



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:09 PM EDT

PDB ID : 4AW6 / pdb_00004aw6
Title : Crystal structure of the human nuclear membrane zinc metalloprotease ZMP-STE24 (FACE1)
Authors : Pike, A.C.W.; Dong, Y.Y.; Quigley, A.; Dong, L.; Cooper, C.D.O.; Chaikuad, A.; Goubin, S.; Shrestha, L.; Li, Q.; Mukhopadhyay, S.; Yang, J.; Xia, X.; Shintre, C.A.; Barr, A.J.; Berridge, G.; Chalk, R.; Bray, J.E.; von Delft, F.; Bullock, A.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Burgess-Brown, N.; Carpenter, E.P.
Deposited on : 2012-05-31
Resolution : 3.40 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

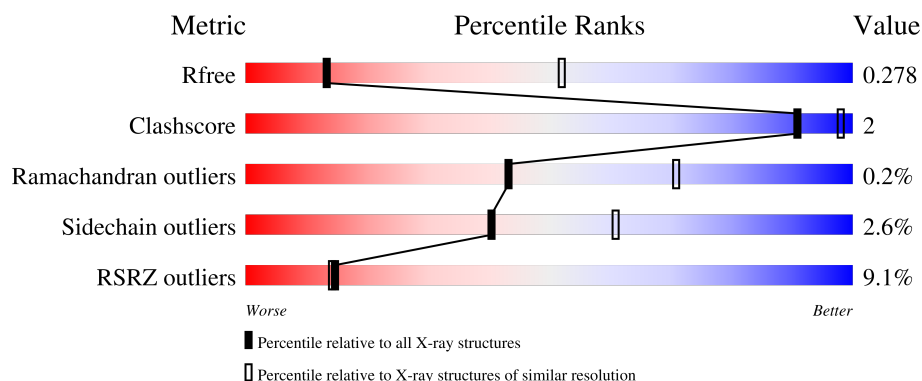
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	482	7% 81% 7% 11%
1	B	482	10% 81% 6% 13%
1	D	482	7% 78% 9% 13%

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

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Mol	Chain	Length	Quality of chain
1	E	482	8% 82% 5% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12978 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 CAAX PRENYL PROTEASE 1 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	1	0
			3281	2198	497	578	8			
1	B	419	Total	C	N	O	S	0	1	0
			3199	2140	490	561	8			
1	D	418	Total	C	N	O	S	0	1	0
			3252	2175	497	571	9			
1	E	418	Total	C	N	O	S	0	1	0
			3134	2091	478	558	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	THR	variant	UNP O75844
A	476	ALA	-	expression tag	UNP O75844
A	477	GLU	-	expression tag	UNP O75844
A	478	ASN	-	expression tag	UNP O75844
A	479	LEU	-	expression tag	UNP O75844
A	480	TYR	-	expression tag	UNP O75844
A	481	PHE	-	expression tag	UNP O75844
A	482	GLN	-	expression tag	UNP O75844
B	137	ALA	THR	variant	UNP O75844
B	476	ALA	-	expression tag	UNP O75844
B	477	GLU	-	expression tag	UNP O75844
B	478	ASN	-	expression tag	UNP O75844
B	479	LEU	-	expression tag	UNP O75844
B	480	TYR	-	expression tag	UNP O75844
B	481	PHE	-	expression tag	UNP O75844
B	482	GLN	-	expression tag	UNP O75844
D	137	ALA	THR	variant	UNP O75844
D	476	ALA	-	expression tag	UNP O75844
D	477	GLU	-	expression tag	UNP O75844
D	478	ASN	-	expression tag	UNP O75844
D	479	LEU	-	expression tag	UNP O75844

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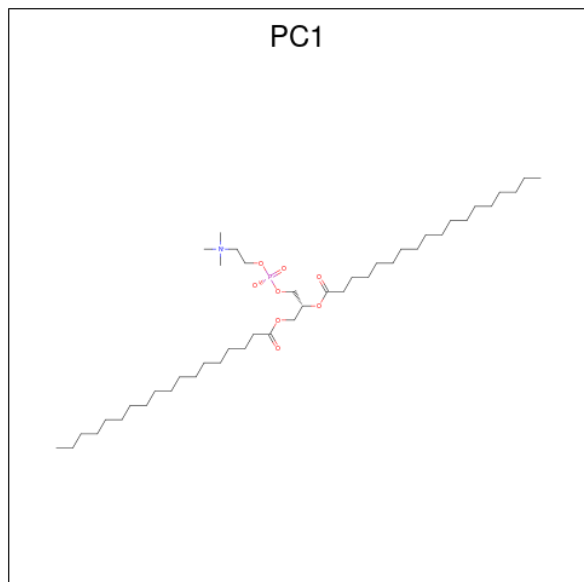
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Chain	Residue	Modelled	Actual	Comment	Reference
D	480	TYR	-	expression tag	UNP O75844
D	481	PHE	-	expression tag	UNP O75844
D	482	GLN	-	expression tag	UNP O75844
E	137	ALA	THR	variant	UNP O75844
E	476	ALA	-	expression tag	UNP O75844
E	477	GLU	-	expression tag	UNP O75844
E	478	ASN	-	expression tag	UNP O75844
E	479	LEU	-	expression tag	UNP O75844
E	480	TYR	-	expression tag	UNP O75844
E	481	PHE	-	expression tag	UNP O75844
E	482	GLN	-	expression tag	UNP O75844

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).

