



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 2NWX / pdb_00002nwx
Title : Crystal structure of GltPh in complex with L-aspartate and sodium ions
Authors : Gouaux, E.; Boudker, O.; Ryan, R.; Yernool, D.; Shimamoto, K.
Deposited on : 2006-11-16
Resolution : 3.29 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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

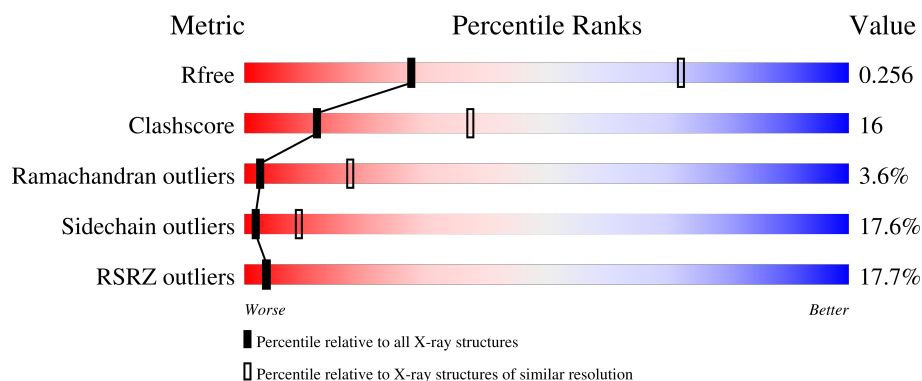
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	422	
1	B	422	
1	C	422	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PLM	C	425	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8596 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			2846	1871	456	502	17			
1	B	396	Total	C	N	O	S	0	0	0
			2816	1853	450	496	17			
1	C	401	Total	C	N	O	S	0	0	0
			2847	1872	456	502	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	cloning artifact	UNP O59010
A	419	LEU	-	cloning artifact	UNP O59010
A	420	VAL	-	cloning artifact	UNP O59010
A	421	PRO	-	cloning artifact	UNP O59010
A	422	ARG	-	cloning artifact	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	cloning artifact	UNP O59010
B	419	LEU	-	cloning artifact	UNP O59010
B	420	VAL	-	cloning artifact	UNP O59010
B	421	PRO	-	cloning artifact	UNP O59010

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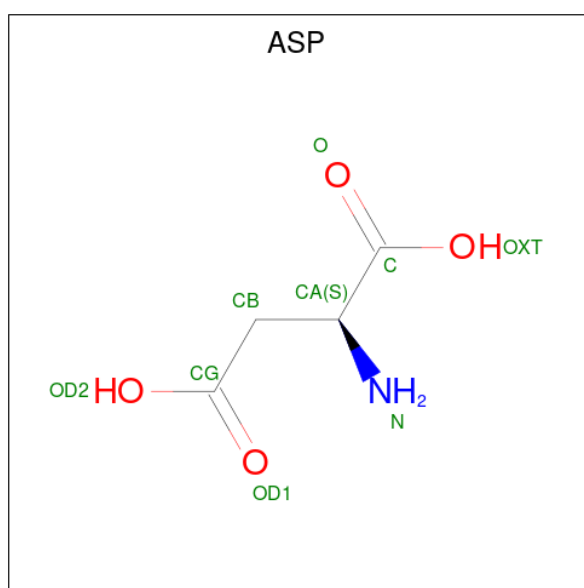
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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	cloning artifact	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	cloning artifact	UNP O59010
C	419	LEU	-	cloning artifact	UNP O59010
C	420	VAL	-	cloning artifact	UNP O59010
C	421	PRO	-	cloning artifact	UNP O59010
C	422	ARG	-	cloning artifact	UNP O59010

