



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2023 – 04:27 pm BST

PDB ID : 8AG1
Title : Crystal structure of a novel OX40 antibody
Authors : Gao, H.; Zhou, A.
Deposited on : 2022-07-19
Resolution : 3.30 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

<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
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.34
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

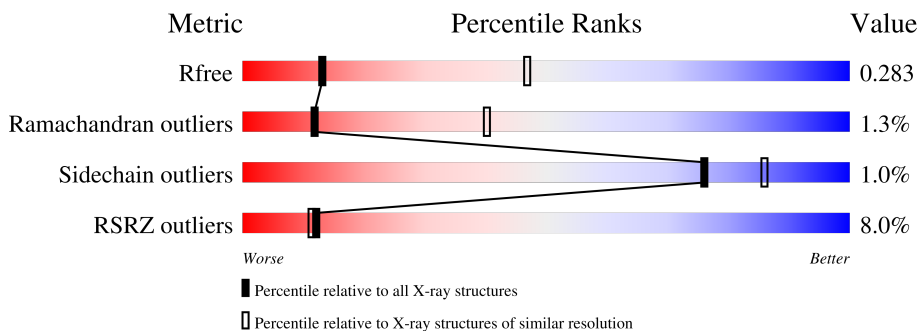
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 $\leq 5\%$. 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	L	216	 97%
1	l	216	 97%
2	H	240	 90% 9%
2	h	240	 89% 10%
3	A	156	 86% 12%
3	a	156	 45% 53%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8038 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 Novel OX40 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	215	Total 1637	C 1024	N 277	O 332	S 4	0	1	0
1	l	216	Total 1636	C 1026	N 273	O 332	S 5	0	1	0

- Molecule 2 is a protein called Novel OX40 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	Total 1657	C 1048	N 275	O 330	S 4	0	0	0
2	h	215	Total 1631	C 1033	N 271	O 323	S 4	0	0	0

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	138	Total 973	C 584	N 177	O 194	S 18	0	0	0
3	a	73	Total 488	C 295	N 84	O 97	S 12	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

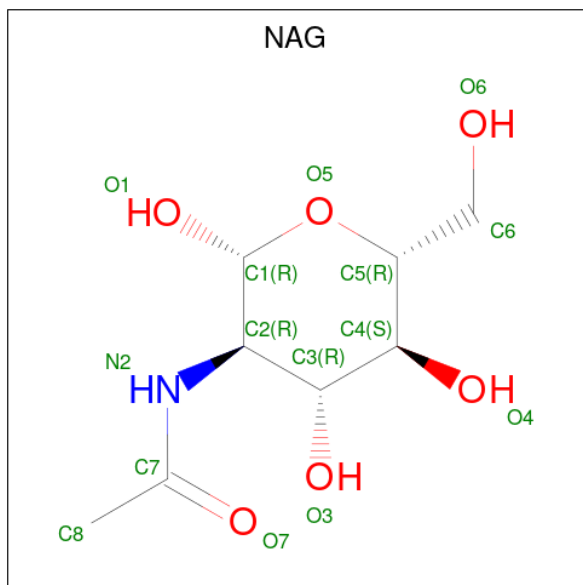
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	LEU	MET	conflict	UNP P43489
A	171	MET	-	expression tag	UNP P43489
A	172	ASP	-	expression tag	UNP P43489
A	173	PRO	-	expression tag	UNP P43489
A	174	GLY	-	expression tag	UNP P43489
A	175	GLY	-	expression tag	UNP P43489
A	176	SER	-	expression tag	UNP P43489
A	177	HIS	-	expression tag	UNP P43489