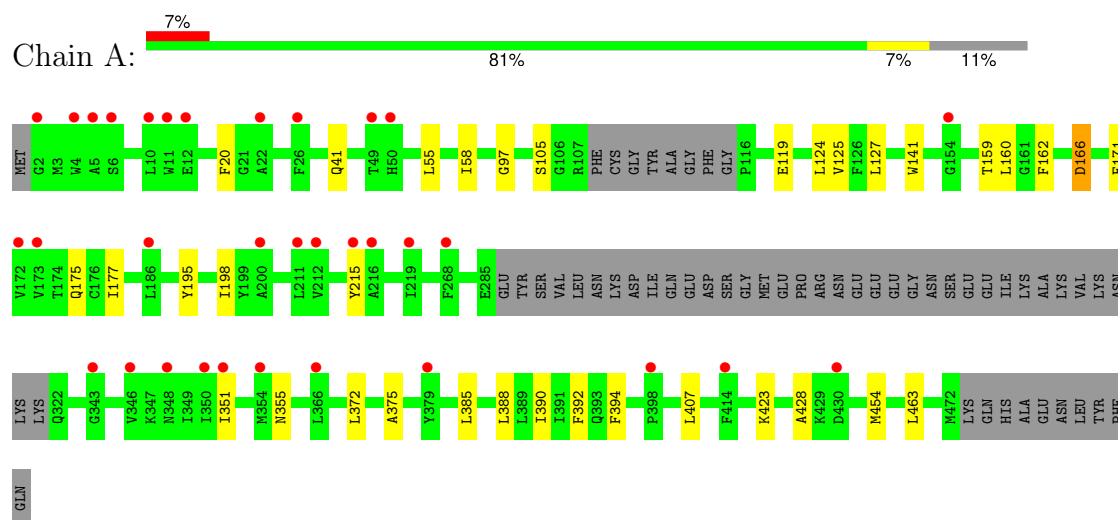


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 28	C 28	0	0
3	B	1	Total 27	C 27	0	0
3	D	1	Total 26	C 26	0	0
3	E	1	Total 27	C 27	0	0

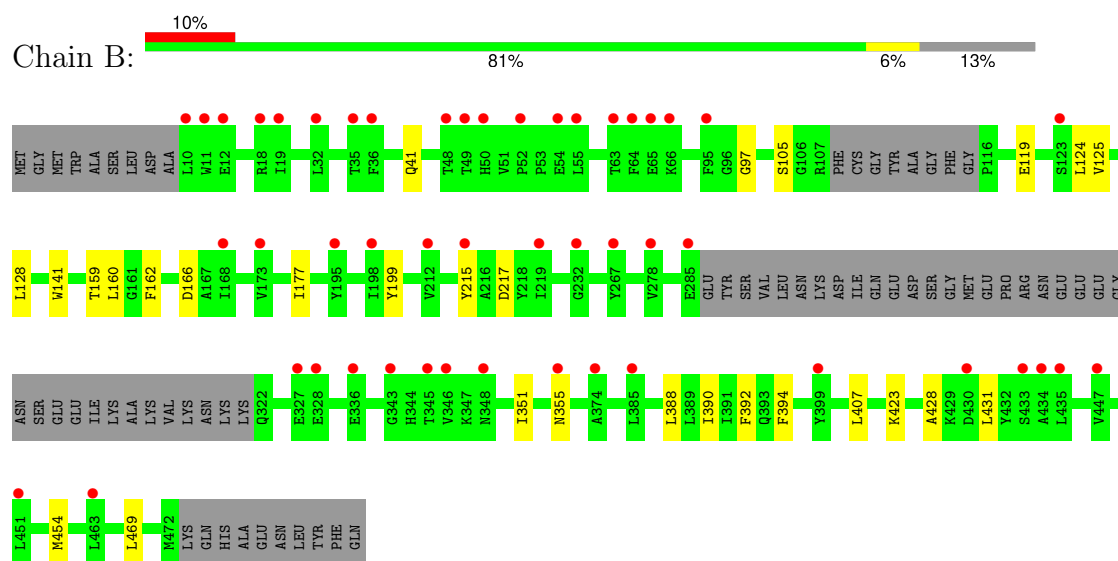
3 Residue-property plots [i](#)

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.

