



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 PM GMT

PDB ID : 4RWL  
Title : Crystal structure of FGFR1 (C488A, C584C) in complex with 6-(7-((1-amino cyclopropyl) methoxy)-6-methoxyquinolin-4-yloxy)-N-methyl-1-naphthamide (E3810)  
Authors : Sohl, C.D.; Anderson, K.S.  
Deposited on : 2014-12-04  
Resolution : 2.19 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](mailto: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.

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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

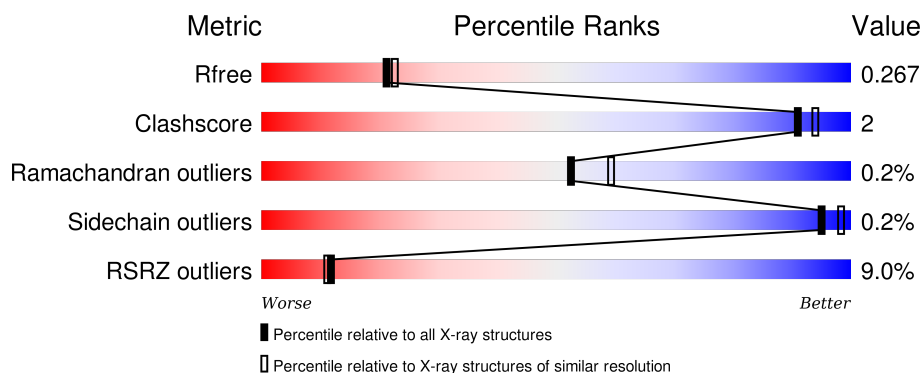
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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	317	 5% 86% 11%
1	B	317	 11% 84% 6% 10%

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
3	SO4	B	802	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4451 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 1.

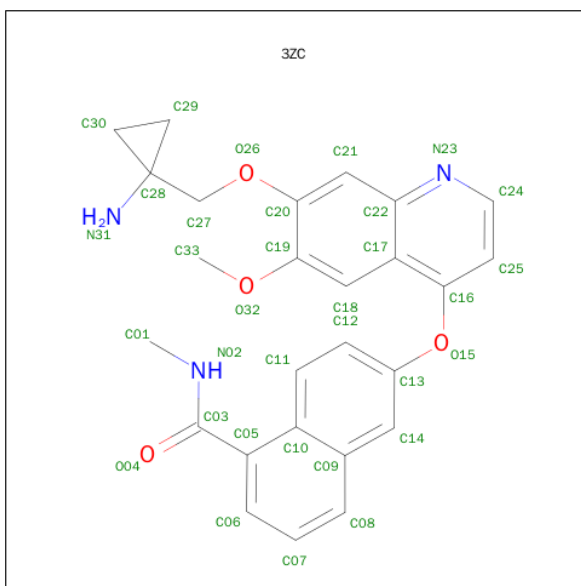
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2166	1378	370	401	17			
1	B	285	Total	C	N	O	S	0	0	0
			2197	1397	374	410	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	MET	-	EXPRESSION TAG	UNP P11362
A	450	GLY	-	EXPRESSION TAG	UNP P11362
A	451	HIS	-	EXPRESSION TAG	UNP P11362
A	452	HIS	-	EXPRESSION TAG	UNP P11362
A	453	HIS	-	EXPRESSION TAG	UNP P11362
A	454	HIS	-	EXPRESSION TAG	UNP P11362
A	455	HIS	-	EXPRESSION TAG	UNP P11362
A	456	HIS	-	EXPRESSION TAG	UNP P11362
A	457	MET	-	EXPRESSION TAG	UNP P11362
A	488	ALA	CYS	ENGINEERED MUTATION	UNP P11362
A	584	SER	CYS	ENGINEERED MUTATION	UNP P11362
B	449	MET	-	EXPRESSION TAG	UNP P11362
B	450	GLY	-	EXPRESSION TAG	UNP P11362
B	451	HIS	-	EXPRESSION TAG	UNP P11362
B	452	HIS	-	EXPRESSION TAG	UNP P11362
B	453	HIS	-	EXPRESSION TAG	UNP P11362
B	454	HIS	-	EXPRESSION TAG	UNP P11362
B	455	HIS	-	EXPRESSION TAG	UNP P11362
B	456	HIS	-	EXPRESSION TAG	UNP P11362
B	457	MET	-	EXPRESSION TAG	UNP P11362
B	488	ALA	CYS	ENGINEERED MUTATION	UNP P11362
B	584	SER	CYS	ENGINEERED MUTATION	UNP P11362

