



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:31 pm BST

PDB ID : 3RDE
Title : Crystal structure of the catalytic domain of porcine leukocyte 12-lipoxygenase
Authors : Funk, M.O.; Xu, S.; Marnett, L.J.; Mueser, T.C.
Deposited on : 2011-04-01
Resolution : 1.89 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

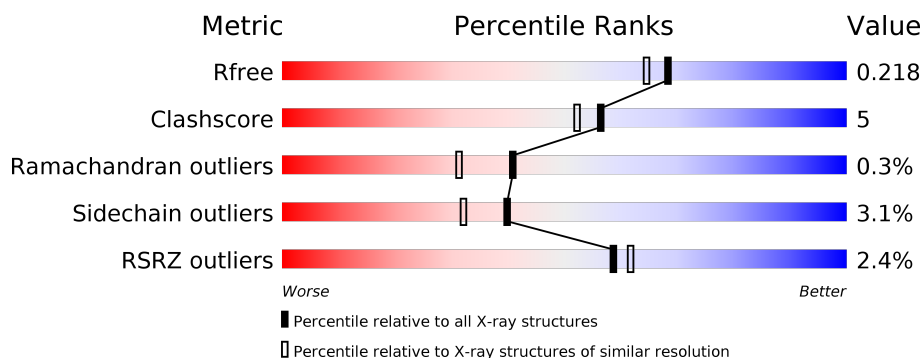
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	573	<div> <div>83%</div> <div>12%</div> <div>• •</div> </div>
1	B	573	<div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	C	573	<div> <div>6%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>
1	D	573	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>• •</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19031 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	552	Total	C	N	O	S	13	3	0
			4412	2824	760	804	24			
1	B	552	Total	C	N	O	S	9	4	0
			4421	2829	762	806	24			
1	C	552	Total	C	N	O	S	43	1	0
			4398	2816	756	802	24			
1	D	552	Total	C	N	O	S	35	4	0
			4416	2826	758	808	24			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	-	INITIATING METHIONINE	UNP P16469
A	92	GLY	-	EXPRESSION TAG	UNP P16469
A	93	SER	-	EXPRESSION TAG	UNP P16469
A	94	SER	-	EXPRESSION TAG	UNP P16469
A	95	HIS	-	EXPRESSION TAG	UNP P16469
A	96	HIS	-	EXPRESSION TAG	UNP P16469
A	97	HIS	-	EXPRESSION TAG	UNP P16469
A	98	HIS	-	EXPRESSION TAG	UNP P16469
A	99	HIS	-	EXPRESSION TAG	UNP P16469
A	100	HIS	-	EXPRESSION TAG	UNP P16469
A	101	SER	-	EXPRESSION TAG	UNP P16469
A	102	SER	-	EXPRESSION TAG	UNP P16469
A	103	GLY	-	EXPRESSION TAG	UNP P16469
A	104	LEU	-	EXPRESSION TAG	UNP P16469
A	105	VAL	-	EXPRESSION TAG	UNP P16469
A	106	PRO	-	EXPRESSION TAG	UNP P16469
A	107	ARG	-	EXPRESSION TAG	UNP P16469
A	108	GLY	-	EXPRESSION TAG	UNP P16469
A	109	SER	-	EXPRESSION TAG	UNP P16469
A	110	HIS	-	EXPRESSION TAG	UNP P16469
A	111	MET	-	EXPRESSION TAG	UNP P16469

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Chain	Residue	Modelled	Actual	Comment	Reference
A	210	SER	CYS	ENGINEERED MUTATION	UNP P16469
A	218	ARG	GLN	ENGINEERED MUTATION	UNP P16469
A	292	SER	CYS	ENGINEERED MUTATION	UNP P16469
B	91	MET	-	INITIATING METHIONINE	UNP P16469
B	92	GLY	-	EXPRESSION TAG	UNP P16469
B	93	SER	-	EXPRESSION TAG	UNP P16469
B	94	SER	-	EXPRESSION TAG	UNP P16469
B	95	HIS	-	EXPRESSION TAG	UNP P16469
B	96	HIS	-	EXPRESSION TAG	UNP P16469
B	97	HIS	-	EXPRESSION TAG	UNP P16469
B	98	HIS	-	EXPRESSION TAG	UNP P16469
B	99	HIS	-	EXPRESSION TAG	UNP P16469
B	100	HIS	-	EXPRESSION TAG	UNP P16469
B	101	SER	-	EXPRESSION TAG	UNP P16469
B	102	SER	-	EXPRESSION TAG	UNP P16469
B	103	GLY	-	EXPRESSION TAG	UNP P16469
B	104	LEU	-	EXPRESSION TAG	UNP P16469
B	105	VAL	-	EXPRESSION TAG	UNP P16469
B	106	PRO	-	EXPRESSION TAG	UNP P16469
B	107	ARG	-	EXPRESSION TAG	UNP P16469
B	108	GLY	-	EXPRESSION TAG	UNP P16469
B	109	SER	-	EXPRESSION TAG	UNP P16469
B	110	HIS	-	EXPRESSION TAG	UNP P16469
B	111	MET	-	EXPRESSION TAG	UNP P16469
B	210	SER	CYS	ENGINEERED MUTATION	UNP P16469
B	218	ARG	GLN	ENGINEERED MUTATION	UNP P16469
B	292	SER	CYS	ENGINEERED MUTATION	UNP P16469
C	91	MET	-	INITIATING METHIONINE	UNP P16469
C	92	GLY	-	EXPRESSION TAG	UNP P16469
C	93	SER	-	EXPRESSION TAG	UNP P16469
C	94	SER	-	EXPRESSION TAG	UNP P16469
C	95	HIS	-	EXPRESSION TAG	UNP P16469
C	96	HIS	-	EXPRESSION TAG	UNP P16469
C	97	HIS	-	EXPRESSION TAG	UNP P16469
C	98	HIS	-	EXPRESSION TAG	UNP P16469
C	99	HIS	-	EXPRESSION TAG	UNP P16469
C	100	HIS	-	EXPRESSION TAG	UNP P16469
C	101	SER	-	EXPRESSION TAG	UNP P16469
C	102	SER	-	EXPRESSION TAG	UNP P16469
C	103	GLY	-	EXPRESSION TAG	UNP P16469
C	104	LEU	-	EXPRESSION TAG	UNP P16469
C	105	VAL	-	EXPRESSION TAG	UNP P16469

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Chain	Residue	Modelled	Actual	Comment	Reference
C	106	PRO	-	EXPRESSION TAG	UNP P16469
C	107	ARG	-	EXPRESSION TAG	UNP P16469
C	108	GLY	-	EXPRESSION TAG	UNP P16469
C	109	SER	-	EXPRESSION TAG	UNP P16469
C	110	HIS	-	EXPRESSION TAG	UNP P16469
C	111	MET	-	EXPRESSION TAG	UNP P16469
C	210	SER	CYS	ENGINEERED MUTATION	UNP P16469
C	218	ARG	GLN	ENGINEERED MUTATION	UNP P16469
C	292	SER	CYS	ENGINEERED MUTATION	UNP P16469
D	91	MET	-	INITIATING METHIONINE	UNP P16469
D	92	GLY	-	EXPRESSION TAG	UNP P16469
D	93	SER	-	EXPRESSION TAG	UNP P16469
D	94	SER	-	EXPRESSION TAG	UNP P16469
D	95	HIS	-	EXPRESSION TAG	UNP P16469
D	96	HIS	-	EXPRESSION TAG	UNP P16469
D	97	HIS	-	EXPRESSION TAG	UNP P16469
D	98	HIS	-	EXPRESSION TAG	UNP P16469
D	99	HIS	-	EXPRESSION TAG	UNP P16469
D	100	HIS	-	EXPRESSION TAG	UNP P16469
D	101	SER	-	EXPRESSION TAG	UNP P16469
D	102	SER	-	EXPRESSION TAG	UNP P16469
D	103	GLY	-	EXPRESSION TAG	UNP P16469
D	104	LEU	-	EXPRESSION TAG	UNP P16469
D	105	VAL	-	EXPRESSION TAG	UNP P16469
D	106	PRO	-	EXPRESSION TAG	UNP P16469
D	107	ARG	-	EXPRESSION TAG	UNP P16469
D	108	GLY	-	EXPRESSION TAG	UNP P16469
D	109	SER	-	EXPRESSION TAG	UNP P16469
D	110	HIS	-	EXPRESSION TAG	UNP P16469
D	111	MET	-	EXPRESSION TAG	UNP P16469
D	210	SER	CYS	ENGINEERED MUTATION	UNP P16469
D	218	ARG	GLN	ENGINEERED MUTATION	UNP P16469
D	292	SER	CYS	ENGINEERED MUTATION	UNP P16469

