

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 24, 2023 – 05:29 AM EDT

PDB ID	:	5TRC
Title	:	Crystal structure of phosphorylated AC3-AC5 domains of yeast acetyl-CoA
		carboxylase
Authors	:	Wei, J.; Tong, L.
Deposited on	:	2016-10-26
Resolution	:	2.90 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R <sub>free</sub>	130704	1957 (2.90-2.90)		
Clashscore	141614	2172 (2.90-2.90)		
Ramachandran outliers	138981	2115 (2.90-2.90)		
Sidechain outliers	138945	2117 (2.90-2.90)		
RSRZ outliers	127900	1906 (2.90-2.90)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	474	2% 	37%	5% 10%		
1	В	474	37%	42%	5% 16%		



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6628 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Δ	496	Total	С	Ν	0	Р	$\mathbf{S}$	0	0	0
1		420	3414	2178	581	648	1	6		0	0
1	В	308	Total	С	Ν	0	Р	S	0	0	0
	D	590	3212	2051	549	605	1	6	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	1504	HIS	-	expression tag	UNP Q00955
А	1505	HIS	-	expression tag	UNP Q00955
A	1506	HIS	-	expression tag	UNP Q00955
A	1507	HIS	-	expression tag	UNP Q00955
А	1508	HIS	-	expression tag	UNP Q00955
A	1509	HIS	-	expression tag	UNP Q00955
В	1504	HIS	-	expression tag	UNP Q00955
В	1505	HIS	-	expression tag	UNP Q00955
В	1506	HIS	-	expression tag	UNP Q00955
В	1507	HIS	-	expression tag	UNP Q00955
В	1508	HIS	-	expression tag	UNP Q00955
В	1509	HIS	-	expression tag	UNP Q00955

There are 12 discrepancies between the modelled and reference sequences:

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Cl 1 1	0	0
2	В	1	Total Cl 1 1	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.



PPRO SER ALA ALA ALA ALA PHE PHE PHE PHE CVS SER VAL VAL VAL VAL VAL CVS SER ALA AASN

• Molecule 1: Acetyl-CoA carboxylase







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	56.43Å 93.19Å 110.94Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.57^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	46.57 - 2.90	Depositor
Resolution (A)	46.57 - 2.88	EDS
% Data completeness	97.5 (46.57-2.90)	Depositor
(in resolution range)	97.5(46.57-2.88)	EDS
$R_{merge}$	0.05	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
B B.	0.223 , $0.287$	Depositor
$\Pi, \Pi_{free}$	0.227 , $0.287$	DCC
$R_{free}$ test set	1272 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	82.6	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , $61.1$	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6628	wwPDB-VP
Average B, all atoms $(Å^2)$	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, 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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.61	0/3470	0.71	1/4703~(0.0%)	
1	В	0.53	0/3260	0.69	0/4410	
All	All	0.57	0/6730	0.70	1/9113~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	1293	GLU	C-N-CD	5.04	138.98	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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	А	3414	0	3409	166	0
1	В	3212	0	3213	221	0
2	А	1	0	0	1	0
2	В	1	0	0	1	0
All	All	6628	0	6622	383	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 29.



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:1275:TYR:O	1:A:1290:ARG:O	1.66	1.14	
1:B:1221:VAL:HG11	1:B:1260:ARG:NH1	1.70	1.07	
1:A:1445:ASN:OD1	1:A:1447:VAL:HG22	1.59	1.01	
1:B:1221:VAL:HG13	1:B:1260:ARG:CG	1.97	0.94	
1:A:1189:ILE:O	1:A:1193:SER:OG	1.85	0.94	
1:B:1221:VAL:HG13	1:B:1260:ARG:HG3	1.49	0.93	
1:B:1221:VAL:CG1	1:B:1260:ARG:HG3	2.00	0.89	
1:B:1482:PRO:O	1:B:1485:THR:HG22	1.73	0.88	
1:B:1313:ILE:HD11	1:B:1324:GLU:HB2	1.56	0.88	
1:B:1305:LEU:HD12	1:B:1310:ILE:HD11	1.55	0.88	
1:B:1221:VAL:HG11	1:B:1260:ARG:CZ	2.06	0.85	
1:B:1275:TYR:O	1:B:1290:ARG:O	1.96	0.84	
1:B:1373:GLU:OE2	1:B:1414:ARG:NH2	2.12	0.83	
1:B:1106:ILE:HD11	1:B:1177:LEU:HD22	1.59	0.83	
1:A:1044:ILE:HD12	1:A:1085:VAL:HG12	1.63	0.80	
1:B:1088:GLN:OE1	1:B:1268:LYS:HG2	1.81	0.80	
1:A:1421:SER:O	1:A:1446:ASN:HB3	1.83	0.78	
1:B:1088:GLN:HE21	1:B:1089:PHE:HE1	1.29	0.78	
1:B:1406:GLY:HA2	1:B:1409:GLU:HG3	1.64	0.78	
1:A:1445:ASN:CG	1:A:1447:VAL:HG22	2.04	0.77	
1:B:1272:TYR:O	1:B:1318:ARG:NH2	2.18	0.75	
1:B:1461:LYS:HG2	1:B:1467:TRP:CD1	2.22	0.75	
1:B:1305:LEU:CD1	1:B:1310:ILE:HD11	2.18	0.74	
1:A:1408:LEU:O	1:A:1411:PHE:N	2.18	0.73	
1:A:1329:THR:CG2	1:A:1494:GLN:HG2	2.19	0.73	
1:B:1221:VAL:HG13	1:B:1260:ARG:HG2	1.70	0.73	
1:A:1448:SER:O	1:A:1450:TYR:N	2.21	0.72	
1:A:1108:ARG:NH1	2:A:1601:CL:CL	2.60	0.72	
1:A:1117:ASP:OD1	1:A:1132:LYS:HE2	1.89	0.71	
1:A:1045:GLU:HG3	1:A:1089:PHE:HE2	1.54	0.71	
1:A:1141:SER:OG	1:A:1426:ARG:NH1	2.24	0.70	
1:B:1039:GLU:O	1:B:1043:GLN:HG3	1.90	0.70	
1:B:1063:LYS:HE2	1:B:1064:ARG:HG3	1.71	0.70	
1:A:1421:SER:O	1:A:1446:ASN:CB	2.39	0.69	
1:A:1113:TYR:OH	1:A:1158:VAL:HG23	1.93	0.69	
1:B:1341:ILE:CG2	1:B:1390:ILE:HD11	2.22	0.69	
1:B:1380:SER:HB2	1:B:1383:ASN:HD21	1.58	0.69	
1:A:1045:GLU:HG3	1:A:1089:PHE:CE2	2.28	0.69	
1:A:1342:ILE:HD11	1:A:1364:LEU:HD12	1.74	0.69	
1:A:1329:THR:HG23	1:A:1494:GLN:HG2	1.75	0.68	

