Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2024 – 12:06 PM EDT

PDB ID	:	8UF4
Title	:	Crystal structure of wildtype dystroglycan proteolytic domain (juxtamembrane domain)
Authors	:	Anderson, M.J.M.; Shi, K.; Hayward, A.N.; Uhlens, C.; Evans III, R.L.; Grant, E.; Greenberg, L.; Aihara, H.; Gordon, W.R.
Deposited on	:	2023-10-03
Resolution	:	2.43 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

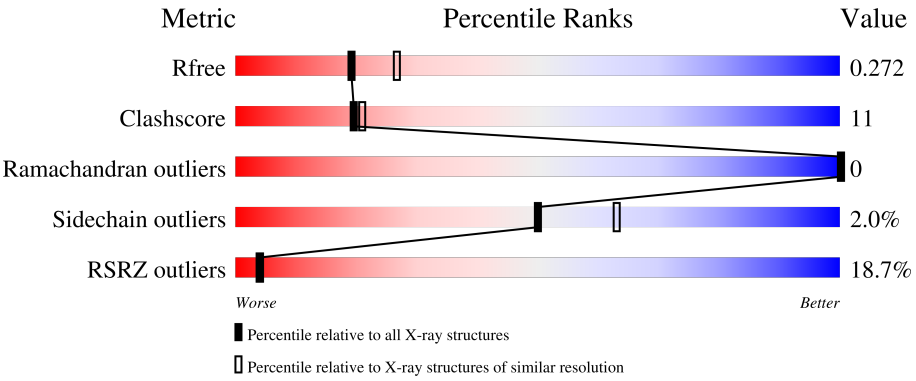
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.43 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	163	10% 74% 22%
1	C	163	23% 66% 31%
2	B	95	21% 61% 9% 28%
2	D	95	11% 66% 29%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3700 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 a-dystroglycan.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1284	815	230	236	3			
1	C	159	Total	C	N	O	S	0	0	0
			1275	810	228	234	3			

- Molecule 2 is a protein called Beta-dystroglycan.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	68	Total	C	N	O	S	0	0	0
			520	327	91	100	2			
2	D	67	Total	C	N	O	S	0	0	0
			513	322	90	99	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		

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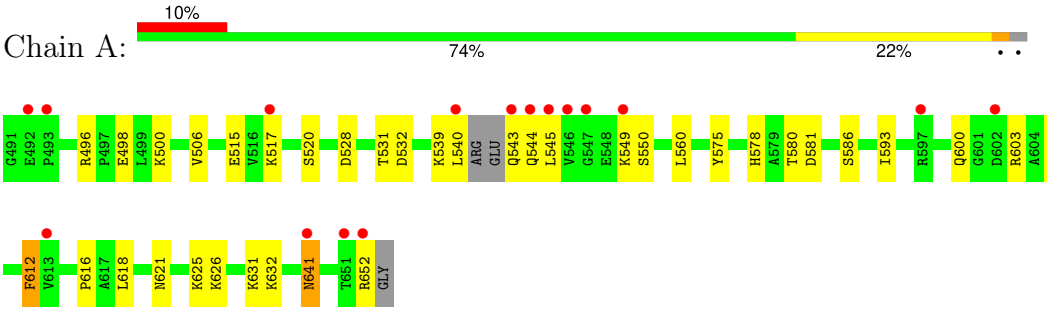
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	6	Total O 6 6	0	0
5	C	39	Total O 39 39	0	0
5	D	12	Total O 12 12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

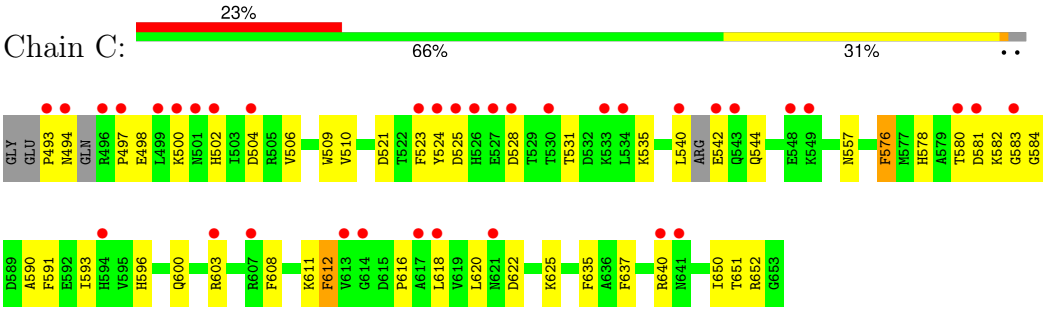
• Molecule 1: a-dystroglycan

Chain A:



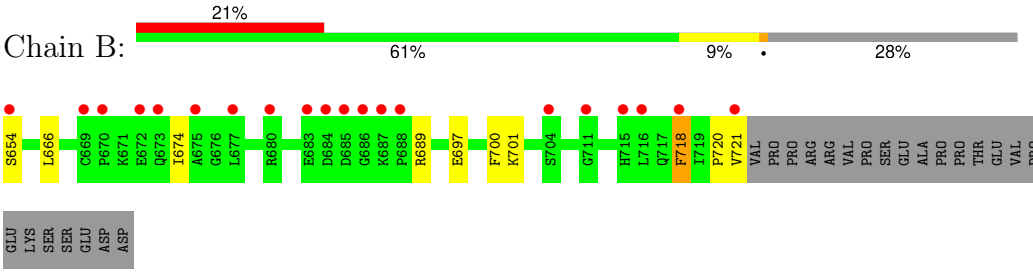
• Molecule 1: a-dystroglycan

Chain C:



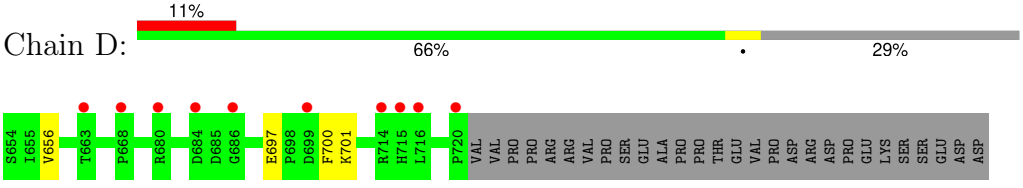
• Molecule 2: Beta-dystroglycan

Chain B:



• Molecule 2: Beta-dystroglycan

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.95Å 86.58Å 128.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.43 – 2.43 51.43 – 2.43	Depositor EDS
% Data completeness (in resolution range)	85.5 (51.43-2.43) 85.4 (51.43-2.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.275 0.223 , 0.272	Depositor DCC
R_{free} test set	968 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3700	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, CL

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	0.41	0/1314	0.68	0/1774
1	C	0.43	0/1304	0.68	0/1758
2	B	0.37	0/532	0.60	0/725
2	D	0.38	0/525	0.60	0/715
All	All	0.41	0/3675	0.66	0/4972

There are no bond length outliers.

There are no bond angle outliers.