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Chain	Residue	Modelled	Actual	Comment	Reference
A	178	HIS	-	expression tag	UNP P43489
A	179	HIS	-	expression tag	UNP P43489
A	180	HIS	-	expression tag	UNP P43489
A	181	HIS	-	expression tag	UNP P43489
A	182	HIS	-	expression tag	UNP P43489
A	183	HIS	-	expression tag	UNP P43489
A	184	HIS	-	expression tag	UNP P43489
a	52	LEU	MET	conflict	UNP P43489
a	171	MET	-	expression tag	UNP P43489
a	172	ASP	-	expression tag	UNP P43489
a	173	PRO	-	expression tag	UNP P43489
a	174	GLY	-	expression tag	UNP P43489
a	175	GLY	-	expression tag	UNP P43489
a	176	SER	-	expression tag	UNP P43489
a	177	HIS	-	expression tag	UNP P43489
a	178	HIS	-	expression tag	UNP P43489
a	179	HIS	-	expression tag	UNP P43489
a	180	HIS	-	expression tag	UNP P43489
a	181	HIS	-	expression tag	UNP P43489
a	182	HIS	-	expression tag	UNP P43489
a	183	HIS	-	expression tag	UNP P43489
a	184	HIS	-	expression tag	UNP P43489

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	O	0	0
			1	1		
5	A	1	Total	O	0	0
			1	1		

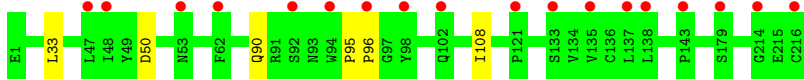
3 Residue-property plots

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.

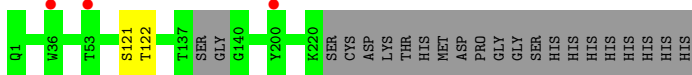
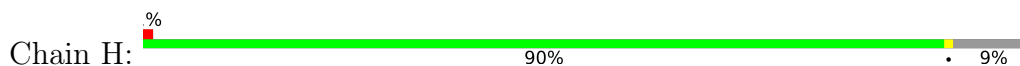
- Molecule 1: Novel OX40 antibody light chain



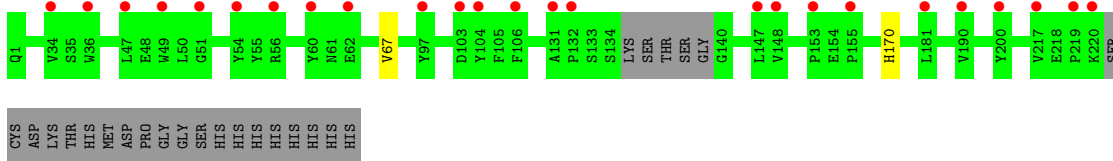
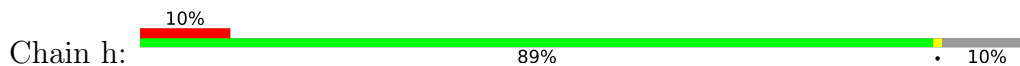
- Molecule 1: Novel OX40 antibody light chain



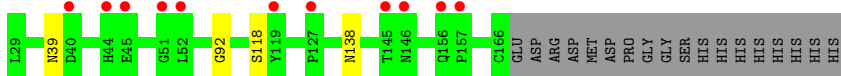
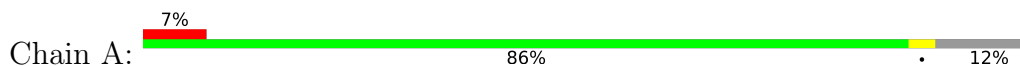
- Molecule 2: Novel OX40 antibody heavy chain



