



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GRW
Title : FGFR3 in complex with a Fab
Authors : Wiesmann, C.
Deposited on : 2009-03-26
Resolution : 2.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

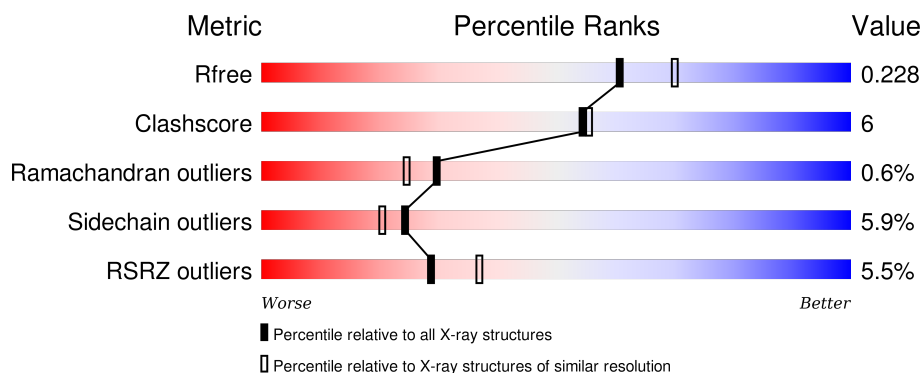
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. 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	241	
2	L	214	
3	H	235	

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
5	SO4	H	222	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5274 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1629	1030	298	295	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ALA	-	EXPRESSION TAG	UNP Q8NI16
A	141	ASP	-	EXPRESSION TAG	UNP Q8NI16
A	142	PRO	-	EXPRESSION TAG	UNP Q8NI16
A	375	HIS	-	EXPRESSION TAG	UNP Q8NI16
A	376	HIS	-	EXPRESSION TAG	UNP Q8NI16
A	377	HIS	-	EXPRESSION TAG	UNP Q8NI16
A	378	HIS	-	EXPRESSION TAG	UNP Q8NI16
A	379	HIS	-	EXPRESSION TAG	UNP Q8NI16
A	380	HIS	-	EXPRESSION TAG	UNP Q8NI16

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1636	1024	271	335	6			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	230	Total	C	N	O	S	0	0	0
			1716	1083	282	344	7			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total 77	O 77	0	0
6	L	82	Total 82	O 82	0	0
6	H	115	Total 115	O 115	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.05Å 99.33Å 143.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 24.83 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.10) 99.3 (24.83-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.228 0.194 , 0.228	Depositor DCC
R_{free} test set	2500 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 49782 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5274	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, 0.375 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: NAG, SO4

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	0.53	0/1671	0.72	1/2272 (0.0%)
2	L	0.57	1/1672 (0.1%)	0.71	1/2273 (0.0%)
3	H	0.58	0/1757	0.70	0/2398
All	All	0.56	1/5100 (0.0%)	0.71	2/6943 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	194	CYS	CB-SG	-5.51	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ASN	N-CA-C	6.27	127.92	111.00
2	L	201	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	302	GLY	Peptide

