Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:28 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

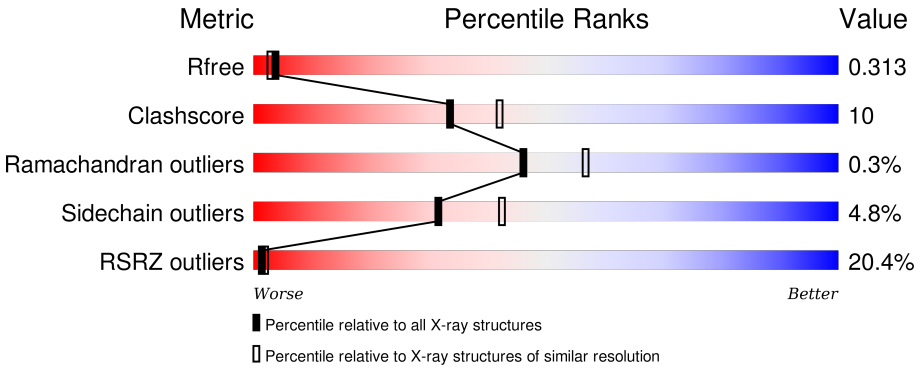
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	11% 81% 16%
1	B	500	10% 81% 17%
1	C	500	37% 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
2	MN	A	601	-	-	-	X
2	MN	B	601	-	-	-	X
3	RB0	A	602	-	-	-	X
3	RB0	B	602	-	-	-	X
3	RB0	C	602	-	-	-	X
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			

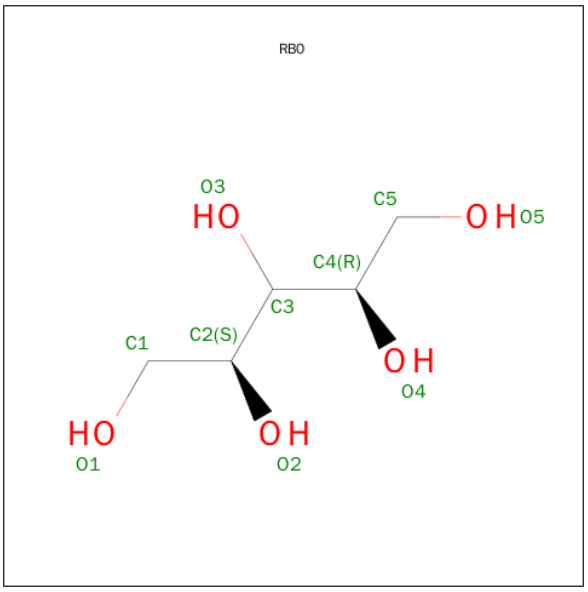
There are 6 discrepancies between the modelled and reference sequences:

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).

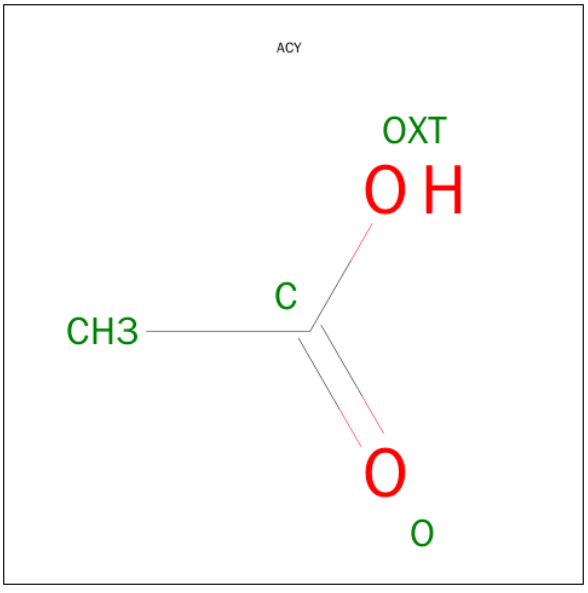
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is SUGAR (D-RIBULOSE) (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.

