HA	1:B:90:GLU:HB2	1.90	0.54
1:A:475:LEU:C	1:A:477:SER:H	2.10	0.54
1:B:430:LEU:O	1:B:434:ILE:HG13	2.08	0.53
1:A:53:ASP:N	1:A:54:PRO:HD3	2.23	0.53
1:A:56:LYS:HE2	1:A:69:ASP:OD1	2.07	0.53
1:B:92:SER:O	1:B:93:GLY:O	2.26	0.53
1:B:448:THR:HG22	2:B:607:HOH:O	2.09	0.53
1:B:104:TYR:C	1:B:106:ASP:H	2.11	0.53
1:B:13:LEU:HD21	1:B:75:HIS:CD2	2.45	0.52
1:A:162:ILE:HD11	1:A:204:LEU:HD21	1.90	0.52
1:A:432:GLN:NE2	1:B:219:GLU:OE1	2.43	0.52
1:B:189:GLU:H	1:B:189:GLU:CD	2.11	0.51
1:B:74:GLN:NE2	1:B:79:ASP:HA	2.25	0.51
1:A:446:LEU:HD23	1:A:446:LEU:C	2.31	0.51
1:B:198:SER:HB3	1:B:201:LYS:HB3	1.93	0.51
1:A:51:VAL:HG11	1:A:73:VAL:HG21	1.92	0.51
1:B:162:ILE:HD11	1:B:204:LEU:HD21	1.92	0.51
1:A:303:GLN:HG2	2:A:579:HOH:O	2.11	0.51
1:B:303:GLN:NE2	1:B:303:GLN:H	2.09	0.51
1:B:419:GLY:N	1:B:450:MSE:HE2	2.26	0.51
1:A:70:LEU:HD23	1:A:126:LEU:HD21	1.94	0.50
1:B:51:VAL:HG13	1:B:73:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:SER:HA	1:B:242:HIS:O	2.12	0.50
1:A:292:PRO:HG3	1:A:441:TYR:CD2	2.47	0.50
1:A:446:LEU:HD21	1:A:450:MSE:SE	2.63	0.49
1:A:220:GLU:HB3	1:A:226:PHE:CD2	2.47	0.49
1:B:419:GLY:N	1:B:450:MSE:CE	2.75	0.49
1:A:458:ASP:OD2	1:A:463:LYS:HD3	2.12	0.49
1:B:13:LEU:HD13	1:B:47:VAL:HG13	1.95	0.49
1:A:436:ARG:HD2	1:A:440:TYR:OH	2.13	0.49
1:B:56:LYS:HZ3	1:B:59:GLU:HB2	1.78	0.48
1:B:104:TYR:C	1:B:106:ASP:N	2.67	0.48
1:B:117:ALA:O	1:B:121:ILE:HG13	2.13	0.48
1:B:220:GLU:HB3	1:B:226:PHE:CD2	2.49	0.48
1:B:56:LYS:HE2	1:B:69:ASP:OD1	2.13	0.48
1:B:52:THR:HG23	1:B:53:ASP:OD1	2.14	0.48
1:B:124:GLY:C	1:B:126:LEU:H	2.17	0.48
1:A:129:TRP:CH2	1:A:131:PRO:HG3	2.48	0.48
1:B:51:VAL:HG11	1:B:73:VAL:HG11	1.96	0.47
1:B:424:PRO:HB2	1:B:426:THR:HG23	1.96	0.47
1:B:418:THR:C	1:B:450:MSE:HE2	2.34	0.47
1:B:417:ALA:HB1	1:B:450:MSE:HE3	1.96	0.47
1:A:104:TYR:C	1:A:106:ASP:N	2.68	0.47
1:B:245:VAL:HG12	1:B:246:ASN:O	2.14	0.47
1:B:11:TYR:CD1	1:B:12:PRO:HA	2.50	0.47
1:A:191:ILE:HD12	1:A:197:VAL:HG13	1.95	0.47
1:A:222:LEU:HD22	1:A:235:GLY:HA2	1.96	0.47
1:B:1:MSE:HE1	1:B:476:ILE:HD12	1.94	0.47
1:B:75:HIS:O	1:B:76:GLU:C	2.48	0.47
1:A:191:ILE:HG22	1:A:202:GLY:HA3	1.95	0.47
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.79	0.46
1:A:11:TYR:CD1	1:A:12:PRO:HA	2.51	0.46
1:B:134:VAL:HG23	1:B:156:ILE:HD11	1.95	0.46
1:B:420:VAL:HG13	1:B:436:ARG:NH2	2.31	0.46
1:B:56:LYS:NZ	1:B:59:GLU:HB2	2.31	0.46
1:A:86:PRO:HA	1:A:90:GLU:HB2	1.97	0.46
1:B:58:PHE:CB	1:B:126:LEU:HD21	2.44	0.46
1:B:222:LEU:HD22	1:B:235:GLY:HA2	1.97	0.46
1:A:76:GLU:OE1	1:A:76:GLU:HA	2.15	0.46
1:A:300:LEU:HA	1:A:306:ILE:HG13	1.97	0.46
