



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 AM UTC

PDB ID : 8QDQ / pdb_00008qdq
Title : Vitis vinifera dimeric 13S-lipoxygenase LOXA in the closed conformation
Authors : Wild, K.; Sinning, I.
Deposited on : 2023-08-30
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

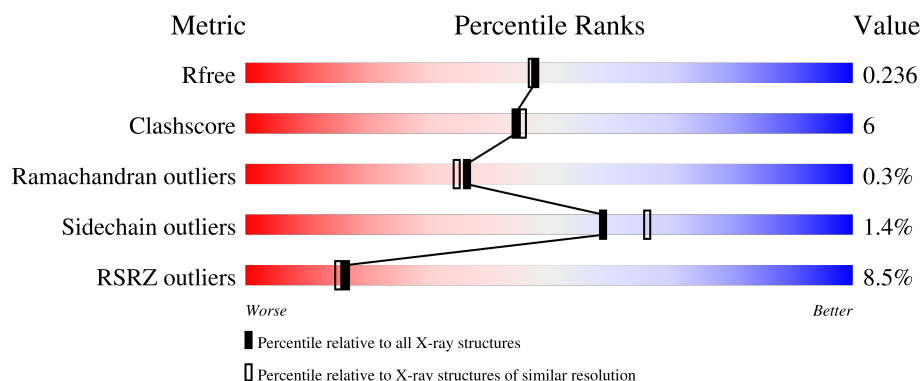
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	863	4% 85% 10% .
1	B	863	12% 80% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13989 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 Lipoxxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	S	0	0	0
			6616	4255	1108	1241	12			
1	B	827	Total	C	N	O	S	0	0	0
			6612	4252	1107	1241	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	MET	-	initiating methionine	UNP D7SLA9
A	40	HIS	-	expression tag	UNP D7SLA9
A	41	HIS	-	expression tag	UNP D7SLA9
A	42	HIS	-	expression tag	UNP D7SLA9
A	43	HIS	-	expression tag	UNP D7SLA9
A	44	HIS	-	expression tag	UNP D7SLA9
A	45	HIS	-	expression tag	UNP D7SLA9
A	46	GLY	-	expression tag	UNP D7SLA9
A	47	SER	-	expression tag	UNP D7SLA9
A	379	ALA	SER	conflict	UNP D7SLA9
B	39	MET	-	initiating methionine	UNP D7SLA9
B	40	HIS	-	expression tag	UNP D7SLA9
B	41	HIS	-	expression tag	UNP D7SLA9
B	42	HIS	-	expression tag	UNP D7SLA9
B	43	HIS	-	expression tag	UNP D7SLA9
B	44	HIS	-	expression tag	UNP D7SLA9
B	45	HIS	-	expression tag	UNP D7SLA9
B	46	GLY	-	expression tag	UNP D7SLA9
B	47	SER	-	expression tag	UNP D7SLA9
B	379	ALA	SER	conflict	UNP D7SLA9

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	429	Total 429	O 429	0	0
3	B	330	Total 330	O 330	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.77Å 110.65Å 91.17Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	46.49 – 2.00 46.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.49-2.00) 98.4 (46.49-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.199 , 0.235 0.199 , 0.236	Depositor DCC
R_{free} test set	5909 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13989	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/6797	0.50	0/9249
1	B	0.32	0/6793	0.49	0/9243
All	All	0.32	0/13590	0.50	0/18492

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

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	6616	0	6529	62	1
1	B	6612	0	6521	97	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	429	0	0	14	0
3	B	330	0	0	30	0
All	All	13989	0	13050	157	1

