



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 02:41 AM EDT

PDB ID : 1NO3
Title : REFINED STRUCTURE OF SOYBEAN LIPOXYGENASE-3 WITH 4-NITROCATECHOL AT 2.15 ANGSTROM RESOLUTION
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Deposited on : 2003-01-15
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

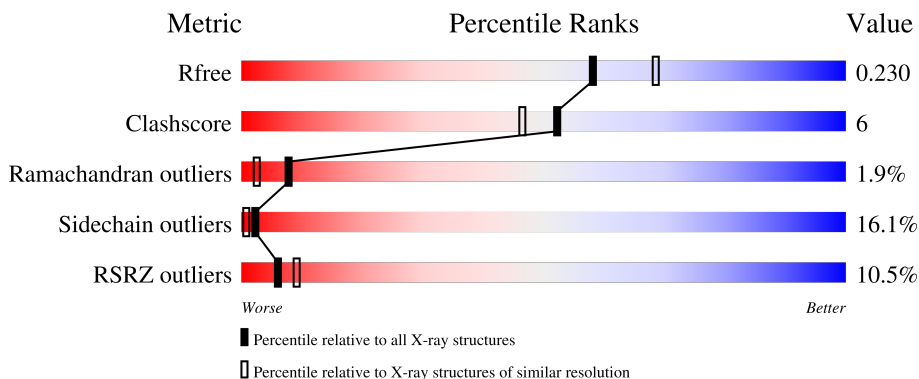
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	857	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7315 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.

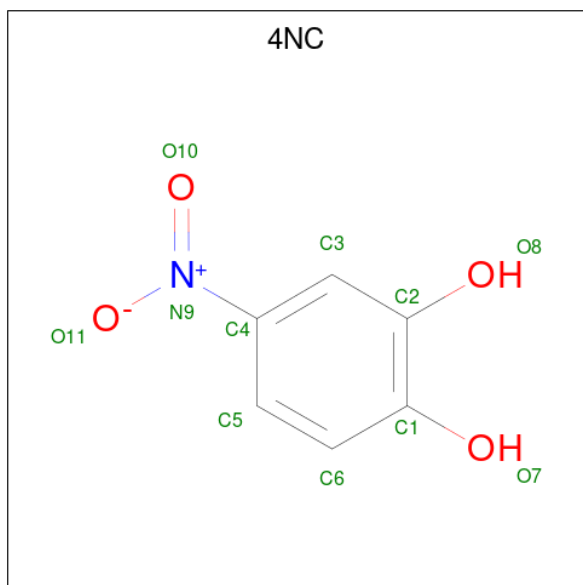
- Molecule 1 is a protein called Lipoxygenase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	851	6809	4347	1173	1271	18	0	1	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 4-NITROCATÉCHOL (three-letter code: 4NC) (formula: C₆H₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	6	1	4	0	0

