



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:31 PM UTC

PDB ID : 1KMP / pdb_00001kmp
Title : Crystal structure of the Outer Membrane Transporter FecA Complexed with Ferric Citrate
Authors : Ferguson, A.D.; Chakraborty, R.; Smith, B.S.; Esser, L.; van der Helm, D.; Deisenhofer, J.
Deposited on : 2001-12-17
Resolution : 2.50 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 : 4-5-2 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

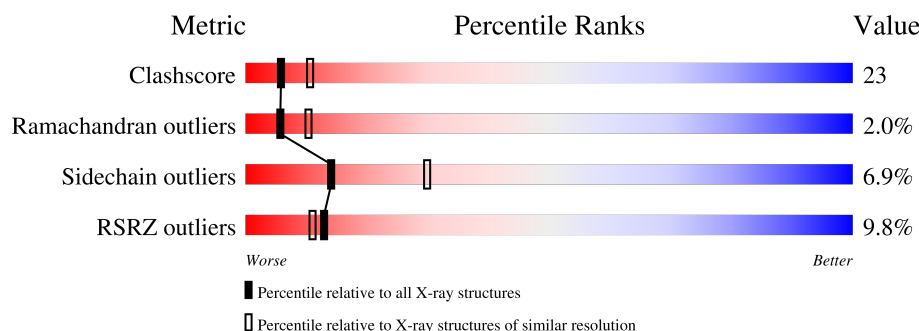
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	774	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5615 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.

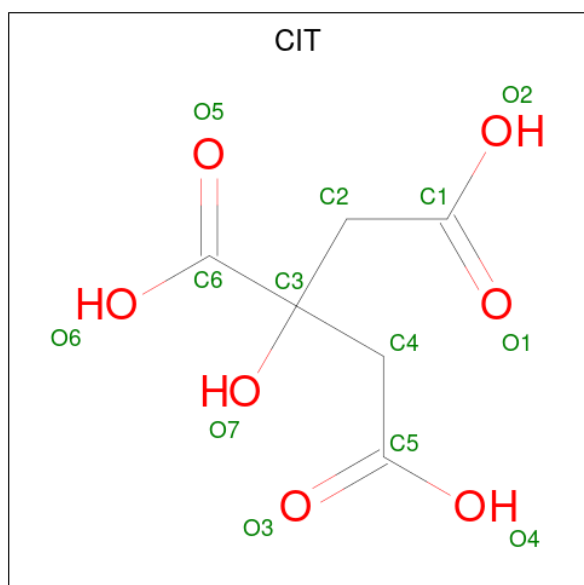
- Molecule 1 is a protein called IRON(III) DICITRATE TRANSPORT PROTEIN FECA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	Se	0	0	0
			5079	3178	894	993	14			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

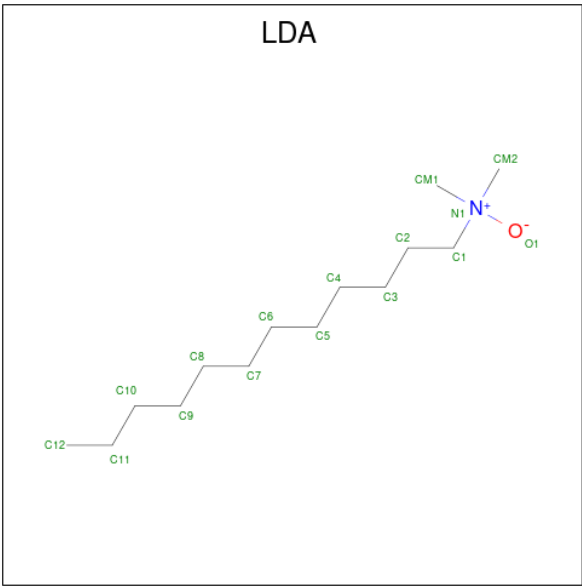
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		

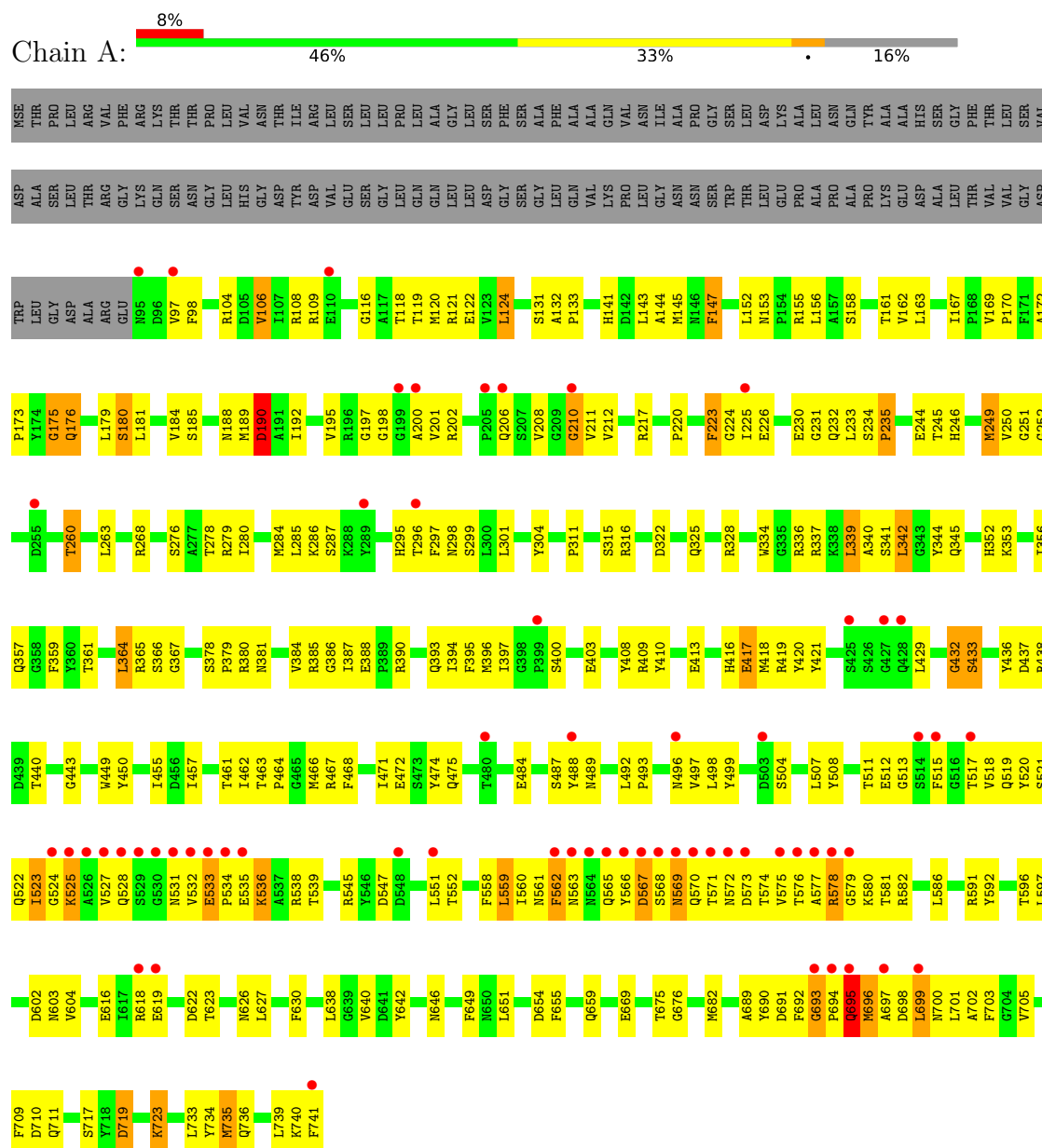
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		

