



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 12:35 PM EDT

PDB ID : 1KMP
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

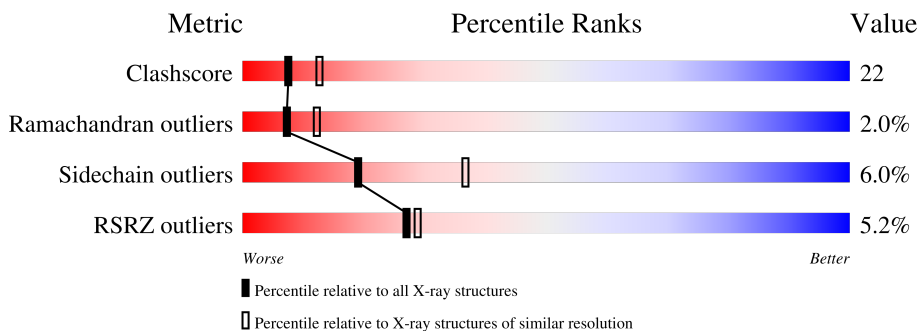
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	

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	LDA	A	753	-	-	-	X
4	LDA	A	757	-	-	-	X

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.

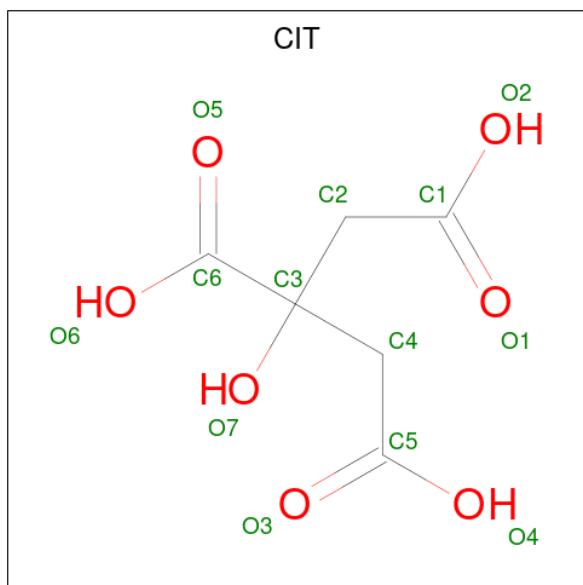
- Molecule 1 is a protein called IRON(III) DICITRATE TRANSPORT PROTEIN FECA.

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

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

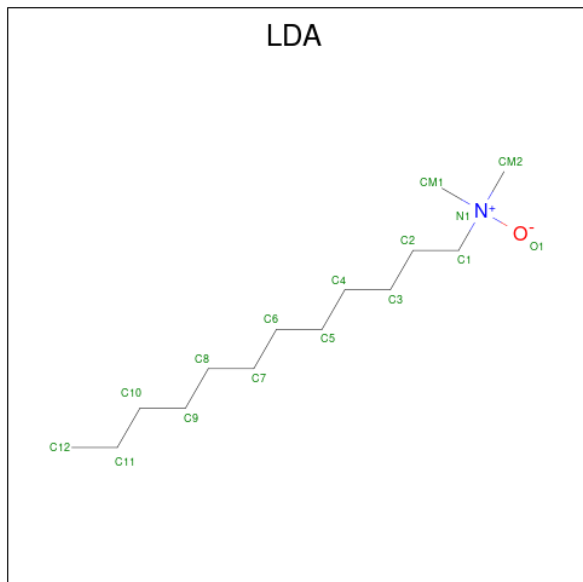
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is CITRIC ACID (three-letter code: 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 (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
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		
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 i

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

• Molecule 1: 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 – 2.49	Depositor EDS
% Data completeness (in resolution range)	86.5 (36.95-2.50) 93.4 (36.95-2.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.48Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.282 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.257	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/5194	0.64	0/7031

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5079	0	4798	236	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	236	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 22.

