



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:03 PM GMT

PDB ID : 3D3L
Title : The 2.6 Å crystal structure of the lipoxygenase domain of human arachidonate 12-lipoxygenase, 12S-type (CASP Target)
Authors : Tresaugues, L.; Moche, M.; Arrowsmith, C.H.; Berglund, H.; Busam, R.D.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Herman, M.D.; Johansson, A.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Lehtio, L.; Nilsson, M.E.; Nyman, T.; Olesen, K.; Persson, C.; Sagemark, J.; Schueler, H.; Svensson, L.; Thorsell, A.G.; Van Den Berg, S.; Welin, M.; Weigelt, J.; Wikstrom, M.; Nordlund, P.; Structural Genomics Consortium (SGC)
Deposited on : 2008-05-12
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

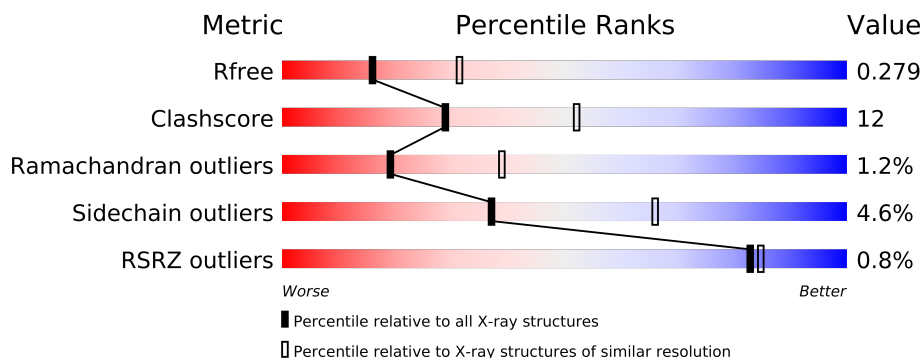
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	541	
1	B	541	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7268 atoms, of which 0 are hydrogen and 0 are deuterium.

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 12-lipoxygenase, 12S-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3595	2312	612	644	27			
1	B	447	Total	C	N	O	S	0	0	0
			3565	2293	608	637	27			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	MET	-	EXPRESSION TAG	UNP P18054
A	156	HIS	-	EXPRESSION TAG	UNP P18054
A	157	HIS	-	EXPRESSION TAG	UNP P18054
A	158	HIS	-	EXPRESSION TAG	UNP P18054
A	159	HIS	-	EXPRESSION TAG	UNP P18054
A	160	HIS	-	EXPRESSION TAG	UNP P18054
A	161	HIS	-	EXPRESSION TAG	UNP P18054
A	162	SER	-	EXPRESSION TAG	UNP P18054
A	163	SER	-	EXPRESSION TAG	UNP P18054
A	164	GLY	-	EXPRESSION TAG	UNP P18054
A	165	VAL	-	EXPRESSION TAG	UNP P18054
A	166	ASP	-	EXPRESSION TAG	UNP P18054
A	167	LEU	-	EXPRESSION TAG	UNP P18054
A	168	GLY	-	EXPRESSION TAG	UNP P18054
A	169	THR	-	EXPRESSION TAG	UNP P18054
A	170	GLU	-	EXPRESSION TAG	UNP P18054
A	171	ASN	-	EXPRESSION TAG	UNP P18054
A	261	ARG	GLN	VARIANT	UNP P18054
A	663	SER	ILE	ENGINEERED	UNP P18054
A	664	ASP	-	EXPRESSION TAG	UNP P18054
A	665	SER	-	EXPRESSION TAG	UNP P18054
A	666	LYS	-	EXPRESSION TAG	UNP P18054
A	667	GLY	-	EXPRESSION TAG	UNP P18054
A	668	GLY	-	EXPRESSION TAG	UNP P18054
A	669	TYR	-	EXPRESSION TAG	UNP P18054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	670	GLY	-	EXPRESSION TAG	UNP P18054
A	671	SER	-	EXPRESSION TAG	UNP P18054
A	672	GLU	-	EXPRESSION TAG	UNP P18054
A	673	PHE	-	EXPRESSION TAG	UNP P18054