3 Residue-property plots

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: IRON(III) DICITRATE TRANSPORT PROTEIN FECA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.47Å 88.76Å 95.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.95 – 2.50 36.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.5 (36.95-2.50) 88.4 (36.95-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.282 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, CIT, FE

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	0.45	0/5194	0.92	19/7031 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	SER	N-CA-C	-7.61	102.96	111.71
1	A	315	SER	N-CA-C	-7.24	101.51	110.41
1	A	190	ASP	N-CA-C	-6.31	105.74	113.50
1	A	717	SER	N-CA-C	-6.31	98.23	108.52
1	A	328	ARG	CA-C-N	6.30	126.21	119.28
1	A	328	ARG	C-N-CA	6.30	126.21	119.28
1	A	158	SER	N-CA-C	6.08	120.69	113.16
1	A	176	GLN	CA-C-N	5.63	125.24	119.56
1	A	176	GLN	C-N-CA	5.63	125.24	119.56
1	A	429	LEU	N-CA-C	-5.61	101.85	110.32
1	A	432	GLY	N-CA-C	-5.51	103.32	111.03
1	A	654	ASP	N-CA-C	-5.41	100.95	109.50
1	A	234	SER	CA-C-N	5.33	126.50	119.84
1	A	234	SER	C-N-CA	5.33	126.50	119.84
1	A	719	ASP	N-CA-C	5.30	119.81	113.23
1	A	175	GLY	N-CA-C	5.26	120.42	113.37
1	A	172	ALA	CA-C-N	5.12	125.42	119.47
1	A	172	ALA	C-N-CA	5.12	125.42	119.47
1	A	523	ILE	N-CA-C	-5.06	105.46	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5079	0	4798	246	0
2	A	2	0	0	0	0
3	A	26	0	8	1	0
4	A	256	0	496	12	0
5	A	252	0	0	18	0
All	All	5615	0	5302	246	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 23.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASP:HB2	1:A:576:THR:HB	1.46	0.98
1:A:519:GLN:H	1:A:522:GLN:HE21	1.13	0.91
1:A:225:ILE:HD11	1:A:250:VAL:HG13	1.57	0.84
1:A:533:GLU:HB3	1:A:534:PRO:HA	1.59	0.84
1:A:533:GLU:OE1	1:A:535:GLU:HG3	1.79	0.83
1:A:504:SER:HB2	1:A:547:ASP:O	1.80	0.81
1:A:698:ASP:HB2	1:A:740:LYS:HB2	1.63	0.81
1:A:579:GLY:HA3	1:A:619:GLU:HB2	1.62	0.80
1:A:202:ARG:HB2	5:A:777:HOH:O	1.83	0.77
1:A:525:LYS:HE3	1:A:531:ASN:HB3	1.67	0.76
1:A:210:GLY:HA2	5:A:856:HOH:O	1.85	0.75
1:A:719:ASP:HB2	5:A:907:HOH:O	1.87	0.74
1:A:175:GLY:HA3	1:A:520:TYR:CE2	2.22	0.74
1:A:578:ARG:HA	5:A:925:HOH:O	1.88	0.73
1:A:523:ILE:O	1:A:525:LYS:HG3	1.89	0.72
1:A:231:GLY:HA3	4:A:756:LDA:H112	1.71	0.71
1:A:339:LEU:C	1:A:339:LEU:HD23	2.16	0.71
1:A:225:ILE:HD12	1:A:250:VAL:HG22	1.72	0.70
1:A:220:PRO:HG2	1:A:249:MSE:HE1	1.71	0.70
1:A:394:ILE:HG12	1:A:403:GLU:HG3	1.72	0.70
1:A:579:GLY:HA3	1:A:619:GLU:CB	2.21	0.70
1:A:651:LEU:HB2	4:A:745:LDA:HM12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:OG1	1:A:245:THR:HG21	1.93	0.69
1:A:519:GLN:HB2	1:A:522:GLN:NE2	2.07	0.69
1:A:649:PHE:HB3	4:A:745:LDA:HM22	1.74	0.69
1:A:145:MSE:HE3	1:A:147:PHE:CD2	2.28	0.68
1:A:202:ARG:HH11	1:A:202:ARG:HG2	1.58	0.68
1:A:488:TYR:OH	1:A:517:THR:HB	1.93	0.68
1:A:449:TRP:HB3	4:A:755:LDA:H51	1.76	0.67
1:A:569:ASN:HA	1:A:719:ASP:HB3	1.75	0.66
1:A:438:ARG:HD3	5:A:799:HOH:O	1.96	0.66
1:A:570:GLN:HE21	1:A:570:GLN:HA	1.60	0.66
1:A:339:LEU:HD23	1:A:340:ALA:N	2.10	0.66
1:A:220:PRO:CG	1:A:249:MSE:HE1	2.26	0.66
1:A:198:GLY:HA2	1:A:496:ASN:HD21	1.59	0.65
1:A:535:GLU:HB3	1:A:562:PHE:HE1	1.62	0.65
1:A:696:MSE:HG2	1:A:697:ALA:N	2.11	0.64
1:A:388:GLU:HB2	1:A:409:ARG:HG2	1.79	0.63
1:A:118:THR:HG23	1:A:119:THR:HG23	1.80	0.62
1:A:378:SER:HB3	5:A:771:HOH:O	1.99	0.62
1:A:316:ARG:HD3	1:A:669:GLU:OE1	1.99	0.62
1:A:395:PHE:HE1	1:A:397:ILE:HD11	1.65	0.62
1:A:109:ARG:HE	1:A:217:ARG:HD3	1.66	0.61
1:A:695:GLN:CD	1:A:696:MSE:H	2.08	0.60
1:A:498:LEU:HD12	1:A:507:LEU:O	2.01	0.60
1:A:655:PHE:HB3	1:A:682:MSE:HG3	1.83	0.60
1:A:225:ILE:HD13	1:A:250:VAL:HA	1.82	0.60
1:A:552:THR:HG23	1:A:552:THR:O	2.01	0.60
1:A:108:ARG:HH11	1:A:108:ARG:HB3	1.68	0.58
1:A:316:ARG:HB3	5:A:937:HOH:O	2.03	0.58
1:A:562:PHE:O	1:A:580:LYS:HG3	2.04	0.58
1:A:518:VAL:HG13	1:A:533:GLU:HB2	1.84	0.58
1:A:735:MSE:SE	4:A:756:LDA:H91	2.53	0.58
1:A:380:ARG:HG2	1:A:417:GLU:HB3	1.86	0.57
1:A:118:THR:HG21	1:A:232:GLN:HE22	1.68	0.57
1:A:98:PHE:HA	1:A:545:ARG:HD2	1.85	0.57
1:A:580:LYS:HG2	5:A:904:HOH:O	2.04	0.57
1:A:188:ASN:HB3	1:A:284:MSE:HE2	1.87	0.57