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 (157) 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:279:THR:OG1	3:B:1101:HOH:O	1.82	0.97
1:B:163:HIS:N	3:B:1104:HOH:O	2.01	0.85
1:A:379:ALA:N	3:A:1105:HOH:O	2.12	0.82
1:B:363:LYS:O	3:B:1105:HOH:O	2.01	0.77
1:B:103:LYS:HG2	1:B:104:THR:HG23	1.69	0.73
1:A:502:ASP:OD2	3:A:1102:HOH:O	2.05	0.72
1:B:246:ASP:O	3:B:1106:HOH:O	2.07	0.71
1:A:498:PHE:HB2	1:A:508:LEU:HD11	1.74	0.69
1:B:362:HIS:O	1:B:364:VAL:N	2.26	0.69
1:A:625:GLU:HG3	3:A:1215:HOH:O	1.92	0.68
1:A:121:GLU:OE2	3:A:1104:HOH:O	2.11	0.68
1:B:362:HIS:C	1:B:364:VAL:H	2.02	0.68
1:A:424:TRP:O	3:A:1103:HOH:O	2.10	0.68
1:B:867:ASN:ND2	3:B:1123:HOH:O	2.25	0.68
1:B:439:GLU:O	1:B:524:LYS:NZ	2.26	0.67
1:A:448:GLU:HG2	1:A:457:VAL:HG23	1.76	0.66
1:A:390:GLN:HG2	3:A:1118:HOH:O	1.96	0.65
1:B:200:ARG:HA	3:B:1340:HOH:O	1.97	0.65
1:B:235:GLU:HA	1:B:280:GLY:HA3	1.78	0.64
1:A:183:GLU:O	3:A:1106:HOH:O	2.15	0.64
1:B:246:ASP:C	3:B:1106:HOH:O	2.40	0.63
1:B:109:VAL:HG13	1:B:154:ILE:HD12	1.82	0.62
1:A:174:LEU:HB2	1:A:182:ILE:HB	1.82	0.61
1:A:514:ARG:HG2	1:A:515:PRO:HD2	1.82	0.61
1:B:441:ALA:HB3	1:B:526:VAL:HG23	1.82	0.61
1:B:108:GLU:OE2	1:B:199:LYS:NZ	2.33	0.61
1:B:102:GLY:O	1:B:131:ARG:HD2	1.99	0.60
1:B:102:GLY:HA3	1:B:163:HIS:HB2	1.83	0.59
1:B:314:SER:HB2	1:B:901:ILE:HD13	1.83	0.59
1:A:125:ILE:HD13	1:A:148:PRO:HD2	1.84	0.59
1:B:74:VAL:HG22	1:B:172:ILE:HG12	1.84	0.58
1:B:783:GLU:OE2	3:B:1108:HOH:O	2.17	0.58
1:B:480:SER:N	3:B:1102:HOH:O	2.00	0.57
1:B:821:SER:O	3:B:1109:HOH:O	2.18	0.57
1:B:851:ARG:HD3	3:B:1157:HOH:O	2.03	0.57
1:B:163:HIS:CD2	1:B:165:LYS:HB2	2.39	0.57
1:B:247:VAL:HA	3:B:1106:HOH:O	2.04	0.57
1:B:359:LEU:HB2	1:B:382:SER:HB2	1.87	0.56
1:B:695:LYS:NZ	3:B:1119:HOH:O	2.23	0.56
1:B:255:ASP:HA	1:B:286:ILE:HD12	1.88	0.56
1:A:74:VAL:HG22	1:A:172:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ASP:OD2	3:A:1107:HOH:O	2.18	0.55
1:B:78:LEU:HD21	1:B:97:VAL:HG13	1.88	0.55
1:B:84:LEU:HD12	1:B:311:LEU:HD22	1.89	0.55
1:A:470:ASP:OD1	3:A:1108:HOH:O	2.18	0.54
1:B:246:ASP:HB2	1:B:278:ARG:HG3	1.90	0.54
1:B:103:LYS:NZ	3:B:1127:HOH:O	2.27	0.54
1:B:371:ARG:O	1:B:374:ARG:NH2	2.40	0.54
1:B:448:GLU:HG2	1:B:457:VAL:HG23	1.89	0.54
1:B:514:ARG:HG2	1:B:515:PRO:HD2	1.90	0.53
1:B:236:ARG:NE	1:B:236:ARG:HA	2.24	0.53
1:A:531:TRP:CZ2	1:B:506:LYS:HD2	2.45	0.52
1:A:293:ARG:NH1	3:A:1113:HOH:O	2.26	0.52
1:B:310:GLU:O	1:B:316:ASN:ND2	2.42	0.52
1:B:236:ARG:NH1	3:B:1113:HOH:O	2.38	0.51