A	674	GLU	-	EXPRESSION TAG	UNP P18054
A	675	LEU	-	EXPRESSION TAG	UNP P18054
A	676	ARG	-	EXPRESSION TAG	UNP P18054
A	677	ARG	-	EXPRESSION TAG	UNP P18054
A	678	GLN	-	EXPRESSION TAG	UNP P18054
A	679	ALA	-	EXPRESSION TAG	UNP P18054
A	680	CYS	-	EXPRESSION TAG	UNP P18054
A	681	GLY	-	EXPRESSION TAG	UNP P18054
A	682	ARG	-	EXPRESSION TAG	UNP P18054
A	683	THR	-	EXPRESSION TAG	UNP P18054
A	684	ARG	-	EXPRESSION TAG	UNP P18054
A	685	ALA	-	EXPRESSION TAG	UNP P18054
A	686	PRO	-	EXPRESSION TAG	UNP P18054
A	687	PRO	-	EXPRESSION TAG	UNP P18054
A	688	PRO	-	EXPRESSION TAG	UNP P18054
A	689	PRO	-	EXPRESSION TAG	UNP P18054
A	690	PRO	-	EXPRESSION TAG	UNP P18054
A	691	LEU	-	EXPRESSION TAG	UNP P18054
A	692	ARG	-	EXPRESSION TAG	UNP P18054
A	693	SER	-	EXPRESSION TAG	UNP P18054
A	694	GLY	-	EXPRESSION TAG	UNP P18054
A	695	CYS	-	EXPRESSION TAG	UNP P18054
B	155	MET	-	EXPRESSION TAG	UNP P18054
B	156	HIS	-	EXPRESSION TAG	UNP P18054
B	157	HIS	-	EXPRESSION TAG	UNP P18054
B	158	HIS	-	EXPRESSION TAG	UNP P18054
B	159	HIS	-	EXPRESSION TAG	UNP P18054
B	160	HIS	-	EXPRESSION TAG	UNP P18054
B	161	HIS	-	EXPRESSION TAG	UNP P18054
B	162	SER	-	EXPRESSION TAG	UNP P18054
B	163	SER	-	EXPRESSION TAG	UNP P18054
B	164	GLY	-	EXPRESSION TAG	UNP P18054
B	165	VAL	-	EXPRESSION TAG	UNP P18054
B	166	ASP	-	EXPRESSION TAG	UNP P18054
B	167	LEU	-	EXPRESSION TAG	UNP P18054
B	168	GLY	-	EXPRESSION TAG	UNP P18054
B	169	THR	-	EXPRESSION TAG	UNP P18054
B	170	GLU	-	EXPRESSION TAG	UNP P18054

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Chain	Residue	Modelled	Actual	Comment	Reference
B	171	ASN	-	EXPRESSION TAG	UNP P18054
B	261	ARG	GLN	VARIANT	UNP P18054
B	663	SER	ILE	ENGINEERED	UNP P18054
B	664	ASP	-	EXPRESSION TAG	UNP P18054
B	665	SER	-	EXPRESSION TAG	UNP P18054
B	666	LYS	-	EXPRESSION TAG	UNP P18054
B	667	GLY	-	EXPRESSION TAG	UNP P18054
B	668	GLY	-	EXPRESSION TAG	UNP P18054
B	669	TYR	-	EXPRESSION TAG	UNP P18054
B	670	GLY	-	EXPRESSION TAG	UNP P18054
B	671	SER	-	EXPRESSION TAG	UNP P18054
B	672	GLU	-	EXPRESSION TAG	UNP P18054
B	673	PHE	-	EXPRESSION TAG	UNP P18054
B	674	GLU	-	EXPRESSION TAG	UNP P18054
B	675	LEU	-	EXPRESSION TAG	UNP P18054
B	676	ARG	-	EXPRESSION TAG	UNP P18054
B	677	ARG	-	EXPRESSION TAG	UNP P18054
B	678	GLN	-	EXPRESSION TAG	UNP P18054
B	679	ALA	-	EXPRESSION TAG	UNP P18054
B	680	CYS	-	EXPRESSION TAG	UNP P18054
B	681	GLY	-	EXPRESSION TAG	UNP P18054
B	682	ARG	-	EXPRESSION TAG	UNP P18054
