



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:01 PM GMT

PDB ID : 1RRH  
Title : Soybean Lipoxygenase (LOX-3) at ambient temperatures at 2.0 Å resolution  
Authors : Borbulevych, O.Y.; Jankun, J.; Skrzypczak-Jankun, E.  
Deposited on : 2003-12-08  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

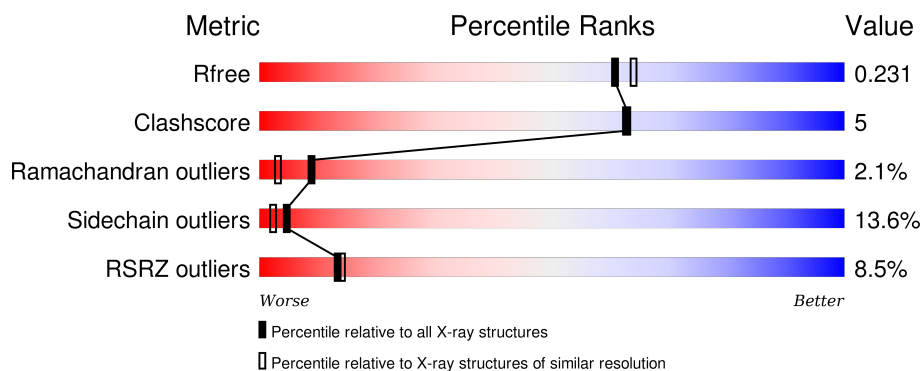
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div>8%</div> <div>75%</div> <div>19%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7339 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 Seed lipoxygenase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6789	4335	1167	1269	18			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	HIS	SEE REMARK 999	UNP P09186
A	57	SER	PRO	SEE REMARK 999	UNP P09186
A	112	PRO	LEU	SEE REMARK 999	UNP P09186
A	201	ILE	VAL	SEE REMARK 999	UNP P09186
A	382	ASP	GLU	SEE REMARK 999	UNP P09186
A	428	ASP	GLY	SEE REMARK 999	UNP P09186
A	630	THR	ALA	SEE REMARK 999	UNP P09186

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

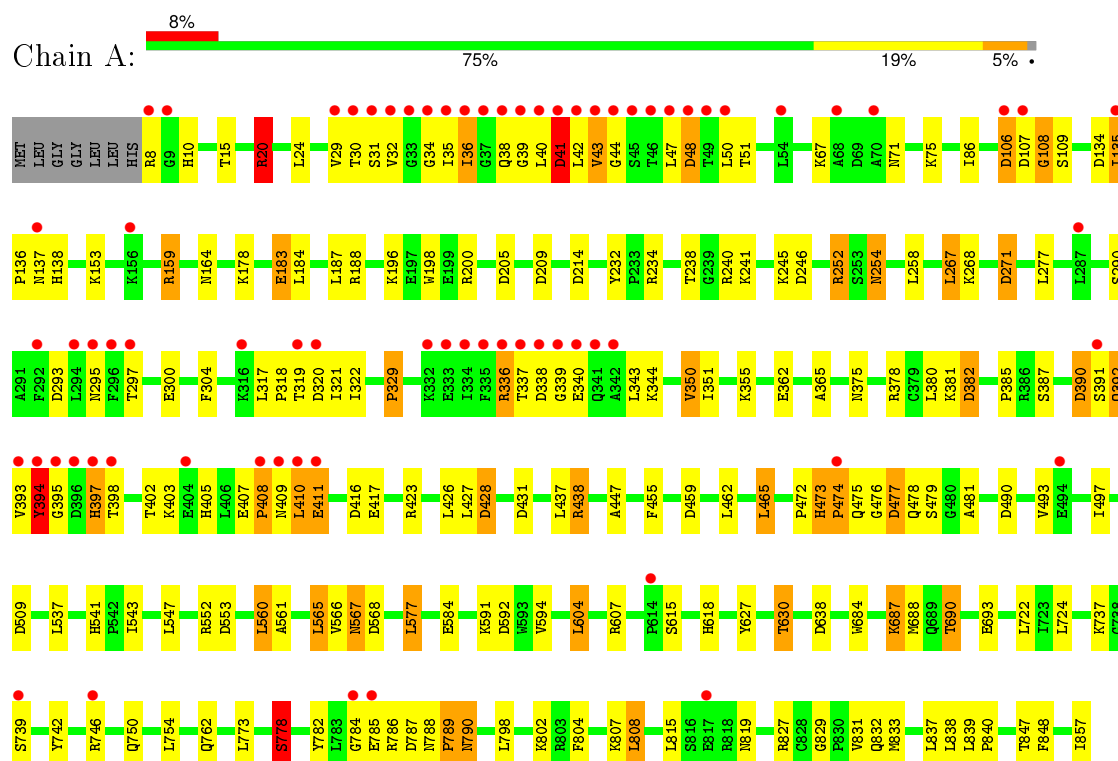
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	549	Total	O	0	0
			549	549		

### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Seed lipoxygenase-3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.71Å 137.21Å 61.79Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.5 (10.00-2.00) 86.5 (10.00-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.231 0.181 , 0.231	Depositor DCC
$R_{free}$ test set	2744 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53997 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FE2

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	0.74	2/6961 (0.0%)	1.07	44/9453 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	394	TYR	CD2-CE2	-8.38	1.26	1.39
1	A	394	TYR	CE2-CZ	-5.54	1.31	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	A	234	ARG	NE-CZ-NH1	11.83	126.22	120.30
1	A	607	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	A	607	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	209	ASP	CB-CG-OD2	9.76	127.08	118.30
1	A	209	ASP	CB-CG-OD1	-9.51	109.74	118.30
1	A	787	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	159	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	238	THR	C-N-CA	-8.12	105.25	122.30
1	A	789	PRO	N-CD-CG	-7.91	91.34	103.20
1	A	459	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	20	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	20	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	847	THR	C-N-CA	-7.36	103.29	121.70
1	A	246	ASP	CB-CG-OD2	7.34	124.90	118.30
1	A	159	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	431	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	293	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	390	ASP	CB-CG-OD2	6.70	124.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	428	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	205	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	778	SER	CB-CA-C	-6.14	98.44	110.10
1	A	490	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	214	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	592	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	416	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	107	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	320	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	477	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	785	GLU	N-CA-C	-5.54	96.03	111.00
1	A	252	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	560	LEU	CA-CB-CG	-5.48	102.70	115.30
1	A	108	GLY	N-CA-C	-5.41	99.58	113.10
1	A	48	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	584	GLU	CB-CA-C	-5.36	99.67	110.40
1	A	848	PHE	CB-CA-C	5.31	121.02	110.40
1	A	200	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	271	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	577	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	A	509	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	790	ASN	CB-CA-C	-5.10	100.20	110.40
1	A	687	LYS	C-N-CA	-5.02	109.14	121.70
1	A	240	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	6789	0	6714	72	0
2	A	1	0	0	0	0
3	A	549	0	0	9	0
All	All	7339	0	6714	72	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 5.

