



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 05:04 PM EDT

PDB ID : 7TTL
Title : Stable-5-LOX elongated Ha2 (4 copies ASU)
Authors : Gilbert, N.C.; Newcomer, M.E.
Deposited on : 2022-02-01
Resolution : 2.43 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
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
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

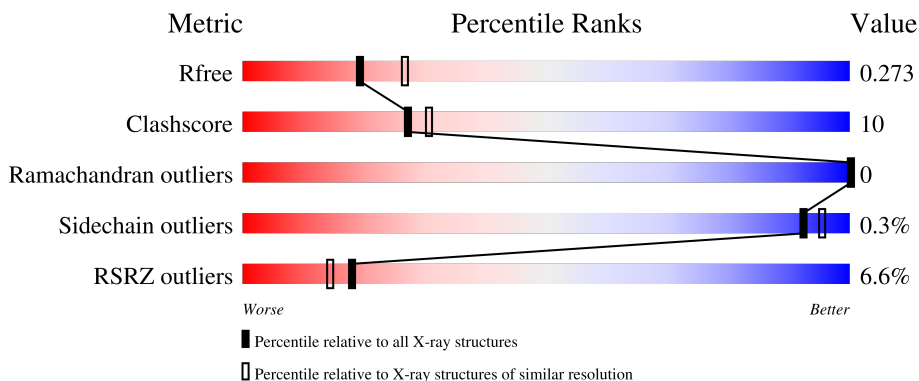
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	691	 4% 77% 20%
1	B	691	 % 76% 17% 7%
1	C	691	 7% 72% 17% 11%
1	D	691	 13% 75% 22%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 42420 atoms, of which 20733 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 Arachidonate 5-lipoxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	674	10837	3509	5354	932	1014	28	0	2	0
1	C	617	9902	3199	4904	849	929	21	0	1	0
1	D	673	10823	3507	5345	933	1011	27	0	1	0
1	B	643	10378	3368	5130	887	970	23	0	0	0

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP P09917
A	-13	GLY	-	expression tag	UNP P09917
A	-12	SER	-	expression tag	UNP P09917
A	-11	SER	-	expression tag	UNP P09917
A	-10	HIS	-	expression tag	UNP P09917
A	-9	HIS	-	expression tag	UNP P09917
A	-8	HIS	-	expression tag	UNP P09917
A	-7	HIS	-	expression tag	UNP P09917
A	-6	HIS	-	expression tag	UNP P09917
A	-6A	HIS	-	expression tag	UNP P09917
A	-6B	SER	-	expression tag	UNP P09917
A	-6C	SER	-	expression tag	UNP P09917
A	-6D	GLY	-	expression tag	UNP P09917
A	-6E	LEU	-	expression tag	UNP P09917
A	-6F	VAL	-	expression tag	UNP P09917
A	-6G	PRO	-	expression tag	UNP P09917
A	-6H	ARG	-	expression tag	UNP P09917
A	-6I	GLY	-	expression tag	UNP P09917
A	-6J	SER	-	expression tag	UNP P09917
A	-6K	HIS	-	expression tag	UNP P09917
A	16	GLU	TRP	conflict	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	HIS	PHE	conflict	UNP P09917
A	?	-	PRO	deletion	UNP P09917
A	?	-	PHE	deletion	UNP P09917
A	?	-	TYR	deletion	UNP P09917
A	43	GLY	ASN	conflict	UNP P09917
A	44	SER	ASP	conflict	UNP P09917
A	75	GLY	TRP	conflict	UNP P09917
A	76	SER	LEU	conflict	UNP P09917
A	240	ALA	CYS	conflict	UNP P09917
A	561	ALA	CYS	conflict	UNP P09917
A	653	GLU	LYS	conflict	UNP P09917
A	654	ASN	LYS	conflict	UNP P09917
A	655	LEU	LYS	conflict	UNP P09917
C	-17	MET	-	initiating methionine	UNP P09917
C	-16	GLY	-	expression tag	UNP P09917
C	-15	SER	-	expression tag	UNP P09917
C	-14	SER	-	expression tag	UNP P09917
C	-13	HIS	-	expression tag	UNP P09917
C	-12	HIS	-	expression tag	UNP P09917
C	-11	HIS	-	expression tag	UNP P09917
C	-10	HIS	-	expression tag	UNP P09917
C	-9	HIS	-	expression tag	UNP P09917
C	-8	HIS	-	expression tag	UNP P09917
C	-7	SER	-	expression tag	UNP P09917
C	-6	SER	-	expression tag	UNP P09917
C	-5	GLY	-	expression tag	UNP P09917
C	-4	LEU	-	expression tag	UNP P09917
C	-3	VAL	-	expression tag	UNP P09917
C	-2	PRO	-	expression tag	UNP P09917
C	-1	ARG	-	expression tag	UNP P09917
C	0	GLY	-	expression tag	UNP P09917
C	1	SER	-	expression tag	UNP P09917
C	2	HIS	-	expression tag	UNP P09917
C	16	GLU	TRP	conflict	UNP P09917
C	17	HIS	PHE	conflict	UNP P09917
C	?	-	PRO	deletion	UNP P09917
C	?	-	PHE	deletion	UNP P09917
C	?	-	TYR	deletion	UNP P09917
C	43	GLY	ASN	conflict	UNP P09917
C	44	SER	ASP	conflict	UNP P09917
C	75	GLY	TRP	conflict	UNP P09917
C	76	SER	LEU	conflict	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
C	240	ALA	CYS	conflict	UNP P09917
C	561	ALA	CYS	conflict	UNP P09917
C	653	GLU	LYS	conflict	UNP P09917
C	654	ASN	LYS	conflict	UNP P09917
C	655	LEU	LYS	conflict	UNP P09917
D	-15	MET	-	initiating methionine	UNP P09917
D	-14	GLY	-	expression tag	UNP P09917
D	-13	SER	-	expression tag	UNP P09917
D	-12	SER	-	expression tag	UNP P09917
D	-11	HIS	-	expression tag	UNP P09917
D	-10	HIS	-	expression tag	UNP P09917
D	-9	HIS	-	expression tag	UNP P09917
D	-8	HIS	-	expression tag	UNP P09917
D	-7	HIS	-	expression tag	UNP P09917
D	-6	HIS	-	expression tag	UNP P09917
D	-6A	SER	-	expression tag	UNP P09917
D	-6B	SER	-	expression tag	UNP P09917
D	-6C	GLY	-	expression tag	UNP P09917
D	-6D	LEU	-	expression tag	UNP P09917
D	-6E	VAL	-	expression tag	UNP P09917
D	-6F	PRO	-	expression tag	UNP P09917
D	-6G	ARG	-	expression tag	UNP P09917
D	-6H	GLY	-	expression tag	UNP P09917
D	-6I	SER	-	expression tag	UNP P09917
D	-6J	HIS	-	expression tag	UNP P09917
D	16	GLU	TRP	conflict	UNP P09917
D	17	HIS	PHE	conflict	UNP P09917
D	?	-	PRO	deletion	UNP P09917
D	?	-	PHE	deletion	UNP P09917
D	?	-	TYR	deletion	UNP P09917
D	43	GLY	ASN	conflict	UNP P09917
D	44	SER	ASP	conflict	UNP P09917
D	75	GLY	TRP	conflict	UNP P09917
D	76	SER	LEU	conflict	UNP P09917
D	240	ALA	CYS	conflict	UNP P09917
D	561	ALA	CYS	conflict	UNP P09917
D	653	GLU	LYS	conflict	UNP P09917
D	654	ASN	LYS	conflict	UNP P09917
D	655	LEU	LYS	conflict	UNP P09917
B	-17	MET	-	initiating methionine	UNP P09917
B	-16	GLY	-	expression tag	UNP P09917
B	-15	SER	-	expression tag	UNP P09917

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	SER	-	expression tag	UNP P09917
B	-13	HIS	-	expression tag	UNP P09917
B	-12	HIS	-	expression tag	UNP P09917
B	-11	HIS	-	expression tag	UNP P09917
B	-10	HIS	-	expression tag	UNP P09917
B	-9	HIS	-	expression tag	UNP P09917
B	-8	HIS	-	expression tag	UNP P09917
B	-7	SER	-	expression tag	UNP P09917
B	-6	SER	-	expression tag	UNP P09917
B	-5	GLY	-	expression tag	UNP P09917
B	-4	LEU	-	expression tag	UNP P09917
B	-3	VAL	-	expression tag	UNP P09917
B	-2	PRO	-	expression tag	UNP P09917
B	-1	ARG	-	expression tag	UNP P09917
B	0	GLY	-	expression tag	UNP P09917
B	1	SER	-	expression tag	UNP P09917
B	2	HIS	-	expression tag	UNP P09917
B	16	GLU	TRP	conflict	UNP P09917
B	17	HIS	PHE	conflict	UNP P09917
B	?	-	PRO	deletion	UNP P09917
B	?	-	PHE	deletion	UNP P09917
B	?	-	TYR	deletion	UNP P09917
B	43	GLY	ASN	conflict	UNP P09917
B	44	SER	ASP	conflict	UNP P09917
B	75	GLY	TRP	conflict	UNP P09917
B	76	SER	LEU	conflict	UNP P09917
B	240	ALA	CYS	conflict	UNP P09917
B	561	ALA	CYS	conflict	UNP P09917
B	653	GLU	LYS	conflict	UNP P09917
B	654	ASN	LYS	conflict	UNP P09917
B	655	LEU	LYS	conflict	UNP P09917