1:A:396:MSE:HG3	1:A:400:SER:O	2.03	0.57
1:A:527:VAL:CG2	1:A:577:ALA:HB2	2.36	0.56
1:A:173:PRO:HD2	1:A:413:GLU:OE1	2.06	0.56
1:A:322:ASP:O	1:A:325:GLN:HG2	2.06	0.56
1:A:225:ILE:CD1	1:A:250:VAL:HG13	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:TYR:OH	1:A:597:LEU:HD21	2.06	0.56
1:A:552:THR:CG2	1:A:591:ARG:HB3	2.36	0.55
1:A:697:ALA:HB1	1:A:741:PHE:HE2	1.70	0.55
1:A:511:THR:HA	1:A:539:THR:O	2.07	0.55
1:A:695:GLN:NE2	1:A:696:MSE:H	2.03	0.55
1:A:184:VAL:CG2	1:A:189:MSE:HE3	2.37	0.55
1:A:586:LEU:HD23	1:A:586:LEU:C	2.32	0.54
1:A:202:ARG:NH2	1:A:390:ARG:NE	2.56	0.54
1:A:699:LEU:CD2	1:A:739:LEU:HD13	2.38	0.54
1:A:175:GLY:HA3	1:A:520:TYR:CZ	2.43	0.54
1:A:143:LEU:HD12	1:A:280:ILE:HD11	1.88	0.54
1:A:202:ARG:HG2	1:A:202:ARG:NH1	2.22	0.53
1:A:703:PHE:CE2	1:A:735:MSE:HG3	2.43	0.53
1:A:124:LEU:HD11	1:A:192:ILE:HG21	1.88	0.53
1:A:208:VAL:HG21	1:A:562:PHE:CE2	2.43	0.53
1:A:120:MSE:HE1	1:A:185:SER:C	2.32	0.53
1:A:167:ILE:HD11	1:A:341:SER:CB	2.38	0.53
1:A:417:GLU:HG2	1:A:440:THR:OG1	2.09	0.53
1:A:249:MSE:HE2	1:A:249:MSE:C	2.34	0.53
1:A:366:SER:HB3	1:A:379:PRO:HA	1.91	0.53
1:A:418:MSE:HA	1:A:438:ARG:O	2.09	0.53
1:A:223:PHE:H	1:A:252:GLY:HA2	1.74	0.52
1:A:364:LEU:C	1:A:364:LEU:HD13	2.34	0.52
1:A:638:LEU:C	1:A:638:LEU:HD12	2.33	0.52
1:A:579:GLY:HA3	1:A:619:GLU:HG2	1.90	0.52
1:A:276:SER:HB3	1:A:311:PRO:HG3	1.92	0.52
1:A:184:VAL:HG23	1:A:189:MSE:HE3	1.91	0.52
1:A:462:ILE:HG22	1:A:464:PRO:HD3	1.90	0.52
1:A:565:GLN:NE2	1:A:581:THR:OG1	2.42	0.52
1:A:525:LYS:HE3	1:A:531:ASN:CB	2.37	0.52
1:A:552:THR:HG22	1:A:591:ARG:HB3	1.91	0.52
1:A:200:ALA:HB3	1:A:512:GLU:HB3	1.92	0.51
1:A:457:ILE:HG23	1:A:457:ILE:O	2.10	0.51
1:A:147:PHE:CZ	1:A:212:VAL:HG21	2.46	0.51
1:A:278:THR:HG22	1:A:279:ARG:N	2.26	0.51
1:A:551:LEU:HD13	1:A:551:LEU:C	2.35	0.51
1:A:580:LYS:HE3	5:A:904:HOH:O	2.10	0.51
1:A:450:TYR:HD2	5:A:886:HOH:O	1.94	0.51
1:A:579:GLY:HA3	1:A:619:GLU:CG	2.41	0.51
1:A:511:THR:HG23	1:A:511:THR:O	2.10	0.51
1:A:578:ARG:HB2	5:A:810:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ASP:O	1:A:603:ASN:HB2	2.09	0.50
1:A:462:ILE:HD12	1:A:462:ILE:N	2.26	0.50
1:A:675:THR:HG22	1:A:676:GLY:N	2.24	0.50
1:A:695:GLN:CG	1:A:696:MSE:H	2.24	0.50
1:A:145:MSE:HE3	1:A:147:PHE:HD2	1.75	0.50
1:A:472:GLU:HG2	1:A:487:SER:HB2	1.93	0.50
1:A:630:PHE:HA	1:A:659:GLN:OE1	2.12	0.50
1:A:120:MSE:CE	1:A:184:VAL:HG22	2.42	0.50
1:A:519:GLN:N	1:A:522:GLN:HE21	1.94	0.50
1:A:532:VAL:O	1:A:533:GLU:O	2.29	0.49
1:A:533:GLU:HB3	1:A:534:PRO:CA	2.38	0.49
1:A:169:VAL:N	1:A:170:PRO:CD	2.75	0.49
1:A:287:SER:HB2	1:A:299:SER:OG	2.12	0.49
1:A:535:GLU:HB3	1:A:562:PHE:CE1	2.47	0.49
1:A:559:LEU:HD23	1:A:560:ILE:N	2.27	0.49
1:A:225:ILE:CD1	1:A:250:VAL:HA	2.42	0.49
1:A:515:PHE:HA	1:A:535:GLU:O	2.12	0.49
1:A:120:MSE:HE3	1:A:184:VAL:HG22	1.94	0.49
1:A:176:GLN:HE21	1:A:176:GLN:HA	1.77	0.49
1:A:566:TYR:N	1:A:566:TYR:CD1	2.80	0.49
1:A:417:GLU:HG3	5:A:799:HOH:O	2.13	0.49
1:A:570:GLN:NE2	3:A:2001:CIT:O4	2.45	0.49
1:A:104:ARG:HG3	1:A:195:VAL:HG22	1.94	0.48
1:A:380:ARG:HG2	1:A:417:GLU:CB	2.42	0.48
1:A:387:ILE:HG22	1:A:410:TYR:HB3	1.95	0.48
1:A:249:MSE:HG2	1:A:263:LEU:HD23	1.94	0.48
1:A:97:VAL:HG11	1:A:106:VAL:HG12	1.95	0.48
1:A:419:ARG:HH21	1:A:438:ARG:HH21	1.61	0.48
1:A:357:GLN:NE2	5:A:953:HOH:O	2.41	0.48
1:A:520:TYR:C	1:A:522:GLN:H	2.21	0.48
1:A:263:LEU:HD12	1:A:284:MSE:HE3	1.96	0.48
1:A:463:THR:HG22	1:A:463:THR:O	2.14	0.48
1:A:740:LYS:HE2	5:A:866:HOH:O	2.13	0.48
1:A:420:TYR:HA	1:A:436:TYR:HA	1.95	0.48
1:A:511:THR:HG21	4:A:753:LDA:H92	1.96	0.48
1:A:561:ASN:ND2	4:A:757:LDA:HM22	2.29	0.48
1:A:468:PHE:CZ	1:A:489:ASN:HB3	2.49	0.47
1:A:519:GLN:O	1:A:522:GLN:HG2	2.14	0.47
1:A:566:TYR:HB3	1:A:575:VAL:CG1	2.44	0.47
1:A:570:GLN:HE21	1:A:570:GLN:CA	2.23	0.47
1:A:366:SER:CB	1:A:379:PRO:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:O	1:A:467:ARG:HD2	2.15	0.47
1:A:334:TRP:CZ3	1:A:367:GLY:HA2	2.49	0.47
1:A:571:THR:HG21	1:A:723:LYS:HZ1	1.80	0.47
1:A:691:ASP:OD2	1:A:694:PRO:HG3	2.14	0.47
1:A:692:PHE:O	1:A:693:GLY:C	2.57	0.46
1:A:190:ASP:OD2	1:A:217:ARG:HA	2.15	0.46
1:A:116:GLY:HA2	1:A:736:GLN:NE2	2.30	0.46
1:A:296:THR:HG23	1:A:345:GLN:HB3	1.96	0.46