1:B:284:SER:HA	3:B:1132:HOH:O	2.10	0.51
1:A:78:LEU:HD21	1:A:101:LEU:HD11	1.90	0.51
1:A:820:HIS:NE2	1:A:893:LYS:O	2.42	0.51
1:A:84:LEU:HD13	1:A:311:LEU:HD22	1.93	0.51
1:B:254:PRO:HB3	1:B:261:THR:HG23	1.93	0.51
1:B:498:PHE:HB2	1:B:508:LEU:HD11	1.93	0.51
1:B:371:ARG:NH1	3:B:1107:HOH:O	2.16	0.51
1:A:101:LEU:HD11	1:A:139:VAL:HG21	1.91	0.50
1:B:275:ARG:HA	3:B:1106:HOH:O	2.11	0.50
1:A:79:THR:OG1	1:A:80:VAL:N	2.42	0.50
1:A:68:VAL:HG23	1:A:149:ASP:OD1	2.12	0.50
1:B:781:PRO:O	3:B:1111:HOH:O	2.19	0.50
1:B:256:SER:O	3:B:1110:HOH:O	2.18	0.50
1:B:284:SER:HB3	1:B:287:ASP:O	2.11	0.50
1:A:869:LYS:HE2	3:A:1382:HOH:O	2.10	0.50
1:B:366:GLN:NE2	3:B:1124:HOH:O	2.25	0.49
1:A:357:PRO:HA	1:A:381:ASP:HB3	1.93	0.49
1:B:233:GLN:O	3:B:1113:HOH:O	2.20	0.49
1:A:379:ALA:HB1	3:A:1114:HOH:O	2.13	0.49
1:B:851:ARG:HD2	3:B:1393:HOH:O	2.13	0.49
1:B:447:VAL:HG13	1:B:508:LEU:HD13	1.94	0.48
1:B:746:VAL:HA	1:B:750:HIS:HB3	1.93	0.48
1:B:236:ARG:NH2	3:B:1113:HOH:O	2.28	0.48
1:B:401:ARG:NH1	1:B:403:GLU:OE2	2.43	0.48
1:A:838:ASP:OD2	3:A:1109:HOH:O	2.20	0.48
1:A:401:ARG:HD2	1:A:403:GLU:OE2	2.14	0.48
1:A:83:PHE:CE2	1:A:87:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TRP:C	3:A:1103:HOH:O	2.56	0.48
1:B:234:GLY:O	1:B:278:ARG:NH2	2.40	0.48
1:B:612:ILE:HG21	1:B:813:VAL:HG21	1.96	0.48
1:B:234:GLY:HA3	3:B:1113:HOH:O	2.14	0.47
1:B:625:GLU:OE1	3:B:1112:HOH:O	2.20	0.47
1:A:87:LEU:HD13	1:A:311:LEU:HD11	1.96	0.47
1:A:314:SER:HB2	1:A:901:ILE:HD13	1.96	0.47
1:A:70:VAL:HG21	1:A:147:ILE:HD12	1.97	0.47
1:B:514:ARG:NH2	1:B:780:ASP:OD2	2.43	0.46
1:A:109:VAL:HG13	1:A:154:ILE:HG23	1.96	0.46
1:B:355:ASN:OD1	1:B:381:ASP:HB3	2.15	0.46
1:A:374:ARG:NH1	1:A:385:GLN:HB3	2.30	0.45
1:A:777:PRO:O	1:A:781:PRO:HB3	2.17	0.45
1:B:353:GLY:HA3	1:B:383:LEU:HD11	1.99	0.45
1:B:141:TYR:OH	1:B:167:MET:HE1	2.17	0.45
1:A:129:ALA:HB2	1:A:143:SER:HB2	1.99	0.45
1:B:121:GLU:OE2	1:B:219:GLU:HB2	2.16	0.45
1:B:163:HIS:O	1:B:192:SER:HB2	2.17	0.44
1:A:394:ARG:HD2	1:A:394:ARG:HA	1.71	0.44
1:A:506:LYS:HD2	1:B:531:TRP:CZ2	2.53	0.44
1:B:332:VAL:HG13	1:B:333:ILE:H	1.83	0.44
1:B:532:GLU:CD	1:B:535:GLY:H	2.25	0.44
1:A:401:ARG:NH1	1:A:403:GLU:OE2	2.47	0.44
1:A:351:ASN:O	1:A:385:GLN:NE2	2.50	0.44
1:A:359:LEU:HD12	1:A:359:LEU:HA	1.75	0.44
1:A:607:ILE:HG22	1:A:613:ILE:HD12	2.00	0.44
1:B:145:PHE:CE2	1:B:147:ILE:HD11	2.52	0.44
1:A:886:SER:HB2	1:A:893:LYS:HG3	1.99	0.44
1:B:71:LYS:HE3	1:B:142:GLU:OE1	2.17	0.44
1:A:255:ASP:HA	1:A:286:ILE:HD12	1.99	0.43
