Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:40 AM GMT

PDB ID	:	2DWY
Title	:	Crystal Structure Analysis of GGA1-GAE
Authors	:	Inoue, M.; Shiba, T.; Yamada, Y.; Ihara, K.; Kawasaki, M.; Kato, R.; Nakayama, K.; Wakatsuki, S.
Deposited on	:	2006-08-21
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:

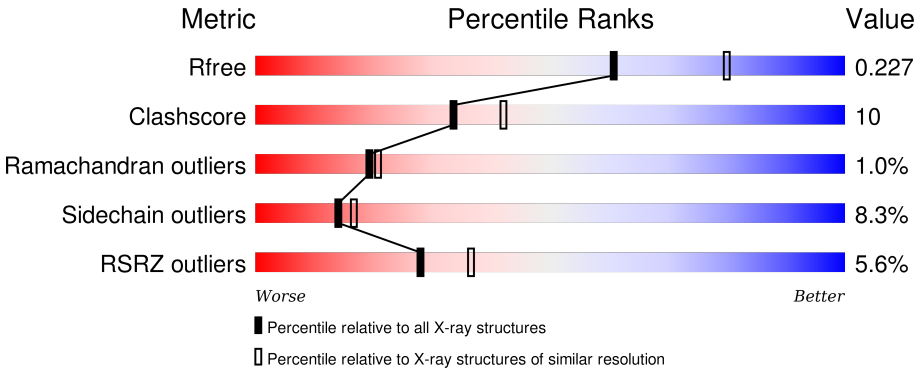
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	133	9% 74% 20%
1	B	133	4% 69% 23% 5%
1	C	133	5% 63% 32%
1	D	133	4% 69% 23% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4231 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 ADP-RIBOSYLATION FACTOR BINDING PROTEIN GGA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1020	662	173	181	4			
1	B	126	Total	C	N	O	S	0	0	0
			1001	651	170	176	4			
1	C	132	Total	C	N	O	S	0	0	0
			1042	678	176	184	4			
1	D	129	Total	C	N	O	S	0	0	0
			1020	662	173	181	4			

- Molecule 2 is water.

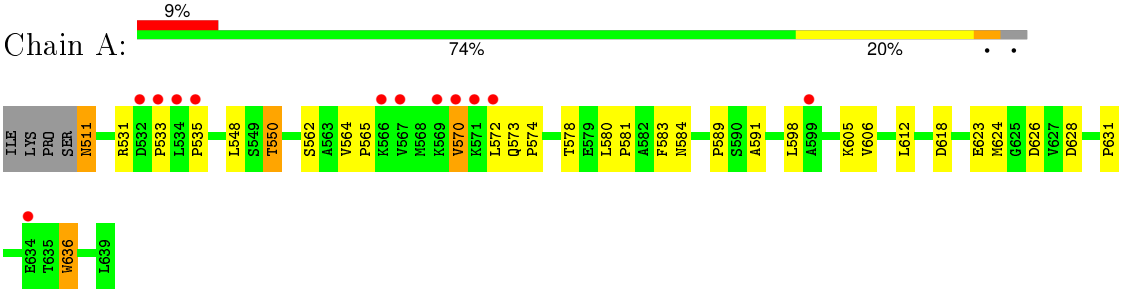
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		
2	B	31	Total	O	0	0
			31	31		
2	C	37	Total	O	0	0
			37	37		
2	D	39	Total	O	0	0
			39	39		

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.

