Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:08 AM GMT

PDB ID	:	2W29
Title	:	GLY102THR MUTANT OF RV3291C
Authors	:	Shrivastava, T.; Dey, S.; Ravishankar, R.
Deposited on	:	2008-10-25
Resolution	:	4.10 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:

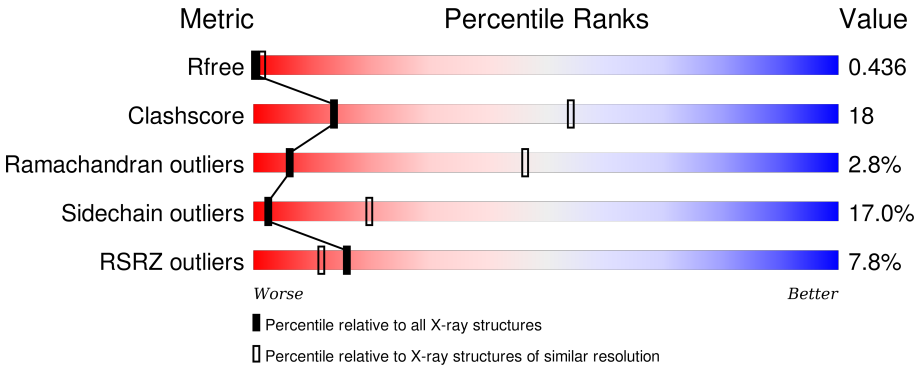
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.10 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	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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	150	7% 67% 23% 5%
1	B	150	9% 62% 25% 9%
1	C	150	7% 63% 27% 5%
1	D	150	9% 59% 30% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4488 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 PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1130	699	209	221	1			
1	B	147	Total	C	N	O	S	0	0	0
			1114	691	203	219	1			
1	C	147	Total	C	N	O	S	0	0	0
			1130	699	209	221	1			
1	D	147	Total	C	N	O	S	0	0	0
			1114	691	203	219	1			

There are 4 discrepancies between the modelled and reference sequences:

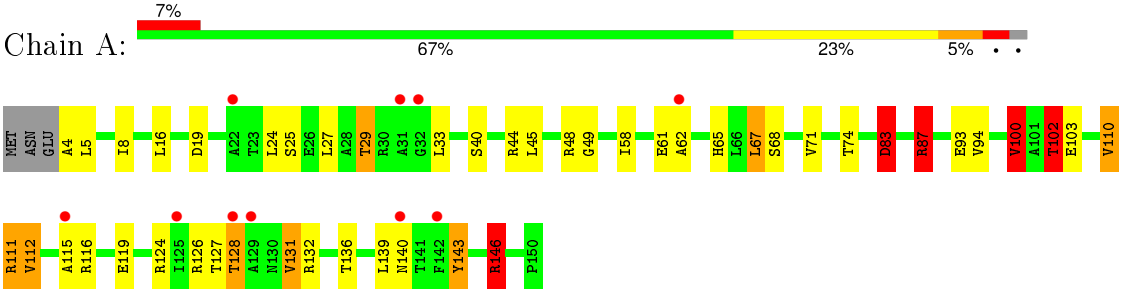
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	THR	GLY	ENGINEERED MUTATION	UNP P96896
B	102	THR	GLY	ENGINEERED MUTATION	UNP P96896
C	102	THR	GLY	ENGINEERED MUTATION	UNP P96896
D	102	THR	GLY	ENGINEERED MUTATION	UNP P96896

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.

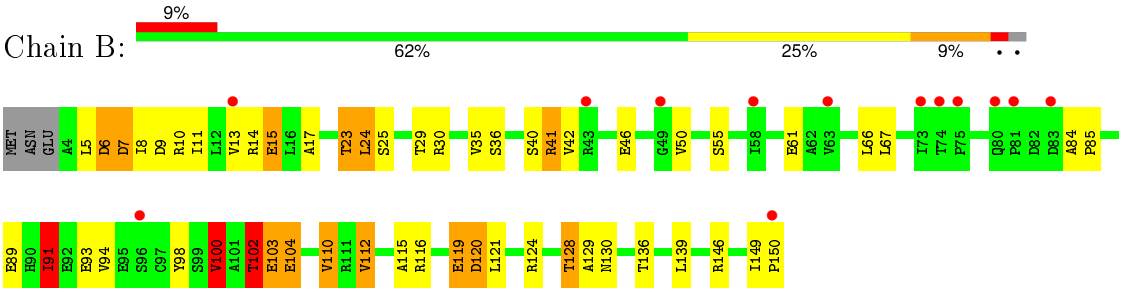
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN

Chain A:



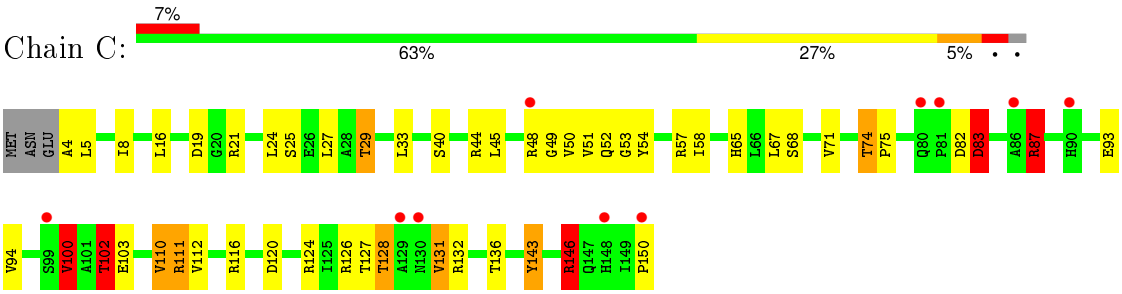
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN

Chain B:



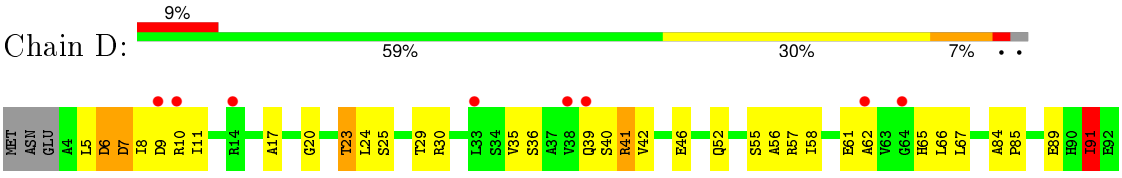
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN

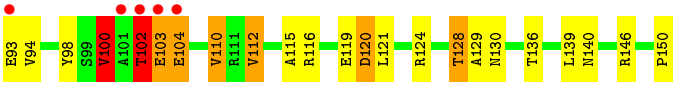
Chain C:



• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN

Chain D:




E93
V94
Y98
S99
V100
A101
T102
E103
E104
V110
R111
V112
A115
R116
E119
D120
L121
R124
T128
A129
N130
T136
L139
N140
R146
P150