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

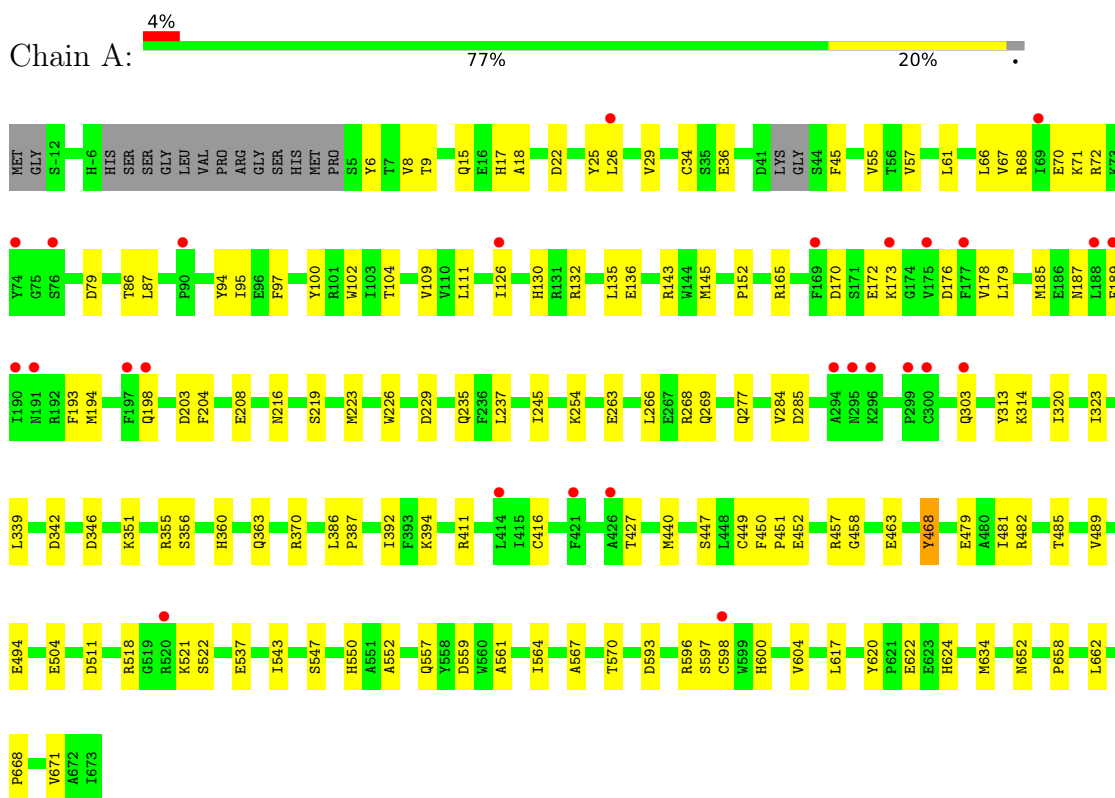
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		
3	C	82	Total	O	0	0
			82	82		
3	D	77	Total	O	0	0
			77	77		
3	B	156	Total	O	0	0
			156	156		

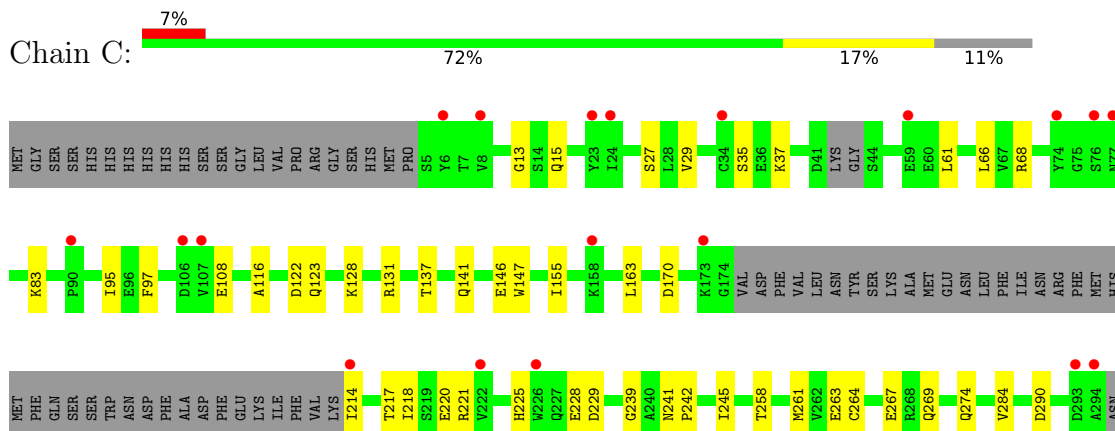
3 Residue-property plots i

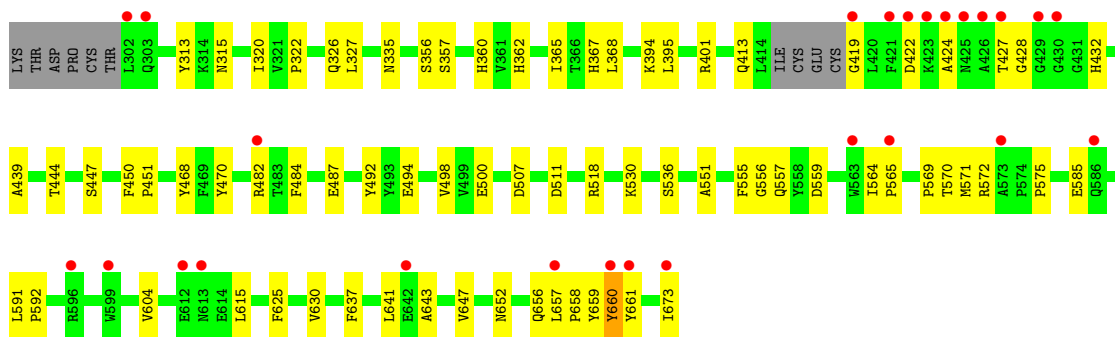
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arachidonate 5-lipoxygenase

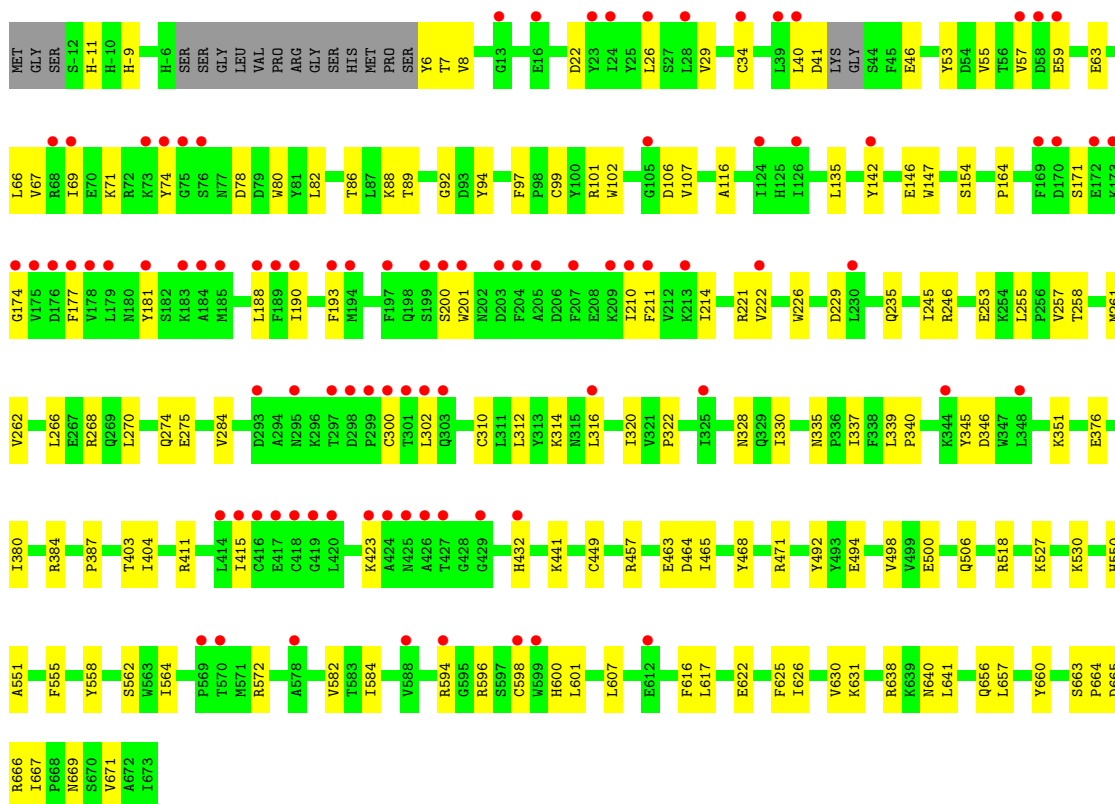
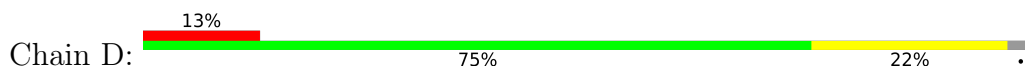


• Molecule 1: Arachidonate 5-lipoxygenase

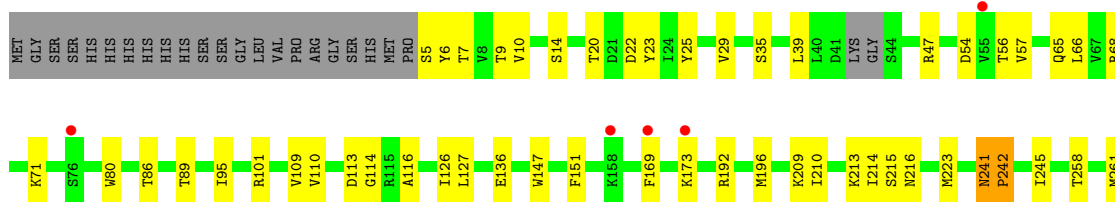
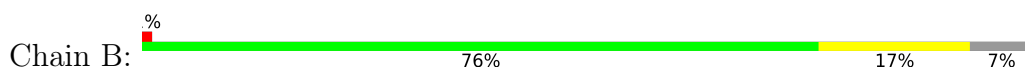