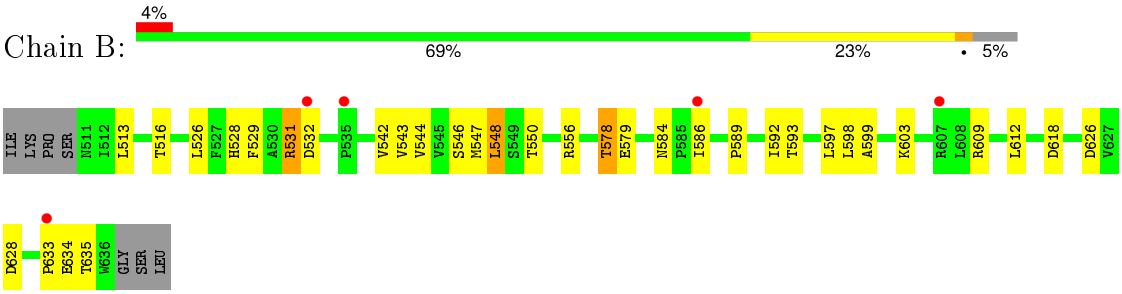
- Molecule 1: ADP-RIBOSYLATION FACTOR BINDING PROTEIN GGA1

Chain A:



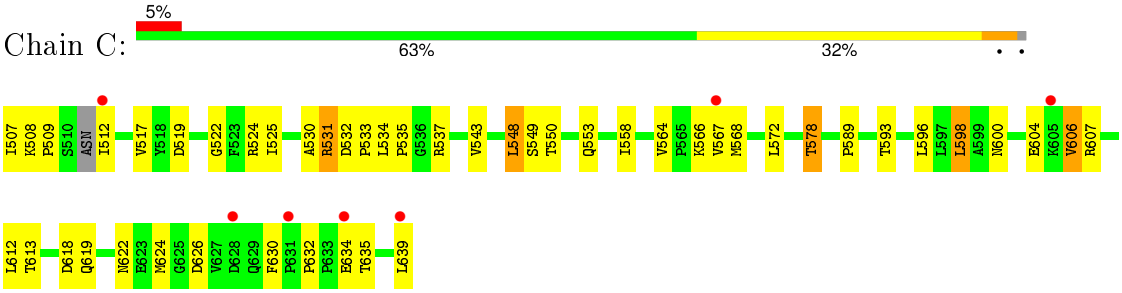
- Molecule 1: ADP-RIBOSYLATION FACTOR BINDING PROTEIN GGA1

Chain B:



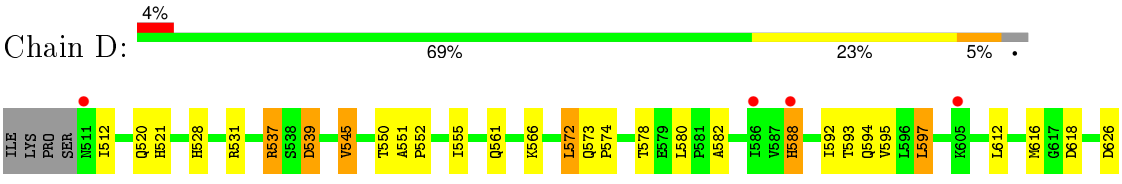
- Molecule 1: ADP-RIBOSYLATION FACTOR BINDING PROTEIN GGA1

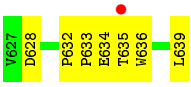
Chain C:



- Molecule 1: ADP-RIBOSYLATION FACTOR BINDING PROTEIN GGA1

Chain D:




