Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 07:47 AM EDT

PDB ID	:	4F2D
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*
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:

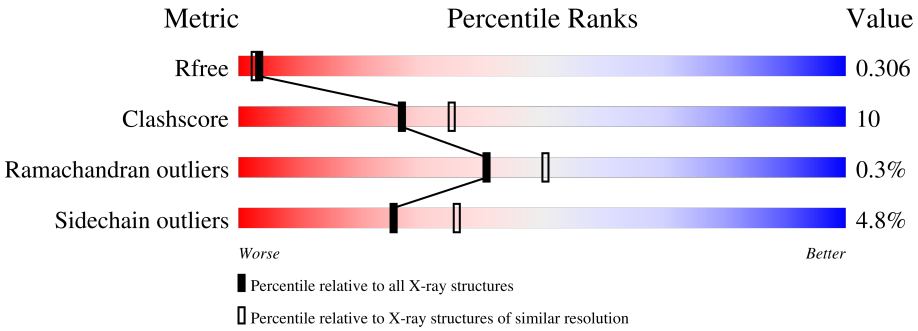
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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%

Mol	Chain	Length	Quality of chain
1	A	500	81% 16% .
1	B	500	81% 17% .
1	C	500	81% 16% .

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
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
1	A	498	Total	C	N	O	S	Se	0	0	0
			3861	2451	677	710	7	16			
1	B	498	Total	C	N	O	S	Se	0	1	0
			3901	2478	681	718	7	17			
1	C	498	Total	C	N	O	S	Se	0	1	0
			3767	2379	658	706	7	17			

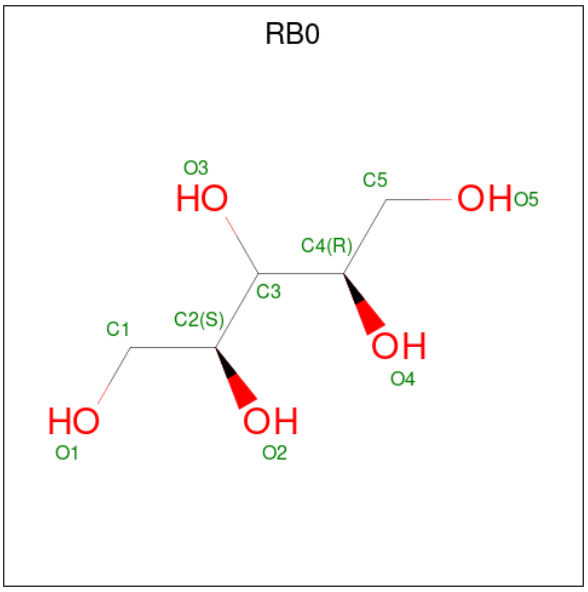
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: MN) (formula: Mn).

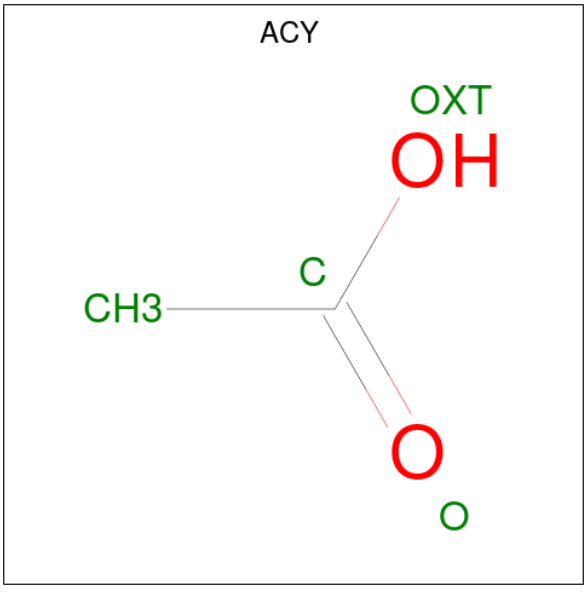
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is D-ribitol (three-letter code: RB0) (formula: $C_5H_{12}O_5$).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is water.

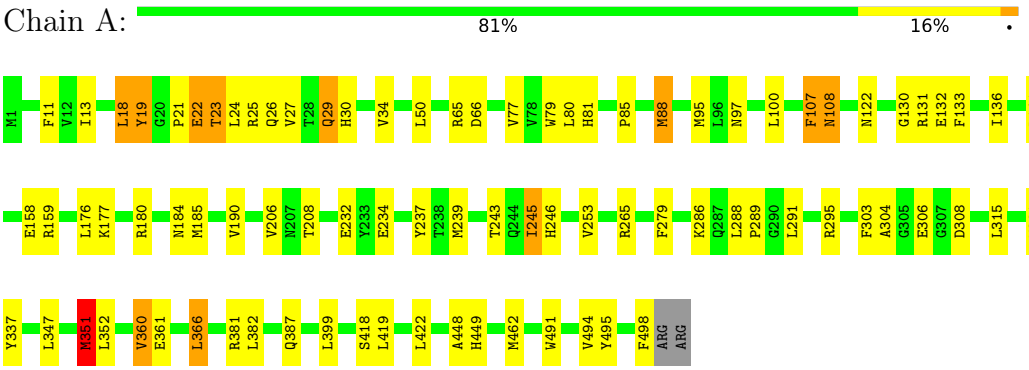
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	95	Total O 95 95	0	0
5	C	34	Total O 34 34	0	0

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. 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. 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.