All (72) 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:394:TYR:CD1	1:A:481:ALA:HB2	2.15	0.79
1:A:541:HIS:HD2	1:A:543:ILE:H	1.31	0.78
1:A:438:ARG:NH1	1:A:477:ASP:OD1	2.23	0.71
1:A:36:ILE:HG13	1:A:267:LEU:HB3	1.72	0.71
1:A:784:GLY:HA3	1:A:808:LEU:HD23	1.78	0.64
1:A:438:ARG:HD2	1:A:473:HIS:HE1	1.64	0.61
1:A:473:HIS:HB2	1:A:476:GLY:H	1.68	0.58
1:A:271:ASP:OD2	1:A:778:SER:HB2	2.02	0.58
1:A:319:THR:HA	1:A:322:ILE:HB	1.85	0.57
1:A:394:TYR:HD1	1:A:481:ALA:HB2	1.64	0.57
1:A:560:LEU:HG	1:A:560:LEU:O	2.00	0.57
1:A:618:HIS:ND1	1:A:638:ASP:OD2	2.27	0.57
1:A:567:ASN:H	1:A:567:ASN:HD22	1.53	0.57
1:A:819:ASN:ND2	1:A:827:ARG:HE	2.04	0.56
1:A:394:TYR:HD2	1:A:394:TYR:N	2.04	0.55
1:A:690:THR:HG22	1:A:693:GLU:H	1.72	0.55
1:A:106:ASP:OD1	1:A:106:ASP:N	2.40	0.55
1:A:784:GLY:HA2	1:A:804:PHE:CE2	2.41	0.55
1:A:336:ARG:HB2	1:A:344:LYS:HB2	1.89	0.55
1:A:561:ALA:HA	1:A:565:LEU:HB2	1.87	0.55
1:A:394:TYR:HD2	1:A:394:TYR:H	1.53	0.54
1:A:394:TYR:N	1:A:394:TYR:CD2	2.77	0.52
1:A:392:GLN:HB2	1:A:394:TYR:HE2	1.75	0.51
1:A:393:VAL:HB	3:A:1385:HOH:O	2.11	0.51
1:A:365:ALA:HB1	1:A:462:LEU:HB3	1.94	0.50
1:A:438:ARG:HG2	3:A:1262:HOH:O	2.11	0.50
1:A:20:ARG:HH11	1:A:20:ARG:H	1.61	0.49
1:A:541:HIS:CD2	1:A:543:ILE:H	2.22	0.49
1:A:159:ARG:HA	1:A:159:ARG:HD2	1.63	0.48
1:A:30:THR:HG21	1:A:329:PRO:HB3	1.96	0.48
1:A:782:TYR:H	1:A:786:ARG:HD2	1.78	0.48
1:A:183:GLU:OE1	3:A:1259:HOH:O	2.20	0.48
1:A:407:GLU:HA	1:A:408:PRO:HD3	1.56	0.47
1:A:394:TYR:HA	1:A:397:HIS:HB2	1.97	0.47
1:A:552:ARG:NH1	3:A:1206:HOH:O	2.48	0.47
1:A:497:ILE:HD11	1:A:742:TYR:HE2	1.80	0.47
1:A:408:PRO:HB3	3:A:1375:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.96	0.46
1:A:36:ILE:HG21	1:A:268:LYS:HB2	1.98	0.46
1:A:473:HIS:HA	1:A:474:PRO:HD2	1.88	0.46
1:A:408:PRO:HB2	1:A:409:ASN:H	1.53	0.45
1:A:455:PHE:HB2	1:A:465:LEU:HD22	1.99	0.45
1:A:304:PHE:H	1:A:750:GLN:NE2	2.15	0.44
1:A:438:ARG:HD2	1:A:473:HIS:CE1	2.49	0.44
1:A:447:ALA:HB2	1:A:577:LEU:HD11	1.99	0.44
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.74	0.43
1:A:38:GLN:HB3	1:A:39:GLY:H	1.68	0.43
1:A:378:ARG:NH1	1:A:428:ASP:H	2.16	0.43
1:A:380:LEU:HD11	1:A:385:PRO:HG3	2.00	0.43
1:A:10:HIS:HD2	1:A:135:ILE:HG12	1.83	0.43
1:A:604:LEU:HD11	1:A:630:THR:OG1	2.18	0.43
1:A:36:ILE:HD13	1:A:36:ILE:HA	1.87	0.42
1:A:39:GLY:O	1:A:41:ASP:N	2.52	0.42
1:A:350:VAL:HG13	1:A:351:ILE:HG23	2.01	0.42
1:A:36:ILE:HB	1:A:268:LYS:HG3	2.00	0.42
1:A:402:THR:HG22	1:A:405:HIS:ND1	2.35	0.42
1:A:829:GLY:O	1:A:832:GLN:NE2	2.53	0.42
1:A:788:ASN:HD22	1:A:788:ASN:HA	1.60	0.41
1:A:380:LEU:HD13	1:A:426:LEU:HB2	2.02	0.41
1:A:382:ASP:OD1	1:A:382:ASP:N	2.53	0.41
1:A:338:ASP:HB2	1:A:344:LYS:HE3	2.02	0.41
1:A:784:GLY:HA3	1:A:808:LEU:CD2	2.50	0.41
1:A:411:GLU:HG3	1:A:423:ARG:HH22	1.86	0.41
1:A:136:PRO:O	1:A:138:HIS:N	2.54	0.41
1:A:159:ARG:NE	3:A:1282:HOH:O	2.28	0.41
1:A:318:PRO:HG2	1:A:321:ILE:HD12	2.03	0.41
1:A:594:VAL:HB	1:A:684:TRP:CE2	2.56	0.40
1:A:340:GLU:N	3:A:1323:HOH:O	2.52	0.40
1:A:790:ASN:HA	3:A:1270:HOH:O	2.20	0.40
1:A:403:LYS:NZ	3:A:1347:HOH:O	2.43	0.40
1:A:839:LEU:HA	1:A:840:PRO:HD3	1.86	0.40
1:A:254:ASN:HD22	1:A:254:ASN:HA	1.68	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	848/857 (99%)	792 (93%)	38 (4%)	18 (2%)	9 3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	42	LEU
1	A	43	VAL
1	A	295	ASN
1	A	408	PRO
1	A	789	PRO
1	A	137	ASN
1	A	410	LEU
1	A	737	LYS
1	A	329	PRO
1	A	472	PRO
1	A	108	GLY
1	A	135	ILE
1	A	390	ASP
1	A	44	GLY
1	A	339	GLY
1	A	474	PRO
1	A	34	GLY