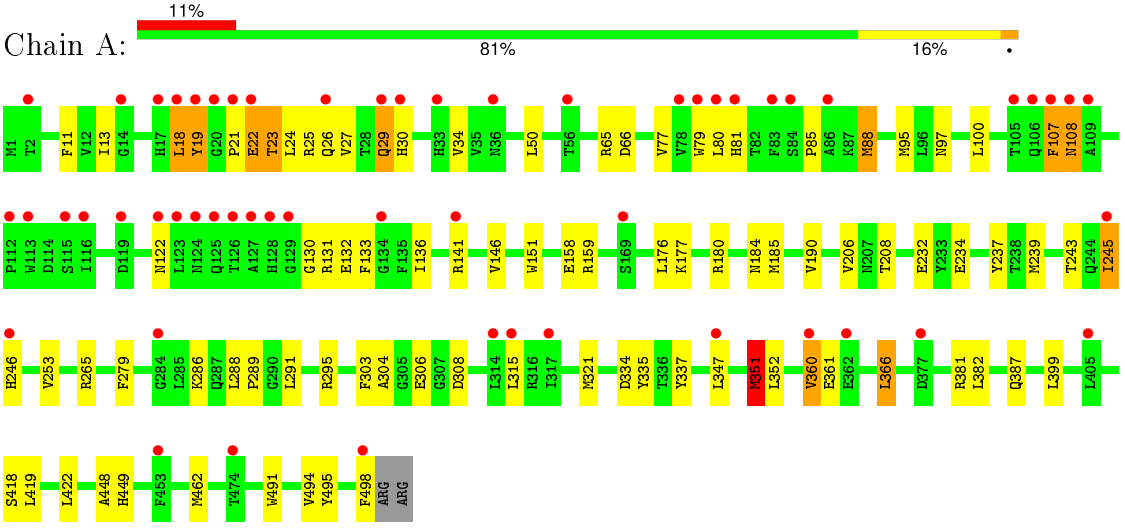
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	95	Total O 95 95	0	0
5	C	34	Total O 34 34	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

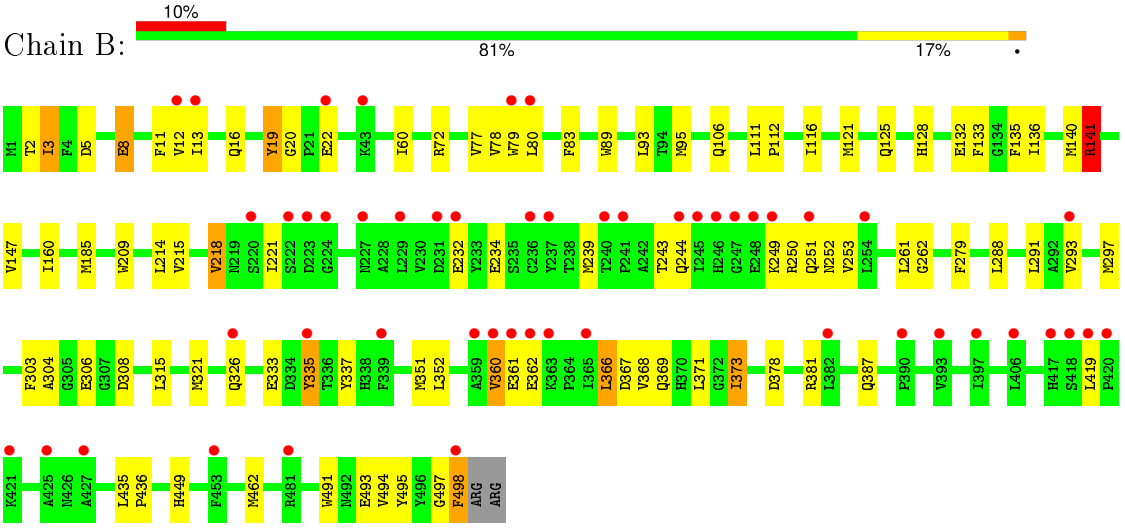
- Molecule 1: L-arabinose isomerase

Chain A:



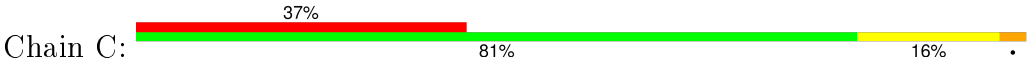
- Molecule 1: L-arabinose isomerase

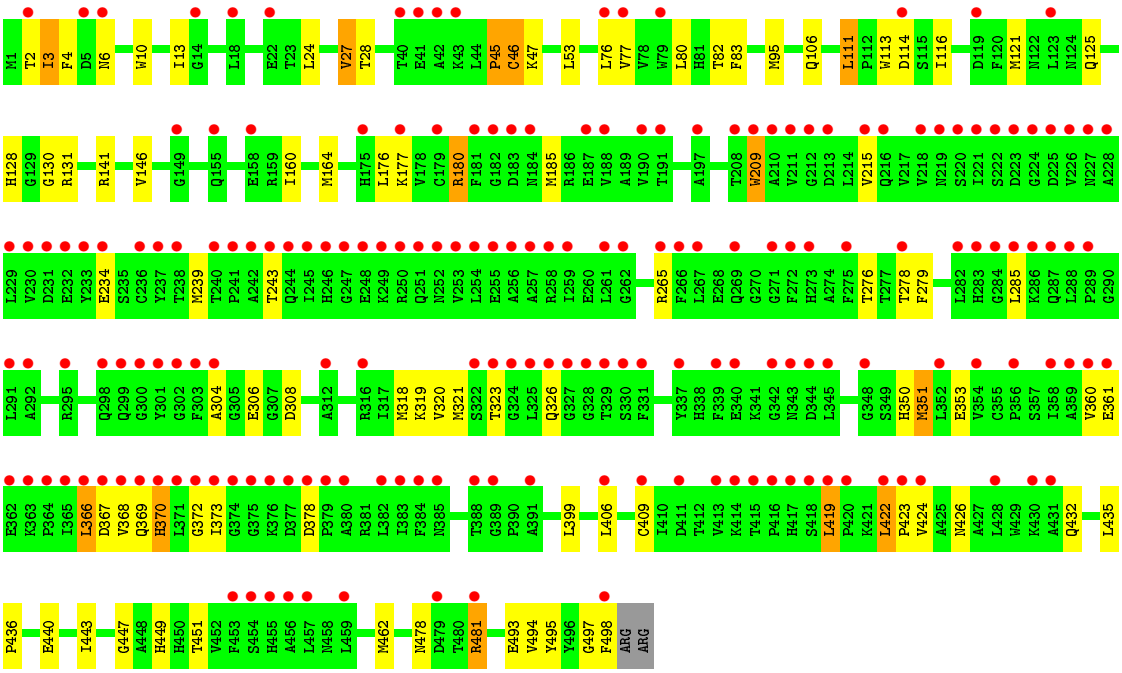
Chain B:



- Molecule 1: L-arabinose isomerase

Chain C:




M1 T2 I3 F4 D5 N6 W10 I13 G14 L18 E22 T23 L24 V27 T28 T40 E41 A42 K43 L44 P45 C46 K47 L53 L76 V77 V78 W79 L80 H81 T82 F83 M95 Q106 L111 P112 W113 D114 S115 I116 D119 F120 M121 N122 L123 N124 Q125
H128 G129 G130 R131 R141 V146 G149 Q155 E158 R159 I160 M164 H175 L176 K177 V178 C179 R180 F181 G182 D183 N184 M185 R186 E187 V188 A189 V190 T191 A197 T208 W209 A210 V211 G212 D213 L214 V215 Q216 V217 V218 N219 S220 I221 S222 D223 G224 D225 V226 N227 A228
L229 V230 D231 E232 Y233 E234 S235 C236 Y237 T238 M239 T240 P241 A242 T243 Q244 I245 H246 G247 E248 K249 R250 Q251 N252 V253 L254 E255 A256 A257 R258 I259 E260 L261 G262 R265 F266 L267 E268 Q269 G270 G271 F272 H273 A274 F275 T276 T277 T278 F279 L282 H283 G284 L285 K286 Q287 L288 P289 G290
L291 A292 R295 Q298 Q299 G300 Y301 G302 F303 A304 G305 E306 G307 D308 A312 R316 I317 M318 K319 V320 M321 S322 T323 G324 L325 Q326 G327 G328 T329 S330 F331 Y337 H338 F339 E340 K341 G342 N343 D344 L345 G348 S349 H350 M351 L352 E353 V354 C355 P356 S357 I358 A359 V360 E361
E362 K363 P364 I365 L366 D367 V368 Q369 H370 L371 G372 I373 G374 G375 K376 D377 D378 P379 A380 R381 L382 I383 F384 N385 T388 G389 P390 A391 L399 L406 C409 I410 D411 T412 V413 K414 T415 P416 H417 S418 L419 P420 K421 L422 P423 V424 A425 N426 A427 L428 W429 K430 A431 Q432 L435
P436 E440 I443 G447 A448 H449 H450 T451 V452 F453 S454 H455 A456 L457 N458 L459 M462 N478 D479 T480 R481 E493 V494 Y495 Y496 G497 F498 ARG ARG

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 0.281 , 0.313	Depositor DCC
R_{free} test set	3793 reflections (5.38%)	DCC
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
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 74254 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

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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:B:288:LEU:HD21	1:B:351:MSE:HE2	1.47	0.95
1:A:321:MSE:SE	1:A:462:MSE:HE1	2.16	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:HD12	1:B:366:LEU:C	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

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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:C:146:VAL:CG2	5:C:716:HOH:O	2.41	0.67
1:A:495:TYR:HA	1:C:494:VAL:HG11	1.77	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:C:3:ILE:HD11	1:C:320:VAL:HG13	1.79	0.65
1:A:190:VAL:HG22	1:B:135:PHE:CB	2.26	0.65
1:A:27:VAL:HG23	1:A:81:HIS:CG	2.31	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:243:THR:HG23	1:A:253:VAL:HG21	1.80	0.62
1:A:180:ARG:HB2	1:A:208:THR:HG22	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

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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:C:373:ILE:CG2	1:C:373:ILE:O	2.54	0.55
1:B:369:GLN:O	1:B:378:ASP:HB3	2.06	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:C	1:C:366:LEU:HD12	2.28	0.54
1:C:497:GLY:O	1:C:498:PHE:HB3	2.07	0.54
1:A:366:LEU:C	1:A:366:LEU:HD12	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:CD1	1:B:366:LEU:C	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:82:THR:HG22	1:C:83:PHE:O	2.10	0.50
1:C:46:CYS:SG	1:C:164:MSE:HE3	2.51	0.50
1:B:8:GLU:OE1	1:B:72:ARG:NH1	2.44	0.50
1:A:304:ALA:HB3	1:A:308:ASP:O	2.11	0.50
1:B:12:VAL:HG22	1:B:78:VAL:HG22	1.93	0.50
1:B:304:ALA:HB3	1:B:308:ASP:O	2.12	0.50
1:A:65:ARG:NH1	1:A:66:ASP:OD1	2.45	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