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	83.00Å 185.70Å 119.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 34.10 – 3.97	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-4.10) 87.4 (34.10-3.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.388 , (Not available) 0.450 , 0.436	Depositor DCC
R_{free} test set	333 reflections (4.70%)	DCC
Wilson B-factor (Å^2)	110.1	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 7.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 7243 reflections	Xtriage
F_o,F_c correlation	0.64	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	1.32	4/1144 (0.3%)	1.58	13/1557 (0.8%)
1	B	1.20	3/1128 (0.3%)	1.33	11/1538 (0.7%)
1	C	1.31	2/1144 (0.2%)	1.36	15/1557 (1.0%)
1	D	1.20	3/1128 (0.3%)	1.33	11/1538 (0.7%)
All	All	1.26	12/4544 (0.3%)	1.40	50/6190 (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	0	2
1	C	0	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	THR	CA-CB	13.63	1.88	1.53
1	D	102	THR	CA-CB	13.04	1.87	1.53
1	B	102	THR	CA-CB	12.98	1.87	1.53
1	C	102	THR	CA-CB	12.59	1.86	1.53
1	A	132	ARG	CG-CD	6.33	1.67	1.51
1	C	132	ARG	CG-CD	6.33	1.67	1.51
1	D	98	TYR	CG-CD1	5.89	1.46	1.39
1	B	98	TYR	CG-CD1	5.86	1.46	1.39
1	B	55	SER	CA-CB	5.59	1.61	1.52
1	D	55	SER	CA-CB	5.53	1.61	1.52
1	A	143	TYR	CD2-CE2	5.03	1.46	1.39
1	A	112	VAL	CB-CG2	-5.02	1.42	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	THR	CA-CB-CG2	-28.37	72.69	112.40
1	A	102	THR	CA-CB-OG1	19.34	149.61	109.00
1	D	102	THR	N-CA-CB	-11.72	88.03	110.30
1	B	102	THR	N-CA-CB	-11.69	88.08	110.30
1	B	102	THR	CB-CA-C	-11.47	80.62	111.60
1	D	102	THR	CB-CA-C	-11.47	80.63	111.60
1	C	102	THR	CB-CA-C	-11.38	80.88	111.60
1	C	102	THR	N-CA-CB	-11.17	89.07	110.30
1	A	102	THR	N-CA-CB	9.64	128.62	110.30
1	B	129	ALA	C-N-CA	-8.34	100.85	121.70
1	D	129	ALA	C-N-CA	-8.30	100.95	121.70
1	A	126	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	C	126	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	C	100	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	A	100	VAL	CG1-CB-CG2	7.39	122.73	110.90
1	A	126	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	C	126	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	131	VAL	CG1-CB-CG2	6.59	121.44	110.90
1	C	131	VAL	CG1-CB-CG2	6.55	121.38	110.90
1	C	110	VAL	CG1-CB-CG2	6.50	121.30	110.90
1	A	110	VAL	CG1-CB-CG2	6.49	121.28	110.90
1	D	91	ILE	CB-CA-C	6.46	124.53	111.60
1	B	91	ILE	CB-CA-C	6.40	124.41	111.60
1	D	100	VAL	CG1-CB-CG2	6.37	121.10	110.90
1	B	100	VAL	CG1-CB-CG2	6.32	121.01	110.90
1	C	83	ASP	N-CA-CB	-6.29	99.28	110.60
1	A	83	ASP	N-CA-CB	-6.24	99.37	110.60
1	D	130	ASN	CB-CA-C	5.76	121.92	110.40
1	D	112	VAL	CG1-CB-CG2	5.73	120.07	110.90
1	B	110	VAL	CG1-CB-CG2	5.72	120.06	110.90
1	D	110	VAL	CG1-CB-CG2	5.72	120.05	110.90
1	B	130	ASN	CB-CA-C	5.71	121.82	110.40
1	B	112	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	C	146	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	19	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	87	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	19	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	146	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	129	ALA	O-C-N	-5.31	114.21	122.70
1	A	87	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	129	ALA	O-C-N	-5.30	114.22	122.70
1	B	146	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	146	ARG	NE-CZ-NH2	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ARG	CB-CA-C	5.14	120.69	110.40
1	B	120	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	120	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	146	ARG	CB-CA-C	5.10	120.61	110.40
1	C	120	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	C	82	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	C	116	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	GLY	Peptide
1	A	83	ASP	Peptide
1	C	49	GLY	Peptide
1	C	83	ASP	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	1130	0	1134	33	31
1	B	1114	0	1108	71	0
1	C	1130	0	1133	51	0
1	D	1114	0	1108	83	7
All	All	4488	0	4483	166	38

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 18.

