



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:20 AM GMT

PDB ID : 3I2A  
Title : Crystal structure of a chimeric trypsin inhibitor protein STI(L)-WCI(S)  
Authors : Sen, U.; Khamrui, S.  
Deposited on : 2009-06-29  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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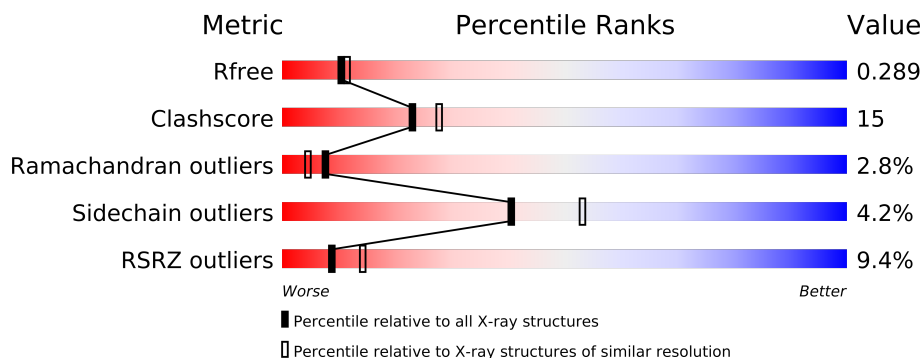
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	187	
1	B	187	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2970 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Chymotrypsin inhibitor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1408	892	248	263	5			
1	B	180	Total	C	N	O	S	0	0	0
			1399	887	246	261	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P10822
A	1	SER	-	EXPRESSION TAG	UNP P10822
A	2	HIS	-	EXPRESSION TAG	UNP P10822
A	3	MET	-	EXPRESSION TAG	UNP P10822
A	66	PRO	GLN	ENGINEERED	UNP P10822
A	67	TYR	PHE	ENGINEERED	UNP P10822
A	68	ARG	LEU	ENGINEERED	UNP P10822
A	69	ILE	SER	ENGINEERED	UNP P10822
A	70	ARG	LEU	ENGINEERED	UNP P10822
B	200	GLY	-	EXPRESSION TAG	UNP P10822
B	201	SER	-	EXPRESSION TAG	UNP P10822
B	202	HIS	-	EXPRESSION TAG	UNP P10822
B	203	MET	-	EXPRESSION TAG	UNP P10822
B	266	PRO	GLN	ENGINEERED	UNP P10822
B	267	TYR	PHE	ENGINEERED	UNP P10822
B	268	ARG	LEU	ENGINEERED	UNP P10822
B	269	ILE	SER	ENGINEERED	UNP P10822
B	270	ARG	LEU	ENGINEERED	UNP P10822

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

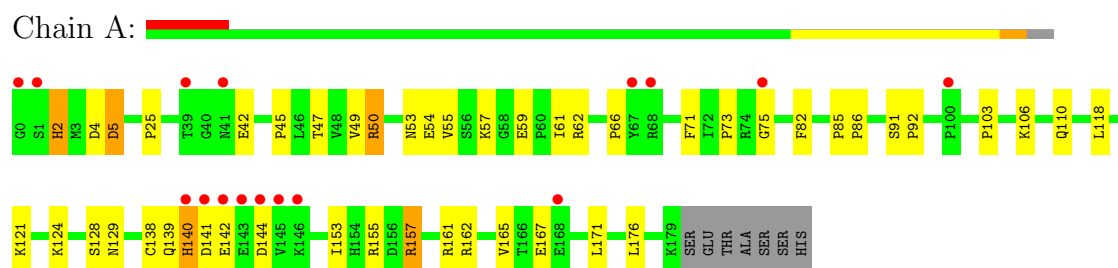
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	80	Total	O	0	0
			80	80		

