



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:47 AM UTC

PDB ID : 4F2D / pdb\_00004f2d  
Title : Crystal Structure of Escherichia coli L-arabinose Isomerase (ECAI) complexed with Ribitol  
Authors : Manjasetty, B.A.; Burley, S.K.; Almo, S.C.; Chance, M.R.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2012-05-07  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	B	603	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11787 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	498	3861	2451	677	710	7	16	0	0	0
1	B	498	3901	2478	681	718	7	17	0	1	0
1	C	498	3767	2379	658	706	7	17	0	1	0

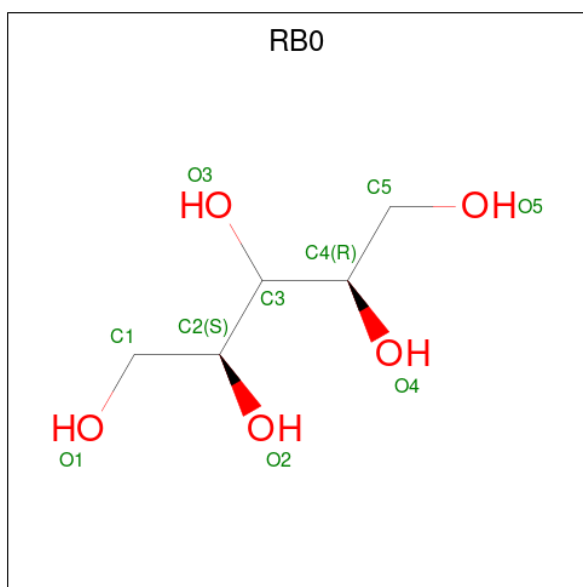
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLU	LYS	conflict	UNP P08202
A	360	VAL	ALA	conflict	UNP P08202
B	248	GLU	LYS	conflict	UNP P08202
B	360	VAL	ALA	conflict	UNP P08202
C	248	GLU	LYS	conflict	UNP P08202
C	360	VAL	ALA	conflict	UNP P08202

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

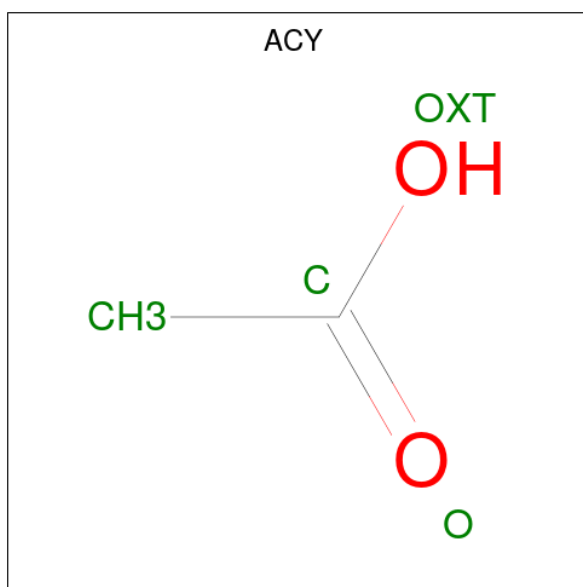
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is D-ribitol (CCD ID: RB0) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

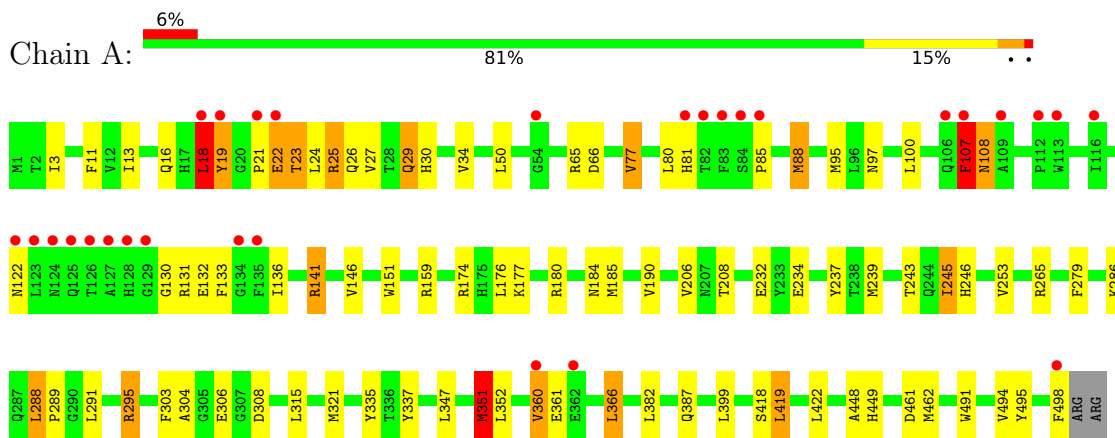
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	95	Total O 95 95	0	0
5	C	34	Total O 34 34	0	0

