Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:35 PM GMT

PDB ID	:	1GAF
Title	:	48G7 HYBRIDOMA LINE FAB COMPLEXED WITH HAPTEN 5-(PARA-NITROPHENYL PHOSPHONATE)-PENTANOIC ACID
Authors	:	Wedemayer, G.J.; Patten, P.A.; Stevens, R.C.; Schultz, P.G.
Deposited on	:	1996-02-06
Resolution	:	1.95 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:

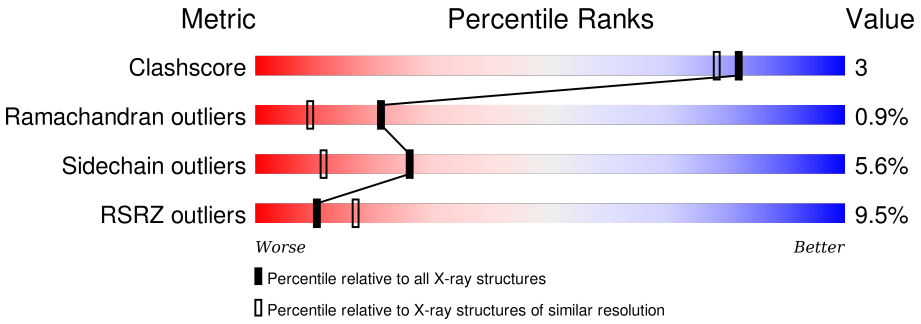
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	L	214	6% 92% 7%
2	H	217	13% 84% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4538 atoms, of which 1085 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 CHIMERIC 48G7 FAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	214	Total	C	H	N	O	S	0	0	0
			2045	1027	395	280	337	6			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	15	LEU	VAL	CONFLICT	GB 4768677
L	17	GLU	ASP	CONFLICT	GB 4768677
L	20	SER	THR	CONFLICT	GB 4768677
L	21	LEU	ILE	CONFLICT	GB 4768677
L	24	ARG	GLN	CONFLICT	GB 4768677
L	28	GLU	ASP	CONFLICT	GB 4768677
L	31	GLY	ASN	CONFLICT	GB 4768677
L	34	GLY	ASN	CONFLICT	GB 4768677
L	36	LEU	TYR	CONFLICT	GB 4768677
L	41	ASP	GLY	CONFLICT	GB 4768677
L	42	GLY	LYS	CONFLICT	GB 4768677
L	44	ILE	PRO	CONFLICT	GB 4768677
L	46	ARG	LEU	CONFLICT	GB 4768677
L	50	ALA	GLY	CONFLICT	GB 4768677
L	53	THR	ASN	CONFLICT	GB 4768677
L	55	HIS	GLU	CONFLICT	GB 4768677
L	56	SER	THR	CONFLICT	GB 4768677
L	60	LYS	SER	CONFLICT	GB 4768677
L	66	ARG	GLY	CONFLICT	GB 4768677
L	69	SER	THR	CONFLICT	GB 4768677
L	71	TYR	PHE	CONFLICT	GB 4768677
L	72	SER	ILE	CONFLICT	GB 4768677
L	73	LEU	PHE	CONFLICT	GB 4768677
L	79	GLU	GLN	CONFLICT	GB 4768677
L	80	SER	PRO	CONFLICT	GB 4768677
L	83	PHE	ILE	CONFLICT	GB 4768677
L	85	ASP	THR	CONFLICT	GB 4768677

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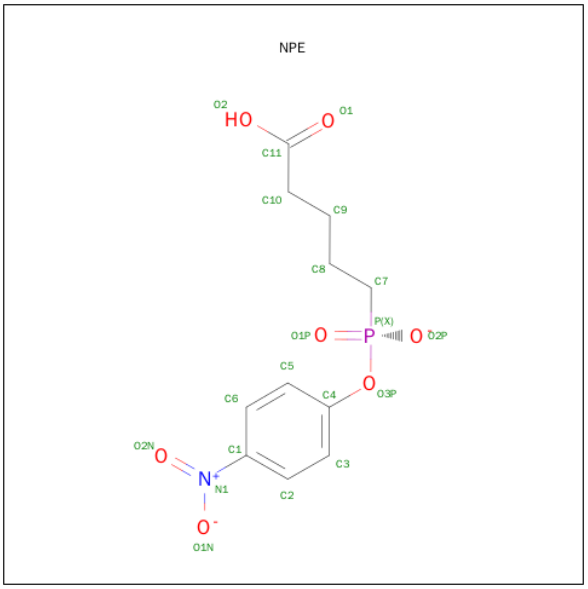
Chain	Residue	Modelled	Actual	Comment	Reference
L	89	LEU	GLN	CONFLICT	GB 4768677
L	92	ALA	ASP	CONFLICT	GB 4768677
L	93	SER	ASN	CONFLICT	GB 4768677
L	94	TYR	LEU	CONFLICT	GB 4768677
L	96	ARG	LEU	CONFLICT	GB 4768677
L	177	SER	ASN	CONFLICT	GB 4768677