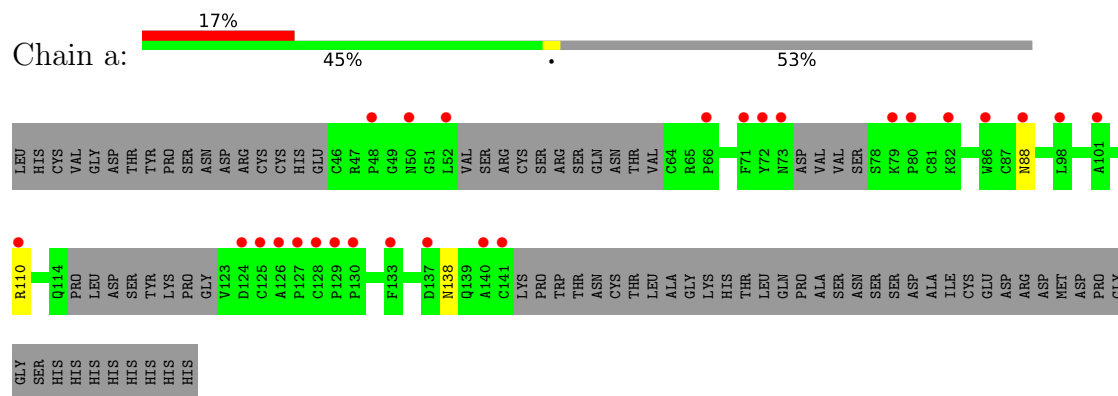
- Molecule 2: Novel OX40 antibody heavy chain



- Molecule 3: Tumor necrosis factor receptor superfamily member 4



- Molecule 3: Tumor necrosis factor receptor superfamily member 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.36Å 162.36Å 232.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.50 – 3.30 77.38 – 3.30	Depositor EDS
% Data completeness (in resolution range)	80.1 (77.50-3.30) 80.2 (77.38-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.33Å)	Xtrriage
Refinement program	REFMAC 8.0.002	Depositor
R, R_{free}	0.194 , 0.268 0.209 , 0.283	Depositor DCC
R_{free} test set	1132 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	97.9	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	L	0.28	0/1678	0.45	0/2287
1	l	0.28	0/1677	0.44	0/2285
2	H	0.28	0/1699	0.48	0/2325
2	h	0.28	0/1673	0.46	0/2291
3	A	0.28	0/998	0.46	0/1370
3	a	0.33	0/499	0.48	0/681
All	All	0.28	0/8224	0.46	0/11239

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	L	214/216 (99%)	191 (89%)	19 (9%)	4 (2%)	8	34
1	l	215/216 (100%)	189 (88%)	23 (11%)	3 (1%)	11	38
2	H	214/240 (89%)	190 (89%)	22 (10%)	2 (1%)	17	48
2	h	211/240 (88%)	192 (91%)	19 (9%)	0	100	100
3	A	136/156 (87%)	121 (89%)	12 (9%)	3 (2%)	6	30
3	a	65/156 (42%)	55 (85%)	8 (12%)	2 (3%)	4	23
All	All	1055/1224 (86%)	938 (89%)	103 (10%)	14 (1%)	12	40