V627
D628
P632
P633
E634
T635
W636
L639

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.48Å 88.24Å 67.22Å 90.00° 96.10° 90.00°	Depositor
Resolution (Å)	41.52 – 2.30 41.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (41.52-2.30) 94.7 (41.63-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.257 0.221 , 0.227	Depositor DCC
R_{free} test set	1156 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.3	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 23246 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4231	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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	0.61	0/1049	0.85	4/1433 (0.3%)
1	B	0.59	0/1030	0.84	4/1409 (0.3%)
1	C	0.56	0/1071	0.79	3/1461 (0.2%)
1	D	0.59	0/1049	0.80	4/1433 (0.3%)
All	All	0.59	0/4199	0.82	15/5736 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	539	ASP	CB-CG-OD2	7.41	124.97	118.30
1	C	519	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	618	ASP	CB-CG-OD2	6.96	124.56	118.30
1	D	618	ASP	CB-CG-OD2	6.94	124.55	118.30
1	B	626	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	532	ASP	CB-CG-OD2	6.37	124.03	118.30
1	D	628	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	626	ASP	CB-CG-OD2	5.68	123.42	118.30
1	C	626	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	550	THR	OG1-CB-CG2	-5.28	97.85	110.00
1	B	628	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	628	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	626	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	618	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	532	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1020	0	1042	23	0
1	B	1001	0	1023	23	0
1	C	1042	0	1071	34	0
1	D	1020	0	1042	25	0
2	A	41	0	0	0	0
2	B	31	0	0	0	0
2	C	37	0	0	4	0
2	D	39	0	0	0	0
All	All	4231	0	4178	84	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 10.

