



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 10:06 am BST

PDB ID : 7O07
Title : 14-3-3sigma covalently bound to peptide (chloroacetamide-Cys interaction)
Authors : Somsen, B.A.; Ottmann, C.
Deposited on : 2021-03-25
Resolution : 1.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

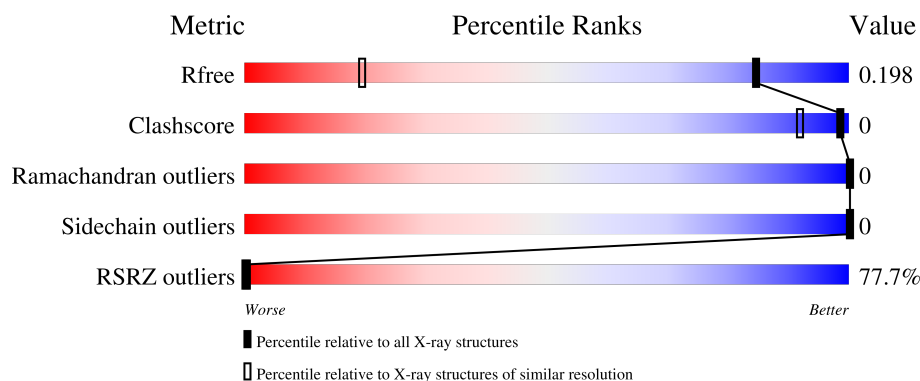
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	A	236	<div> <div>77%</div> <div> <div></div> <div>97%</div> <div>..</div> </div> </div>
2	P	12	<div> <div>58%</div> <div> <div>75%</div> <div>17%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2401 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 14-3-3 protein sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1987	1238	334	401	14	0	22	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P31947
A	-3	ALA	-	expression tag	UNP P31947
A	-2	MET	-	expression tag	UNP P31947
A	-1	GLY	-	expression tag	UNP P31947
A	0	SER	-	expression tag	UNP P31947

- Molecule 2 is a protein called Transcriptional coactivator YAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	11	94	55	19	19	1	0	1	1

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		

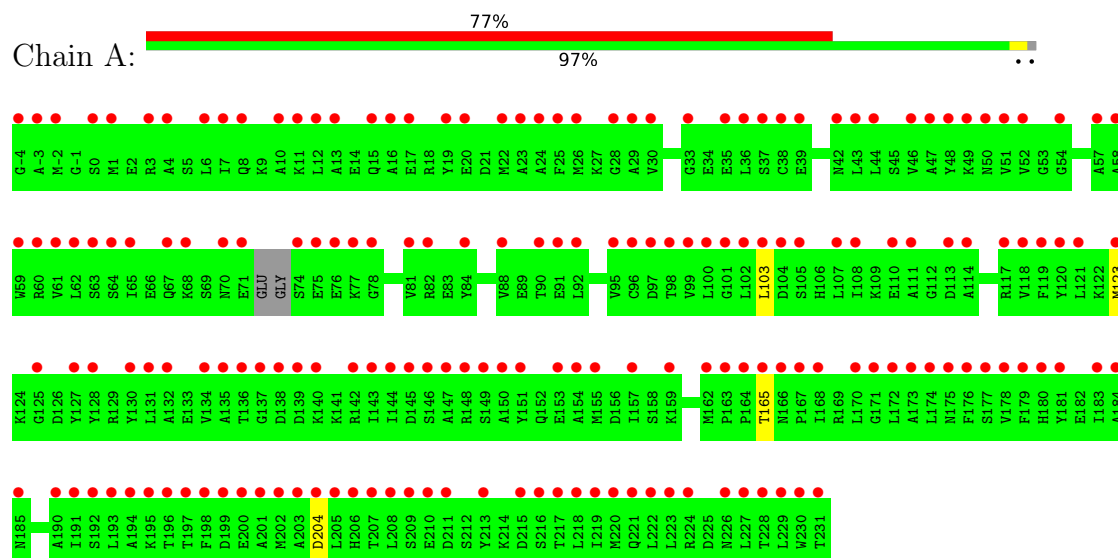
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	P	21	Total	O	0	0
			21	21		