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	121	SER
1	l	50	ASP
3	A	39	ASN
1	L	50	ASP
3	a	138	ASN
2	H	122	THR
3	A	118	SER
1	L	98	TYR
1	L	96	PRO
3	A	92	GLY
3	a	110	ARG
1	L	95	PRO
1	l	95	PRO
1	l	96	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	L	181/186 (97%)	179 (99%)	2 (1%)	73	85
1	l	181/186 (97%)	178 (98%)	3 (2%)	60	78
2	H	192/214 (90%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	188/214 (88%)	186 (99%)	2 (1%)	73	85
3	A	109/136 (80%)	108 (99%)	1 (1%)	78	87
3	a	52/136 (38%)	51 (98%)	1 (2%)	57	77
All	All	903/1072 (84%)	894 (99%)	9 (1%)	76	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	46	LEU
1	L	110	ARG
2	h	67	VAL
2	h	170	HIS
1	l	33	LEU
1	l	90	GLN
1	l	108	ILE
3	A	138	ASN
3	a	88	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	140	ASN
2	H	41	GLN
2	H	161	ASN
2	h	3	GLN
2	h	41	GLN
2	h	161	ASN
1	l	38	GLN
1	l	126	GLN
3	A	114	GLN
3	A	138	ASN
3	A	139	GLN
3	a	88	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	201	3	14,14,15	0.38	0	17,19,21	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	201	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	NAG	C8-C7-N2-C2
4	A	201	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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	L	215/216 (99%)	0.52	3 (1%) 75 75	53, 80, 105, 117	0
1	l	216/216 (100%)	0.52	18 (8%) 11 11	72, 120, 149, 174	0
2	H	218/240 (90%)	0.43	3 (1%) 75 75	57, 84, 119, 138	0
2	h	215/240 (89%)	0.85	25 (11%) 4 4	66, 91, 129, 159	0
3	A	138/156 (88%)	0.55	11 (7%) 12 11	66, 94, 132, 150	0
3	a	73/156 (46%)	1.63	26 (35%) 0 0	90, 130, 150, 151	2 (2%)
All	All	1075/1224 (87%)	0.65	86 (8%) 12 11	53, 95, 140, 174	2 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	l	216	CYS	16.4
3	a	141	CYS	5.9
3	a	129	PRO	5.1
2	h	131	ALA	5.1
3	a	140	ALA	5.1
3	a	110	ARG	5.1
2	h	60	TYR	4.4
3	a	137	ASP	4.0
3	a	128	CYS	4.0
3	a	73	ASN	4.0
3	a	124	ASP	4.0
3	A	146	ASN	3.9
1	l	98	TYR	3.6
3	a	80	PRO	3.6
2	h	106	PHE	3.6
1	l	47	LEU	3.5
3	A	51	GLY	3.4
3	a	126	ALA	3.4
3	a	127	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	62	PHE	3.3
3	a	133	PHE	3.3
1	l	62	PHE	3.3
3	a	48	PRO	3.2
2	h	51	GLY	3.1
2	h	34	VAL	3.1
2	h	220	LYS	3.1
3	A	40	ASP	3.1
3	a	79	LYS	3.0
2	h	190	VAL	3.0
3	a	50	ASN	3.0
3	A	156	GLN	3.0
2	h	49	TRP	3.0
3	a	86	TRP	2.9
1	l	121	PRO	2.9
1	l	102	GLN	2.9
3	A	119	TYR	2.9
1	L	75	ILE	2.8
3	a	71	PHE	2.8
2	h	104	TYR	2.8
2	h	217	VAL	2.8
1	l	94	TRP	2.8
3	a	72	TYR	2.8
3	A	44	HIS	2.8
1	l	96	PRO	2.7
1	l	137	LEU	2.7
2	h	36	TRP	2.7
1	l	135	VAL	2.6
2	h	103	ASP	2.6
2	h	219	PRO	2.6
2	h	97	TYR	2.6
1	l	53	ASN	2.6
3	A	145	THR	2.6
3	a	130	PRO	2.5
3	a	82	LYS	2.5
2	h	155	PRO	2.5
2	h	153	PRO	2.4
2	h	147	LEU	2.4
1	l	133	SER	2.4
2	h	54	TYR	2.4
3	A	52	LEU	2.4
2	H	36	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	45	GLU	2.3
3	a	101	ALA	2.3
1	l	48	ILE	2.3
2	h	181	LEU	2.3
3	a	52	LEU	2.3
2	h	132	PRO	2.3
1	l	214	GLY	2.2
3	a	66	PRO	2.2
2	h	200	TYR	2.2
1	l	138	LEU	2.2
3	A	157	PRO	2.2
3	a	88	ASN	2.2
1	l	179	SER	2.1
2	h	62	GLU	2.1
2	h	148	VAL	2.1
2	h	56	ARG	2.1
1	L	48	ILE	2.1
3	a	125	CYS	2.1
2	H	200	TYR	2.1
3	a	98	LEU	2.1
1	l	143	PRO	2.0
2	h	47	LEU	2.0
2	H	53	THR	2.0
1	l	92	SER	2.0
3	A	127	PRO	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, 95th 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(\AA^2)	Q<0.9
4	NAG	A	201	14/15	0.84	0.17	88,107,115,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.