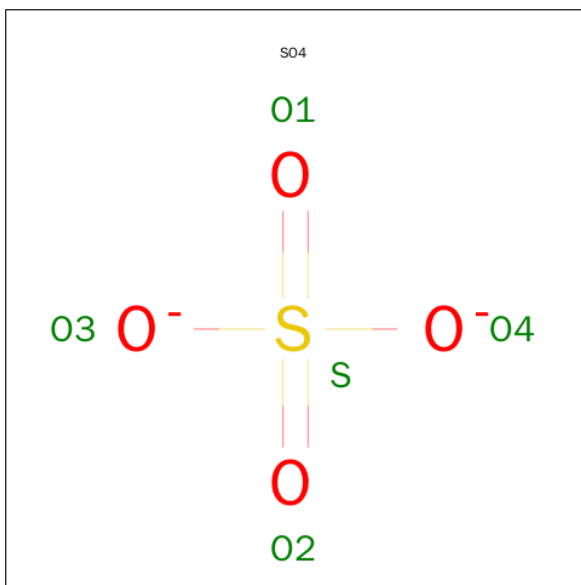
- Molecule 2 is 6-({7-[(1-AMINOCYCLOPROPYL)METHOXY]-6-METHOXYQUINOLIN-4-YL}OXY)-N-METHYLNAPHTHALENE-1-CARBOXAMIDE (three-letter code: 3ZC)

(formula: C<sub>26</sub>H<sub>25</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			33	26	3	4		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



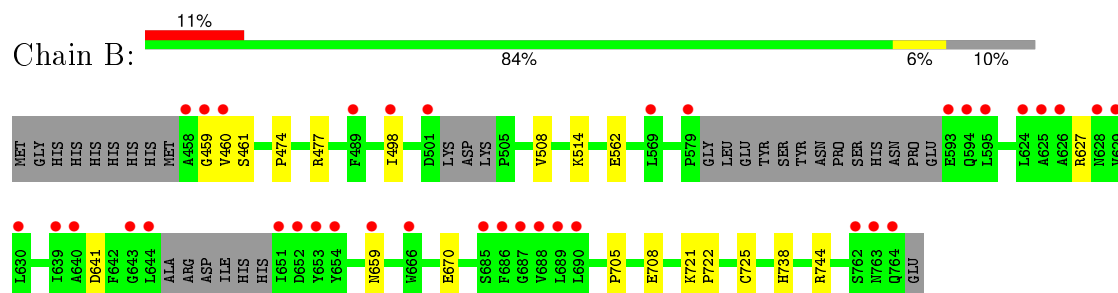
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total 25	O 25	0	0
4	B	25	Total 25	O 25	0	0



- Molecule 1: Fibroblast growth factor receptor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.17Å 57.86Å 65.66Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	32.99 – 2.19 32.99 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.99-2.19) 95.7 (32.99-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.207 , 0.256 0.220 , 0.267	Depositor DCC
$R_{free}$ test set	1915 reflections (5.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.2	EDS
Estimated twinning fraction	0.021 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38180 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4451	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3ZC, 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	0.43	0/2209	0.56	0/2998
1	B	0.41	0/2241	0.54	0/3039
All	All	0.42	0/4450	0.55	0/6037

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	2166	0	2099	4	0
1	B	2197	0	2134	14	0
2	B	33	0	25	6	0
3	B	5	0	0	2	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
All	All	4451	0	4258	19	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 (19) 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:721:LYS:NZ	1:A:727:ASN:OD1	2.23	0.71
1:B:498:ILE:HG12	1:B:508:VAL:HG12	1.89	0.54
2:B:801:3ZC:O04	2:B:801:3ZC:H10	2.06	0.54
1:B:459:GLY:C	1:B:461:SER:H	2.12	0.54
1:B:562:GLU:O	2:B:801:3ZC:H2	2.09	0.52
1:B:670:GLU:OE2	1:B:744:ARG:NH1	2.33	0.50
1:B:514:LYS:HB2	2:B:801:3ZC:H9	1.95	0.48
1:B:514:LYS:HB2	2:B:801:3ZC:C08	2.45	0.47
1:B:474:PRO:HB2	1:B:477:ARG:HG3	1.98	0.46
1:B:627:ARG:HD3	3:B:802:SO4:O2	2.17	0.45
1:B:641:ASP:HA	2:B:801:3ZC:H5	1.98	0.45
1:A:694:PHE:CZ	1:A:729:LEU:HD13	2.51	0.45
1:B:721:LYS:HE3	1:B:725:CYS:O	2.18	0.44
1:A:672:LEU:HD21	1:A:710:PHE:CE1	2.53	0.43
1:A:578:PRO:HA	1:A:579:PRO:HD3	1.86	0.43
1:B:659:ASN:HB3	3:B:802:SO4:O4	2.19	0.42
1:B:705:PRO:HD2	1:B:708:GLU:HB2	2.02	0.41
1:B:721:LYS:HA	1:B:722:PRO:HD3	1.88	0.41
1:B:641:ASP:CA	2:B:801:3ZC:H5	2.51	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	274/317 (86%)	270 (98%)	4 (2%)	0	100	100
1	B	277/317 (87%)	274 (99%)	2 (1%)	1 (0%)	39	42
All	All	551/634 (87%)	544 (99%)	6 (1%)	1 (0%)	52	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	460	VAL