All (166) 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:102:THR:CA	1:B:102:THR:CB	1.87	1.53
1:D:102:THR:CA	1:D:102:THR:CB	1.87	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:CB	1:A:102:THR:CA	1.88	1.48
1:C:102:THR:CA	1:C:102:THR:CB	1.86	1.47
1:A:102:THR:CG2	1:A:102:THR:CA	2.04	1.33
1:A:136:THR:CG2	1:B:102:THR:HG23	1.61	1.28
1:C:136:THR:CG2	1:D:102:THR:HG23	1.68	1.22
1:C:136:THR:HG23	1:D:102:THR:HG23	1.26	1.17
1:B:14:ARG:HD3	1:B:149:ILE:HB	1.29	1.13
1:B:139:LEU:HD13	1:D:119:GLU:HB2	1.32	1.10
1:A:102:THR:CG2	1:A:102:THR:HA	1.82	1.10
1:B:102:THR:HB	1:B:103:GLU:N	1.67	1.09
1:D:102:THR:C	1:D:102:THR:CB	2.20	1.09
1:D:102:THR:HB	1:D:103:GLU:N	1.67	1.09
1:C:102:THR:HB	1:C:103:GLU:N	1.68	1.09
1:B:102:THR:C	1:B:102:THR:CB	2.20	1.09
1:B:139:LEU:HD22	1:D:115:ALA:O	1.51	1.08
1:C:102:THR:C	1:C:102:THR:CB	2.20	1.08
1:A:136:THR:HG23	1:B:102:THR:HG23	1.03	1.00
1:A:102:THR:HG23	1:A:102:THR:HA	1.40	0.99
1:B:139:LEU:CD1	1:D:119:GLU:HB2	1.97	0.94
1:C:102:THR:CB	1:C:103:GLU:N	2.31	0.93
1:A:136:THR:CG2	1:B:102:THR:CG2	2.46	0.93
1:C:136:THR:CG2	1:D:102:THR:CG2	2.50	0.90
1:D:102:THR:CB	1:D:102:THR:N	2.35	0.89
1:B:102:THR:N	1:B:102:THR:CB	2.35	0.89
1:C:136:THR:HG21	1:D:102:THR:HG23	1.53	0.89
1:B:100:VAL:HG13	1:B:102:THR:OG1	1.75	0.87
1:A:102:THR:CA	1:A:102:THR:HG22	2.02	0.86
1:A:136:THR:HG23	1:B:102:THR:CG2	1.98	0.86
1:C:136:THR:HG21	1:D:102:THR:CG2	2.08	0.82
1:B:139:LEU:O	1:D:116:ARG:HB3	1.80	0.82
1:B:66:LEU:CD1	1:D:66:LEU:CD1	2.56	0.82
1:D:100:VAL:HG13	1:D:102:THR:OG1	1.79	0.81
1:B:102:THR:CB	1:B:103:GLU:N	2.38	0.81
1:D:124:ARG:O	1:D:128:THR:HG23	1.82	0.80
1:B:66:LEU:HD12	1:D:66:LEU:HD13	1.64	0.80
1:B:14:ARG:CZ	1:B:149:ILE:O	2.29	0.79
1:C:136:THR:HG23	1:D:102:THR:CG2	2.11	0.79
1:B:66:LEU:HD13	1:D:66:LEU:CD1	2.12	0.78
1:A:136:THR:HG21	1:B:102:THR:HG23	1.60	0.78
1:B:124:ARG:O	1:B:128:THR:HG23	1.82	0.78
1:D:102:THR:CB	1:D:103:GLU:N	2.39	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:HB	1:C:103:GLU:H	1.45	0.76
1:B:66:LEU:HD13	1:D:66:LEU:HD12	1.66	0.76
1:B:139:LEU:HD13	1:D:119:GLU:CB	2.13	0.76
1:A:136:THR:HG21	1:B:102:THR:CG2	2.14	0.76
1:C:146:ARG:HH21	1:D:89:GLU:HG2	1.50	0.76
1:C:102:THR:C	1:C:102:THR:HB	1.95	0.74
1:C:124:ARG:O	1:C:128:THR:HG23	1.88	0.73
1:D:42:VAL:O	1:D:46:GLU:HG3	1.89	0.73
1:A:124:ARG:O	1:A:128:THR:HG23	1.88	0.73
1:B:42:VAL:O	1:B:46:GLU:HG3	1.89	0.73
