wwPDB X-ray Structure Validation Summary Report (i)

Mar 7, 2026 – 12:39 AM UTC

PDB ID	:	3D3L / pdb_00003d3l
Title	:	The 2.6 A crystal structure of the lipoxygenase domain of human arachidonate 12-lipoxygenase, 12S-type
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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

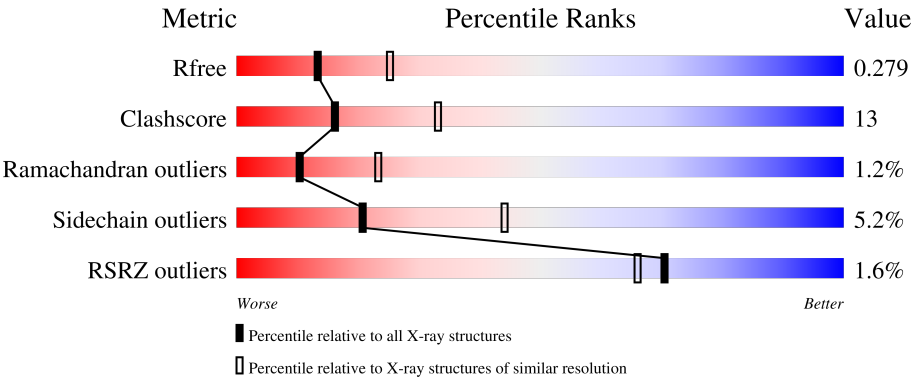
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12

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 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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 <=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	541	% 60% 21% • • 17%
1	B	541	% 60% 19% • • 17%

Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7268 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 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 mutation	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 mutation	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 (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is water.

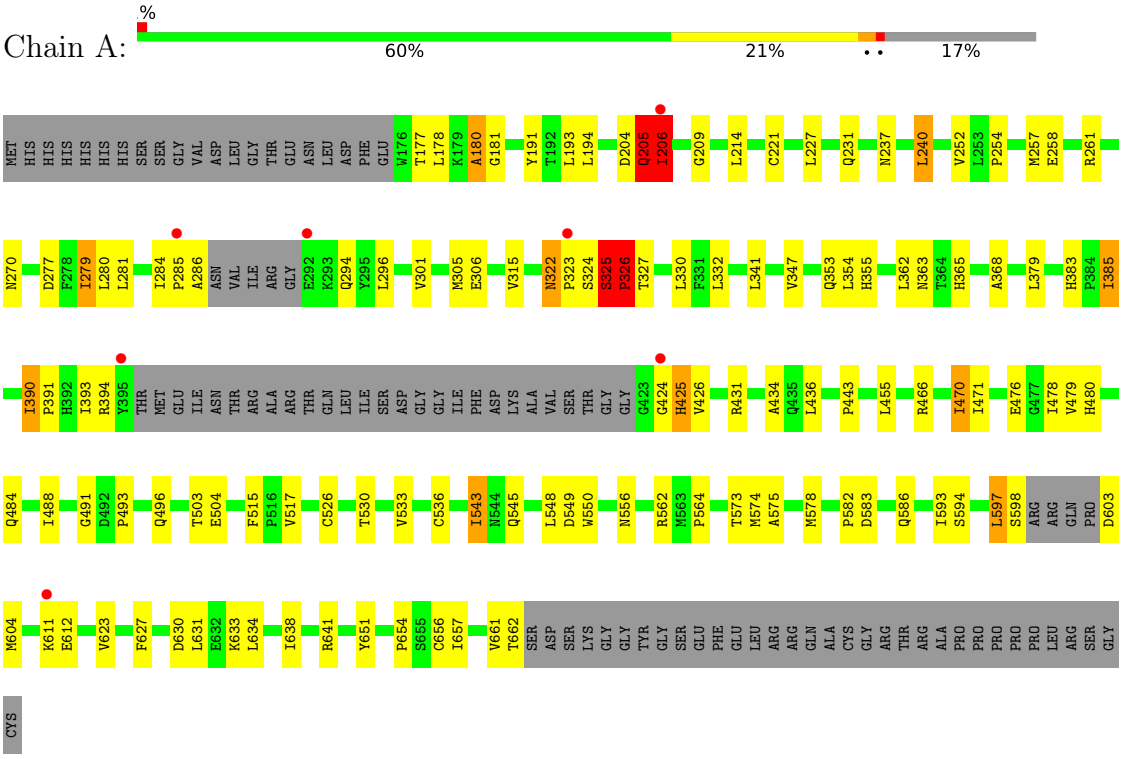
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	B	45	Total O 45 45	0	0

3 Residue-property plots (i)

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

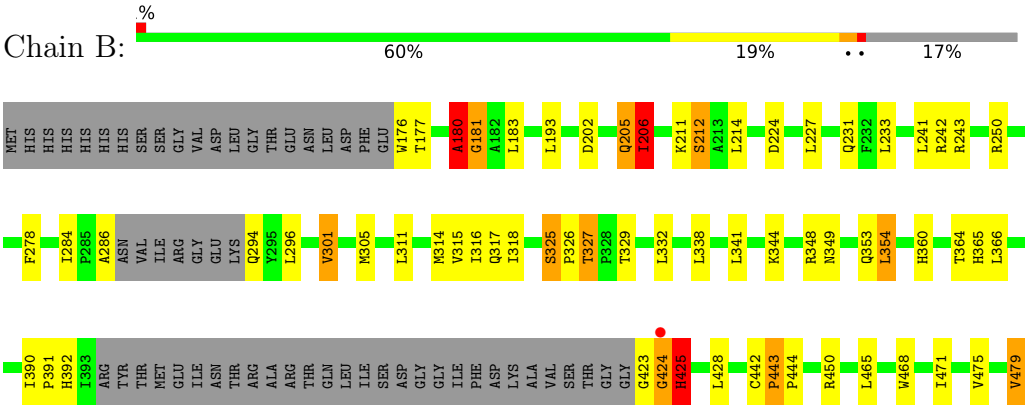
• Molecule 1: Arachidonate 12-lipoxygenase, 12S-type

