



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:52 AM GMT

PDB ID : 2YO1  
Title : Salmonella enterica SadA 1049-1304 fused to GCN4 adaptors (SadAK9- cflI)  
Authors : Hartmann, M.D.; Hernandez Alvarez, B.; Lupas, A.N.  
Deposited on : 2012-10-20  
Resolution : 3.10 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](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.

---

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

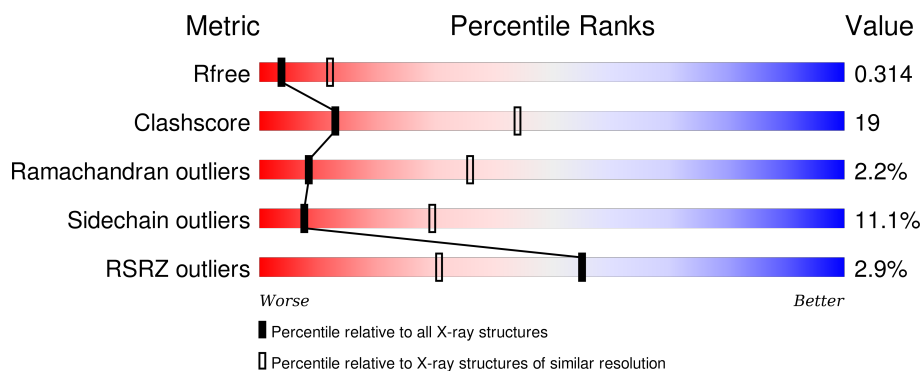
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	322	<div> <div>57%</div> <div>24%</div> <div>•</div> <div>15%</div> </div>
1	B	322	<div> <div>4%</div> <div>55%</div> <div>27%</div> <div>•</div> <div>15%</div> </div>
1	C	322	<div> <div>3%</div> <div>50%</div> <div>30%</div> <div>•</div> <div>15%</div> </div>

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
2	CL	C	2334	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5775 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 GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			1929	1159	347	418	5			
1	B	273	Total	C	N	O	S	0	0	0
			1919	1157	344	414	4			
1	C	273	Total	C	N	O	S	0	0	0
			1926	1152	348	421	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1023	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
A	1027	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
A	1030	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
A	1034	ILE	ASN	ENGINEERED MUTATION	UNP Q8ZL64
A	1037	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
A	1041	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
A	1044	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
A	1048	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
A	1308	ILE	LEU	ENGINEERED MUTATION	UNP P03069
A	1312	ILE	VAL	ENGINEERED MUTATION	UNP P03069
A	1315	ILE	LEU	ENGINEERED MUTATION	UNP P03069
A	1319	ILE	ASN	ENGINEERED MUTATION	UNP P03069
A	1322	ILE	LEU	ENGINEERED MUTATION	UNP P03069
A	1326	ILE	VAL	ENGINEERED MUTATION	UNP P03069
A	1329	ILE	LEU	ENGINEERED MUTATION	UNP P03069
A	1333	ILE	VAL	ENGINEERED MUTATION	UNP P03069
A	1334	LYS	-	EXPRESSION TAG	UNP Q8ZL64
A	1335	LEU	-	EXPRESSION TAG	UNP Q8ZL64
A	1336	HIS	-	EXPRESSION TAG	UNP Q8ZL64
A	1337	HIS	-	EXPRESSION TAG	UNP Q8ZL64
A	1338	HIS	-	EXPRESSION TAG	UNP Q8ZL64
A	1339	HIS	-	EXPRESSION TAG	UNP Q8ZL64