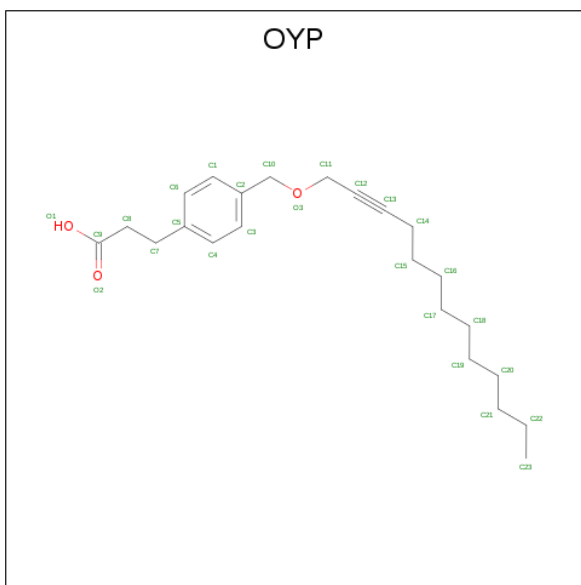
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 4 is 3-{4-[(tridec-2-yn-1-yloxy)methyl]phenyl}propanoic acid (three-letter code: OYP) (formula: C₂₃H₃₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			26	23	3		
4	B	1	Total	C	O	0	0
			26	23	3		
4	C	1	Total	C	O	0	0
			26	23	3		
4	D	1	Total	C	O	0	0
			26	23	3		

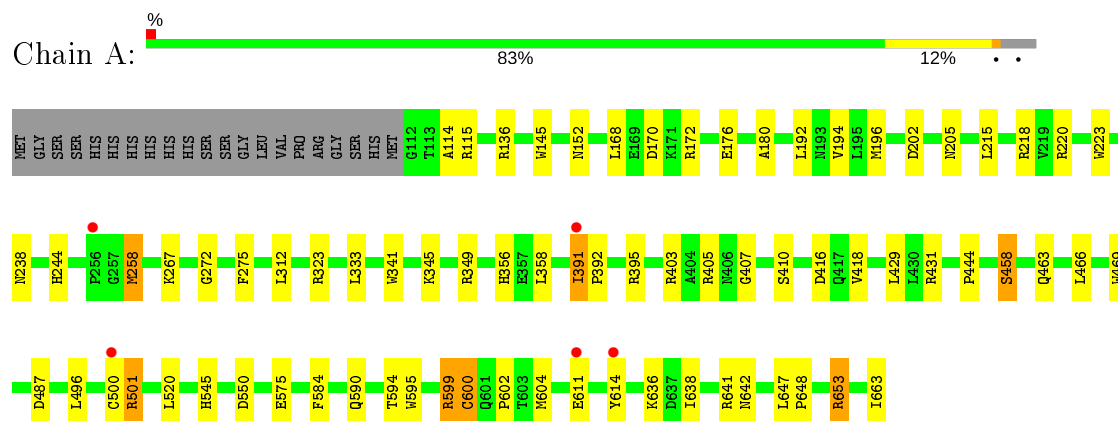
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	393	Total 393	O 393	0	0
5	B	386	Total 386	O 386	0	0
5	C	187	Total 187	O 187	0	0
5	D	308	Total 308	O 308	0	0

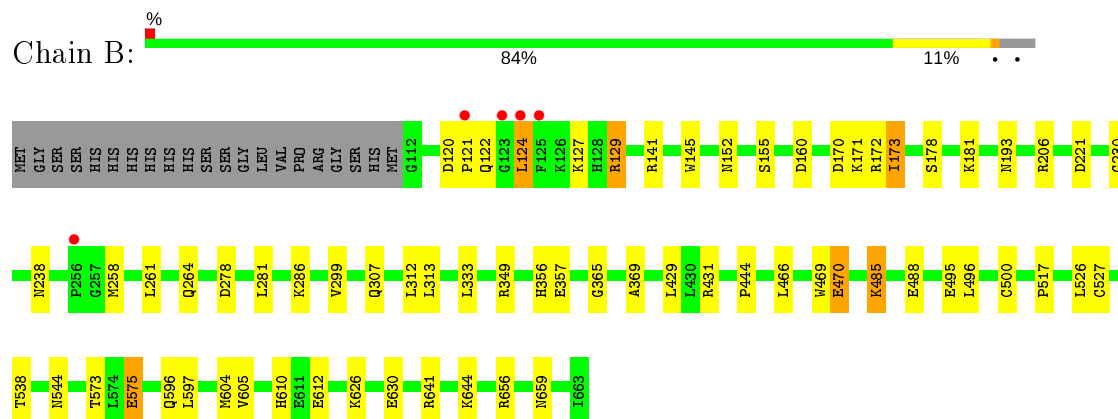
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

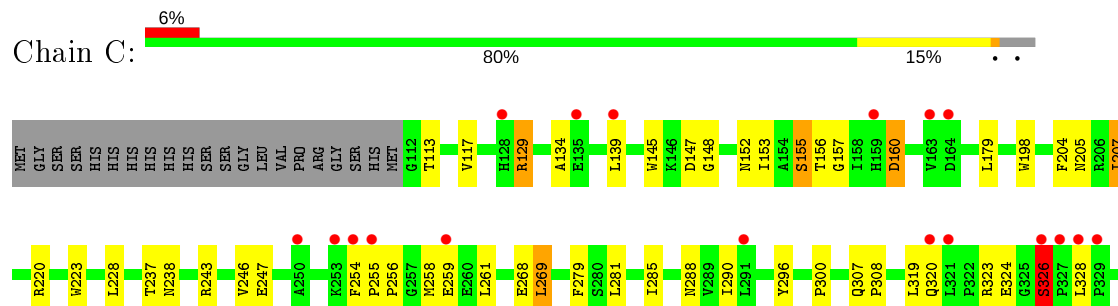
- Molecule 1: Arachidonate 12-lipoxygenase, 12S-type

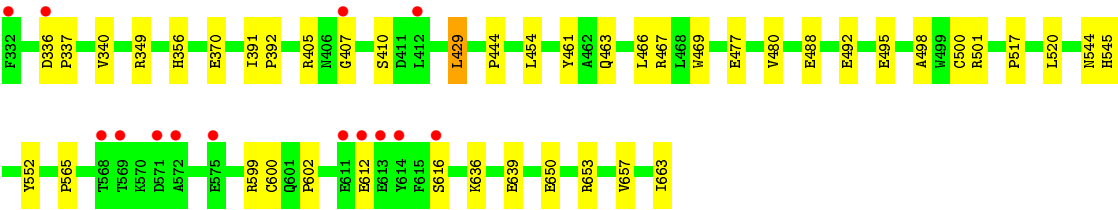


- Molecule 1: Arachidonate 12-lipoxygenase, 12S-type

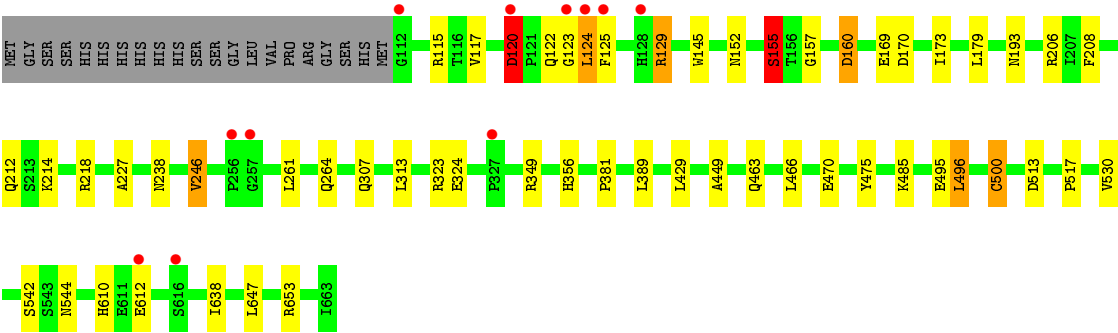
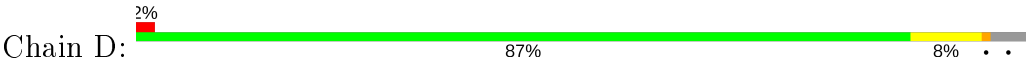


