Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:25 PM GMT

PDB ID	:	4EMU
Title	:	Crystal structure of ligand free human STING
Authors	:	Li, P.
Deposited on	:	2012-04-12
Resolution	:	1.90 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:

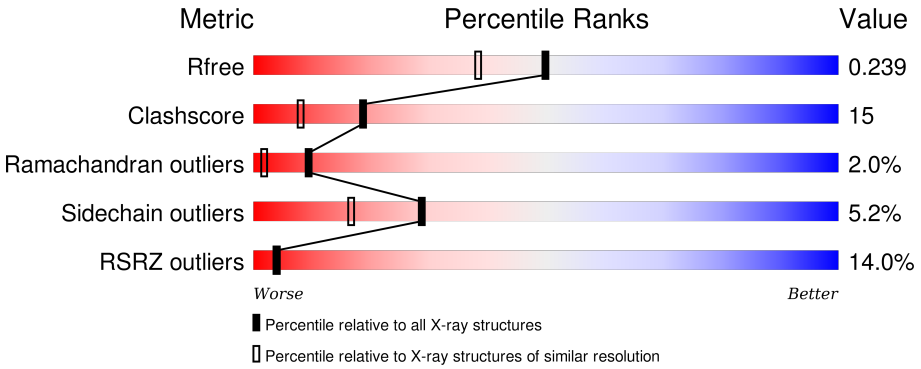
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	188	16% 66% 23% • 7%
1	B	188	10% 68% 22% • • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2977 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 Transmembrane protein 173.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1415	890	248	271	6			
1	B	175	Total	C	N	O	S	0	0	0
			1415	890	248	271	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	SER	-	EXPRESSION TAG	UNP Q86WV6
B	154	SER	-	EXPRESSION TAG	UNP Q86WV6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

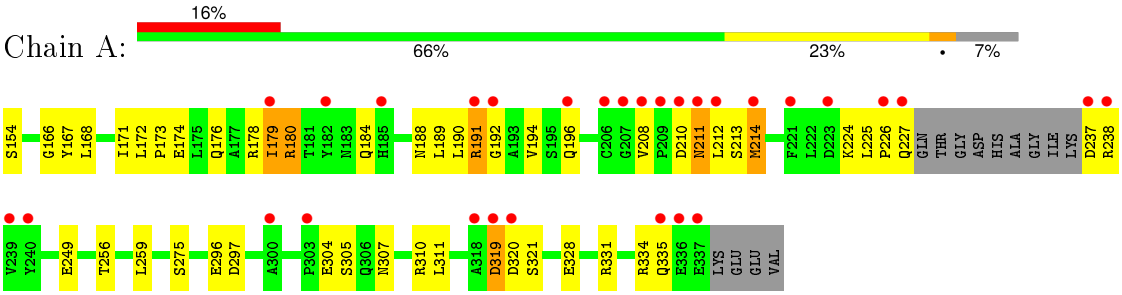
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	89	Total	O	0	0
			89	89		

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.

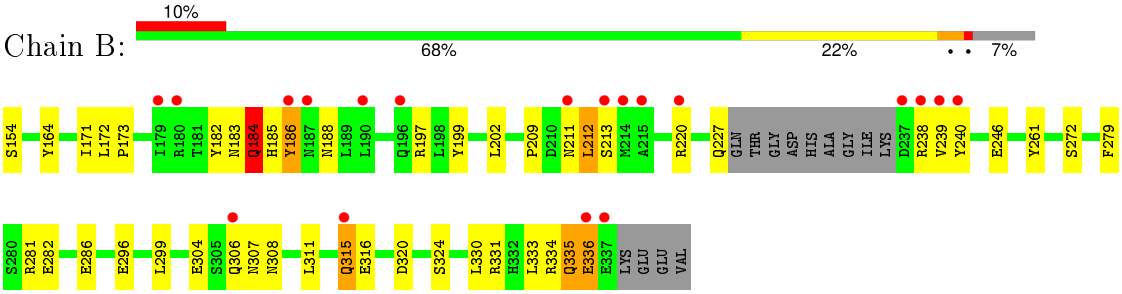
- Molecule 1: Transmembrane protein 173

Chain A:



- Molecule 1: Transmembrane protein 173

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.93Å 78.11Å 127.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.35 – 1.90 37.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (37.35-1.90) 91.3 (37.35-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.211 , 0.248 0.204 , 0.239	Depositor DCC
R_{free} test set	1830 reflections (7.17%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 27798 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2977	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: CA

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	0.31	0/1442	0.51	1/1955 (0.1%)
1	B	0.38	0/1442	0.53	0/1955
All	All	0.35	0/2884	0.52	1/3910 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	GLY	N-CA-C	-5.53	99.29	113.10

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	1415	0	1380	39	1
1	B	1415	0	1380	47	1
2	B	1	0	0	0	0
3	A	57	0	0	3	0
3	B	89	0	0	12	2
All	All	2977	0	2760	86	3

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 15.

All (86) 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:180:ARG:HG3	1:A:180:ARG:HH11	1.27	0.99
1:A:319:ASP:O	1:A:321:SER:N	1.99	0.95
1:B:197:ARG:HG3	1:B:197:ARG:HH11	1.32	0.93
1:B:315:GLN:NE2	3:B:565:HOH:O	2.02	0.92
1:A:166:GLY:O	1:A:238:ARG:NH1	2.07	0.88
1:A:328:GLU:OE2	1:A:331:ARG:NH2	2.13	0.81
1:A:180:ARG:HG3	1:A:180:ARG:NH1	1.96	0.79
1:B:211:ASN:OD1	1:B:212:LEU:N	2.19	0.75
1:B:315:GLN:HA	1:B:315:GLN:OE1	1.89	0.73
1:A:179:ILE:HD12	1:A:196:GLN:HA	1.70	0.73
1:B:227:GLN:HE21	1:B:240:TYR:H	1.39	0.71
1:A:188:ASN:HA	1:A:191:ARG:HH12	1.56	0.71
1:B:334:ARG:NE	3:B:579:HOH:O	2.15	0.69
1:B:315:GLN:CD	1:B:316:GLU:H	1.96	0.68
1:B:197:ARG:HD2	1:B:336:GLU:OE1	1.92	0.68
1:B:246:GLU:OE1	3:B:555:HOH:O	2.12	0.67
1:A:275:SER:OG	3:A:416:HOH:O	2.13	0.65
1:A:213:SER:O	1:A:214:MET:HB2	1.96	0.65
1:A:178:ARG:HD2	1:A:227:GLN:OE1	1.97	0.65
1:B:296:GLU:HG2	1:B:311:LEU:HD12	1.81	0.63
1:B:238:ARG:NH1	1:B:239:VAL:O	2.32	0.62
1:B:227:GLN:NE2	1:B:240:TYR:O	2.33	0.62
1:A:296:GLU:HG2	1:A:311:LEU:HD12	1.82	0.61
1:A:328:GLU:CD	1:A:331:ARG:HH22	2.04	0.60
1:A:174:GLU:N	1:A:174:GLU:OE1	2.35	0.59
1:A:188:ASN:HA	1:A:191:ARG:NH1	2.17	0.59
1:B:227:GLN:NE2	1:B:240:TYR:H	2.00	0.59
1:B:154:SER:N	3:B:513:HOH:O	2.36	0.59
1:A:171:ILE:HA	1:A:174:GLU:OE2	2.04	0.58
1:B:184:GLN:HG2	1:B:185:HIS:H	1.68	0.58
1:B:197:ARG:HG3	1:B:197:ARG:NH1	2.08	0.58
1:B:211:ASN:CG	1:B:212:LEU:N	2.58	0.56