All (84) 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:D:531:ARG:NH2	1:D:639:LEU:O	2.09	0.84
1:C:512:ILE:HD12	1:C:639:LEU:HD22	1.65	0.79
1:A:550:THR:HG22	1:B:589:PRO:HD2	1.66	0.76
1:C:531:ARG:HD2	1:C:639:LEU:O	1.86	0.75
1:C:635:THR:HG22	1:C:639:LEU:HD21	1.75	0.67
1:C:524:ARG:HD3	2:C:109:HOH:O	1.95	0.65
1:B:528:HIS:HE1	1:B:546:SER:OG	1.80	0.65
1:A:550:THR:HG21	1:B:589:PRO:HB2	1.78	0.65
1:B:550:THR:HG22	1:B:550:THR:O	1.98	0.64
1:C:535:PRO:HB3	1:D:573:GLN:HE22	1.64	0.62
1:C:606:VAL:HG21	1:C:630:PHE:HB2	1.83	0.59
1:C:567:VAL:HG21	1:C:604:GLU:HG3	1.86	0.58
1:D:512:ILE:HD11	1:D:635:THR:HG21	1.86	0.57
1:D:537:ARG:HB2	1:D:539:ASP:OD1	2.04	0.57
1:A:589:PRO:HG3	1:B:548:LEU:HD13	1.85	0.57
1:A:564:VAL:HG22	1:A:570:VAL:HG13	1.87	0.56
1:A:583:PHE:CE1	1:B:589:PRO:HG2	2.42	0.55
1:C:564:VAL:HG11	1:C:598:LEU:HD21	1.89	0.55
1:C:517:VAL:HG22	1:C:525:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:PRO:CD	1:D:550:THR:HG21	2.37	0.55
1:A:574:PRO:O	1:B:531:ARG:NH2	2.39	0.55
1:A:550:THR:HG21	1:B:589:PRO:CB	2.37	0.54
1:A:550:THR:O	1:A:550:THR:HG22	2.07	0.54
1:C:530:ALA:HB2	1:D:593:THR:HG21	1.91	0.53
1:D:555:ILE:HD11	1:D:616:MET:CE	2.37	0.53
1:C:589:PRO:HD2	1:D:550:THR:CG2	2.39	0.52
1:A:598:LEU:HD21	1:A:606:VAL:HG11	1.92	0.52
1:D:580:LEU:HD21	1:D:592:ILE:HG12	1.91	0.52
1:C:548:LEU:HD23	1:C:549:SER:H	1.75	0.52
1:C:635:THR:HG22	1:C:639:LEU:CD2	2.39	0.51
1:C:593:THR:HG22	1:D:528:HIS:CE1	2.45	0.51
1:B:603:LYS:HB3	1:B:633:PRO:HB2	1.93	0.51
1:C:613:THR:OG1	1:C:622:ASN:ND2	2.44	0.50
1:A:623:GLU:HB3	1:D:561:GLN:HG3	1.94	0.49
1:C:589:PRO:HG2	1:D:550:THR:CG2	2.42	0.49
1:C:507:ILE:HA	1:C:531:ARG:HH12	1.78	0.48
1:C:632:PRO:O	1:C:635:THR:HB	2.14	0.48
1:D:555:ILE:HD11	1:D:616:MET:HE2	1.94	0.48
1:C:548:LEU:HD23	1:C:549:SER:N	2.28	0.48
1:C:589:PRO:HD2	1:D:550:THR:HG21	1.94	0.47
1:D:573:GLN:HB3	1:D:574:PRO:HD2	1.97	0.47
1:B:547:MET:HB2	1:B:592:ILE:HB	1.97	0.46
1:D:552:PRO:O	1:D:582:ALA:HB1	2.15	0.46
1:D:633:PRO:HA	1:D:636:TRP:CD1	2.51	0.45
1:D:521:HIS:O	1:D:551:ALA:HB2	2.17	0.45
1:B:544:VAL:HG13	1:B:593:THR:HG23	1.98	0.45
1:A:631:PRO:O	1:A:636:TRP:CZ3	2.70	0.45
1:A:573:GLN:HB2	1:B:531:ARG:HH12	1.82	0.45
1:A:598:LEU:HD21	1:A:606:VAL:CG1	2.46	0.45
1:B:516:THR:HA	1:B:526:LEU:HD23	1.98	0.45
1:C:553:GLN:HB2	2:C:114:HOH:O	2.17	0.45
1:A:533:PRO:HG2	1:B:599:ALA:HB2	1.99	0.45
1:A:511:ASN:N	1:A:511:ASN:ND2	2.65	0.45
1:A:550:THR:CG2	1:B:589:PRO:HD2	2.41	0.44
1:C:558:ILE:HA	1:C:613:THR:O	2.17	0.44
1:B:529:PHE:CD2	1:B:543:VAL:HG22	2.52	0.44
1:B:584:ASN:OD1	1:B:586:ILE:HG22	2.18	0.44
1:B:542:VAL:HG22	1:B:597:LEU:HD12	2.00	0.44
1:C:572:LEU:HD21	1:C:596:LEU:HD12	2.00	0.43
1:C:543:VAL:HB	1:C:596:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:PRO:HB3	1:D:595:VAL:HG11	2.01	0.43
1:A:580:LEU:HA	1:A:581:PRO:HD3	1.90	0.43
1:C:578:THR:HG22	2:C:123:HOH:O	2.19	0.43
1:C:618:ASP:HB3	1:C:619:GLN:HE21	1.83	0.43
1:D:545:VAL:HG13	1:D:594:GLN:O	2.18	0.43
1:B:542:VAL:HG22	1:B:597:LEU:CD1	2.49	0.43
1:D:632:PRO:HA	1:D:633:PRO:HD3	1.95	0.43
1:A:562:SER:HB2	1:A:572:LEU:HD21	2.00	0.43
1:C:568:MET:HE3	1:C:600:ASN:HB2	2.00	0.42
1:A:548:LEU:HD12	1:A:591:ALA:HB2	2.02	0.42
1:D:537:ARG:CB	1:D:539:ASP:OD1	2.67	0.42
1:C:568:MET:HE2	1:C:598:LEU:HD11	2.01	0.42
1:C:522:GLY:HA2	1:C:524:ARG:HH12	1.84	0.42
1:C:534:LEU:HD23	1:C:534:LEU:HA	1.95	0.41
1:D:597:LEU:HD23	1:D:597:LEU:HA	1.98	0.41
1:A:550:THR:HG22	1:B:589:PRO:CD	2.45	0.41
1:A:550:THR:HA	1:A:583:PHE:HB2	2.03	0.41
1:B:550:THR:CG2	1:B:550:THR:O	2.67	0.41
1:A:624:MET:HG3	1:D:572:LEU:HD13	2.03	0.41
1:A:550:THR:CG2	1:B:589:PRO:CG	2.99	0.41
1:C:524:ARG:CD	2:C:109:HOH:O	2.62	0.41
1:D:578:THR:O	1:D:578:THR:CG2	2.69	0.41
1:C:534:LEU:HD12	1:C:537:ARG:NH2	2.36	0.40
1:B:578:THR:CG2	1:B:578:THR:O	2.70	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	127/133 (96%)	120 (94%)	5 (4%)	2 (2%)	12 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	124/133 (93%)	116 (94%)	7 (6%)	1 (1%)	24 27
1	C	128/133 (96%)	119 (93%)	8 (6%)	1 (1%)	24 27
1	D	127/133 (96%)	124 (98%)	2 (2%)	1 (1%)	24 27
All	All	506/532 (95%)	479 (95%)	22 (4%)	5 (1%)	19 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	PRO
1	C	509	PRO
1	B	635	THR
1	D	588	HIS
1	A	565	PRO