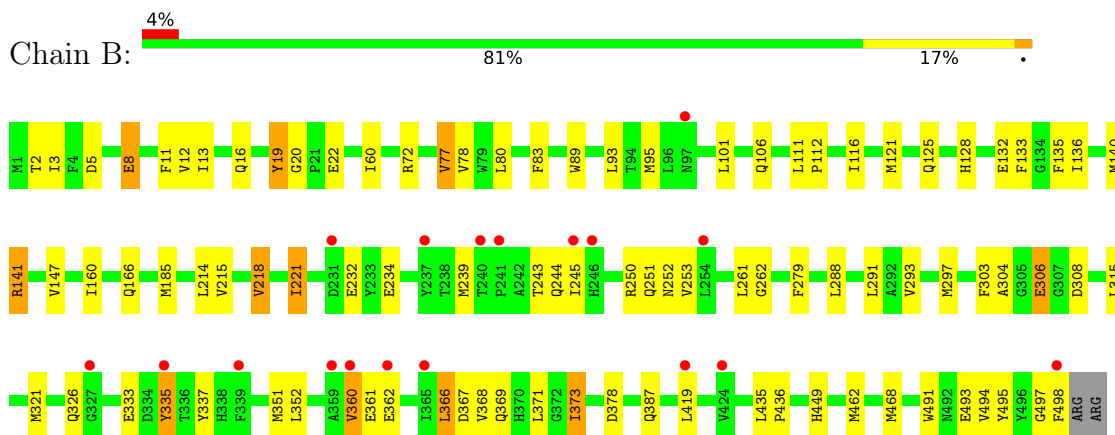
### 3 Residue-property plots i

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.

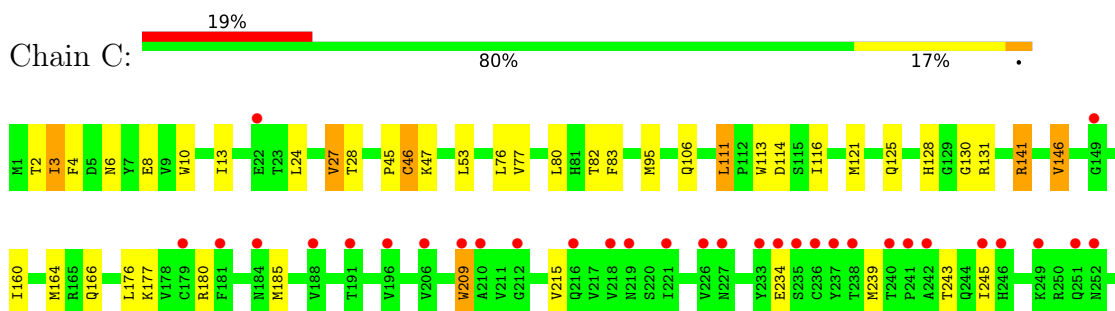
- Molecule 1: L-arabinose isomerase

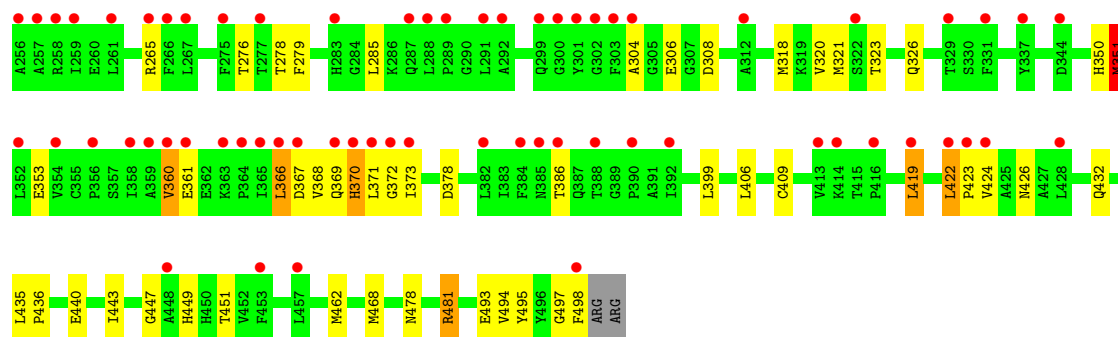


- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.47Å 116.47Å 214.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.30) 98.3 (20.00-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.30Å)	Xtrriage
Refinement program	REFMAC 5.6.0116	Depositor
R, $R_{free}$	0.212 , 0.255 0.277 , 0.307	Depositor DCC
$R_{free}$ test set	3793 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RB0, ACY, MN

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	0.73	1/3940 (0.0%)	0.83	9/5328 (0.2%)
1	B	0.71	0/3984	0.77	1/5388 (0.0%)
1	C	0.72	0/3847	0.82	4/5203 (0.1%)
All	All	0.72	1/11771 (0.0%)	0.81	14/15919 (0.1%)

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	3
1	B	0	1
1	C	0	3
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ARG	C-N	7.75	1.44	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLU	N-CA-C	15.16	127.86	111.03
1	C	47	LYS	N-CA-C	-11.24	90.58	108.90
1	C	370	HIS	N-CA-C	-10.07	94.28	110.20
1	A	23	THR	CA-C-N	8.05	131.88	120.28
1	A	23	THR	C-N-CA	8.05	131.88	120.28
1	A	108	ASN	N-CA-C	7.73	127.26	110.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ARG	O-C-N	7.00	129.28	122.07
1	C	245	ILE	N-CA-C	6.86	117.37	110.23
1	A	23	THR	O-C-N	-6.46	114.00	122.59
1	A	351	MSE	N-CA-CB	-6.05	100.27	110.49
1	A	107	PHE	N-CA-C	5.92	123.41	110.80
1	C	371	LEU	N-CA-C	5.90	118.53	108.02
1	B	245	ILE	N-CA-C	5.85	116.31	110.23
1	A	18	LEU	N-CA-C	5.44	119.40	112.87