### 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	744/749 (99%)	643 (86%)	101 (14%)	5 2

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	15	THR
1	A	20	ARG
1	A	24	LEU
1	A	29	VAL
1	A	31	SER
1	A	32	VAL
1	A	35	ILE
1	A	36	ILE
1	A	41	ASP
1	A	43	VAL
1	A	47	LEU
1	A	48	ASP
1	A	50	LEU
1	A	51	THR
1	A	67	LYS
1	A	71	ASN
1	A	75	LYS
1	A	86	ILE
1	A	106	ASP
1	A	109	SER
1	A	134	ASP
1	A	153	LYS
1	A	164	ASN
1	A	178	LYS
1	A	183	GLU
1	A	184	LEU
1	A	187	LEU
1	A	196	LYS
1	A	198	TRP
1	A	232	TYR
1	A	241	LYS
1	A	245	LYS
1	A	252	ARG
1	A	254	ASN
1	A	258	LEU
1	A	267	LEU
1	A	277	LEU

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Mol	Chain	Res	Type
1	A	290	SER
1	A	297	THR
1	A	300	GLU
1	A	317	LEU
1	A	336	ARG
1	A	337	THR
1	A	343	LEU
1	A	350	VAL
1	A	355	LYS
1	A	362	GLU
1	A	375	ASN
1	A	381	LYS
1	A	382	ASP
1	A	391	SER
1	A	392	GLN
1	A	394	TYR
1	A	397	HIS
1	A	398	THR
1	A	410	LEU
1	A	411	GLU
1	A	417	GLU
1	A	427	LEU
1	A	437	LEU
1	A	438	ARG
1	A	465	LEU
1	A	473	HIS
1	A	475	GLN
1	A	478	GLN
1	A	479	SER
1	A	493	VAL
1	A	537	LEU
1	A	547	LEU
1	A	553	ASP
1	A	565	LEU
1	A	566	VAL
1	A	567	ASN
1	A	568	ASP
1	A	591	LYS
1	A	604	LEU
1	A	615	SER
1	A	627	TYR
1	A	630	THR