B	683	THR	-	EXPRESSION TAG	UNP P18054
B	684	ARG	-	EXPRESSION TAG	UNP P18054
B	685	ALA	-	EXPRESSION TAG	UNP P18054
B	686	PRO	-	EXPRESSION TAG	UNP P18054
B	687	PRO	-	EXPRESSION TAG	UNP P18054
B	688	PRO	-	EXPRESSION TAG	UNP P18054
B	689	PRO	-	EXPRESSION TAG	UNP P18054
B	690	PRO	-	EXPRESSION TAG	UNP P18054
B	691	LEU	-	EXPRESSION TAG	UNP P18054
B	692	ARG	-	EXPRESSION TAG	UNP P18054
B	693	SER	-	EXPRESSION TAG	UNP P18054
B	694	GLY	-	EXPRESSION TAG	UNP P18054
B	695	CYS	-	EXPRESSION TAG	UNP P18054

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total 61	O 61	0	0
3	B	45	Total 45	O 45	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.59Å 70.15Å 77.87Å 65.37° 88.01° 69.82°	Depositor
Resolution (Å)	47.19 – 2.60 47.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.19-2.60) 97.8 (47.19-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.276 0.211 , 0.279	Depositor DCC
R_{free} test set	1628 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 25.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 32072 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7268	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.47	0/3692	0.64	3/5026 (0.1%)
1	B	0.47	0/3661	0.63	2/4983 (0.0%)
All	All	0.47	0/7353	0.63	5/10009 (0.0%)

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	1	4
1	B	1	2
All	All	2	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	SER	C-N-CD	-7.40	104.32	120.60
1	B	181	GLY	N-CA-C	-5.85	98.47	113.10
1	A	325	SER	C-N-CA	5.71	145.99	122.00
1	B	206	ILE	CB-CA-C	5.35	122.30	111.60
1	A	326	PRO	CA-N-CD	-5.23	104.17	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	206	ILE	CA
1	B	206	ILE	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	GLN	Peptide
1	A	322	ASN	Peptide
1	A	324	SER	Peptide
1	A	325	SER	Peptide
1	B	180	ALA	Peptide
1	B	325	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3595	0	3566	98	0
1	B	3565	0	3549	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	61	0	0	2	0
3	B	45	0	0	0	1
All	All	7268	0	7115	177	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (177) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:ASP:O	1:B:206:ILE:CG2	1.87	1.22
1:A:479:VAL:HG11	1:A:526:CYS:SG	2.00	1.00
1:B:315:VAL:HG22	1:B:332:LEU:CD2	1.94	0.98
1:B:202:ASP:O	1:B:206:ILE:HG22	1.67	0.94
1:A:573:THR:HG22	1:A:575:ALA:H	1.32	0.93
1:A:180:ALA:HB3	1:A:181:GLY:HA3	1.51	0.90
1:A:379:LEU:HD13	1:A:385:ILE:HD11	1.53	0.90