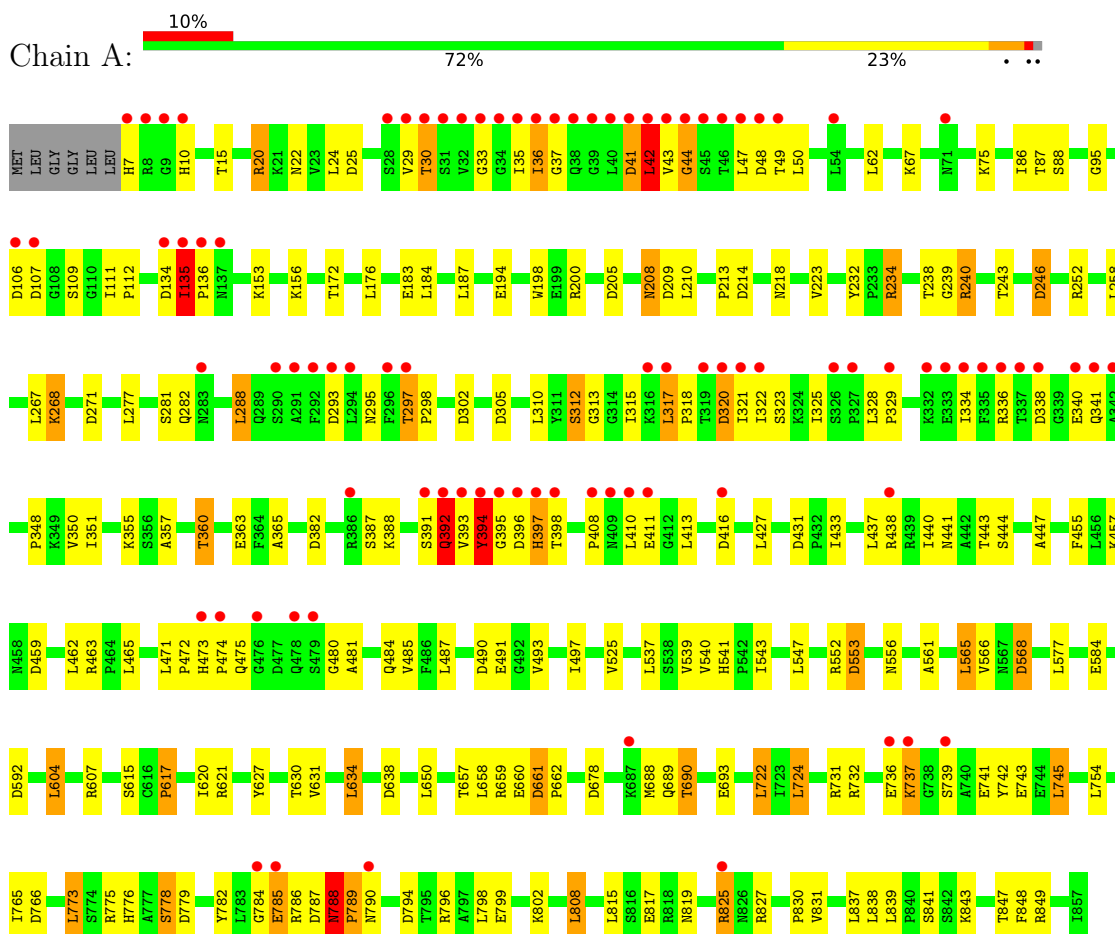
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	494	Total 494	O 494	0	0

3 Residue-property plots i

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

- Molecule 1: Lipoxxygenase-3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.91Å 137.53Å 61.88Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	10.00 – 2.15 10.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (10.00-2.15) 99.1 (10.00-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.15Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.186 , 0.233 0.188 , 0.230	Depositor DCC
R_{free} test set	2543 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7315	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: 4NC, 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	0.71	2/6983 (0.0%)	1.09	50/9483 (0.5%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	394	TYR	CD2-CE2	-6.55	1.29	1.39
1	A	394	TYR	CE2-CZ	-5.41	1.31	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	A	234	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	A	240	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	A	787	ASP	CB-CG-OD2	10.08	127.37	118.30
1	A	607	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	607	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	A	293	ASP	CB-CG-OD2	8.58	126.03	118.30
1	A	205	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	238	THR	C-N-CA	-7.54	106.47	122.30
1	A	246	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	459	ASP	CB-CG-OD2	7.14	124.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	200	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	42	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	37	GLY	N-CA-C	-6.43	97.02	113.10
1	A	592	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	240	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	25	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	214	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	107	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	338	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	305	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	847	THR	C-N-CA	-6.02	106.65	121.70
1	A	724	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	490	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	47	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	678	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	320	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	650	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	722	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	302	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	413	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	794	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	785	GLU	N-CA-C	-5.62	95.83	111.00
1	A	48	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	766	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	790	ASN	N-CA-C	5.45	125.72	111.00
1	A	638	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	584	GLU	CB-CA-C	-5.34	99.72	110.40
1	A	416	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	295	ASN	N-CA-C	5.27	125.23	111.00
1	A	745	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	568	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	779	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	661	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	209	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	848	PHE	CB-CA-C	5.08	120.56	110.40
1	A	553	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	431	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	480	GLY	N-CA-C	5.01	125.63	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ARG	Sidechain

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	6809	0	6727	75	0
2	A	1	0	0	0	0
3	A	11	0	3	1	0
4	A	494	0	0	4	0
All	All	7315	0	6730	75	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 6.