1:B:126:LEU:HB2	2:B:606:HOH:O	2.15	0.45
1:A:51:VAL:CG1	1:A:73:VAL:HG21	2.46	0.45
1:A:91:ARG:NH2	1:A:106:ASP:OD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:VAL:O	1:A:421:GLN:HA	2.16	0.45
1:B:125:VAL:O	1:B:127:PRO:HD3	2.16	0.45
1:A:96:TYR:O	1:A:103:ASP:HA	2.16	0.45
1:A:92:SER:OG	1:A:99:GLN:NE2	2.50	0.45
1:B:26:LEU:N	1:B:27:PRO:CD	2.79	0.45
1:B:340:ALA:HA	1:B:343:ARG:CZ	2.47	0.44
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.17	0.44
1:A:265:TYR:CZ	1:A:273:ARG:HG2	2.52	0.44
1:A:345:HIS:CD2	2:A:688:HOH:O	2.70	0.44
1:B:278:LYS:HG3	1:B:288:ASP:OD1	2.18	0.44
1:A:51:VAL:CG1	1:A:52:THR:N	2.80	0.43
1:B:286:ILE:HB	1:B:346:GLY:O	2.18	0.43
1:B:201:LYS:C	1:B:201:LYS:HD3	2.38	0.43
1:B:92:SER:OG	1:B:99:GLN:HG3	2.18	0.43
1:A:93:GLY:O	1:A:94:GLY:O	2.37	0.43
1:B:53:ASP:N	1:B:54:PRO:HD3	2.34	0.43
1:A:31:GLU:C	1:A:33:HIS:H	2.22	0.43
1:A:319:LEU:HD13	1:A:438:VAL:HG21	2.01	0.43
1:B:51:VAL:HG21	1:B:82:ILE:HD11	1.99	0.43
1:A:45:PRO:HD3	1:A:89:TYR:O	2.19	0.43
1:B:124:GLY:C	1:B:126:LEU:N	2.72	0.42
1:A:295:CYS:HB3	1:A:366:CYS:SG	2.59	0.42
1:A:66:GLU:OE1	1:A:66:GLU:HA	2.19	0.42
1:A:277:LYS:HG2	2:A:514:HOH:O	2.19	0.41
1:A:371:ILE:HB	1:A:394:VAL:HG12	2.01	0.41
1:A:248:ILE:HG13	1:A:459:VAL:O	2.21	0.41
1:B:273:ARG:NH2	2:B:488:HOH:O	2.53	0.41
1:A:13:LEU:HD21	1:A:75:HIS:CE1	2.56	0.41
1:B:92:SER:O	1:B:93:GLY:C	2.59	0.41
1:B:143:MSE:O	1:B:146:VAL:HB	2.20	0.41
1:B:330:ASP:O	1:B:334:GLU:HG3	2.21	0.41
1:A:385:ALA:HB1	1:A:390:CYS:O	2.21	0.41
1:A:216:SER:O	1:A:220:GLU:HG3	2.19	0.41
1:A:475:LEU:C	1:A:477:SER:N	2.74	0.41
1:A:430:LEU:O	1:A:434:ILE:HG13	2.20	0.41
1:A:144:THR:HB	1:A:145:PRO:HD3	2.02	0.41
1:A:265:TYR:CE2	1:A:273:ARG:HG2	2.56	0.41
1:B:391:ILE:HG13	1:B:447:TRP:CZ2	2.56	0.41
1:A:13:LEU:HD21	1:A:75:HIS:ND1	2.36	0.40
1:B:295:CYS:HB3	1:B:366:CYS:SG	2.61	0.40
1:B:189:GLU:HA	1:B:205:GLN:NE2	2.36	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	475/485 (98%)	449 (94%)	20 (4%)	6 (1%)	15 15
1	B	475/485 (98%)	453 (95%)	20 (4%)	2 (0%)	39 48
All	All	950/970 (98%)	902 (95%)	40 (4%)	8 (1%)	24 27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	92	SER
1	A	94	GLY
1	B	93	GLY
1	A	270	LEU
1	B	125	VAL
1	A	138	ASP
1	A	213	VAL

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	372/369 (101%)	362 (97%)	10 (3%)	52 70
1	B	372/369 (101%)	367 (99%)	5 (1%)	76 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	744/738 (101%)	729 (98%)	15 (2%)	63 79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	97	LEU
1	A	192	GLU
1	A	269	ASN
1	A	273	ARG