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

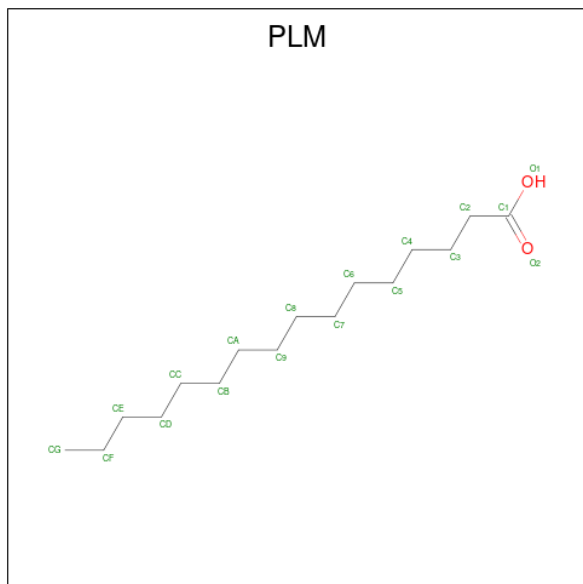
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 4 1 4	0	0
3	A	1	Total C N O 9 4 1 4	0	0
3	A	1	Total C N O 9 4 1 4	0	0

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 17 16 1	0	0
4	B	1	Total C O 17 16 1	0	0
4	C	1	Total C O 17 16 1	0	0

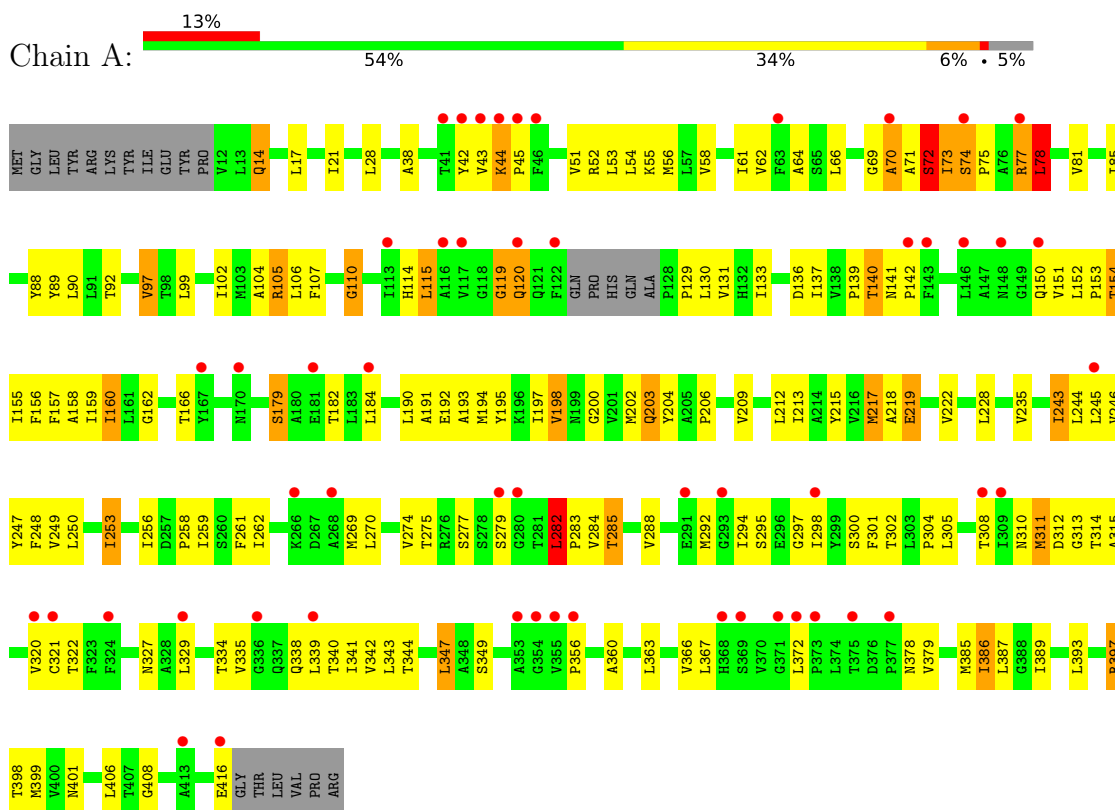
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0