- Molecule 1: Arachidonate 12-lipoxygenase, 12S-type





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 181.54Å 91.61Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	48.97 – 1.89 48.97 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.97-1.89) 99.4 (48.97-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.214 0.179 , 0.218	Depositor DCC
R_{free} test set	6468 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19031	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: K, FE2, OYP

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	1.27	9/4527 (0.2%)	1.04	14/6144 (0.2%)
1	B	1.24	10/4536 (0.2%)	1.01	11/6156 (0.2%)
1	C	1.17	6/4510 (0.1%)	0.96	5/6122 (0.1%)
1	D	1.17	5/4531 (0.1%)	0.99	12/6150 (0.2%)
All	All	1.22	30/18104 (0.2%)	1.00	42/24572 (0.2%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	488	GLU	CD-OE1	5.95	1.32	1.25
1	C	498	ALA	CA-CB	5.94	1.65	1.52
1	A	600	CYS	CB-SG	5.91	1.92	1.82
1	C	461	TYR	CE2-CZ	-5.86	1.30	1.38
1	C	155	SER	C-N	-5.84	1.20	1.34
1	D	227	ALA	CA-CB	5.75	1.64	1.52
1	B	612	GLU	CB-CG	5.60	1.62	1.52
1	B	369	ALA	CA-CB	5.57	1.64	1.52
1	B	641	ARG	CG-CD	-5.57	1.38	1.51
1	A	653	ARG	CB-CG	-5.53	1.37	1.52
1	A	223	TRP	NE1-CE2	-5.53	1.30	1.37
1	A	431	ARG	CG-CD	5.50	1.65	1.51
1	A	575	GLU	CG-CD	5.50	1.60	1.51
1	C	480	VAL	CB-CG1	5.45	1.64	1.52
1	A	275	PHE	CE2-CZ	5.43	1.47	1.37
1	B	470	GLU	C-N	-5.40	1.21	1.34
1	C	148	GLY	N-CA	5.32	1.54	1.46
1	A	458	SER	CB-OG	-5.28	1.35	1.42
1	D	475	TYR	CD1-CE1	5.26	1.47	1.39
1	A	180	ALA	CA-CB	5.18	1.63	1.52
1	C	134	ALA	CA-CB	5.17	1.63	1.52
1	B	365	GLY	C-O	5.16	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	VAL	CB-CG2	5.13	1.63	1.52
1	D	449	ALA	CA-CB	5.12	1.63	1.52
1	B	605	VAL	CB-CG2	5.12	1.63	1.52
1	D	463	GLN	CG-CD	5.11	1.62	1.51
1	D	160	ASP	CB-CG	-5.08	1.41	1.51
1	B	181	LYS	CD-CE	5.06	1.64	1.51
1	B	575	GLU	CG-CD	5.06	1.59	1.51
1	A	418	VAL	CB-CG2	5.04	1.63	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	D	129	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	129	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	B	129	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	D	170	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	221	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	202	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	496	LEU	CA-CB-CG	5.91	128.88	115.30
1	A	312	LEU	CB-CG-CD1	5.87	120.98	111.00
1	A	501	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	136	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	416	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	170	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	349	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	513	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	431	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	395[A]	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	395[B]	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	349	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	246	VAL	CG1-CB-CG2	5.51	119.71	110.90
1	A	604	MET	CG-SD-CE	5.47	108.96	100.20
1	D	513	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	D	123	GLY	N-CA-C	5.43	126.69	113.10
1	B	172	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	170	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	D	429	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	A	496	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	538	THR	O-C-N	-5.36	114.10	123.20
1	D	349	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	487	ASP	CB-CG-OD1	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	115	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	431	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	403	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	141	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	597	LEU	CB-CG-CD2	5.13	119.72	111.00
1	B	278	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	326	SER	C-N-CD	-5.09	109.39	120.60
1	C	254	PHE	C-N-CD	-5.09	109.41	120.60
1	C	599	ARG	CG-CD-NE	-5.07	101.15	111.80
1	C	243	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	349	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4412	0	4407	42	0
1	B	4421	0	4414	43	0
1	C	4398	0	4389	56	0
1	D	4416	0	4404	36	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	33	0	0
4	B	26	0	33	0	0
4	C	26	0	33	1	0
4	D	26	0	33	0	0
5	A	393	0	0	1	0
5	B	386	0	0	2	0
5	C	187	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	308	0	0	3	0
All	All	19031	0	17746	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ILE:CG2	1:A:392:PRO:HD3	1.54	1.37
1:B:485:LYS:HD3	1:B:485:LYS:N	1.47	1.14
1:B:485:LYS:H	1:B:485:LYS:CD	1.63	1.09
1:B:485:LYS:HD3	1:B:485:LYS:H	0.91	1.07
1:A:391:ILE:CG2	1:A:392:PRO:CD	2.31	1.07
1:A:500[B]:CYS:SG	1:A:520:LEU:HG	2.00	1.01
1:A:391:ILE:HG22	1:A:392:PRO:HD3	1.03	1.00
1:A:391:ILE:HG22	1:A:392:PRO:CD	1.90	0.99
1:C:129:ARG:HD3	1:C:495:GLU:OE2	1.65	0.96
1:A:391:ILE:HG23	1:A:392:PRO:HD3	1.48	0.95
1:C:288:ASN:ND2	1:C:290:ILE:HD11	1.85	0.92
1:A:391:ILE:HG23	1:A:392:PRO:CD	1.99	0.91
1:D:542:SER:HB3	5:D:764:HOH:O	1.71	0.90
1:A:192:LEU:HG	1:A:196:MET:HE1	1.55	0.88
1:B:656[B]:ARG:HG3	1:B:656[B]:ARG:HH11	1.39	0.87
1:C:157:GLY:O	1:C:160:ASP:HB2	1.76	0.86
1:D:117:VAL:O	1:D:120:ASP:HB2	1.77	0.85
1:C:204:PHE:O	1:C:207:ILE:HD13	1.76	0.84
1:A:114:ALA:O	1:A:115:ARG:HD2	1.79	0.83
1:C:255:PRO:HD3	1:C:328:LEU:HD13	1.60	0.82
1:A:391:ILE:HG23	1:A:392:PRO:N	1.95	0.79
1:D:124:LEU:HD13	1:D:125:PHE:CE1	2.19	0.78
1:D:124:LEU:HD13	1:D:125:PHE:CD1	2.19	0.77
1:C:207:ILE:H	1:C:207:ILE:HD13	1.47	0.77
1:D:145:TRP:H	1:D:152:ASN:HD21	1.35	0.73
1:C:145:TRP:H	1:C:152:ASN:HD21	1.36	0.72
1:A:220:ARG:HD3	5:A:758:HOH:O	1.87	0.72
1:A:145:TRP:H	1:A:152:ASN:HD21	1.36	0.71
1:A:192:LEU:CG	1:A:196:MET:HE1	2.19	0.71
1:A:500[B]:CYS:HG	1:A:520:LEU:HG	1.55	0.69
1:B:307:GLN:NE2	1:B:313:LEU:HD12	2.08	0.68
1:A:391:ILE:HG21	1:A:614:TYR:CE1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HD22	4:C:664:OYP:O2	1.93	0.67
1:C:204:PHE:O	1:C:207:ILE:CD1	2.43	0.67
1:A:192:LEU:CD1	1:A:196:MET:HE1	2.26	0.66
1:C:500[B]:CYS:SG	1:C:517:PRO:HB2	2.36	0.66
1:C:356:HIS:HE1	1:C:544:ASN:O	1.79	0.66
1:B:656[B]:ARG:NH1	1:B:656[B]:ARG:HG3	2.08	0.65
1:D:466:LEU:O	1:D:470:GLU:HG3	1.98	0.63
1:D:542:SER:CB	5:D:764:HOH:O	2.39	0.63
1:A:172:ARG:O	1:A:176:GLU:HG3	1.99	0.63
1:A:205:ASN:ND2	1:A:220:ARG:HH11	1.97	0.63