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	PHE	Peptide
1	A	18	LEU	Peptide
1	A	21	PRO	Peptide
1	B	326	GLN	Peptide
1	C	369	GLN	Peptide
1	C	370	HIS	Peptide
1	C	46	CYS	Peptide

## 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	A	3861	0	3723	79	0
1	B	3901	0	3790	96	0
1	C	3767	0	3524	92	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	10	0	11	1	0
3	B	10	0	11	1	0
3	C	10	0	12	0	0
4	B	4	0	3	6	0
5	A	92	0	0	2	0
5	B	95	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	34	0	0	5	0
All	All	11787	0	11074	237	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 10.

All (237) 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:288:LEU:CD2	1:B:351:MSE:HE2	1.68	1.22
1:B:288:LEU:HD22	1:B:351:MSE:CE	1.75	1.17
1:C:2:THR:HG23	1:C:323:THR:HG21	1.20	1.16
1:A:122:ASN:HD21	1:C:373:ILE:HD11	1.09	1.12
1:C:239:MSE:HE3	1:C:366:LEU:HG	1.37	1.04
1:B:288:LEU:HD22	1:B:351:MSE:HE2	1.28	1.03
1:B:351:MSE:HE3	1:B:371:LEU:HD21	1.37	1.01
1:C:239:MSE:HE2	1:C:243:THR:HG22	1.45	0.96
1:A:190:VAL:HG23	1:B:132:GLU:OE1	1.66	0.95
1:A:321:MSE:SE	1:A:462:MSE:HE1	2.16	0.95
1:B:288:LEU:HD21	1:B:351:MSE:HE2	1.47	0.95
1:C:2:THR:CG2	1:C:323:THR:HG21	1.97	0.93
1:B:288:LEU:HD23	1:B:352:LEU:HD12	1.50	0.93
1:B:321:MSE:SE	1:B:462:MSE:HE1	2.19	0.92
1:B:491:TRP:O	4:B:603:ACY:H1	1.73	0.89
1:C:321:MSE:SE	1:C:462:MSE:HE1	2.23	0.88
1:B:366:LEU:C	1:B:366:LEU:HD12	2.00	0.86
1:A:122:ASN:ND2	1:C:373:ILE:HD11	1.91	0.83
1:A:337:TYR:H	1:B:106:GLN:HE22	1.27	0.83
1:A:494:VAL:HG21	4:B:603:ACY:H3	1.60	0.82
1:B:288:LEU:CD2	1:B:351:MSE:CE	2.46	0.81
1:C:95[B]:MSE:SE	5:C:703:HOH:O	2.48	0.80
1:B:185:MSE:HE1	1:B:306:GLU:OE1	1.82	0.80
1:C:146:VAL:HG22	5:C:716:HOH:O	1.83	0.79
1:A:122:ASN:HD21	1:C:373:ILE:CD1	1.93	0.79
1:B:243:THR:HG23	1:B:253:VAL:HG21	1.65	0.79
1:C:373:ILE:HG22	1:C:373:ILE:O	1.81	0.78
1:A:24:LEU:HA	1:A:27:VAL:HG12	1.65	0.76
1:A:239:MSE:HE3	1:A:243:THR:HG22	1.68	0.76
1:B:111:LEU:HD11	1:B:116:ILE:HD12	1.68	0.75
1:C:368:VAL:CG1	1:C:378:ASP:OD2	2.34	0.75
1:C:239:MSE:HE2	1:C:243:THR:CG2	2.15	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:602:RB0:C1	1:B:16:GLN:HE22	2.01	0.74
1:A:360:VAL:HG13	1:A:387:GLN:HG2	1.70	0.73
1:B:239:MSE:HE3	1:B:243:THR:HG22	1.70	0.73
1:B:360:VAL:HG13	1:B:387:GLN:HG2	1.71	0.72
1:B:493:GLU:OE2	1:C:141:ARG:HD3	1.88	0.72
1:B:368:VAL:C	1:B:369:GLN:HG2	2.16	0.71
1:B:337:TYR:H	1:C:106:GLN:HE22	1.38	0.71
1:C:180:ARG:HG3	1:C:276:THR:OG1	1.91	0.70
1:A:190:VAL:HG22	1:B:135:PHE:CG	2.27	0.70
1:B:321:MSE:SE	1:B:462:MSE:CE	2.90	0.69
1:A:245:ILE:HG23	1:A:246:HIS:CD2	2.27	0.69
1:B:12:VAL:CG2	1:B:78:VAL:HG22	2.22	0.69
1:C:239:MSE:HE3	1:C:366:LEU:CG	2.21	0.68
1:A:494:VAL:CG2	4:B:603:ACY:H3	2.24	0.68
1:B:494:VAL:HG11	1:C:495:TYR:HA	1.76	0.67
1:A:449:HIS:HB2	1:B:128:HIS:HB2	1.76	0.67
1:A:495:TYR:HA	1:C:494:VAL:HG11	1.77	0.67
1:C:146:VAL:CG2	5:C:716:HOH:O	2.41	0.67