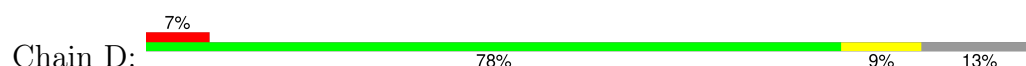
• Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG

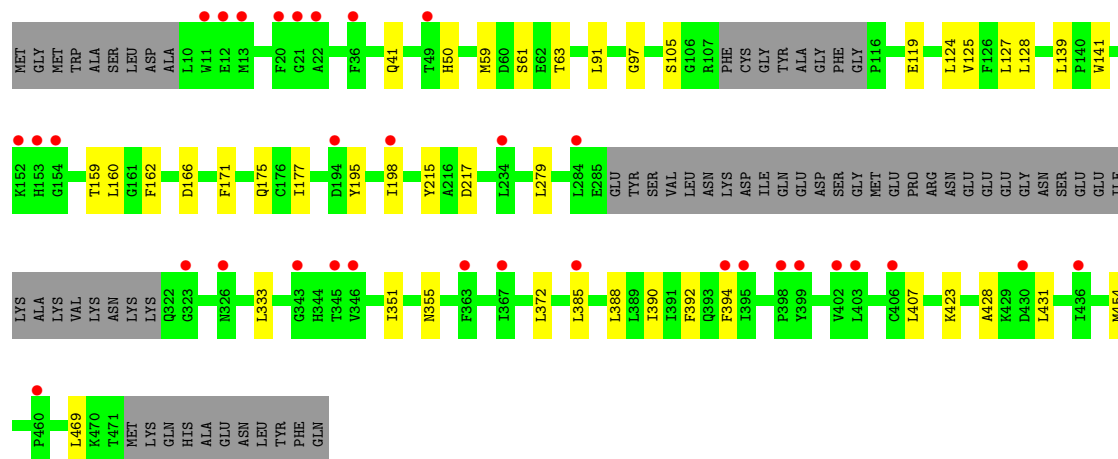


• Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG

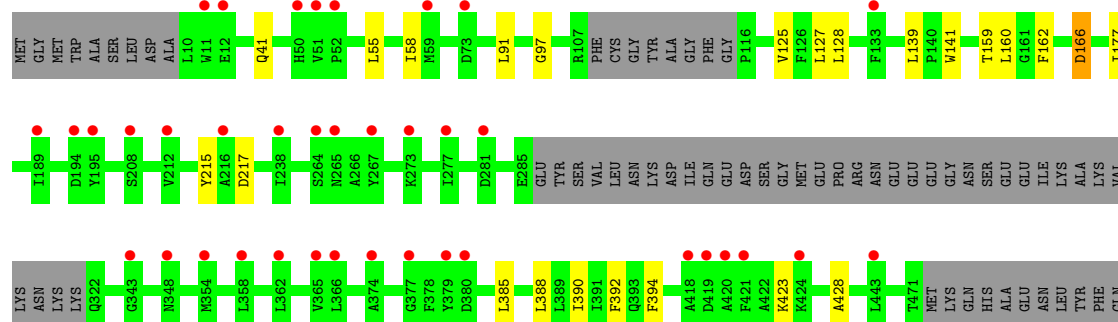
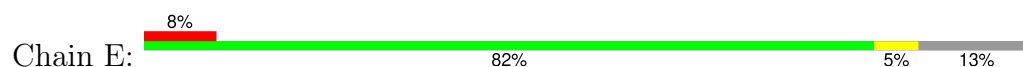


• Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG





• Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.99Å 95.45Å 131.09Å 76.73° 79.64° 72.61°	Depositor
Resolution (Å)	37.96 – 3.40 37.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.96-3.40) 99.9 (37.96-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.40Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2	Depositor
R, R_{free}	0.246 , 0.264 0.261 , 0.278	Depositor DCC
R_{free} test set	1927 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	115.4	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12978	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: PC1, ZN

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	0.78	0/3383	1.37	6/4626 (0.1%)
1	B	0.77	0/3298	1.38	5/4509 (0.1%)
1	D	0.76	0/3353	1.38	5/4577 (0.1%)
1	E	0.78	0/3232	1.39	5/4429 (0.1%)
All	All	0.77	0/13266	1.38	21/18141 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	GLY	CA-C-N	6.08	126.27	120.43
1	B	97	GLY	C-N-CA	6.08	126.27	120.43
1	A	97	GLY	CA-C-N	6.02	126.21	120.43
1	A	97	GLY	C-N-CA	6.02	126.21	120.43
1	D	97	GLY	CA-C-N	5.92	126.11	120.43
1	D	97	GLY	C-N-CA	5.92	126.11	120.43
1	E	97	GLY	CA-C-N	5.86	126.05	120.43
1	E	97	GLY	C-N-CA	5.86	126.05	120.43
1	B	177	ILE	N-CA-C	-5.42	107.15	111.81
1	D	177	ILE	N-CA-C	-5.42	107.15	111.81
1	A	141	TRP	CA-C-N	5.23	127.28	120.28
1	A	141	TRP	C-N-CA	5.23	127.28	120.28
1	D	141	TRP	CA-C-N	5.22	127.27	120.28
1	D	141	TRP	C-N-CA	5.22	127.27	120.28
1	E	141	TRP	CA-C-N	5.21	127.27	120.28
1	E	141	TRP	C-N-CA	5.21	127.27	120.28
1	B	141	TRP	CA-C-N	5.14	127.17	120.28
1	B	141	TRP	C-N-CA	5.14	127.17	120.28
1	A	177	ILE	CA-C-N	5.05	127.01	120.44
1	A	177	ILE	C-N-CA	5.05	127.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	ILE	N-CA-C	-5.00	107.51	111.81

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	3281	0	3078	12	0
1	B	3199	0	2980	8	0
1	D	3252	0	3074	15	0
1	E	3134	0	2833	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	28	0	48	0	0
3	B	27	0	46	0	0
3	D	26	0	44	0	0
3	E	27	0	46	0	0
All	All	12978	0	12149	43	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 2.