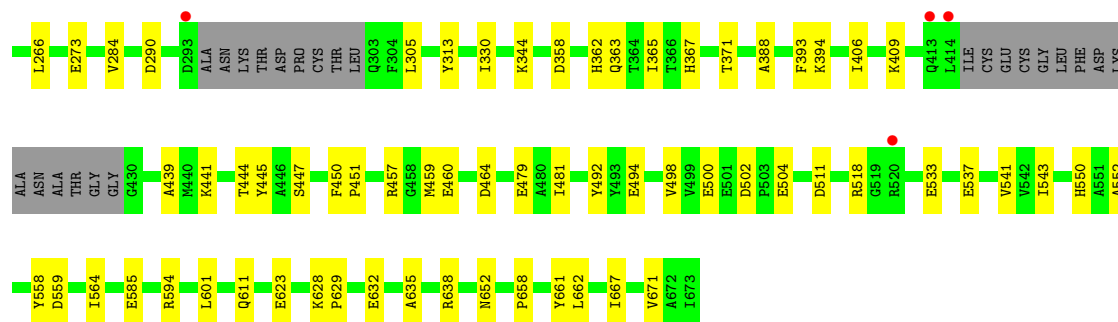


● Molecule 1: Arachidonate 5-lipoxygenase



● Molecule 1: Arachidonate 5-lipoxygenase





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.79Å 204.55Å 106.77Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	102.27 – 2.43 102.27 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.7 (102.27-2.43) 78.3 (102.27-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.215 , 0.275 0.215 , 0.273	Depositor DCC
R_{free} test set	1851 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtrriage
Anisotropy	0.854	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	42420	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6466e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.73	3/5629 (0.1%)	0.81	1/7636 (0.0%)
1	B	0.75	5/5380 (0.1%)	0.80	2/7297 (0.0%)
1	C	0.64	0/5122	0.75	0/6949
1	D	0.64	2/5622 (0.0%)	0.75	0/7627
All	All	0.69	10/21753 (0.0%)	0.78	3/29509 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	PRO	N-CA	12.85	1.69	1.47
1	D	449	CYS	CB-SG	5.97	1.92	1.82
1	A	449	CYS	CB-SG	5.80	1.92	1.82
1	A	452	GLU	CG-CD	5.77	1.60	1.51
1	B	241	ASN	C-N	5.62	1.45	1.34
1	A	463	GLU	CG-CD	5.45	1.60	1.51
1	D	102	TRP	CB-CG	-5.44	1.40	1.50
1	B	136	GLU	CG-CD	5.39	1.60	1.51
1	B	445	TYR	CD2-CE2	-5.16	1.31	1.39
1	B	533	GLU	CG-CD	5.11	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASP	CB-CG-OD2	6.94	124.55	118.30
1	B	242	PRO	CA-N-CD	-6.48	102.43	111.50
1	B	464	ASP	CB-CG-OD1	5.06	122.86	118.30