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1340	HIS	-	EXPRESSION TAG	UNP Q8ZL64
A	1341	HIS	-	EXPRESSION TAG	UNP Q8ZL64
B	1023	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
B	1027	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
B	1030	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
B	1034	ILE	ASN	ENGINEERED MUTATION	UNP Q8ZL64
B	1037	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
B	1041	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
B	1044	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
B	1048	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
B	1308	ILE	LEU	ENGINEERED MUTATION	UNP P03069
B	1312	ILE	VAL	ENGINEERED MUTATION	UNP P03069
B	1315	ILE	LEU	ENGINEERED MUTATION	UNP P03069
B	1319	ILE	ASN	ENGINEERED MUTATION	UNP P03069
B	1322	ILE	LEU	ENGINEERED MUTATION	UNP P03069
B	1326	ILE	VAL	ENGINEERED MUTATION	UNP P03069
B	1329	ILE	LEU	ENGINEERED MUTATION	UNP P03069
B	1333	ILE	VAL	ENGINEERED MUTATION	UNP P03069
B	1334	LYS	-	EXPRESSION TAG	UNP Q8ZL64
B	1335	LEU	-	EXPRESSION TAG	UNP Q8ZL64
B	1336	HIS	-	EXPRESSION TAG	UNP Q8ZL64
B	1337	HIS	-	EXPRESSION TAG	UNP Q8ZL64
B	1338	HIS	-	EXPRESSION TAG	UNP Q8ZL64
B	1339	HIS	-	EXPRESSION TAG	UNP Q8ZL64
B	1340	HIS	-	EXPRESSION TAG	UNP Q8ZL64
B	1341	HIS	-	EXPRESSION TAG	UNP Q8ZL64
C	1023	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
C	1027	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
C	1030	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
C	1034	ILE	ASN	ENGINEERED MUTATION	UNP Q8ZL64
C	1037	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
C	1041	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
C	1044	ILE	LEU	ENGINEERED MUTATION	UNP Q8ZL64
C	1044	ILE	VAL	ENGINEERED MUTATION	UNP Q8ZL64
C	1308	ILE	LEU	ENGINEERED MUTATION	UNP P03069
C	1312	ILE	VAL	ENGINEERED MUTATION	UNP P03069
C	1315	ILE	LEU	ENGINEERED MUTATION	UNP P03069
C	1319	ILE	ASN	ENGINEERED MUTATION	UNP P03069
C	1322	ILE	LEU	ENGINEERED MUTATION	UNP P03069
C	1326	ILE	VAL	ENGINEERED MUTATION	UNP P03069
C	1329	ILE	LEU	ENGINEERED MUTATION	UNP P03069
C	1333	ILE	VAL	ENGINEERED MUTATION	UNP P03069

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1334	LYS	-	EXPRESSION TAG	UNP Q8ZL64
C	1335	LEU	-	EXPRESSION TAG	UNP Q8ZL64
C	1336	HIS	-	EXPRESSION TAG	UNP Q8ZL64
C	1337	HIS	-	EXPRESSION TAG	UNP Q8ZL64
C	1338	HIS	-	EXPRESSION TAG	UNP Q8ZL64
C	1339	HIS	-	EXPRESSION TAG	UNP Q8ZL64
C	1340	HIS	-	EXPRESSION TAG	UNP Q8ZL64
C	1341	HIS	-	EXPRESSION TAG	UNP Q8ZL64

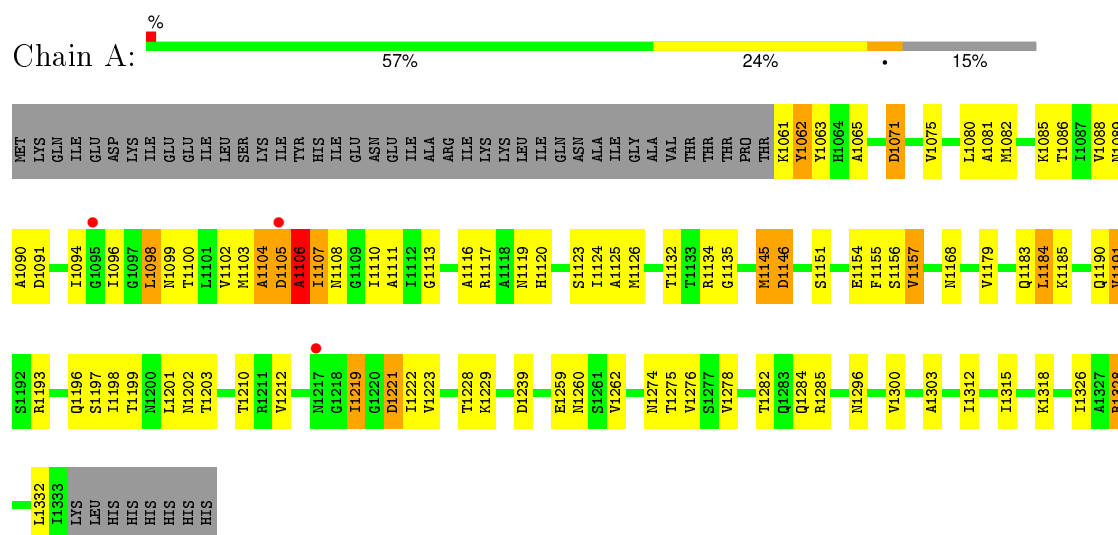
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