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1291:HIS:CD2	1:A:1318:ARG:HG2	2.29	0.68
1:B:1040:ARG:NH1	1:B:1084:ASP:OD2	2.26	0.68
1:B:1343:ARG:HH11	1:B:1343:ARG:HG2	1.56	0.68
1:A:1126:VAL:CG2	1:A:1127:PRO:HD2	2.24	0.67
1:B:1036:SER:HA	1:B:1039:GLU:OE1	1.95	0.67
1:A:1315:THR:HB	1:A:1371:ASN:HD21	1.60	0.67
1:A:1315:THR:HB	1:A:1371:ASN:ND2	2.10	0.67
1:B:1313:ILE:CD1	1:B:1324:GLU:HB2	2.23	0.67
1:B:1461:LYS:HG2	1:B:1467:TRP:HD1	1.58	0.66
1:A:1293:GLU:OE2	1:A:1294:PRO:HD2	1.95	0.66
1:B:1109:ALA:O	1:B:1295:ALA:HB1	1.96	0.66
1:B:1220:ASN:O	1:B:1259:ARG:N	2.29	0.65
1:A:1126:VAL:HG22	1:A:1127:PRO:HD2	1.78	0.65
1:A:1339:ARG:HG2	1:A:1339:ARG:HH11	1.62	0.65
1:A:1350:ASP:OD1	1:A:1350:ASP:N	2.28	0.65
1:B:1299:GLN:OE1	1:B:1390:ILE:HD13	1.98	0.64
1:B:1109:ALA:O	1:B:1295:ALA:CB	2.46	0.64
1:A:1232:PHE:HE2	1:A:1241:ARG:HG3	1.63	0.64
1:A:1106:ILE:HD13	1:A:1131:TRP:CE3	2.33	0.64
1:B:1040:ARG:NH2	1:B:1084:ASP:OD2	2.30	0.63
1:B:1469:PHE:O	1:B:1479:HIS:O	2.16	0.63
1:B:1221:VAL:CG1	1:B:1260:ARG:NH1	2.55	0.63
1:B:1369:LEU:O	1:B:1373:GLU:HG3	1.98	0.63
1:A:1121:HIS:CE1	1:A:1196:VAL:HG11	2.34	0.63
1:A:1445:ASN:OD1	1:A:1447:VAL:CG2	2.43	0.63
1:B:1174:GLU:H	1:B:1220:ASN:ND2	1.97	0.63
1:A:1044:ILE:HD12	1:A:1085:VAL:CG1	2.28	0.62
1:B:1309:ASN:N	1:B:1326:VAL:O	2.31	0.62
1:B:1288:THR:HG22	1:B:1312:PRO:HD3	1.80	0.62
1:B:1174:GLU:O	1:B:1220:ASN:ND2	2.34	0.61
1:B:1344:THR:HG22	1:B:1356:TYR:OH	2.00	0.61
1:A:1088:GLN:HG3	1:A:1089:PHE:CD1	2.35	0.61
1:A:1457:TYR:CD2	1:A:1469:PHE:HB3	2.35	0.61
1:B:1440:LEU:HD23	1:B:1458:THR:HG22	1.81	0.61
1:B:1106:ILE:HD11	1:B:1177:LEU:CD2	2.28	0.61
1:B:1460:VAL:HG12	1:B:1461:LYS:H	1.65	0.61
1:B:1460:VAL:O	1:B:1468:VAL:N	2.23	0.61
1:B:1376:ASP:OD1	1:B:1378:SER:HB3	2.01	0.61
1:B:1408:LEU:HD12	1:B:1444:ILE:CG2	2.30	0.61
1:B:1342:ILE:HD12	1:B:1389:PHE:CZ	2.36	0.61
1:B:1272:TYR:CG	1:B:1273:PRO:HD2	2.36	0.60



			Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1234:SER:O	1:B:1238:ILE:HG13	2.01	0.60
1:A:1221:VAL:HG22	1:A:1260:ARG:HG3	1.83	0.60
1:A:1358:THR:OG1	1:A:1403:ALA:HB1	2.01	0.60
1:B:1242:LEU:HD21	1:B:1263:PHE:CD1	2.36	0.60
1:B:1108:ARG:NH1	2:B:1601:CL:CL	2.71	0.60
1:A:1226:VAL:O	1:A:1226:VAL:HG12	2.01	0.60
1:A:1278:PHE:CE2	1:A:1285:GLU:HB2	2.37	0.60
1:B:1289:ILE:O	1:B:1289:ILE:HG13	2.01	0.60
1:A:1226:VAL:HG11	1:A:1265:PHE:CE2	2.36	0.60
1:B:1289:ILE:HD11	1:B:1292:ILE:CG2	2.32	0.60
1:B:1087:LEU:HD12	1:B:1266:GLY:CA	2.32	0.59
1:A:1408:LEU:HD22	1:A:1415:LEU:HD11	1.84	0.59
1:B:1189:ILE:O	1:B:1193:SER:OG	2.20	0.59
1:A:1124:VAL:HG13	1:A:1192:GLN:HG2	1.85	0.59
1:A:1343:ARG:HG3	1:A:1343:ARG:HH11	1.68	0.59
1:B:1443:LEU:HD22	1:B:1457:TYR:HE1	1.68	0.58
1:A:1445:ASN:OD1	1:A:1447:VAL:HG13	2.02	0.58
1:A:1282:ASN:O	1:A:1284:ASN:N	2.30	0.58
1:A:1406:GLY:HA2	1:A:1409:GLU:OE1	2.03	0.58
1:A:1196:VAL:HG12	1:A:1196:VAL:O	2.04	0.58
1:A:1342:ILE:CD1	1:A:1364:LEU:HD12	2.34	0.58
1:B:1041:THR:HA	1:B:1085:VAL:HG11	1.85	0.58
1:B:1108:ARG:O	1:B:1111:ARG:HB2	2.04	0.58
1:B:1301:GLU:OE1	1:B:1441:ARG:NH2	2.37	0.58
1:A:1289:ILE:HG13	1:A:1289:ILE:O	2.03	0.58
1:A:1353:ILE:HD11	1:A:1394:ASP:HB3	1.86	0.58
1:A:1353:ILE:CD1	1:A:1394:ASP:HB3	2.34	0.58
1:A:1447:VAL:O	1:A:1448:SER:HB2	2.04	0.58
1:A:1344:THR:HB	1:A:1356:TYR:OH	2.04	0.57
1:B:1491:GLU:O	1:B:1494:GLN:HG3	2.04	0.57
1:B:1091:THR:HG21	1:B:1227:ALA:HB2	1.85	0.57
1:B:1106:ILE:CD1	1:B:1177:LEU:HD22	2.32	0.57
1:B:1408:LEU:HD12	1:B:1444:ILE:HG21	1.87	0.57
1:B:1235:GLU:OE2	1:B:1276:TYR:OH	2.20	0.57
1:B:1443:LEU:HD22	1:B:1457:TYR:CE1	2.39	0.57
1:A:1458:THR:HG22	1:A:1459:GLU:H	1.69	0.57
1:A:1156:VAL:HG12	1:A:1163:TYR:O	2.05	0.57
1:A:1175:GLY:HA2	1:A:1221:VAL:O	2.06	0.56
1:A:1401:GLU:HB2	1:A:1456:MET:SD	2.44	0.56
1:B:1052:VAL:HG22	1:B:1067:PRO:CA	2.35	0.56
1:B:1089:PHE:N	1:B:1089:PHE:CD1	2.72	0.56



			Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1185:ASP:O	1:A:1189:ILE:HG12	2.05	0.56
1:B:1124:VAL:HG22	1:B:1192:GLN:CD	2.26	0.56
1:B:1128:ILE:CD1	1:B:1193:SER:HB3	2.36	0.56
1:B:1341:ILE:HG23	1:B:1390:ILE:HD11	1.86	0.56
1:A:1399:ASP:O	1:A:1402:ALA:HB3	2.06	0.56
1:A:1232:PHE:CE2	1:A:1241:ARG:HG3	2.40	0.56
1:B:1353:ILE:HG21	1:B:1394:ASP:OD1	2.06	0.56
1:A:1091:THR:HG21	1:A:1180:VAL:O	2.06	0.56
1:A:1491:GLU:HB3	1:A:1494:GLN:NE2	2.21	0.56
1:B:1243:ARG:HA	1:B:1246:LEU:HD12	1.87	0.55
1:A:1088:GLN:HE21	1:A:1089:PHE:HE1	1.53	0.55
1:A:1194:LEU:O	1:A:1197:ILE:HG23	2.06	0.55
1:A:1257:SER:O	1:A:1257:SER:OG	2.23	0.55
1:B:1356:TYR:CZ	1:B:1360:GLU:HG3	2.41	0.55
1:B:1114:THR:O	1:B:1133:PHE:HA	2.07	0.55
1:B:1040:ARG:HH12	1:B:1084:ASP:CG	2.10	0.55
1:B:1242:LEU:HA	1:B:1245:ILE:HD12	1.88	0.55
1:A:1040:ARG:HA	1:A:1043:GLN:HB2	1.89	0.55
1:B:1052:VAL:CG2	1:B:1067:PRO:HB3	2.37	0.55
1:B:1285:GLU:OE2	1:B:1290:ARG:CD	2.55	0.55
1:A:1194:LEU:HD11	1:A:1253:LEU:HD23	1.88	0.54
1:A:1339:ARG:HG2	1:A:1339:ARG:NH1	2.21	0.54
1:A:1441:ARG:HG3	1:A:1469:PHE:HE1	1.72	0.54
1:A:1057:TYR:CE1	1:B:1040:ARG:HB3	2.43	0.54
1:B:1052:VAL:HG22	1:B:1067:PRO:HA	1.89	0.54
1:B:1102:ALA:HB1	1:B:1177:LEU:HD23	1.89	0.54
1:A:1235:GLU:O	1:A:1238:ILE:N	2.41	0.54
1:B:1089:PHE:HD1	1:B:1089:PHE:H	1.55	0.54
1:B:1425:ILE:HB	1:B:1442:ALA:HB3	1.90	0.54
1:A:1354:GLN:HB2	1:A:1395:ILE:HD11	1.90	0.54
1:A:1395:ILE:HG12	1:A:1396:SER:H	1.72	0.54
1:B:1289:ILE:CD1	1:B:1292:ILE:CG2	2.86	0.53
1:B:1194:LEU:O	1:B:1196:VAL:N	2.41	0.53
1:A:1342:ILE:CG1	1:A:1364:LEU:HD12	2.38	0.53
1:B:1310:ILE:CG2	1:B:1311:LYS:N	2.71	0.53
1:B:1354:GLN:N	1:B:1395:ILE:HD11	2.24	0.53
1:B:1395:ILE:HG22	1:B:1400:VAL:HG23	1.91	0.52
1:B:1460:VAL:HG21	1:B:1470:LYS:HD2	1.91	0.52
1:A:1049:LYS:O	1:A:1053:VAL:HG23	2.09	0.52
1:B:1406:GLY:CA	1:B:1409:GLU:HG3	2.36	0.52
1:B:1088:GLN:HG3	1:B:1089:PHE:CD1	2.43	0.52