All (236) 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: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
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:C	1:A:339:LEU:HD23	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HE	1:A:217:ARG:HD3	1.66	0.61
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:695:GLN:CD	1:A:696:MSE:H	2.08	0.56
1:A:225:ILE:CD1	1:A:250:VAL:HG13	2.33	0.56
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: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: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: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:579:GLY:HA3	1:A:619:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:586:LEU:HD23	1:A:586:LEU:C	2.32	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:120:MSE:HE1	1:A:185:SER:C	2.32	0.48
1:A:380:ARG:HG2	1:A:417:GLU:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:249:MSE:HE2	1:A:249:MSE:C	2.34	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:638:LEU:C	1:A:638:LEU:HD12	2.33	0.48
1:A:364:LEU:C	1:A:364:LEU:HD13	2.34	0.47
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
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:190:ASP:OD2	1:A:217:ARG:HA	2.15	0.46
1:A:551:LEU:HD13	1:A:551:LEU:C	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:520:TYR:C	1:A:522:GLN:H	2.21	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:692:PHE:O	1:A:693:GLY:C	2.57	0.42
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:524:GLY:C	1:A:525:LYS:HG3	2.40	0.41
1:A:339:LEU:C	1:A:339:LEU:CD2	2.88	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
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: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: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: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%)	7 12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	GLU
1	A	210	GLY
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 [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	534/621 (86%)	502 (94%)	32 (6%)	19 37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	124	LEU
1	A	147	PHE
1	A	156	LEU
1	A	162	VAL
1	A	190	ASP

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Mol	Chain	Res	Type
1	A	244	GLU
1	A	249	MSE
1	A	337	ARG
1	A	342	LEU
1	A	365	ARG
1	A	385	ARG
1	A	417	GLU
1	A	466	MSE
1	A	475	GLN
1	A	528	GLN
1	A	536	LYS
1	A	559	LEU
1	A	562	PHE
1	A	569	ASN
1	A	570	GLN
1	A	596	THR
1	A	622	ASP
1	A	695	GLN
1	A	698	ASP
1	A	699	LEU
1	A	700	ASN
1	A	701	LEU
1	A	711	GLN
1	A	712	ASP
1	A	723	LYS
1	A	735	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	A	603	ASN
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 monosaccharides 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
4	LDA	A	752	-	12,15,15	2.03	1 (8%)	14,17,17	1.65	4 (28%)
4	LDA	A	748	-	12,15,15	2.09	1 (8%)	14,17,17	1.64	4 (28%)
4	LDA	A	743	-	12,15,15	2.12	1 (8%)	14,17,17	1.62	4 (28%)
4	LDA	A	756	-	12,15,15	2.05	1 (8%)	14,17,17	1.71	4 (28%)
4	LDA	A	758	-	12,15,15	2.09	1 (8%)	14,17,17	1.74	4 (28%)
4	LDA	A	749	-	12,15,15	2.06	1 (8%)	14,17,17	1.69	4 (28%)
4	LDA	A	757	-	12,15,15	1.97	1 (8%)	14,17,17	1.76	4 (28%)
4	LDA	A	754	-	12,15,15	2.05	1 (8%)	14,17,17	1.64	4 (28%)
3	CIT	A	2003	2	12,12,12	1.84	4 (33%)	17,17,17	2.21	7 (41%)