All (43) 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:E:127:LEU:HD13	1:E:385:LEU:HD21	1.77	0.66
1:A:105:SER:HB2	1:A:125:VAL:HG13	1.81	0.62
1:D:105:SER:HB2	1:D:125:VAL:HG13	1.82	0.61
1:B:105:SER:HB2	1:B:125:VAL:HG13	1.84	0.59
1:A:55:LEU:HA	1:A:58:ILE:HD12	1.87	0.56
1:E:55:LEU:HA	1:E:58:ILE:HD12	1.89	0.53
1:D:195:TYR:HB3	1:D:198:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:LEU:O	1:E:392:PHE:HB2	2.10	0.52
1:A:388:LEU:O	1:A:392:PHE:HB2	2.11	0.51
1:D:388:LEU:O	1:D:392:PHE:HB2	2.11	0.51
1:A:127:LEU:HD13	1:A:385:LEU:HD21	1.93	0.50
1:B:388:LEU:O	1:B:392:PHE:HB2	2.11	0.50
1:A:195:TYR:HB3	1:A:198:ILE:HD12	1.93	0.50
1:B:351:ILE:HG21	1:B:407:LEU:HD21	1.95	0.49
1:E:125:VAL:HA	1:E:128:LEU:HD12	1.93	0.49
1:D:127:LEU:HD13	1:D:385:LEU:HD21	1.97	0.47
1:A:171:PHE:O	1:A:175:GLN:HG2	2.14	0.47
1:D:351:ILE:HG21	1:D:407:LEU:HD21	1.97	0.47
1:A:351:ILE:HG21	1:A:407:LEU:HD21	1.97	0.46
1:D:59:MET:HE2	1:D:63:THR:HG22	1.98	0.45
1:D:139:LEU:HB3	1:E:91:LEU:HD13	1.99	0.45
1:B:423:LYS:HA	1:B:428:ALA:HB2	2.00	0.43
1:D:423:LYS:HA	1:D:428:ALA:HB2	2.00	0.43
1:E:423:LYS:HA	1:E:428:ALA:HB2	2.00	0.43
1:A:423:LYS:HA	1:A:428:ALA:HB2	2.01	0.43
1:B:125:VAL:HA	1:B:128:LEU:HD12	1.99	0.43
1:D:279:LEU:HD21	1:D:333:LEU:HD21	2.01	0.42
1:B:390:ILE:HA	1:B:394:PHE:HD2	1.85	0.42
1:D:431:LEU:HD23	1:D:469:LEU:HD21	2.02	0.42
1:D:125:VAL:HA	1:D:128:LEU:HD12	2.01	0.42
1:B:159:THR:HG23	1:B:162:PHE:H	1.85	0.41
1:D:171:PHE:O	1:D:175:GLN:HG2	2.20	0.41
1:A:159:THR:HG23	1:A:162:PHE:H	1.85	0.41
1:E:159:THR:HG23	1:E:162:PHE:H	1.86	0.41
1:A:162:PHE:O	1:A:166:ASP:HB2	2.21	0.41
1:D:91:LEU:HD13	1:E:139:LEU:HB3	2.02	0.41
1:D:390:ILE:HA	1:D:394:PHE:HD2	1.86	0.41
1:A:390:ILE:HA	1:A:394:PHE:HD2	1.86	0.41
1:A:20:PHE:HB2	1:A:375:ALA:HB1	2.03	0.40
1:D:159:THR:HG23	1:D:162:PHE:H	1.86	0.40
1:B:431:LEU:HD23	1:B:469:LEU:HD21	2.02	0.40
1:E:162:PHE:O	1:E:166:ASP:HB2	2.22	0.40
1:E:390:ILE:HA	1:E:394:PHE:HD2	1.85	0.40

There are no symmetry-related clashes.

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	422/482 (88%)	409 (97%)	12 (3%)	1 (0%)	43	71
1	B	414/482 (86%)	398 (96%)	15 (4%)	1 (0%)	43	71
1	D	413/482 (86%)	400 (97%)	12 (3%)	1 (0%)	43	71
1	E	413/482 (86%)	397 (96%)	15 (4%)	1 (0%)	43	71
All	All	1662/1928 (86%)	1604 (96%)	54 (3%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	TYR
1	B	215	TYR
1	D	215	TYR
1	E	215	TYR

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	323/425 (76%)	314 (97%)	9 (3%)	38	60
1	B	311/425 (73%)	302 (97%)	9 (3%)	37	60
1	D	325/425 (76%)	314 (97%)	11 (3%)	32	57
1	E	295/425 (69%)	291 (99%)	4 (1%)	59	70
All	All	1254/1700 (74%)	1221 (97%)	33 (3%)	40	61