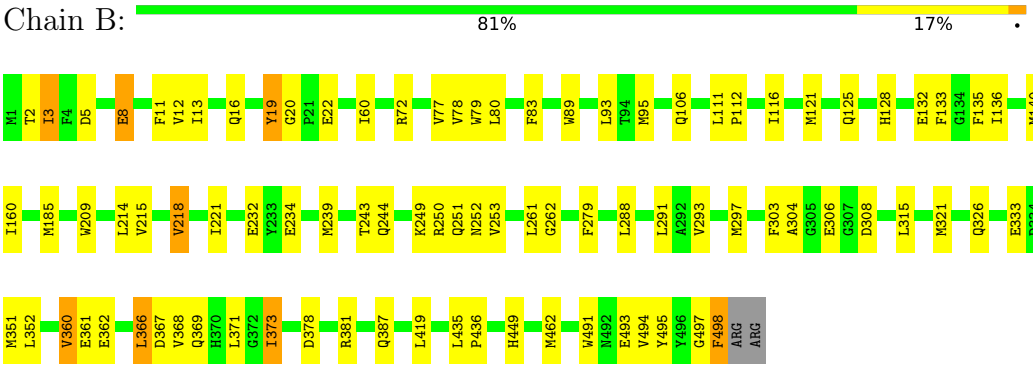
• Molecule 1: L-arabinose isomerase

Chain A:



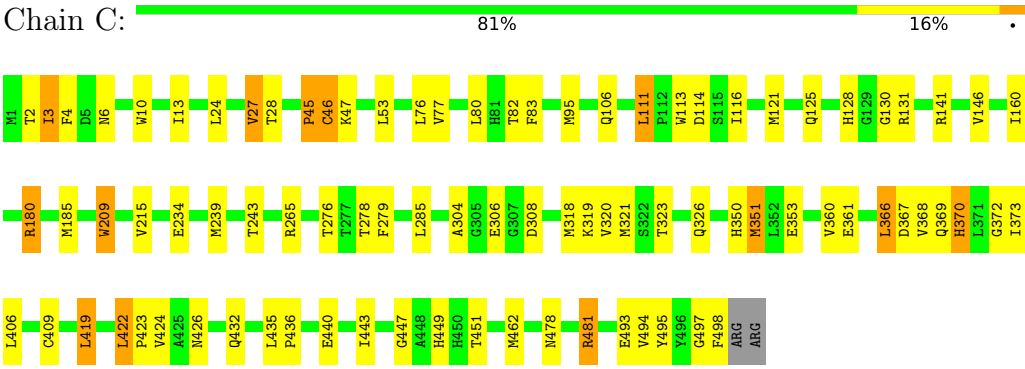
• Molecule 1: L-arabinose isomerase

Chain B:



• Molecule 1: L-arabinose isomerase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.47Å 116.47Å 214.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.30) 98.5 (19.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.212 , 0.255 0.276 , 0.306	Depositor DCC
R_{free} test set	3746 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11787	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, RB0, 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	0.53	1/3940 (0.0%)	0.61	4/5328 (0.1%)
1	B	0.52	2/3984 (0.1%)	0.59	2/5388 (0.0%)
1	C	0.53	0/3847	0.60	2/5203 (0.0%)
All	All	0.53	3/11771 (0.0%)	0.60	8/15919 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	TRP	CD2-CE2	5.03	1.47	1.41
1	A	79	TRP	CD2-CE2	5.00	1.47	1.41
1	B	79	TRP	CD2-CE2	5.00	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	47	LYS	N-CA-C	-7.56	90.58	111.00
1	B	141	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	22	GLU	N-CA-C	6.24	127.86	111.00
1	C	370	HIS	N-CA-C	-6.19	94.28	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASN	N-CA-C	6.02	127.26	111.00
1	B	141	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	351	MSE	N-CA-CB	-5.74	100.27	110.60
1	A	23	THR	O-C-N	-5.44	114.00	122.70