All (75) 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:541:HIS:HD2	1:A:543:ILE:H	1.18	0.89
1:A:785:GLU:OE2	1:A:786:ARG:NH1	2.22	0.73
1:A:773:LEU:HD21	3:A:859:4NC:H6	1.71	0.73
1:A:604:LEU:HD21	1:A:630:THR:HG23	1.71	0.72
1:A:42:LEU:HB3	1:A:95:GLY:H	1.53	0.72
1:A:36:ILE:HB	1:A:268:LYS:HG3	1.74	0.68
1:A:541:HIS:CD2	1:A:543:ILE:H	2.08	0.68
1:A:360:THR:HG22	1:A:363:GLU:H	1.58	0.68
1:A:788:ASN:HB3	1:A:789:PRO:HD3	1.75	0.67
1:A:357:ALA:O	1:A:360:THR:HB	1.98	0.63
1:A:785:GLU:HA	4:A:1041:HOH:O	1.99	0.62
1:A:441:ASN:HD21	1:A:447:ALA:H	1.46	0.62
1:A:194:GLU:HA	1:A:239:GLY:HA3	1.82	0.61
1:A:208:ASN:HD22	1:A:208:ASN:H	1.49	0.61
1:A:243:THR:HG22	1:A:246:ASP:H	1.65	0.60
1:A:784:GLY:HA3	1:A:808:LEU:HD23	1.84	0.59
1:A:825:ARG:HA	1:A:825:ARG:HE	1.68	0.58
1:A:360:THR:HG21	1:A:830:PRO:HG3	1.85	0.58
1:A:20:ARG:NH1	1:A:49:THR:OG1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD2	1:A:778:SER:HB2	2.07	0.55
1:A:819:ASN:ND2	1:A:827:ARG:HE	2.05	0.54
1:A:839:LEU:HD23	1:A:849:ARG:HH11	1.74	0.53
1:A:657:THR:HG21	4:A:993:HOH:O	2.09	0.53
1:A:106:ASP:N	1:A:106:ASP:OD1	2.42	0.52
1:A:394:TYR:HA	1:A:397:HIS:HB3	1.91	0.52
1:A:457:LYS:HE2	1:A:463:ARG:HB2	1.91	0.52
1:A:394:TYR:HB3	1:A:481:ALA:H	1.75	0.51
1:A:33:GLY:HA2	1:A:268:LYS:HG2	1.93	0.51
1:A:213:PRO:HG2	1:A:243:THR:HG21	1.93	0.50
1:A:690:THR:HG22	1:A:693:GLU:H	1.76	0.50
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.92	0.49
1:A:22:ASN:H	1:A:22:ASN:HD22	1.61	0.49
1:A:365:ALA:HB1	1:A:462:LEU:HB3	1.95	0.49
1:A:541:HIS:HE1	1:A:661:ASP:OD2	1.95	0.49
1:A:317:LEU:HB3	1:A:322:ILE:HG12	1.95	0.49
1:A:561:ALA:HA	1:A:565:LEU:HB2	1.95	0.48
1:A:440:ILE:O	1:A:443:THR:OG1	2.32	0.48
1:A:394:TYR:HA	1:A:397:HIS:CB	2.44	0.47
1:A:10:HIS:CD2	1:A:135:ILE:HB	2.50	0.47
1:A:473:HIS:HA	1:A:474:PRO:HD2	1.63	0.46
1:A:776:HIS:NE2	1:A:849:ARG:O	2.43	0.46
1:A:447:ALA:HB2	1:A:577:LEU:HD11	1.97	0.46
1:A:782:TYR:HB2	1:A:786:ARG:HE	1.80	0.46
1:A:825:ARG:HA	1:A:825:ARG:NE	2.31	0.46
1:A:392:GLN:H	1:A:392:GLN:HG2	1.51	0.45
1:A:75:LYS:HB2	1:A:75:LYS:HE2	1.65	0.45
1:A:788:ASN:HD22	1:A:788:ASN:HA	1.40	0.45
1:A:392:GLN:HB2	1:A:394:TYR:HE2	1.81	0.44
1:A:135:ILE:HG23	1:A:136:PRO:HD3	2.00	0.44
1:A:22:ASN:H	1:A:22:ASN:ND2	2.16	0.44
1:A:312:SER:HB2	1:A:313:GLY:H	1.61	0.44
1:A:765:ILE:HD13	1:A:765:ILE:HG21	1.65	0.44
1:A:497:ILE:HD11	1:A:742:TYR:HE2	1.83	0.44
1:A:433:ILE:HG12	1:A:437:LEU:HD13	1.99	0.44
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.80	0.43
1:A:786:ARG:NH2	1:A:841:SER:OG	2.51	0.43
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.94	0.43
1:A:318:PRO:HG2	1:A:321:ILE:HD12	2.00	0.43
1:A:541:HIS:HD2	1:A:543:ILE:N	2.01	0.43
1:A:393:VAL:C	1:A:395:GLY:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HD13	1:A:36:ILE:HA	1.81	0.42
1:A:288:LEU:HD12	1:A:288:LEU:HA	1.74	0.42
1:A:690:THR:HG21	4:A:1147:HOH:O	2.20	0.42
1:A:297:THR:HG21	1:A:315:ILE:HD11	2.01	0.42
1:A:42:LEU:C	1:A:44:GLY:H	2.22	0.42
1:A:297:THR:HA	1:A:298:PRO:HD2	1.74	0.41
1:A:659:ARG:NH1	1:A:689:GLN:O	2.52	0.41
1:A:819:ASN:HD22	1:A:819:ASN:HA	1.71	0.41
1:A:348:PRO:HD2	1:A:351:ILE:HD11	2.03	0.41
1:A:441:ASN:ND2	1:A:447:ALA:H	2.16	0.41
1:A:240:ARG:NH2	4:A:1064:HOH:O	2.48	0.40
1:A:315:ILE:HG21	1:A:315:ILE:HD13	1.79	0.40
1:A:620:ILE:HD11	1:A:634:LEU:HD21	2.03	0.40
1:A:455:PHE:HB2	1:A:465:LEU:HD22	2.03	0.40
1:A:660:GLU:O	1:A:662:PRO:HD3	2.21	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	850/857 (99%)	785 (92%)	49 (6%)	16 (2%)	8 2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
1	A	394	TYR
1	A	408	PRO
1	A	789	PRO
1	A	41	ASP
1	A	42	LEU