1:B:111:LEU:HD12	1:B:112:PRO:HD2	1.77	0.66
1:B:2:THR:HG22	1:B:5:ASP:OD2	1.95	0.66
1:A:27:VAL:HG23	1:A:81:HIS:CG	2.31	0.65
1:A:190:VAL:HG22	1:B:135:PHE:CB	2.26	0.65
1:C:3:ILE:HD11	1:C:320:VAL:HG13	1.79	0.65
1:C:24:LEU:HA	1:C:27:VAL:HG13	1.79	0.65
1:A:422:LEU:HD11	1:B:121:MSE:HE2	1.79	0.64
1:C:2:THR:HG23	1:C:323:THR:CG2	2.13	0.63
1:B:214:LEU:O	1:B:218:VAL:HG12	1.98	0.62
1:A:180:ARG:HB2	1:A:208:THR:HG22	1.80	0.62
1:A:243:THR:HG23	1:A:253:VAL:HG21	1.80	0.62
1:A:418:SER:C	1:A:419:LEU:HD23	2.25	0.62
1:B:215:VAL:HA	1:B:218:VAL:HG13	1.81	0.62
1:B:185:MSE:CE	1:B:306:GLU:OE1	2.47	0.62
1:A:22:GLU:O	1:A:25:ARG:N	2.33	0.61
1:C:82:THR:HG23	1:C:125:GLN:NE2	2.15	0.61
1:C:368:VAL:HG11	1:C:378:ASP:OD2	1.99	0.61
1:A:208:THR:HG23	5:A:719:HOH:O	2.01	0.60
1:C:28:THR:HG23	1:C:53:LEU:HD11	1.82	0.60
1:A:491:TRP:CD1	4:B:603:ACY:H2	2.37	0.59
1:B:306:GLU:HG3	5:B:787:HOH:O	2.02	0.59
1:A:366:LEU:HD12	1:A:366:LEU:C	2.27	0.59
1:A:27:VAL:HG23	1:A:81:HIS:CD2	2.37	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLU:HG3	5:A:765:HOH:O	2.03	0.59
1:B:83:PHE:H	1:B:125:GLN:HE21	1.51	0.59
1:B:333:GLU:OE1	3:B:602:RB0:O5	2.20	0.58
1:A:80:LEU:HD13	1:A:130:GLY:HA2	1.86	0.58
1:C:366:LEU:HD12	1:C:366:LEU:C	2.28	0.58
1:A:494:VAL:HG11	1:B:495:TYR:HA	1.86	0.58
1:B:111:LEU:HD11	1:B:116:ILE:CD1	2.33	0.57
1:B:335:TYR:HD2	1:C:121:MSE:SE	2.38	0.57
1:B:93:LEU:HD13	1:B:140:MSE:HE1	1.86	0.57
1:A:159:ARG:NH2	1:C:440:GLU:OE2	2.38	0.56
1:A:24:LEU:O	1:A:27:VAL:HG12	2.06	0.56
1:A:146:VAL:HG11	1:C:443:ILE:HG21	1.87	0.56
1:B:366:LEU:C	1:B:366:LEU:CD1	2.73	0.56
1:B:369:GLN:O	1:B:378:ASP:HB3	2.06	0.55
1:C:373:ILE:O	1:C:373:ILE:CG2	2.54	0.55
1:A:234:GLU:HG2	1:A:239:MSE:HE2	1.89	0.54
1:B:215:VAL:HA	1:B:218:VAL:CG1	2.37	0.54
1:B:111:LEU:CD1	1:B:116:ILE:HD12	2.36	0.54
1:C:111:LEU:HD13	1:C:116:ILE:HD12	1.88	0.54
1:C:497:GLY:O	1:C:498:PHE:HB3	2.07	0.54
1:C:304:ALA:HB3	1:C:308:ASP:O	2.08	0.54
1:A:347:LEU:HD22	1:B:121:MSE:HE1	1.90	0.53
1:B:221:ILE:HD11	1:B:262:GLY:N	2.23	0.53
1:C:351:MSE:HE2	1:C:373:ILE:HG21	1.90	0.53
1:A:180:ARG:NH2	1:A:184:ASN:OD1	2.42	0.53
1:A:185:MSE:HE3	1:A:306:GLU:HG3	1.91	0.53
1:C:111:LEU:HD12	1:C:111:LEU:C	2.34	0.52
1:C:279:PHE:CE2	1:C:351:MSE:HE1	2.44	0.52
1:B:19:TYR:OH	1:B:125:GLN:NE2	2.40	0.52
1:A:18:LEU:H	1:A:19:TYR:HD2	1.58	0.52
1:C:409:CYS:HB3	1:C:432:GLN:NE2	2.25	0.52
1:B:351:MSE:SE	1:B:373:ILE:HD12	2.60	0.52
1:A:190:VAL:HG22	1:B:135:PHE:CD2	2.44	0.52
1:C:116:ILE:HD11	1:C:121:MSE:HE2	1.93	0.52
1:B:288:LEU:HD23	1:B:352:LEU:CD1	2.33	0.51
1:A:22:GLU:O	1:A:23:THR:C	2.52	0.51
1:A:24:LEU:CA	1:A:27:VAL:HG12	2.36	0.51
1:B:449:HIS:HB2	1:C:128:HIS:HB2	1.92	0.51
1:C:239:MSE:CE	1:C:243:THR:HG22	2.29	0.51
1:A:347:LEU:CD2	1:B:121:MSE:HE1	2.41	0.51
1:C:46:CYS:SG	1:C:164:MSE:HE3	2.51	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:THR:HG22	1:C:83:PHE:O	2.10	0.50
1:A:304:ALA:HB3	1:A:308:ASP:O	2.11	0.50