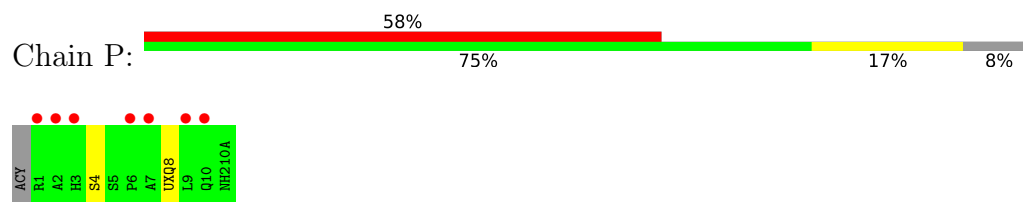
3 Residue-property plots

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: 14-3-3 protein sigma



• Molecule 2: Transcriptional coactivator YAP1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	82.59Å 112.58Å 63.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 1.20 66.59 – 1.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.88-1.20) 95.9 (66.59-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.20Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.184 , 0.196 0.186 , 0.198	Depositor DCC
R_{free} test set	4633 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2401	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 5.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, NH2, MG, UXQ

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	0.30	0/2012	0.50	0/2705
2	P	0.26	0/66	0.48	0/86
All	All	0.30	0/2078	0.50	0/2791

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	1987	0	1915	2	0
2	P	94	0	71	0	0
3	A	4	0	0	0	0
4	A	295	0	0	0	0
4	P	21	0	0	0	0
All	All	2401	0	1986	2	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 0.

All (2) 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:A:103:LEU:HD21	1:A:123[A]:MET:HE2	1.82	0.62
1:A:165:THR:HG23	1:A:204:ASP:HB3	1.95	0.49

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	252/236 (107%)	248 (98%)	4 (2%)	0	100	100
2	P	8/12 (67%)	8 (100%)	0	0	100	100
All	All	260/248 (105%)	256 (98%)	4 (2%)	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	208/198 (105%)	208 (100%)	0	100	100
2	P	7/6 (117%)	7 (100%)	0	100	100
All	All	215/204 (105%)	215 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
2	SEP	P	4	2	8,9,10	1.25	1 (12%)	8,12,14	0.95	0
2	UXQ	P	8	1,2	15,16,18	0.34	0	17,20,23	0.83	1 (5%)