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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:141:ARG:NH2	1:C:399:LEU:O	2.45	0.48
1:A:30:HIS:O	1:A:34:VAL:HG23	2.12	0.48
1:C:209:TRP:CE3	1:C:209:TRP:HA	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:C:82:THR:HG22	1:C:83:PHE:N	2.29	0.48
1:B:221:ILE:HD11	1:B:262:GLY:CA	2.44	0.48
1:C:3:ILE:HA	1:C:6:ASN:HD22	1.78	0.48
1:A:131:ARG:HD3	1:C:449:HIS:HA	1.96	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:46:CYS:O	1:C:164:MSE:HE1	2.15	0.47
1:C:10:TRP:HB2	1:C:76:LEU:HD22	1.97	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:C:131:ARG:NE	5:C:733:HOH:O	2.48	0.46
1:A:133:PHE:O	1:A:136:ILE:HG22	2.16	0.46
1:A:146:VAL:HG21	1:C:443:ILE:HG22	1.98	0.46
1:C:366:LEU:HD12	1:C:367:ASP:N	2.31	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: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:HE3	1:C:209:TRP:HA	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

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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:HD23	1:C:419:LEU:N	2.32	0.44
1:C:185:MSE:HE2	1:C:279:PHE:CE2	2.53	0.44
1:B:133:PHE:O	1:B:136:ILE:HG22	2.17	0.44
1:C:278:THR:HG21	5:C:728:HOH:O	2.17	0.44
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.87	0.44
1:A:399:LEU:O	1:B:141:ARG:NH2	2.50	0.44
1:B:83:PHE:H	1:B:125:GLN:NE2	2.13	0.44
1:A:30:HIS:CD2	1:A:107:PHE:CZ	3.06	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:C:2:THR:HG22	1:C:4:PHE:H	1.83	0.43
1:B:234:GLU:HG2	1:B:239:MSE:HE2	2.00	0.43
1:A:107:PHE:O	1:A:151:TRP:NE1	2.36	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:B:221:ILE:HD11	1:B:261:LEU:C	2.39	0.43
1:B:93:LEU:CD1	1:B:140:MSE:HE1	2.48	0.43
1:A:288:LEU:HD22	1:A:352:LEU:HD12	2.00	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:C:24:LEU:HA	1:C:27:VAL:CG1	2.49	0.42
1:B:13:ILE:N	1:B:13:ILE:HD12	2.33	0.42
1:C:234:GLU:HG2	1:C:239:MSE:SE	2.70	0.42
1:B:337:TYR:OH	1:C:131:ARG:NH1	2.50	0.42
1:A:176:LEU:HD23	1:A:177:LYS:N	2.33	0.42
1:C:239:MSE:CE	1:C:243:THR:CG2	2.92	0.42
1:A:237:TYR:OH	1:A:295:ARG:HD2	2.19	0.42
1:A:13:ILE:HD12	1:A:13:ILE:N	2.34	0.42
1:B:60:ILE:HD13	1:B:89:TRP:CE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:THR:OG1	1:B:3:ILE:N	2.52	0.42
1:A:419:LEU:HD23	1:A:419:LEU:N	2.35	0.42
1:B:80:LEU:HD11	1:B:133:PHE:CG	2.54	0.42
1:B:494:VAL:HG23	4:B:603:ACY:CH3	2.49	0.42
1:B:221:ILE:CD1	1:B:261:LEU:HB3	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:C:180:ARG:CG	1:C:276:THR:OG1	2.66	0.41
1:C:160:ILE:O	1:C:164:MSE:HG3	2.20	0.41
1:B:435:LEU:HB3	1:B:436:PRO:HD3	2.02	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:C:82:THR:HG23	1:C:125:GLN:HE21	1.85	0.40
1:A:185:MSE:HE2	1:A:279:PHE:CE2	2.55	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%)	39	48
1	B	497/500 (99%)	484 (97%)	12 (2%)	1 (0%)	52	64
1	C	497/500 (99%)	479 (96%)	16 (3%)	2 (0%)	39	48
All	All	1490/1500 (99%)	1443 (97%)	42 (3%)	5 (0%)	46	57

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%)	34	46
1	B	411/402 (102%)	389 (95%)	22 (5%)	27	36
1	C	379/402 (94%)	361 (95%)	18 (5%)	32	43
All	All	1191/1206 (99%)	1133 (95%)	58 (5%)	31	41

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

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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

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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

