



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:47 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 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

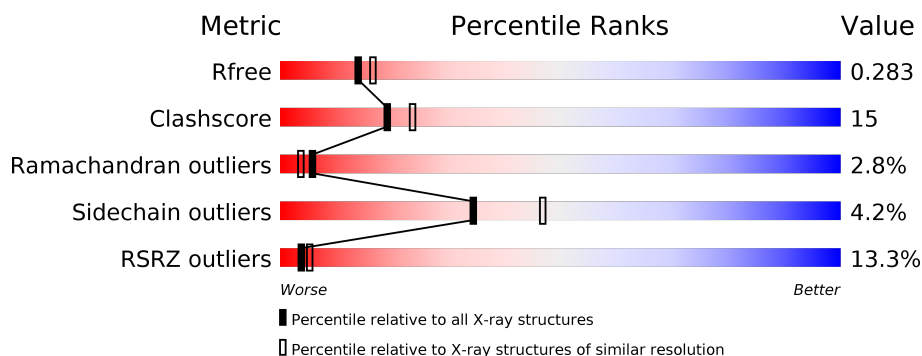
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	187	 10% 71% 23% . .
1	B	187	 16% 66% 28% . . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2970 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 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		

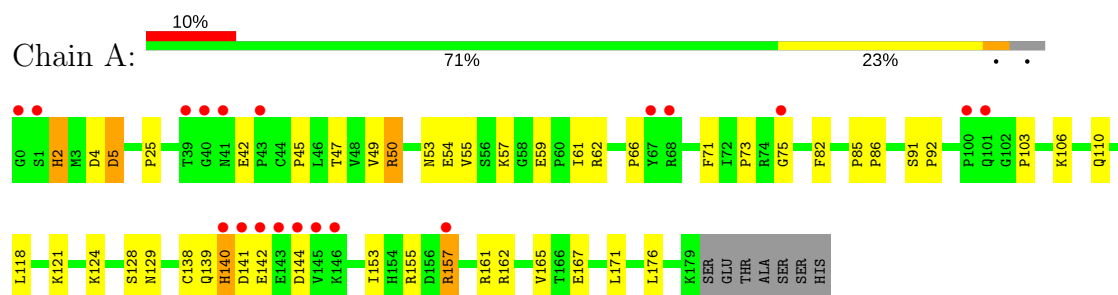
- Molecule 3 is water.

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

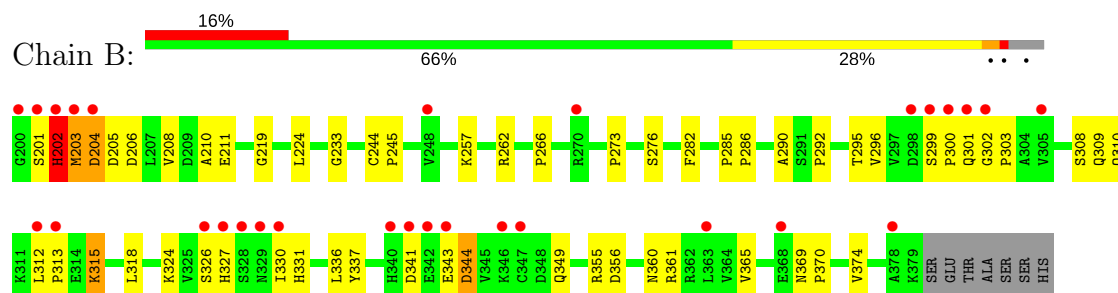
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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) 96.1 (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 0.229 , 0.283	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> )	0.32 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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 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	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
All	All	2970	0	2752	81	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 15.

All (81) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:59:GLU:O	1:A:61:ILE:HG13	2.15	0.46
1:B:266:PRO:HG3	1:B:318:LEU:HD21	1.98	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:A:2:HIS:HB2	1:A:5:ASP:OD1	2.17	0.45
1:B:355:ARG:HG2	1:B:361:ARG:HG2	1.98	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
1:A:141:ASP:CG	1:A:141:ASP:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	178/187 (95%)	159 (89%)	15 (8%)	4 (2%)	8	6
1	B	178/187 (95%)	162 (91%)	10 (6%)	6 (3%)	4	2
All	All	356/374 (95%)	321 (90%)	25 (7%)	10 (3%)	6	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%)	20	26
1	B	153/163 (94%)	150 (98%)	3 (2%)	60	77
All	All	308/326 (94%)	295 (96%)	13 (4%)	34	47

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 [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](#)

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.

No monomer is involved in short contacts.

## 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	180/187 (96%)	0.68	19 (10%) 7 10	16, 35, 101, 154	0
1	B	180/187 (96%)	0.88	29 (16%) 2 3	21, 41, 116, 146	0
All	All	360/374 (96%)	0.78	48 (13%) 4 5	16, 39, 111, 154	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	GLU	12.1
1	B	202	HIS	11.2
1	B	201	SER	10.2
1	A	140	HIS	10.0
1	B	300	PRO	9.0
1	B	200	GLY	8.5
1	B	327	HIS	8.0
1	A	100	PRO	7.3
1	B	203	MET	7.2
1	A	145	VAL	6.8
1	B	329	ASN	6.2
1	B	342	GLU	6.1
1	A	144	ASP	5.3
1	A	1	SER	5.3
1	B	301	GLN	5.0
1	A	143	GLU	5.0
1	A	141	ASP	4.9
1	A	75	GLY	4.7
1	A	0	GLY	4.3
1	A	41	ASN	4.1
1	B	298	ASP	3.6
1	A	146	LYS	3.5
1	A	68	ARG	3.3
1	B	326	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	341	ASP	3.2
1	B	313	PRO	3.0
1	A	39	THR	2.9
1	B	347	CYS	2.8
1	B	328	SER	2.8
1	B	343	GLU	2.8
1	B	378	ALA	2.8
1	A	40	GLY	2.7
1	B	302	GLY	2.6
1	B	299	SER	2.6
1	A	43	PRO	2.5
1	B	346	LYS	2.4
1	B	248	VAL	2.4
1	B	340	HIS	2.4
1	A	67	TYR	2.4
1	B	368	GLU	2.3
1	B	312	LEU	2.3
1	B	330	ILE	2.2
1	A	101	GLN	2.2
1	B	270	ARG	2.1
1	B	363	LEU	2.1
1	B	305	VAL	2.1
1	A	157	ARG	2.1
1	B	204	ASP	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<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( $\text{\AA}^2$ )	Q<0.9
2	CL	A	402	1/1	0.96	0.17	0.41	36,36,36,36	0
2	CL	B	401	1/1	0.97	0.08	-2.15	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.