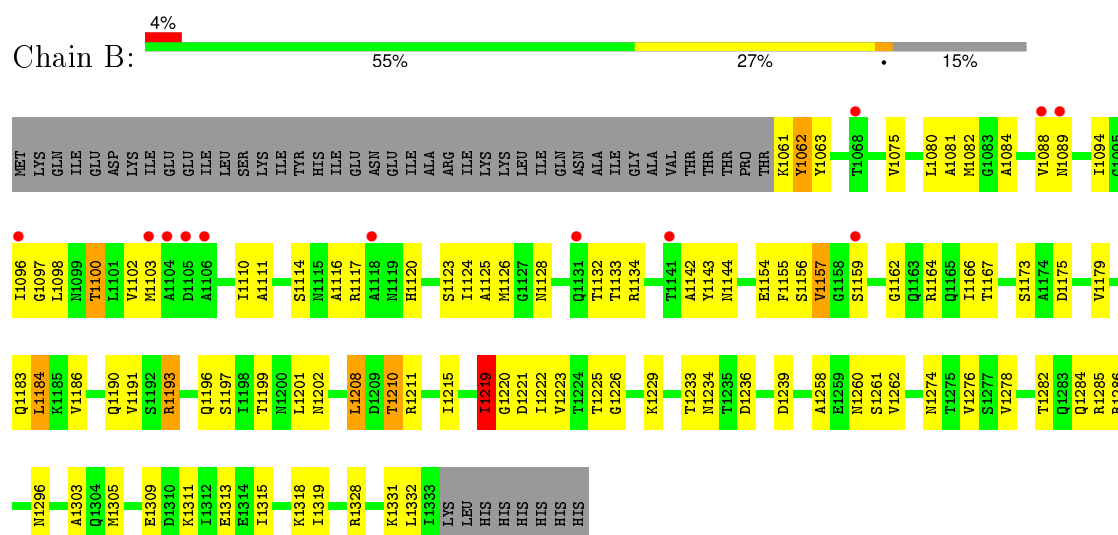
### 3 Residue-property plots

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.

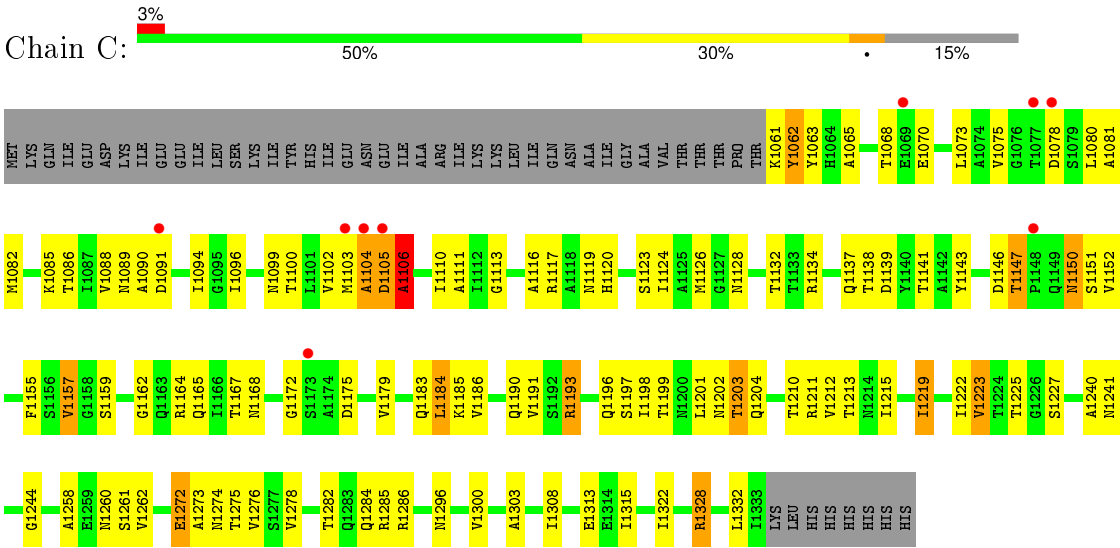
- Molecule 1: GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN



- Molecule 1: GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN



- Molecule 1: GENERAL CONTROL PROTEIN GCN4, PUTATIVE INNER MEMBRANE PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.03Å 48.78Å 135.83Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	38.64 – 3.10 37.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (38.64-3.10) 97.0 (37.48-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.265 , 0.320 0.270 , 0.314	Depositor DCC
$R_{free}$ test set	971 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 40.9	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	15 of 18781 reflections (0.080%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	5775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: 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	0.63	0/1940	0.69	0/2641
1	B	0.67	0/1930	0.72	0/2628
1	C	0.65	1/1936 (0.1%)	0.70	0/2637
All	All	0.65	1/5806 (0.0%)	0.70	0/7906

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	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1272	GLU	CD-OE1	6.36	1.32	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1106	ALA	Peptide
1	C	1106	ALA	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	1929	0	1840	90	0
1	B	1919	0	1830	89	0
1	C	1926	0	1823	114	0
2	C	1	0	0	0	0
All	All	5775	0	5493	215	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 19.