1:A:298:ASN:O	1:A:342:LEU:HD23	2.15	0.46
1:A:144:ALA:HB2	1:A:180:SER:O	2.15	0.46
1:A:263:LEU:CD1	1:A:284:MSE:HE3	2.45	0.46
1:A:572:ASN:O	1:A:574:THR:HG23	2.14	0.46
1:A:703:PHE:HD2	4:A:756:LDA:H22	1.81	0.46
1:A:524:GLY:C	1:A:525:LYS:HG3	2.40	0.46
1:A:118:THR:HG21	1:A:232:GLN:NE2	2.29	0.46
1:A:118:THR:HG22	1:A:122:GLU:OE1	2.16	0.46
1:A:198:GLY:HA2	1:A:496:ASN:ND2	2.26	0.46
1:A:296:THR:CG2	1:A:345:GLN:HB3	2.46	0.46
1:A:226:GLU:OE2	1:A:740:LYS:HD2	2.16	0.45
1:A:155:ARG:NH2	1:A:570:GLN:OE1	2.50	0.45
1:A:225:ILE:HB	1:A:741:PHE:HB2	1.99	0.45
1:A:108:ARG:HB3	1:A:108:ARG:NH1	2.30	0.45
1:A:246:HIS:HB2	4:A:743:LDA:H52	1.97	0.45
1:A:571:THR:HG21	1:A:723:LYS:NZ	2.32	0.45
1:A:233:LEU:O	1:A:235:PRO:HD3	2.16	0.45
1:A:582:ARG:NH2	1:A:618:ARG:HD2	2.31	0.45
1:A:386:GLY:HA2	1:A:410:TYR:O	2.16	0.45
1:A:408:TYR:CG	1:A:409:ARG:N	2.85	0.45
1:A:432:GLY:O	1:A:433:SER:CB	2.63	0.45
1:A:570:GLN:HA	1:A:570:GLN:NE2	2.28	0.45
1:A:131:SER:HB2	5:A:969:HOH:O	2.17	0.45
1:A:233:LEU:C	1:A:235:PRO:HD3	2.41	0.45
1:A:695:GLN:NE2	1:A:696:MSE:N	2.65	0.45
1:A:223:PHE:HA	1:A:251:GLY:O	2.18	0.44
1:A:296:THR:HG22	5:A:796:HOH:O	2.17	0.44
1:A:121:ARG:HG3	1:A:132:ALA:HB1	1.98	0.44
1:A:224:GLY:O	1:A:225:ILE:HD13	2.17	0.44
1:A:697:ALA:O	1:A:698:ASP:C	2.61	0.44
1:A:152:LEU:O	1:A:153:ASN:C	2.60	0.44
1:A:268:ARG:HG2	1:A:268:ARG:HH11	1.83	0.44
1:A:693:GLY:O	1:A:695:GLN:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HG12	4:A:758:LDA:HM11	1.99	0.44
1:A:361:THR:OG1	1:A:384:VAL:HB	2.17	0.44
1:A:231:GLY:O	1:A:734:TYR:HA	2.18	0.44
1:A:364:LEU:HD23	1:A:381:ASN:OD1	2.17	0.44
1:A:524:GLY:O	1:A:525:LYS:HB2	2.18	0.43
1:A:499:TYR:CE2	4:A:747:LDA:H61	2.53	0.43
1:A:552:THR:O	1:A:552:THR:CG2	2.64	0.43
1:A:188:ASN:HB3	1:A:284:MSE:CE	2.49	0.43
1:A:533:GLU:CD	1:A:535:GLU:HG3	2.41	0.43
1:A:124:LEU:CD1	1:A:192:ILE:HG21	2.49	0.43
1:A:206:GLN:NE2	1:A:517:THR:HG23	2.34	0.43
1:A:295:HIS:HD2	1:A:344:TYR:OH	2.02	0.43
1:A:455:ILE:O	1:A:461:THR:HA	2.19	0.43
1:A:520:TYR:O	1:A:522:GLN:N	2.52	0.43
1:A:359:PHE:HE1	1:A:384:VAL:HG12	1.83	0.43
1:A:508:TYR:CD1	1:A:508:TYR:C	2.97	0.43
1:A:220:PRO:HB2	1:A:252:GLY:HA2	2.00	0.43
1:A:195:VAL:HB	1:A:211:VAL:HG13	2.01	0.43
1:A:230:GLU:HA	1:A:735:MSE:O	2.19	0.43
1:A:161:THR:O	1:A:211:VAL:HG23	2.19	0.42
1:A:573:ASP:HB2	5:A:828:HOH:O	2.19	0.42
1:A:524:GLY:O	1:A:525:LYS:CB	2.66	0.42
1:A:646:ASN:HB2	1:A:690:TYR:CE1	2.55	0.42
1:A:141:HIS:CE1	1:A:143:LEU:HB2	2.55	0.42
1:A:260:THR:HA	1:A:286:LYS:O	2.20	0.42
1:A:570:GLN:NE2	1:A:570:GLN:CA	2.82	0.42
1:A:695:GLN:HE21	1:A:695:GLN:HB3	1.59	0.42
1:A:197:GLY:HA2	1:A:512:GLU:OE2	2.20	0.42
1:A:285:LEU:HD12	1:A:285:LEU:HA	1.92	0.42
1:A:352:HIS:CD2	1:A:393:GLN:HG3	2.54	0.42
1:A:536:LYS:N	1:A:563:ASN:OD1	2.52	0.42
1:A:627:LEU:HD21	5:A:759:HOH:O	2.20	0.42
1:A:492:LEU:HD22	1:A:513:GLY:C	2.45	0.41
1:A:604:VAL:HG22	1:A:642:TYR:CD1	2.56	0.41
1:A:698:ASP:CB	1:A:740:LYS:HB2	2.43	0.41
1:A:179:LEU:C	1:A:181:LEU:N	2.74	0.41
1:A:416:HIS:CE1	1:A:418:MSE:HE2	2.55	0.41
1:A:623:THR:HA	1:A:626:ASN:ND2	2.35	0.41
1:A:421:TYR:CE2	1:A:437:ASP:HB3	2.55	0.41
1:A:304:TYR:O	1:A:336:ARG:HA	2.21	0.41
1:A:689:ALA:CB	1:A:702:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HD2	1:A:133:PRO:O	2.20	0.41
1:A:299:SER:HA	1:A:341:SER:O	2.20	0.41
1:A:443:GLY:HA3	1:A:474:TYR:CZ	2.56	0.41
1:A:520:TYR:C	1:A:522:GLN:N	2.79	0.41
1:A:522:GLN:HB2	1:A:532:VAL:HG11	2.03	0.41
1:A:739:LEU:HD11	1:A:741:PHE:CE2	2.55	0.41
1:A:616:GLU:OE1	1:A:618:ARG:NH2	2.54	0.40
1:A:693:GLY:C	1:A:695:GLN:N	2.79	0.40
1:A:709:PHE:O	1:A:710:ASP:C	2.64	0.40
1:A:739:LEU:HD21	1:A:741:PHE:CZ	2.56	0.40
1:A:297:PHE:CD1	1:A:297:PHE:N	2.89	0.40
1:A:493:PRO:HD2	1:A:538:ARG:HH22	1.85	0.40
1:A:558:PHE:CD1	1:A:558:PHE:C	2.98	0.40
1:A:566:TYR:HB3	1:A:575:VAL:HG12	2.01	0.40
1:A:449:TRP:HH2	4:A:748:LDA:H21	1.86	0.40
1:A:167:ILE:HD11	1:A:341:SER:HB2	2.03	0.40
1:A:705:VAL:HG22	1:A:733:LEU:HD23	2.03	0.40
1:A:285:LEU:HD23	1:A:301:LEU:HD12	2.03	0.40
1:A:471:ILE:O	1:A:487:SER:HA	2.22	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	645/774 (83%)	581 (90%)	51 (8%)	13 (2%)	6 10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	GLU
1	A	210	GLY