1:A:379:LEU:CD1	1:A:385:ILE:HD11	2.05	0.86
1:B:471:ILE:HG22	1:B:530:THR:HG23	1.58	0.84
1:B:364:THR:HG21	1:B:540:HIS:HD2	1.45	0.82
1:A:281:LEU:HD22	1:A:296:LEU:HD22	1.61	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:ALA:HB3	1:A:181:GLY:CA	2.12	0.79
1:B:202:ASP:O	1:B:206:ILE:HG23	1.82	0.79
1:A:286:ALA:HB2	1:A:296:LEU:HD12	1.66	0.78
1:B:364:THR:HG21	1:B:540:HIS:CD2	2.18	0.77
1:B:205:GLN:HB2	1:B:206:ILE:HG22	1.70	0.73
1:B:315:VAL:HG22	1:B:332:LEU:HD22	1.68	0.73
1:B:424:GLY:HA3	1:B:425:HIS:HB2	1.71	0.73
1:A:476:GLU:HA	1:A:479:VAL:HG12	1.72	0.72
1:B:318:ILE:HG21	1:B:565:PRO:HB3	1.73	0.70
1:B:231:GLN:HE22	1:B:556:ASN:HD21	1.38	0.70
1:B:260:LEU:CD2	1:B:315:VAL:HG21	2.22	0.69
1:B:211:LYS:O	1:B:212:SER:HB3	1.92	0.69
1:B:214:LEU:HD23	1:B:549:ASP:HB3	1.76	0.67
1:A:180:ALA:CB	1:A:181:GLY:CA	2.73	0.66
1:B:286:ALA:HB1	1:B:294:GLN:HB2	1.77	0.66
1:B:424:GLY:CA	1:B:425:HIS:HB2	2.26	0.66
1:A:231:GLN:HE22	1:A:556:ASN:HD21	1.44	0.65
1:B:639:THR:O	1:B:643:GLU:HG2	1.96	0.65
1:A:286:ALA:HB2	1:A:296:LEU:CD1	2.25	0.65
1:B:250:ARG:HH21	1:B:317:GLN:HE21	1.45	0.65
1:B:260:LEU:HD21	1:B:315:VAL:HG21	1.79	0.64
1:A:470:ILE:HD13	1:A:630:ASP:HB3	1.79	0.64
1:A:548:LEU:HB2	1:A:598:SER:OG	1.99	0.63
1:B:202:ASP:O	1:B:206:ILE:HG21	1.91	0.63
1:A:573:THR:HG22	1:A:575:ALA:N	2.11	0.62
1:B:390:ILE:CG2	1:B:391:PRO:HD3	2.29	0.62
1:B:211:LYS:O	1:B:212:SER:CB	2.47	0.61
1:B:233:LEU:HD11	1:B:311:LEU:HD22	1.81	0.61
1:A:379:LEU:HD13	1:A:385:ILE:CD1	2.27	0.60
1:B:390:ILE:HG22	1:B:391:PRO:HD3	1.83	0.60
1:A:286:ALA:HB3	1:A:294:GLN:O	2.01	0.60
1:B:205:GLN:N	1:B:206:ILE:HG22	2.17	0.60
1:A:315:VAL:HG21	1:A:330:LEU:HD22	1.83	0.60
1:A:254:PRO:HD2	1:A:330:LEU:HD12	1.85	0.59
1:B:284:ILE:HG23	1:B:424:GLY:O	2.03	0.58
1:A:385:ILE:C	1:A:385:ILE:HD12	2.24	0.58
1:B:479:VAL:HG21	1:B:526:CYS:SG	2.43	0.58
1:A:322:ASN:O	1:A:325:SER:N	2.36	0.57
1:A:471:ILE:CG2	1:A:530:THR:HG23	2.34	0.57
1:A:471:ILE:HG22	1:A:530:THR:HG23	1.85	0.57
1:A:279:ILE:HD12	1:A:280:LEU:N	2.20	0.57
1:B:205:GLN:CB	1:B:206:ILE:HG22	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:GLN:H	1:B:206:ILE:HG22	1.72	0.55
1:B:305:MET:HE3	1:B:311:LEU:HD13	1.88	0.55
1:B:305:MET:CE	1:B:311:LEU:HD13	2.37	0.54
1:A:301:VAL:HG21	1:A:347:VAL:HG11	1.89	0.54
1:B:258:GLU:HA	1:B:261:ARG:HB2	1.90	0.54
1:A:424:GLY:HA2	1:A:425:HIS:HB2	1.90	0.54
1:B:424:GLY:HA3	1:B:425:HIS:CB	2.38	0.53
1:A:177:THR:HG22	1:A:178:LEU:H	1.73	0.53