- Molecule 2 is a protein called CHIMERIC 48G7 FAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	217	Total	C	H	N	O	S	0	0	0
			2008	1031	376	267	328	6			

- Molecule 3 is 5-(PARA-NITROPHENYL PHOSPHONATE)-PENTANOIC ACID (three-letter code: NPE) (formula: $C_{11}H_{13}NO_7P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	H	1	Total	C	H	N	O	P	0	0
			32	11	12	1	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	78	Total	H	O	0	0
			234	156	78		

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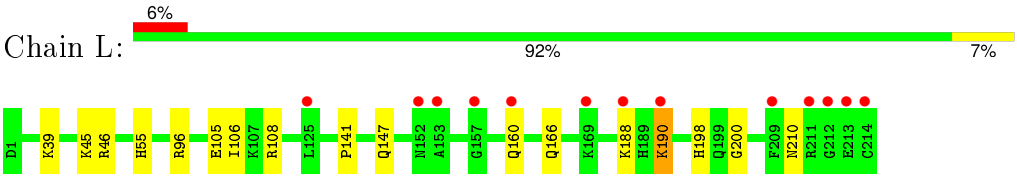
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	73	Total 219	H 146	O 73	0	0

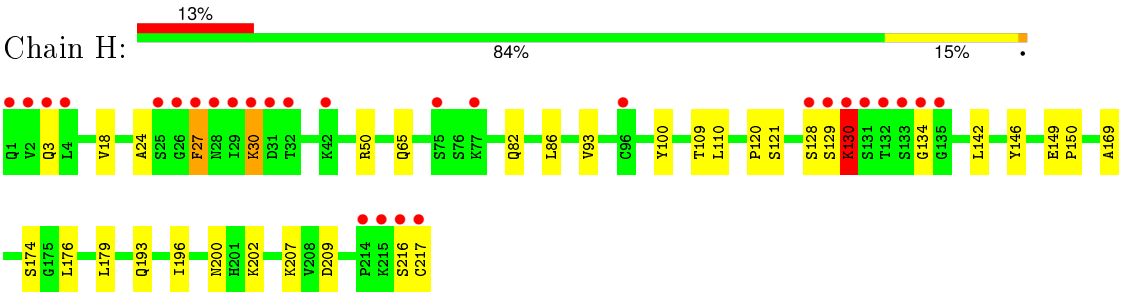
3 Residue-property plots (i)

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: CHIMERIC 48G7 FAB



- Molecule 2: CHIMERIC 48G7 FAB



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.26Å 44.85Å 85.45Å 90.00° 121.55° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.60 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.95) 96.8 (19.60-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 1.94Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.244 , 0.307 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 32279 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4538	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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

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

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	0.35	0/1683	0.64	0/2277
2	H	0.34	0/1671	0.65	0/2278
All	All	0.35	0/3354	0.65	0/4555

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	L	1650	395	1601	10	0
2	H	1632	376	1611	11	1
3	H	20	12	12	1	0
4	H	78	156	0	1	0
4	L	73	146	0	3	1
All	All	3453	1085	3224	21	1

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 3.

All (21) 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)
2:H:196:ILE:HD11	2:H:209:ASP:HB3	1.61	0.82
2:H:149:GLU:HB2	2:H:150:PRO:HA	1.78	0.65
2:H:93:VAL:HG22	2:H:109:THR:HG22	1.83	0.60
1:L:106:ILE:H	1:L:166:GLN:HE22	1.50	0.58
1:L:190:LYS:N	1:L:190:LYS:HD2	2.19	0.58
2:H:120:PRO:HB3	2:H:146:TYR:HB3	1.86	0.58
1:L:46:ARG:HE	1:L:55:HIS:HD2	1.51	0.56
2:H:216:SER:N	4:H:279:HOH:O	2.38	0.56
1:L:45:LYS:HG2	4:L:283:HOH:O	2.05	0.56
2:H:24:ALA:HB1	2:H:27:PHE:HD2	1.74	0.53
1:L:198:HIS:CD2	1:L:200:GLY:H	2.27	0.53
2:H:30:LYS:H	2:H:30:LYS:HD2	1.74	0.52
1:L:190:LYS:HD2	1:L:190:LYS:H	1.76	0.49
1:L:141:PRO:O	1:L:198:HIS:HE1	1.97	0.48
1:L:39:LYS:HG3	4:L:283:HOH:O	2.15	0.47
1:L:106:ILE:HD12	4:L:275:HOH:O	2.15	0.47
2:H:169:ALA:HB2	2:H:179:LEU:HD23	1.97	0.45
2:H:129:SER:O	2:H:130:LYS:HB3	2.16	0.44
2:H:18:VAL:HG22	2:H:86:LEU:HD11	2.00	0.44
1:L:96:ARG:NH2	3:H:218:NPE:H81	2.35	0.41
2:H:200:ASN:HD22	2:H:202:LYS:NZ	2.19	0.41

