Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:57 PM GMT

PDB ID	:	4QIN
Title	:	Structure of the human smoothened receptor in complex with SAG1.5
Authors	:	Wang, C.; Wu, H.; Evron, T.; Vardy, E.; Han, G.W.; Huang, X.-P.; Hufeisen, S.J.; Mangano, T.J.; Urban, D.J.; Katritch, V.; Cherezov, V.; Caron, M.G.; Roth, B.L.; Stevens, R.C.; GPCR Network (GPCR)
Deposited on	:	2014-05-31
Resolution	:	2.60 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:

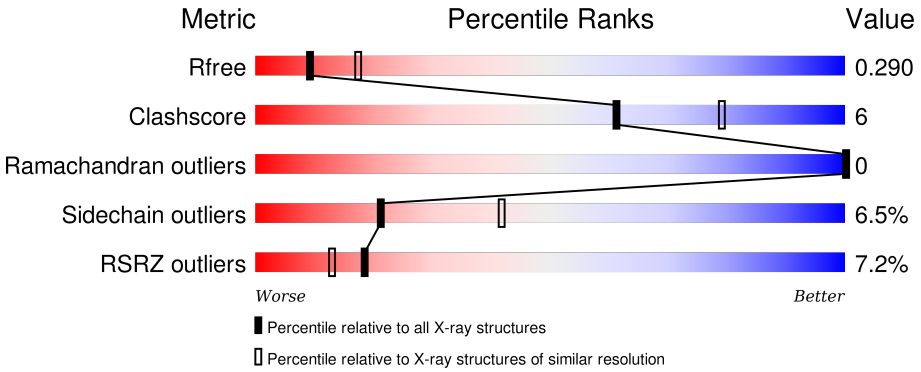
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	A	468	7% 80% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3454 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.

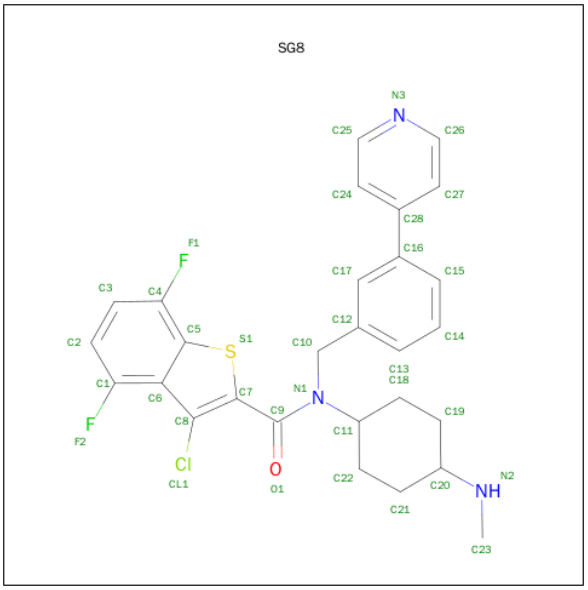
- Molecule 1 is a protein called Smoothened homolog/Soluble cytochrome b562 chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3411	2215	556	619	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	EXPRESSION TAG	UNP Q99835
A	188	GLY	-	EXPRESSION TAG	UNP Q99835
A	189	THR	-	EXPRESSION TAG	UNP Q99835
A	1007	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7
A	1102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
A	1106	LEU	ARG	ENGINEERED MUTATION	UNP P0ABE7

- Molecule 2 is 3-CHLORO-4,7-DIFLUORO-N-[TRANS-4-(METHYLAMINO)CYCLOHEXYL]-N-[3-(PYRIDIN-4-YL)BENZYL]-1-BENZOTHIOPHENE-2-CARBOXAMIDE (three-letter code: SG8) (formula: $C_{28}H_{26}ClF_2N_3OS$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			36	28	1	2	3	1	1		