1:A:574:MET:HE3	1:A:578:MET:HG2	1.90	0.53
1:B:510:ALA:HB1	1:B:515:PHE:CD1	2.43	0.52
1:A:322:ASN:O	1:A:326:PRO:HD2	2.09	0.52
1:B:301:VAL:HG13	1:B:316:ILE:HG12	1.91	0.52
1:A:305:MET:CE	1:A:455:LEU:CD2	2.87	0.52
1:B:257:MET:CE	1:B:332:LEU:HD11	2.40	0.51
1:A:305:MET:CE	1:A:455:LEU:HD22	2.41	0.51
1:A:654:PRO:HA	1:A:657:ILE:HD12	1.93	0.51
1:A:379:LEU:HD11	1:A:385:ILE:HD11	1.88	0.51
1:A:284:ILE:HG22	1:A:285:PRO:O	2.11	0.51
1:A:325:SER:N	1:A:326:PRO:HD2	2.25	0.51
1:A:305:MET:HE1	1:A:455:LEU:HD21	1.93	0.51
1:B:284:ILE:HG22	1:B:296:LEU:HD12	1.93	0.50
1:A:638:ILE:HG23	1:A:641:ARG:NH2	2.26	0.50
1:B:284:ILE:CG2	1:B:424:GLY:O	2.58	0.50
1:B:423:GLY:O	1:B:424:GLY:C	2.50	0.50
1:A:305:MET:HE1	1:A:455:LEU:CD2	2.42	0.50
1:B:360:HIS:O	1:B:364:THR:HB	2.11	0.50
1:A:322:ASN:N	1:A:325:SER:O	2.43	0.49
1:B:475:VAL:O	1:B:479:VAL:HG13	2.13	0.49
1:A:257:MET:CE	1:A:332:LEU:HD11	2.42	0.49
1:B:492:ASP:O	1:B:496:GLN:HG2	2.13	0.49
1:B:180:ALA:N	1:B:181:GLY:HA3	2.28	0.49
1:A:471:ILE:HD12	1:A:533:VAL:HG11	1.95	0.49
1:A:466:ARG:CG	1:A:634:LEU:HD13	2.43	0.49
1:B:577:VAL:HG12	1:B:581:LEU:HD12	1.95	0.48
1:B:296:LEU:HD21	1:B:353:GLN:HG3	1.95	0.48
1:B:542:ALA:HB2	1:B:652:LEU:HD21	1.95	0.48
1:B:206:ILE:HD11	1:B:592:ALA:HA	1.95	0.48
1:A:221:CYS:HB2	1:A:227:LEU:HD22	1.96	0.48
1:A:254:PRO:CD	1:A:330:LEU:HD12	2.43	0.48
1:B:344:LYS:O	1:B:348:ARG:HG2	2.13	0.48
1:A:194:LEU:HD13	1:A:593:ILE:HD13	1.95	0.47
1:B:260:LEU:HD22	1:B:315:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:237:ASN:HB2	1:A:355:HIS:CD2	2.50	0.47
1:B:364:THR:HG22	1:B:365:HIS:N	2.28	0.47
1:B:205:GLN:CA	1:B:206:ILE:HG22	2.44	0.47
1:A:279:ILE:HD12	1:A:280:LEU:H	1.80	0.47
1:A:545:GLN:HE22	1:A:656:CYS:HB3	1.79	0.47
1:A:424:GLY:HA3	1:A:426:VAL:N	2.31	0.46
1:A:466:ARG:HG2	1:A:634:LEU:HD13	1.97	0.46
1:B:183:LEU:CD2	1:B:366:LEU:HD13	2.46	0.46
1:A:315:VAL:CG2	1:A:330:LEU:HD22	2.46	0.46
1:B:503:THR:HG23	1:B:515:PHE:HB3	1.96	0.46
1:A:431:ARG:O	1:A:434:ALA:HB3	2.16	0.46
1:B:193:LEU:HD12	1:B:193:LEU:O	2.16	0.46
1:A:476:GLU:HA	1:A:479:VAL:CG1	2.44	0.46
1:A:504:GLU:OE2	1:A:517:VAL:HG13	2.16	0.46
1:A:390:ILE:CG2	1:A:391:PRO:HD3	2.46	0.46
1:B:517:VAL:HG12	1:B:517:VAL:O	2.15	0.45
1:A:355:HIS:CD2	1:A:543:ILE:HD12	2.51	0.45
1:A:536:CYS:O	1:A:661:VAL:HG23	2.17	0.45
1:A:593:ILE:HG22	1:A:597:LEU:HD22	1.98	0.45
1:A:193:LEU:HD12	1:A:193:LEU:O	2.17	0.45
1:A:631:LEU:HD22	1:A:654:PRO:HB3	1.99	0.44
1:B:444:PRO:HG3	1:B:468:TRP:NE1	2.32	0.44