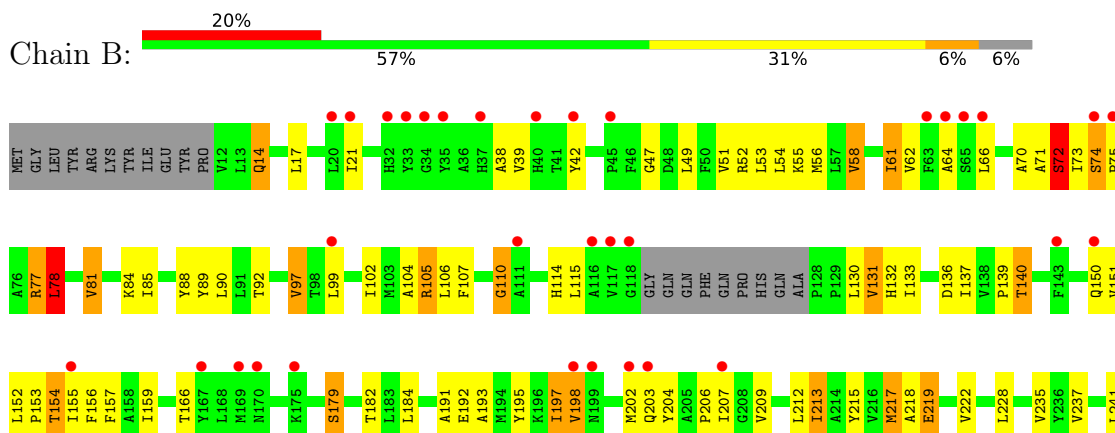
3 Residue-property plots

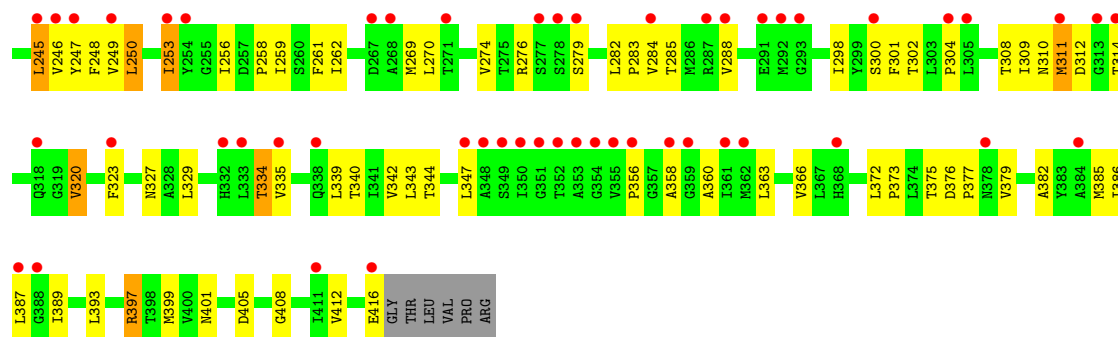
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 425aa long hypothetical proton glutamate symport protein