1:B:395:ASP:OD2	1:B:401:ARG:NH2	2.33	0.43
1:A:362:HIS:O	1:A:366:GLN:HG3	2.17	0.43
1:A:69:SER:HA	1:A:146:VAL:HG22	2.00	0.43
1:B:381:ASP:OD2	3:B:1114:HOH:O	2.20	0.43
1:A:840:LEU:HD23	1:A:840:LEU:HA	1.81	0.43
1:B:281:ARG:O	3:B:1115:HOH:O	2.21	0.43
1:B:608:ASN:OD1	1:B:608:ASN:N	2.37	0.43
1:B:95:ASP:O	1:B:96:ASP:HB2	2.18	0.43
1:B:320:SER:HB3	1:B:365:LEU:CD2	2.49	0.42
1:B:362:HIS:O	1:B:364:VAL:HG23	2.17	0.42
1:A:706:LEU:HG	1:A:730:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PRO:C	1:B:359:LEU:H	2.27	0.42
1:B:440:SER:OG	1:B:511:GLU:OE1	2.25	0.42
1:B:695:LYS:HA	1:B:695:LYS:HD2	1.96	0.42
1:A:366:GLN:HG2	1:A:373:VAL:HG12	2.00	0.42
1:B:344:THR:HG23	3:B:1385:HOH:O	2.19	0.42
1:A:750:HIS:CD2	1:A:750:HIS:C	2.97	0.42
1:B:430:LEU:HB3	1:B:435:TYR:CD2	2.55	0.42
1:B:362:HIS:C	1:B:364:VAL:N	2.67	0.42
1:B:259:GLU:C	1:B:261:THR:H	2.26	0.42
1:B:324:ALA:HB1	1:B:365:LEU:HD11	2.01	0.42
1:B:481:GLU:HB3	1:B:622:TYR:CZ	2.54	0.42
1:B:344:THR:O	1:B:348:GLU:HG3	2.19	0.42
1:B:360:LYS:C	1:B:362:HIS:H	2.27	0.42
1:B:777:PRO:O	1:B:781:PRO:HB3	2.20	0.41
1:A:67:SER:HB3	1:A:146:VAL:CG1	2.49	0.41
1:A:102:GLY:HA3	1:A:163:HIS:HB2	2.02	0.41
1:A:121:GLU:OE2	1:A:219:GLU:HB2	2.20	0.41
1:B:259:GLU:O	1:B:262:ARG:NH1	2.50	0.41
1:A:746:VAL:HA	1:A:750:HIS:HB3	2.01	0.41
1:B:161:ASN:HB3	1:B:191:ALA:O	2.21	0.41
1:B:306:SER:HB2	1:B:316:ASN:OD1	2.20	0.41
1:A:710:TRP:HZ2	1:A:728:PRO:HD2	1.84	0.41
1:A:486:LYS:HE2	1:A:486:LYS:HB2	1.90	0.41
1:B:247:VAL:HG23	1:B:249:ASP:OD2	2.21	0.41
1:B:866:LYS:HA	1:B:872:HIS:ND1	2.36	0.41
1:A:424:TRP:HA	1:A:425:PRO:C	2.45	0.41
1:A:448:GLU:O	1:A:452:LYS:HB2	2.21	0.41
1:B:514:ARG:HB3	1:B:523:TRP:HB3	2.03	0.41
1:A:359:LEU:HB3	1:A:362:HIS:HB3	2.02	0.41
1:A:449:ARG:HB3	1:A:449:ARG:HH11	1.86	0.41
1:B:73:THR:OG1	1:B:173:VAL:HB	2.21	0.40
1:B:256:SER:OG	3:B:1110:HOH:O	2.22	0.40
1:A:350:TYR:OH	1:A:764:TYR:HA	2.22	0.40
1:B:617:PHE:HA	1:B:770:THR:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:NE2	1:B:98:SER:OG[2_444]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	822/863 (95%)	797 (97%)	24 (3%)	1 (0%)	48	46
1	B	821/863 (95%)	774 (94%)	43 (5%)	4 (0%)	24	21
All	All	1643/1726 (95%)	1571 (96%)	67 (4%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	363	LYS
1	B	127	ALA
1	B	358	ASN
1	A	127	ALA
1	B	357	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	720/749 (96%)	715 (99%)	5 (1%)	76	82
1	B	720/749 (96%)	705 (98%)	15 (2%)	47	52
All	All	1440/1498 (96%)	1420 (99%)	20 (1%)	59	66