All (215) 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:1201:LEU:HD11	1:B:1202:ASN:OD1	1.43	1.15
1:A:1124:ILE:HD13	1:C:1126:MET:CE	1.77	1.14
1:A:1124:ILE:HD13	1:C:1126:MET:HE3	1.38	1.04
1:A:1090:ALA:HB3	1:A:1102:VAL:HG11	1.45	0.99
1:C:1090:ALA:HB3	1:C:1102:VAL:HG11	1.46	0.97
1:B:1219:ILE:HG22	1:B:1220:GLY:N	1.80	0.96
1:A:1126:MET:HE3	1:B:1124:ILE:HD13	1.49	0.95
1:A:1103:MET:O	1:A:1104:ALA:O	1.89	0.91
1:A:1107:ILE:HG23	1:A:1108:ASN:HB2	1.53	0.90
1:C:1103:MET:O	1:C:1104:ALA:O	1.89	0.89
1:A:1124:ILE:HD13	1:C:1126:MET:HE2	1.53	0.88
1:C:1090:ALA:CB	1:C:1102:VAL:HG11	2.04	0.87
1:B:1219:ILE:CG2	1:B:1220:GLY:N	2.36	0.86
1:B:1219:ILE:HG22	1:B:1220:GLY:H	1.38	0.84
1:A:1202:ASN:OD1	1:C:1201:LEU:HD11	1.78	0.83
1:A:1278:VAL:O	1:A:1285:ARG:HD2	1.79	0.83
1:A:1315:ILE:HG21	1:C:1315:ILE:HD13	1.60	0.82
1:A:1094:ILE:HD13	1:C:1096:ILE:HG22	1.61	0.82
1:B:1278:VAL:O	1:B:1285:ARG:HD2	1.81	0.80
1:A:1126:MET:CE	1:B:1124:ILE:HD13	2.13	0.79
1:C:1278:VAL:O	1:C:1285:ARG:HD2	1.84	0.78
1:A:1111:ALA:HB1	1:A:1116:ALA:HB1	1.66	0.77
1:B:1219:ILE:HD12	1:C:1223:VAL:HG23	1.66	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1201:LEU:CD2	1:C:1201:LEU:HB3	2.18	0.74
1:A:1090:ALA:CB	1:A:1102:VAL:HG11	2.18	0.73
1:A:1100:THR:HG22	1:A:1113:GLY:O	1.88	0.72
1:C:1111:ALA:HB1	1:C:1116:ALA:HB1	1.69	0.72
1:C:1081:ALA:HB2	1:C:1088:VAL:HG21	1.71	0.72
1:B:1111:ALA:HB1	1:B:1116:ALA:HB1	1.69	0.72
1:A:1124:ILE:CD1	1:C:1126:MET:HE2	2.20	0.72
1:B:1081:ALA:HB2	1:B:1088:VAL:HG21	1.74	0.70
1:C:1134:ARG:HD2	1:C:1137:GLN:HE21	1.56	0.70
1:A:1061:LYS:O	1:A:1062:TYR:HB2	1.92	0.70
1:C:1073:LEU:HG	1:C:1075:VAL:HG23	1.73	0.69
1:B:1126:MET:HE3	1:C:1124:ILE:HD13	1.76	0.68
1:A:1104:ALA:O	1:A:1106:ALA:N	2.27	0.68
1:B:1167:THR:HG22	1:C:1134:ARG:NH2	2.09	0.67
1:C:1090:ALA:CB	1:C:1102:VAL:CG1	2.73	0.67
1:B:1219:ILE:CD1	1:C:1223:VAL:HG23	2.24	0.67
1:C:1203:THR:HG22	1:C:1204:GLN:N	2.08	0.67
1:A:1090:ALA:HB3	1:A:1102:VAL:CG1	2.23	0.67
1:B:1061:LYS:O	1:B:1062:TYR:HB2	1.94	0.67
1:A:1090:ALA:CB	1:A:1102:VAL:CG1	2.74	0.66
1:B:1233:THR:O	1:B:1233:THR:HG23	1.95	0.66
1:C:1061:LYS:O	1:C:1062:TYR:HB2	1.96	0.66
1:B:1296:ASN:HB3	1:C:1303:ALA:HB2	1.76	0.65
1:A:1296:ASN:HB3	1:B:1303:ALA:HB2	1.78	0.65
1:B:1201:LEU:HD11	1:C:1202:ASN:OD1	1.96	0.65
1:B:1219:ILE:O	1:B:1222:ILE:HB	1.98	0.64
1:C:1134:ARG:HD2	1:C:1137:GLN:NE2	2.13	0.64
1:A:1086:THR:HG23	1:A:1100:THR:OG1	1.98	0.63
1:B:1210:THR:HG22	1:B:1211:ARG:N	2.13	0.63
1:C:1090:ALA:HB2	1:C:1102:VAL:CG1	2.29	0.63
1:B:1126:MET:CE	1:C:1124:ILE:HD13	2.29	0.63
1:C:1104:ALA:O	1:C:1106:ALA:N	2.33	0.62
1:B:1098:LEU:HD11	1:C:1078:ASP:HB3	1.81	0.62
1:C:1081:ALA:HB2	1:C:1088:VAL:CG2	2.29	0.62
1:C:1086:THR:HG23	1:C:1100:THR:OG1	2.01	0.61
1:A:1094:ILE:CD1	1:C:1096:ILE:HG22	2.30	0.60
1:A:1081:ALA:HB2	1:A:1088:VAL:HG21	1.84	0.60
1:B:1167:THR:HG22	1:C:1134:ARG:CZ	2.31	0.60
1:A:1096:ILE:HG22	1:B:1094:ILE:HD13	1.82	0.60
1:C:1222:ILE:N	1:C:1222:ILE:HD12	2.17	0.59
1:B:1081:ALA:HB2	1:B:1088:VAL:CG2	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1222:ILE:HG22	1:B:1223:VAL:N	2.18	0.58
1:A:1303:ALA:HB2	1:C:1296:ASN:HB3	1.85	0.58
1:B:1222:ILE:O	1:B:1226:GLY:N	2.36	0.58
1:A:1312:ILE:HD11	1:C:1308:ILE:HG23	1.85	0.58
1:A:1262:VAL:HB	1:A:1276:VAL:HG13	1.85	0.58
1:A:1219:ILE:HG23	1:C:1219:ILE:HD11	1.86	0.58
1:B:1111:ALA:HB1	1:B:1116:ALA:CB	2.35	0.57
1:C:1111:ALA:HB1	1:C:1116:ALA:CB	2.34	0.57
1:B:1063:TYR:CZ	1:C:1063:TYR:HB3	2.38	0.57
1:B:1219:ILE:CD1	1:C:1219:ILE:HG23	2.35	0.57