Some 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

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Mol	Chain	Res	Type
1	C	343	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	RB0	A	602	2	9,9,9	0.30	0	10,11,11	0.94	0
3	RB0	B	602	2	9,9,9	0.23	0	10,11,11	0.46	0
4	ACY	B	603	-	1,3,3	0.68	0	0,3,3	0.00	-
3	RB0	C	602	2	9,9,9	0.26	0	10,11,11	0.54	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
3	RB0	A	602	2	-	0/12/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RB0	B	602	2	-	0/12/12/12	0/0/0/0
4	ACY	B	603	-	-	0/0/0/0	0/0/0/0
3	RB0	C	602	2	-	0/12/12/12	0/0/0/0

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.

3 monomers are involved in 8 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	481/500 (96%)	0.85	56 (11%)	6	10	16, 26, 59, 77	2 (0%)
1	B	481/500 (96%)	0.79	51 (10%)	8	12	17, 27, 35, 60	1 (0%)
1	C	481/500 (96%)	2.13	187 (38%)	0	0	20, 43, 74, 81	1 (0%)
All	All	1443/1500 (96%)	1.26	294 (20%)	1	2	16, 29, 69, 81	4 (0%)

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	HIS	14.1
1	C	219	ASN	13.2
1	C	251	GLN	12.6
1	C	416	PRO	10.4
1	C	234	GLU	10.4
1	C	373	ILE	9.9
1	C	267	LEU	9.8
1	C	360	VAL	9.5
1	C	365	ILE	8.9
1	C	371	LEU	8.8
1	C	299	GLN	8.5
1	C	241	PRO	8.3
1	C	377	ASP	7.5
1	C	237	TYR	7.3
1	C	245	ILE	7.3
1	C	227	ASN	7.3
1	C	265	ARG	7.3
1	C	413	VAL	7.1
1	C	304	ALA	6.9
1	C	236	CYS	6.8
1	C	420	PRO	6.8
1	C	363	LYS	6.8
1	C	303	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	414	LYS	6.5
1	C	247	GLY	6.4
1	C	291	LEU	6.4
1	B	360	VAL	6.4
1	A	21	PRO	6.3
1	C	369	GLN	6.3
1	C	240	THR	6.3
1	C	229	LEU	6.1
1	C	261	LEU	6.1
1	C	370	HIS	6.0
1	C	361	GLU	5.9
1	C	364	PRO	5.9
1	C	382	LEU	5.9
1	C	220	SER	5.9
1	C	233	TYR	5.8
1	C	422	LEU	5.8
1	C	367	ASP	5.6
1	C	248	GLU	5.6
1	C	352	LEU	5.6
1	C	249	LYS	5.6
1	C	213	ASP	5.6
1	C	269	GLN	5.5
1	C	366	LEU	5.5
1	C	358	ILE	5.5
1	C	385	ASN	5.3
1	B	246	HIS	5.3
1	C	384	PHE	5.2
1	B	245	ILE	5.2
1	A	115	SER	5.2
1	C	209	TRP	5.1
1	C	417	HIS	5.1
1	A	360	VAL	5.1
1	C	215	VAL	5.0
1	B	362	GLU	4.9
1	C	242	ALA	4.9
1	B	421	LYS	4.9
1	C	216	GLN	4.9
1	B	241	PRO	4.9
1	C	184	ASN	4.8
1	C	326	GLN	4.8
1	A	112	PRO	4.7
1	C	223	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	230	VAL	4.7