1:C:155:SER:OG	1:C:160:ASP:HB3	1.99	0.62
1:B:178:SER:C	1:B:596[B]:GLN:HE22	2.03	0.61
1:D:169:GLU:HG2	1:D:173:ILE:HD12	1.82	0.61
1:C:288:ASN:CG	1:C:290:ILE:HD11	2.21	0.61
1:A:114:ALA:O	1:A:115:ARG:CD	2.50	0.60
1:A:205:ASN:HD22	1:A:220:ARG:HH11	1.50	0.59
1:B:145:TRP:H	1:B:152:ASN:HD21	1.49	0.58
1:B:193:ASN:HD22	1:B:206:ARG:HH21	1.49	0.58
1:C:600:CYS:O	1:C:602:PRO:HD3	2.02	0.58
1:A:642:ASN:HB3	1:A:648:PRO:HB3	1.85	0.58
1:D:169:GLU:CG	1:D:173:ILE:HD12	2.34	0.58
1:D:117:VAL:O	1:D:120:ASP:CB	2.51	0.57
1:D:124:LEU:CD1	1:D:125:PHE:CD1	2.86	0.57
1:B:281:LEU:HG	1:B:429:LEU:HD11	1.85	0.57
1:D:117:VAL:C	1:D:120:ASP:HB2	2.25	0.57
1:C:545:HIS:CE1	1:C:663:ILE:HG23	2.41	0.56
1:C:454:LEU:CD2	1:C:466:LEU:HD11	2.35	0.55
1:C:444:PRO:HD2	1:C:469:TRP:CE3	2.42	0.54
1:B:281:LEU:HG	1:B:429:LEU:CD1	2.37	0.54
1:D:124:LEU:CD1	1:D:125:PHE:HD1	2.20	0.54
1:C:429:LEU:HD12	1:C:429:LEU:O	2.07	0.54
1:B:178:SER:OG	1:B:596[B]:GLN:OE1	2.25	0.54
1:C:223:TRP:HA	1:C:228:LEU:HD23	1.88	0.54
1:C:129:ARG:NH1	1:C:495:GLU:OE1	2.41	0.54
1:C:356:HIS:CE1	1:C:544:ASN:O	2.60	0.54
1:A:194:VAL:HG12	1:A:584:PHE:HZ	1.73	0.53
1:D:356:HIS:HE1	1:D:544:ASN:O	1.91	0.53
1:C:650:GLU:OE1	1:C:653:ARG:HD3	2.10	0.52
1:A:391:ILE:HG21	1:A:614:TYR:CD1	2.45	0.52
1:D:129:ARG:CD	1:D:495:GLU:OE2	2.58	0.52
1:C:205:ASN:HD21	1:C:220:ARG:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:THR:OG1	1:B:575:GLU:HG2	2.10	0.52
1:B:124:LEU:CD1	1:B:124:LEU:C	2.78	0.51
1:B:129:ARG:CD	1:B:495:GLU:OE2	2.57	0.51
1:B:356:HIS:HE1	1:B:544:ASN:O	1.94	0.51
1:B:124:LEU:CD1	1:B:124:LEU:O	2.59	0.51
1:B:124:LEU:HD13	1:B:124:LEU:O	2.10	0.51
1:C:156:THR:OG1	1:C:160:ASP:OD2	2.28	0.51
1:D:129:ARG:HD3	1:D:495:GLU:OE2	2.11	0.50
1:C:204:PHE:HA	1:C:207:ILE:CD1	2.41	0.50
1:D:307:GLN:NE2	1:D:313:LEU:HD12	2.27	0.50
1:B:485:LYS:CE	1:B:485:LYS:H	2.22	0.50
1:C:405:ARG:O	1:C:410:SER:HB3	2.11	0.50
1:C:336:ASP:HB3	1:C:337:PRO:HD2	1.93	0.50
1:D:238:ASN:HB2	1:D:356:HIS:HB2	1.93	0.49
1:C:205:ASN:ND2	1:C:220:ARG:HD2	2.27	0.49
1:D:208:PHE:CZ	1:D:212:GLN:HG3	2.47	0.49
1:B:258:MET:CE	1:B:333:LEU:HD11	2.43	0.49
1:D:193:ASN:HD22	1:D:206:ARG:HH21	1.60	0.48
1:A:500[B]:CYS:SG	1:A:520:LEU:CG	2.89	0.48
1:B:466:LEU:O	1:B:470:GLU:HG3	2.13	0.48
1:A:600:CYS:O	1:A:602:PRO:HD3	2.12	0.48
1:B:160:ASP:C	1:B:160:ASP:OD1	2.52	0.48
1:B:193:ASN:ND2	1:B:206:ARG:HH21	2.11	0.48
1:C:391:ILE:CG2	1:C:392:PRO:HD3	2.44	0.48
1:D:193:ASN:ND2	1:D:206:ARG:HH21	2.12	0.48
1:A:341:TRP:CD1	1:A:345:LYS:HE2	2.48	0.47
1:C:285:ILE:HG13	1:C:429:LEU:HD22	1.95	0.47
1:C:500[B]:CYS:SG	1:C:520:LEU:HG	2.54	0.47
1:A:358:LEU:HD12	1:A:429:LEU:HD23	1.95	0.47
1:C:356:HIS:CD2	1:C:552:TYR:OH	2.67	0.47
1:C:153:ILE:HG22	1:C:370:GLU:OE2	2.14	0.47
1:C:307:GLN:HB3	1:C:308:PRO:HD2	1.96	0.47
1:B:170:ASP:OD1	1:B:171:LYS:N	2.38	0.47
1:B:129:ARG:HD2	1:B:495:GLU:OE2	2.15	0.46
1:D:124:LEU:HD13	1:D:125:PHE:HE1	1.79	0.46
1:D:157:GLY:O	1:D:160:ASP:HB2	2.15	0.46
1:B:129:ARG:HD3	1:B:495:GLU:OE2	2.14	0.46
1:C:117:VAL:HG13	1:C:129:ARG:NH1	2.31	0.46
1:C:155:SER:OG	1:C:160:ASP:CB	2.63	0.46
1:A:463:GLN:NE2	1:A:641:ARG:HH11	2.14	0.46
1:C:281:LEU:HG	1:C:429:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:HH11	1:C:495:GLU:CD	2.18	0.46
1:A:194:VAL:HG12	1:A:584:PHE:CZ	2.51	0.45
1:A:638:ILE:HG21	1:A:653:ARG:HG2	1.98	0.45
1:B:173:ILE:HA	1:B:173:ILE:HD12	1.67	0.45
1:C:207:ILE:H	1:C:207:ILE:CD1	2.21	0.45
1:A:238:ASN:HB2	1:A:356:HIS:HB2	1.98	0.45
1:B:444:PRO:HD2	1:B:469:TRP:CE3	2.52	0.45
1:A:258:MET:HE1	1:A:333:LEU:HD11	1.97	0.45
1:C:337:PRO:HG2	1:C:340:VAL:CG2	2.47	0.45
1:A:444:PRO:HD2	1:A:469:TRP:CE3	2.52	0.44
1:B:610:HIS:HD2	1:B:659:ASN:HD21	1.65	0.44
1:C:204:PHE:HA	1:C:207:ILE:HD11	1.98	0.44
1:C:237:THR:HG22	1:C:356:HIS:CE1	2.52	0.44
1:A:405:ARG:O	1:A:410:SER:HB3	2.17	0.44
1:B:656[B]:ARG:NH1	1:B:656[B]:ARG:CG	2.76	0.44
1:A:192:LEU:O	1:A:196:MET:HE2	2.18	0.44
1:B:527:CYS:HB3	5:B:832:HOH:O	2.18	0.44
1:C:279:PHE:HB2	1:C:300:PRO:HD2	2.00	0.44
1:C:198:TRP:HH2	1:C:207:ILE:HD12	1.82	0.44
1:D:638:ILE:HG21	1:D:653:ARG:HG2	1.99	0.44
1:C:255:PRO:CD	1:C:328:LEU:HD13	2.42	0.43
1:A:244:HIS:HE1	1:A:272:GLY:O	2.01	0.43
1:A:545:HIS:CE1	1:A:663:ILE:HG23	2.53	0.43
1:B:356:HIS:CE1	1:B:544:ASN:O	2.71	0.43
1:D:323:ARG:HA	1:D:323:ARG:HD3	1.75	0.43
1:B:496:LEU:HD21	1:B:526:LEU:HD13	1.99	0.43
1:B:500[B]:CYS:SG	1:B:517:PRO:HB2	2.58	0.43
1:C:337:PRO:HG2	1:C:340:VAL:HG21	2.00	0.43
1:D:117:VAL:HA	1:D:120:ASP:HB2	1.99	0.43
1:D:129:ARG:HD2	1:D:495:GLU:OE2	2.19	0.43
1:A:595:TRP:CZ2	1:A:599:ARG:HD2	2.54	0.43
1:D:389:LEU:HD23	1:D:530:VAL:HG11	2.01	0.43
1:D:610:HIS:CD2	1:D:610:HIS:H	2.36	0.43
1:B:610:HIS:HE1	5:B:836:HOH:O	2.02	0.42
1:C:205:ASN:ND2	1:C:220:ARG:HH11	2.17	0.42
1:C:246:VAL:C	1:C:269:LEU:HD21	2.39	0.42
1:C:319:LEU:HA	1:C:319:LEU:HD23	1.85	0.42
1:D:500[A]:CYS:SG	1:D:517:PRO:HG2	2.59	0.42
1:A:215:LEU:HD23	1:A:550:ASP:HB3	2.00	0.42
1:C:238:ASN:HB2	1:C:356:HIS:HB2	2.01	0.42
1:C:463:GLN:O	1:C:467:ARG:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:HIS:CD2	1:B:610:HIS:H	2.36	0.42
1:B:626:LYS:HE3	1:B:630:GLU:OE2	2.19	0.42
1:B:261:LEU:HA	1:B:264:GLN:HG2	2.01	0.42
1:A:145:TRP:CG	1:A:405:ARG:HD2	2.54	0.42
1:C:653:ARG:O	1:C:657:VAL:HG23	2.20	0.42
1:B:307:GLN:NE2	1:B:313:LEU:CD1	2.82	0.41
1:C:247:GLU:N	1:C:269:LEU:HD21	2.35	0.41
1:B:238:ASN:HB2	1:B:356:HIS:HB2	2.01	0.41
1:D:206:ARG:HD3	5:D:757:HOH:O	2.20	0.41
1:B:124:LEU:HD12	1:B:124:LEU:C	2.41	0.41
1:D:356:HIS:CE1	1:D:544:ASN:O	2.73	0.41
1:C:296:TYR:CE2	1:C:565:PRO:HG3	2.56	0.41
1:D:261:LEU:HA	1:D:264:GLN:HG2	2.02	0.41
1:C:488:GLU:HG3	1:C:492:GLU:OE2	2.20	0.41
1:C:205:ASN:HD22	1:C:220:ARG:HH11	1.68	0.41
1:A:590:GLN:O	1:A:594:THR:HG23	2.21	0.41
1:B:357:GLU:OE1	1:B:357:GLU:HA	2.21	0.41
1:D:124:LEU:HG	1:D:124:LEU:H	1.48	0.41
1:D:129:ARG:HD3	1:D:381:PRO:HG3	2.02	0.41
1:D:155[B]:SER:O	1:D:155[B]:SER:OG	2.24	0.41
1:B:230:GLY:HA3	1:B:312:LEU:O	2.21	0.40
1:A:638:ILE:HG21	1:A:653:ARG:CG	2.52	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	553/573 (96%)	539 (98%)	13 (2%)	1 (0%)	47	38
1	B	554/573 (97%)	543 (98%)	10 (2%)	1 (0%)	47	38
1	C	551/573 (96%)	531 (96%)	17 (3%)	3 (0%)	29	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	554/573 (97%)	540 (98%)	11 (2%)	3 (0%)	29	18
All	All	2212/2292 (96%)	2153 (97%)	51 (2%)	8 (0%)	41	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	PRO
1	D	155[A]	SER
1	D	155[B]	SER
1	C	256	PRO
1	C	326	SER
1	A	407	GLY
1	D	120	ASP
1	C	407	GLY