### 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	224/277 (81%)	224 (100%)	0	100	100
1	B	228/277 (82%)	227 (100%)	1 (0%)	93	97
All	All	452/554 (82%)	451 (100%)	1 (0%)	95	98

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

Mol	Chain	Res	Type
1	B	738	HIS

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

Mol	Chain	Res	Type
1	B	679	HIS
1	B	727	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

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	$\# Z  > 2$
2	3ZC	B	801	-	36,37,37	2.26	10 (27%)	48,54,54	1.50	11 (22%)
3	SO4	B	802	-	4,4,4	0.31	0	6,6,6	0.13	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	3ZC	B	801	-	-	0/17/22/22	0/4/5/5
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	3ZC	C17-C22	-3.38	1.37	1.42
2	B	801	3ZC	C10-C09	-3.04	1.37	1.42
2	B	801	3ZC	C21-C22	2.21	1.45	1.41
2	B	801	3ZC	O15-C16	2.29	1.42	1.38
2	B	801	3ZC	C18-C19	2.34	1.40	1.36
2	B	801	3ZC	C25-C16	2.46	1.44	1.38
2	B	801	3ZC	O26-C20	2.62	1.42	1.37
2	B	801	3ZC	C21-C20	2.81	1.41	1.36
2	B	801	3ZC	O32-C19	3.68	1.43	1.37
2	B	801	3ZC	C03-N02	8.74	1.43	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	3ZC	C16-O15-C13	-3.28	112.23	118.50
2	B	801	3ZC	O32-C19-C18	-2.97	121.26	125.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	3ZC	C17-C22-N23	-2.62	120.09	122.88
2	B	801	3ZC	C33-O32-C19	-2.51	113.74	117.54
2	B	801	3ZC	C01-N02-C03	-2.35	119.00	121.80
2	B	801	3ZC	C11-C12-C13	-2.21	117.38	120.14
2	B	801	3ZC	C11-C10-C05	-2.16	120.07	123.27
2	B	801	3ZC	C18-C17-C22	2.31	121.88	118.94
2	B	801	3ZC	O32-C19-C20	2.75	119.33	115.40
2	B	801	3ZC	C24-N23-C22	2.92	121.81	116.87
2	B	801	3ZC	C21-C22-N23	3.05	121.32	117.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	3ZC	6	0
3	B	802	SO4	2	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	282/317 (88%)	0.40	15 (5%) 30 29	32, 44, 72, 92	0
1	B	285/317 (89%)	0.68	36 (12%) 5 5	34, 46, 70, 81	0
All	All	567/634 (89%)	0.54	51 (8%) 12 11	32, 46, 72, 92	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	PHE	6.7
1	B	458	ALA	6.2
1	A	520	ALA	5.4
1	B	653	TYR	4.8
1	B	501	ASP	4.7
1	B	624	LEU	4.4
1	B	639	ILE	4.4
1	B	579	PRO	4.0
1	B	763	ASN	4.0
1	A	518	SER	3.9
1	B	689	LEU	3.9
1	A	521	THR	3.8
1	B	688	VAL	3.6
1	B	651	ILE	3.6
1	B	625	ALA	3.5
1	B	644	LEU	3.5
1	B	654	TYR	3.5
1	B	498	ILE	3.4
1	B	762	SER	3.4
1	A	654	TYR	3.3
1	B	594	GLN	3.2
1	A	516	LEU	3.1
1	A	485	GLY	3.0
1	B	652	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	687	GLY	2.8
1	B	629	VAL	2.8
1	A	556	PRO	2.8
1	B	685	SER	2.7
1	A	501	ASP	2.6
1	B	640	ALA	2.6
1	B	626	ALA	2.6
1	B	595	LEU	2.5
1	B	643	GLY	2.5
1	B	666	TRP	2.5
1	A	688	VAL	2.4
1	A	502	LYS	2.4
1	B	593	GLU	2.4
1	A	579	PRO	2.4
1	B	460	VAL	2.4
1	A	525	LEU	2.3
1	B	630	LEU	2.3
1	B	659	ASN	2.3
1	A	592	GLU	2.3
1	A	724	ASN	2.3
1	B	690	LEU	2.1
1	B	628	ASN	2.1
1	B	686	PHE	2.1
1	B	764	GLN	2.1
1	B	459	GLY	2.0
1	A	503	ASP	2.0
1	B	569	LEU	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	3ZC	B	801	33/33	0.88	0.18	0.24	40,45,52,54	0
3	SO4	B	802	5/5	0.99	0.09	-2.30	52,54,59,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.