1:B:8:GLU:OE1	1:B:72:ARG:NH1	2.44	0.50
1:B:12:VAL:HG22	1:B:78:VAL:HG22	1.93	0.50
1:A:65:ARG:NH1	1:A:66:ASP:OD1	2.45	0.50
1:B:304:ALA:HB3	1:B:308:ASP:O	2.12	0.50
1:B:221:ILE:HD13	1:B:261:LEU:HB3	1.92	0.49
1:A:190:VAL:HG22	1:B:135:PHE:HB3	1.92	0.49
1:A:185:MSE:HE3	1:A:306:GLU:CG	2.42	0.49
1:B:367:ASP:OD1	1:B:369:GLN:NE2	2.45	0.49
1:B:221:ILE:HD11	1:B:262:GLY:HA2	1.94	0.48
1:B:497:GLY:O	1:B:498:PHE:C	2.55	0.48
1:A:30:HIS:O	1:A:34:VAL:HG23	2.12	0.48
1:A:141:ARG:NH2	1:C:399:LEU:O	2.45	0.48
1:C:209:TRP:HA	1:C:209:TRP:CE3	2.48	0.48
1:C:3:ILE:CD1	1:C:320:VAL:HG13	2.43	0.48
1:B:494:VAL:HG23	4:B:603:ACY:H1	1.96	0.48
1:C:82:THR:CG2	1:C:83:PHE:N	2.75	0.48
1:B:293:VAL:HG12	1:B:297:MSE:HE2	1.94	0.48
1:B:221:ILE:HD11	1:B:262:GLY:CA	2.44	0.48
1:C:82:THR:HG22	1:C:83:PHE:N	2.29	0.48
1:A:131:ARG:HD3	1:C:449:HIS:HA	1.96	0.48
1:B:221:ILE:HD11	1:B:261:LEU:C	2.39	0.48
1:C:3:ILE:HA	1:C:6:ASN:HD22	1.78	0.48
1:B:2:THR:CG2	1:B:5:ASP:OD2	2.62	0.47
1:C:422:LEU:HD22	1:C:424:VAL:H	1.78	0.47
1:B:147:VAL:HG21	1:B:160:ILE:HD13	1.96	0.47
1:A:245:ILE:CG2	1:A:246:HIS:CD2	2.98	0.47
1:B:185:MSE:HE3	1:B:306:GLU:CB	2.44	0.47
1:C:422:LEU:CD2	1:C:424:VAL:HG22	2.43	0.47
1:C:10:TRP:HB2	1:C:76:LEU:HD22	1.97	0.47
1:C:46:CYS:O	1:C:164:MSE:HE1	2.15	0.47
1:B:185:MSE:HE2	1:B:279:PHE:CE2	2.50	0.46
1:B:243:THR:HG23	1:B:253:VAL:CG2	2.42	0.46
1:C:2:THR:HG22	1:C:3:ILE:N	2.30	0.46
1:B:419:LEU:HD21	1:C:113:TRP:HE3	1.80	0.46
1:B:5:ASP:O	1:B:72:ARG:NH2	2.49	0.46
1:A:24:LEU:C	1:A:27:VAL:HG12	2.41	0.46
1:A:133:PHE:O	1:A:136:ILE:HG22	2.16	0.46
1:C:131:ARG:NE	5:C:733:HOH:O	2.48	0.46
1:A:146:VAL:HG21	1:C:443:ILE:HG22	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASN:N	1:B:252:ASN:HD22	2.13	0.46
1:C:13:ILE:N	1:C:13:ILE:HD12	2.31	0.46
1:C:366:LEU:HD12	1:C:367:ASP:N	2.31	0.46
1:B:147:VAL:HB	1:B:160:ILE:HD11	1.98	0.45
1:A:141:ARG:HD3	1:C:493:GLU:OE2	2.16	0.45
1:A:100:LEU:C	1:A:100:LEU:HD23	2.42	0.45
1:C:209:TRP:HA	1:C:209:TRP:HE3	1.82	0.45
1:C:46:CYS:SG	1:C:164:MSE:CE	3.05	0.45
1:A:24:LEU:HA	1:A:27:VAL:CG1	2.40	0.45
1:C:422:LEU:HD23	1:C:423:PRO:HD2	1.98	0.45
1:C:478:ASN:O	1:C:481:ARG:NH2	2.50	0.45
1:B:239:MSE:CE	1:B:243:THR:HG22	2.41	0.45
1:B:11:PHE:CD1	1:B:77:VAL:HG22	2.52	0.44
1:C:215:VAL:HG22	1:C:285:LEU:CD2	2.46	0.44
1:C:419:LEU:N	1:C:419:LEU:HD23	2.32	0.44
1:A:16:GLN:C	1:A:19:TYR:CD2	2.96	0.44
1:A:461:ASP:C	1:A:462:MSE:HE2	2.42	0.44
1:B:133:PHE:O	1:B:136:ILE:HG22	2.17	0.44
1:C:185:MSE:HE2	1:C:279:PHE:CE2	2.53	0.44
1:C:278:THR:HG21	5:C:728:HOH:O	2.17	0.44
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.87	0.44
1:A:399:LEU:O	1:B:141:ARG:NH2	2.50	0.44
1:A:30:HIS:CD2	1:A:107:PHE:CZ	3.06	0.44
1:B:83:PHE:H	1:B:125:GLN:NE2	2.13	0.44
1:B:185:MSE:HE3	1:B:306:GLU:CG	2.48	0.44
1:C:406:LEU:HD22	1:C:447:GLY:HA3	1.99	0.44
1:C:24:LEU:O	1:C:28:THR:HG23	2.18	0.44
1:C:419:LEU:HD13	1:C:426:ASN:ND2	2.33	0.44