1:A:583:ASP:H	1:A:586:GLN:NE2	2.14	0.44
1:B:548:LEU:HD13	1:B:548:LEU:C	2.37	0.44
1:A:296:LEU:HD23	3:A:837:HOH:O	2.16	0.44
1:A:543:ILE:HD13	1:A:543:ILE:HA	1.90	0.44
1:B:471:ILE:CG2	1:B:530:THR:HG23	2.38	0.44
1:B:315:VAL:HG22	1:B:332:LEU:HD23	1.93	0.44
1:A:365:HIS:O	1:A:368:ALA:HB3	2.18	0.44
1:B:370:VAL:HG13	1:B:506:GLY:HA3	1.98	0.44
1:B:383:HIS:HD2	1:B:385:ILE:H	1.66	0.44
1:A:180:ALA:CB	1:A:181:GLY:HA3	2.27	0.44
1:A:379:LEU:HD22	1:A:383:HIS:CD2	2.52	0.44
1:A:214:LEU:HD23	1:A:549:ASP:HB3	1.99	0.44
1:A:305:MET:HE3	1:A:455:LEU:CD2	2.48	0.44
1:B:385:ILE:HD12	1:B:385:ILE:O	2.18	0.44
1:A:476:GLU:O	1:A:479:VAL:HG12	2.18	0.43
1:A:478:ILE:HG12	1:A:623:VAL:HG11	1.98	0.43
1:B:503:THR:HG23	1:B:515:PHE:CB	2.47	0.43
1:A:634:LEU:HD11	1:A:638:ILE:HD11	2.00	0.43
1:A:390:ILE:HG23	1:A:391:PRO:HD3	1.99	0.43
1:A:476:GLU:CA	1:A:479:VAL:HG12	2.47	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:491:GLY:O	1:A:493:PRO:HD3	2.17	0.43
1:A:305:MET:HE3	1:A:455:LEU:HD22	2.00	0.43
1:B:483:TYR:CD1	1:B:488:ILE:HG22	2.53	0.43
1:B:278:PHE:HD2	1:B:354:LEU:HD22	1.84	0.43
1:A:362:LEU:HG	1:A:363:ASN:HD22	1.84	0.42
1:A:177:THR:HG22	1:A:178:LEU:N	2.34	0.42
1:A:582:PRO:HB3	1:A:586:GLN:HE21	1.85	0.42
1:A:503:THR:HG23	1:A:515:PHE:CB	2.49	0.42
1:A:252:VAL:HG12	1:A:327:THR:HG23	2.02	0.42
1:B:227:LEU:HD11	1:B:550:TRP:CH2	2.54	0.42
1:A:204:ASP:O	1:A:209:GLY:N	2.47	0.42
1:B:495:LEU:HD21	1:B:525:LEU:HD22	2.01	0.42
1:A:479:VAL:HG13	1:A:480:HIS:N	2.34	0.42
1:A:573:THR:HG22	1:A:574:MET:N	2.35	0.42
1:A:277:ASP:OD1	1:A:279:ILE:HG23	2.20	0.42
1:B:176:TRP:O	1:B:177:THR:HG23	2.20	0.42
1:B:582:PRO:HB3	1:B:586:GLN:HE21	1.85	0.42
1:A:479:VAL:CG1	1:A:526:CYS:SG	2.91	0.42
1:B:231:GLN:OE1	1:B:348:ARG:NH2	2.52	0.42
1:A:562:ARG:HD3	1:A:586:GLN:HE22	1.85	0.42
1:B:241:LEU:O	1:B:450:ARG:HD2	2.19	0.42
1:B:537:THR:OG1	1:B:538:ALA:N	2.52	0.42
1:B:214:LEU:HD23	1:B:549:ASP:CB	2.46	0.42
1:A:322:ASN:O	1:A:325:SER:C	2.59	0.42
1:A:279:ILE:HG21	3:A:857:HOH:O	2.19	0.41
1:B:499:CYS:HB2	1:B:519:PHE:CE2	2.55	0.41
1:B:661:VAL:HG13	1:B:661:VAL:O	2.21	0.41
1:A:574:MET:HE3	1:A:578:MET:CG	2.50	0.41
1:A:296:LEU:HD21	1:A:353:GLN:HG3	2.02	0.41
1:A:573:THR:CG2	1:A:574:MET:N	2.83	0.41
1:A:470:ILE:HG22	1:A:627:PHE:CD1	2.55	0.41
1:A:363:ASN:ND2	1:A:436:LEU:HD13	2.36	0.41
1:A:634:LEU:O	1:A:638:ILE:HG12	2.20	0.41
1:A:240:LEU:HD21	1:A:354:LEU:HD12	2.03	0.41
1:A:484:GLN:H	1:A:488:ILE:HD12	1.85	0.41
