

Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 05:46 PM EDT

PDB ID : 4LSC

Title: Isolated SERK1 co-receptor ectodomain at high resolution

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Deposited on : 2013-07-22

Resolution : 1.53 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 (i) 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 (1)) 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 : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

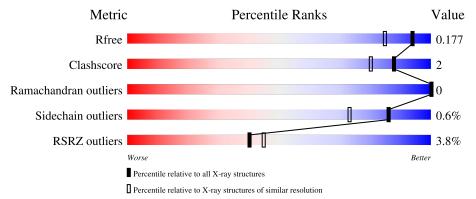
 $Validation\ Pipeline\ (wwPDB-VP) \quad : \quad 2.35.1$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.53 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 $(\#\text{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	223	81%	·	17%
2	В	4	50%	50%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	В	3	_	-	-	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3136 atoms, of which 1463 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 Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	186	Total 2911	C 922	H 1463	N 244	O 277	S 5	0	10	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP Q94AG2
A	20	GLY	-	expression tag	UNP Q94AG2
A	21	SER	-	expression tag	UNP Q94AG2
A	22	SER	_	expression tag	UNP Q94AG2
A	23	MET	-	expression tag	UNP Q94AG2
A	115	ASP	ASN	engineered mutation	UNP Q94AG2
A	163	GLN	ASN	engineered mutation	UNP Q94AG2
A	214	LEU	-	expression tag	UNP Q94AG2
A	215	GLU	-	expression tag	UNP Q94AG2
A	216	ASN	-	expression tag	UNP Q94AG2
A	217	LEU	-	expression tag	UNP Q94AG2
A	218	TYR	-	expression tag	UNP Q94AG2
A	219	PHE	-	expression tag	UNP Q94AG2
A	220	GLN	-	expression tag	UNP Q94AG2
A	221	GLY	-	expression tag	UNP Q94AG2
A	222	ALA	-	expression tag	UNP Q94AG2
A	223	TRP	-	expression tag	UNP Q94AG2
A	224	SER	-	expression tag	UNP Q94AG2
A	225	HIS	-	expression tag	UNP Q94AG2
A	226	PRO	-	expression tag	UNP Q94AG2
A	227	GLN	-	expression tag	UNP Q94AG2
A	228	PHE	-	expression tag	UNP Q94AG2
A	229	GLU		expression tag	UNP Q94AG2
A	230	LYS		expression tag	UNP Q94AG2
A	231	GLY		expression tag	UNP Q94AG2
A	232	SER		expression tag	UNP Q94AG2
A	233	HIS	-	expression tag	UNP Q94AG2

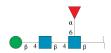
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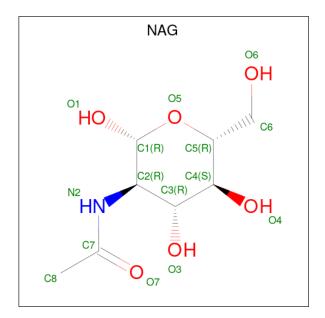
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	HIS	-	expression tag	UNP Q94AG2
A	235	HIS	-	expression tag	UNP Q94AG2
A	236	HIS	-	expression tag	UNP Q94AG2
A	237	HIS	-	expression tag	UNP Q94AG2
A	238	HIS	-	expression tag	UNP Q94AG2
A	239	HIS	-	expression tag	UNP Q94AG2
A	240	HIS	=	expression tag	UNP Q94AG2
A	241	HIS	-	expression tag	UNP Q94AG2

• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	4	Total 49	C 28	N 2	O 19	0	0	0

 \bullet Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$





\mathbf{Mol}	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
3	A	1	Total 14			O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0

\bullet Molecule 4 is water.

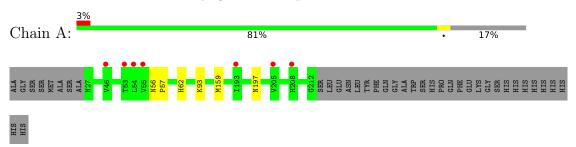
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	148	Total O 148 148	0	0



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: Somatic embryogenesis receptor kinase 1



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50% 50%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	72.63Å 72.63Å 80.97Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.67 - 1.53	Depositor
Resolution (A)	49.67 - 1.53	EDS
% Data completeness	100.0 (49.67-1.53)	Depositor
(in resolution range)	100.0 (49.67-1.53)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	2.08 (at 1.53Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1334)	Depositor
D.D.	0.167 , 0.177	Depositor
R, R_{free}	0.166 , 0.177	DCC
R_{free} test set	1830 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.48, 50.6	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: BMA, NAG, FUC

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	0/1510	0.63	0/2074	

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)

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	1448	1463	1450	6	0
2	В	49	0	43	0	0
3	A	28	0	26	4	0
4	A	148	0	0	1	0
All	All	1673	1463	1519	6	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 2.

All (6) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\left(\operatorname{\mathring{A}} ight)$	$ ext{overlap }(ext{Å})$
1:A:159:MET:CE	3:A:1005:NAG:H5	2.11	0.80
1:A:159:MET:HE2	3:A:1005:NAG:H5	1.83	0.58
1:A:159:MET:HE3	3:A:1005:NAG:H5	1.88	0.51
1:A:62:HIS:ND1	4:A:1212:HOH:O	2.35	0.48
1:A:197:ASN:ND2	3:A:1004:NAG:O6	2.47	0.47
1:A:56:ASN:HB2	1:A:57:PRO:HD2	1.99	0.44

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	194/223 (87%)	188 (97%)	6 (3%)	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.