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Mol	Chain	Res	Type
1	A	223	PHE
1	A	433	SER
1	A	521	SER
1	A	525	LYS
1	A	568	SER
1	A	569	ASN
1	A	693	GLY
1	A	578	ARG
1	A	696	MSE
1	A	567	ASP
1	A	695	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	534/621 (86%)	497 (93%)	37 (7%)	14	30

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	124	LEU
1	A	147	PHE
1	A	156	LEU
1	A	162	VAL
1	A	163	LEU
1	A	190	ASP
1	A	235	PRO
1	A	244	GLU
1	A	249	MSE
1	A	260	THR
1	A	337	ARG
1	A	339	LEU
1	A	342	LEU
1	A	353	LYS

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Mol	Chain	Res	Type
1	A	364	LEU
1	A	365	ARG
1	A	385	ARG
1	A	417	GLU
1	A	466	MSE
1	A	475	GLN
1	A	484	GLU
1	A	497	VAL
1	A	528	GLN
1	A	536	LYS
1	A	559	LEU
1	A	562	PHE
1	A	596	THR
1	A	622	ASP
1	A	640	VAL
1	A	695	GLN
1	A	699	LEU
1	A	700	ASN
1	A	701	LEU
1	A	711	GLN
1	A	723	LYS
1	A	735	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	232	GLN
1	A	240	ASN
1	A	246	HIS
1	A	247	ASN
1	A	295	HIS
1	A	362	GLN
1	A	412	ASN
1	A	416	HIS
1	A	475	GLN
1	A	522	GLN
1	A	528	GLN
1	A	561	ASN
1	A	565	GLN
1	A	569	ASN
1	A	603	ASN

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Mol	Chain	Res	Type
1	A	656	GLN
1	A	695	GLN

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	CIT	A	2001	2	12,12,12	2.02	5 (41%)	17,17,17	1.69	3 (17%)
4	LDA	A	746	-	13,15,15	1.95	1 (7%)	14,17,17	1.76	4 (28%)
4	LDA	A	752	-	13,15,15	1.89	1 (7%)	14,17,17	1.65	4 (28%)
3	CIT	A	2003	2	12,12,12	1.86	3 (25%)	17,17,17	1.98	6 (35%)
4	LDA	A	744	-	13,15,15	1.96	1 (7%)	14,17,17	1.65	4 (28%)
4	LDA	A	749	-	13,15,15	1.91	1 (7%)	14,17,17	1.69	4 (28%)
4	LDA	A	758	-	13,15,15	1.94	1 (7%)	14,17,17	1.74	4 (28%)
4	LDA	A	755	-	13,15,15	1.79	1 (7%)	14,17,17	1.65	4 (28%)
4	LDA	A	747	-	13,15,15	1.92	1 (7%)	14,17,17	1.68	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	A	750	-	13,15,15	1.82	1 (7%)	14,17,17	1.69	4 (28%)
4	LDA	A	757	-	13,15,15	1.82	1 (7%)	14,17,17	1.76	4 (28%)
4	LDA	A	753	-	13,15,15	1.85	1 (7%)	14,17,17	1.68	4 (28%)
4	LDA	A	748	-	13,15,15	1.94	1 (7%)	14,17,17	1.64	4 (28%)
4	LDA	A	743	-	13,15,15	1.97	1 (7%)	14,17,17	1.62	4 (28%)
4	LDA	A	751	-	13,15,15	1.93	1 (7%)	14,17,17	1.64	4 (28%)
4	LDA	A	745	-	13,15,15	1.89	1 (7%)	14,17,17	1.72	4 (28%)
4	LDA	A	754	-	13,15,15	1.90	1 (7%)	14,17,17	1.64	4 (28%)
4	LDA	A	756	-	13,15,15	1.92	1 (7%)	14,17,17	1.71	4 (28%)