1:A:107:PHE:O	1:A:151:TRP:NE1	2.36	0.43
1:B:234:GLU:HG2	1:B:239:MSE:HE2	2.00	0.43
1:C:2:THR:HG22	1:C:4:PHE:H	1.83	0.43
1:B:221:ILE:CD1	1:B:262:GLY:N	2.81	0.43
1:C:28:THR:CG2	1:C:53:LEU:HD11	2.47	0.43
1:C:80:LEU:HD13	1:C:130:GLY:HA2	2.01	0.43
1:C:2:THR:CG2	1:C:323:THR:CG2	2.84	0.43
1:A:288:LEU:HD22	1:A:352:LEU:HD12	2.00	0.43
1:B:93:LEU:CD1	1:B:140:MSE:HE1	2.48	0.43
1:C:360:VAL:HG22	1:C:386:THR:C	2.44	0.43
1:A:11:PHE:CD1	1:A:77:VAL:HG22	2.54	0.43
1:A:291:LEU:CD1	1:A:382:LEU:HG	2.48	0.43
1:B:303:PHE:H	1:B:315:LEU:HD23	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HD12	1:B:13:ILE:N	2.33	0.42
1:B:221:ILE:CD1	1:B:261:LEU:C	2.92	0.42
1:C:24:LEU:HA	1:C:27:VAL:CG1	2.49	0.42
1:A:176:LEU:HD23	1:A:177:LYS:N	2.33	0.42
1:B:337:TYR:OH	1:C:131:ARG:NH1	2.50	0.42
1:C:234:GLU:HG2	1:C:239:MSE:SE	2.70	0.42
1:A:13:ILE:N	1:A:13:ILE:HD12	2.34	0.42
1:A:237:TYR:OH	1:A:295:ARG:HD2	2.19	0.42
1:C:239:MSE:CE	1:C:243:THR:CG2	2.92	0.42
1:B:60:ILE:HD13	1:B:89:TRP:CE2	2.54	0.42
1:C:166:GLN:C	1:C:468:MSE:HE3	2.45	0.42
1:B:80:LEU:HD11	1:B:133:PHE:CG	2.54	0.42
1:B:166:GLN:C	1:B:468:MSE:HE3	2.45	0.42
1:C:4:PHE:HD2	1:C:45:PRO:HB2	1.84	0.42
1:C:318:MSE:HE3	1:C:462:MSE:SE	2.69	0.42
1:B:101:LEU:C	1:B:101:LEU:HD23	2.45	0.42
1:B:221:ILE:CD1	1:B:261:LEU:HB3	2.49	0.42
1:B:494:VAL:HG23	4:B:603:ACY:CH3	2.49	0.42
1:A:366:LEU:C	1:A:366:LEU:CD1	2.93	0.42
1:A:419:LEU:HD23	1:A:419:LEU:N	2.35	0.42
1:A:180:ARG:HD2	1:A:206:VAL:CG1	2.50	0.42
1:B:221:ILE:CD1	1:B:261:LEU:CB	2.98	0.42
1:C:350:HIS:ND1	1:C:353:GLU:OE1	2.44	0.42
1:C:176:LEU:HD23	1:C:177:LYS:N	2.35	0.42
1:C:116:ILE:HD11	1:C:121:MSE:CE	2.50	0.41
1:A:449:HIS:CB	1:B:128:HIS:HB2	2.48	0.41
1:A:288:LEU:HD11	1:A:351:MSE:HE3	2.03	0.41
1:A:288:LEU:HD23	1:A:289:PRO:N	2.36	0.41
1:C:185:MSE:HE3	1:C:306:GLU:HG3	2.03	0.41
1:C:435:LEU:HB3	1:C:436:PRO:HD3	2.02	0.41
1:B:221:ILE:HD12	1:B:261:LEU:HB2	2.03	0.41
1:B:435:LEU:HB3	1:B:436:PRO:HD3	2.02	0.41
1:C:160:ILE:O	1:C:164:MSE:HG3	2.20	0.41
1:C:180:ARG:CG	1:C:276:THR:OG1	2.66	0.41
1:A:303:PHE:H	1:A:315:LEU:HD23	1.86	0.40
1:A:185:MSE:HE2	1:A:279:PHE:CE2	2.55	0.40
1:C:82:THR:HG23	1:C:125:GLN:HE21	1.85	0.40
1:A:13:ILE:HD13	1:A:50:LEU:CD1	2.51	0.40
1:A:26:GLN:O	1:A:29:GLN:HG2	2.22	0.40
1:A:85:PRO:O	1:A:88:MSE:HB2	2.21	0.40
1:A:190:VAL:HG11	1:A:448:ALA:HB2	2.04	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	496/500 (99%)	480 (97%)	14 (3%)	2 (0%)	30	38
1	B	497/500 (99%)	484 (97%)	12 (2%)	1 (0%)	43	55
1	C	497/500 (99%)	479 (96%)	16 (3%)	2 (0%)	30	38
All	All	1490/1500 (99%)	1443 (97%)	42 (3%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	20	GLY
1	C	372	GLY
1	A	351	MSE
1	C	351	MSE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/402 (100%)	379 (94%)	22 (6%)	19	28
1	B	411/402 (102%)	389 (95%)	22 (5%)	20	29
1	C	379/402 (94%)	360 (95%)	19 (5%)	22	33
All	All	1191/1206 (99%)	1128 (95%)	63 (5%)	21	30