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	483/498 (97%)	470 (97%)	13 (3%)	44	38
1	B	484/498 (97%)	474 (98%)	10 (2%)	53	48
1	C	481/498 (97%)	459 (95%)	22 (5%)	27	17
1	D	484/498 (97%)	468 (97%)	16 (3%)	38	29
All	All	1932/1992 (97%)	1871 (97%)	61 (3%)	40	30

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	A	218	ARG
1	A	258	MET
1	A	267	LYS
1	A	323	ARG
1	A	391	ILE

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Mol	Chain	Res	Type
1	A	458	SER
1	A	466	LEU
1	A	501	ARG
1	A	599	ARG
1	A	611	GLU
1	A	636	LYS
1	A	647	LEU
1	B	120	ASP
1	B	122	GLN
1	B	124	LEU
1	B	127	LYS
1	B	155	SER
1	B	173	ILE
1	B	286	LYS
1	B	485	LYS
1	B	604	MET
1	B	644	LYS
1	C	113	THR
1	C	129	ARG
1	C	139	LEU
1	C	147	ASP
1	C	160	ASP
1	C	207	ILE
1	C	258	MET
1	C	259	GLU
1	C	261	LEU
1	C	268	GLU
1	C	269	LEU
1	C	320	GLN
1	C	323	ARG
1	C	324	GLU
1	C	326	SER
1	C	429	LEU
1	C	477	GLU
1	C	501	ARG
1	C	612	GLU
1	C	616	SER
1	C	636	LYS
1	C	639	GLU
1	D	120	ASP
1	D	122	GLN
1	D	124	LEU

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Mol	Chain	Res	Type
1	D	155[A]	SER
1	D	155[B]	SER
1	D	179	LEU
1	D	214	LYS
1	D	218	ARG
1	D	246	VAL
1	D	324	GLU
1	D	485	LYS
1	D	496	LEU
1	D	500[A]	CYS
1	D	500[B]	CYS
1	D	612	GLU
1	D	647	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	159	HIS
1	A	205	ASN
1	A	244	HIS
1	A	463	GLN
1	A	548	GLN
1	B	152	ASN
1	B	193	ASN
1	B	205	ASN
1	B	244	HIS
1	B	270	GLN
1	B	307	GLN
1	B	356	HIS
1	B	463	GLN
1	B	610	HIS
1	C	152	ASN
1	C	205	ASN
1	C	244	HIS
1	C	307	GLN
1	C	356	HIS
1	C	540	GLN
1	C	548	GLN
1	C	610	HIS
1	D	128	HIS
1	D	152	ASN