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	1284	0	1265	31	0
1	C	1275	0	1257	45	0
2	B	520	0	515	10	0
2	D	513	0	506	3	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	48	0	0	4	0
5	B	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	39	0	0	5	0
5	D	12	0	0	0	0
All	All	3700	0	3543	81	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 (81) 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:C:493:PRO:HA	1:C:583:GLY:HA3	1.33	1.05
1:A:515:GLU:HG2	1:A:560:LEU:HD11	1.61	0.82
1:C:540:LEU:HB2	1:C:544:GLN:HG3	1.70	0.73
1:A:603:ARG:HG3	2:B:666:LEU:HD22	1.71	0.72
1:C:502:HIS:NE2	1:C:591:PHE:HA	2.03	0.72
1:C:493:PRO:HA	1:C:583:GLY:CA	2.16	0.72
1:C:612:PHE:CD2	2:D:700:PHE:HB3	2.26	0.71
2:D:697:GLU:OE2	2:D:701:LYS:HG2	1.92	0.68
1:C:611:LYS:HG2	2:D:656:VAL:HG22	1.76	0.68
1:C:635:PHE:HD1	1:C:640:ARG:HB2	1.57	0.68
1:A:517:LYS:HG2	1:A:560:LEU:HD13	1.75	0.67
1:A:517:LYS:HB3	5:A:847:HOH:O	1.95	0.67
1:C:502:HIS:CD2	1:C:504:ASP:H	2.13	0.67
1:A:631:LYS:HE3	1:A:641:ASN:HD21	1.61	0.66
1:A:612:PHE:CD2	2:B:700:PHE:HB3	2.32	0.64
2:B:697:GLU:OE2	2:B:701:LYS:HG2	1.98	0.64
1:C:500:LYS:N	5:C:802:HOH:O	2.28	0.60
1:A:506:VAL:HB	1:A:593:ILE:HG12	1.84	0.59
1:A:580:THR:HG22	1:A:586:SER:OG	2.03	0.58
1:A:616:PRO:HG2	1:A:652:ARG:HG2	1.84	0.58
1:C:497:PRO:HG3	1:C:581:ASP:HB3	1.84	0.58
1:A:600:GLN:HG2	2:B:666:LEU:HD21	1.86	0.57
1:A:520:SER:HA	1:A:531:THR:HB	1.86	0.57
1:C:600:GLN:O	1:C:603:ARG:HG2	2.04	0.56
2:B:654:SER:N	5:B:801:HOH:O	2.38	0.56
1:A:496:ARG:HD3	1:A:586:SER:O	2.06	0.56
1:C:502:HIS:NE2	1:C:590:ALA:O	2.40	0.55
1:C:582:LYS:N	1:C:582:LYS:HD2	2.20	0.55
1:A:606:ALA:HB2	2:B:674:ILE:HD13	1.89	0.53
1:C:580:THR:HG22	1:C:586:SER:OG	2.09	0.53
1:A:626:LYS:NZ	5:A:801:HOH:O	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LEU:HD13	1:A:575:TYR:CZ	2.45	0.52
1:A:544:GLN:HE22	1:A:550:SER:HB2	1.74	0.51
1:C:494:ASN:OD1	1:C:585:LEU:HD12	2.11	0.51
1:A:498:GLU:OE1	1:A:500:LYS:NZ	2.42	0.51
1:C:616:PRO:HG2	1:C:652:ARG:HB3	1.93	0.51
1:C:523:PHE:HD2	1:C:531:THR:HG23	1.76	0.50
1:A:532:ASP:N	1:A:532:ASP:OD1	2.43	0.50
1:A:528:ASP:OD2	1:A:581:ASP:HB2	2.12	0.50
1:C:584:GLY:HA2	5:C:837:HOH:O	2.11	0.49
1:A:544:GLN:HB3	1:A:545:LEU:H	1.38	0.49
1:A:605:PRO:HB2	2:B:674:ILE:HD11	1.94	0.49
1:C:528:ASP:OD2	1:C:581:ASP:HB2	2.13	0.49
1:C:578:HIS:CD2	1:C:588:VAL:HG22	2.48	0.48
1:A:632:LYS:NZ	5:A:813:HOH:O	2.46	0.48
1:C:509:TRP:CD1	1:C:596:HIS:HB2	2.50	0.47
1:C:510:VAL:HG23	1:C:596:HIS:O	2.13	0.47
1:C:587:ALA:HB1	5:C:823:HOH:O	2.15	0.47
1:C:651:THR:HG22	1:C:652:ARG:H	1.80	0.47
1:C:502:HIS:CE1	1:C:504:ASP:HA	2.51	0.46
1:A:543:GLN:O	1:A:544:GLN:HG2	2.16	0.46
2:B:689:ARG:HH21	1:C:521:ASP:CG	2.20	0.45
1:C:498:GLU:HB2	1:C:524:TYR:O	2.17	0.45
1:C:576:PHE:CD1	1:C:576:PHE:N	2.84	0.45
1:C:535:LYS:HB3	1:C:580:THR:OG1	2.17	0.44
1:A:517:LYS:HG2	1:A:560:LEU:CD1	2.46	0.44
1:A:600:GLN:O	1:A:603:ARG:HG2	2.18	0.44
1:A:618:LEU:HD11	1:A:625:LYS:HE3	2.00	0.44
1:C:506:VAL:HB	1:C:593:ILE:HG12	2.00	0.44
1:C:651:THR:HG22	1:C:652:ARG:N	2.34	0.43
2:B:718:PHE:N	2:B:718:PHE:CD1	2.87	0.43
1:C:557:ASN:ND2	5:C:803:HOH:O	2.29	0.42
1:A:549:LYS:HB3	1:A:549:LYS:HE2	1.87	0.42
1:C:494:ASN:HD22	1:C:525:ASP:CG	2.23	0.42
1:C:622:ASP:CB	1:C:625:LYS:HE3	2.50	0.42
1:C:494:ASN:OD1	1:C:494:ASN:N	2.50	0.42
1:C:612:PHE:CD1	1:C:612:PHE:N	2.88	0.42
1:C:618:LEU:HD22	5:C:804:HOH:O	2.19	0.42
1:A:608:PHE:CD1	1:A:608:PHE:N	2.88	0.41
2:B:720:PRO:O	2:B:721:VAL:HG22	2.19	0.41
1:C:523:PHE:N	1:C:531:THR:OG1	2.50	0.41
1:C:622:ASP:HB3	1:C:625:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ASN:HD21	1:C:497:PRO:HD3	1.84	0.41
1:C:635:PHE:CD1	1:C:640:ARG:HB2	2.44	0.41
1:C:581:ASP:CG	1:C:583:GLY:H	2.23	0.41
1:C:620:LEU:HD21	1:C:650:ILE:HB	2.02	0.40
1:A:496:ARG:HH11	1:A:586:SER:H	1.69	0.40
1:A:621:ASN:HB3	5:A:839:HOH:O	2.22	0.40
1:C:542:GLU:HG3	1:C:542:GLU:O	2.21	0.40
1:A:539:LYS:HD2	1:A:578:HIS:CD2	2.57	0.40
1:C:635:PHE:CD1	1:C:640:ARG:HD3	2.57	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	156/163 (96%)	143 (92%)	13 (8%)	0	100	100
1	C	153/163 (94%)	148 (97%)	5 (3%)	0	100	100
2	B	66/95 (70%)	63 (96%)	3 (4%)	0	100	100
2	D	65/95 (68%)	62 (95%)	3 (5%)	0	100	100
All	All	440/516 (85%)	416 (94%)	24 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	139/141 (99%)	136 (98%)	3 (2%)	47	60
1	C	138/141 (98%)	134 (97%)	4 (3%)	37	49
2	B	59/85 (69%)	58 (98%)	1 (2%)	56	69
2	D	58/85 (68%)	58 (100%)	0	100	100
All	All	394/452 (87%)	386 (98%)	8 (2%)	50	63