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	19	TYR
1	A	29	GLN
1	A	77	VAL
1	A	88	MSE
1	A	95	MSE
1	A	97	ASN
1	A	132	GLU
1	A	141	ARG
1	A	174	ARG
1	A	232	GLU
1	A	245	ILE
1	A	265	ARG
1	A	286	LYS
1	A	288	LEU
1	A	295	ARG
1	A	335	TYR
1	A	360	VAL
1	A	361	GLU
1	A	366	LEU
1	A	419	LEU
1	A	498	PHE
1	B	3	ILE
1	B	8	GLU
1	B	19	TYR
1	B	22	GLU
1	B	77	VAL
1	B	95[A]	MSE
1	B	95[B]	MSE
1	B	141	ARG
1	B	218	VAL
1	B	221	ILE
1	B	232	GLU
1	B	244	GLN
1	B	250	ARG
1	B	251	GLN
1	B	291	LEU
1	B	306	GLU
1	B	335	TYR
1	B	360	VAL
1	B	361	GLU
1	B	362	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	366	LEU
1	B	373	ILE
1	C	3	ILE
1	C	8	GLU
1	C	27	VAL
1	C	77	VAL
1	C	111	LEU
1	C	114	ASP
1	C	141	ARG
1	C	146	VAL
1	C	209	TRP
1	C	265	ARG
1	C	326	GLN
1	C	351	MSE
1	C	360	VAL
1	C	361	GLU
1	C	366	LEU
1	C	419	LEU
1	C	422	LEU
1	C	451	THR
1	C	481	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	29	GLN
1	A	68	ASN
1	A	122	ASN
1	A	124	ASN
1	A	125	GLN
1	A	150	HIS
1	A	246	HIS
1	A	251	GLN
1	A	273	HIS
1	A	298	GLN
1	A	299	GLN
1	A	343	ASN
1	A	426	ASN
1	A	469	HIS
1	A	478	ASN
1	B	6	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	16	GLN
1	B	29	GLN
1	B	102	GLN
1	B	104	HIS
1	B	106	GLN
1	B	124	ASN
1	B	125	GLN
1	B	244	GLN
1	B	252	ASN
1	B	269	GLN
1	B	283	HIS
1	B	298	GLN
1	B	299	GLN
1	B	338	HIS
1	B	343	ASN
1	B	369	GLN
1	B	455	HIS
1	B	469	HIS
1	B	478	ASN
1	C	6	ASN
1	C	29	GLN
1	C	106	GLN
1	C	124	ASN
1	C	125	GLN
1	C	244	GLN
1	C	298	GLN
1	C	299	GLN
1	C	338	HIS
1	C	370	HIS
1	C	387	GLN
1	C	426	ASN
1	C	469	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACY	B	603	-	3,3,3	0.81	0	3,3,3	0.62	0
3	RB0	C	602	2	9,9,9	0.28	0	11,11,11	0.78	0
3	RB0	B	602	2	9,9,9	0.24	0	11,11,11	0.60	0
3	RB0	A	602	2	9,9,9	0.30	0	11,11,11	1.40	1 (9%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RB0	C	602	2	-	5/12/12/12	-
3	RB0	B	602	2	-	2/12/12/12	-
3	RB0	A	602	2	-	0/12/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	RB0	C4-C3-C2	-3.44	107.84	113.57