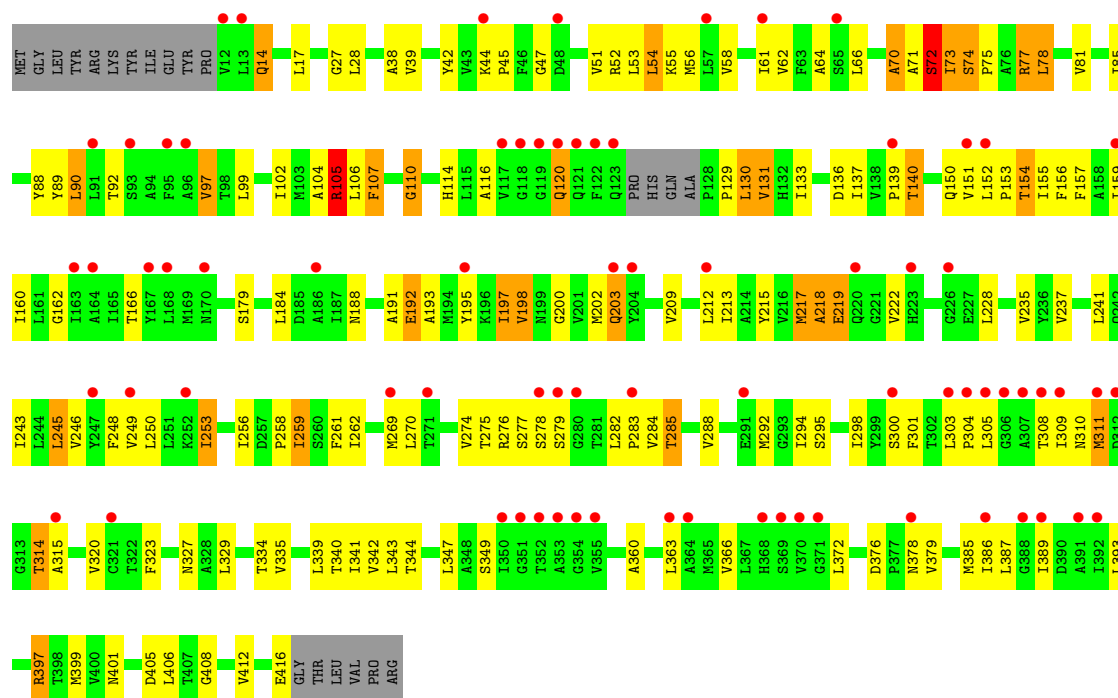


- Molecule 1: 425aa long hypothetical proton glutamate symport protein





- Molecule 1: 425aa long hypothetical proton glutamate symport protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	115.47Å 115.47Å 324.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.29 100.00 – 3.29	Depositor EDS
% Data completeness (in resolution range)	69.2 (100.00-3.29) 69.2 (100.00-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	9.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.263 , 0.286 0.250 , 0.256	Depositor DCC
R_{free} test set	1155 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	123.4	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8596	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: PLM, NA

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	1.02	2/2896 (0.1%)	1.21	9/3960 (0.2%)
1	B	0.85	1/2866 (0.0%)	1.14	4/3920 (0.1%)
1	C	0.83	1/2897 (0.0%)	1.14	7/3962 (0.2%)
All	All	0.90	4/8659 (0.0%)	1.16	20/11842 (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	0	2
1	B	0	1
1	C	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	ILE	CA-CB	6.29	1.61	1.54
1	A	378	ASN	CA-C	6.08	1.60	1.52
1	A	73	ILE	CA-CB	5.71	1.62	1.54
1	B	320	VAL	CA-CB	5.26	1.60	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLN	N-CA-C	9.01	122.67	109.69
1	A	14	GLN	N-CA-C	-6.90	104.53	114.12
1	B	14	GLN	N-CA-C	-6.57	105.18	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	GLN	N-CA-C	-6.21	104.30	113.61
1	C	120	GLN	N-CA-C	5.79	123.14	110.80
1	C	105	ARG	N-CA-C	-5.78	105.33	112.90
1	B	58	VAL	CB-CA-C	-5.54	104.88	111.97
1	C	282	LEU	N-CA-C	5.47	121.90	109.81
1	C	72	SER	N-CA-C	5.42	122.34	110.80
1	A	72	SER	N-CA-C	5.41	122.33	110.80
1	A	107	PHE	N-CA-C	-5.29	102.45	110.28
1	B	358	ALA	N-CA-C	5.29	122.06	110.80
1	A	105	ARG	N-CA-C	-5.24	106.04	112.90
1	A	312	ASP	N-CA-C	-5.15	105.29	112.45
1	B	72	SER	N-CA-C	5.12	121.70	110.80
1	A	282	LEU	CA-C-N	-5.11	113.66	118.97
1	A	282	LEU	C-N-CA	-5.11	113.66	118.97
1	C	107	PHE	N-CA-C	-5.10	102.15	110.20
1	C	292	MET	N-CA-C	-5.05	105.21	113.19
1	A	292	MET	N-CA-C	-5.02	105.26	113.19

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLY	Peptide
1	A	70	ALA	Peptide
1	B	70	ALA	Peptide
1	C	376	ASP	Peptide
1	C	70	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	2846	0	2902	103	0
1	B	2816	0	2872	89	0
1	C	2847	0	2898	98	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
3	A	27	0	9	8	0
4	A	17	0	31	0	0
4	B	17	0	31	0	0
4	C	17	0	31	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	8596	0	8774	272	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 16.