1:B:139:LEU:HD23	1:D:115:ALA:HB1	1.71	0.73
1:B:14:ARG:HD3	1:B:149:ILE:CB	2.13	0.72
1:B:124:ARG:O	1:B:128:THR:CG2	2.38	0.71
1:C:146:ARG:NH2	1:D:89:GLU:O	2.21	0.71
1:B:102:THR:HB	1:B:103:GLU:H	1.56	0.71
1:C:51:VAL:HG22	1:D:58:ILE:CD1	2.22	0.70
1:D:124:ARG:O	1:D:128:THR:CG2	2.38	0.70
1:D:102:THR:HB	1:D:103:GLU:H	1.54	0.69
1:B:66:LEU:CD1	1:D:66:LEU:HD13	2.22	0.68
1:B:116:ARG:HD2	1:D:140:ASN:CG	2.15	0.66
1:B:100:VAL:CG1	1:B:102:THR:OG1	2.45	0.65
1:B:139:LEU:CD2	1:D:115:ALA:O	2.36	0.64
1:C:50:VAL:HG22	1:D:62:ALA:HB1	1.80	0.63
1:B:139:LEU:O	1:D:116:ARG:CB	2.47	0.63
1:C:146:ARG:NH2	1:D:89:GLU:HG2	2.14	0.62
1:A:102:THR:CB	1:A:103:GLU:N	2.62	0.62
1:D:100:VAL:CG1	1:D:102:THR:OG1	2.48	0.62
1:A:102:THR:C	1:A:102:THR:CB	2.66	0.62
1:D:91:ILE:HD11	1:D:93:GLU:HG2	1.82	0.62
1:C:102:THR:CB	1:C:103:GLU:H	2.04	0.61
1:B:91:ILE:HD11	1:B:93:GLU:HG2	1.82	0.61
1:A:102:THR:HG23	1:A:102:THR:CA	2.02	0.61
1:B:116:ARG:HA	1:D:139:LEU:O	2.01	0.60
1:A:146:ARG:NH2	1:B:89:GLU:O	2.34	0.60
1:D:7:ASP:HA	1:D:10:ARG:HB2	1.85	0.59
1:C:54:TYR:CE2	1:D:56:ALA:HB2	2.38	0.58
1:B:15:GLU:OE2	1:B:15:GLU:HA	2.02	0.58
1:C:51:VAL:HG22	1:D:58:ILE:HD13	1.84	0.58
1:B:116:ARG:CA	1:D:139:LEU:O	2.51	0.58
1:C:16:LEU:HD21	1:C:27:LEU:HD11	1.85	0.57
1:A:16:LEU:HD21	1:A:27:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASP:O	1:B:9:ASP:HB2	2.06	0.56
1:D:102:THR:HB	1:D:102:THR:C	2.01	0.56
1:C:54:TYR:CD2	1:D:56:ALA:HB2	2.40	0.56
1:B:7:ASP:HA	1:B:10:ARG:HB2	1.85	0.56
1:D:102:THR:OG1	1:D:102:THR:N	2.39	0.56
1:B:102:THR:N	1:B:102:THR:OG1	2.38	0.55
1:D:6:ASP:O	1:D:9:ASP:HB2	2.05	0.55
1:C:100:VAL:HG22	1:D:136:THR:HG22	1.88	0.55
1:B:116:ARG:HD2	1:D:140:ASN:OD1	2.07	0.55
1:A:146:ARG:HH21	1:B:89:GLU:HG2	1.71	0.55
1:C:124:ARG:O	1:C:128:THR:CG2	2.54	0.54
1:C:150:PRO:HG3	1:D:65:HIS:CE1	2.42	0.54
1:A:102:THR:C	1:A:102:THR:HG22	2.28	0.54
1:B:67:LEU:HD11	1:D:67:LEU:HD21	1.89	0.54
1:A:124:ARG:O	1:A:128:THR:CG2	2.54	0.54
1:C:68:SER:OG	1:C:111:ARG:HD3	2.08	0.54
1:C:146:ARG:HH21	1:D:89:GLU:CG	2.20	0.53
1:C:83:ASP:HB3	1:C:87:ARG:HD2	1.91	0.53
1:B:115:ALA:HB2	1:D:67:LEU:HD23	1.90	0.53
1:C:102:THR:CA	1:C:102:THR:CG2	2.82	0.53
1:B:139:LEU:HA	1:D:115:ALA:HB1	1.90	0.53
1:A:68:SER:OG	1:A:111:ARG:HD3	2.08	0.53
1:C:146:ARG:HH22	1:D:89:GLU:C	2.12	0.53
1:A:83:ASP:HB3	1:A:87:ARG:HD2	1.90	0.53
1:A:102:THR:CB	1:A:103:GLU:H	2.21	0.52