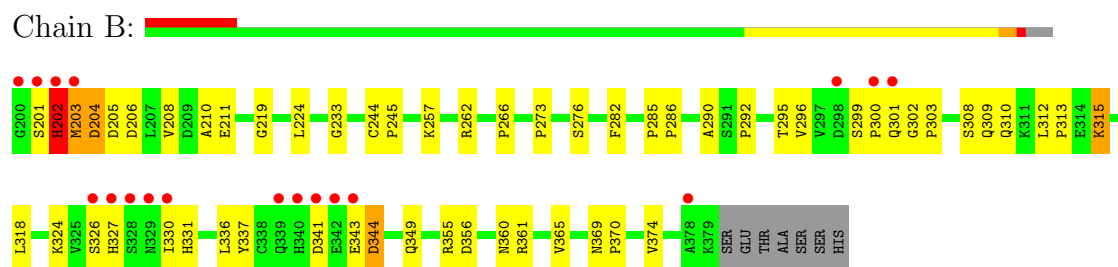
### 3 Residue-property plots

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: Chymotrypsin inhibitor 3



#### • Molecule 1: Chymotrypsin inhibitor 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.38Å 141.38Å 46.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.30 19.96 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.96-2.30) 96.2 (19.96-2.25)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.26Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.234 , 0.289 0.233 , 0.289	Depositor DCC
$R_{free}$ test set	1037 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.2	EDS
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 21427 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2970	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 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.35	0/1444	0.71	0/1966
1	B	0.35	0/1434	0.76	1/1953 (0.1%)
All	All	0.35	0/2878	0.73	1/3919 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ASP	N-CA-C	-5.72	95.56	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1408	0	1382	34	0
1	B	1399	0	1370	47	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	81	0	0	3	0
3	B	80	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2970	0	2752	81	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:203:MET:O	1:B:205:ASP:N	1.90	1.04
1:A:157:ARG:HD2	1:A:157:ARG:H	1.23	1.00
1:B:201:SER:O	1:B:202:HIS:HB2	1.66	0.93
1:B:303:PRO:HG2	1:B:365:VAL:HB	1.51	0.92
1:B:295:THR:HG21	1:B:312:LEU:HG	1.57	0.86
1:B:203:MET:C	1:B:205:ASP:H	1.81	0.82
1:A:25:PRO:HG2	1:A:50:ARG:HD3	1.64	0.80
1:A:75:GLY:HA2	1:A:121:LYS:HD3	1.65	0.77
1:A:140:HIS:CD2	1:A:140:HIS:O	2.38	0.77
1:A:157:ARG:H	1:A:157:ARG:CD	2.00	0.71
1:B:202:HIS:O	1:B:204:ASP:N	2.25	0.70
1:B:349:GLN:HB2	3:B:500:HOH:O	1.91	0.70
1:B:203:MET:HA	1:B:203:MET:CE	2.21	0.69
1:A:141:ASP:O	1:A:142:GLU:HB3	1.96	0.66
1:A:140:HIS:CG	1:A:140:HIS:O	2.49	0.65
1:B:308:SER:HB3	1:B:312:LEU:HD21	1.79	0.65
1:B:273:PRO:HG2	1:B:276:SER:HB2	1.81	0.62
1:B:349:GLN:HG2	3:B:513:HOH:O	2.01	0.60
1:A:53:ASN:OD1	1:A:55:VAL:HG22	2.01	0.60
1:A:153:ILE:HD11	1:A:171:LEU:HD21	1.82	0.59
1:A:157:ARG:HD2	1:A:157:ARG:N	2.06	0.59
1:B:282:PHE:O	1:B:292:PRO:HB3	2.02	0.59
1:A:157:ARG:HH11	1:A:157:ARG:N	2.02	0.57
1:A:66:PRO:HG3	1:A:118:LEU:HD11	1.86	0.57
1:A:161:ARG:HD3	2:A:402:CL:CL	2.43	0.56
1:B:203:MET:C	1:B:205:ASP:N	2.44	0.56
1:A:153:ILE:CD1	1:A:171:LEU:HD21	2.37	0.55
1:B:330:ILE:HD13	3:B:466:HOH:O	2.04	0.55
1:B:204:ASP:OD1	1:B:324:LYS:NZ	2.39	0.55
1:B:300:PRO:HB2	1:B:301:GLN:NE2	2.22	0.55
1:B:211:GLU:HG2	3:B:493:HOH:O	2.07	0.54
1:A:66:PRO:HD3	1:A:118:LEU:HD21	1.90	0.54
1:B:266:PRO:HD3	1:B:318:LEU:HD11	1.89	0.54
1:B:203:MET:HA	1:B:203:MET:HE2	1.90	0.54
1:B:300:PRO:HB2	1:B:301:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:313:PRO:HB2	1:B:315:LYS:HZ2	1.73	0.53
1:B:313:PRO:HB2	1:B:315:LYS:NZ	2.24	0.52
1:A:140:HIS:O	1:A:142:GLU:N	2.42	0.52
1:A:91:SER:HB2	1:A:92:PRO:HD2	1.91	0.52
1:B:303:PRO:CG	1:B:365:VAL:HB	2.31	0.51
1:B:310:GLN:HB3	3:B:559:HOH:O	2.10	0.51
1:A:124:LYS:HG3	3:A:542:HOH:O	2.12	0.50
1:A:129:ASN:N	1:A:129:ASN:HD22	2.10	0.49
1:A:57:LYS:HD3	1:A:176:LEU:HD23	1.94	0.48
1:B:300:PRO:HD2	3:B:453:HOH:O	2.14	0.48
1:A:128:SER:O	1:A:129:ASN:HB2	2.13	0.48
1:B:356:ASP:OD2	1:B:360:ASN:HB2	2.15	0.47
1:B:369:ASN:N	1:B:370:PRO:HD3	2.30	0.47
1:B:203:MET:HA	1:B:205:ASP:OD1	2.16	0.46
1:B:224:LEU:HD21	1:B:257:LYS:HA	1.97	0.46
1:B:266:PRO:HG3	1:B:318:LEU:HD21	1.98	0.46
1:A:59:GLU:O	1:A:61:ILE:HG13	2.15	0.46
1:A:157:ARG:HH11	1:A:157:ARG:H	1.64	0.46
1:A:54:GLU:HG3	3:A:546:HOH:O	2.16	0.46
1:B:336:LEU:HD12	1:B:336:LEU:N	2.32	0.45
1:A:49:VAL:HG12	1:A:162:ARG:HA	1.99	0.45
1:A:82:PHE:O	1:A:85:PRO:HD3	2.16	0.45
1:B:355:ARG:HG2	1:B:361:ARG:HG2	1.98	0.45
1:A:2:HIS:HB2	1:A:5:ASP:OD1	2.17	0.45
1:B:299:SER:O	1:B:302:GLY:N	2.43	0.45
1:B:233:GLY:HA3	1:B:257:LYS:O	2.18	0.44
1:B:208:VAL:HG11	1:B:331:HIS:CE1	2.52	0.44
1:A:45:PRO:O	1:A:86:PRO:HG2	2.18	0.44
1:A:47:THR:OG1	1:A:106:LYS:NZ	2.51	0.44
1:B:343:GLU:HB3	1:B:344:ASP:H	1.64	0.43
1:B:244:CYS:HB2	1:B:245:PRO:CD	2.49	0.43
1:B:355:ARG:HA	1:B:360:ASN:O	2.18	0.43
1:A:103:PRO:HB2	1:A:165:VAL:HB	2.01	0.42
1:B:208:VAL:HB	1:B:331:HIS:CG	2.53	0.42
1:B:290:ALA:HB2	1:B:309:GLN:C	2.39	0.42
1:B:210:ALA:HB2	1:B:374:VAL:HG12	2.02	0.42
1:A:71:PHE:O	1:A:73:PRO:HD3	2.19	0.42
1:B:262:ARG:HE	1:B:262:ARG:HB2	1.64	0.42
1:A:66:PRO:HD2	3:A:547:HOH:O	2.18	0.42
1:B:296:VAL:HG21	1:B:337:TYR:CD1	2.55	0.42
1:B:285:PRO:HA	1:B:286:PRO:HD3	1.92	0.41
1:B:219:GLY:O	1:B:262:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:ASP:CG	1:A:141:ASP:O	2.57	0.41
1:A:129:ASN:ND2	1:A:129:ASN:N	2.69	0.41
1:B:330:ILE:O	1:B:330:ILE:HG23	2.21	0.41
1:B:301:GLN:CD	1:B:301:GLN:H	2.24	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	178/187 (95%)	159 (89%)	15 (8%)	4 (2%)	10	7
1	B	178/187 (95%)	162 (91%)	10 (6%)	6 (3%)	6	3
All	All	356/374 (95%)	321 (90%)	25 (7%)	10 (3%)	8	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	B	202	HIS
1	B	203	MET
1	B	204	ASP
1	B	326	SER
1	B	327	HIS
1	A	2	HIS
1	A	144	ASP
1	B	341	ASP
1	A	42	GLU