All (1) 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)
2:H:174:SER:HG	4:L:222:HOH:H1[4_555]	1.05	0.55

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	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	34 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	215/217 (99%)	203 (94%)	9 (4%)	3 (1%)	14 4
All	All	427/431 (99%)	406 (95%)	17 (4%)	4 (1%)	21 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	130	LYS
2	H	128	SER
1	L	210	ASN
2	H	134	GLY

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	187/187 (100%)	181 (97%)	6 (3%)	46 33
2	H	187/187 (100%)	172 (92%)	15 (8%)	15 4
All	All	374/374 (100%)	353 (94%)	21 (6%)	26 11

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	105	GLU
1	L	108	ARG
1	L	147	GLN
1	L	160	GLN
1	L	188	LYS
1	L	190	LYS
2	H	3	GLN
2	H	27	PHE
2	H	30	LYS
2	H	50	ARG
2	H	65	GLN
2	H	82	GLN

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Mol	Chain	Res	Type
2	H	100	TYR
2	H	110	LEU
2	H	121	SER
2	H	130	LYS
2	H	142	LEU
2	H	176	LEU
2	H	193	GLN
2	H	207	LYS
2	H	217	CYS

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

Mol	Chain	Res	Type
1	L	6	GLN
1	L	55	HIS
1	L	137	ASN
1	L	166	GLN
1	L	198	HIS
2	H	65	GLN
2	H	156	ASN
2	H	165	HIS
2	H	200	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 carbohydrates 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	$\#\|Z\| > 2$
3	NPE	H	218	-	14,20,20	3.19	5 (35%)	19,27,27	1.15	2 (10%)

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
3	NPE	H	218	-	-	0/14/17/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	218	NPE	P-O2P	-3.96	1.43	1.52
3	H	218	NPE	P-O3P	-3.81	1.52	1.62
3	H	218	NPE	P-O1P	-3.81	1.42	1.51
3	H	218	NPE	C6-C1	2.26	1.43	1.38
3	H	218	NPE	O2N-N1	8.94	1.40	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	218	NPE	C6-C1-N1	2.21	121.26	119.48
3	H	218	NPE	O1P-P-C7	3.02	114.11	108.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	218	NPE	1	0

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	L	214/214 (100%)	0.53	13 (6%) 25 34	5, 16, 37, 104	0
2	H	217/217 (100%)	1.04	28 (12%) 5 8	6, 16, 73, 100	0
All	All	431/431 (100%)	0.79	41 (9%) 10 17	5, 16, 55, 104	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	GLY	20.3
2	H	217	CYS	19.1
2	H	27	PHE	17.5
1	L	213	GLU	17.5
2	H	216	SER	15.0
2	H	132	THR	13.5
1	L	214	CYS	11.7
2	H	130	LYS	9.8
2	H	1	GLN	8.5
2	H	129	SER	8.4
2	H	26	GLY	8.0
2	H	29	ILE	8.0
2	H	133	SER	7.9
2	H	134	GLY	7.6
2	H	2	VAL	5.5
2	H	215	LYS	5.3
2	H	131	SER	5.1
1	L	211	ARG	5.1
2	H	30	LYS	4.8
2	H	128	SER	4.8
2	H	31	ASP	4.8
2	H	3	GLN	4.6
2	H	135	GLY	3.5
2	H	28	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	209	PHE	3.1
2	H	4	LEU	3.1
1	L	169	LYS	3.0
1	L	160	GLN	2.8
2	H	25	SER	2.8
1	L	157	GLY	2.7
1	L	153	ALA	2.6
2	H	32	THR	2.5
2	H	214	PRO	2.4
2	H	75	SER	2.3
1	L	190	LYS	2.3
1	L	125	LEU	2.3
1	L	152	ASN	2.2
2	H	96	CYS	2.2
1	L	188	LYS	2.2
2	H	42	LYS	2.2
2	H	77	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	NPE	H	218	20/20	0.95	0.13	0.02	0,14,45,48	0

6.5 Other polymers (i)

There are no such residues in this entry.