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	CIT	A	2001	2	-	2/16/16/16	-
4	LDA	A	746	-	-	9/13/13/13	-
4	LDA	A	752	-	-	5/13/13/13	-
3	CIT	A	2003	2	-	2/16/16/16	-
4	LDA	A	744	-	-	7/13/13/13	-
4	LDA	A	749	-	-	10/13/13/13	-
4	LDA	A	758	-	-	10/13/13/13	-
4	LDA	A	755	-	-	12/13/13/13	-
4	LDA	A	747	-	-	10/13/13/13	-
4	LDA	A	750	-	-	10/13/13/13	-
4	LDA	A	757	-	-	8/13/13/13	-
4	LDA	A	753	-	-	9/13/13/13	-
4	LDA	A	748	-	-	10/13/13/13	-
4	LDA	A	743	-	-	8/13/13/13	-
4	LDA	A	751	-	-	7/13/13/13	-
4	LDA	A	745	-	-	10/13/13/13	-
4	LDA	A	754	-	-	8/13/13/13	-
4	LDA	A	756	-	-	10/13/13/13	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	743	LDA	O1-N1	-6.68	1.25	1.42
4	A	744	LDA	O1-N1	-6.63	1.25	1.42
4	A	748	LDA	O1-N1	-6.62	1.25	1.42
4	A	746	LDA	O1-N1	-6.61	1.25	1.42
4	A	758	LDA	O1-N1	-6.60	1.26	1.42
4	A	747	LDA	O1-N1	-6.57	1.26	1.42
4	A	756	LDA	O1-N1	-6.57	1.26	1.42
4	A	751	LDA	O1-N1	-6.50	1.26	1.42
4	A	749	LDA	O1-N1	-6.50	1.26	1.42
4	A	754	LDA	O1-N1	-6.45	1.26	1.42
4	A	745	LDA	O1-N1	-6.42	1.26	1.42
4	A	752	LDA	O1-N1	-6.41	1.26	1.42
4	A	757	LDA	O1-N1	-6.26	1.26	1.42
4	A	753	LDA	O1-N1	-6.23	1.26	1.42
4	A	750	LDA	O1-N1	-6.20	1.26	1.42
4	A	755	LDA	O1-N1	-6.01	1.27	1.42
3	A	2001	CIT	C3-C6	4.53	1.58	1.53
3	A	2003	CIT	O7-C3	3.70	1.50	1.43
3	A	2003	CIT	C3-C6	3.32	1.56	1.53
3	A	2001	CIT	O1-C1	2.57	1.30	1.22
3	A	2001	CIT	O7-C3	2.53	1.48	1.43
3	A	2001	CIT	O6-C6	-2.20	1.22	1.30
3	A	2001	CIT	O2-C1	-2.16	1.23	1.30
3	A	2003	CIT	O4-C5	-2.10	1.23	1.30

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	CIT	O6-C6-C3	3.98	120.77	113.14
3	A	2001	CIT	O5-C6-C3	-3.85	114.62	122.09
4	A	746	LDA	CM1-N1-C1	-3.82	102.21	110.23
3	A	2003	CIT	O5-C6-C3	-3.66	115.00	122.09
4	A	757	LDA	CM1-N1-C1	-3.65	102.56	110.23
4	A	745	LDA	CM1-N1-C1	-3.60	102.68	110.23
4	A	758	LDA	CM1-N1-C1	-3.58	102.70	110.23
4	A	753	LDA	CM1-N1-C1	-3.53	102.82	110.23
3	A	2003	CIT	O6-C6-C3	3.53	119.91	113.14
4	A	750	LDA	CM1-N1-C1	-3.48	102.92	110.23
4	A	756	LDA	CM1-N1-C1	-3.45	102.98	110.23
4	A	749	LDA	CM1-N1-C1	-3.43	103.03	110.23
4	A	744	LDA	CM1-N1-C1	-3.41	103.08	110.23
4	A	751	LDA	CM1-N1-C1	-3.33	103.24	110.23
4	A	755	LDA	CM1-N1-C1	-3.32	103.25	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	747	LDA	CM1-N1-C1	-3.32	103.26	110.23
4	A	748	LDA	CM1-N1-C1	-3.31	103.29	110.23
4	A	754	LDA	CM1-N1-C1	-3.24	103.42	110.23
4	A	752	LDA	CM1-N1-C1	-3.23	103.44	110.23
4	A	743	LDA	CM1-N1-C1	-3.18	103.56	110.23
4	A	757	LDA	O1-N1-C1	3.08	116.84	109.27
3	A	2003	CIT	O7-C3-C4	2.95	116.12	109.38
4	A	753	LDA	O1-N1-C1	2.86	116.28	109.27
4	A	745	LDA	O1-N1-C1	2.84	116.24	109.27
4	A	758	LDA	O1-N1-C1	2.83	116.22	109.27
4	A	744	LDA	O1-N1-C1	2.83	116.20	109.27
4	A	748	LDA	O1-N1-C1	2.81	116.18	109.27
4	A	746	LDA	O1-N1-C1	2.79	116.11	109.27
4	A	754	LDA	O1-N1-C1	2.75	116.01	109.27
4	A	756	LDA	O1-N1-C1	2.74	115.99	109.27
4	A	750	LDA	O1-N1-C1	2.71	115.92	109.27
4	A	749	LDA	O1-N1-C1	2.69	115.87	109.27
4	A	751	LDA	O1-N1-C1	2.68	115.85	109.27
4	A	747	LDA	O1-N1-C1	2.66	115.81	109.27
4	A	755	LDA	O1-N1-C1	2.66	115.81	109.27
4	A	746	LDA	CM2-N1-C1	2.64	115.77	110.23
4	A	752	LDA	O1-N1-C1	2.63	115.73	109.27
4	A	743	LDA	O1-N1-C1	2.61	115.68	109.27
4	A	758	LDA	CM2-N1-C1	2.49	115.47	110.23
4	A	747	LDA	CM2-N1-C1	2.42	115.31	110.23
4	A	749	LDA	CM2-N1-C1	2.39	115.26	110.23
4	A	755	LDA	C9-C8-C7	-2.36	102.42	114.37
4	A	743	LDA	CM2-N1-C1	2.36	115.18	110.23
4	A	745	LDA	CM2-N1-C1	2.34	115.16	110.23
4	A	752	LDA	CM2-N1-C1	2.33	115.13	110.23
4	A	745	LDA	C9-C8-C7	-2.33	102.61	114.37
4	A	751	LDA	CM2-N1-C1	2.31	115.09	110.23
4	A	756	LDA	C9-C8-C7	-2.31	102.69	114.37
4	A	750	LDA	CM2-N1-C1	2.30	115.06	110.23
4	A	757	LDA	CM2-N1-C1	2.28	115.03	110.23
4	A	756	LDA	CM2-N1-C1	2.28	115.03	110.23
4	A	750	LDA	C9-C8-C7	-2.26	102.92	114.37
4	A	754	LDA	C9-C8-C7	-2.26	102.92	114.37
4	A	755	LDA	CM2-N1-C1	2.26	114.98	110.23
3	A	2001	CIT	O7-C3-C4	2.26	114.52	109.38
4	A	757	LDA	C9-C8-C7	-2.24	103.03	114.37
4	A	744	LDA	CM2-N1-C1	2.24	114.94	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	758	LDA	C9-C8-C7	-2.23	103.12	114.37
4	A	747	LDA	C9-C8-C7	-2.21	103.18	114.37
4	A	752	LDA	C9-C8-C7	-2.21	103.19	114.37
4	A	749	LDA	C9-C8-C7	-2.21	103.22	114.37
4	A	753	LDA	CM2-N1-C1	2.20	114.86	110.23
4	A	753	LDA	C9-C8-C7	-2.18	103.36	114.37
4	A	748	LDA	CM2-N1-C1	2.17	114.80	110.23
4	A	743	LDA	C9-C8-C7	-2.15	103.50	114.37
4	A	751	LDA	C9-C8-C7	-2.15	103.51	114.37
4	A	754	LDA	CM2-N1-C1	2.15	114.74	110.23
4	A	746	LDA	C9-C8-C7	-2.13	103.62	114.37
3	A	2003	CIT	O1-C1-C2	-2.09	117.03	122.95
4	A	748	LDA	C9-C8-C7	-2.09	103.81	114.37
3	A	2003	CIT	O7-C3-C2	-2.06	104.67	109.38
4	A	744	LDA	C9-C8-C7	-2.05	104.03	114.37
3	A	2003	CIT	O4-C5-C4	2.03	120.78	114.35