1:A:167:TYR:CZ	1:A:171:ILE:HD13	2.41	0.55
1:B:182:TYR:O	1:B:184:GLN:N	2.38	0.55
1:B:164:TYR:OH	3:B:577:HOH:O	2.17	0.55
1:B:182:TYR:C	1:B:184:GLN:H	2.11	0.54
1:B:197:ARG:CG	1:B:197:ARG:HH11	2.10	0.53
1:B:331:ARG:NE	3:B:523:HOH:O	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ARG:NH2	3:B:579:HOH:O	2.42	0.53
1:A:176:GLN:HA	1:A:179:ILE:HD11	1.91	0.52
1:B:188:ASN:ND2	3:B:571:HOH:O	2.43	0.51
1:B:335:GLN:HG2	3:B:560:HOH:O	2.10	0.50
1:B:272:SER:HA	1:B:279:PHE:O	2.11	0.50
1:B:212:LEU:HD23	1:B:212:LEU:O	2.12	0.50
1:B:286:GLU:OE2	3:B:544:HOH:O	2.19	0.49
1:A:179:ILE:HD11	1:A:196:GLN:HG2	1.95	0.49
1:B:334:ARG:CZ	3:B:579:HOH:O	2.58	0.49
1:B:197:ARG:CG	1:B:197:ARG:NH1	2.71	0.49
1:A:210:ASP:N	1:A:210:ASP:OD1	2.38	0.49
1:B:299:LEU:O	1:B:306:GLN:HB2	2.12	0.48
1:B:209:PRO:HB2	1:B:211:ASN:ND2	2.29	0.48
1:B:197:ARG:CD	1:B:336:GLU:OE1	2.60	0.46
1:B:238:ARG:HG3	1:B:239:VAL:N	2.31	0.46
1:A:172:LEU:N	1:A:173:PRO:CD	2.77	0.46
1:A:307:ASN:HA	1:A:310:ARG:HH12	1.81	0.46
1:B:172:LEU:N	1:B:173:PRO:CD	2.78	0.46
1:B:315:GLN:CD	1:B:316:GLU:N	2.67	0.46
1:A:211:ASN:CG	1:A:213:SER:HB2	2.36	0.46
1:A:297:ASP:OD2	3:A:444:HOH:O	2.21	0.45
1:B:306:GLN:NE2	3:B:533:HOH:O	2.46	0.45
1:B:330:LEU:O	1:B:334:ARG:HG3	2.16	0.45
1:B:197:ARG:NE	1:B:307:ASN:O	2.49	0.45
1:A:237:ASP:C	1:A:238:ARG:HG3	2.37	0.45
1:A:331:ARG:O	1:A:335:GLN:HG3	2.16	0.45
1:B:304:GLU:N	1:B:304:GLU:OE1	2.43	0.44
1:A:237:ASP:O	1:A:238:ARG:HG2	2.18	0.44
1:B:209:PRO:HD2	1:B:261:TYR:CE2	2.52	0.44
1:A:194:VAL:HA	1:A:256:THR:OG1	2.18	0.44
1:A:237:ASP:O	1:A:238:ARG:CG	2.66	0.44
1:A:225:LEU:HD12	1:A:226:PRO:HD2	1.99	0.44
1:A:180:ARG:HD2	1:A:180:ARG:HA	1.59	0.43
1:B:220:ARG:NH2	1:B:246:GLU:OE2	2.43	0.43
1:B:202:LEU:CD1	1:B:311:LEU:HB3	2.47	0.43
1:B:184:GLN:O	1:B:186:TYR:N	2.51	0.43
1:A:212:LEU:HD13	1:A:259:LEU:HD23	2.00	0.43
1:B:282:GLU:OE1	1:B:282:GLU:N	2.46	0.43
1:A:224:LYS:O	1:A:226:PRO:HD3	2.19	0.42
1:A:249:GLU:CD	1:A:334:ARG:HH22	2.21	0.42
1:A:208:VAL:N	3:A:448:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:ND2	1:A:213:SER:HB2	2.34	0.42
1:A:237:ASP:C	1:A:238:ARG:CG	2.87	0.42
1:B:199:TYR:CZ	1:B:333:LEU:HD13	2.56	0.41
1:A:168:LEU:O	1:A:172:LEU:HG	2.20	0.41
1:A:304:GLU:HG2	1:A:305:SER:N	2.35	0.41
1:A:190:LEU:O	1:A:191:ARG:O	2.39	0.41
1:B:184:GLN:CG	1:B:185:HIS:N	2.85	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:521:HOH:O	3:B:538:HOH:O[3_756]	1.90	0.30
1:A:189:LEU:O	1:B:188:ASN:ND2[4_556]	2.03	0.17
3:B:526:HOH:O	3:B:529:HOH:O[7_646]	2.18	0.02