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	119	GLU
1	A	124	LEU
1	A	160	LEU
1	A	166	ASP
1	A	355	ASN
1	A	372	LEU
1	A	454	MET
1	A	463	LEU
1	B	41	GLN
1	B	119	GLU
1	B	124	LEU
1	B	160	LEU
1	B	166	ASP
1	B	199	TYR
1	B	217	ASP
1	B	355	ASN
1	B	454	MET
1	D	41	GLN
1	D	50	HIS
1	D	61	SER
1	D	119	GLU
1	D	124	LEU
1	D	160	LEU
1	D	166	ASP
1	D	217	ASP
1	D	355	ASN
1	D	372	LEU
1	D	454	MET
1	E	41	GLN
1	E	160	LEU
1	E	166	ASP
1	E	217	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	353	GLN
1	A	355	ASN
1	A	467	GLN

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Mol	Chain	Res	Type
1	B	274	ASN
1	B	353	GLN
1	D	50	HIS
1	D	175	GLN
1	D	274	ASN
1	D	353	GLN
1	D	355	ASN
1	D	467	GLN
1	E	353	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 8 ligands modelled in this entry, 4 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	$\# Z > 2$
3	PC1	E	1473	-	25,25,53	0.18	0	23,23,61	0.19	0
3	PC1	A	1474	-	26,26,53	0.23	0	24,24,61	0.16	0
3	PC1	D	1473	-	24,24,53	0.22	0	22,22,61	0.16	0
3	PC1	B	1474	-	25,25,53	0.20	0	23,23,61	0.18	0

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
3	PC1	E	1473	-	-	1/21/21/57	-
3	PC1	A	1474	-	-	1/22/22/57	-
3	PC1	D	1473	-	-	1/20/20/57	-
3	PC1	B	1474	-	-	1/21/21/57	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

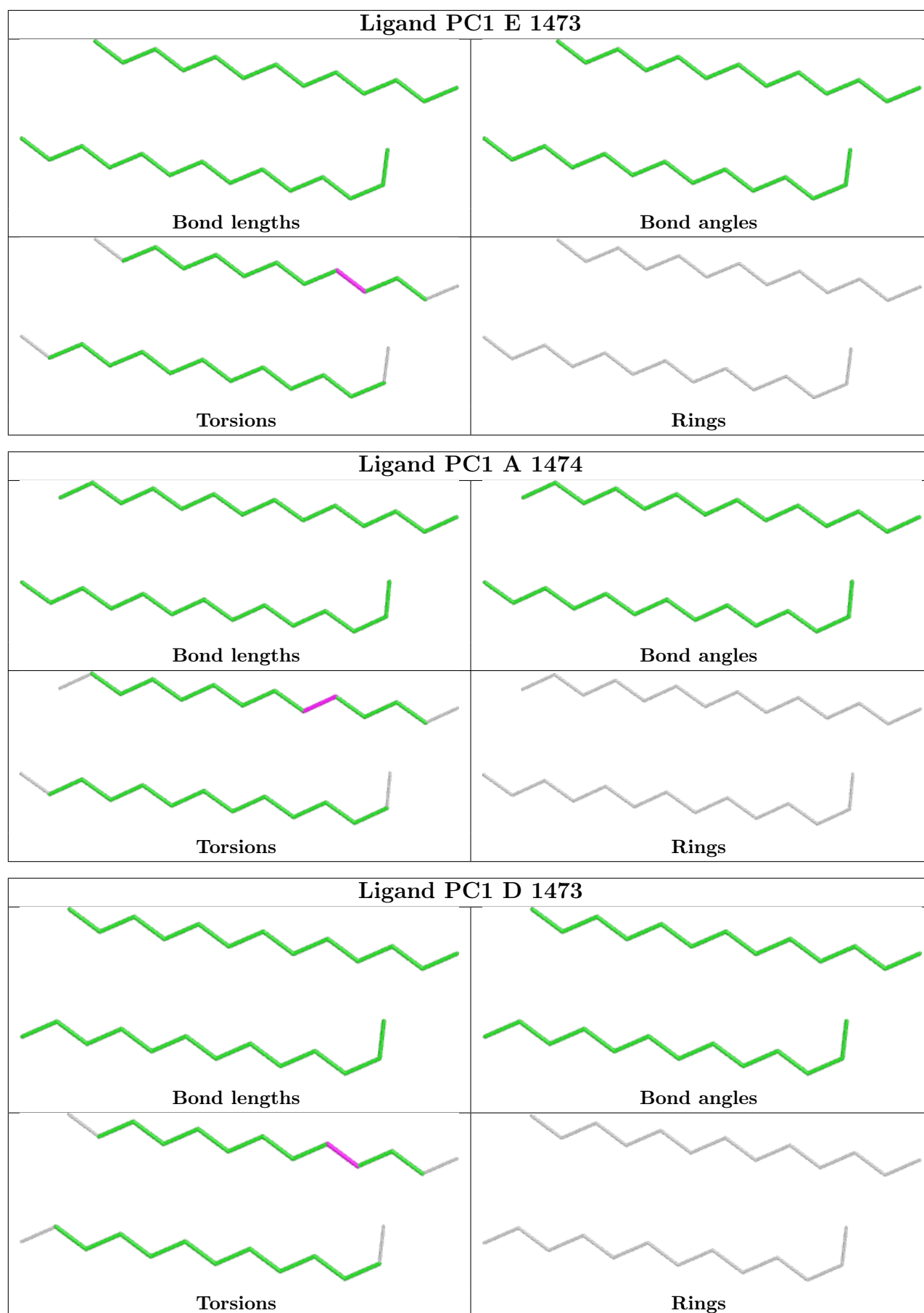
All (4) torsion outliers are listed below:

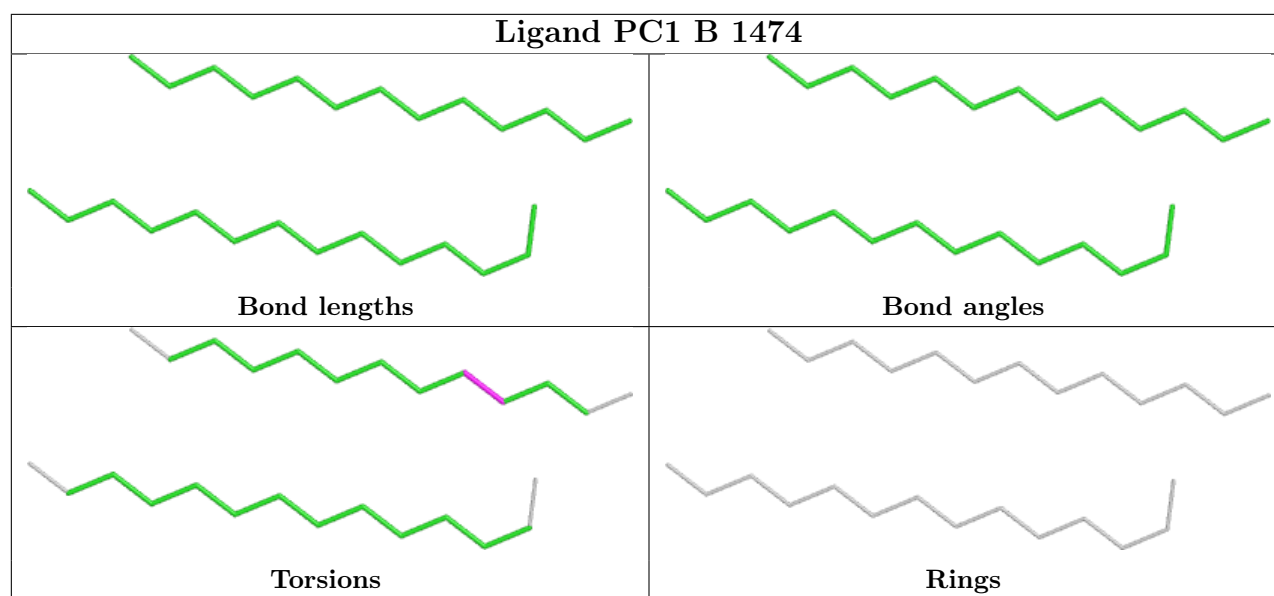
Mol	Chain	Res	Type	Atoms
3	E	1473	PC1	C23-C24-C25-C26
3	B	1474	PC1	C23-C24-C25-C26
3	D	1473	PC1	C23-C24-C25-C26
3	A	1474	PC1	C24-C25-C26-C27

There are no ring outliers.

No monomer is involved in short contacts.