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	757	LDA	C11-C10-C9-C8
4	A	746	LDA	C2-C3-C4-C5
4	A	748	LDA	C11-C10-C9-C8
4	A	750	LDA	C3-C4-C5-C6
4	A	748	LDA	C3-C4-C5-C6
4	A	756	LDA	C4-C5-C6-C7
4	A	757	LDA	C2-C3-C4-C5
4	A	753	LDA	C6-C7-C8-C9
4	A	754	LDA	C2-C3-C4-C5
4	A	755	LDA	C7-C8-C9-C10
4	A	758	LDA	C3-C4-C5-C6
4	A	746	LDA	C3-C4-C5-C6
4	A	753	LDA	C5-C6-C7-C8
4	A	751	LDA	C5-C6-C7-C8
4	A	757	LDA	C7-C8-C9-C10
4	A	746	LDA	C6-C7-C8-C9
4	A	753	LDA	C7-C8-C9-C10
4	A	745	LDA	C5-C6-C7-C8
4	A	753	LDA	C3-C4-C5-C6
4	A	755	LDA	C4-C5-C6-C7
4	A	745	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	758	LDA	C2-C3-C4-C5
4	A	744	LDA	C4-C5-C6-C7
4	A	748	LDA	C6-C7-C8-C9
4	A	752	LDA	C11-C10-C9-C8
4	A	756	LDA	C6-C7-C8-C9
4	A	743	LDA	C5-C6-C7-C8
4	A	756	LDA	C3-C4-C5-C6
4	A	747	LDA	C2-C3-C4-C5
4	A	755	LDA	C11-C10-C9-C8
4	A	758	LDA	C6-C7-C8-C9
4	A	745	LDA	C2-C3-C4-C5
4	A	756	LDA	C5-C6-C7-C8
4	A	745	LDA	C4-C5-C6-C7
4	A	750	LDA	C5-C6-C7-C8
4	A	745	LDA	C7-C8-C9-C10
4	A	744	LDA	C3-C4-C5-C6
4	A	744	LDA	C5-C6-C7-C8
4	A	745	LDA	C1-C2-C3-C4
4	A	756	LDA	C1-C2-C3-C4
4	A	754	LDA	C5-C6-C7-C8
4	A	752	LDA	C3-C4-C5-C6
4	A	753	LDA	C2-C3-C4-C5
4	A	755	LDA	C6-C7-C8-C9
4	A	746	LDA	C1-C2-C3-C4
3	A	2003	CIT	O1-C1-C2-C3
3	A	2003	CIT	O2-C1-C2-C3
4	A	747	LDA	C6-C7-C8-C9
4	A	751	LDA	C3-C4-C5-C6
4	A	747	LDA	C1-C2-C3-C4
4	A	747	LDA	C5-C6-C7-C8
4	A	748	LDA	C5-C6-C7-C8
4	A	743	LDA	C4-C5-C6-C7
4	A	750	LDA	C2-C3-C4-C5
4	A	754	LDA	C3-C4-C5-C6
4	A	750	LDA	C11-C10-C9-C8
4	A	749	LDA	C1-C2-C3-C4
4	A	755	LDA	C1-C2-C3-C4
4	A	754	LDA	C9-C10-C11-C12
4	A	746	LDA	C7-C8-C9-C10
4	A	744	LDA	C11-C10-C9-C8
4	A	751	LDA	C6-C7-C8-C9
4	A	748	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	A	745	LDA	C9-C10-C11-C12
4	A	755	LDA	C9-C10-C11-C12
4	A	748	LDA	C9-C10-C11-C12
4	A	753	LDA	C9-C10-C11-C12
4	A	758	LDA	C9-C10-C11-C12
4	A	754	LDA	C7-C8-C9-C10
4	A	757	LDA	C6-C7-C8-C9
4	A	747	LDA	C3-C4-C5-C6
4	A	747	LDA	C4-C5-C6-C7
4	A	749	LDA	C5-C6-C7-C8
4	A	749	LDA	C4-C5-C6-C7
4	A	749	LDA	C6-C7-C8-C9
4	A	743	LDA	C9-C10-C11-C12
4	A	746	LDA	C5-C6-C7-C8
4	A	755	LDA	C3-C4-C5-C6
4	A	755	LDA	C5-C6-C7-C8
4	A	751	LDA	C11-C10-C9-C8
4	A	743	LDA	C2-C1-N1-CM1
4	A	743	LDA	C2-C1-N1-CM2
4	A	744	LDA	C2-C1-N1-CM1
4	A	744	LDA	C2-C1-N1-CM2
4	A	745	LDA	C2-C1-N1-CM1
4	A	745	LDA	C2-C1-N1-CM2
4	A	746	LDA	C2-C1-N1-CM1
4	A	746	LDA	C2-C1-N1-CM2
4	A	747	LDA	C2-C1-N1-CM1
4	A	747	LDA	C2-C1-N1-CM2
4	A	748	LDA	C2-C1-N1-CM1
4	A	748	LDA	C2-C1-N1-CM2
4	A	749	LDA	C2-C1-N1-CM1
4	A	749	LDA	C2-C1-N1-CM2
4	A	750	LDA	C2-C1-N1-CM1
4	A	750	LDA	C2-C1-N1-CM2
4	A	751	LDA	C2-C1-N1-CM1
4	A	751	LDA	C2-C1-N1-CM2
4	A	752	LDA	C2-C1-N1-CM1
4	A	752	LDA	C2-C1-N1-CM2
4	A	753	LDA	C2-C1-N1-CM1
4	A	753	LDA	C2-C1-N1-CM2
4	A	754	LDA	C2-C1-N1-CM1
4	A	754	LDA	C2-C1-N1-CM2
4	A	755	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
4	A	755	LDA	C2-C1-N1-CM2
4	A	756	LDA	C2-C1-N1-CM1
4	A	756	LDA	C2-C1-N1-CM2
4	A	757	LDA	C2-C1-N1-CM1
4	A	757	LDA	C2-C1-N1-CM2
4	A	758	LDA	C2-C1-N1-CM1
4	A	758	LDA	C2-C1-N1-CM2
4	A	748	LDA	C7-C8-C9-C10
4	A	758	LDA	C7-C8-C9-C10
4	A	758	LDA	C4-C5-C6-C7
4	A	757	LDA	C9-C10-C11-C12
4	A	758	LDA	C11-C10-C9-C8
4	A	743	LDA	C2-C1-N1-O1
4	A	744	LDA	C2-C1-N1-O1
4	A	745	LDA	C2-C1-N1-O1
4	A	746	LDA	C2-C1-N1-O1
4	A	747	LDA	C2-C1-N1-O1
4	A	748	LDA	C2-C1-N1-O1
4	A	749	LDA	C2-C1-N1-O1
4	A	750	LDA	C2-C1-N1-O1
4	A	751	LDA	C2-C1-N1-O1
4	A	752	LDA	C2-C1-N1-O1
4	A	753	LDA	C2-C1-N1-O1
4	A	754	LDA	C2-C1-N1-O1
4	A	755	LDA	C2-C1-N1-O1
4	A	756	LDA	C2-C1-N1-O1
4	A	757	LDA	C2-C1-N1-O1
4	A	758	LDA	C2-C1-N1-O1
4	A	747	LDA	C9-C10-C11-C12
4	A	750	LDA	C9-C10-C11-C12
4	A	755	LDA	C2-C3-C4-C5
4	A	749	LDA	C11-C10-C9-C8
3	A	2001	CIT	C3-C4-C5-O3
3	A	2001	CIT	C3-C4-C5-O4
4	A	756	LDA	C2-C3-C4-C5
4	A	743	LDA	C2-C3-C4-C5
4	A	756	LDA	C7-C8-C9-C10
4	A	750	LDA	C7-C8-C9-C10
4	A	749	LDA	C9-C10-C11-C12
4	A	743	LDA	C3-C4-C5-C6
4	A	750	LDA	C1-C2-C3-C4
4	A	749	LDA	C3-C4-C5-C6