1:A:1219:ILE:HD11	1:B:1219:ILE:HG13	1.86	0.57
1:A:1094:ILE:HD13	1:C:1096:ILE:CG2	2.32	0.57
1:B:1219:ILE:HD13	1:C:1219:ILE:HG23	1.88	0.56
1:C:1219:ILE:HA	1:C:1222:ILE:HD13	1.86	0.56
1:B:1123:SER:OG	1:B:1132:THR:HG21	2.06	0.56
1:C:1100:THR:HG22	1:C:1113:GLY:O	2.07	0.55
1:A:1260:ASN:HD22	1:A:1274:ASN:HD22	1.52	0.55
1:A:1312:ILE:CD1	1:C:1308:ILE:HG23	2.36	0.55
1:A:1145:MET:HE2	1:B:1186:VAL:HG21	1.89	0.55
1:B:1084:ALA:HB3	1:B:1098:LEU:HD23	1.89	0.55
1:B:1102:VAL:HG12	1:B:1102:VAL:O	2.07	0.55
1:B:1211:ARG:O	1:B:1215:ILE:HD12	2.06	0.55
1:A:1111:ALA:HB1	1:A:1116:ALA:CB	2.34	0.54
1:B:1097:GLY:O	1:B:1100:THR:HG23	2.08	0.54
1:A:1094:ILE:O	1:A:1110:ILE:HA	2.08	0.54
1:B:1159:SER:N	1:B:1162:GLY:O	2.40	0.54
1:A:1085:LYS:O	1:A:1099:ASN:HA	2.07	0.54
1:A:1104:ALA:O	1:A:1106:ALA:HB3	2.08	0.54
1:A:1184:LEU:HD12	1:B:1143:TYR:HE2	1.72	0.54
1:A:1104:ALA:O	1:A:1105:ASP:C	2.47	0.53
1:A:1201:LEU:HD23	1:B:1201:LEU:HB3	1.90	0.53
1:A:1120:HIS:CE1	1:A:1134:ARG:HA	2.44	0.53
1:B:1260:ASN:HD22	1:B:1274:ASN:HD22	1.56	0.53
1:B:1258:ALA:O	1:B:1261:SER:OG	2.22	0.53
1:B:1075:VAL:HG11	1:B:1089:ASN:HD22	1.74	0.53
1:B:1120:HIS:CE1	1:B:1134:ARG:HA	2.44	0.53
1:A:1081:ALA:HB2	1:A:1088:VAL:CG2	2.38	0.52
1:C:1260:ASN:HD22	1:C:1274:ASN:HD22	1.57	0.52
1:A:1156:SER:OG	1:C:1168:ASN:ND2	2.39	0.52
1:C:1102:VAL:HG12	1:C:1102:VAL:O	2.09	0.52
1:C:1328:ARG:O	1:C:1332:LEU:HD13	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:LEU:CD2	1:B:1201:LEU:HB3	2.40	0.52
1:C:1120:HIS:CE1	1:C:1134:ARG:HA	2.45	0.51
1:A:1065:ALA:CB	1:B:1080:LEU:HD23	2.41	0.51
1:B:1096:ILE:HG22	1:C:1094:ILE:HD13	1.93	0.51
1:C:1146:ASP:O	1:C:1147:THR:HG23	2.10	0.51
1:A:1123:SER:OG	1:A:1132:THR:HG21	2.10	0.50
1:A:1198:ILE:HD13	1:C:1197:SER:HB2	1.92	0.50
1:C:1159:SER:N	1:C:1162:GLY:O	2.43	0.50
1:A:1222:ILE:N	1:A:1222:ILE:HD13	2.27	0.50
1:B:1133:THR:H	1:B:1154:GLU:CD	2.14	0.50
1:A:1063:TYR:OH	1:C:1080:LEU:HD22	2.11	0.50
1:A:1065:ALA:HB2	1:B:1080:LEU:CD2	2.42	0.50
1:B:1315:ILE:HD13	1:C:1315:ILE:HG21	1.93	0.49
1:C:1203:THR:CG2	1:C:1204:GLN:N	2.75	0.49
1:C:1241:ASN:OD1	1:C:1241:ASN:C	2.50	0.49
1:C:1219:ILE:O	1:C:1222:ILE:N	2.43	0.49
1:C:1075:VAL:HG11	1:C:1089:ASN:HD22	1.77	0.49
1:B:1201:LEU:HD23	1:C:1201:LEU:HB3	1.90	0.49
1:C:1094:ILE:O	1:C:1110:ILE:HA	2.13	0.49
1:C:1211:ARG:O	1:C:1215:ILE:HD13	2.13	0.49
1:A:1326:ILE:CD1	1:C:1322:ILE:HG23	2.43	0.49
1:A:1065:ALA:HB2	1:B:1080:LEU:HD23	1.94	0.48
1:B:1184:LEU:HD12	1:C:1143:TYR:HE2	1.78	0.48
1:A:1124:ILE:HG22	1:A:1125:ALA:N	2.29	0.48
1:A:1090:ALA:HB2	1:A:1102:VAL:CG1	2.42	0.48
1:C:1104:ALA:O	1:C:1105:ASP:C	2.51	0.48
1:A:1086:THR:HG23	1:A:1100:THR:HG1	1.77	0.48
1:A:1075:VAL:HG11	1:A:1089:ASN:HD22	1.79	0.48
1:C:1155:PHE:CE1	1:C:1157:VAL:HG13	2.48	0.48
1:C:1278:VAL:O	1:C:1285:ARG:CD	2.58	0.48
1:A:1102:VAL:O	1:A:1102:VAL:HG12	2.13	0.48
1:A:1326:ILE:HD12	1:C:1322:ILE:HG23	1.96	0.48
1:C:1150:ASN:OD1	1:C:1150:ASN:N	2.47	0.48
1:A:1155:PHE:CE1	1:A:1157:VAL:HG13	2.49	0.48
1:C:1104:ALA:O	1:C:1106:ALA:HB3	2.14	0.48
1:B:1211:ARG:NH2	1:C:1212:VAL:HG12	2.29	0.48
1:A:1145:MET:CE	1:B:1186:VAL:HG21	2.44	0.47
1:B:1262:VAL:HB	1:B:1276:VAL:HG13	1.96	0.47
1:C:1222:ILE:H	1:C:1222:ILE:HD12	1.78	0.47
1:A:1315:ILE:HD13	1:B:1315:ILE:HG21	1.94	0.47
1:C:1184:LEU:O	1:C:1185:LYS:C	2.52	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:LYS:NZ	1:B:1223:VAL:O	2.47	0.47
1:B:1142:ALA:HB1	1:C:1172:GLY:O	2.14	0.47
1:B:1221:ASP:O	1:B:1225:THR:HG23	2.15	0.47
1:A:1328:ARG:O	1:A:1332:LEU:HD13	2.15	0.47