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1391:ALA:HB3	1:B:1393:PHE:CZ	2.44	0.52
1:A:1058:GLY:HA2	1:B:1040:ARG:HG2	1.90	0.52
1:B:1182:HIS:HE2	1:B:1231:GLY:N	2.08	0.52
1:B:1279:ASN:HD21	1:B:1286:ASN:HD22	1.57	0.52
1:B:1439:PRO:HG2	1:B:1459:GLU:HB2	1.92	0.52
1:B:1180:VAL:HG12	1:B:1189:ILE:HD12	1.92	0.52
1:B:1225:CYS:SG	1:B:1226:VAL:N	2.83	0.52
1:A:1178:MET:HE2	1:A:1193:SER:HB2	1.90	0.52
1:B:1341:ILE:HG21	1:B:1390:ILE:HD11	1.92	0.52
1:B:1460:VAL:HG12	1:B:1461:LYS:N	2.25	0.52
1:A:1055:VAL:HG12	1:A:1061:ASN:HB3	1.92	0.52
1:A:1158:VAL:HG11	1:A:1298:PHE:HD2	1.75	0.52
1:A:1458:THR:HG22	1:A:1459:GLU:N	2.23	0.52
1:A:1395:ILE:CG1	1:A:1396:SER:H	2.22	0.51
1:B:1086:LEU:HG	1:B:1086:LEU:O	2.08	0.51
1:B:1064:ARG:O	1:B:1065:SER:OG	2.25	0.51
1:B:1106:ILE:HD12	1:B:1131:TRP:CZ3	2.45	0.51
1:B:1156:VAL:HG13	1:B:1157:SEP:N	2.25	0.51
1:B:1357:LEU:HD22	1:B:1427:ILE:HD11	1.92	0.51
1:A:1055:VAL:HG22	1:A:1056:ALA:N	2.26	0.51
1:B:1289:ILE:CD1	1:B:1292:ILE:HG22	2.40	0.51
1:B:1293:GLU:OE2	1:B:1294:PRO:HD2	2.10	0.51
1:B:1285:GLU:OE2	1:B:1290:ARG:HD2	2.11	0.51
1:B:1338:THR:HG21	1:B:1368:ILE:HG12	1.92	0.51
1:B:1180:VAL:HB	1:B:1185:ASP:CB	2.41	0.50
1:B:1124:VAL:HG23	1:B:1125:THR:OG1	2.10	0.50
1:B:1334:LYS:O	1:B:1380:SER:HA	2.11	0.50
1:B:1440:LEU:CD2	1:B:1458:THR:HG22	2.42	0.50
1:B:1489:VAL:CG1	1:B:1490:LYS:N	2.75	0.50
1:A:1045:GLU:CG	1:A:1089:PHE:HE2	2.21	0.50
1:B:1132:LYS:HA	1:B:1173:ARG:O	2.11	0.50
1:B:1220:ASN:O	1:B:1258:ILE:HA	2.11	0.50
1:B:1236:GLU:O	1:B:1240:VAL:HG12	2.12	0.50
1:B:1353:ILE:HD12	1:B:1353:ILE:H	1.75	0.50
1:A:1113:TYR:CZ	1:A:1158:VAL:HG23	2.46	0.50
1:A:1353:ILE:HD13	1:A:1395:ILE:N	2.26	0.50
1:B:1369:LEU:HD22	1:B:1418:LEU:HD12	1.94	0.50
1:B:1429:ILE:HB	1:B:1438:VAL:HG13	1.94	0.50
1:A:1240:VAL:O	1:A:1244:GLU:HG3	2.12	0.49
1:B:1194:LEU:HD11	1:B:1253:LEU:HD23	1.94	0.49
1:A:1092:HIS:ND1	1:A:1093:GLN:N	2.61	0.49