1:B:8:ILE:HB	1:B:41:ARG:NH2	2.24	0.52
1:A:4:ALA:O	1:A:48:ARG:NH2	2.43	0.52
1:C:65:HIS:CE1	1:D:150:PRO:HG3	2.44	0.52
1:B:91:ILE:HD12	1:B:91:ILE:C	2.31	0.51
1:D:8:ILE:HB	1:D:41:ARG:NH2	2.24	0.51
1:C:4:ALA:O	1:C:48:ARG:NH2	2.43	0.51
1:D:91:ILE:HD12	1:D:91:ILE:C	2.31	0.51
1:C:52:GLN:N	1:D:57:ARG:O	2.31	0.51
1:B:102:THR:C	1:B:102:THR:HB	2.00	0.51
1:A:100:VAL:HG22	1:B:136:THR:HG22	1.93	0.50
1:A:146:ARG:NH2	1:B:89:GLU:HG2	2.26	0.50
1:A:65:HIS:CE1	1:B:150:PRO:HG3	2.46	0.50
1:C:54:TYR:HA	1:D:56:ALA:HA	1.94	0.50
1:B:115:ALA:HB2	1:D:67:LEU:CD2	2.42	0.49
1:C:146:ARG:NH2	1:D:89:GLU:CG	2.75	0.49
1:B:116:ARG:HB2	1:D:139:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HA	1:D:115:ALA:CB	2.43	0.48
1:C:100:VAL:HG13	1:C:102:THR:OG1	2.13	0.48
1:A:62:ALA:HB1	1:B:50:VAL:HG22	1.95	0.48
1:C:8:ILE:HG21	1:C:33:LEU:HD11	1.96	0.48
1:A:102:THR:CG2	1:A:102:THR:C	2.81	0.47
1:C:21:ARG:NH1	1:D:20:GLY:O	2.47	0.47
1:C:57:ARG:O	1:D:52:GLN:HG3	2.15	0.47
1:C:58:ILE:HD12	1:D:17:ALA:HB2	1.97	0.47
1:B:119:GLU:HB2	1:D:139:LEU:HD13	1.97	0.47
1:C:54:TYR:CD2	1:D:56:ALA:CB	2.99	0.46
1:B:102:THR:HB	1:B:104:GLU:H	1.81	0.45
1:A:8:ILE:HG21	1:A:33:LEU:HD11	1.96	0.45
1:A:58:ILE:HD13	1:B:13:VAL:HB	1.98	0.45
1:B:119:GLU:HB2	1:D:139:LEU:CD1	2.47	0.45
1:C:50:VAL:HG22	1:D:62:ALA:CB	2.47	0.45
1:C:53:GLY:O	1:D:57:ARG:N	2.34	0.45
1:B:102:THR:CG2	1:B:102:THR:CA	2.84	0.45
1:D:8:ILE:HB	1:D:41:ARG:HH21	1.83	0.44
1:A:58:ILE:HD12	1:B:17:ALA:HB2	1.98	0.44
1:C:74:THR:HA	1:C:75:PRO:HD3	1.91	0.44
1:D:102:THR:HB	1:D:104:GLU:H	1.83	0.43
1:D:102:THR:CG2	1:D:102:THR:CA	2.84	0.43
1:C:146:ARG:NH2	1:D:89:GLU:HA	2.34	0.43
1:D:23:THR:O	1:D:24:LEU:C	2.57	0.43
1:B:91:ILE:HD11	1:B:121:LEU:HD11	2.01	0.42
1:B:149:ILE:HA	1:B:150:PRO:HD3	1.86	0.42
1:B:14:ARG:NE	1:B:149:ILE:O	2.52	0.42
1:D:91:ILE:HD11	1:D:121:LEU:HD11	2.01	0.42
1:C:146:ARG:HH22	1:D:89:GLU:HA	1.84	0.42
1:B:124:ARG:O	1:B:128:THR:HG22	2.18	0.42
1:C:143:TYR:OH	1:D:85:PRO:O	2.26	0.42
1:C:146:ARG:HH22	1:D:89:GLU:CA	2.33	0.42
1:C:54:TYR:CE2	1:D:56:ALA:CB	3.02	0.42
1:B:8:ILE:HB	1:B:41:ARG:HH21	1.83	0.42
1:B:23:THR:O	1:B:24:LEU:C	2.57	0.41
1:B:67:LEU:HD12	1:B:115:ALA:HA	2.02	0.41
1:B:84:ALA:N	1:B:85:PRO:CD	2.84	0.41
1:A:25:SER:O	1:A:29:THR:HG23	2.21	0.41
1:D:84:ALA:N	1:D:85:PRO:CD	2.84	0.41
1:D:124:ARG:O	1:D:128:THR:HG22	2.18	0.41
1:C:25:SER:O	1:C:29:THR:HG23	2.20	0.41