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	CIT	1	0
4	A	758	LDA	1	0
4	A	755	LDA	1	0
4	A	747	LDA	1	0
4	A	757	LDA	1	0
4	A	753	LDA	1	0
4	A	748	LDA	1	0
4	A	743	LDA	1	0
4	A	745	LDA	2	0
4	A	756	LDA	3	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, 95th 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	633/774 (81%)	0.61	62 (9%) 13 11	7, 21, 47, 82	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	GLU	6.5
1	A	694	PRO	5.8
1	A	532	VAL	5.8
1	A	741	PHE	4.8
1	A	526	ALA	4.8
1	A	567	ASP	4.6
1	A	199	GLY	4.5
1	A	697	ALA	4.4
1	A	525	LYS	4.2
1	A	527	VAL	4.0
1	A	693	GLY	4.0
1	A	95	ASN	3.9
1	A	503	ASP	3.8
1	A	568	SER	3.7
1	A	529	SER	3.7
1	A	575	VAL	3.7
1	A	534	PRO	3.6
1	A	515	PHE	3.5
1	A	577	ALA	3.4
1	A	524	GLY	3.4
1	A	255	ASP	3.2
1	A	528	GLN	3.1
1	A	695	GLN	3.1
1	A	427	GLY	3.1
1	A	572	ASN	3.1
1	A	573	ASP	3.0
1	A	548	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	619	GLU	2.8
1	A	699	LEU	2.8
1	A	97	VAL	2.8
1	A	576	THR	2.7
1	A	562	PHE	2.7
1	A	578	ARG	2.6
1	A	428	GLN	2.6
1	A	571	THR	2.6
1	A	564	ASN	2.5
1	A	531	ASN	2.5
1	A	530	GLY	2.4
1	A	569	ASN	2.4
1	A	551	LEU	2.3
1	A	225	ILE	2.3
1	A	566	TYR	2.3
1	A	205	PRO	2.3
1	A	517	THR	2.3
1	A	210	GLY	2.3
1	A	425	SER	2.2
1	A	618	ARG	2.2
1	A	289	TYR	2.2
1	A	579	GLY	2.2
1	A	563	ASN	2.1
1	A	565	GLN	2.1
1	A	110	GLU	2.1
1	A	535	GLU	2.1
1	A	496	ASN	2.1
1	A	206	GLN	2.0
1	A	200	ALA	2.0
1	A	480	THR	2.0
1	A	399	PRO	2.0
1	A	570	GLN	2.0
1	A	296	THR	2.0
1	A	488	TYR	2.0
1	A	514	SER	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, 95th 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($\text{\AA}^2$)	Q<0.9
4	LDA	A	757	16/16	0.59	0.26	39,42,48,49	0
4	LDA	A	753	16/16	0.63	0.24	40,42,54,54	0
4	LDA	A	756	16/16	0.66	0.28	52,53,55,57	0
4	LDA	A	752	16/16	0.68	0.22	45,48,54,54	0
4	LDA	A	745	16/16	0.68	0.25	42,44,51,52	0
4	LDA	A	744	16/16	0.70	0.24	38,44,50,52	0
4	LDA	A	755	16/16	0.70	0.23	39,41,49,50	0
4	LDA	A	754	16/16	0.72	0.21	41,43,47,49	0
4	LDA	A	746	16/16	0.72	0.25	40,44,46,48	0
4	LDA	A	747	16/16	0.73	0.22	34,37,47,48	0
4	LDA	A	758	16/16	0.74	0.22	39,43,48,50	0
4	LDA	A	751	16/16	0.76	0.21	46,49,50,50	0
4	LDA	A	750	16/16	0.76	0.19	30,33,48,48	0
4	LDA	A	748	16/16	0.77	0.19	37,41,44,44	0
4	LDA	A	743	16/16	0.78	0.21	40,45,47,51	0
3	CIT	A	2003	13/13	0.81	0.26	53,55,58,60	0
2	FE	A	2002	1/1	0.82	0.14	58,58,58,58	0
3	CIT	A	2001	13/13	0.82	0.22	51,52,57,58	0
4	LDA	A	749	16/16	0.87	0.16	34,41,54,56	0
2	FE	A	2000	1/1	0.96	0.08	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.