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Mol	Chain	Res	Type
1	A	687	LYS
1	A	688	MET
1	A	690	THR
1	A	722	LEU
1	A	724	LEU
1	A	739	SER
1	A	746	ARG
1	A	754	LEU
1	A	762	GLN
1	A	773	LEU
1	A	778	SER
1	A	798	LEU
1	A	802	LYS
1	A	807	LYS
1	A	808	LEU
1	A	815	LEU
1	A	831	VAL
1	A	833	MET
1	A	837	LEU
1	A	838	LEU
1	A	857	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	22	ASN
1	A	137	ASN
1	A	164	ASN
1	A	254	ASN
1	A	282	GLN
1	A	295	ASN
1	A	375	ASN
1	A	421	ASN
1	A	458	ASN
1	A	473	HIS
1	A	478	GLN
1	A	521	ASN
1	A	541	HIS
1	A	567	ASN
1	A	574	GLN
1	A	750	GLN

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Mol	Chain	Res	Type
1	A	762	GLN
1	A	788	ASN
1	A	806	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	850/857 (99%)	0.09	72 (8%) 13 14	11, 21, 45, 65	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	10.9
1	A	32	VAL	10.1
1	A	393	VAL	10.1
1	A	33	GLY	9.6
1	A	395	GLY	8.9
1	A	46	THR	8.8
1	A	341	GLN	7.9
1	A	49	THR	7.7
1	A	40	LEU	7.7
1	A	9	GLY	7.4
1	A	31	SER	7.2
1	A	396	ASP	7.1
1	A	35	ILE	7.0
1	A	36	ILE	6.9
1	A	409	ASN	6.6
1	A	39	GLY	6.4
1	A	42	LEU	6.1
1	A	8	ARG	6.0
1	A	107	ASP	5.7
1	A	135	ILE	5.3
1	A	47	LEU	5.2
1	A	48	ASP	5.2
1	A	137	ASN	5.1
1	A	43	VAL	5.1
1	A	45	SER	4.9
1	A	333	GLU	4.8
1	A	410	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	394	TYR	4.7
1	A	296	PHE	4.6
1	A	41	ASP	4.6
1	A	397	HIS	4.5
1	A	44	GLY	4.5
1	A	337	THR	4.4
1	A	297	THR	4.0
1	A	294	LEU	4.0
1	A	342	ALA	3.7
1	A	338	ASP	3.6
1	A	332	LYS	3.6
1	A	156	LYS	3.6
1	A	408	PRO	3.5
1	A	474	PRO	3.5
1	A	391	SER	3.4
1	A	316	LYS	3.4
1	A	339	GLY	3.1
1	A	411	GLU	3.1
1	A	29	VAL	3.0
1	A	739	SER	3.0
1	A	336	ARG	2.9
1	A	340	GLU	2.8
1	A	54	LEU	2.7
1	A	746	ARG	2.7
1	A	398	THR	2.7
1	A	320	ASP	2.6
1	A	37	GLY	2.6
1	A	50	LEU	2.4
1	A	404	GLU	2.4
1	A	334	ILE	2.4
1	A	292	PHE	2.4
1	A	784	GLY	2.3
1	A	785	GLU	2.3
1	A	614	PRO	2.2
1	A	70	ALA	2.2
1	A	68	ALA	2.2
1	A	106	ASP	2.2
1	A	38	GLN	2.2
1	A	319	THR	2.2
1	A	335	PHE	2.2
1	A	817	GLU	2.2
1	A	494	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	287	LEU	2.0
1	A	30	THR	2.0
1	A	295	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	A	858	1/1	0.98	0.07	-1.36	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.