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	RB0	O1-C1-C2-O2
3	C	602	RB0	O4-C4-C5-O5
3	C	602	RB0	C3-C4-C5-O5
3	C	602	RB0	O1-C1-C2-C3
3	B	602	RB0	O1-C1-C2-O2
3	C	602	RB0	C2-C3-C4-O4
3	B	602	RB0	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	ACY	6	0
3	B	602	RB0	1	0
3	A	602	RB0	1	0

## 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	481/500 (96%)	0.45	29 (6%) 27 29	16, 26, 59, 77	2 (0%)
1	B	481/500 (96%)	0.40	18 (3%) 45 48	17, 27, 35, 60	1 (0%)
1	C	481/500 (96%)	1.22	96 (19%) 3 3	20, 43, 74, 81	1 (0%)
All	All	1443/1500 (96%)	0.69	143 (9%) 13 14	16, 29, 69, 81	4 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	ALA	5.4
1	C	283	HIS	4.6
1	C	219	ASN	4.5
1	C	360	VAL	4.5
1	A	84	SER	4.4
1	C	367	ASP	4.4
1	C	365	ILE	4.3
1	C	371	LEU	4.1
1	C	251	GLN	4.1
1	C	369	GLN	4.0
1	C	267	LEU	4.0
1	A	81	HIS	3.9
1	C	364	PRO	3.9
1	C	373	ILE	3.8
1	C	237	TYR	3.8
1	C	382	LEU	3.8
1	A	83	PHE	3.7
1	B	498	PHE	3.7
1	C	249	LYS	3.6
1	C	358	ILE	3.5
1	C	366	LEU	3.5
1	C	291	LEU	3.5
1	C	233	TYR	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	246	HIS	3.5
1	C	303	PHE	3.5
1	C	245	ILE	3.5
1	B	360	VAL	3.4
1	C	218	VAL	3.4
1	C	413	VAL	3.4
1	B	245	ILE	3.4
1	C	257	ALA	3.3
1	C	302	GLY	3.3
1	B	254	LEU	3.3
1	A	109	ALA	3.3
1	A	21	PRO	3.3
1	C	238	THR	3.3
1	C	331	PHE	3.3
1	C	210	ALA	3.3
1	C	354	VAL	3.3
1	A	112	PRO	3.3
1	C	259	ILE	3.3
1	C	498	PHE	3.2
1	C	209	TRP	3.2
1	C	416	PRO	3.2
1	C	266	PHE	3.1
1	C	242	ALA	3.1
1	C	370	HIS	3.1
1	C	288	LEU	3.0
1	A	19	TYR	3.0
1	A	125	GLN	3.0
1	C	363	LYS	3.0
1	C	240	THR	3.0
1	A	124	ASN	3.0
1	C	422	LEU	2.9
1	C	221	ILE	2.9
1	B	419	LEU	2.9
1	C	256	ALA	2.9
1	B	362	GLU	2.9
1	C	428	LEU	2.8
1	C	457	LEU	2.8
1	C	275	PHE	2.8
1	A	360	VAL	2.8
1	A	134	GLY	2.8
1	B	246	HIS	2.8
1	C	289	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	234	GLU	2.8
1	C	292	ALA	2.8
1	C	241	PRO	2.8
1	C	212	GLY	2.7
1	C	390	PRO	2.7
1	C	299	GLN	2.7
1	B	241	PRO	2.7
1	C	287	GLN	2.7
1	C	181	PHE	2.7
1	C	384	PHE	2.7
1	B	365	ILE	2.6
1	A	18	LEU	2.6
1	C	337	TYR	2.6
1	C	359	ALA	2.6
1	A	126	THR	2.6
1	C	453	PHE	2.6
1	C	423	PRO	2.5
1	A	22	GLU	2.5
1	C	448	ALA	2.5
1	C	191	THR	2.5
1	C	388	THR	2.5
1	C	261	LEU	2.5
1	C	419	LEU	2.5
1	A	127	ALA	2.5
1	C	385	ASN	2.5
1	C	322	SER	2.5
1	A	113	TRP	2.5
1	C	352	LEU	2.5
1	A	54	GLY	2.5
1	A	362	GLU	2.4
1	C	424	VAL	2.4
1	C	344	ASP	2.4
1	C	277	THR	2.4
1	C	301	TYR	2.4
1	C	179	CYS	2.4
1	A	128	HIS	2.4
1	C	216	GLN	2.4
1	C	149	GLY	2.4
1	A	498	PHE	2.4
1	B	335	TYR	2.3
1	C	329	THR	2.3
1	A	107	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	359	ALA	2.3
1	C	235	SER	2.3
1	C	22	GLU	2.3
1	A	135	PHE	2.3
1	A	122	ASN	2.3
1	B	231	ASP	2.3
1	C	361	GLU	2.3
1	C	258	ARG	2.2
1	B	339	PHE	2.2
1	C	265	ARG	2.2
1	C	414	LYS	2.2
1	C	206	VAL	2.2
1	A	123	LEU	2.2
1	C	226	VAL	2.2
1	C	236	CYS	2.2
1	C	392	ILE	2.1
1	B	97	ASN	2.1
1	C	356	PRO	2.1
1	A	106	GLN	2.1
1	A	129	GLY	2.1
1	C	300	GLY	2.1
1	C	184	ASN	2.1
1	A	85	PRO	2.1
1	B	424	VAL	2.1
1	C	372	GLY	2.1
1	A	82	THR	2.1
1	C	227	ASN	2.1
1	B	327	GLY	2.1
1	C	196	VAL	2.1
1	B	240	THR	2.0
1	C	252	ASN	2.0
1	B	237	TYR	2.0
1	C	188	VAL	2.0
1	C	386	THR	2.0
1	C	312	ALA	2.0
1	A	116	ILE	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 [i](#)

There are no oligosaccharides 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
3	RB0	C	602	10/10	0.81	0.33	48,54,59,63	10
4	ACY	B	603	4/4	0.91	0.11	25,35,37,39	0
3	RB0	B	602	10/10	0.94	0.20	37,52,62,65	2
2	MN	C	601	1/1	0.94	0.15	80,80,80,80	1
3	RB0	A	602	10/10	0.94	0.19	37,43,50,52	2
2	MN	B	601	1/1	0.96	0.15	52,52,52,52	0
2	MN	A	601	1/1	0.97	0.18	45,45,45,45	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.