1:A:1145:MET:O	1:A:1146:ASP:HB2	2.15	0.46
1:C:1198:ILE:HG22	1:C:1202:ASN:HD21	1.80	0.46
1:C:1103:MET:SD	1:C:1119:ASN:ND2	2.88	0.46
1:A:1315:ILE:CG2	1:C:1315:ILE:HD13	2.36	0.46
1:B:1100:THR:HB	1:B:1116:ALA:HB3	1.98	0.46
1:B:1155:PHE:CE1	1:B:1157:VAL:HG13	2.49	0.46
1:A:1126:MET:CE	1:B:1124:ILE:HG21	2.46	0.45
1:C:1179:VAL:HG22	1:C:1183:GLN:HB2	1.97	0.45
1:A:1212:VAL:HG12	1:C:1211:ARG:NH2	2.31	0.45
1:B:1166:ILE:HG23	1:C:1155:PHE:HD1	1.81	0.45
1:C:1085:LYS:O	1:C:1099:ASN:HA	2.16	0.45
1:A:1124:ILE:CD1	1:C:1126:MET:CE	2.68	0.45
1:A:1080:LEU:HD23	1:C:1065:ALA:HB2	1.98	0.45
1:B:1175:ASP:OD1	1:C:1185:LYS:NZ	2.45	0.45
1:B:1201:LEU:HD21	1:C:1201:LEU:HB3	1.99	0.44
1:A:1201:LEU:HB3	1:C:1201:LEU:HD23	1.99	0.44
1:A:1098:LEU:HD12	1:A:1098:LEU:H	1.82	0.44
1:B:1286:ARG:HB2	1:C:1275:THR:HG22	2.00	0.44
1:A:1104:ALA:C	1:A:1106:ALA:N	2.70	0.44
1:B:1094:ILE:O	1:B:1110:ILE:HA	2.17	0.44
1:A:1103:MET:HB2	1:A:1119:ASN:HA	2.00	0.44
1:C:1272:GLU:O	1:C:1273:ALA:C	2.56	0.44
1:A:1135:GLY:HA2	1:A:1154:GLU:HB3	2.00	0.43
1:B:1144:ASN:O	1:C:1186:VAL:HG11	2.18	0.43
1:A:1105:ASP:O	1:A:1106:ALA:C	2.56	0.43
1:B:1179:VAL:HG22	1:B:1183:GLN:HB2	2.00	0.43
1:B:1128:ASN:N	1:B:1164:ARG:HH22	2.16	0.43
1:A:1190:GLN:O	1:A:1191:VAL:C	2.55	0.43
1:B:1124:ILE:HG22	1:B:1125:ALA:N	2.33	0.43
1:B:1162:GLY:HA3	1:C:1152:VAL:HG21	2.01	0.43
1:B:1305:MET:CE	1:B:1309:GLU:OE2	2.66	0.43
1:C:1105:ASP:O	1:C:1106:ALA:C	2.57	0.43
1:C:1128:ASN:HD22	1:C:1164:ARG:NH2	2.17	0.43
1:A:1134:ARG:NH2	1:C:1167:THR:HG22	2.34	0.42
1:A:1168:ASN:ND2	1:B:1156:SER:OG	2.50	0.42
1:B:1219:ILE:HD13	1:C:1219:ILE:CG2	2.49	0.42
1:A:1179:VAL:HG22	1:A:1183:GLN:HB2	2.00	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1225:THR:OG1	1:C:1227:SER:HB2	2.18	0.42
1:A:1103:MET:SD	1:A:1119:ASN:ND2	2.93	0.42
1:B:1190:GLN:HA	1:B:1193:ARG:HH11	1.85	0.42
1:C:1123:SER:OG	1:C:1132:THR:HG21	2.20	0.42
1:B:1233:THR:O	1:B:1233:THR:CG2	2.64	0.42
1:B:1157:VAL:O	1:B:1164:ARG:CD	2.68	0.42
1:C:1258:ALA:O	1:C:1261:SER:OG	2.31	0.42
1:C:1081:ALA:CB	1:C:1088:VAL:CG2	2.97	0.42
1:C:1190:GLN:HA	1:C:1193:ARG:HH11	1.85	0.42
1:B:1234:ASN:ND2	1:C:1244:GLY:O	2.50	0.42
1:A:1185:LYS:NZ	1:C:1175:ASP:OD1	2.51	0.42
1:A:1278:VAL:O	1:A:1285:ARG:CD	2.59	0.41
1:A:1259:GLU:OE1	1:A:1260:ASN:HB2	2.19	0.41
1:B:1167:THR:CG2	1:C:1134:ARG:CZ	2.99	0.41
1:B:1328:ARG:O	1:B:1332:LEU:HD13	2.20	0.41
1:A:1179:VAL:HG13	1:C:1179:VAL:HG12	2.01	0.41
1:C:1262:VAL:HB	1:C:1276:VAL:HG13	2.03	0.41
1:C:1141:THR:O	1:C:1141:THR:HG23	2.21	0.41
1:B:1229:LYS:O	1:C:1240:ALA:N	2.52	0.41
1:B:1208:LEU:HD23	1:C:1212:VAL:HG21	2.03	0.41
1:A:1275:THR:HA	1:C:1286:ARG:O	2.21	0.41
1:C:1070:GLU:HG2	1:C:1085:LYS:HG2	2.02	0.41
1:A:1197:SER:O	1:A:1201:LEU:HD13	2.21	0.41
1:B:1197:SER:HB2	1:C:1198:ILE:HD13	2.03	0.41
1:A:1318:LYS:HD2	1:B:1319:ILE:HG21	2.03	0.41
1:B:1173:SER:N	1:C:1165:GLN:HE22	2.18	0.41
1:A:1071:ASP:OD1	1:A:1071:ASP:N	2.53	0.41
1:C:1128:ASN:ND2	1:C:1164:ARG:NH2	2.69	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	271/322 (84%)	236 (87%)	26 (10%)	9 (3%)	5	26
1	B	271/322 (84%)	235 (87%)	32 (12%)	4 (2%)	13	46
1	C	271/322 (84%)	238 (88%)	28 (10%)	5 (2%)	11	42
All	All	813/966 (84%)	709 (87%)	86 (11%)	18 (2%)	8	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1062	TYR
1	A	1104	ALA
1	A	1105	ASP
1	B	1062	TYR
1	C	1062	TYR
1	C	1104	ALA
1	C	1105	ASP
1	A	1106	ALA
1	A	1145	MET
1	A	1146	ASP
1	B	1103	MET
1	B	1219	ILE
1	B	1239	ASP
1	C	1106	ALA
1	A	1098	LEU
1	A	1223	VAL
1	A	1221	ASP
1	C	1147	THR