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	1629	0	1609	43	0
2	L	1636	0	1587	13	0
3	H	1716	0	1672	10	0
4	A	14	0	13	0	0
5	H	5	0	0	0	0
6	A	77	0	0	3	0
6	H	115	0	0	1	0
6	L	82	0	0	1	0
All	All	5274	0	4881	63	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 (63) 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:341:THR:HG23	6:A:2:HOH:O	1.65	0.94
1:A:255:LEU:CD2	1:A:277:VAL:HG22	2.12	0.80
1:A:312:TRP:HZ2	1:A:321:VAL:HG12	1.50	0.76
2:L:123:GLU:HG3	6:H:263:HOH:O	1.86	0.74
1:A:285:ILE:HG21	1:A:321:VAL:HG11	1.70	0.73
1:A:159:MET:HE1	6:A:13:HOH:O	1.92	0.67
1:A:261:ALA:HB1	1:A:351:PHE:CD1	2.30	0.66
1:A:163:LEU:HD13	1:A:242:THR:HB	1.79	0.64
1:A:312:TRP:CZ2	1:A:321:VAL:HG12	2.31	0.64
2:L:112:ALA:HB1	2:L:201:LEU:HD13	1.79	0.63
2:L:198:HIS:CD2	2:L:200:GLY:H	2.17	0.62
1:A:275:CYS:O	1:A:321:VAL:HG22	2.01	0.61
1:A:291:VAL:HG11	1:A:307:THR:HG23	1.81	0.60
1:A:261:ALA:CB	1:A:351:PHE:CD1	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:O	1:A:301:ASP:N	2.34	0.59
1:A:293:VAL:HG12	1:A:296:SER:HB3	1.86	0.58
1:A:296:SER:OG	1:A:298:VAL:O	2.15	0.57
1:A:296:SER:C	1:A:298:VAL:H	2.08	0.56
1:A:255:LEU:HD21	1:A:277:VAL:HG22	1.85	0.56
2:L:138:ASN:N	2:L:138:ASN:HD22	2.03	0.56
1:A:312:TRP:HZ2	1:A:321:VAL:CG1	2.19	0.55
1:A:220:PRO:O	1:A:223:ARG:HG3	2.08	0.54
1:A:155:ARG:HB3	1:A:158:ARG:HG3	1.90	0.53
2:L:28:ASP:OD1	2:L:68:GLY:HA2	2.07	0.53
3:H:67:PHE:CZ	3:H:82:MET:HE2	2.44	0.53
3:H:63:VAL:HG13	3:H:67:PHE:HB2	1.91	0.53
1:A:312:TRP:CZ2	1:A:321:VAL:CG1	2.93	0.52
1:A:291:VAL:CG1	1:A:307:THR:HG23	2.40	0.51
2:L:123:GLU:OE2	3:H:209:LYS:NZ	2.34	0.51
1:A:259:LEU:HG	1:A:260:PRO:HD3	1.93	0.50
1:A:288:LEU:HB3	1:A:306:VAL:CG2	2.41	0.50
3:H:199:ASN:HD22	3:H:200:HIS:N	2.10	0.49
1:A:166:VAL:HG12	1:A:243:LEU:HD21	1.94	0.49
1:A:166:VAL:CG1	1:A:243:LEU:HD21	2.42	0.48
2:L:22:THR:HG22	2:L:72:THR:HG22	1.94	0.48
1:A:289:LYS:HD3	1:A:336:TYR:CE2	2.48	0.48
1:A:298:VAL:HG22	1:A:299:GLY:H	1.79	0.47
1:A:163:LEU:HD22	1:A:163:LEU:N	2.29	0.47
1:A:261:ALA:CB	1:A:351:PHE:HD1	2.26	0.47
1:A:289:LYS:HD3	1:A:336:TYR:CZ	2.49	0.47
3:H:123:PRO:HD3	3:H:209:LYS:HE2	1.97	0.47
1:A:291:VAL:HG11	1:A:307:THR:CG2	2.44	0.46
1:A:275:CYS:HB3	1:A:321:VAL:CG2	2.46	0.46
3:H:54:ASN:C	3:H:54:ASN:HD22	2.19	0.46
1:A:275:CYS:HB3	1:A:321:VAL:HG23	1.98	0.46
1:A:177:PRO:HG2	3:H:100(B):TYR:CZ	2.52	0.45
2:L:48:ILE:HD12	2:L:73:LEU:HD23	1.99	0.45
1:A:341:THR:HB	1:A:346:VAL:HG22	1.99	0.45
2:L:198:HIS:HD2	2:L:200:GLY:H	1.65	0.44
1:A:166:VAL:HG12	1:A:243:LEU:CD2	2.48	0.44
1:A:163:LEU:CD2	1:A:163:LEU:N	2.80	0.43
1:A:269:SER:O	1:A:328:VAL:HG22	2.19	0.43
1:A:312:TRP:CH2	1:A:321:VAL:HB	2.53	0.42
1:A:163:LEU:HD23	6:A:35:HOH:O	2.19	0.42
1:A:166:VAL:HG11	1:A:172:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3:GLN:HB2	6:L:248:HOH:O	2.19	0.42
2:L:116:PHE:CD1	3:H:130:SER:HA	2.55	0.41
3:H:63:VAL:HG22	3:H:67:PHE:CD2	2.55	0.41
2:L:141:PRO:O	2:L:198:HIS:HE1	2.03	0.41
2:L:124:GLN:HG2	2:L:129:THR:O	2.20	0.41
3:H:82:MET:HE2	3:H:82(C):LEU:HD21	2.02	0.41
1:A:298:VAL:HA	1:A:304:PRO:HA	2.02	0.41
1:A:261:ALA:HB2	1:A:351:PHE:CD1	2.54	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	204/241 (85%)	193 (95%)	7 (3%)	4 (2%)	9	4
2	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
3	H	228/235 (97%)	223 (98%)	5 (2%)	0	100	100
All	All	644/690 (93%)	623 (97%)	17 (3%)	4 (1%)	30	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	PRO
1	A	301	ASP
1	A	262	ASN
1	A	298	VAL