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	5483	5354	5355	109	0
1	B	5248	5130	5135	100	0
1	C	4998	4904	4904	100	0
1	D	5478	5345	5347	123	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	161	0	0	25	0
3	B	156	0	0	20	0
3	C	82	0	0	13	0
3	D	77	0	0	20	0
All	All	21687	20733	20741	425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PRO:N	1:B:242:PRO:CA	1.69	1.37
1:B:192:ARG:O	1:B:196:MET:CE	2.00	1.09
1:D:34[B]:CYS:SG	3:D:868:HOH:O	2.19	0.98
1:B:500:GLU:OE1	3:B:801:HOH:O	1.87	0.91
1:B:367:HIS:O	1:B:371:THR:HG22	1.70	0.91
1:C:487:GLU:OE2	3:C:801:HOH:O	1.86	0.91
1:B:192:ARG:O	1:B:196:MET:HE3	1.71	0.90
1:C:660:TYR:OH	3:C:802:HOH:O	1.89	0.89
1:A:518:ARG:NH1	1:C:290:ASP:OD2	2.05	0.88
1:B:10:VAL:O	3:B:802:HOH:O	1.92	0.87
1:A:8:VAL:HG11	1:A:26:LEU:CD2	2.05	0.86
1:B:504:GLU:OE2	3:B:803:HOH:O	1.95	0.84
1:D:403:THR:OG1	3:D:801:HOH:O	1.94	0.84
1:C:482:ARG:NH1	1:C:536:SER:OG	2.10	0.83
1:A:9:THR:CG2	1:A:86:THR:HB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ASP:HA	1:D:74:TYR:HB3	1.61	0.80
1:B:147:TRP:CD1	3:B:810:HOH:O	2.34	0.80
1:B:216:ASN:ND2	3:B:811:HOH:O	2.16	0.79
1:B:173:LYS:NZ	1:B:611:GLN:OE1	2.16	0.78
1:B:192:ARG:O	1:B:196:MET:HE1	1.84	0.78
1:B:147:TRP:NE1	3:B:810:HOH:O	2.15	0.77
1:A:356:SER:OG	3:A:802:HOH:O	2.02	0.76
1:A:198:GLN:OE1	3:A:803:HOH:O	2.02	0.76
1:D:246:ARG:NH2	3:D:809:HOH:O	2.17	0.74
1:B:661:TYR:O	3:B:804:HOH:O	2.06	0.73
1:D:640:ASN:O	3:D:805:HOH:O	2.07	0.73
1:A:34[A]:CYS:SG	1:A:68:ARG:NH1	2.63	0.71
1:B:479:GLU:OE1	3:B:805:HOH:O	2.06	0.71
1:D:527:LYS:NZ	3:D:804:HOH:O	2.05	0.71
1:C:394:LYS:C	1:C:625:PHE:HE2	1.95	0.71
1:D:270:LEU:O	3:D:807:HOH:O	2.09	0.71
1:B:552:ALA:O	3:B:806:HOH:O	2.08	0.71
1:A:537:GLU:OE2	3:A:806:HOH:O	2.09	0.70
1:A:458:GLY:O	3:A:805:HOH:O	2.09	0.70
1:D:63:GLU:OE2	3:D:806:HOH:O	2.08	0.70
1:A:130:HIS:ND1	3:A:801:HOH:O	1.98	0.70
1:A:9:THR:HG23	1:A:86:THR:HB	1.74	0.69
1:C:27:SER:OG	1:C:37:LYS:HG2	1.92	0.69
1:A:303:GLN:OE1	1:A:570:THR:OG1	2.03	0.69
1:D:146:GLU:OE2	1:D:518:ARG:NH2	2.22	0.69
1:C:427:THR:O	1:C:432:HIS:N	2.26	0.68
1:B:623:GLU:O	3:B:807:HOH:O	2.11	0.68
1:A:193:PHE:HB2	1:A:598[B]:CYS:SG	2.34	0.68
1:B:29:VAL:HB	1:B:66:LEU:HB2	1.75	0.68
1:A:269:GLN:NE2	3:A:819:HOH:O	2.27	0.67
1:B:215:SER:O	3:B:808:HOH:O	2.12	0.67
1:B:169:PHE:HZ	1:B:406:ILE:HD13	1.61	0.66
1:D:26:LEU:HD12	1:D:69:ILE:HD11	1.78	0.66
1:A:504:GLU:OE1	3:A:807:HOH:O	2.12	0.66
1:C:357:SER:OG	3:C:804:HOH:O	2.14	0.65
1:C:367:HIS:HE1	3:C:807:HOH:O	1.78	0.65
1:D:193:PHE:HB2	1:D:598:CYS:SG	2.35	0.65
1:C:394:LYS:CB	1:C:625:PHE:CE2	2.80	0.65
1:D:201:TRP:CH2	1:D:210:ILE:HD13	2.31	0.65
1:D:669:ASN:HB2	3:D:839:HOH:O	1.96	0.65
1:C:394:LYS:C	1:C:625:PHE:CE2	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ARG:NH2	1:C:108:GLU:OE2	2.29	0.64
1:A:216:ASN:H	1:A:219:SER:HG	1.46	0.64
1:A:552:ALA:HB2	1:A:662:LEU:HD21	1.80	0.64
1:D:41:ASP:N	3:D:808:HOH:O	2.11	0.64
1:A:86:THR:HG21	1:A:94:TYR:CE1	2.32	0.64
1:B:358:ASP:OD1	3:B:809:HOH:O	2.15	0.64
1:C:95:ILE:HG22	1:C:97:PHE:CE2	2.33	0.64
1:C:95:ILE:CG2	1:C:97:PHE:CE2	2.81	0.63
1:A:363:GLN:NE2	1:A:557:GLN:OE1	2.29	0.62
1:A:617:LEU:O	3:A:808:HOH:O	2.16	0.62
1:A:518:ARG:NH2	3:A:818:HOH:O	2.26	0.62
1:D:314:LYS:HD2	1:D:464:ASP:O	2.00	0.62
1:D:518:ARG:NH1	1:B:290:ASP:OD1	2.32	0.62
1:A:26:LEU:HD11	1:A:67:VAL:HG13	1.81	0.62
1:D:494:GLU:HG2	1:D:498:VAL:HG21	1.81	0.62
1:A:8:VAL:HG11	1:A:26:LEU:HD21	1.81	0.61
1:D:246:ARG:NH1	3:D:813:HOH:O	2.25	0.61
1:D:660:TYR:O	1:D:666:ARG:HD3	1.99	0.61
1:D:270:LEU:N	3:D:807:HOH:O	2.34	0.61
1:C:643:ALA:O	1:C:647:VAL:HG13	2.01	0.60
1:D:190:ILE:HG22	1:D:190:ILE:O	2.02	0.60
1:A:86:THR:HG21	1:A:94:TYR:CZ	2.36	0.60
1:A:518:ARG:NE	3:A:818:HOH:O	2.30	0.60
1:D:80:TRP:CZ3	1:D:82:LEU:HD12	2.37	0.60
1:A:593:ASP:OD2	1:A:596:ARG:NH1	2.31	0.60
1:C:395:LEU:N	1:C:625:PHE:HE2	1.99	0.60
1:C:625:PHE:CD1	1:C:630:VAL:HG21	2.37	0.60
1:D:258:THR:HG22	1:D:261:MET:SD	2.42	0.59
1:B:213:LYS:O	1:B:214:ILE:HD13	2.02	0.59
1:A:235:GLN:NE2	3:A:810:HOH:O	2.18	0.59
1:A:237:LEU:HD11	1:A:320:ILE:HD12	1.84	0.59
1:C:572:ARG:HD3	1:C:591:LEU:O	2.03	0.59
1:B:35:SER:HB2	1:B:57:VAL:HG11	1.83	0.59
1:A:593:ASP:O	1:A:597:SER:OG	2.19	0.59
1:A:17:HIS:O	3:A:809:HOH:O	2.17	0.59
1:C:263:GLU:O	3:C:805:HOH:O	2.17	0.59
1:C:394:LYS:HB2	1:C:625:PHE:CZ	2.38	0.59
1:D:190:ILE:HG23	1:D:193:PHE:HD2	1.66	0.59
1:A:550:HIS:NE2	1:A:671:VAL:HG13	2.18	0.58
1:C:559:ASP:OD2	1:C:661:TYR:OH	2.19	0.58
1:A:356:SER:O	1:A:360:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:ILE:HD13	1:D:600:HIS:CD2	2.38	0.58
1:C:274:GLN:NE2	3:C:803:HOH:O	1.97	0.58
1:A:102:TRP:CG	1:A:165:ARG:HG3	2.39	0.58
1:D:6:TYR:N	1:D:55:VAL:O	2.37	0.58
1:B:564:ILE:HD11	1:B:601:LEU:HD21	1.86	0.58
1:A:79:ASP:OD1	1:A:104:THR:HG22	2.04	0.58
1:A:521:LYS:HG3	3:A:870:HOH:O	2.03	0.58
1:D:518:ARG:HA	1:B:330:ILE:CD1	2.34	0.58
1:D:270:LEU:C	3:D:807:HOH:O	2.42	0.57
1:D:29:VAL:HB	1:D:66:LEU:HB2	1.86	0.57
1:C:559:ASP:HB2	1:C:661:TYR:OH	2.05	0.56
1:B:585:GLU:OE2	3:B:812:HOH:O	2.18	0.56
1:D:221:ARG:HD2	1:D:657:LEU:HD12	1.87	0.56
1:C:444:THR:HG23	1:C:447:SER:H	1.70	0.56
1:A:109:VAL:CG1	1:A:111:LEU:HD21	2.35	0.55
1:C:444:THR:CG2	1:C:447:SER:HB3	2.36	0.55
1:C:394:LYS:HB3	1:C:625:PHE:CE2	2.42	0.55
1:C:395:LEU:N	1:C:625:PHE:CE2	2.75	0.55
1:A:15:GLN:HG2	1:A:18:ALA:HB2	1.88	0.55
1:A:100:TYR:CD2	1:A:622:GLU:HG2	2.42	0.55
1:A:229:ASP:OD1	1:A:351:LYS:NZ	2.34	0.55
1:B:22:ASP:OD2	1:B:71:LYS:HE3	2.07	0.55
1:D:320:ILE:O	1:D:320:ILE:HD12	2.06	0.55
1:D:101:ARG:NH1	3:D:803:HOH:O	2.02	0.55
1:D:626:ILE:HA	1:D:631:LYS:HE3	1.88	0.55
1:A:102:TRP:CZ2	1:A:165:ARG:NH2	2.75	0.54
1:D:6:TYR:HB2	1:D:55:VAL:HG23	1.88	0.54
1:B:14:SER:O	1:B:47:ARG:HD3	2.08	0.54
1:B:450:PHE:HB3	1:B:451:PRO:HD3	1.90	0.54
1:C:413:GLN:O	1:C:419:GLY:HA3	2.08	0.54
1:A:185:MET:CE	1:A:194:MET:HG2	2.38	0.54
1:A:652:ASN:HB3	1:A:658:PRO:HB3	1.90	0.54
1:D:284:VAL:HG12	1:D:310:CYS:HB3	1.89	0.54
1:C:29:VAL:HB	1:C:66:LEU:HB2	1.90	0.53
1:A:145:MET:HE1	3:A:841:HOH:O	2.09	0.53
1:C:122:ASP:OD1	1:C:131:ARG:NH1	2.41	0.53
1:D:664:PRO:HA	1:D:667:ILE:HD12	1.89	0.53
1:B:68:ARG:HG3	1:B:110:VAL:HG22	1.90	0.53
1:D:193:PHE:CD1	1:D:594:ARG:HD2	2.43	0.53
1:C:422:ASP:HA	1:C:428:GLY:HA3	1.91	0.53
1:D:57:VAL:HG23	1:D:59:GLU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASP:OD2	1:A:71:LYS:NZ	2.34	0.53
1:A:494:GLU:HG2	3:A:893:HOH:O	2.09	0.53
1:A:550:HIS:CG	1:A:671:VAL:HG22	2.44	0.53
1:C:269:GLN:HB2	1:D:300:CYS:SG	2.49	0.52
1:D:441:LYS:HG3	1:B:441:LYS:HZ2	1.74	0.52
1:C:368:LEU:HD12	1:C:368:LEU:O	2.10	0.52
1:A:29:VAL:HB	1:A:66:LEU:HB2	1.91	0.52
1:A:176:ASP:OD2	1:A:179:LEU:HD13	2.09	0.52
1:B:35:SER:HB2	1:B:57:VAL:CG1	2.39	0.52
1:D:550:HIS:CD2	1:D:671:VAL:HG22	2.45	0.52
1:D:214:ILE:O	1:D:558:TYR:OH	2.24	0.52
1:A:26:LEU:HD11	1:A:67:VAL:CG1	2.40	0.51
1:B:20:THR:HB	1:B:80:TRP:HB2	1.93	0.51
1:A:8:VAL:HG11	1:A:26:LEU:HD22	1.89	0.51
1:D:46:GLU:OE2	3:D:810:HOH:O	2.19	0.51
1:D:562:SER:O	1:D:601:LEU:HD21	2.11	0.51
1:B:23:TYR:HD1	1:B:39:LEU:HD11	1.76	0.51
1:D:99:CYS:O	1:D:101:ARG:HG3	2.11	0.51
1:B:388:ALA:HA	1:B:393:PHE:CD2	2.46	0.51
1:D:550:HIS:CG	1:D:671:VAL:HG22	2.46	0.51
1:A:339:LEU:N	1:A:342:ASP:OD1	2.36	0.51
1:A:457:ARG:NH2	1:A:468:TYR:OH	2.37	0.51
1:D:211:PHE:HA	1:D:214:ILE:HG12	1.93	0.50
1:D:222:VAL:O	1:D:226:TRP:HB3	2.11	0.50
1:A:411:ARG:O	1:A:416:CYS:HB3	2.11	0.50
1:C:146:GLU:OE2	1:C:518:ARG:NH2	2.35	0.50
1:C:258:THR:HG22	1:C:261:MET:HG3	1.93	0.50
1:C:570:THR:HG22	1:C:571:MET:N	2.26	0.50
1:D:302:LEU:O	1:D:572:ARG:HA	2.11	0.50
1:D:229:ASP:OD1	1:D:351:LYS:NZ	2.34	0.50
1:A:386:LEU:HD13	1:A:392:ILE:HG22	1.94	0.50
1:D:80:TRP:CH2	1:D:82:LEU:HD12	2.46	0.50
1:C:482:ARG:CZ	1:C:536:SER:OG	2.60	0.50
1:B:214:ILE:HG22	3:B:821:HOH:O	2.11	0.50
1:C:267:GLU:OE2	1:C:315:ASN:HB2	2.12	0.50
1:C:327:LEU:HD13	1:C:575:PRO:HB3	1.94	0.50
1:D:135:LEU:HD21	1:D:387:PRO:HD3	1.93	0.50
1:D:262:VAL:HG23	1:D:266:LEU:HD13	1.94	0.50
1:D:423:LYS:O	1:D:596:ARG:HG2	2.12	0.50
1:B:367:HIS:O	1:B:371:THR:CG2	2.50	0.50
1:D:-11:HIS:NE2	1:D:-9:HIS:HB2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HA	1:A:313:TYR:CE2	2.47	0.49
1:C:258:THR:CG2	1:C:261:MET:HG3	2.43	0.49
1:C:556:GLY:CA	1:C:661:TYR:CZ	2.95	0.49
1:D:235:GLN:O	3:D:811:HOH:O	2.20	0.49
1:D:8:VAL:HG11	1:D:26:LEU:HD13	1.94	0.49
1:D:171:SER:OG	1:D:174:GLY:CA	2.60	0.49
1:D:245:ILE:O	1:D:457:ARG:HD2	2.12	0.49
1:A:522:SER:OG	3:A:811:HOH:O	2.20	0.49
1:A:360:HIS:HE1	3:A:802:HOH:O	1.95	0.49
1:B:460:GLU:OE2	1:B:460:GLU:N	2.39	0.49
1:A:8:VAL:HG22	1:A:87:LEU:HD22	1.95	0.49
1:A:178:VAL:HG13	1:A:179:LEU:HD12	1.94	0.49
1:D:190:ILE:CG2	1:D:598:CYS:SG	3.01	0.49
1:C:569:PRO:HD2	1:C:592:PRO:HG2	1.94	0.49
1:D:625:PHE:CD1	1:D:630:VAL:HG11	2.48	0.49
1:A:204:PHE:CE1	1:A:226:TRP:CZ2	3.00	0.49
1:C:245:ILE:HA	1:C:284:VAL:HG22	1.94	0.49
1:B:126:ILE:O	3:B:813:HOH:O	2.20	0.48
1:A:277:GLN:NE2	3:A:835:HOH:O	2.42	0.48
1:C:27:SER:HB2	1:C:68:ARG:HB2	1.93	0.48
1:C:394:LYS:HB2	1:C:625:PHE:CE2	2.47	0.48
1:D:335:ASN:ND2	3:D:823:HOH:O	2.46	0.48
1:B:95:ILE:CG2	1:B:113:ASP:OD1	2.61	0.48
1:D:177:PHE:HE1	1:D:607:LEU:HD11	1.78	0.48
1:A:132:ARG:O	1:A:136:GLU:HG3	2.14	0.48
1:D:656:GLN:OE1	1:D:656:GLN:HA	2.13	0.48
1:B:169:PHE:CZ	1:B:406:ILE:HA	2.48	0.48
1:C:394:LYS:HB3	1:C:625:PHE:CD2	2.49	0.48
1:C:585:GLU:N	1:C:585:GLU:OE1	2.47	0.48
1:B:169:PHE:CE1	1:B:406:ILE:HG12	2.49	0.48
1:A:86:THR:CG2	1:A:94:TYR:CE1	2.97	0.48
1:D:86:THR:HG21	1:D:94:TYR:CE1	2.49	0.48
1:B:25:TYR:CZ	1:B:39:LEU:HD12	2.49	0.47
1:B:652:ASN:HB3	1:B:658:PRO:HB3	1.95	0.47
1:C:217:THR:O	1:C:220:GLU:HG2	2.14	0.47
1:D:320:ILE:HD12	1:D:320:ILE:C	2.34	0.47
1:A:268:ARG:O	1:A:269:GLN:HB2	2.14	0.47