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Mol	Chain	Res	Type
1	D	193	ASN
1	D	205	ASN
1	D	244	HIS
1	D	270	GLN
1	D	295	GLN
1	D	307	GLN
1	D	356	HIS
1	D	540	GLN
1	D	610	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OYP	A	664	-	23,26,26	0.72	1 (4%)	26,29,29	1.19	4 (15%)
4	OYP	D	664	-	23,26,26	0.64	0	26,29,29	2.30	6 (23%)
4	OYP	B	664	-	23,26,26	0.65	0	26,29,29	1.32	3 (11%)
4	OYP	C	664	-	23,26,26	0.75	0	26,29,29	1.38	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OYP	A	664	-	-	4/18/20/20	0/1/1/1
4	OYP	D	664	-	-	6/18/20/20	0/1/1/1
4	OYP	B	664	-	-	3/18/20/20	0/1/1/1
4	OYP	C	664	-	-	3/18/20/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	664	OYP	O3-C10	-2.48	1.33	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	664	OYP	C7-C8-C9	-9.37	96.95	112.67
4	C	664	OYP	C10-O3-C11	3.52	119.53	113.34
4	D	664	OYP	C7-C5-C4	-3.36	112.73	121.23
4	C	664	OYP	O3-C11-C12	-3.34	100.63	112.06
4	C	664	OYP	C7-C8-C9	-3.06	107.53	112.67
4	D	664	OYP	C1-C6-C5	-2.94	116.99	121.03
4	D	664	OYP	C3-C2-C1	2.93	122.78	118.17
4	A	664	OYP	C10-O3-C11	2.83	118.32	113.34
4	D	664	OYP	C4-C3-C2	-2.66	117.37	121.03
4	A	664	OYP	C10-C2-C1	-2.60	114.55	120.66
4	B	664	OYP	C3-C2-C1	2.57	122.20	118.17
4	B	664	OYP	C10-C2-C3	-2.50	114.80	120.66
4	A	664	OYP	C4-C3-C2	-2.32	117.83	121.03
4	B	664	OYP	C6-C1-C2	-2.31	117.85	121.03
4	A	664	OYP	C10-C2-C3	2.08	125.53	120.66
4	D	664	OYP	C6-C5-C4	2.01	121.33	118.17

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	664	OYP	O3-C11-C12-C13
4	C	664	OYP	C12-C13-C14-C15
4	A	664	OYP	O3-C11-C12-C13

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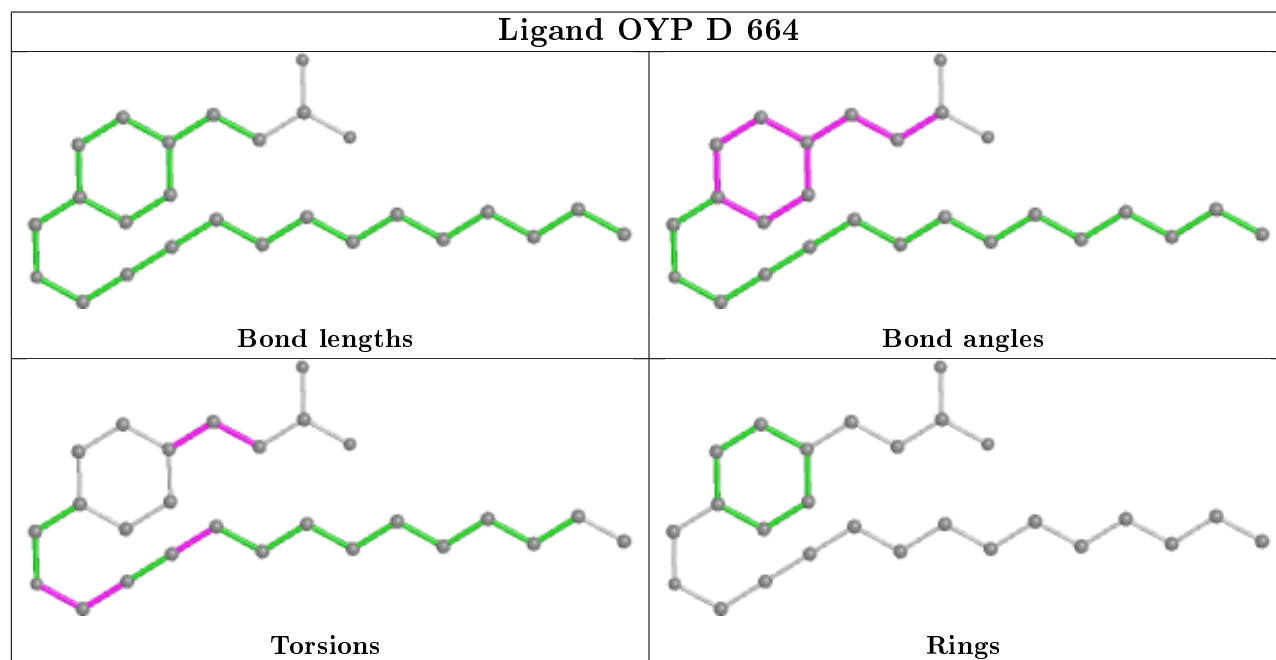
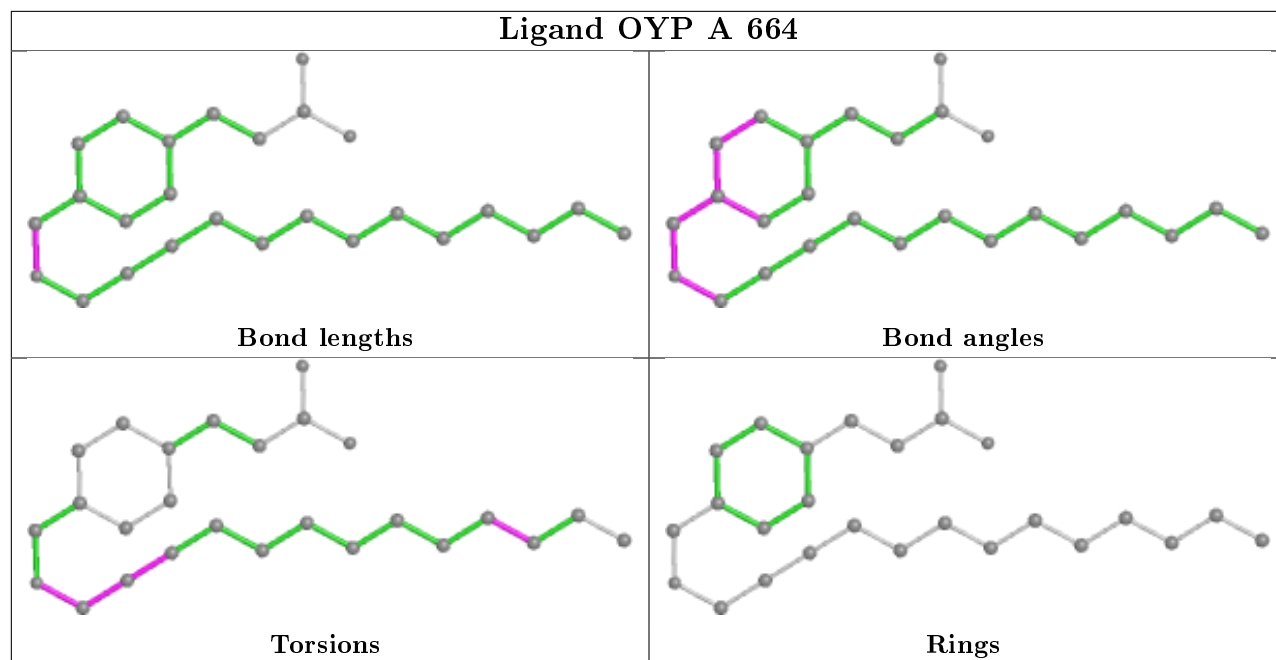
Mol	Chain	Res	Type	Atoms
4	D	664	OYP	C5-C7-C8-C9
4	D	664	OYP	C12-C13-C14-C15
4	A	664	OYP	C12-C11-O3-C10
4	D	664	OYP	C12-C11-O3-C10
4	B	664	OYP	C19-C20-C21-C22
4	C	664	OYP	C12-C11-O3-C10
4	B	664	OYP	O3-C11-C12-C13
4	A	664	OYP	C11-C12-C13-C14
4	D	664	OYP	O3-C11-C12-C13
4	D	664	OYP	C4-C5-C7-C8
4	D	664	OYP	C6-C5-C7-C8
4	A	664	OYP	C19-C20-C21-C22
4	B	664	OYP	C5-C7-C8-C9