5.3.2 Protein sidechains ⓘ

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	176/202 (87%)	165 (94%)	11 (6%)	22	18
2	L	188/188 (100%)	179 (95%)	9 (5%)	31	29
3	H	192/197 (98%)	179 (93%)	13 (7%)	20	16
All	All	556/587 (95%)	523 (94%)	33 (6%)	24	20

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ARG
1	A	213	LEU
1	A	243	LEU
1	A	262	ASN
1	A	271	VAL
1	A	276	LYS
1	A	307	THR
1	A	323	LEU
1	A	341	THR
1	A	349	LYS
1	A	352	TRP
2	L	39	LYS
2	L	73	LEU
2	L	125	LEU
2	L	126	LYS
2	L	135	LEU
2	L	138	ASN
2	L	154	LEU
2	L	181	LEU
2	L	201	LEU
3	H	1	GLU
3	H	11	LEU
3	H	18	LEU
3	H	54	ASN
3	H	63	VAL
3	H	108	LEU

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Mol	Chain	Res	Type
3	H	150	VAL
3	H	170	LEU
3	H	175	LEU
3	H	189	LEU
3	H	199	ASN
3	H	201	LYS
3	H	206	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	274	HIS
1	A	290	HIS
2	L	3	GLN
2	L	138	ASN
2	L	198	HIS
3	H	54	ASN
3	H	76	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](#)

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1	1	14,14,15	0.59	0	15,19,21	1.13	1 (6%)
5	SO4	H	222	-	4,4,4	0.11	0	6,6,6	0.20	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	1	1	-	0/6/23/26	0/1/1/1
5	SO4	H	222	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1	NAG	C1-O5-C5	3.12	116.21	112.25

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

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, 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	206/241 (85%)	0.50	27 (13%) 5 6	26, 43, 125, 149	0
2	L	214/214 (100%)	-0.27	4 (1%) 70 75	26, 35, 53, 106	0
3	H	230/235 (97%)	-0.32	5 (2%) 65 71	25, 34, 59, 111	0
All	All	650/690 (94%)	-0.05	36 (5%) 29 37	25, 36, 71, 149	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	GLY	8.8
1	A	305	TYR	7.7
1	A	293	VAL	7.1
2	L	214	CYS	7.1
1	A	292	GLU	6.8
1	A	259	LEU	6.4
1	A	294	ASN	6.2
1	A	299	GLY	5.8
1	A	295	GLY	5.3
3	H	216	CYS	5.2
1	A	260	PRO	5.1
1	A	234	PHE	5.0
1	A	298	VAL	5.0
1	A	301	ASP	4.5
3	H	215	SER	4.4
1	A	291	VAL	4.3
1	A	266	VAL	4.3
1	A	304	PRO	3.9
1	A	300	PRO	3.8
1	A	352	TRP	3.4
1	A	297	LYS	3.2
1	A	303	THR	3.2
1	A	193	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	3.1
1	A	296	SER	2.8
1	A	354	SER	2.8
3	H	214	LYS	2.7
3	H	42	GLY	2.5
2	L	135	LEU	2.3
1	A	233	LYS	2.3
1	A	355	VAL	2.1
2	L	133	VAL	2.1
1	A	230	VAL	2.1
3	H	1	GLU	2.1
1	A	312	TRP	2.1
2	L	127	SER	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	H	222	5/5	0.96	0.14	7.03	66,68,69,70	0
4	NAG	A	1	14/15	0.86	0.18	-	52,58,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.