1:A:485:THR:O	1:A:489:VAL:HG13	2.14	0.47
1:D:346:ASP:OD1	1:D:582:VAL:HG22	2.14	0.47
1:C:450:PHE:HB3	1:C:451:PRO:HD3	1.97	0.47
1:D:345:TYR:CZ	1:D:584:ILE:HB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:GLN:HB3	1:C:604:VAL:HG13	1.95	0.47
1:B:101:ARG:NH1	1:B:109:VAL:HG13	2.29	0.47
1:B:628:LYS:N	1:B:629:PRO:CD	2.77	0.47
1:A:36:GLU:OE2	3:A:812:HOH:O	2.21	0.47
1:C:13:GLY:HA2	1:C:83:LYS:HD3	1.97	0.47
1:C:556:GLY:HA3	1:C:661:TYR:CZ	2.50	0.47
1:D:71:LYS:HE3	1:D:78:ASP:O	2.15	0.47
1:A:95:ILE:HG22	1:A:97:PHE:CE2	2.50	0.47
1:D:201:TRP:CE2	1:D:594:ARG:HG2	2.50	0.47
1:B:169:PHE:HZ	1:B:406:ILE:HA	1.79	0.47
1:B:558:TYR:O	1:B:559:ASP:C	2.53	0.47
1:A:564:ILE:HD13	1:A:600:HIS:CD2	2.50	0.46
1:D:201:TRP:HH2	1:D:210:ILE:HD13	1.77	0.46
1:C:637:PHE:O	1:C:641:LEU:HG	2.15	0.46
1:D:268:ARG:NE	3:D:814:HOH:O	2.28	0.46
1:C:362:HIS:HE1	1:C:557:GLN:HG2	1.80	0.46
1:C:559:ASP:CB	1:C:661:TYR:OH	2.64	0.46
1:B:95:ILE:HG23	1:B:113:ASP:OD1	2.15	0.46
1:C:214:ILE:N	3:C:820:HOH:O	2.47	0.46
1:B:196:MET:HB2	1:B:196:MET:HE2	1.83	0.46
1:B:457:ARG:O	1:B:459:MET:HG2	2.15	0.46
1:B:479:GLU:O	1:B:479:GLU:HG2	2.15	0.46
1:B:192:ARG:HB2	1:B:209:LYS:HG2	1.97	0.46
1:B:213:LYS:HG2	1:B:223:MET:HE2	1.98	0.46
1:B:242:PRO:N	1:B:242:PRO:C	2.61	0.46
1:D:106:ASP:OD1	1:D:107:VAL:N	2.48	0.46
1:B:169:PHE:CZ	1:B:406:ILE:HD13	2.46	0.46
1:C:401:ARG:NE	3:C:821:HOH:O	2.49	0.46
1:D:40:LEU:HB3	1:D:53:TYR:CZ	2.51	0.46
1:D:415:ILE:HG23	1:D:432:HIS:HE2	1.81	0.46
1:A:479:GLU:HG2	1:B:196:MET:HE3	1.98	0.45
1:A:482:ARG:HH11	1:B:192:ARG:NH2	2.14	0.45
1:D:380:ILE:HG22	1:D:384:ARG:HD2	1.99	0.45
1:B:245:ILE:O	1:B:245:ILE:HG23	2.15	0.45
1:A:313:TYR:HB2	1:A:323:ILE:HD13	1.98	0.45
1:C:564:ILE:HB	1:C:565:PRO:HD3	1.98	0.45
1:D:506:GLN:OE1	1:D:506:GLN:HA	2.16	0.45
1:D:284:VAL:O	1:D:284:VAL:HG13	2.16	0.45
1:A:102:TRP:CE2	1:A:165:ARG:CZ	2.99	0.45
1:D:284:VAL:O	1:D:284:VAL:CG1	2.65	0.45
1:B:365:ILE:HD12	1:B:439:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:GLU:O	1:B:635:ALA:HB3	2.16	0.45
1:A:450:PHE:HB3	1:A:451:PRO:HD3	1.98	0.45
1:D:339:LEU:HB3	1:D:340:PRO:HD2	1.98	0.45
1:D:465:ILE:O	1:D:471:ARG:NH2	2.32	0.45
1:B:537:GLU:O	1:B:541:VAL:HG23	2.16	0.45
1:C:225:HIS:CD2	1:C:228:GLU:OE2	2.70	0.45
1:C:673:ILE:OXT	3:C:807:HOH:O	2.21	0.45
1:B:494:GLU:HG2	1:B:498:VAL:HG21	1.98	0.45
1:B:564:ILE:CD1	1:B:601:LEU:HD21	2.46	0.45
1:A:245:ILE:HA	1:A:284:VAL:HG22	1.98	0.45
1:A:254:LYS:NZ	1:A:285:ASP:OD1	2.37	0.45
1:C:470:TYR:HA	1:C:659:TYR:CE2	2.52	0.45
1:D:22:ASP:HA	1:D:74:TYR:CB	2.41	0.45
1:D:312:LEU:HD23	1:D:322:PRO:HA	1.98	0.45
1:D:463:GLU:OE1	1:D:463:GLU:N	2.48	0.45
1:B:344:LYS:O	3:B:814:HOH:O	2.21	0.45
1:A:481:ILE:HD13	1:A:543:ILE:HG22	1.99	0.45
1:D:116:ALA:HB3	1:D:492:TYR:CE1	2.51	0.45
1:C:95:ILE:HG21	1:C:97:PHE:CE2	2.52	0.45
1:D:638:ARG:HG2	3:D:854:HOH:O	2.16	0.45
1:B:6:TYR:HE2	1:B:89:THR:HG22	1.81	0.45
1:B:65:GLN:HB3	1:B:127:LEU:HD21	1.99	0.45
1:C:572:ARG:NH1	1:C:591:LEU:O	2.40	0.44
1:D:6:TYR:CE1	1:D:89:THR:HG22	2.52	0.44
1:B:241:ASN:HB2	1:B:362:HIS:CD2	2.52	0.44
1:B:481:ILE:HD13	1:B:543:ILE:HG22	1.99	0.44
1:C:68:ARG:NE	1:C:108:GLU:OE2	2.50	0.44
1:C:264:CYS:C	3:C:805:HOH:O	2.55	0.44
1:B:213:LYS:C	1:B:214:ILE:HD13	2.36	0.44
1:B:305:LEU:HD12	1:B:305:LEU:O	2.18	0.44
1:C:356:SER:O	1:C:360:HIS:CD2	2.70	0.44
1:C:556:GLY:HA2	1:C:661:TYR:CZ	2.51	0.44
1:D:258:THR:HG22	1:D:261:MET:HG3	2.00	0.44
1:A:8:VAL:HG22	1:A:87:LEU:CD2	2.47	0.44
1:A:25:TYR:CE2	1:A:72:ARG:HG3	2.53	0.44
1:C:241:ASN:N	1:C:242:PRO:CD	2.80	0.44
1:C:570:THR:CG2	1:C:571:MET:N	2.79	0.44
1:C:241:ASN:N	1:C:242:PRO:HD3	2.32	0.44
1:C:494:GLU:HG2	1:C:498:VAL:HG21	2.00	0.44
1:B:151:PHE:O	1:B:518:ARG:NH1	2.48	0.44
1:A:6:TYR:N	1:A:55:VAL:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:THR:HG22	1:C:261:MET:CG	2.48	0.44
1:D:314:LYS:CD	1:D:464:ASP:O	2.65	0.44
1:D:617:LEU:HG	1:D:641:LEU:HD11	1.99	0.44
1:B:245:ILE:HA	1:B:284:VAL:HG22	1.98	0.44
1:B:273:GLU:CD	1:B:273:GLU:H	2.21	0.43
1:C:551:ALA:HA	1:C:555:PHE:CD1	2.52	0.43
1:D:258:THR:HG22	1:D:261:MET:CG	2.48	0.43
1:B:9:THR:CG2	1:B:86:THR:OG1	2.65	0.43
1:B:550:HIS:CG	1:B:671:VAL:HG22	2.54	0.43
1:C:123:GLN:O	1:C:128:LYS:HE2	2.19	0.43
1:C:365:ILE:HD12	1:C:439:ALA:CB	2.48	0.43
1:A:360:HIS:CD2	1:A:427:THR:HG23	2.54	0.43
1:C:116:ALA:HB3	1:C:492:TYR:CE1	2.53	0.43
1:C:229:ASP:HB3	1:C:322:PRO:HD2	2.01	0.43
1:C:274:GLN:HG2	3:C:803:HOH:O	2.19	0.43
1:B:502:ASP:OD1	1:B:502:ASP:C	2.57	0.43
1:B:266:LEU:HA	1:B:313:TYR:CE2	2.53	0.43
1:A:208:GLU:HG3	1:A:223:MET:SD	2.59	0.43
1:A:518:ARG:CZ	3:A:818:HOH:O	2.61	0.43
1:A:559:ASP:N	3:A:842:HOH:O	2.46	0.43
1:C:15:GLN:HG2	1:C:170:ASP:CG	2.39	0.43
1:C:155:ILE:HG21	1:C:163:LEU:HD21	2.00	0.43
1:C:239:GLY:O	1:C:242:PRO:HD3	2.18	0.43
1:D:328:ASN:H	1:D:335:ASN:HD21	1.65	0.43
1:D:330:ILE:CB	3:D:802:HOH:O	2.67	0.43
1:B:22:ASP:OD2	1:B:71:LYS:CE	2.67	0.43
1:C:221:ARG:NH1	1:C:656:GLN:O	2.50	0.42
1:D:257:VAL:CG2	1:D:337:ILE:HD13	2.49	0.42
1:C:313:TYR:O	1:C:320:ILE:HA	2.19	0.42
1:D:7:THR:OG1	1:D:88:LYS:HB2	2.19	0.42
1:D:147:TRP:CH2	1:D:415:ILE:O	2.72	0.42
1:D:415:ILE:HG23	1:D:432:HIS:NE2	2.33	0.42
1:B:444:THR:OG1	1:B:447:SER:HB3	2.20	0.42
1:A:152:PRO:HD3	1:A:440:MET:HE1	2.01	0.42
1:A:165:ARG:HH22	1:A:170:ASP:HA	1.84	0.42
1:C:326:GLN:HG2	1:C:335:ASN:HD21	1.83	0.42
1:D:564:ILE:HD13	1:D:600:HIS:HD2	1.82	0.42
1:C:401:ARG:NH1	1:C:615:LEU:HD12	2.34	0.42
1:D:88:LYS:NZ	1:D:92:GLY:O	2.40	0.42
1:D:200:SER:CB	1:D:572:ARG:HH22	2.32	0.42
1:D:270:LEU:HB3	1:D:274:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PHE:HZ	1:B:406:ILE:CD1	2.31	0.42
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.84	0.42
1:A:394:LYS:HG2	1:A:624:HIS:HB3	2.00	0.42
1:C:221:ARG:HD2	1:C:657:LEU:HD12	2.02	0.42
1:D:154:SER:HB2	1:D:411:ARG:NH1	2.34	0.42
1:D:255:LEU:HG	1:D:257:VAL:HG23	2.01	0.42
1:D:663:SER:O	1:D:665:ASP:N	2.52	0.42
1:B:7:THR:HG22	1:B:54:ASP:OD1	2.19	0.42
1:A:172:GLU:HG3	1:A:173:LYS:HG3	2.01	0.42
1:A:229:ASP:OD2	3:A:813:HOH:O	2.21	0.42
1:A:263:GLU:HG3	3:A:938:HOH:O	2.20	0.42
1:D:500:GLU:HG3	1:D:530:LYS:HG2	2.01	0.42
1:B:258:THR:OG1	1:B:261:MET:HG3	2.19	0.42
1:A:57:VAL:HG11	1:A:61:LEU:HD11	2.02	0.42
1:A:102:TRP:CD1	1:A:165:ARG:HG3	2.54	0.42
1:C:484:PHE:HB2	1:C:637:PHE:CD1	2.54	0.42
1:C:625:PHE:CE1	1:C:630:VAL:HG21	2.55	0.42
1:D:551:ALA:HA	1:D:555:PHE:CD1	2.55	0.42
1:B:216:ASN:OD1	1:B:216:ASN:O	2.37	0.42
1:A:355:ARG:NH1	3:A:837:HOH:O	2.43	0.42
1:A:600:HIS:O	1:A:604:VAL:HG22	2.19	0.42
1:D:190:ILE:HG22	1:D:598:CYS:SG	2.60	0.42
1:D:376:GLU:OE2	1:D:411:ARG:NH2	2.52	0.42
1:B:362:HIS:ND1	1:B:363:GLN:OE1	2.48	0.42
1:B:216:ASN:O	1:B:216:ASN:CG	2.59	0.42
1:C:218:ILE:HG21	1:C:559:ASP:HB3	2.02	0.41
1:C:362:HIS:CE1	1:C:557:GLN:HG2	2.55	0.41
1:D:622:GLU:OE2	3:D:812:HOH:O	2.22	0.41
1:B:116:ALA:HB3	1:B:492:TYR:CE1	2.55	0.41
1:B:169:PHE:HE1	1:B:406:ILE:HG12	1.82	0.41
1:D:339:LEU:N	1:D:339:LEU:HD12	2.35	0.41
1:B:623:GLU:HB2	3:B:807:HOH:O	2.19	0.41
1:A:143:ARG:NH1	3:A:852:HOH:O	2.53	0.41
1:B:5:SER:N	1:B:56:THR:HG22	2.36	0.41
1:A:70:GLU:OE2	1:A:72:ARG:NE	2.42	0.41
1:A:550:HIS:CD2	1:A:671:VAL:HG13	2.55	0.41
1:A:561:ALA:HA	1:A:567:ALA:HB3	2.01	0.41
1:D:345:TYR:CE2	1:D:584:ILE:HD13	2.55	0.41
1:A:254:LYS:HZ1	1:A:285:ASP:CG	2.20	0.41
1:C:68:ARG:CZ	1:C:108:GLU:OE2	2.68	0.41
1:B:47:ARG:N	3:B:826:HOH:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:O	1:B:394:LYS:HE3	2.20	0.41
1:B:409:LYS:HA	1:B:409:LYS:HD2	1.91	0.41
1:A:268:ARG:NH2	1:A:314:LYS:O	2.53	0.41
1:A:370:ARG:HH22	1:A:447:SER:CB	2.33	0.41
1:A:620:TYR:CD2	1:A:634:MET:HE2	2.56	0.41
1:A:45:PHE:CD2	1:A:45:PHE:N	2.89	0.41
1:C:258:THR:HG23	1:C:261:MET:H	1.84	0.41
1:C:507:ASP:O	1:C:511:ASP:HB2	2.21	0.41
1:D:316:LEU:HD23	1:D:316:LEU:HA	1.90	0.41
1:B:173:LYS:CE	1:B:611:GLN:OE1	2.69	0.41
1:A:135:LEU:HD21	1:A:387:PRO:HD3	2.01	0.41
1:C:35:SER:HB3	1:C:61:LEU:HD11	2.03	0.41
1:D:253:GLU:OE2	1:D:253:GLU:HA	2.21	0.41
1:D:415:ILE:HG23	1:D:432:HIS:CD2	2.55	0.41
1:D:616:PHE:O	1:D:617:LEU:C	2.59	0.41
1:B:210:ILE:HD13	1:B:594:ARG:HB3	2.03	0.41
1:B:638:ARG:HD2	3:B:901:HOH:O	2.20	0.41
1:A:547:SER:HB2	1:A:668:PRO:O	2.21	0.41
1:D:67:VAL:HG23	1:D:97:PHE:CE1	2.55	0.41
1:D:558:TYR:O	1:D:562:SER:OG	2.38	0.41
1:B:25:TYR:OH	1:B:39:LEU:HD12	2.21	0.41
1:B:39:LEU:C	1:B:39:LEU:HD23	2.41	0.41
1:C:147:TRP:N	3:C:806:HOH:O	2.19	0.40
1:A:126:ILE:N	1:A:126:ILE:HD12	2.35	0.40
1:A:254:LYS:HG2	3:C:815:HOH:O	2.21	0.40
1:D:177:PHE:O	1:D:181:TYR:HB2	2.22	0.40
1:C:424:ALA:O	1:C:569:PRO:HB2	2.21	0.40
1:C:625:PHE:HD1	1:C:630:VAL:HG11	1.86	0.40
1:C:652:ASN:HB3	1:C:658:PRO:HB3	2.03	0.40
1:D:142:TYR:CE2	1:D:164:PRO:HG2	2.56	0.40
1:D:188:LEU:HD23	1:D:214:ILE:HD12	2.03	0.40
1:B:662:LEU:HA	1:B:667:ILE:HD11	2.02	0.40
1:C:500:GLU:HG3	1:C:530:LYS:HG2	2.04	0.40
1:D:266:LEU:HD23	1:D:275:GLU:HG3	2.03	0.40
1:D:376:GLU:HG3	1:D:404:ILE:HG12	2.04	0.40
1:A:126:ILE:HD12	1:A:126:ILE:H	1.87	0.40
1:A:187:ASN:O	1:A:189:PHE:CE2	2.75	0.40
1:C:137:THR:O	1:C:141:GLN:HG2	2.22	0.40
1:D:337:ILE:O	1:D:339:LEU:CD1	2.70	0.40
1:B:216:ASN:N	3:B:821:HOH:O	2.31	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	670/691 (97%)	644 (96%)	26 (4%)	0	100	100
1	B	635/691 (92%)	606 (95%)	29 (5%)	0	100	100
1	C	608/691 (88%)	592 (97%)	16 (3%)	0	100	100
1	D	668/691 (97%)	639 (96%)	29 (4%)	0	100	100
All	All	2581/2764 (93%)	2481 (96%)	100 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	597/608 (98%)	594 (100%)	3 (0%)	88	93
1	B	570/608 (94%)	569 (100%)	1 (0%)	93	96
1	C	541/608 (89%)	539 (100%)	2 (0%)	91	94
1	D	595/608 (98%)	594 (100%)	1 (0%)	93	96
All	All	2303/2432 (95%)	2296 (100%)	7 (0%)	92	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASP
1	A	468	TYR