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	117/121 (97%)	109 (93%)	8 (7%)	20 25
1	B	115/121 (95%)	105 (91%)	10 (9%)	13 15
1	C	120/121 (99%)	108 (90%)	12 (10%)	9 11
1	D	117/121 (97%)	108 (92%)	9 (8%)	16 20
All	All	469/484 (97%)	430 (92%)	39 (8%)	14 17

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	ASN
1	A	531	ARG
1	A	570	VAL
1	A	578	THR
1	A	584	ASN
1	A	605	LYS

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Mol	Chain	Res	Type
1	A	612	LEU
1	A	636	TRP
1	B	513	LEU
1	B	531	ARG
1	B	548	LEU
1	B	556	ARG
1	B	578	THR
1	B	579	GLU
1	B	598	LEU
1	B	609	ARG
1	B	612	LEU
1	B	634	GLU
1	C	508	LYS
1	C	531	ARG
1	C	548	LEU
1	C	550	THR
1	C	566	LYS
1	C	578	THR
1	C	598	LEU
1	C	606	VAL
1	C	607	ARG
1	C	612	LEU
1	C	624	MET
1	C	634	GLU
1	D	520	GLN
1	D	537	ARG
1	D	545	VAL
1	D	566	LYS
1	D	572	LEU
1	D	588	HIS
1	D	597	LEU
1	D	612	LEU
1	D	634	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	511	ASN
1	A	561	GLN
1	A	573	GLN
1	B	528	HIS
1	B	594	GLN

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Mol	Chain	Res	Type
1	B	602	GLN
1	C	553	GLN
1	C	619	GLN
1	C	622	ASN
1	D	573	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	129/133 (96%)	0.57	12 (9%)	11	16	26, 41, 71, 81	0
1	B	126/133 (94%)	0.32	5 (3%)	42	51	28, 43, 65, 69	0
1	C	132/133 (99%)	0.39	7 (5%)	30	39	31, 49, 69, 83	0
1	D	129/133 (96%)	0.21	5 (3%)	43	52	31, 46, 64, 75	0
All	All	516/532 (96%)	0.38	29 (5%)	28	36	26, 45, 68, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	570	VAL	9.6
1	A	535	PRO	4.1
1	D	586	ILE	4.0
1	A	567	VAL	3.9
1	D	588	HIS	3.8
1	A	533	PRO	3.2
1	D	635	THR	3.1
1	A	571	LYS	2.9
1	A	569	LYS	2.9
1	D	511	ASN	2.8
1	C	605	LYS	2.7
1	C	512	ILE	2.7
1	B	633	PRO	2.7
1	A	566	LYS	2.7
1	B	586	ILE	2.7
1	A	572	LEU	2.6
1	B	535	PRO	2.6
1	C	628	ASP	2.5
1	A	599	ALA	2.5
1	C	639	LEU	2.5
1	A	532	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	631	PRO	2.4
1	B	532	ASP	2.4
1	A	634	GLU	2.3
1	C	634	GLU	2.3
1	C	567	VAL	2.1
1	D	605	LYS	2.1
1	A	534	LEU	2.0
1	B	607	ARG	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.