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	2.00	5 (41%)	17,17,17	1.98	3 (17%)
4	LDA	A	747	-	12,15,15	2.08	1 (8%)	14,17,17	1.67	5 (35%)
4	LDA	A	746	-	12,15,15	2.10	1 (8%)	14,17,17	1.75	4 (28%)
4	LDA	A	753	-	12,15,15	1.99	1 (8%)	14,17,17	1.68	4 (28%)
4	LDA	A	755	-	12,15,15	1.92	1 (8%)	14,17,17	1.65	4 (28%)
4	LDA	A	744	-	12,15,15	2.10	1 (8%)	14,17,17	1.65	4 (28%)
4	LDA	A	745	-	12,15,15	2.03	1 (8%)	14,17,17	1.72	4 (28%)
4	LDA	A	750	-	12,15,15	1.96	1 (8%)	14,17,17	1.69	4 (28%)
4	LDA	A	751	-	12,15,15	2.07	1 (8%)	14,17,17	1.64	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
4	LDA	A	752	-	-	5/13/13/13	-
4	LDA	A	748	-	-	10/13/13/13	-
4	LDA	A	743	-	-	8/13/13/13	-
4	LDA	A	756	-	-	10/13/13/13	-
4	LDA	A	758	-	-	10/13/13/13	-
4	LDA	A	749	-	-	10/13/13/13	-
4	LDA	A	757	-	-	8/13/13/13	-
4	LDA	A	754	-	-	8/13/13/13	-
3	CIT	A	2003	2	-	2/16/16/16	-
3	CIT	A	2001	2	-	2/16/16/16	-
4	LDA	A	747	-	-	10/13/13/13	-
4	LDA	A	746	-	-	9/13/13/13	-
4	LDA	A	753	-	-	9/13/13/13	-
4	LDA	A	755	-	-	12/13/13/13	-
4	LDA	A	744	-	-	7/13/13/13	-
4	LDA	A	745	-	-	10/13/13/13	-
4	LDA	A	750	-	-	10/13/13/13	-
4	LDA	A	751	-	-	7/13/13/13	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	743	LDA	O1-N1	-7.00	1.25	1.42
4	A	744	LDA	O1-N1	-6.95	1.25	1.42
4	A	748	LDA	O1-N1	-6.94	1.25	1.42
4	A	746	LDA	O1-N1	-6.94	1.25	1.42
4	A	758	LDA	O1-N1	-6.92	1.26	1.42
4	A	747	LDA	O1-N1	-6.89	1.26	1.42
4	A	756	LDA	O1-N1	-6.89	1.26	1.42
4	A	751	LDA	O1-N1	-6.82	1.26	1.42
4	A	749	LDA	O1-N1	-6.81	1.26	1.42
4	A	754	LDA	O1-N1	-6.77	1.26	1.42
4	A	745	LDA	O1-N1	-6.74	1.26	1.42
4	A	752	LDA	O1-N1	-6.72	1.26	1.42
4	A	757	LDA	O1-N1	-6.56	1.26	1.42
4	A	753	LDA	O1-N1	-6.54	1.26	1.42
4	A	750	LDA	O1-N1	-6.51	1.26	1.42
4	A	755	LDA	O1-N1	-6.30	1.27	1.42
3	A	2001	CIT	C3-C6	4.58	1.58	1.53
3	A	2003	CIT	O7-C3	3.60	1.50	1.43
3	A	2003	CIT	C3-C6	3.37	1.56	1.53
3	A	2001	CIT	O1-C1	2.52	1.30	1.22
3	A	2001	CIT	O7-C3	2.45	1.48	1.43
3	A	2001	CIT	O2-C1	-2.10	1.23	1.30
3	A	2001	CIT	O6-C6	-2.08	1.22	1.30
3	A	2003	CIT	C4-C3	2.07	1.56	1.53
3	A	2003	CIT	O4-C5	-2.04	1.23	1.30

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	CIT	O5-C6-C3	-5.39	114.62	122.25
3	A	2003	CIT	O5-C6-C3	-5.12	115.00	122.25
3	A	2001	CIT	O6-C6-C3	4.45	120.77	113.05
3	A	2003	CIT	O6-C6-C3	3.95	119.91	113.05
4	A	746	LDA	CM1-N1-C1	-3.82	102.21	110.23
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	755	LDA	CM1-N1-C1	-3.32	103.25	110.23
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	2.87	116.12	109.40
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	-2.37	102.42	114.42
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	114.42
4	A	751	LDA	CM2-N1-C1	2.31	115.09	110.23
4	A	756	LDA	C9-C8-C7	-2.31	102.69	114.42
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	-2.27	102.92	114.42
4	A	754	LDA	C9-C8-C7	-2.27	102.92	114.42
4	A	755	LDA	CM2-N1-C1	2.26	114.98	110.23
4	A	757	LDA	C9-C8-C7	-2.24	103.03	114.42
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	114.42
4	A	747	LDA	C9-C8-C7	-2.21	103.18	114.42
4	A	752	LDA	C9-C8-C7	-2.21	103.19	114.42
4	A	749	LDA	C9-C8-C7	-2.21	103.22	114.42
4	A	753	LDA	CM2-N1-C1	2.20	114.86	110.23
3	A	2001	CIT	O7-C3-C4	2.19	114.52	109.40
4	A	753	LDA	C9-C8-C7	-2.18	103.36	114.42
4	A	748	LDA	CM2-N1-C1	2.17	114.80	110.23
4	A	743	LDA	C9-C8-C7	-2.15	103.50	114.42
4	A	751	LDA	C9-C8-C7	-2.15	103.51	114.42
4	A	754	LDA	CM2-N1-C1	2.15	114.74	110.23
4	A	746	LDA	C9-C8-C7	-2.13	103.62	114.42
4	A	748	LDA	C9-C8-C7	-2.09	103.81	114.42
4	A	744	LDA	C9-C8-C7	-2.05	104.03	114.42
3	A	2003	CIT	O1-C1-C2	-2.02	117.03	122.94
3	A	2003	CIT	O7-C3-C2	-2.02	104.67	109.40
3	A	2003	CIT	O7-C3-C6	2.02	111.69	108.86
3	A	2003	CIT	O4-C5-C4	2.00	120.78	114.35
4	A	747	LDA	C6-C5-C4	-2.00	104.26	114.42

There are no chirality outliers.