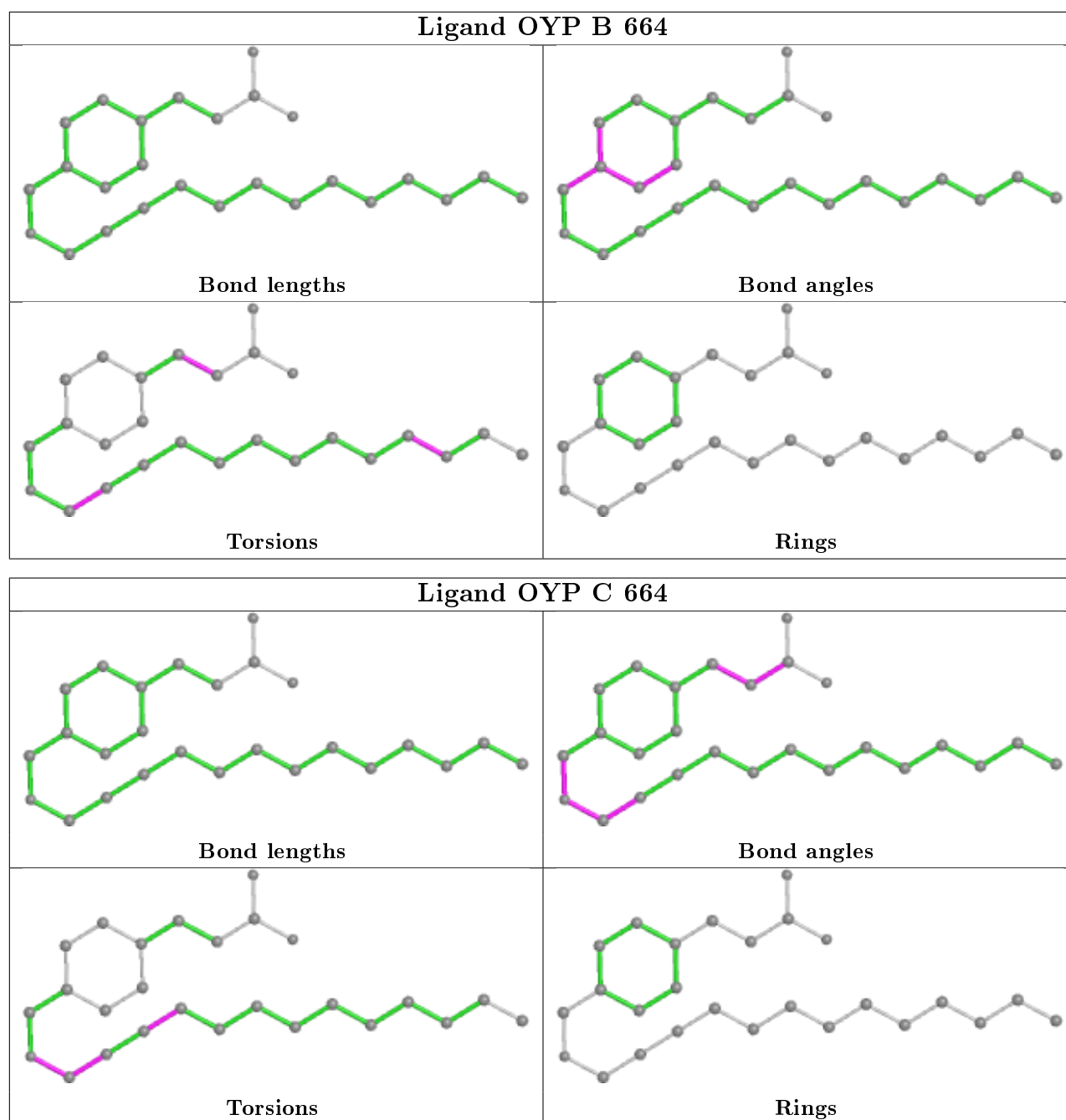
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	664	OYP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	550/573 (95%)	-0.24	5 (0%) 84 85	8, 16, 31, 47	0
1	B	551/573 (96%)	-0.24	5 (0%) 84 85	7, 17, 32, 53	0
1	C	546/573 (95%)	0.31	32 (5%) 22 25	16, 28, 46, 63	0
1	D	547/573 (95%)	-0.19	11 (2%) 65 68	11, 20, 36, 56	0
All	All	2194/2292 (95%)	-0.09	53 (2%) 59 62	7, 20, 39, 63	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	GLY	7.4
1	D	120	ASP	6.8
1	B	121	PRO	6.0
1	D	124	LEU	5.7
1	C	614	TYR	5.0
1	C	328	LEU	4.3
1	C	327	PRO	4.2
1	C	163	VAL	4.2
1	C	255	PRO	3.9
1	C	254	PHE	3.8
1	C	571	ASP	3.6
1	B	124	LEU	3.6
1	B	256	PRO	3.6
1	C	128	HIS	3.4
1	C	569	THR	3.4
1	C	326	SER	3.2
1	C	616	SER	3.1
1	C	259	GLU	3.1
1	D	112	GLY	3.0
1	D	327	PRO	3.0
1	C	329	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	139	LEU	2.9
1	B	123	GLY	2.8
1	D	256	PRO	2.8
1	C	568	THR	2.8
1	A	256	PRO	2.8
1	C	336	ASP	2.7
1	C	407	GLY	2.7
1	C	572	ALA	2.7
1	C	291	LEU	2.7
1	D	125	PHE	2.7
1	C	611	GLU	2.7
1	D	257	GLY	2.6
1	A	611	GLU	2.5
1	C	253	LYS	2.5
1	A	614	TYR	2.5
1	C	575	GLU	2.4
1	B	125	PHE	2.4
1	C	613	GLU	2.4
1	A	500[A]	CYS	2.3
1	C	332	PHE	2.3
1	C	250	ALA	2.2
1	A	391	ILE	2.2
1	C	135	GLU	2.2
1	D	128	HIS	2.2
1	D	616	SER	2.2
1	C	321	LEU	2.1
1	C	612	GLU	2.1
1	D	612	GLU	2.1
1	C	164	ASP	2.1
1	C	320	GLN	2.0
1	C	412	LEU	2.0
1	C	159	HIS	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 ⓘ

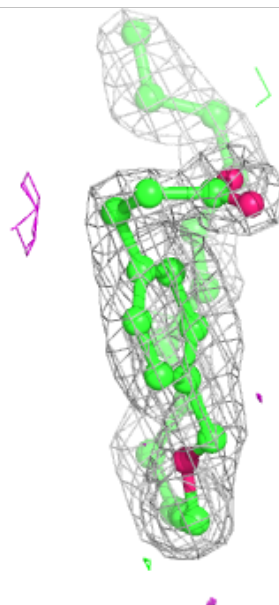
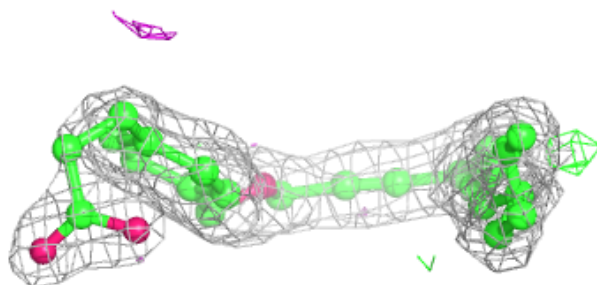
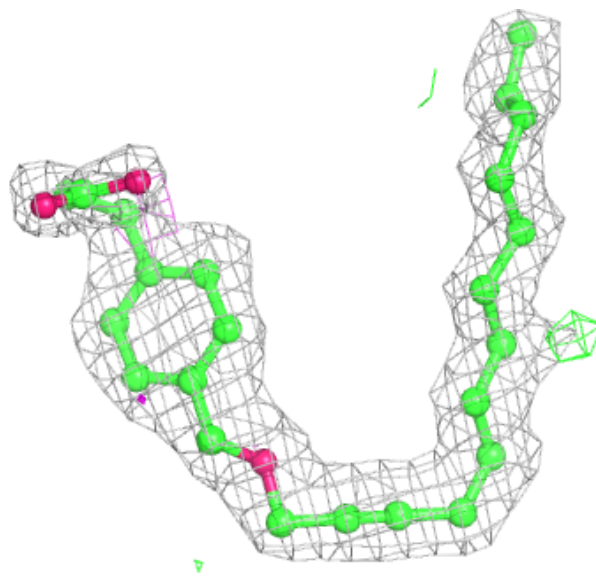
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OYP	C	664	26/26	0.94	0.13	15,27,30,30	4
4	OYP	D	664	26/26	0.95	0.12	12,19,29,30	3
4	OYP	B	664	26/26	0.96	0.14	9,19,26,30	3
2	K	D	1	1/1	0.96	0.17	53,53,53,53	0
4	OYP	A	664	26/26	0.97	0.12	8,16,21,24	3
2	K	A	2	1/1	0.98	0.29	57,57,57,57	0
3	FE2	D	4	1/1	1.00	0.10	12,12,12,12	0
3	FE2	B	2	1/1	1.00	0.11	9,9,9,9	0
3	FE2	A	1	1/1	1.00	0.10	8,8,8,8	0
3	FE2	C	3	1/1	1.00	0.08	17,17,17,17	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.