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL

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Mol	Chain	Res	Type
1	A	382	SER
1	A	392	LEU
1	A	480	SER
1	A	484	GLN
1	B	84	LEU
1	B	90	LEU
1	B	139	VAL
1	B	154	ILE
1	B	157	VAL
1	B	162	GLU
1	B	192	SER
1	B	268	SER
1	B	308	VAL
1	B	332	VAL
1	B	336	THR
1	B	608	ASN
1	B	618	THR
1	B	657	SER
1	B	831	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	198	GLN
1	A	408	GLN
1	A	767	ASN
1	B	161	ASN
1	B	163	HIS
1	B	362	HIS
1	B	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	828/863 (95%)	0.13	34 (4%) 41 40	18, 33, 68, 89	0
1	B	827/863 (95%)	0.65	107 (12%) 7 6	20, 40, 77, 89	0
All	All	1655/1726 (95%)	0.39	141 (8%) 16 15	18, 37, 73, 89	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ILE	4.9
1	B	311	LEU	4.2
1	B	78	LEU	4.2
1	B	373	VAL	4.0
1	B	232	GLY	3.7
1	B	375	ALA	3.7
1	B	288	PRO	3.6
1	B	359	LEU	3.6
1	B	292	THR	3.6
1	B	72	ALA	3.6
1	A	139	VAL	3.5
1	B	285	LYS	3.5
1	B	74	VAL	3.5
1	B	140	THR	3.5
1	B	254	PRO	3.4
1	A	133	ALA	3.4
1	B	109	VAL	3.4
1	A	146	VAL	3.4
1	B	107	LEU	3.3
1	B	73	THR	3.2
1	B	83	PHE	3.2
1	B	290	ALA	3.2
1	B	133	ALA	3.1
1	B	101	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	88	ILE	3.1
1	A	450	GLU	3.1
1	B	177	PHE	3.1
1	A	379	ALA	3.1
1	B	154	ILE	3.1
1	B	365	LEU	3.1
1	B	286	ILE	3.0
1	B	100	TRP	3.0
1	B	130	HIS	3.0
1	B	321	ALA	3.0
1	A	359	LEU	3.0
1	B	190	VAL	3.0
1	B	253	ASP	3.0
1	B	141	TYR	2.9
1	B	400	PHE	2.9
1	A	127	ALA	2.9
1	B	265	LEU	2.9
1	B	239	TYR	2.9
1	B	158	LEU	2.8
1	B	104	THR	2.8
1	B	255	ASP	2.8
1	B	139	VAL	2.8
1	B	147	ILE	2.8
1	A	126	GLY	2.8
1	A	375	ALA	2.8
1	B	368	ILE	2.8
1	B	424	TRP	2.8
1	B	332	VAL	2.7
1	A	783	GLU	2.7
1	B	127	ALA	2.7
1	B	271	TYR	2.7
1	A	147	ILE	2.7
1	B	87	LEU	2.7
1	B	261	THR	2.7
1	A	100	TRP	2.7
1	B	103	LYS	2.6
1	B	609	ALA	2.6
1	A	87	LEU	2.6
1	A	116	PRO	2.6
1	B	430	LEU	2.6
1	B	80	VAL	2.6
1	B	146	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	325	VAL	2.6
1	B	125	ILE	2.5
1	B	79	THR	2.5
1	B	426	LEU	2.5
1	B	194	PHE	2.5
1	A	70	VAL	2.5
1	B	97	VAL	2.5
1	B	75	THR	2.5
1	B	382	SER	2.5
1	B	84	LEU	2.5
1	A	99	ASP	2.4
1	A	103	LYS	2.4
1	B	90	LEU	2.4
1	B	70	VAL	2.4
1	A	692	PHE	2.4
1	B	270	GLN	2.4
1	B	159	VAL	2.4
1	A	531	TRP	2.4
1	B	129	ALA	2.4
1	B	176	GLY	2.4
1	B	367	ASP	2.4
1	A	104	THR	2.4
1	B	145	PHE	2.3
1	B	132	ALA	2.3
1	A	179	ASN	2.3
1	A	78	LEU	2.3
1	A	145	PHE	2.3
1	B	148	PRO	2.3
1	B	105	LEU	2.3
1	B	324	ALA	2.3
1	A	101	LEU	2.3
1	A	107	LEU	2.3
1	B	167	MET	2.3
1	A	83	PHE	2.2
1	B	137	GLY	2.2
1	B	252	GLY	2.2
1	B	622	TYR	2.2
1	B	164	HIS	2.2
1	B	362	HIS	2.2
1	B	284	SER	2.2
1	B	258	PRO	2.2
1	B	356	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	482	VAL	2.2
1	A	130	HIS	2.2
1	A	400	PHE	2.2
1	B	157	VAL	2.2
1	B	383	LEU	2.2
1	B	170	ARG	2.2
1	B	296	THR	2.2
1	B	312	THR	2.2
1	B	329	ILE	2.1
1	B	82	GLY	2.1
1	B	621	LYS	2.1
1	B	162	GLU	2.1
1	B	172	ILE	2.1
1	B	287	ASP	2.1
1	B	126	GLY	2.1
1	B	193	LYS	2.1
1	A	140	THR	2.1
1	A	176	GLY	2.1
1	B	519	GLY	2.1
1	B	717	GLY	2.1
1	B	450	GLU	2.0
1	A	84	LEU	2.0
1	B	161	ASN	2.0
1	A	144	ASP	2.0
1	B	521	PRO	2.0
1	A	97	VAL	2.0
1	B	76	VAL	2.0
1	B	264	VAL	2.0
1	B	256	SER	2.0
1	B	283	MET	2.0
1	B	337	SER	2.0
1	B	838	ASP	2.0
1	B	319	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