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Mol	Chain	Res	Type
1	A	44	GLY
1	A	320	ASP
1	A	392	GLN
1	A	43	VAL
1	A	135	ILE
1	A	788	ASN
1	A	30	THR
1	A	472	PRO
1	A	737	LYS
1	A	617	PRO

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	746/749 (100%)	626 (84%)	120 (16%)	2 1

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	15	THR
1	A	20	ARG
1	A	24	LEU
1	A	29	VAL
1	A	30	THR
1	A	35	ILE
1	A	36	ILE
1	A	41	ASP
1	A	42	LEU
1	A	50	LEU
1	A	62	LEU
1	A	67	LYS
1	A	86	ILE
1	A	87	THR
1	A	88	SER

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Mol	Chain	Res	Type
1	A	109	SER
1	A	134	ASP
1	A	135	ILE
1	A	153	LYS
1	A	156	LYS
1	A	172	THR
1	A	176	LEU
1	A	183	GLU
1	A	184	LEU
1	A	187	LEU
1	A	198	TRP
1	A	208	ASN
1	A	210	LEU
1	A	218	ASN
1	A	223	VAL
1	A	232	TYR
1	A	252	ARG
1	A	258	LEU
1	A	267	LEU
1	A	268	LYS
1	A	277	LEU
1	A	281	SER
1	A	282	GLN
1	A	288	LEU
1	A	297	THR
1	A	310	LEU
1	A	312	SER
1	A	317	LEU
1	A	323	SER
1	A	325	ILE
1	A	328	LEU
1	A	334	ILE
1	A	336	ARG
1	A	340	GLU
1	A	341	GLN
1	A	350	VAL
1	A	355	LYS
1	A	360	THR
1	A	382	ASP
1	A	388	LYS
1	A	391	SER
1	A	392	GLN

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Mol	Chain	Res	Type
1	A	394	TYR
1	A	397	HIS
1	A	398	THR
1	A	410	LEU
1	A	411	GLU
1	A	427	LEU
1	A	438	ARG
1	A	444	SER
1	A	475	GLN
1	A	484	GLN
1	A	485	VAL
1	A	487	LEU
1	A	491	GLU
1	A	493	VAL
1	A	525	VAL
1	A	537	LEU
1	A	539	VAL
1	A	540	VAL
1	A	547	LEU
1	A	552	ARG
1	A	553	ASP
1	A	556	ASN
1	A	565	LEU
1	A	566	VAL
1	A	568	ASP
1	A	604	LEU
1	A	615	SER
1	A	617	PRO
1	A	621	ARG
1	A	627	TYR
1	A	631	VAL
1	A	634	LEU
1	A	658	LEU
1	A	688	MET
1	A	690	THR
1	A	722	LEU
1	A	724	LEU
1	A	731	ARG
1	A	732	ARG
1	A	736	GLU
1	A	737	LYS
1	A	739	SER

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Mol	Chain	Res	Type
1	A	741	GLU
1	A	743	GLU
1	A	745	LEU
1	A	754	LEU
1	A	773	LEU
1	A	775	ARG
1	A	778	SER
1	A	788	ASN
1	A	796	ARG
1	A	798	LEU
1	A	799	GLU
1	A	802	LYS
1	A	808	LEU
1	A	815	LEU
1	A	817	GLU
1	A	825	ARG
1	A	831	VAL
1	A	837	LEU
1	A	838	LEU
1	A	843	LYS