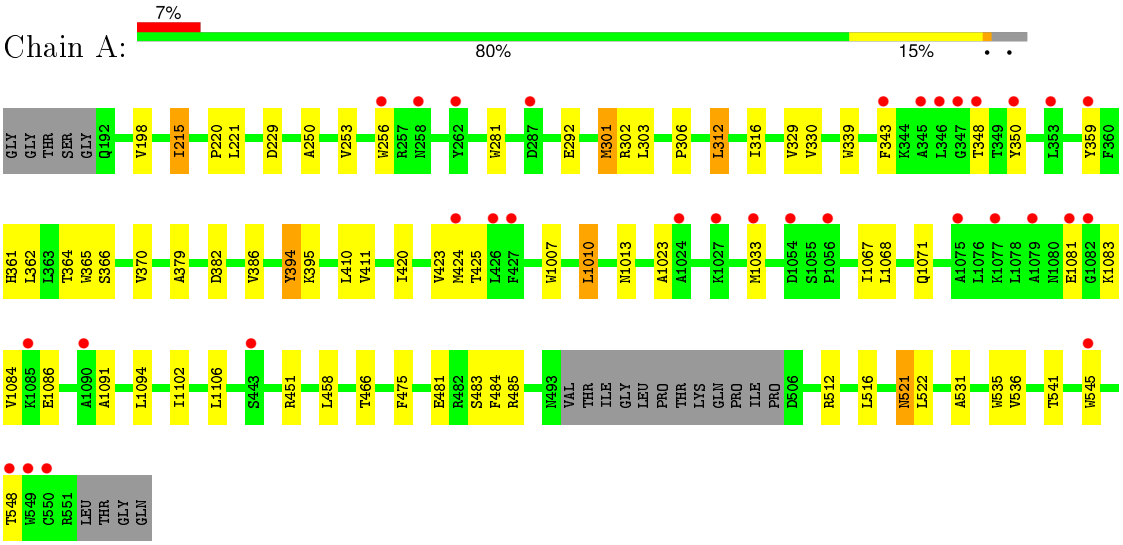
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

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: Smoothened homolog/Soluble cytochrome b562 chimeric protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.22Å 158.93Å 60.02Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	44.42 – 2.60 44.42 – 2.59	Depositor EDS
% Data completeness (in resolution range)	72.1 (44.42-2.60) 72.5 (44.42-2.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.99 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.225 , 0.260 0.249 , 0.290	Depositor DCC
R_{free} test set	754 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.7	EDS
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Outliers	0 of 15154 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3454	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% 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: SG8

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	0.51	0/3498	0.66	0/4772

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	3411	0	3220	37	0
2	A	36	0	26	3	0
3	A	7	0	0	0	0
All	All	3454	0	3246	37	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 6.

All (37) 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:382:ASP:HB2	1:A:394:TYR:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD11	1:A:220:PRO:HG2	1.62	0.80
1:A:312:LEU:HD13	1:A:312:LEU:H	1.55	0.72
1:A:329:VAL:HB	1:A:411:VAL:HG21	1.71	0.71
1:A:306:PRO:HD2	1:A:379:ALA:HA	1.75	0.69
1:A:301:MET:HE3	2:A:1201:SG8:H8	1.77	0.65
1:A:215:ILE:HD11	1:A:220:PRO:CG	2.28	0.64
1:A:221:LEU:O	1:A:512:ARG:HD2	1.96	0.64
1:A:343:PHE:HB3	1:A:425:THR:HG21	1.85	0.58
1:A:215:ILE:CD1	1:A:220:PRO:HG2	2.33	0.57
1:A:215:ILE:HD13	1:A:484:PHE:HZ	1.71	0.56
1:A:420:ILE:O	1:A:424:MET:HG3	2.08	0.54
1:A:330:VAL:HG21	1:A:364:THR:HA	1.91	0.53
1:A:281:TRP:CH2	1:A:522:LEU:HD21	2.44	0.53
1:A:301:MET:CE	2:A:1201:SG8:H8	2.39	0.52
1:A:312:LEU:O	1:A:316:ILE:HG12	2.09	0.52
1:A:536:VAL:HB	1:A:541:THR:HG21	1.92	0.52
1:A:366:SER:O	1:A:370:VAL:HG23	2.10	0.52
1:A:451:ARG:NH1	1:A:535:TRP:O	2.45	0.50
1:A:1023:ALA:HB2	1:A:1084:VAL:HG22	1.94	0.50
1:A:303:LEU:HD13	1:A:395:LYS:HD2	1.94	0.50
1:A:250:ALA:HA	1:A:253:VAL:HG12	1.95	0.48
1:A:330:VAL:CG2	1:A:364:THR:HA	2.42	0.48
1:A:1010:LEU:HD11	1:A:1068:LEU:HD21	1.95	0.48
1:A:458:LEU:HD23	1:A:531:ALA:HB1	1.94	0.48
1:A:481:GLU:HG2	2:A:1201:SG8:H25	1.94	0.48
1:A:1068:LEU:HD22	1:A:1102:ILE:HD11	1.96	0.47
1:A:339:TRP:HH2	1:A:423:VAL:HG13	1.79	0.47
1:A:1091:ALA:O	1:A:1094:LEU:HB2	2.14	0.47
1:A:1013:ASN:HD22	1:A:1033:MET:HG3	1.80	0.47
1:A:1083:LYS:HB3	1:A:1086:GLU:HB2	1.97	0.45
1:A:466:THR:HG23	1:A:521:ASN:HD21	1.81	0.45
1:A:215:ILE:HD13	1:A:484:PHE:CZ	2.50	0.45
1:A:1067:ILE:O	1:A:1071:GLN:HG2	2.18	0.43
1:A:361:HIS:O	1:A:365:TRP:HD1	2.01	0.43
1:A:545:TRP:HA	1:A:548:THR:HG22	2.03	0.40
1:A:348:THR:C	1:A:350:TYR:H	2.25	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	443/468 (95%)	420 (95%)	23 (5%)	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	338/390 (87%)	316 (94%)	22 (6%)	21 42