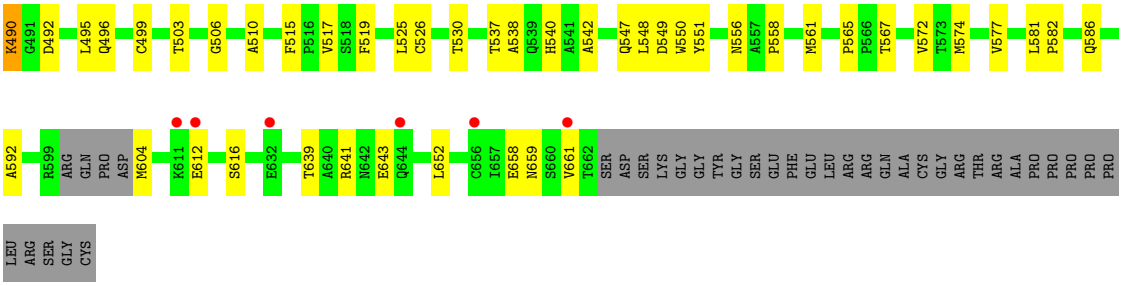
Chain A:



• Molecule 1: Arachidonate 12-lipoxygenase, 12S-type

Chain B:




K490 G491 D492 L495 Q496 C499 T503 G506 A510 F515 P516 V517 S518 F519 L525 C526 T530 T537 A538 Q539 H540 A541 A542 Q547 L548 D549 W550 Y551 N556 A557 P558 M561 P565 P566 T567 V572 T573 M574 V577 L581 P582 Q586
A592 R599 ARG GLN PRO ASP M604 K611 E612 S616 E632 T639 A640 R641 N642 E643 Q644 L652 C656 I657 E658 N659 S660 V661 T662 SER ASP SER LYS GLY GLY TYR GLY SER GLU PHE GLU LEU ARG ARG GLN ALA CYS GLY ARG THR ARG ALA PRO PRO PRO PRO PRO
LEU ARG SER GLY CYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.276 0.210 , 0.279	Depositor DCC
R_{free} test set	1628 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.62	1/3692 (0.0%)	0.99	10/5026 (0.2%)
1	B	0.62	0/3661	0.91	10/4983 (0.2%)
All	All	0.62	1/7353 (0.0%)	0.95	20/10009 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	ILE	CA-CB	7.49	1.58	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	SER	CA-C-N	20.92	145.99	119.84
1	A	325	SER	C-N-CA	20.92	145.99	119.84
1	B	205	GLN	N-CA-C	11.36	123.22	111.07
1	B	326	PRO	N-CA-C	-9.05	104.15	114.92
1	A	205	GLN	N-CA-C	8.18	123.82	112.04

All (2) chirality outliers are listed below:

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

5 of 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

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	3595	0	3566	98	0
1	B	3565	0	3549	89	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	187	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 13.

The worst 5 of 187 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:202:ASP:O	1:B:206:ILE:CG2	1.87	1.22
1:A:574:MET:HE1	1:A:578:MET:HE2	1.33	1.09
1:A:479:VAL:HG11	1:A:526:CYS:SG	2.00	1.00
1:B:305:MET:HE3	1:B:311:LEU:HD13	1.43	1.00
1:A:305:MET:HE1	1:A:455:LEU:CD2	1.93	0.99

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:833:HOH:O	3:B:840:HOH:O[1_565]	2.11	0.09

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	443/541 (82%)	406 (92%)	32 (7%)	5 (1%)	11 25
1	B	439/541 (81%)	409 (93%)	24 (6%)	6 (1%)	9 19
All	All	882/1082 (82%)	815 (92%)	56 (6%)	11 (1%)	10 23

5 of 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

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	392/468 (84%)	369 (94%)	23 (6%)	18 38
1	B	390/468 (83%)	372 (95%)	18 (5%)	24 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	782/936 (84%)	741 (95%)	41 (5%)	21 44

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	301	VAL
1	B	465	LEU
1	B	327	THR
1	B	385	ILE
1	B	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	317	GLN
1	B	383	HIS
1	B	363	ASN
1	B	425	HIS
1	A	520	GLN

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 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.04	7 (1%)	70	66	13, 24, 37, 49	0
1	B	447/541 (82%)	0.01	7 (1%)	70	66	13, 23, 38, 52	0
All	All	898/1082 (82%)	0.02	14 (1%)	70	66	13, 23, 38, 52	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	TYR	3.5
1	B	424	GLY	3.1
1	A	611	LYS	2.8
1	B	611	LYS	2.6
1	B	644	GLN	2.5

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	A	801	1/1	0.99	0.01	13,13,13,13	0
2	FE	B	801	1/1	0.99	0.03	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.