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	22	ASN
1	A	208	ASN
1	A	400	GLN
1	A	441	ASN
1	A	458	ASN
1	A	475	GLN
1	A	521	ASN
1	A	541	HIS
1	A	556	ASN
1	A	574	GLN
1	A	618	HIS
1	A	665	GLN
1	A	725	ASN
1	A	750	GLN
1	A	788	ASN
1	A	790	ASN
1	A	813	ASN
1	A	819	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	4NC	A	859	-	10,11,11	0.94	1 (10%)	13,15,15	1.54	3 (23%)

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	4NC	A	859	-	-	2/2/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	859	4NC	C3-C2	-2.19	1.35	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	859	4NC	C5-C4-N9	3.17	121.76	119.38
3	A	859	4NC	C3-C4-N9	-2.63	116.42	118.75
3	A	859	4NC	C6-C5-C4	-2.05	117.22	120.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	859	4NC	C3-C4-N9-O10
3	A	859	4NC	C5-C4-N9-O10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	859	4NC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	851/857 (99%)	0.29	89 (10%) 6 9	14, 23, 39, 57	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	SER	12.1
1	A	341	GLN	11.4
1	A	35	ILE	9.5
1	A	39	GLY	9.3
1	A	36	ILE	8.5
1	A	294	LEU	8.1
1	A	9	GLY	8.0
1	A	33	GLY	7.9
1	A	8	ARG	7.6
1	A	7	HIS	7.3
1	A	48	ASP	7.3
1	A	395	GLY	7.2
1	A	296	PHE	7.2
1	A	396	ASP	7.1
1	A	44	GLY	6.8
1	A	34	GLY	6.8
1	A	46	THR	6.8
1	A	409	ASN	6.6
1	A	332	LYS	6.5
1	A	32	VAL	6.4
1	A	40	LEU	6.4
1	A	393	VAL	6.3
1	A	43	VAL	5.8
1	A	45	SER	5.6
1	A	49	THR	5.5
1	A	42	LEU	5.2
1	A	47	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	4.8
1	A	337	THR	4.7
1	A	107	ASP	4.5
1	A	391	SER	4.5
1	A	135	ILE	4.5
1	A	137	ASN	4.5
1	A	71	ASN	4.4
1	A	37	GLY	4.3
1	A	394	TYR	4.2
1	A	334	ILE	4.1
1	A	38	GLN	4.1
1	A	739	SER	4.1
1	A	30	THR	3.9
1	A	340	GLU	3.9
1	A	292	PHE	3.9
1	A	338	ASP	3.8
1	A	410	LEU	3.7
1	A	336	ARG	3.7
1	A	333	GLU	3.6
1	A	479	SER	3.6
1	A	784	GLY	3.6
1	A	397	HIS	3.6
1	A	293	ASP	3.5
1	A	398	THR	3.5
1	A	136	PRO	3.4
1	A	408	PRO	3.3
1	A	737	LYS	3.3
1	A	474	PRO	3.2
1	A	438	ARG	3.2
1	A	736	GLU	3.1
1	A	327	PRO	3.1
1	A	790	ASN	3.1
1	A	392	GLN	3.0
1	A	322	ILE	3.0
1	A	785	GLU	2.8
1	A	342	ALA	2.8
1	A	320	ASP	2.7
1	A	54	LEU	2.7
1	A	411	GLU	2.7
1	A	317	LEU	2.7
1	A	329	PRO	2.6
1	A	321	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	28	SER	2.6
1	A	316	LYS	2.6
1	A	10	HIS	2.5
1	A	290	SER	2.5
1	A	283	ASN	2.5
1	A	825	ARG	2.4
1	A	326	SER	2.4
1	A	29	VAL	2.4
1	A	386	ARG	2.3
1	A	319	THR	2.3
1	A	416	ASP	2.3
1	A	106	ASP	2.2
1	A	473	HIS	2.2
1	A	291	ALA	2.2
1	A	297	THR	2.2
1	A	134	ASP	2.2
1	A	335	PHE	2.2
1	A	476	GLY	2.2
1	A	478	GLN	2.0
1	A	687	LYS	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
3	4NC	A	859	11/11	0.76	0.40	34,37,39,40	11
2	FE	A	858	1/1	0.98	0.17	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.