A 4 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1128:ILE:CG2	1:B:1176:ILE:HG23	2.41	0.49
1:B:1071:ILE:HD12	1:B:1071:ILE:N	2.27	0.49
1:B:1265:PHE:N	1:B:1265:PHE:CD1	2.78	0.49
1:A:1441:ARG:HG3	1:A:1469:PHE:CE1	2.48	0.49
1:B:1183:LEU:HD12	1:B:1186:VAL:HG21	1.93	0.49
1:B:1391:ALA:HB3	1:B:1393:PHE:CE2	2.47	0.49
1:A:1220:ASN:N	1:A:1257:SER:O	2.41	0.49
1:B:1481:ARG:HG3	1:B:1481:ARG:HH11	1.77	0.49
1:B:1301:GLU:CD	1:B:1441:ARG:HH22	2.16	0.49
1:A:1329:THR:HG21	1:A:1494:GLN:OE1	2.13	0.48
1:B:1074:ASP:O	1:B:1078:SER:HB2	2.13	0.48
1:A:1246:LEU:HD13	1:A:1283:TYR:HB3	1.95	0.48
1:B:1126:VAL:HG21	1:B:1189:ILE:HD13	1.94	0.48
1:B:1194:LEU:CD2	1:B:1258:ILE:HD11	2.43	0.48
1:B:1260:ARG:HB3	1:B:1279:ASN:HB3	1.95	0.48
1:B:1468:VAL:HG12	1:B:1469:PHE:N	2.27	0.48
1:B:1089:PHE:O	1:B:1092:HIS:HB3	2.14	0.48
1:B:1489:VAL:HG12	1:B:1490:LYS:N	2.28	0.48
1:A:1278:PHE:CD2	1:A:1285:GLU:HA	2.48	0.48
1:A:1283:TYR:CD1	1:A:1283:TYR:N	2.82	0.48
1:B:1174:GLU:H	1:B:1220:ASN:HD21	1.62	0.48
1:B:1260:ARG:HG3	1:B:1260:ARG:HH11	1.78	0.48
1:B:1393:PHE:O	1:B:1430:LYS:N	2.41	0.48
1:A:1364:LEU:HD13	1:A:1387:ILE:HG12	1.94	0.47
1:B:1242:LEU:HD21	1:B:1263:PHE:CE1	2.49	0.47
1:B:1258:ILE:O	1:B:1258:ILE:HG22	2.14	0.47
1:B:1102:ALA:O	1:B:1106:ILE:HG12	2.13	0.47
1:B:1272:TYR:CD1	1:B:1273:PRO:HD2	2.49	0.47
1:B:1395:ILE:CG2	1:B:1396:SER:N	2.78	0.47
1:B:1441:ARG:HG2	1:B:1469:PHE:HE1	1.79	0.47
1:B:1089:PHE:N	1:B:1089:PHE:HD1	2.11	0.47
1:B:1239:LEU:HD21	1:B:1276:TYR:CD1	2.50	0.47
1:B:1264:MET:O	1:B:1264:MET:HG2	2.14	0.47
1:B:1401:GLU:HB2	1:B:1456:MET:SD	2.55	0.47
1:A:1069:LEU:O	1:A:1073:LYS:HG2	2.15	0.47
1:A:1087:LEU:HD11	1:A:1264:MET:HE2	1.96	0.47
1:A:1408:LEU:HD22	1:A:1415:LEU:CD1	2.45	0.47
1:B:1085:VAL:HG12	1:B:1085:VAL:O	2.14	0.47
1:A:1395:ILE:HD11	1:A:1399:ASP:HB3	1.97	0.47
1:B:1081:VAL:HG12	1:B:1344:THR:O	2.14	0.47
1:A:1090:LEU:HB3	1:A:1179:ALA:HB2	1.97	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1222:ALA:O	1:A:1261:ILE:HA	2.14	0.46
1:A:1468:VAL:HG12	1:A:1469:PHE:O	2.16	0.46
1:A:1041:THR:HG23	1:A:1088:GLN:NE2	2.31	0.46
1:A:1448:SER:C	1:A:1450:TYR:H	2.18	0.46
1:A:1460:VAL:HG21	1:A:1470:LYS:HD3	1.97	0.46
1:B:1343:ARG:HG2	1:B:1343:ARG:NH1	2.28	0.46
1:A:1138:ALA:CB	1:A:1461:LYS:HE2	2.46	0.46
1:B:1180:VAL:HB	1:B:1185:ASP:HB3	1.98	0.46
1:B:1468:VAL:CG1	1:B:1469:PHE:N	2.79	0.46
1:A:1456:MET:HE3	1:A:1456:MET:HB2	1.69	0.46
1:B:1264:MET:C	1:B:1265:PHE:HD1	2.19	0.46
1:B:1310:ILE:HG22	1:B:1311:LYS:N	2.31	0.46
1:A:1279:ASN:O	1:A:1283:TYR:HA	2.17	0.46
1:B:1124:VAL:HG22	1:B:1192:GLN:OE1	2.15	0.46
1:B:1081:VAL:HG12	1:B:1344:THR:C	2.36	0.45
1:B:1249:ASN:OD1	1:B:1252:GLU:HB2	2.16	0.45
1:B:1279:ASN:OD1	1:B:1279:ASN:N	2.49	0.45
1:B:1308:PHE:HA	1:B:1327:SER:HA	1.98	0.45
1:B:1431:ASP:HA	1:B:1432:PRO:HD2	1.78	0.45
1:A:1454:THR:O	1:A:1454:THR:OG1	2.33	0.45
1:B:1260:ARG:HA	1:B:1278:PHE:O	2.17	0.45
1:A:1382:LEU:HD23	1:A:1382:LEU:HA	1.64	0.45
1:B:1239:LEU:HD21	1:B:1276:TYR:CE1	2.51	0.45
1:B:1333:ASP:OD1	1:B:1490:LYS:HE2	2.16	0.45
1:A:1380:SER:HB2	1:A:1383:ASN:HD21	1.81	0.45
1:A:1264:MET:HE2	1:A:1264:MET:HB2	1.65	0.45
1:A:1342:ILE:HG13	1:A:1364:LEU:HD12	1.98	0.45
1:B:1183:LEU:O	1:B:1186:VAL:HG23	2.15	0.45
1:B:1395:ILE:O	1:B:1429:ILE:HG23	2.16	0.45
1:A:1308:PHE:HB3	1:A:1325:ALA:HB1	1.97	0.45
1:A:1329:THR:CG2	1:A:1494:GLN:CG	2.92	0.45
1:B:1180:VAL:HG23	1:B:1181:ASP:N	2.30	0.45
1:B:1348:ARG:HG3	1:B:1348:ARG:HH11	1.82	0.45
1:A:1108:ARG:O	1:A:1111:ARG:NH1	2.49	0.45
1:A:1264:MET:HE3	1:A:1275:TYR:CE2	2.52	0.45
1:B:1040:ARG:CZ	1:B:1084:ASP:OD2	2.64	0.45
1:B:1180:VAL:HG12	1:B:1189:ILE:CD1	2.47	0.45
1:B:1351:ILE:CG2	1:B:1352:SER:N	2.79	0.45
1:A:1084:ASP:OD1	1:A:1085:VAL:N	2.50	0.44
1:A:1451:VAL:HG13	1:A:1452:ILE:N	2.32	0.44
1:B:1092:HIS:NE2	1:B:1094:ASP:HB3	2.31	0.44