1	C	250	ARG	4.7
1	A	116	ILE	4.7
1	C	359	ALA	4.7
1	C	175	HIS	4.7
1	A	123	LEU	4.6
1	A	18	LEU	4.6
1	A	17	HIS	4.5
1	C	191	THR	4.5
1	C	285	LEU	4.5
1	C	376	LYS	4.5
1	C	271	GLY	4.5
1	C	453	PHE	4.5
1	C	284	GLY	4.4
1	B	254	LEU	4.4
1	C	6	ASN	4.3
1	C	5	ASP	4.3
1	A	246	HIS	4.3
1	C	208	THR	4.3
1	A	19	TYR	4.3
1	C	40	THR	4.2
1	C	415	THR	4.2
1	C	331	PHE	4.2
1	C	286	LYS	4.2
1	C	256	ALA	4.2
1	A	125	GLN	4.2
1	C	283	HIS	4.1
1	C	362	GLU	4.1
1	C	337	TYR	4.1
1	C	211	VAL	4.0
1	C	254	LEU	4.0
1	C	430	LYS	4.0
1	C	344	ASP	4.0
1	C	22	GLU	4.0
1	C	275	PHE	4.0
1	C	258	ARG	3.9
1	A	498	PHE	3.9
1	C	221	ILE	3.9
1	C	177	LYS	3.9
1	C	368	VAL	3.9
1	A	127	ALA	3.8
1	A	245	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	218	VAL	3.8
1	C	354	VAL	3.8
1	A	22	GLU	3.8
1	C	255	GLU	3.8
1	B	419	LEU	3.8
1	C	428	LEU	3.8
1	C	222	SER	3.7
1	C	498	PHE	3.7
1	C	302	GLY	3.7
1	C	457	LEU	3.7
1	C	259	ILE	3.7
1	C	378	ASP	3.7
1	C	232	GLU	3.7
1	C	257	ALA	3.7
1	A	124	ASN	3.6
1	C	419	LEU	3.6
1	C	456	ALA	3.6
1	B	365	ILE	3.5
1	C	424	VAL	3.5
1	C	322	SER	3.5
1	C	300	GLY	3.5
1	C	325	LEU	3.5
1	C	379	PRO	3.4
1	A	128	HIS	3.4
1	B	498	PHE	3.4
1	C	375	GLY	3.4
1	A	362	GLU	3.3
1	C	389	GLY	3.3
1	A	83	PHE	3.3
1	A	107	PHE	3.2
1	C	383	ILE	3.2
1	C	252	ASN	3.2
1	C	423	PRO	3.2
1	C	388	THR	3.2
1	A	33	HIS	3.2
1	C	348	GLY	3.2
1	C	298	GLN	3.2
1	A	129	GLY	3.2
1	C	179	CYS	3.2
1	A	126	THR	3.2
1	B	417	HIS	3.2
1	B	326	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	342	GLY	3.1
1	C	187	GLU	3.1
1	C	238	THR	3.1
1	A	29	GLN	3.1
1	A	315	LEU	3.1
1	C	225	ASP	3.1
1	C	278	THR	3.1
1	B	420	PRO	3.1
1	C	228	ALA	3.0
1	C	340	GLU	3.0
1	C	155	GLN	3.0
1	C	372	GLY	3.0
1	A	317	ILE	3.0
1	C	459	LEU	3.0
1	B	223	ASP	3.0
1	B	363	LYS	3.0
1	C	243	THR	3.0
1	C	182	GLY	2.9
1	C	288	LEU	2.9
1	A	84	SER	2.9
1	B	390	PRO	2.9
1	C	323	THR	2.9
1	A	14	GLY	2.9
1	C	212	GLY	2.9
1	A	119	ASP	2.9
1	C	295	ARG	2.8
1	C	324	GLY	2.8
1	A	79	TRP	2.8
1	B	244	GLN	2.8
1	C	292	ALA	2.8
1	C	266	PHE	2.8
1	C	301	TYR	2.8
1	C	41	GLU	2.8
1	A	122	ASN	2.8
1	B	293	VAL	2.7
1	C	123	LEU	2.7
1	A	169	SER	2.7
1	C	272	PHE	2.7
1	B	231	ASP	2.7
1	A	113	TRP	2.7
1	C	312	ALA	2.7
1	C	329	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	20	GLY	2.7
1	C	244	GLN	2.7