1:B:547:GLN:NE2	1:B:551:TYR:CE2	2.89	0.41
1:B:233:LEU:CD1	1:B:311:LEU:HD22	2.51	0.40
1:A:191:TYR:OH	1:A:425:HIS:ND1	2.50	0.40
1:B:392:HIS:ND1	1:B:659:ASN:O	2.46	0.40
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.95	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	Distance(Å)	Clash(Å)
3:B:833:HOH:O	3:B:840:HOH:O[1.565]	2.11	0.09

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	443/541 (82%)	406 (92%)	32 (7%)	5 (1%)	21	42
1	B	439/541 (81%)	409 (93%)	24 (6%)	6 (1%)	16	32
All	All	882/1082 (82%)	815 (92%)	56 (6%)	11 (1%)	19	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ALA
1	A	326	PRO
1	B	206	ILE
1	B	212	SER
1	B	425	HIS
1	B	616	SER
1	A	206	ILE
1	B	424	GLY
1	A	425	HIS
1	A	393	ILE
1	B	443	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	392/468 (84%)	372 (95%)	20 (5%)	33	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	390/468 (83%)	374 (96%)	16 (4%)	41	72
All	All	782/936 (84%)	746 (95%)	36 (5%)	37	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	A	240	LEU
1	A	258	GLU
1	A	261	ARG
1	A	270	ASN
1	A	306	GLU
1	A	326	PRO
1	A	341	LEU
1	A	394	ARG
1	A	470	ILE
1	A	487	ASP
1	A	496	GLN
1	A	543	ILE
1	A	594	SER
1	A	597	LEU
1	A	603	ASP
1	A	604	MET
1	A	612	GLU
1	A	633	LYS
1	A	662	THR
1	B	224	ASP
1	B	242	ARG
1	B	243	ARG
1	B	258	GLU
1	B	259	GLU
1	B	261	ARG
1	B	327	THR
1	B	385	ILE
1	B	425	HIS
1	B	428	LEU
1	B	465	LEU
1	B	512	ASP
1	B	604	MET
1	B	612	GLU
1	B	633	LYS
1	B	641	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	363	ASN
1	A	383	HIS
1	A	520	GLN
1	A	539	GLN
1	A	545	GLN
1	A	556	ASN
1	A	586	GLN
1	B	269	GLN
1	B	270	ASN
1	B	317	GLN
1	B	363	ASN
1	B	383	HIS
1	B	425	HIS
1	B	545	GLN
1	B	547	GLN
1	B	556	ASN
1	B	586	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	451/541 (83%)	-0.32	1 (0%) 93 94	13, 24, 37, 49	0
1	B	447/541 (82%)	-0.33	6 (1%) 74 75	13, 23, 38, 52	0
All	All	898/1082 (82%)	-0.33	7 (0%) 83 85	13, 23, 38, 52	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	662	THR	4.5
1	A	611	LYS	3.5
1	B	611	LYS	2.7
1	B	616	SER	2.5
1	B	614	TYR	2.4
1	B	612	GLU	2.2
1	B	615	PHE	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 carbohydrates 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. 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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FE	B	801	1/1	0.14	-0.01	14,14,14,14	0
2	FE	A	801	1/1	0.11	-2.72	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.