			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1109:ALA:O	1:B:1295:ALA:HB3	2.17	0.44
1:A:1339:ARG:HH11	1:A:1339:ARG:CG	2.29	0.44
1:B:1124:VAL:HG13	1:B:1192:GLN:HG3	1.98	0.44
1:B:1289:ILE:HD12	1:B:1292:ILE:HG22	1.99	0.44
1:A:1041:THR:OG1	1:A:1085:VAL:HG22	2.17	0.44
1:A:1183:LEU:HD23	1:A:1232:PHE:CZ	2.52	0.44
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.48	0.44
1:A:1176:ILE:HG21	1:A:1178:MET:HE2	1.99	0.44
1:B:1107:ARG:NH2	1:B:1118:ILE:HD12	2.31	0.44
1:A:1315:THR:CG2	1:A:1371:ASN:HD22	2.30	0.44
1:A:1418:LEU:O	1:A:1419:ARG:HB2	2.18	0.44
1:A:1438:VAL:HA	1:A:1439:PRO:HD2	1.55	0.44
1:A:1224:VAL:O	1:A:1263:PHE:HA	2.16	0.44
1:B:1424:GLU:HA	1:B:1442:ALA:O	2.18	0.44
1:B:1442:ALA:C	1:B:1443:LEU:HD12	2.38	0.44
1:A:1395:ILE:HG12	1:A:1399:ASP:HB2	1.98	0.44
1:B:1221:VAL:CG1	1:B:1260:ARG:CG	2.72	0.44
1:A:1395:ILE:CG1	1:A:1399:ASP:HB2	2.48	0.44
1:B:1408:LEU:HD12	1:B:1444:ILE:HG22	1.99	0.44
1:A:1076:ILE:HG12	1:A:1107:ARG:HB3	2.00	0.43
1:A:1106:ILE:CD1	1:A:1131:TRP:CE3	3.01	0.43
1:B:1348:ARG:HD2	1:B:1351:ILE:HD12	2.00	0.43
1:A:1054:LYS:NZ	1:A:1066:GLU:O	2.49	0.43
1:A:1195:GLU:C	1:A:1197:ILE:H	2.22	0.43
1:B:1180:VAL:CG1	1:B:1189:ILE:HD12	2.48	0.43
1:A:1395:ILE:HG12	1:A:1396:SER:N	2.34	0.43
1:B:1128:ILE:HD11	1:B:1193:SER:HB3	2.01	0.43
1:B:1356:TYR:CE2	1:B:1360:GLU:HG3	2.53	0.43
1:A:1190:LEU:O	1:A:1193:SER:OG	2.36	0.43
1:B:1249:ASN:O	1:B:1251:GLN:N	2.51	0.43
1:A:1364:LEU:CD2	1:A:1368:ILE:HG13	2.49	0.43
1:A:1246:LEU:HD13	1:A:1283:TYR:CB	2.48	0.43
1:A:1094:ASP:OD1	1:A:1096:VAL:HG23	2.18	0.43
1:A:1450:TYR:N	1:A:1450:TYR:CD1	2.86	0.43
1:A:1088:GLN:HG3	1:A:1089:PHE:CE1	2.54	0.43
1:A:1168:GLN:HG3	1:A:1168:GLN:O	2.19	0.43
1:A:1333:ASP:CG	1:A:1490:LYS:HD2	2.40	0.43
1:B:1285:GLU:OE2	1:B:1290:ARG:HD3	2.18	0.43
1:B:1342:ILE:HD13	1:B:1360:GLU:HB3	2.00	0.43
1:B:1439:PRO:CG	1:B:1459:GLU:HB2	2.49	0.43
1:A:1046:HIS:NE2	1:B:1050:SER:CB	2.82	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1381:ASP:OD1	1:B:1419:ARG:NH2	2.42	0.42
1:A:1386:PHE:HD1	1:A:1424:GLU:O	2.02	0.42
1:B:1481:ARG:HG3	1:B:1481:ARG:NH1	2.35	0.42
1:A:1218:LEU:O	1:A:1259:ARG:HD2	2.20	0.42
1:B:1460:VAL:O	1:B:1467:TRP:HA	2.19	0.42
1:B:1260:ARG:NH1	1:B:1260:ARG:HG3	2.34	0.42
1:A:1057:TYR:HE1	1:B:1040:ARG:HB3	1.83	0.42
1:B:1261:ILE:HD11	1:B:1263:PHE:CZ	2.54	0.42
1:A:1055:VAL:CG2	1:A:1056:ALA:N	2.82	0.42
1:A:1105:TYR:CE1	1:A:1264:MET:HE1	2.55	0.42
1:A:1126:VAL:HG22	1:A:1127:PRO:CD	2.47	0.42
1:A:1176:ILE:HG21	1:A:1178:MET:CE	2.50	0.42
1:A:1448:SER:C	1:A:1450:TYR:N	2.73	0.42
1:B:1404:PHE:O	1:B:1407:PHE:HB2	2.20	0.42
1:A:1092:HIS:CD2	1:A:1097:VAL:HG21	2.54	0.42
1:A:1287:GLU:HB3	1:A:1312:PRO:HG3	2.02	0.42
1:B:1243:ARG:NH1	1:B:1243:ARG:HG2	2.35	0.41
1:A:1096:VAL:O	1:A:1096:VAL:HG12	2.20	0.41
1:A:1299:GLN:NE2	1:A:1390:ILE:HD13	2.35	0.41
1:B:1083:PHE:N	1:B:1083:PHE:CD1	2.86	0.41
1:B:1494:GLN:HA	1:B:1495:PRO:HD2	1.76	0.41
1:B:1132:LYS:HG2	1:B:1174:GLU:HG2	2.01	0.41
1:A:1078:SER:O	1:A:1108:ARG:NH2	2.53	0.41
1:A:1390:ILE:O	1:A:1390:ILE:HG22	2.19	0.41
1:A:1451:VAL:CG1	1:A:1452:ILE:N	2.84	0.41
1:A:1455:GLU:OE1	1:A:1457:TYR:OH	2.32	0.41
1:B:1079:ASN:ND2	1:B:1392:VAL:HB	2.35	0.41
1:A:1041:THR:HG23	1:A:1088:GLN:HE22	1.85	0.41
1:A:1094:ASP:HA	1:A:1095:PRO:HD3	1.91	0.41
1:B:1038:LYS:HE2	1:B:1038:LYS:HB3	1.91	0.41
1:B:1336:PHE:CE1	1:B:1377:THR:HA	2.55	0.41
1:A:1343:ARG:HG3	1:A:1343:ARG:NH1	2.33	0.41
1:B:1317:ASN:HB3	1:B:1320:ILE:HD12	2.02	0.41
1:B:1336:PHE:N	1:B:1383:ASN:OD1	2.49	0.41
1:A:1125:THR:HB	1:A:1126:VAL:H	1.58	0.41
1:B:1120:VAL:HG22	1:B:1129:VAL:HG13	2.03	0.41
1:B:1243:ARG:O	1:B:1247:ASP:N	2.44	0.41
1:B:1332:LEU:HD23	1:B:1332:LEU:HA	1.77	0.41
1:B:1472:LEU:HD22	1:B:1472:LEU:HA	1.82	0.41
1:B:1250:LYS:HA	1:B:1253:LEU:HD12	2.02	0.41
1:B:1349:ASP:OD1	1:B:1349:ASP:N	2.52	0.41