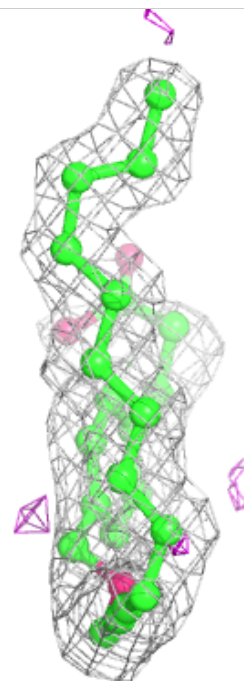
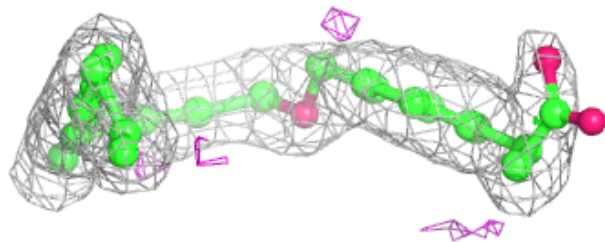
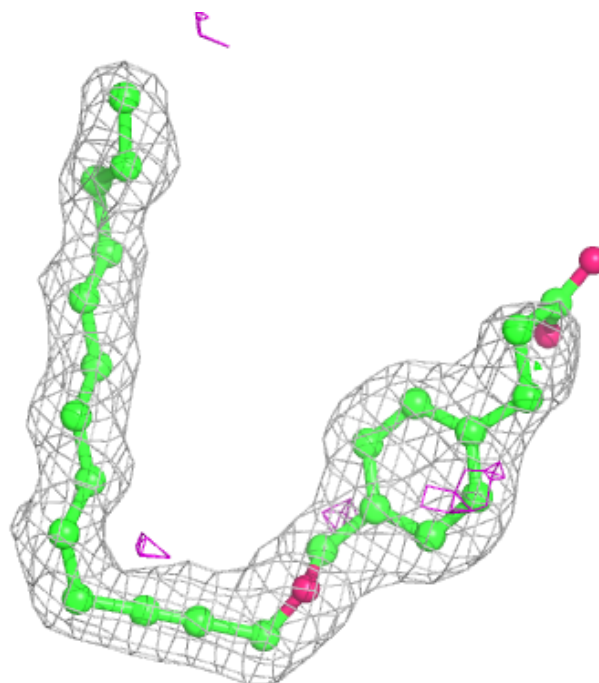
Electron density around OYP C 664:

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



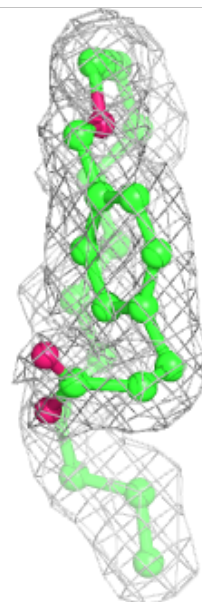
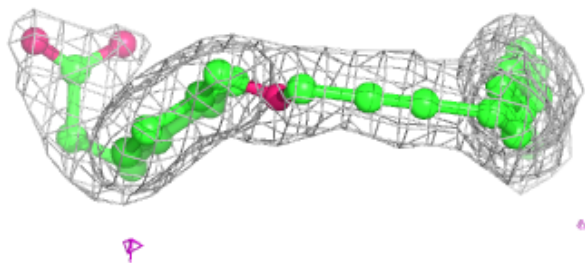
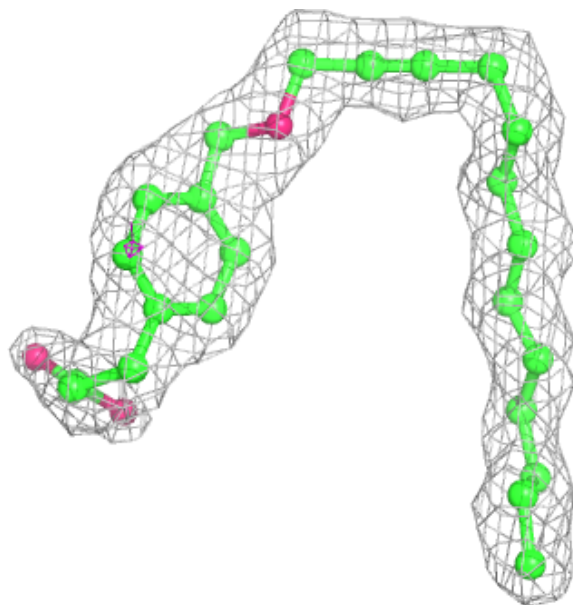
Electron density around OYP D 664:

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



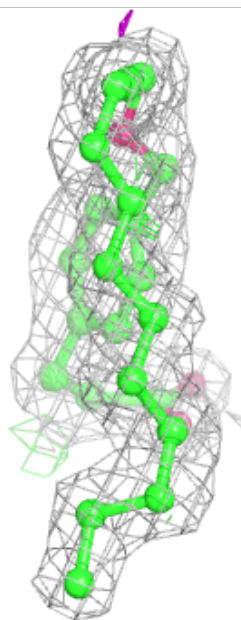
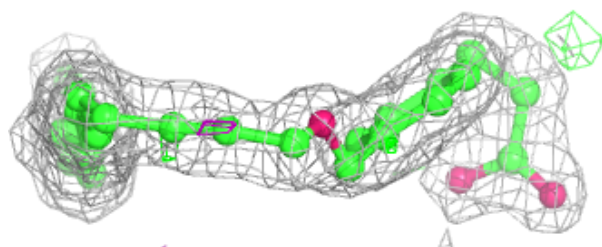
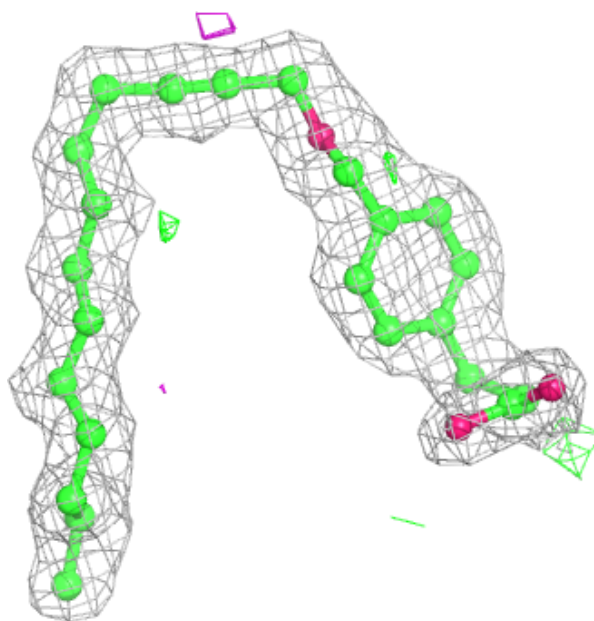
Electron density around OYP B 664:

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



Electron density around OYP A 664:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.