All (272) 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:155:ILE:HD11	1:B:304:PRO:HB2	1.44	0.98
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.47	0.95
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.51	0.91
1:A:136:ASP:HA	1:C:52:ARG:NH2	1.91	0.85
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.60	0.83
1:B:81:VAL:HG21	1:B:298:ILE:HD12	1.63	0.81
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.66	0.77
1:B:249:VAL:O	1:B:253:ILE:HG22	1.85	0.77
1:C:249:VAL:O	1:C:253:ILE:HG22	1.88	0.74
1:A:249:VAL:O	1:A:253:ILE:HG22	1.87	0.74
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.70	0.73
1:A:150:GLN:O	1:A:153:PRO:HD2	1.90	0.71
1:A:344:THR:HB	1:A:366:VAL:HG23	1.72	0.70
1:A:215:TYR:CE1	1:A:219:GLU:HG3	2.27	0.70
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.73	0.69
1:B:38:ALA:O	1:B:42:TYR:HB2	1.92	0.69
1:C:73:ILE:HB	1:C:77:ARG:HG2	1.75	0.69
1:C:150:GLN:O	1:C:153:PRO:HD2	1.93	0.68
1:A:66:LEU:HD13	1:A:300:SER:O	1.93	0.68
1:A:184:LEU:O	1:A:184:LEU:HG	1.93	0.67
1:C:344:THR:HB	1:C:366:VAL:HG23	1.77	0.66
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.10	0.66
1:C:58:VAL:HG22	1:C:283:PRO:HD3	1.76	0.66
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.78	0.66
1:C:215:TYR:CE1	1:C:219:GLU:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:NH1	3:A:425:ASP:OD1	2.29	0.65
1:B:73:ILE:HB	1:B:77:ARG:HG2	1.79	0.65
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.11	0.65
1:A:209:VAL:HG22	1:A:274:VAL:HG11	1.77	0.65
1:C:38:ALA:O	1:C:42:TYR:HB2	1.96	0.65
1:B:215:TYR:CE1	1:B:219:GLU:HG3	2.32	0.64
1:A:73:ILE:HB	1:A:77:ARG:HG2	1.78	0.64
1:B:269:MET:O	1:B:399:MET:HG3	1.98	0.64
1:A:38:ALA:O	1:A:42:TYR:HB2	1.99	0.63
1:C:184:LEU:HG	1:C:184:LEU:O	1.99	0.62
1:B:344:THR:HB	1:B:366:VAL:HG23	1.80	0.62
1:B:64:ALA:HB1	1:B:191:ALA:HB2	1.82	0.62
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.82	0.61
1:A:53:LEU:O	1:A:56:MET:HB3	1.99	0.61
1:A:88:TYR:CE2	1:A:408:GLY:HA3	2.36	0.61
1:C:88:TYR:CE2	1:C:408:GLY:HA3	2.36	0.61
1:B:150:GLN:O	1:B:153:PRO:HD2	2.01	0.60
1:C:193:ALA:O	1:C:197:ILE:HG13	2.01	0.60
1:A:193:ALA:O	1:A:197:ILE:HG13	2.01	0.59
1:B:193:ALA:O	1:B:197:ILE:HG13	2.01	0.59