### 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	155/163 (95%)	145 (94%)	10 (6%)	24	30
1	B	153/163 (94%)	150 (98%)	3 (2%)	68	84
All	All	308/326 (94%)	295 (96%)	13 (4%)	40	53

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	5	ASP
1	A	50	ARG
1	A	62	ARG
1	A	110	GLN
1	A	138	CYS
1	A	140	HIS
1	A	155	ARG
1	A	157	ARG
1	A	167	GLU
1	B	202	HIS
1	B	315	LYS
1	B	344	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	129	ASN
1	A	140	HIS
1	A	158	ASN
1	B	301	GLN
1	B	358	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 2 ligands modelled in this entry, 2 are 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.

## 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<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	180/187 (96%)	0.39	16 (8%) 10 16	16, 35, 101, 154	0
1	B	180/187 (96%)	0.61	18 (10%) 8 13	21, 41, 116, 146	0
All	All	360/374 (96%)	0.50	34 (9%) 9 14	16, 39, 111, 154	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	SER	11.4
1	A	142	GLU	10.6
1	B	202	HIS	10.4
1	B	200	GLY	8.7
1	A	140	HIS	8.6
1	B	203	MET	8.0
1	B	300	PRO	7.3
1	A	100	PRO	7.1
1	B	327	HIS	6.4
1	B	342	GLU	5.7
1	A	145	VAL	5.7
1	A	143	GLU	4.9
1	B	329	ASN	4.3
1	A	144	ASP	4.3
1	A	141	ASP	4.3
1	A	0	GLY	4.2
1	A	75	GLY	4.1
1	A	1	SER	3.7
1	B	341	ASP	3.6
1	A	68	ARG	3.4
1	B	328	SER	3.0
1	B	301	GLN	3.0
1	B	298	ASP	2.9
1	A	146	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	378	ALA	2.8
1	B	339	GLN	2.7
1	A	41	ASN	2.7
1	B	343	GLU	2.4
1	A	39	THR	2.3
1	B	330	ILE	2.3
1	B	340	HIS	2.2
1	B	326	SER	2.2
1	A	168	GLU	2.1
1	A	67	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	A	402	1/1	0.10	-1.57	36,36,36,36	0
2	CL	B	401	1/1	0.04	-3.84	32,32,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.