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Mol	Chain	Res	Type
1	A	511	ASP
1	C	468	TYR
1	C	660	TYR
1	D	468	TYR
1	B	511	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	B	360	HIS

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 4 ligands modelled in this entry, 4 are 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	674/691 (97%)	0.37	27 (4%) 38 35	30, 46, 92, 123	0
1	B	643/691 (93%)	0.24	9 (1%) 75 73	32, 47, 78, 113	0
1	C	617/691 (89%)	0.61	45 (7%) 15 11	39, 60, 107, 154	0
1	D	673/691 (97%)	0.84	90 (13%) 3 1	40, 66, 116, 158	0
All	All	2607/2764 (94%)	0.51	171 (6%) 18 14	30, 55, 103, 158	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	ILE	8.7
1	C	302	LEU	7.6
1	C	74	TYR	7.5
1	D	193	PHE	7.4
1	D	190	ILE	6.9
1	C	429	GLY	6.5
1	D	425	ASN	6.0
1	A	414	LEU	5.7
1	D	429	GLY	5.7
1	D	207	PHE	5.6
1	D	599	TRP	5.5
1	C	76	SER	5.3
1	D	598	CYS	5.1
1	A	189	PHE	5.1
1	D	417	GLU	5.0
1	C	421	PHE	5.0
1	D	201	TRP	4.9
1	D	177	PHE	4.8
1	C	612	GLU	4.7
1	D	188	LEU	4.7
1	C	613	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	176	ASP	4.5
1	C	430	GLY	4.4
1	D	197	PHE	4.4
1	D	427	THR	4.4
1	C	423	LYS	4.4
1	C	599	TRP	4.3
1	D	69	ILE	4.2
1	D	194	MET	4.1
1	C	596	ARG	4.0
1	D	414	LEU	3.9
1	B	414	LEU	3.9
1	C	6	TYR	3.9
1	D	169	PHE	3.9
1	D	126	ILE	3.8
1	A	26	LEU	3.8
1	D	418	CYS	3.8
1	A	299	PRO	3.8
1	C	214	ILE	3.8
1	C	424	ALA	3.7
1	C	77	ASN	3.5
1	D	178	VAL	3.5
1	D	297	THR	3.5
1	A	300	CYS	3.5
1	C	107	VAL	3.5
1	D	298	ASP	3.4
1	D	58	ASP	3.4
1	D	570	THR	3.4
1	D	209	LYS	3.3
1	D	300	CYS	3.2
1	A	188	LEU	3.2
1	D	75	GLY	3.2
1	D	76	SER	3.2
1	D	173	LYS	3.2
1	C	23	TYR	3.2
1	D	26	LEU	3.2
1	D	420	LEU	3.2
1	C	565	PRO	3.2
1	C	660	TYR	3.2
1	C	293	ASP	3.2
1	A	295	ASN	3.2
1	D	588	VAL	3.1
1	D	426	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	74	TYR	3.1
1	D	179	LEU	3.1
1	D	183	LYS	3.1
1	D	569	PRO	3.0
1	C	427	THR	3.0
1	D	316	LEU	3.0
1	D	424	ALA	3.0
1	A	421	PHE	3.0
1	D	181	TYR	3.0
1	A	191	ASN	3.0
1	C	419	GLY	3.0
1	D	105	GLY	3.0
1	A	190	ILE	3.0
1	D	302	LEU	3.0
1	D	419	GLY	3.0
1	D	205	ALA	3.0
1	C	426	ALA	2.9
1	A	177	PHE	2.9
1	D	299	PRO	2.9
1	D	175	VAL	2.9
1	D	68	ARG	2.9
1	D	594	ARG	2.9
1	A	296	LYS	2.8
1	D	184	ALA	2.8
1	D	16	GLU	2.7
1	D	34[A]	CYS	2.7
1	D	210	ILE	2.7
1	C	673	ILE	2.7
1	C	482	ARG	2.7
1	A	169	PHE	2.7
1	B	173	LYS	2.7
1	A	197	PHE	2.7
1	D	295	ASN	2.7
1	A	303	GLN	2.7
1	C	34[A]	CYS	2.6
1	A	173	LYS	2.6
1	A	426	ALA	2.6
1	D	39	LEU	2.6
1	D	432	HIS	2.6
1	C	173	LYS	2.6
1	D	172	GLU	2.6
1	D	170	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	563	TRP	2.6
1	D	213	LYS	2.6
1	D	423	LYS	2.6
1	D	348	LEU	2.5
1	A	175	VAL	2.5
1	D	28	LEU	2.5
1	C	24	ILE	2.5
1	C	422	ASP	2.5
1	D	293	ASP	2.5
1	B	76	SER	2.5
1	B	169	PHE	2.5
1	D	73	LYS	2.5
1	C	90	PRO	2.5
1	C	106	ASP	2.4
1	D	57	VAL	2.4
1	D	200	SER	2.4
1	A	598[A]	CYS	2.4
1	D	204	PHE	2.4
1	D	303	GLN	2.4
1	D	59	GLU	2.4
1	A	126	ILE	2.3
1	D	578	ALA	2.3
1	D	189	PHE	2.3
1	C	59	GLU	2.3
1	D	416	CYS	2.3
1	D	23	TYR	2.3
1	D	142	TYR	2.3
1	A	74	TYR	2.3
1	C	642	GLU	2.3
1	D	40	LEU	2.3
1	A	90	PRO	2.2
1	C	303	GLN	2.2
1	C	586	GLN	2.2
1	C	158	LYS	2.2
1	D	344	LYS	2.2
1	D	13	GLY	2.2
1	C	657	LEU	2.2
1	D	174	GLY	2.2
1	D	230	LEU	2.2
1	D	612	GLU	2.2
1	A	294	ALA	2.2
1	C	294	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	69	ILE	2.2
1	B	293	ASP	2.2
1	B	55	VAL	2.1
1	B	520	ARG	2.1
1	D	203	ASP	2.1
1	D	301	THR	2.1
1	D	199	SER	2.1
1	C	573	ALA	2.1
1	C	661	TYR	2.1
1	C	226	TRP	2.1
1	D	211	PHE	2.1
1	A	198	GLN	2.1
1	D	325	ILE	2.1
1	A	76	SER	2.1
1	C	425	ASN	2.1
1	A	520	ARG	2.1
1	C	222	VAL	2.0
1	D	24	ILE	2.0
1	C	8	VAL	2.0
1	D	222	VAL	2.0
1	B	158	LYS	2.0
1	D	185	MET	2.0
1	B	413	GLN	2.0
1	D	124	ILE	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](#)