All (147) torsion outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atoms
4	A	748	LDA	C4-C5-C6-C7
4	A	748	LDA	C9-C10-C11-C12
4	A	749	LDA	C1-C2-C3-C4
4	A	754	LDA	C9-C10-C11-C12
4	A	755	LDA	C9-C10-C11-C12
4	A	758	LDA	C9-C10-C11-C12
4	A	753	LDA	C9-C10-C11-C12
4	A	754	LDA	C3-C4-C5-C6
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	C5-C6-C7-C8
4	A	751	LDA	C11-C10-C9-C8
4	A	755	LDA	C3-C4-C5-C6
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

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Mol	Chain	Res	Type	Atoms
4	A	754	LDA	C2-C1-N1-CM1
4	A	754	LDA	C2-C1-N1-CM2
4	A	755	LDA	C2-C1-N1-CM1
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	757	LDA	C9-C10-C11-C12
4	A	758	LDA	C4-C5-C6-C7
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	755	LDA	C2-C3-C4-C5
4	A	750	LDA	C9-C10-C11-C12
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	749	LDA	C9-C10-C11-C12
4	A	750	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
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
4	A	748	LDA	1	0
4	A	743	LDA	1	0
4	A	756	LDA	3	0
4	A	758	LDA	1	0
4	A	757	LDA	1	0
3	A	2001	CIT	1	0
4	A	747	LDA	1	0
4	A	753	LDA	1	0
4	A	755	LDA	1	0
4	A	745	LDA	2	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%)	0.27	33 (5%) 27 29	7, 21, 47, 82	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	PRO	6.1
1	A	693	GLY	4.8
1	A	697	ALA	4.6
1	A	527	VAL	4.6
1	A	741	PHE	4.5
1	A	526	ALA	4.2
1	A	572	ASN	4.0
1	A	532	VAL	4.0
1	A	503	ASP	4.0
1	A	427	GLY	4.0
1	A	95	ASN	4.0
1	A	695	GLN	4.0
1	A	533	GLU	3.9
1	A	531	ASN	3.7
1	A	425	SER	3.4
1	A	399	PRO	3.3
1	A	428	GLN	3.3
1	A	528	GLN	3.0
1	A	567	ASP	3.0
1	A	529	SER	2.7
1	A	571	THR	2.7
1	A	524	GLY	2.7
1	A	568	SER	2.6
1	A	549	GLY	2.6
1	A	255	ASP	2.6
1	A	221	GLN	2.4
1	A	254	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	222	ASP	2.3
1	A	400	SER	2.2
1	A	534	PRO	2.2
1	A	574	THR	2.2
1	A	525	LYS	2.1
1	A	575	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
4	LDA	A	757	16/16	0.61	0.41	39,42,48,49	0
4	LDA	A	756	16/16	0.64	0.33	52,53,55,57	0
4	LDA	A	753	16/16	0.64	0.44	40,42,54,54	0
4	LDA	A	755	16/16	0.66	0.36	39,41,49,50	0
4	LDA	A	754	16/16	0.70	0.31	41,43,47,49	0
4	LDA	A	752	16/16	0.70	0.33	45,48,54,54	0
4	LDA	A	751	16/16	0.72	0.30	46,49,50,50	0
4	LDA	A	744	16/16	0.74	0.35	38,44,50,52	0
4	LDA	A	746	16/16	0.75	0.34	40,44,46,48	0
4	LDA	A	750	16/16	0.77	0.30	30,33,48,48	0
2	FE	A	2002	1/1	0.79	0.22	58,58,58,58	0
3	CIT	A	2003	13/13	0.79	0.30	53,55,58,60	0
4	LDA	A	747	16/16	0.80	0.30	34,37,47,48	0
3	CIT	A	2001	13/13	0.80	0.29	51,52,57,58	0
4	LDA	A	743	16/16	0.80	0.30	40,45,47,51	0
4	LDA	A	745	16/16	0.81	0.34	42,44,51,52	0
4	LDA	A	748	16/16	0.82	0.38	37,41,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LDA	A	758	16/16	0.83	0.37	39,43,48,50	0
4	LDA	A	749	16/16	0.86	0.28	34,41,54,56	0
2	FE	A	2000	1/1	0.92	0.11	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.