3:A:426:ASP:N	1:B:356:PRO:HA	2.17	0.59
1:A:51:VAL:O	1:A:55:LYS:HG2	2.03	0.59
1:B:184:LEU:O	1:B:184:LEU:HG	2.02	0.58
1:B:131:VAL:C	1:B:133:ILE:H	2.12	0.58
1:A:64:ALA:HB1	1:A:191:ALA:HB2	1.86	0.57
1:C:131:VAL:C	1:C:133:ILE:H	2.13	0.57
1:A:52:ARG:HH11	1:B:140:THR:HG23	1.71	0.56
1:B:88:TYR:CE2	1:B:408:GLY:HA3	2.39	0.56
1:C:97:VAL:HG21	1:C:342:VAL:HA	1.86	0.56
1:A:269:MET:O	1:A:399:MET:HG3	2.05	0.56
1:B:58:VAL:HG22	1:B:283:PRO:HD3	1.86	0.56
1:A:104:ALA:HB2	1:A:320:VAL:HG23	1.86	0.56
1:C:159:ILE:HD11	1:C:301:PHE:HD1	1.71	0.56
1:C:53:LEU:O	1:C:56:MET:HB3	2.06	0.56
1:B:66:LEU:HD13	1:B:300:SER:O	2.06	0.55
1:A:77:ARG:O	1:A:78:LEU:C	2.49	0.55
1:B:53:LEU:O	1:B:56:MET:HB3	2.07	0.55
1:C:74:SER:HB3	1:C:75:PRO:HD3	1.88	0.54
1:C:104:ALA:HB2	1:C:320:VAL:HG23	1.88	0.54
1:B:241:LEU:O	1:B:245:LEU:HB2	2.07	0.54
1:A:110:GLY:HA3	1:A:327:ASN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ILE:HD11	1:C:301:PHE:CD1	2.43	0.54
1:A:97:VAL:HG21	1:A:342:VAL:HA	1.90	0.54
1:C:269:MET:O	1:C:399:MET:HG3	2.07	0.54
1:B:137:ILE:O	1:B:139:PRO:HD3	2.08	0.53
1:B:74:SER:HB3	1:B:75:PRO:HD3	1.90	0.53
1:A:131:VAL:C	1:A:133:ILE:H	2.16	0.53
1:C:66:LEU:HD13	1:C:300:SER:O	2.08	0.53
1:C:215:TYR:O	1:C:219:GLU:HB2	2.08	0.53
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.44	0.53
1:A:356:PRO:HA	3:A:425:ASP:N	2.23	0.52
1:A:157:PHE:HD1	1:C:56:MET:CE	2.21	0.52
1:A:248:PHE:HE2	1:A:262:ILE:HD11	1.73	0.52
1:C:137:ILE:O	1:C:153:PRO:HA	2.10	0.52
1:C:241:LEU:O	1:C:245:LEU:HB2	2.09	0.52
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.44	0.52
1:C:363:LEU:O	1:C:366:VAL:HG12	2.10	0.52
1:A:246:VAL:O	1:A:250:LEU:HB2	2.10	0.52
3:A:427:ASP:N	1:C:276:ARG:O	2.43	0.51
1:C:311:MET:HG3	1:C:401:ASN:CG	2.34	0.51
1:A:140:THR:HG23	1:C:52:ARG:HH11	1.75	0.51
1:A:159:ILE:HD11	1:A:301:PHE:CD1	2.46	0.51
1:A:329:LEU:HD11	1:A:379:VAL:HG23	1.92	0.51
1:A:66:LEU:HD23	1:A:158:ALA:HB3	1.93	0.51
1:C:315:ALA:HB2	1:C:349:SER:OG	2.11	0.51
1:B:97:VAL:HG21	1:B:342:VAL:HA	1.92	0.51
1:A:136:ASP:HA	1:C:52:ARG:HH22	1.74	0.51
1:C:285:THR:HG22	1:C:406:LEU:HD21	1.93	0.51
1:C:14:GLN:HA	1:C:17:LEU:HD23	1.93	0.50
1:C:66:LEU:HD21	1:C:159:ILE:HG13	1.93	0.50