Atom-1	Atom-1 Atom-2		Clash
		uistance (A)	overlap (A)
1:B:1356:TYR:CZ	1:B:1360:GLU:CG	3.03	0.41
1:B:1395:ILE:HG22	1:B:1396:SER:N	2.35	0.41
1:A:1139:ALA:HB3	1:A:1140:PHE:CD1	2.56	0.41
1:B:1087:LEU:HD12	1:B:1266:GLY:HA2	2.01	0.40
1:A:1443:LEU:HD12	1:A:1443:LEU:N	2.36	0.40
1:B:1302:LEU:HD21	1:B:1323:TYR:CE2	2.56	0.40
1:A:1395:ILE:CG1	1:A:1396:SER:N	2.83	0.40
1:B:1105:TYR:CZ	1:B:1264:MET:HE1	2.56	0.40
1:B:1289:ILE:HD11	1:B:1297:ALA:HB2	2.03	0.40
1:B:1348:ARG:HG3	1:B:1348:ARG:NH1	2.36	0.40
1:B:1485:THR:HA	1:B:1486:PRO:HD3	1.85	0.40
1:B:1036:SER:HB3	1:B:1040:ARG:HG3	2.04	0.40
1:A:1233:GLU:OE1	1:A:1233:GLU:HA	2.22	0.40
1:A:1242:LEU:O	1:A:1246:LEU:HG	2.22	0.40
1:A:1353:ILE:HG21	1:A:1393:PHE:HB3	2.03	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	А	417/474 (88%)	371 (89%)	40 (10%)	6 (1%)	11 36
1	В	381/474~(80%)	350~(92%)	29~(8%)	2~(0%)	29 61
All	All	798/948~(84%)	721 (90%)	69 (9%)	8 (1%)	15 45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1449	GLY
1	В	1195	GLU
1	В	1475	PRO



Continued from previous page...