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	427/482 (88%)	0.57	33 (7%)	19	16	46, 130, 185, 235	1 (0%)
1	B	419/482 (86%)	0.68	49 (11%)	9	10	46, 127, 177, 220	1 (0%)
1	D	418/482 (86%)	0.45	33 (7%)	18	16	53, 118, 165, 188	1 (0%)
1	E	418/482 (86%)	0.57	38 (9%)	15	14	53, 155, 204, 225	1 (0%)
All	All	1682/1928 (87%)	0.57	153 (9%)	15	14	46, 129, 189, 235	4 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	GLU	5.6
1	E	51	VAL	5.3
1	E	195	TYR	4.7
1	A	211	LEU	4.7
1	D	406	CYS	4.7
1	E	212	VAL	4.7
1	B	63	THR	4.5
1	A	346	VAL	4.3
1	D	399	TYR	4.3
1	D	343	GLY	4.2
1	B	215	TYR	4.2
1	B	345	THR	4.1
1	A	26	PHE	4.1
1	B	434	ALA	4.1
1	D	22	ALA	4.1
1	E	11	TRP	4.1
1	D	346	VAL	4.0
1	B	11	TRP	4.0
1	B	430	ASP	3.9
1	E	194	ASP	3.9
1	A	212	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLY	3.8
1	A	430	ASP	3.8
1	A	11	TRP	3.8
1	D	12	GLU	3.8
1	B	385	LEU	3.7
1	E	52	PRO	3.7
1	E	379	TYR	3.6
1	B	52	PRO	3.6
1	B	433	SER	3.6
1	D	11	TRP	3.6
1	E	362	LEU	3.4
1	A	5	ALA	3.4
1	A	348	ASN	3.4
1	B	55	LEU	3.4
1	D	326	ASN	3.3
1	B	346	VAL	3.3
1	D	398	PRO	3.2
1	D	21	GLY	3.2
1	E	12	GLU	3.2
1	A	4	TRP	3.1
1	A	12	GLU	3.1
1	B	173	VAL	3.1
1	B	18	ARG	3.0
1	E	366	LEU	3.0
1	A	215	TYR	2.9
1	B	19	ILE	2.9
1	B	32	LEU	2.9
1	A	398	PRO	2.9
1	D	460	PRO	2.9
1	E	50	HIS	2.8
1	B	168	ILE	2.8
1	A	50	HIS	2.8
1	E	418	ALA	2.8
1	A	2	GLY	2.8
1	A	10	LEU	2.8
1	B	54	GLU	2.8
1	E	358	LEU	2.8
1	B	36	PHE	2.8
1	D	154	GLY	2.8
1	B	10	LEU	2.7
1	B	463	LEU	2.7
1	B	198	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	419	ASP	2.7
1	A	216	ALA	2.7
1	E	421	PHE	2.7
1	B	343	GLY	2.7
1	B	348	ASN	2.7
1	E	238	ILE	2.7
1	D	323	GLY	2.7
1	D	385	LEU	2.7
1	B	328	GLU	2.6
1	B	64	PHE	2.6
1	E	374	ALA	2.6
1	E	420	ALA	2.6
1	D	367	ILE	2.6
1	A	351	ILE	2.6
1	E	281	ASP	2.5
1	A	49	THR	2.5
1	B	35	THR	2.5
1	A	219	ILE	2.5
1	E	277	ILE	2.5
1	D	36	PHE	2.5
1	D	394	PHE	2.5
1	D	345	THR	2.5
1	B	285	GLU	2.4
1	B	267	TYR	2.4
1	D	395	ILE	2.4
1	E	273	LYS	2.4
1	A	22	ALA	2.4
1	A	268	PHE	2.4
1	A	366	LEU	2.4
1	A	6	SER	2.4
1	E	265	ASN	2.4
1	B	50	HIS	2.4
1	D	430	ASP	2.4
1	D	403	LEU	2.4
1	B	232	GLY	2.3
1	D	153	HIS	2.3
1	D	436	ILE	2.3
1	E	348	ASN	2.3
1	E	380	ASP	2.3
1	B	336	GLU	2.3
1	E	365	VAL	2.3
1	D	20	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	73	ASP	2.3
1	E	189	ILE	2.3
1	D	49	THR	2.3
1	A	186	LEU	2.3
1	D	234	LEU	2.3
1	A	350	ILE	2.3
1	E	208	SER	2.2
1	B	355	ASN	2.2
1	D	194	ASP	2.2
1	D	284	LEU	2.2
1	E	59	MET	2.2
1	A	173	VAL	2.2
1	B	195	TYR	2.2
1	A	354	MET	2.2
1	E	216	ALA	2.2
1	A	414	PHE	2.2
1	B	49	THR	2.1
1	B	447	VAL	2.1
1	A	154	GLY	2.1
1	E	377	GLY	2.1
1	B	48	THR	2.1
1	A	379	TYR	2.1
1	D	198	ILE	2.1
1	E	443	LEU	2.1
1	E	354	MET	2.1
1	E	264	SER	2.1
1	E	343	GLY	2.1
1	B	95	PHE	2.1
1	A	172	VAL	2.1
1	B	435	LEU	2.1
1	B	451	LEU	2.1
1	B	123	SER	2.1
1	B	278	VAL	2.1
1	D	152	LYS	2.1
1	B	399	TYR	2.1
1	D	13	MET	2.1
1	B	12	GLU	2.1
1	B	65	GLU	2.1
1	A	200	ALA	2.1
1	B	374	ALA	2.0
1	E	267	TYR	2.0
1	D	363	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	133[A]	PHE	2.0
1	E	424	LYS	2.0
1	B	212	VAL	2.0
1	B	66	LYS	2.0
1	D	402	VAL	2.0
1	B	219	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

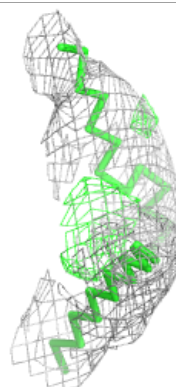
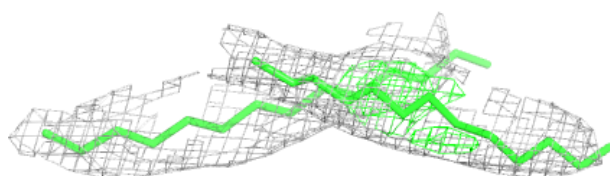
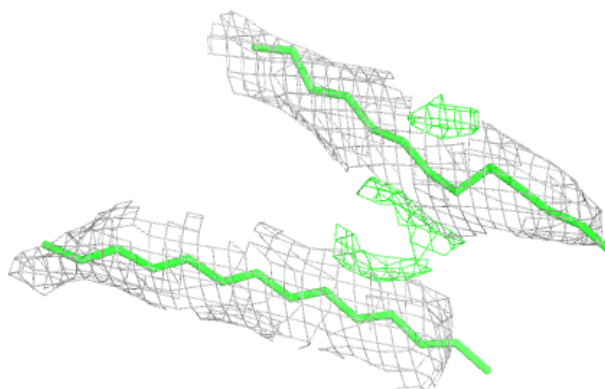
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PC1	E	1473	27/54	0.77	0.26	110,116,142,142	0
3	PC1	A	1474	28/54	0.79	0.24	95,100,136,137	0
3	PC1	B	1474	27/54	0.81	0.26	86,100,108,108	0
3	PC1	D	1473	26/54	0.83	0.24	80,99,113,113	0
2	ZN	B	1473	1/1	0.98	0.08	111,111,111,111	0
2	ZN	E	1472	1/1	0.98	0.07	148,148,148,148	0
2	ZN	D	1472	1/1	0.99	0.05	85,85,85,85	0
2	ZN	A	1473	1/1	0.99	0.05	104,104,104,104	0