1:B:156:PHE:C	1:B:156:PHE:CD2	2.90	0.50
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.47	0.50
1:B:393:LEU:O	1:B:397:ARG:HB3	2.11	0.50
1:A:159:ILE:HD11	1:A:301:PHE:HD1	1.77	0.50
1:B:228:LEU:HD21	1:B:385:MET:HG2	1.94	0.50
1:C:110:GLY:HA3	1:C:327:ASN:HB3	1.94	0.50
1:A:200:GLY:O	1:A:203:GLN:HB2	2.12	0.49
1:B:110:GLY:HA3	1:B:327:ASN:HB3	1.94	0.49
1:C:195:TYR:HA	1:C:198:VAL:CG1	2.42	0.49
1:C:209:VAL:HA	1:C:274:VAL:HG11	1.93	0.49
1:A:55:LYS:HB2	1:B:140:THR:HG22	1.93	0.49
3:A:426:ASP:N	1:B:276:ARG:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:HD1	1:C:56:MET:HE3	1.78	0.49
1:B:209:VAL:HA	1:B:274:VAL:HG11	1.94	0.49
1:C:200:GLY:O	1:C:203:GLN:HB2	2.13	0.49
3:A:427:ASP:OXT	1:C:278:SER:HB2	2.13	0.49
1:B:64:ALA:CB	1:B:191:ALA:HB2	2.42	0.49
1:B:66:LEU:HD21	1:B:159:ILE:HG13	1.95	0.49
1:C:77:ARG:O	1:C:78:LEU:C	2.55	0.48
1:B:209:VAL:HG22	1:B:274:VAL:HG11	1.95	0.48
1:A:360:ALA:O	1:A:363:LEU:HB3	2.13	0.48
1:B:104:ALA:HB2	1:B:320:VAL:HG23	1.96	0.48
1:B:282:LEU:HA	1:B:282:LEU:HD12	1.60	0.48
1:A:311:MET:HG3	1:A:401:ASN:CG	2.39	0.48
1:B:360:ALA:O	1:B:363:LEU:HB3	2.13	0.48
1:C:89:TYR:CD2	1:C:310:ASN:HB2	2.48	0.48
1:B:195:TYR:HA	1:B:198:VAL:CG1	2.43	0.48
1:A:156:PHE:CD2	1:A:156:PHE:C	2.92	0.48
1:C:51:VAL:O	1:C:55:LYS:HG2	2.13	0.48
1:A:89:TYR:CD2	1:A:310:ASN:HB2	2.48	0.48
1:B:137:ILE:O	1:B:153:PRO:HA	2.13	0.47
1:C:209:VAL:HG22	1:C:274:VAL:HG11	1.96	0.47
1:A:363:LEU:O	1:A:366:VAL:HG12	2.14	0.47
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.75	0.47
1:C:311:MET:HG2	1:C:314:THR:HB	1.97	0.47
1:A:156:PHE:CE2	1:C:56:MET:HE1	2.50	0.47
1:A:243:ILE:HG22	1:A:244:LEU:HD23	1.97	0.47
1:C:228:LEU:HD21	1:C:385:MET:HG2	1.97	0.47
1:A:64:ALA:CB	1:A:191:ALA:HB2	2.45	0.47
1:A:137:ILE:O	1:A:139:PRO:HD3	2.14	0.47
1:B:246:VAL:O	1:B:250:LEU:HB2	2.15	0.47
1:A:56:MET:HE1	1:B:156:PHE:HE2	1.78	0.47
1:B:77:ARG:O	1:B:78:LEU:C	2.57	0.47
1:A:74:SER:HB3	1:A:75:PRO:HD3	1.96	0.47
1:A:156:PHE:HE2	1:C:56:MET:HE1	1.80	0.47
1:B:159:ILE:HD11	1:B:301:PHE:CD1	2.49	0.47
1:B:159:ILE:HD11	1:B:301:PHE:HD1	1.79	0.47
1:B:363:LEU:O	1:B:366:VAL:HG12	2.15	0.47
1:B:56:MET:CE	1:C:157:PHE:HD1	2.28	0.47
1:A:294:ILE:HG22	1:A:295:SER:N	2.30	0.46