### 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	199/257 (77%)	177 (89%)	22 (11%)	8	29
1	B	195/257 (76%)	175 (90%)	20 (10%)	9	32
1	C	198/257 (77%)	174 (88%)	24 (12%)	6	24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	592/771 (77%)	526 (89%)	66 (11%)	8	29

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1071	ASP
1	A	1082	MET
1	A	1091	ASP
1	A	1107	ILE
1	A	1117	ARG
1	A	1151	SER
1	A	1157	VAL
1	A	1184	LEU
1	A	1191	VAL
1	A	1193	ARG
1	A	1196	GLN
1	A	1199	THR
1	A	1203	THR
1	A	1210	THR
1	A	1219	ILE
1	A	1221	ASP
1	A	1228	THR
1	A	1239	ASP
1	A	1282	THR
1	A	1284	GLN
1	A	1300	VAL
1	A	1328	ARG
1	B	1082	MET
1	B	1100	THR
1	B	1114	SER
1	B	1117	ARG
1	B	1157	VAL
1	B	1184	LEU
1	B	1191	VAL
1	B	1193	ARG
1	B	1196	GLN
1	B	1199	THR
1	B	1208	LEU
1	B	1210	THR
1	B	1219	ILE
1	B	1236	ASP
1	B	1282	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1284	GLN
1	B	1311	LYS
1	B	1313	GLU
1	B	1318	LYS
1	B	1331	LYS
1	C	1068	THR
1	C	1082	MET
1	C	1091	ASP
1	C	1117	ARG
1	C	1138	THR
1	C	1139	ASP
1	C	1150	ASN
1	C	1151	SER
1	C	1157	VAL
1	C	1184	LEU
1	C	1191	VAL
1	C	1193	ARG
1	C	1196	GLN
1	C	1199	THR
1	C	1203	THR
1	C	1210	THR
1	C	1213	THR
1	C	1219	ILE
1	C	1223	VAL
1	C	1282	THR
1	C	1284	GLN
1	C	1300	VAL
1	C	1313	GLU
1	C	1328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1089	ASN
1	A	1168	ASN
1	A	1196	GLN
1	A	1207	ASN
1	A	1274	ASN
1	B	1089	ASN
1	B	1163	GLN
1	B	1196	GLN
1	B	1274	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1089	ASN
1	C	1115	ASN
1	C	1137	GLN
1	C	1165	GLN
1	C	1168	ASN
1	C	1196	GLN
1	C	1202	ASN
1	C	1274	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 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 [i](#)