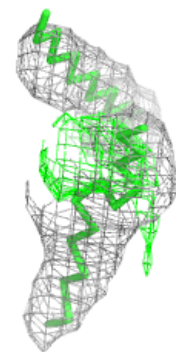
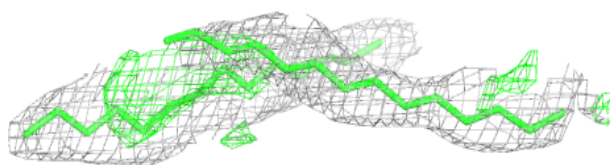
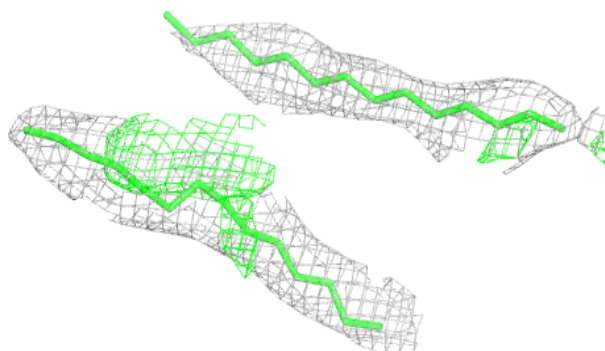
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 E 1473:

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

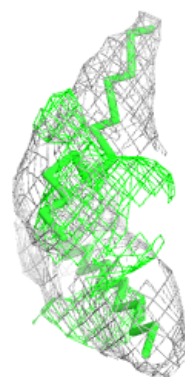
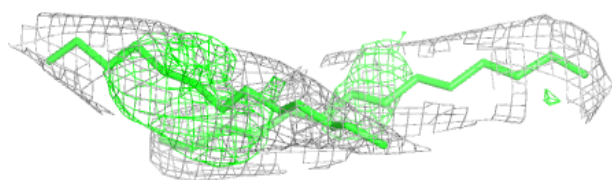
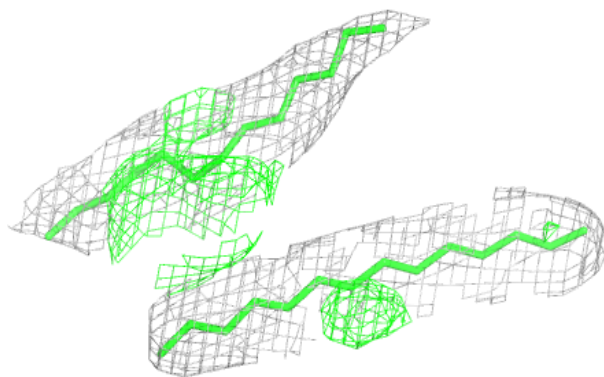
**Electron density around PC1 A 1474:**

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

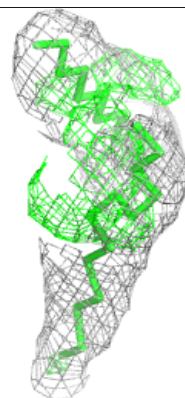
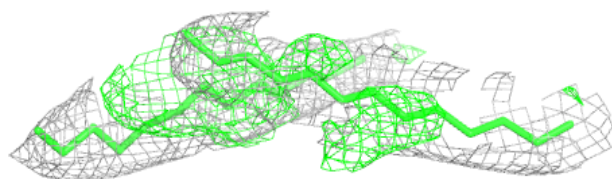
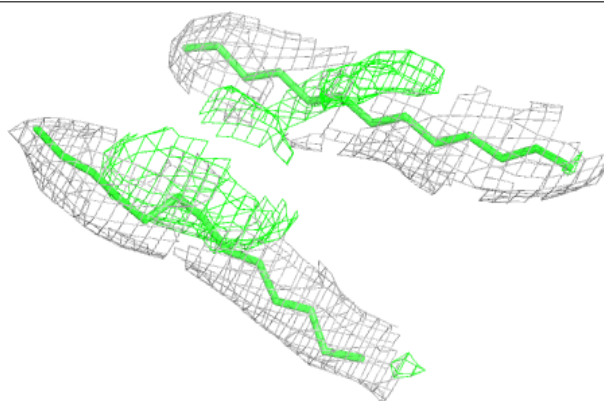


Electron density around PC1 B 1474:

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

**Electron density around PC1 D 1473:**

$2mF_o-DF_c$ (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.