All (38) 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:D:39:GLN:CG	1:D:39:GLN:OE1[4_565]	0.43	1.77
1:A:119:GLU:CD	1:A:139:LEU:CB[3_454]	0.70	1.50
1:A:119:GLU:CG	1:A:139:LEU:CB[3_454]	0.92	1.28
1:A:61:GLU:OE1	1:A:116:ARG:NH2[3_454]	0.95	1.25
1:A:119:GLU:CB	1:A:139:LEU:CG[3_454]	0.97	1.23
1:D:39:GLN:NE2	1:D:39:GLN:NE2[4_565]	1.04	1.16
1:A:61:GLU:OE2	1:A:116:ARG:NE[3_454]	1.07	1.13
1:A:119:GLU:OE2	1:A:139:LEU:CA[3_454]	1.18	1.02
1:A:119:GLU:CB	1:A:139:LEU:CD2[3_454]	1.20	1.00
1:A:119:GLU:OE2	1:A:139:LEU:C[3_454]	1.22	0.98
1:D:39:GLN:CD	1:D:39:GLN:OE1[4_565]	1.23	0.97
1:A:61:GLU:CD	1:A:116:ARG:NH2[3_454]	1.26	0.94
1:A:61:GLU:OE2	1:A:116:ARG:CZ[3_454]	1.27	0.93
1:A:119:GLU:CD	1:A:139:LEU:CA[3_454]	1.35	0.85
1:D:39:GLN:CD	1:D:39:GLN:NE2[4_565]	1.44	0.76
1:A:61:GLU:CD	1:A:116:ARG:CZ[3_454]	1.48	0.72
1:D:39:GLN:CG	1:D:39:GLN:CD[4_565]	1.50	0.70
1:A:119:GLU:OE2	1:A:140:ASN:N[3_454]	1.52	0.68
1:A:119:GLU:CG	1:A:139:LEU:CG[3_454]	1.53	0.67
1:A:119:GLU:CB	1:A:139:LEU:CD1[3_454]	1.59	0.61
1:A:119:GLU:OE1	1:A:139:LEU:CB[3_454]	1.62	0.58
1:A:61:GLU:OE1	1:A:116:ARG:CZ[3_454]	1.65	0.55
1:A:119:GLU:CG	1:A:139:LEU:CA[3_454]	1.70	0.50
1:A:119:GLU:OE2	1:A:139:LEU:CB[3_454]	1.75	0.45
1:D:39:GLN:CB	1:D:39:GLN:OE1[4_565]	1.75	0.45
1:A:119:GLU:CA	1:A:139:LEU:CD2[3_454]	1.79	0.41
1:A:119:GLU:OE2	1:A:139:LEU:N[3_454]	1.81	0.39
1:A:119:GLU:CD	1:A:139:LEU:CG[3_454]	1.90	0.30
1:A:119:GLU:CB	1:A:139:LEU:CB[3_454]	1.91	0.29
1:A:119:GLU:OE1	1:A:139:LEU:CG[3_454]	1.96	0.24
1:D:39:GLN:OE1	1:D:39:GLN:OE1[4_565]	2.00	0.20
1:A:119:GLU:CD	1:A:139:LEU:N[3_454]	2.01	0.19
1:A:119:GLU:CG	1:A:139:LEU:CD2[3_454]	2.02	0.18
1:A:61:GLU:OE2	1:A:116:ARG:NH2[3_454]	2.04	0.16
1:A:61:GLU:CD	1:A:116:ARG:NE[3_454]	2.05	0.15
1:A:61:GLU:OE2	1:A:116:ARG:CD[3_454]	2.11	0.09
1:A:61:GLU:OE1	1:A:116:ARG:NH1[3_454]	2.18	0.02
1:A:67:LEU:CG	1:A:115:ALA:CB[3_454]	2.19	0.01