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	171/188 (91%)	156 (91%)	11 (6%)	4 (2%)	8 1
1	B	171/188 (91%)	157 (92%)	11 (6%)	3 (2%)	11 2
All	All	342/376 (91%)	313 (92%)	22 (6%)	7 (2%)	9 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ARG
1	A	214	MET
1	A	320	ASP
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	212	LEU
1	A	319	ASP
1	B	183	ASN

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	154/164 (94%)	149 (97%)	5 (3%)	46 35
1	B	154/164 (94%)	143 (93%)	11 (7%)	18 8
All	All	308/328 (94%)	292 (95%)	16 (5%)	29 17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	SER
1	A	179	ILE
1	A	180	ARG
1	A	184	GLN
1	A	211	ASN
1	B	171	ILE
1	B	184	GLN
1	B	186	TYR
1	B	213	SER
1	B	281	ARG
1	B	308	ASN
1	B	315	GLN
1	B	320	ASP
1	B	324	SER
1	B	335	GLN
1	B	336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	GLN

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

Of 1 ligands modelled in this entry, 1 is 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

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	175/188 (93%)	1.00	30 (17%)	2	2	27, 49, 103, 167	0
1	B	175/188 (93%)	0.73	19 (10%)	7	8	24, 43, 94, 135	0
All	All	350/376 (93%)	0.86	49 (14%)	4	4	24, 47, 102, 167	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ASP	9.5
1	A	210	ASP	7.8
1	A	337	GLU	7.7
1	A	238	ARG	6.9
1	A	192	GLY	6.3
1	A	239	VAL	6.0
1	B	240	TYR	5.6
1	B	336	GLU	5.6
1	A	240	TYR	5.4
1	B	237	ASP	4.8
1	B	238	ARG	4.5
1	B	214	MET	4.4
1	A	211	ASN	3.9
1	A	227	GLN	3.8
1	A	320	ASP	3.7
1	B	186	TYR	3.7
1	A	185	HIS	3.7
1	A	207	GLY	3.6
1	B	215	ALA	3.5
1	A	191	ARG	3.4
1	A	179	ILE	3.3
1	A	226	PRO	3.2
1	A	319	ASP	3.2
1	A	221	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLN	3.0
1	A	182	TYR	3.0
1	B	337	GLU	2.9
1	B	211	ASN	2.8
1	A	209	PRO	2.8
1	A	318	ALA	2.6
1	A	336	GLU	2.6
1	A	303	PRO	2.5
1	B	315	GLN	2.5
1	B	187	ASN	2.3
1	A	214	MET	2.3
1	B	179	ILE	2.3
1	A	206	CYS	2.3
1	A	208	VAL	2.3
1	B	306	GLN	2.3
1	A	212	LEU	2.3
1	B	190	LEU	2.3
1	B	239	VAL	2.3
1	B	213	SER	2.3
1	B	220	ARG	2.2
1	A	223	ASP	2.1
1	B	180	ARG	2.1
1	A	300	ALA	2.1
1	A	196	GLN	2.1
1	B	196	GLN	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, 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	CA	B	401	1/1	0.99	0.11	-1.58	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.