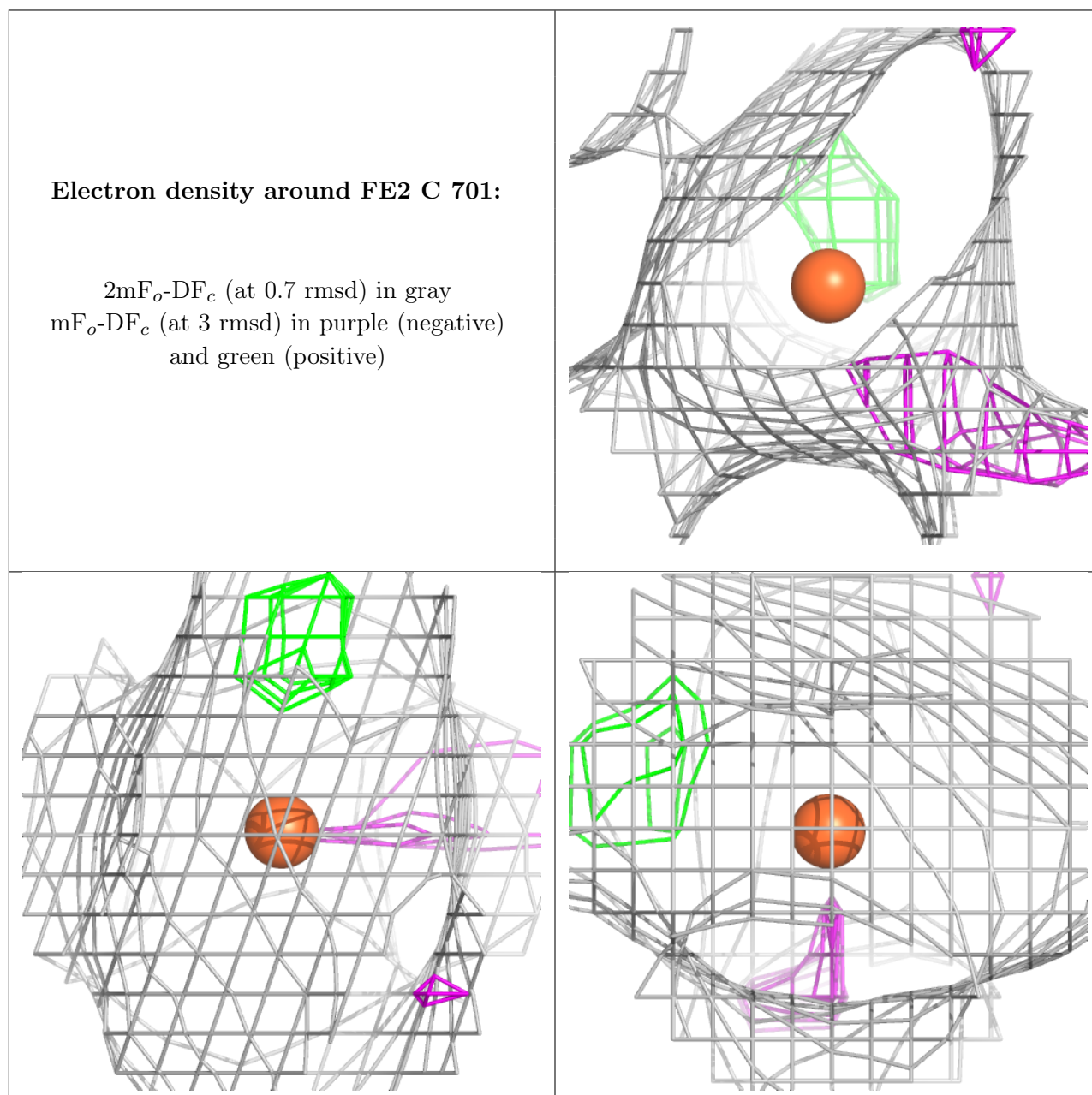
There are no monosaccharides in this entry.

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.