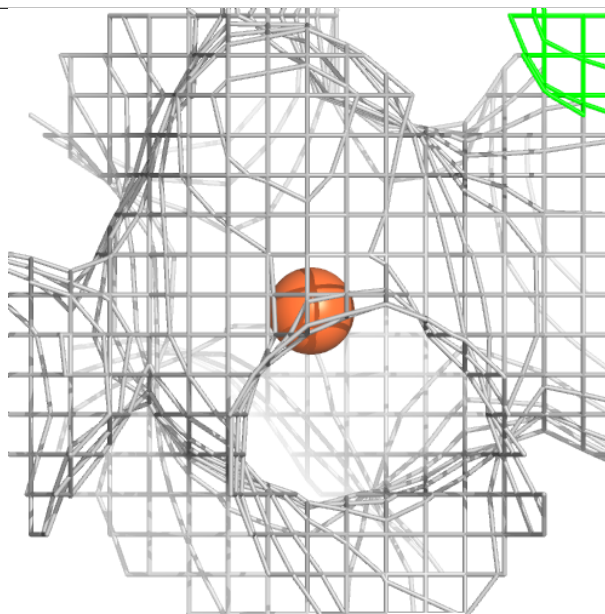
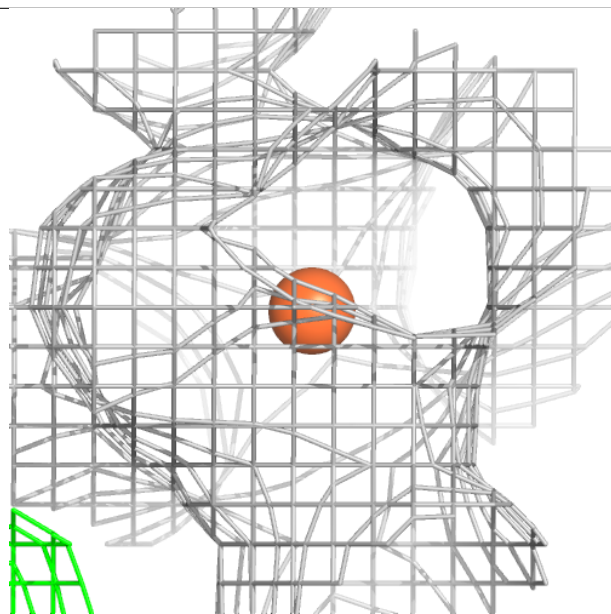
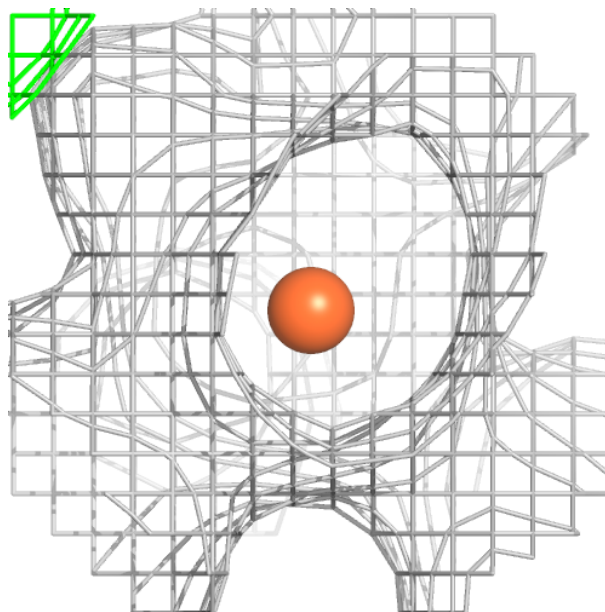
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	B	1001	1/1	0.99	0.03	29,29,29,29	0
2	FE	A	1001	1/1	1.00	0.01	21,21,21,21	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.