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	VAL
1	A	215	ILE
1	A	229	ASP
1	A	256	TRP
1	A	292	GLU
1	A	301	MET
1	A	302	ARG
1	A	312	LEU
1	A	359	TYR
1	A	362	LEU
1	A	386	VAL
1	A	394	TYR
1	A	410	LEU

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Mol	Chain	Res	Type
1	A	1007	TRP
1	A	1010	LEU
1	A	1081	GLU
1	A	1106	LEU
1	A	475	PHE
1	A	483	SER
1	A	485	ARG
1	A	516	LEU
1	A	521	ASN

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

Mol	Chain	Res	Type
1	A	231	HIS
1	A	1013	ASN
1	A	1088	GLN
1	A	521	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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	SG8	A	1201	-	35,40,40	3.12	12 (34%)	44,57,57	1.81	14 (31%)

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	SG8	A	1201	-	-	0/18/32/32	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	SG8	F2-C1	-2.03	1.32	1.35
2	A	1201	SG8	C18-C11	2.26	1.58	1.52
2	A	1201	SG8	C11-N1	2.82	1.52	1.47
2	A	1201	SG8	C2-C1	2.98	1.40	1.36
2	A	1201	SG8	C10-C12	3.67	1.58	1.51
2	A	1201	SG8	C24-C28	4.46	1.48	1.39
2	A	1201	SG8	C25-N3	5.32	1.49	1.33
2	A	1201	SG8	C27-C26	5.56	1.50	1.38
2	A	1201	SG8	C14-C13	6.15	1.51	1.38
2	A	1201	SG8	C15-C16	6.22	1.52	1.39
2	A	1201	SG8	C17-C12	7.42	1.52	1.39
2	A	1201	SG8	C9-N1	8.69	1.49	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	SG8	C3-C4-C5	-3.83	119.59	123.91
2	A	1201	SG8	C2-C1-C6	-2.99	121.63	124.72
2	A	1201	SG8	C10-N1-C11	-2.94	115.08	118.70
2	A	1201	SG8	C24-C25-N3	-2.44	119.38	123.64
2	A	1201	SG8	C27-C26-N3	-2.38	119.49	123.64
2	A	1201	SG8	O1-C9-C7	-2.15	114.58	119.11
2	A	1201	SG8	C21-C22-C11	2.29	114.30	109.54
2	A	1201	SG8	C21-C20-N2	2.30	120.34	111.02
2	A	1201	SG8	C18-C19-C20	2.61	115.08	111.40
2	A	1201	SG8	C10-N1-C9	2.62	124.53	117.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	SG8	C18-C11-C22	2.67	117.51	111.22
2	A	1201	SG8	C19-C18-C11	2.95	115.66	109.54
2	A	1201	SG8	C7-C9-N1	3.73	124.32	119.46
2	A	1201	SG8	C22-C11-N1	3.89	116.84	111.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SG8	3	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	A	447/468 (95%)	0.63	32 (7%) 18 13	23, 56, 107, 120	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1082	GLY	4.3
1	A	1056	PRO	4.1
1	A	1077	LYS	3.9
1	A	1033	MET	3.8
1	A	1075	ALA	3.4
1	A	347	GLY	3.2
1	A	548	THR	3.1
1	A	426	LEU	3.1
1	A	346	LEU	3.0
1	A	545	TRP	3.0
1	A	1085	LYS	3.0
1	A	262	TYR	2.9
1	A	1027	LYS	2.9
1	A	550	CYS	2.8
1	A	348	THR	2.8
1	A	258	ASN	2.7
1	A	443	SER	2.7
1	A	343	PHE	2.6
1	A	287	ASP	2.4
1	A	345	ALA	2.4
1	A	427	PHE	2.4
1	A	1079	ALA	2.3
1	A	353	LEU	2.3
1	A	350	TYR	2.3
1	A	1090	ALA	2.3
1	A	424	MET	2.3
1	A	359	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	256	TRP	2.2
1	A	1024	ALA	2.2
1	A	1054	ASP	2.2
1	A	1081	GLU	2.1
1	A	549	TRP	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 carbohydrates 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. 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
2	SG8	A	1201	36/36	0.91	0.21	0.01	20,46,52,54	0

6.5 Other polymers (i)

There are no such residues in this entry.