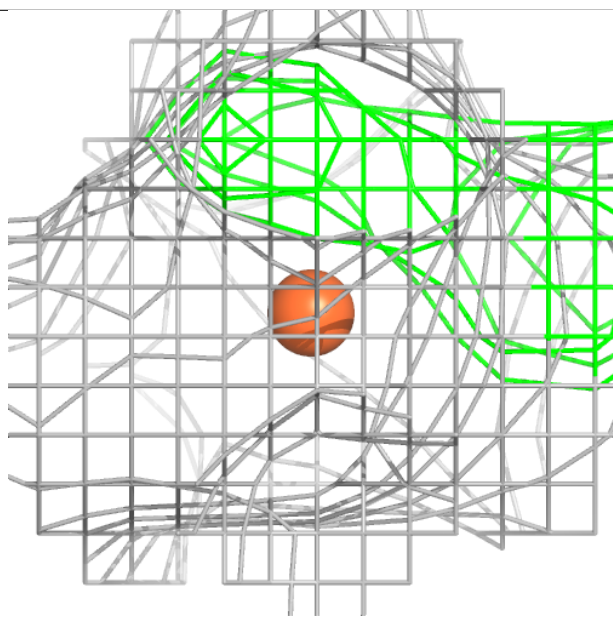
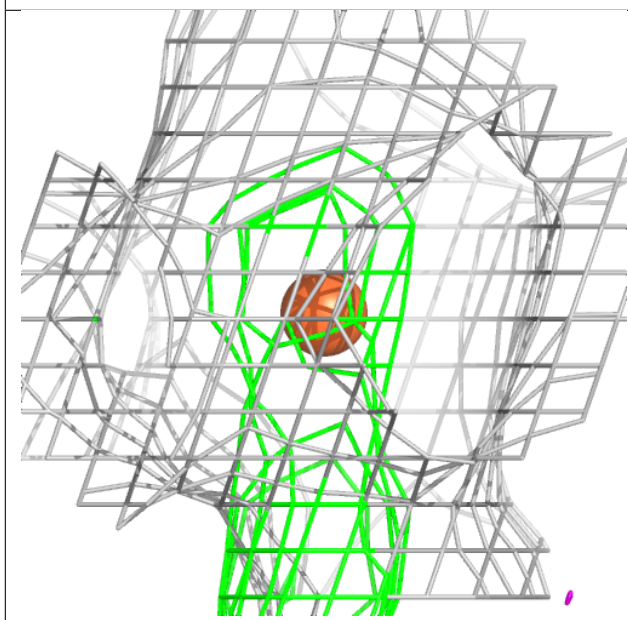
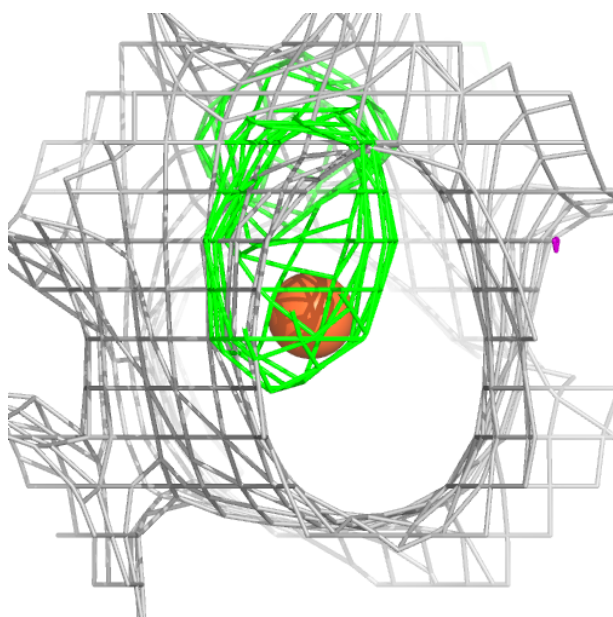
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	C	701	1/1	0.96	0.14	46,46,46,46	0
2	FE2	A	701	1/1	0.99	0.20	37,37,37,37	0
2	FE2	D	701	1/1	0.99	0.17	51,51,51,51	0
2	FE2	B	701	1/1	0.99	0.22	39,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



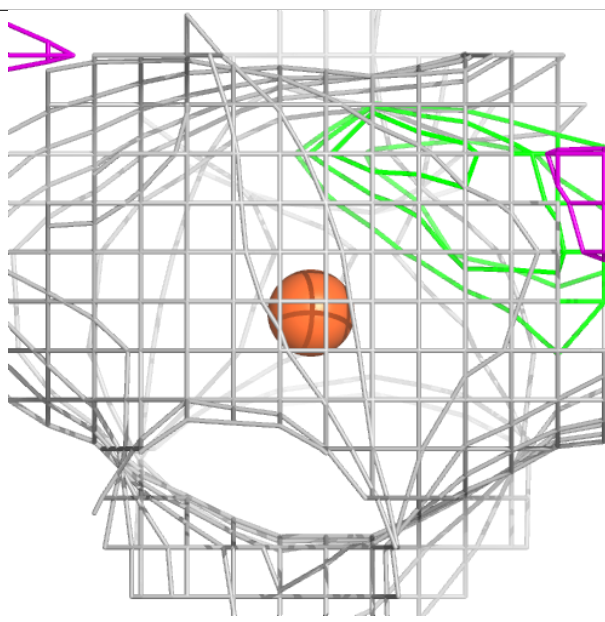
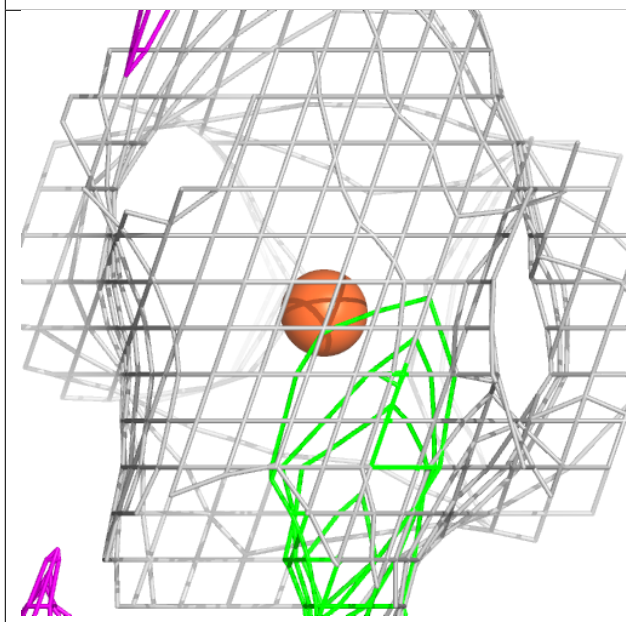
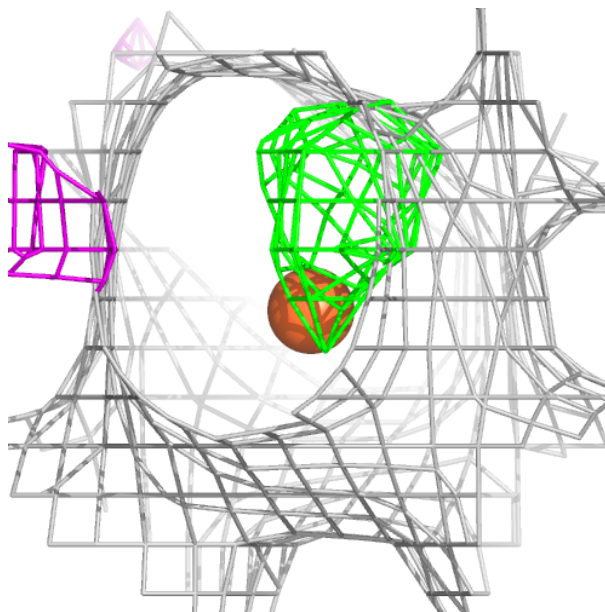
Electron density around FE2 A 701:

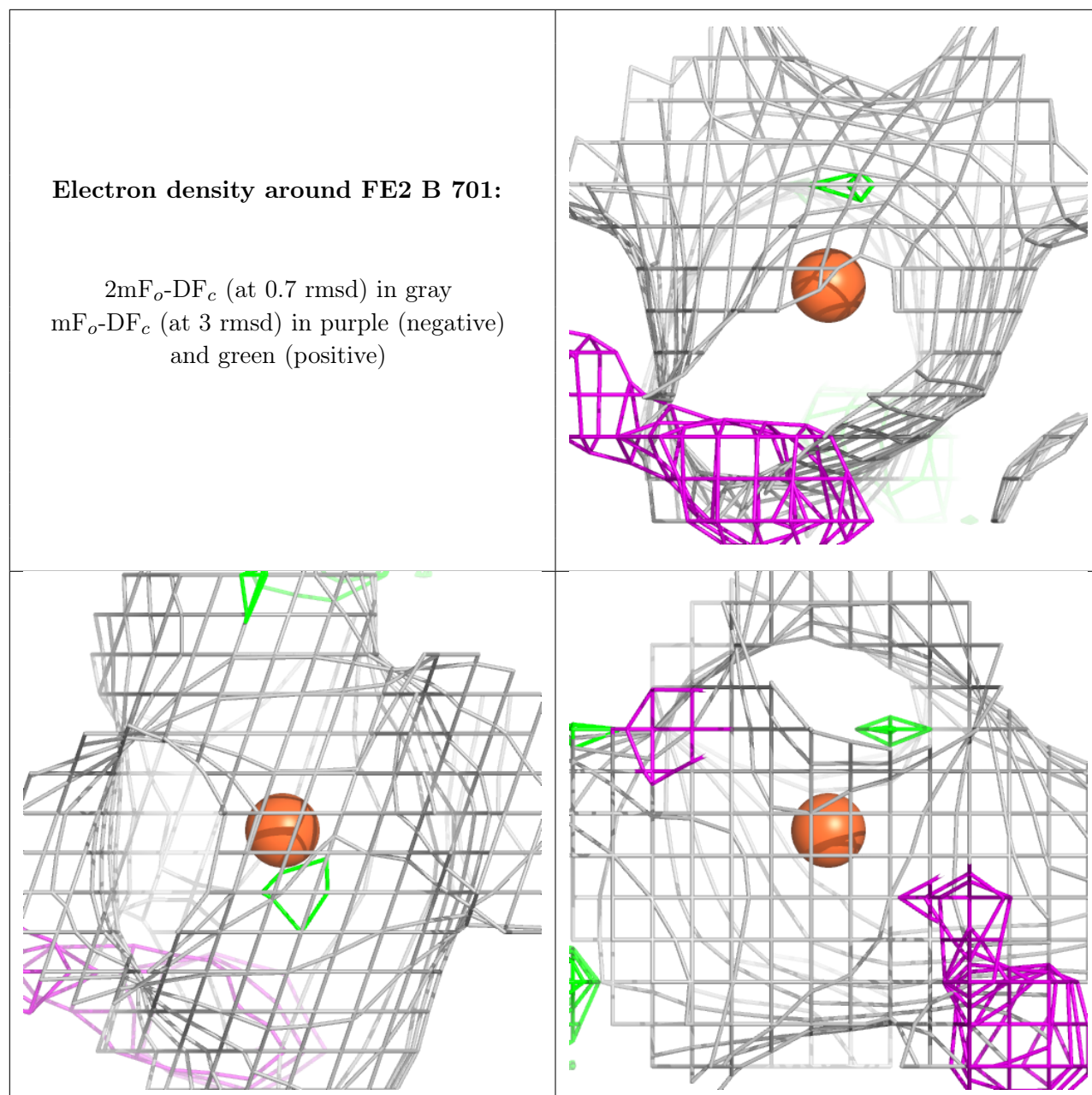
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE2 D 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.