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	76	0
1	B	3901	0	3790	94	0
1	C	3767	0	3524	90	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
5	C	34	0	0	5	0
All	All	11787	0	11074	230	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 (230) 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: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:366:LEU:C	1:B:366:LEU:HD12	2.00	0.81
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
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:337:TYR:H	1:C:106:GLN:HE22	1.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:368:VAL:C	1:B:369:GLN:HG2	2.16	0.66
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: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:27:VAL:HG23	1:A:81:HIS:CD2	2.37	0.59
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:A:494:VAL:HG11	1:B:495:TYR:HA	1.86	0.58
1:A:418:SER:C	1:A:419:LEU:HD23	2.25	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:366:LEU:HD12	1:C:366:LEU:C	2.28	0.54
1:C:497:GLY:O	1:C:498:PHE:HB3	2.07	0.54
1:A:366:LEU:HD12	1:A:366:LEU:C	2.27	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: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:B:366:LEU:C	1:B:366:LEU:CD1	2.73	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:3:ILE:HA	1:C:6:ASN:HD22	1.78	0.48
1:C:111:LEU:HD12	1:C:111:LEU:C	2.34	0.47
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:A:22:GLU:O	1:A:23:THR:C	2.52	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:497:GLY:O	1:B:498:PHE:C	2.55	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:B:221:ILE:HD11	1:B:261:LEU:C	2.39	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: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
1:B:13:ILE:HD12	1:B:13:ILE:N	2.33	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:A:419:LEU:HD23	1:A:419:LEU:N	2.35	0.42
1:B:2:THR:OG1	1:B:3:ILE:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HD11	1:B:133:PHE:CG	2.54	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: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: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:24:LEU:C	1:A:27:VAL:HG12	2.41	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:100:LEU:C	1:A:100:LEU:HD23	2.42	0.40
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%)	34	42
1	B	497/500 (99%)	484 (97%)	12 (2%)	1 (0%)	47	58
1	C	497/500 (99%)	479 (96%)	16 (3%)	2 (0%)	34	42
All	All	1490/1500 (99%)	1443 (97%)	42 (3%)	5 (0%)	41	50

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%)	383 (96%)	18 (4%)	27	39
1	B	411/402 (102%)	389 (95%)	22 (5%)	22	30
1	C	379/402 (94%)	361 (95%)	18 (5%)	26	37
All	All	1191/1206 (99%)	1133 (95%)	58 (5%)	25	35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	29	GLN
1	A	88	MSE
1	A	95	MSE
1	A	97	ASN
1	A	132	GLU
1	A	158	GLU
1	A	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	245	ILE
1	A	265	ARG
1	A	286	LYS
1	A	334	ASP
1	A	335	TYR
1	A	360	VAL
1	A	361	GLU
1	A	366	LEU
1	A	381	ARG
1	A	498	PHE
1	B	3	ILE
1	B	8	GLU
1	B	19	TYR
1	B	22	GLU
1	B	95[A]	MSE
1	B	95[B]	MSE
1	B	141	ARG
1	B	218	VAL
1	B	232	GLU
1	B	244	GLN
1	B	249	LYS
1	B	250	ARG
1	B	251	GLN
1	B	291	LEU
1	B	335	TYR
1	B	360	VAL
1	B	361	GLU
1	B	362	GLU
1	B	366	LEU
1	B	373	ILE
1	B	381	ARG
1	B	498	PHE
1	C	3	ILE
1	C	27	VAL
1	C	45	PRO
1	C	77	VAL
1	C	111	LEU
1	C	114	ASP
1	C	180	ARG
1	C	209	TRP
1	C	265	ARG
1	C	319	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	326	GLN
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 (31) 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	150	HIS
1	A	246	HIS
1	A	273	HIS
1	A	343	ASN
1	A	469	HIS
1	A	478	ASN
1	B	6	ASN
1	B	16	GLN
1	B	29	GLN
1	B	102	GLN
1	B	104	HIS
1	B	106	GLN
1	B	125	GLN
1	B	252	ASN
1	B	269	GLN
1	B	338	HIS
1	B	369	GLN
1	B	464	GLN
1	B	469	HIS
1	B	478	ASN
1	C	6	ASN
1	C	29	GLN
1	C	106	GLN
1	C	125	GLN
1	C	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	343	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 monosaccharides 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	0.76	0	3,3,3	0.61	0
3	RB0	C	602	2	9,9,9	0.28	0	11,11,11	0.67	0
3	RB0	B	602	2	9,9,9	0.24	0	11,11,11	0.52	0
3	RB0	A	602	2	9,9,9	0.30	0	11,11,11	1.20	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. '-' 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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RB0	B	602	2	-	1/12/12/12	-
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(^{o})	Ideal(^{o})
3	A	602	RB0	C4-C3-C2	-2.66	107.84	113.36

There are no chirality outliers.

All (6) 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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.