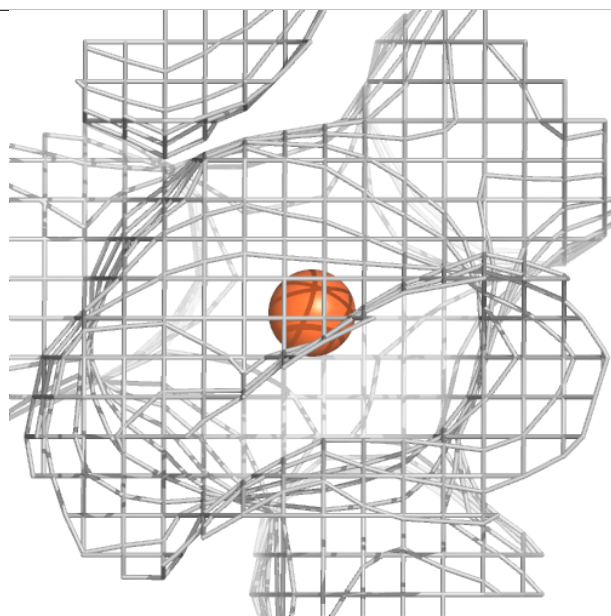
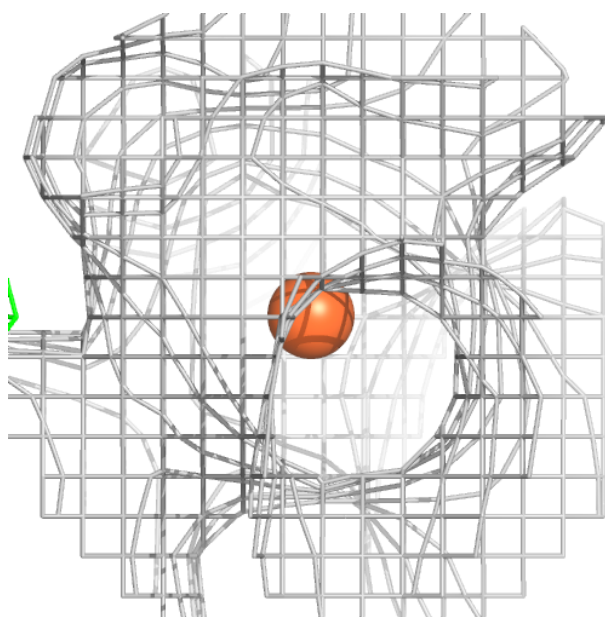
Electron density around FE B 1001:

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



Electron density around FE A 1001:

$2mF_o-DF_c$ (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.