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	145/150 (97%)	141 (97%)	3 (2%)	1 (1%)	26 71
1	B	145/150 (97%)	132 (91%)	6 (4%)	7 (5%)	3 32
1	C	145/150 (97%)	141 (97%)	3 (2%)	1 (1%)	26 71
1	D	145/150 (97%)	133 (92%)	5 (3%)	7 (5%)	3 32
All	All	580/600 (97%)	547 (94%)	17 (3%)	16 (3%)	6 46

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	B	25	SER
1	C	102	THR
1	D	25	SER
1	B	29	THR
1	B	102	THR
1	D	29	THR
1	D	102	THR
1	B	35	VAL
1	D	35	VAL
1	B	5	LEU
1	B	7	ASP
1	B	30	ARG
1	D	5	LEU
1	D	7	ASP
1	D	30	ARG

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	122/127 (96%)	100 (82%)	22 (18%)	2	17
1	B	119/127 (94%)	99 (83%)	20 (17%)	2	20
1	C	122/127 (96%)	99 (81%)	23 (19%)	2	14
1	D	119/127 (94%)	102 (86%)	17 (14%)	4	28
All	All	482/508 (95%)	400 (83%)	82 (17%)	2	20

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	24	LEU
1	A	29	THR
1	A	40	SER
1	A	44	ARG
1	A	45	LEU
1	A	67	LEU
1	A	71	VAL
1	A	74	THR
1	A	83	ASP
1	A	87	ARG
1	A	93	GLU
1	A	94	VAL
1	A	100	VAL
1	A	110	VAL
1	A	111	ARG
1	A	112	VAL
1	A	127	THR
1	A	128	THR
1	A	131	VAL
1	A	143	TYR
1	A	146	ARG
1	B	6	ASP
1	B	11	ILE
1	B	15	GLU
1	B	23	THR
1	B	24	LEU
1	B	36	SER
1	B	40	SER
1	B	41	ARG

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Mol	Chain	Res	Type
1	B	61	GLU
1	B	91	ILE
1	B	94	VAL
1	B	100	VAL
1	B	102	THR
1	B	103	GLU
1	B	104	GLU
1	B	110	VAL
1	B	112	VAL
1	B	119	GLU
1	B	120	ASP
1	B	128	THR
1	C	5	LEU
1	C	24	LEU
1	C	29	THR
1	C	40	SER
1	C	44	ARG
1	C	45	LEU
1	C	67	LEU
1	C	71	VAL
1	C	74	THR
1	C	83	ASP
1	C	87	ARG
1	C	93	GLU
1	C	94	VAL
1	C	100	VAL
1	C	102	THR
1	C	110	VAL
1	C	111	ARG
1	C	112	VAL
1	C	127	THR
1	C	128	THR
1	C	131	VAL
1	C	143	TYR
1	C	146	ARG
1	D	6	ASP
1	D	11	ILE
1	D	23	THR
1	D	36	SER
1	D	40	SER
1	D	41	ARG
1	D	61	GLU

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Mol	Chain	Res	Type
1	D	91	ILE
1	D	94	VAL
1	D	100	VAL
1	D	102	THR
1	D	103	GLU
1	D	104	GLU
1	D	110	VAL
1	D	112	VAL
1	D	120	ASP
1	D	128	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	C	52	GLN
1	C	80	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	147/150 (98%)	0.45	10 (6%) 20 14	15, 33, 56, 69	0
1	B	147/150 (98%)	0.52	13 (8%) 12 9	14, 36, 95, 99	0
1	C	147/150 (98%)	0.40	10 (6%) 20 14	15, 33, 56, 69	0
1	D	147/150 (98%)	0.56	13 (8%) 12 9	14, 36, 95, 99	0
All	All	588/600 (98%)	0.48	46 (7%) 16 11	14, 34, 88, 99	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	39	GLN	10.0
1	D	103	GLU	4.2
1	B	81	PRO	4.1
1	C	130	ASN	4.1
1	A	31	ALA	4.0
1	A	62	ALA	4.0
1	B	80	GLN	3.8
1	B	75	PRO	3.6
1	A	32	GLY	3.4
1	D	62	ALA	3.3
1	B	74	THR	3.3
1	D	102	THR	3.2
1	D	10	ARG	3.2
1	B	49	GLY	3.0
1	A	129	ALA	2.9
1	D	14	ARG	2.9
1	C	148	HIS	2.8
1	C	150	PRO	2.8
1	D	104	GLU	2.7
1	D	101	ALA	2.7
1	D	64	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	81	PRO	2.6
1	A	140	ASN	2.6
1	A	115	ALA	2.5
1	A	142	PHE	2.5
1	B	43	ARG	2.4
1	C	90	HIS	2.4
1	B	83	ASP	2.4
1	D	9	ASP	2.3
1	B	58	ILE	2.3
1	A	22	ALA	2.2
1	C	129	ALA	2.2
1	D	93	GLU	2.2
1	B	96	SER	2.2
1	B	150	PRO	2.2
1	A	125	ILE	2.2
1	C	80	GLN	2.2
1	D	38	VAL	2.2
1	B	13	VAL	2.1
1	C	48	ARG	2.1
1	B	73	ILE	2.1
1	C	86	ALA	2.1
1	B	63	VAL	2.1
1	C	99	SER	2.1
1	D	33	LEU	2.1
1	A	128	THR	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.