Mol	Chain	Res	Type
1	А	1378	SER
1	А	1331	PRO
1	А	1196	VAL
1	А	1475	PRO
1	А	1395	ILE

#### 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	А	380/421~(90%)	340 (90%)	40 (10%)	7 21
1	В	359/421~(85%)	321 (89%)	38 (11%)	6 20
All	All	739/842~(88%)	661 (89%)	78 (11%)	6 20

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1036	SER
1	А	1042	GLU
1	А	1061	ASN
1	А	1076	ILE
1	А	1098	THR
1	А	1122	GLU
1	А	1124	VAL
1	А	1125	THR
1	А	1137	SER
1	А	1141	SER
1	А	1142	THR
1	А	1156	VAL
1	А	1163	TYR
1	А	1172	LEU
1	A	1180	VAL
1	А	1193	SER
1	A	1229	THR
1	А	1237	GLU



Mol	Chain	Res	Type
1	A	1238	ILE
1	A	1239	LEU
1	A	1200	ARG
1	Δ	1211 1243	ARG
1	Δ	1240 1257	SEB
1	Δ	1267	MET
1	Δ	1204	ILE
1	Δ	1292	ILE
1	Δ	1310	ARG
1	Δ	1330	ARG
1	Δ	1344	THR
1	Δ	1344	
1	Λ	1360	CLU
1 1	Λ	1364	LEII
1	Λ Λ	1365	MFT
1	A	1303	
1	A	1360	SER
1	A	1440	IVC
1	A	1400	LIS MET
1	A	1400	
	A	1404	LIS MET
1	A	1478	
1	A	1480	
1	B	1081	VAL
1	B	1089	PHE
1	B	1092	HIS
1	B	1103	GLN
1	B	1111	ARG
1	B	1115	ILE
1	B	1119	ARG
1	B	1125	THR
1	B	1130	GLU
1	B	1134	GLN
1	B	1190	LEU
1	В	1193	SER
1	В	1221	VAL
1	В	1236	GLU
1	В	1237	GLU
1	В	1242	LEU
1	В	1243	ARG
1	В	1251	GLN
1	В	1279	ASN
1	В	1290	ARG



$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type
1	В	1306	SER
1	В	1327	SER
1	В	1329	THR
1	В	1330	SER
1	В	1343	ARG
1	В	1353	ILE
1	В	1367	ASP
1	В	1370	ASP
1	В	1380	SER
1	В	1399	ASP
1	В	1409	GLU
1	В	1410	ARG
1	В	1427	ILE
1	В	1453	LYS
1	В	1454	THR
1	В	1456	MET
1	В	1467	TRP
1	В	1472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	1061	ASN
1	А	1088	GLN
1	А	1121	HIS
1	А	1192	GLN
1	А	1371	ASN
1	В	1134	GLN
1	В	1220	ASN
1	В	1286	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)

2 non-standard protein/DNA/RNA residues 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).

Mal Truna		Chain Bog	Dec Link	B	Bond lengths			Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
1	SEP	А	1157	1	8,9,10	1.29	1 (12%)	8,12,14	1.06	0
1	SEP	В	1157	1	8,9,10	1.49	2 (25%)	8,12,14	1.06	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
1	SEP	А	1157	1	-	2/5/8/10	-
1	SEP	В	1157	1	-	1/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	1157	SEP	P-O1P	3.04	1.60	1.50
1	В	1157	SEP	P-O1P	2.74	1.59	1.50
1	В	1157	SEP	P-O3P	2.15	1.63	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	1157	SEP	N-CA-CB-OG
1	А	1157	SEP	CB-OG-P-O2P
1	В	1157	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	1157	SEP	1	0



#### 5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	425/474~(89%)	0.16	9 (2%) 63 61	39, 77, 116, 143	0
1	В	397/474~(83%)	0.25	10 (2%) 57 55	59, 95, 126, 148	0
All	All	822/948~(86%)	0.21	19 (2%) 60 58	39, 86, 122, 148	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1054	LYS	5.0
1	А	1055	VAL	3.3
1	А	1072	LEU	3.2
1	В	1053	VAL	3.2
1	В	1054	LYS	3.0
1	А	1071	ILE	2.9
1	В	1161	LEU	2.9
1	В	1451	VAL	2.8
1	А	1066	GLU	2.8
1	В	1048	LEU	2.8
1	В	1055	VAL	2.6
1	А	1062	PRO	2.5
1	В	1196	VAL	2.3
1	В	1071	ILE	2.2
1	В	1479	HIS	2.1
1	A	1064	ARG	2.1
1	В	1452	ILE	2.1
1	А	1056	ALA	2.0
1	А	1063	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	SEP	В	1157	10/11	0.93	0.18	83,100,104,105	0
1	SEP	А	1157	10/11	0.97	0.21	55,65,71,75	0

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.

#### 6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	CL	А	1601	1/1	0.94	0.09	71,71,71,71	0
2	CL	В	1601	1/1	0.98	0.12	76,76,76,76	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