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	273/322 (84%)	-0.10	3 (1%) 82 66	20, 65, 119, 151	0
1	B	273/322 (84%)	0.04	12 (4%) 38 17	20, 65, 137, 168	0
1	C	273/322 (84%)	0.04	9 (3%) 50 26	20, 69, 129, 142	0
All	All	819/966 (84%)	-0.00	24 (2%) 55 31	20, 66, 131, 168	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1077	THR	7.9
1	C	1105	ASP	7.6
1	B	1104	ALA	6.2
1	C	1091	ASP	5.2
1	B	1068	THR	5.1
1	C	1148	PRO	4.0
1	C	1078	ASP	3.6
1	A	1217	ASN	3.3
1	B	1105	ASP	3.0
1	C	1104	ALA	2.9
1	B	1089	ASN	2.8
1	A	1105	ASP	2.7
1	B	1106	ALA	2.6
1	B	1103	MET	2.5
1	B	1118	ALA	2.5
1	B	1096	ILE	2.5
1	B	1141	THR	2.4
1	B	1131	GLN	2.4
1	B	1159	SER	2.2
1	C	1173	SER	2.2
1	C	1103	MET	2.2
1	A	1095	GLY	2.1
1	B	1088	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	1069	GLU	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	CL	C	2334	1/1	0.91	0.46	3.02	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.