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
2	SEP	P	4	2	-	0/5/8/10	-
2	UXQ	P	8	1,2	-	0/10/11/15	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	4	SEP	P-O1P	2.67	1.59	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	8	UXQ	O1-C9-C10	-2.54	117.34	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	A	234/236 (99%)	3.03	181 (77%) 0 0	8, 12, 31, 48	0
2	P	8/12 (66%)	4.29	7 (87%) 0 0	12, 16, 27, 42	0
All	All	242/248 (97%)	3.07	188 (77%) 0 0	8, 13, 31, 48	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	SER	10.6
1	A	-3	ALA	9.2
1	A	137	GLY	7.0
2	P	9	LEU	6.6
1	A	229[A]	LEU	6.6
2	P	1	ARG	6.5
1	A	70	ASN	6.0
1	A	219[A]	ILE	5.9
1	A	231	THR	5.6
2	P	2	ALA	5.5
1	A	198	PHE	5.3
1	A	36	LEU	5.3
1	A	52[A]	VAL	5.2
2	P	7	ALA	5.1
1	A	121	LEU	5.0
1	A	7[A]	ILE	5.0
1	A	178	VAL	4.8
1	A	119	PHE	4.7
1	A	218	LEU	4.7
1	A	139	ASP	4.6
1	A	151	TYR	4.6
1	A	127	TYR	4.5
1	A	95	VAL	4.5
1	A	38	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	VAL	4.5
1	A	118	VAL	4.4
1	A	128	TYR	4.4
1	A	172	LEU	4.4
1	A	168	ILE	4.4
1	A	25	PHE	4.4
1	A	30	VAL	4.4
1	A	44	LEU	4.3
1	A	46	VAL	4.3
1	A	99	VAL	4.3
1	A	-4	GLY	4.3
1	A	143	ILE	4.3
1	A	120	TYR	4.3
1	A	130	TYR	4.3
1	A	213	TYR	4.3
1	A	155[A]	MET	4.3
1	A	230	TRP	4.3
1	A	96	CYS	4.2
1	A	76	GLU	4.2
1	A	123[A]	MET	4.2
1	A	62	LEU	4.1
1	A	77	LYS	4.1
1	A	51	VAL	4.1
1	A	6	LEU	4.0
1	A	228	THR	4.0
1	A	157	ILE	4.0
1	A	144	ILE	4.0
1	A	183	ILE	4.0
1	A	176	PHE	3.9
1	A	103	LEU	3.9
1	A	211	ASP	3.9
1	A	191	ILE	3.9
1	A	59	TRP	3.9
1	A	19	TYR	3.9
1	A	100	LEU	3.9
1	A	174	LEU	3.9
1	A	60[A]	ARG	3.8
1	A	84	TYR	3.8
1	A	43	LEU	3.8
1	A	92[A]	LEU	3.8
1	A	207	THR	3.7
1	A	108	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	3.7
1	A	88	VAL	3.7
1	A	75	GLU	3.7
1	A	138	ASP	3.7
1	A	162	MET	3.6
1	A	12	LEU	3.6
1	A	102	LEU	3.6
1	A	170	LEU	3.6
2	P	10	GLN	3.6
1	A	48	TYR	3.6
1	A	134	VAL	3.6
1	A	222	LEU	3.6
1	A	61	VAL	3.5
1	A	202[A]	MET	3.4
1	A	193	LEU	3.4
1	A	208	LEU	3.4
1	A	107	LEU	3.4
1	A	131	LEU	3.4
1	A	78	GLY	3.3
1	A	224	ARG	3.3
1	A	179	PHE	3.3
1	A	165	THR	3.3
1	A	24	ALA	3.3
1	A	181	TYR	3.3
1	A	65	ILE	3.3
1	A	185	ASN	3.2
1	A	184	ALA	3.2
1	A	105	SER	3.2
1	A	140	LYS	3.2
1	A	-2	MET	3.2
1	A	205	LEU	3.1
1	A	227	LEU	3.1
1	A	190	ALA	3.1
1	A	71	GLU	3.1
1	A	22	MET	3.1
1	A	0[A]	SER	3.1
1	A	23	ALA	3.1
1	A	173	ALA	3.1
1	A	26	MET	3.1
1	A	47	ALA	3.0
1	A	194	ALA	3.0
1	A	10	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	98	THR	3.0
1	A	197	THR	3.0
1	A	90	THR	3.0
1	A	136	THR	3.0
1	A	29	ALA	2.9
1	A	113	ASP	2.9
2	P	3	HIS	2.9
1	A	58	ALA	2.9
1	A	217	THR	2.9
1	A	33	GLY	2.9
1	A	154	ALA	2.9
1	A	28	GLY	2.8
1	A	196[A]	THR	2.8
1	A	132	ALA	2.8
1	A	164	PRO	2.8
1	A	209	SER	2.8
1	A	13	ALA	2.8
1	A	145	ASP	2.8
1	A	4	ALA	2.8
1	A	49	LYS	2.8
1	A	159	LYS	2.8
1	A	42	ASN	2.8
1	A	148[A]	ARG	2.7
1	A	97	ASP	2.7
1	A	101	GLY	2.7
1	A	206	HIS	2.7
1	A	57	ALA	2.7
1	A	201	ALA	2.7
1	A	150	ALA	2.7
1	A	175	ASN	2.7
1	A	16	ALA	2.7
1	A	167	PRO	2.6
1	A	142	ARG	2.6
1	A	221	GLN	2.6
1	A	82	ARG	2.6
1	A	1	MET	2.6
1	A	110	GLU	2.6
1	A	117	ARG	2.6
1	A	63[A]	SER	2.5
1	A	149[A]	SER	2.5
1	A	39	GLU	2.5
1	A	146	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	153	GLU	2.5
1	A	203	ALA	2.5
1	A	171	GLY	2.5
1	A	91[A]	GLU	2.5
1	A	192[A]	SER	2.5
1	A	223	LEU	2.4
1	A	64	SER	2.4
1	A	125	GLY	2.4
1	A	50	ASN	2.4
1	A	177[A]	SER	2.4
1	A	163	PRO	2.4
1	A	226	ASN	2.3
1	A	8	GLN	2.3
1	A	199	ASP	2.3
1	A	204	ASP	2.3
1	A	210	GLU	2.3
1	A	17[A]	GLU	2.3
1	A	220	MET	2.3
1	A	200	GLU	2.3
1	A	111	ALA	2.3
1	A	54	GLY	2.3
1	A	67	GLN	2.3
1	A	215	ASP	2.2
2	P	6	PRO	2.2
1	A	20[A]	GLU	2.2
1	A	35	GLU	2.2
1	A	195	LYS	2.2
1	A	180	HIS	2.2
1	A	135	ALA	2.2
1	A	114	ALA	2.1
1	A	166	ASN	2.1
1	A	3	ARG	2.1
1	A	37	SER	2.1
1	A	15	GLN	2.0
1	A	11	LYS	2.0
1	A	68	LYS	2.0
1	A	104	ASP	2.0
1	A	216	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	UXQ	P	8	16/18	0.77	0.24	13,15,20,21	0
2	SEP	P	4	10/11	0.91	0.21	10,12,12,12	0

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(Å ²)	Q<0.9
3	MG	A	301	1/1	0.92	0.17	21,21,21,21	0
3	MG	A	303	1/1	0.96	0.21	11,11,11,11	1
3	MG	A	304	1/1	0.98	0.15	21,21,21,21	0
3	MG	A	302	1/1	0.99	0.23	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.