1	A	285	ARG
1	A	298	SER
1	A	372	PRO
1	A	397	THR
1	A	423	SER
1	B	67	LYS
1	B	298	SER
1	B	303	GLN
1	B	372	PRO
1	B	423	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	432	GLN
1	A	449	GLN
1	B	74	GLN
1	B	99	GLN
1	B	195	ASN
1	B	205	GLN
1	B	283	HIS
1	B	303	GLN

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

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	467/485 (96%)	0.60	43 (9%) 11 16	15, 25, 51, 74	0
1	B	467/485 (96%)	0.86	68 (14%) 3 5	17, 31, 54, 67	0
All	All	934/970 (96%)	0.73	111 (11%) 6 9	15, 28, 53, 74	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	LEU	5.4
1	B	99	GLN	5.1
1	A	100	THR	5.0
1	A	128	GLY	5.0
1	A	98	GLY	5.0
1	B	128	GLY	5.0
1	A	92	SER	4.9
1	A	6	VAL	4.7
1	B	152	GLU	4.6
1	B	345	HIS	4.4
1	B	6	VAL	4.3
1	A	55	VAL	4.1
1	A	93	GLY	4.0
1	A	136	ALA	3.9
1	B	477	SER	3.9
1	B	76	GLU	3.8
1	B	86	PRO	3.7
1	B	136	ALA	3.7
1	A	99	GLN	3.5
1	B	354	TYR	3.5
1	B	49	ALA	3.5
1	B	57	CYS	3.5
1	B	51	VAL	3.4
1	A	102	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	40	LEU	3.4
1	A	105	PRO	3.4
1	B	141	ALA	3.3
1	B	342	SER	3.3
1	B	125	VAL	3.3
1	B	52	THR	3.3
1	A	271	LYS	3.2
1	A	94	GLY	3.2
1	B	67	LYS	3.2
1	B	98	GLY	3.1
1	A	40	LEU	3.1
1	B	104	TYR	3.1
1	B	393	VAL	3.1
1	B	368	ALA	3.0
1	A	141	ALA	3.0
1	B	295	CYS	3.0
1	A	67	LYS	3.0
1	A	114	LEU	3.0
1	B	102	LYS	3.0
1	B	134	VAL	2.9
1	B	5	SER	2.9
1	B	100	THR	2.9
1	B	92	SER	2.9
1	B	55	VAL	2.9
1	B	130	ARG	2.8
1	A	144	THR	2.8
1	A	61	THR	2.8
1	B	339	ALA	2.8
1	A	97	LEU	2.8
1	A	51	VAL	2.7
1	B	124	GLY	2.7
1	A	49	ALA	2.7
1	B	114	LEU	2.7
1	B	366	CYS	2.7
1	B	330	ASP	2.6
1	B	340	ALA	2.6
1	A	477	SER	2.6
1	B	7	SER	2.6
1	B	53	ASP	2.6
1	B	239	HIS	2.6
1	A	369	ILE	2.6
1	B	93	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	2.6
1	B	142	ALA	2.5
1	B	58	PHE	2.5
1	A	4	LEU	2.5
1	B	285	ARG	2.5
1	B	473	SER	2.5
1	B	294	PHE	2.5
1	A	474	GLN	2.5
1	A	101	GLY	2.5
1	B	105	PRO	2.5
1	A	76	GLU	2.5
1	A	127	PRO	2.4
1	B	54	PRO	2.4
1	A	104	TYR	2.4
1	A	371	ILE	2.4
1	B	61	THR	2.4
1	B	420	VAL	2.4
1	A	392	PRO	2.4
1	B	4	LEU	2.4
1	B	144	THR	2.4
1	B	293	LEU	2.3
1	B	329	GLY	2.3
1	B	97	LEU	2.3
1	B	331	VAL	2.2
1	A	142	ALA	2.2
1	A	370	ILE	2.2
1	A	393	VAL	2.2
1	B	434	ILE	2.2
1	B	137	HIS	2.1
1	B	77	ARG	2.1
1	B	369	ILE	2.1
1	B	127	PRO	2.1
1	B	353	GLY	2.1
1	A	32	ALA	2.1
1	A	58	PHE	2.1
1	A	224	ALA	2.1
1	B	41	ILE	2.1
1	B	154	PRO	2.1
1	B	65	GLY	2.0
1	B	229	GLY	2.0
1	B	39	THR	2.0
1	A	137	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	394	VAL	2.0
1	A	46	ALA	2.0
1	A	50	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.