N	Mol	Chain	Analysed	Rotameric	Outliers	F	erce	entiles
	1	A	174/200 (87%)	173 (99%)	1 (1%)		86	73

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LYS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	A	197	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)

4 monosaccharides 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	Tune	Chain	Res	Link	Link Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	0.38	0	17,19,21	0.86	0
2	NAG	В	2	2	14,14,15	0.90	1 (7%)	17,19,21	0.93	2 (11%)
2	BMA	В	3	2	11,11,12	1.64	3 (27%)	15,15,17	1.89	4 (26%)
2	FUC	В	4	2	10,10,11	1.03	0	14,14,16	1.02	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
2	NAG	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1
2	BMA	В	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	В	4	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	В	3	BMA	C4-C3	3.33	1.60	1.52
2	В	2	NAG	O5-C1	-3.28	1.38	1.43
2	В	3	BMA	C4-C5	3.27	1.59	1.53
2	В	3	BMA	O5-C1	-2.54	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
2	В	3	BMA	C1-C2-C3	-4.15	104.57	109.67
2	В	3	BMA	C3-C4-C5	3.84	117.09	110.24
2	В	3	BMA	C1-O5-C5	-2.60	108.68	112.19
2	В	2	NAG	O4-C4-C5	-2.39	103.36	109.30
2	В	3	BMA	C2-C3-C4	2.12	114.56	110.89
2	В	2	NAG	C3-C4-C5	2.05	113.90	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

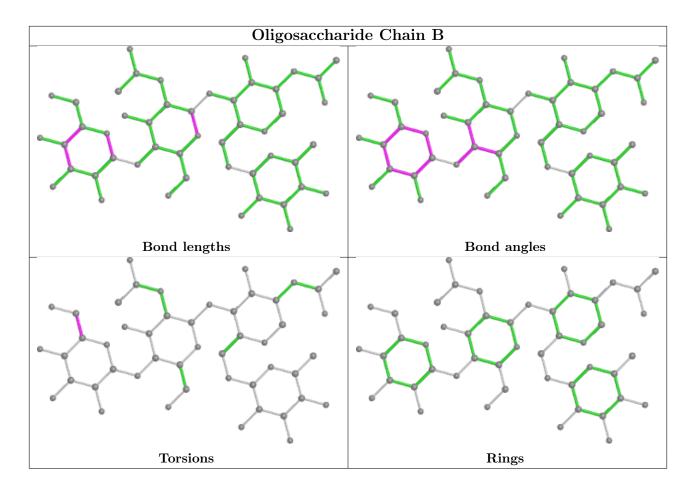
Mol	Chain	Res	Type	Atoms
2	В	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry (i)

2 ligands 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	Trme	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dag	T inle	Bo	ond leng	ths	В	ond ang	les
	Type		Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2									
3	NAG	A	1004	1	14,14,15	0.28	0	17,19,21	0.79	1 (5%)									
3	NAG	A	1005	1	14,14,15	0.22	0	17,19,21	0.44	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
3	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1005	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1004	NAG	C1-O5-C5	2.55	115.64	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	NAG	O5-C5-C6-O6
3	A	1004	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	NAG	1	0
3	A	1005	NAG	3	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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.

\mathbf{N}	Iol	Chain	Analysed	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9	
	1	A	186/223 (83%)	0.22	7 (3%)	40 45		15, 23, 48, 65	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	VAL	5.3
1	A	54	LEU	3.7
1	A	208[A]	HIS	3.5
1	A	53	THR	2.8
1	A	193[A]	ILE	2.7
1	A	205	VAL	2.6
1	A	46[A]	VAL	2.4

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

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

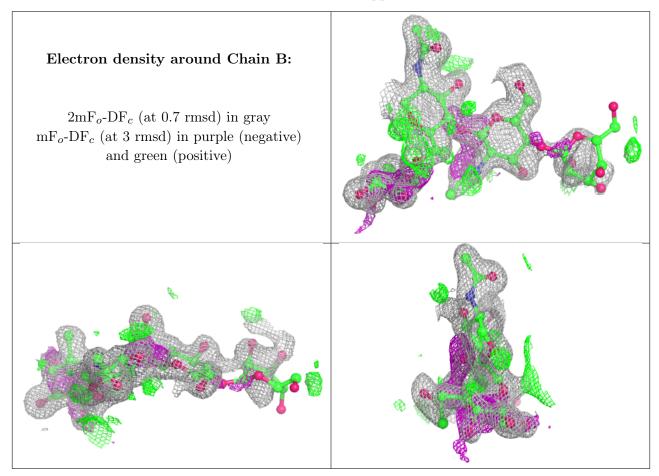
6.3 Carbohydrates (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BMA	В	3	11/12	0.47	0.51	84,89,92,93	0
2	NAG	В	2	14/15	0.74	0.26	33,48,57,79	0
2	NAG	В	1	14/15	0.82	0.11	23,27,30,34	0
2	FUC	В	4	10/11	0.88	0.27	20,27,30,30	0



The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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	${f B-factors(\AA^2)}$	Q<0.9
3	NAG	A	1005	14/15	0.83	0.16	54,65,80,85	0
3	NAG	A	1004	14/15	0.85	0.23	26,36,46,64	0

6.5 Other polymers (i)

There are no such residues in this entry.