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	608	PHE
1	A	612	PHE
1	A	641	ASN
2	B	718	PHE
1	C	576	PHE
1	C	608	PHE
1	C	612	PHE
1	C	637	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	544	GLN
1	A	555	ASN
1	A	641	ASN
1	C	555	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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	160/163 (98%)	0.68	17 (10%)	13	12	27, 44, 84, 119	0
1	C	159/163 (97%)	1.21	38 (23%)	2	2	23, 49, 87, 115	0
2	B	68/95 (71%)	1.61	20 (29%)	1	1	42, 61, 87, 97	0
2	D	67/95 (70%)	1.04	10 (14%)	7	6	31, 51, 75, 89	0
All	All	454/516 (87%)	1.06	85 (18%)	4	4	23, 51, 87, 119	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	721	VAL	5.3
1	C	533	LYS	5.1
1	C	493	PRO	4.7
1	A	545	LEU	4.6
1	C	524	TYR	4.4
1	A	540	LEU	4.1
2	D	720	PRO	4.1
1	C	502	HIS	4.0
2	B	687	LYS	3.8
1	C	581	ASP	3.8
1	C	497	PRO	3.8
2	B	685	ASP	3.6
1	C	530	THR	3.5
2	B	683	GLU	3.3
1	C	494	ASN	3.3
2	B	711	GLY	3.1
1	C	621	ASN	3.1
2	B	715	HIS	3.0
1	C	585	LEU	2.9
1	C	548	GLU	2.9
1	A	602	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	641	ASN	2.9
1	C	523	PHE	2.9
1	A	549	LYS	2.8
1	C	500	LYS	2.8
2	B	677	LEU	2.8
2	B	686	GLY	2.8
1	A	546	VAL	2.8
2	D	716	LEU	2.8
2	B	680	ARG	2.8
1	C	496	ARG	2.7
1	C	640	ARG	2.7
1	C	499	LEU	2.7
1	A	613	VAL	2.7
2	B	675	ALA	2.7
1	C	501	ASN	2.7
1	C	641	ASN	2.6
1	A	544	GLN	2.6
2	D	663	THR	2.6
1	A	651	THR	2.5
1	C	614	GLY	2.5
2	B	669	CYS	2.5
1	A	517	LYS	2.5
1	C	603	ARG	2.5
1	C	534	LEU	2.4
1	C	580	THR	2.4
2	D	714	ARG	2.4
1	A	547	GLY	2.4
1	C	549	LYS	2.4
1	C	618	LEU	2.3
1	C	504	ASP	2.3
1	C	525	ASP	2.3
1	C	526	HIS	2.3
1	C	543	GLN	2.3
1	A	607	ARG	2.3
2	D	668	PRO	2.3
1	C	583	GLY	2.3
1	A	652	ARG	2.3
2	D	680	ARG	2.2
2	B	716	LEU	2.2
1	A	597	ARG	2.2
1	C	528	ASP	2.2
1	C	527	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	594	HIS	2.2
1	A	543	GLN	2.2
1	C	542	GLU	2.2
1	C	617	ALA	2.2
2	D	715	HIS	2.2
2	B	654	SER	2.1
2	B	672	GLU	2.1
2	D	684	ASP	2.1
1	C	586	SER	2.1
2	B	704	SER	2.1
2	B	684	ASP	2.1
2	B	670	PRO	2.1
2	B	718	PHE	2.1
1	A	492	GLU	2.1
1	A	493	PRO	2.1
2	B	688	PRO	2.1
2	D	699	ASP	2.1
1	C	613	VAL	2.0
2	D	686	GLY	2.0
1	C	540	LEU	2.0
2	B	673	GLN	2.0
1	C	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	CL	C	701	1/1	0.88	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	702	1/1	0.98	0.07	44,44,44,44	0
3	CA	A	701	1/1	0.98	0.03	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.