1	C	210	ALA	2.7
1	C	418	SER	2.7
1	A	81	HIS	2.7
1	B	224	GLY	2.7
1	C	14	GLY	2.7
1	B	80	LEU	2.6
1	A	347	LEU	2.6
1	B	339	PHE	2.6
1	B	220	SER	2.6
1	C	190	VAL	2.6
1	C	231	ASP	2.6
1	C	224	GLY	2.6
1	B	251	GLN	2.5
1	C	289	PRO	2.5
1	B	22	GLU	2.5
1	A	108	ASN	2.5
1	C	114	ASP	2.5
1	B	335	TYR	2.5
1	B	229	LEU	2.5
1	A	134	GLY	2.4
1	C	374	GLY	2.4
1	A	106	GLN	2.4
1	B	361	GLU	2.4
1	B	222	SER	2.4
1	A	2	THR	2.4
1	A	377	ASP	2.4
1	C	481	ARG	2.4
1	B	382	LEU	2.4
1	C	454	SER	2.4
1	B	406	LEU	2.4
1	A	78	VAL	2.4
1	C	188	VAL	2.4
1	A	141	ARG	2.4
1	C	77	VAL	2.4
1	C	79	TRP	2.4
1	B	232	GLU	2.4
1	C	406	LEU	2.4
1	C	479	ASP	2.3
1	C	197	ALA	2.3
1	C	43	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	86	ALA	2.3
1	A	474	THR	2.3
1	A	453	PHE	2.3
1	C	2	THR	2.3
1	C	149	GLY	2.3
1	B	236	CYS	2.3
1	C	183	ASP	2.3
1	B	427	ALA	2.3
1	C	380	ALA	2.3
1	C	391	ALA	2.3
1	A	80	LEU	2.3
1	B	79	TRP	2.3
1	B	240	THR	2.3
1	A	36	ASN	2.3
1	B	227	ASN	2.3
1	A	26	GLN	2.2
1	A	284	GLY	2.2
1	C	431	ALA	2.2
1	C	158	GLU	2.2
1	C	76	LEU	2.2
1	C	356	PRO	2.2
1	A	109	ALA	2.2
1	B	12	VAL	2.2
1	C	345	LEU	2.2
1	B	247	GLY	2.2
1	C	327	GLY	2.2
1	C	119	ASP	2.2
1	B	418	SER	2.2
1	B	397	ILE	2.2
1	A	105	THR	2.2
1	C	455	HIS	2.2
1	B	393	VAL	2.2
1	C	181	PHE	2.2
1	B	13	ILE	2.2
1	C	226	VAL	2.2
1	B	481	ARG	2.2
1	B	425	ALA	2.2
1	B	43	LYS	2.1
1	B	453	PHE	2.1
1	B	249	LYS	2.1
1	B	359	ALA	2.1
1	C	409	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	237	TYR	2.1
1	C	42	ALA	2.1
1	C	343	ASN	2.1
1	C	339	PHE	2.1
1	C	282	LEU	2.1
1	C	262	GLY	2.1
1	C	273	HIS	2.1
1	A	314	LEU	2.1
1	C	18	LEU	2.1
1	C	328	GLY	2.1
1	C	316	ARG	2.1
1	C	287	GLN	2.1
1	C	330	SER	2.1
1	A	56	THR	2.0
1	C	411	ASP	2.0
1	A	405	LEU	2.0
1	A	30	HIS	2.0
1	C	253	VAL	2.0
1	B	248	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
3	RB0	A	602	10/10	0.96	0.33	6.25	37,43,50,52	2
2	MN	A	601	1/1	0.97	0.25	4.76	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	B	601	1/1	0.95	0.24	3.65	52,52,52,52	0
3	RB0	B	602	10/10	0.93	0.29	2.28	37,52,62,65	2
3	RB0	C	602	10/10	0.72	0.56	1.92	48,54,59,63	10
4	ACY	B	603	4/4	0.94	0.22	1.16	25,35,37,39	0
2	MN	C	601	1/1	0.95	0.25	0.26	80,80,80,80	1

6.5 Other polymers (i)

There are no such residues in this entry.