1:B:51:VAL:O	1:B:55:LYS:HG2	2.14	0.46
1:A:56:MET:HE1	1:B:156:PHE:CE2	2.50	0.46
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:PRO:O	1:C:261:PHE:HB3	2.16	0.46
1:A:137:ILE:O	1:A:153:PRO:HA	2.15	0.46
1:C:154:THR:HG22	1:C:155:ILE:N	2.30	0.46
1:C:329:LEU:HD11	1:C:379:VAL:HG23	1.97	0.46
1:A:315:ALA:HB2	1:A:349:SER:OG	2.16	0.46
1:B:215:TYR:O	1:B:219:GLU:HB2	2.15	0.46
1:B:154:THR:HG22	1:B:155:ILE:N	2.31	0.46
1:C:310:ASN:HB3	1:C:405:ASP:OD1	2.16	0.46
1:A:398:THR:HG23	3:A:425:ASP:O	2.15	0.46
1:B:39:VAL:HG11	1:B:215:TYR:HA	1.96	0.46
1:C:64:ALA:HB1	1:C:191:ALA:HB2	1.97	0.45
1:C:105:ARG:HD3	1:C:323:PHE:HE2	1.80	0.45
1:C:248:PHE:HE2	1:C:262:ILE:HD11	1.82	0.45
1:A:191:ALA:O	1:A:195:TYR:CD1	2.70	0.45
1:B:329:LEU:HD11	1:B:379:VAL:HG23	1.98	0.45
1:C:39:VAL:HG11	1:C:215:TYR:HA	1.98	0.45
1:C:47:GLY:O	1:C:51:VAL:HG23	2.16	0.45
1:C:61:ILE:CG2	1:C:62:VAL:N	2.79	0.45
1:C:393:LEU:O	1:C:397:ARG:HB3	2.16	0.45
1:A:14:GLN:HA	1:A:17:LEU:HD23	1.98	0.45
1:A:179:SER:O	1:A:182:THR:HB	2.17	0.45
1:B:56:MET:HE2	1:C:157:PHE:HD1	1.82	0.45
1:B:89:TYR:CD2	1:B:310:ASN:HB2	2.52	0.45
1:B:14:GLN:HA	1:B:17:LEU:HD23	1.98	0.45
1:C:130:LEU:O	1:C:133:ILE:HB	2.17	0.44
1:C:156:PHE:CD2	1:C:156:PHE:C	2.95	0.44
1:C:70:ALA:HB3	1:C:162:GLY:HA3	1.98	0.44
1:A:194:MET:O	1:A:198:VAL:HG12	2.17	0.44
1:A:313:GLY:N	1:A:401:ASN:OD1	2.50	0.44
3:A:427:ASP:OD1	1:C:397:ARG:NH1	2.51	0.44
1:C:235:VAL:HG22	1:C:320:VAL:CG1	2.47	0.44
1:B:258:PRO:O	1:B:261:PHE:HB3	2.17	0.44
1:B:311:MET:HG3	1:B:401:ASN:CG	2.43	0.44
1:C:137:ILE:O	1:C:139:PRO:HD3	2.18	0.44
1:B:52:ARG:HH11	1:C:140:THR:HG23	1.82	0.44
1:B:235:VAL:HG22	1:B:320:VAL:CG1	2.44	0.44
1:C:360:ALA:O	1:C:363:LEU:HB3	2.18	0.44
1:C:85:ILE:HD12	1:C:85:ILE:HA	1.82	0.44
1:B:58:VAL:O	1:B:62:VAL:HG23	2.17	0.44
1:A:61:ILE:CG2	1:A:62:VAL:N	2.79	0.44
1:A:154:THR:HG22	1:A:155:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD23	1:B:204:TYR:CZ	2.52	0.44
1:B:61:ILE:CG2	1:B:62:VAL:N	2.79	0.44
1:A:258:PRO:O	1:A:261:PHE:HB3	2.18	0.43
1:B:47:GLY:O	1:B:51:VAL:HG23	2.19	0.43
1:B:77:ARG:HD3	1:B:416:GLU:HG2	2.00	0.43
1:B:107:PHE:CE1	1:B:237:VAL:HG11	2.54	0.43
1:C:107:PHE:CE1	1:C:237:VAL:HG11	2.53	0.43
1:A:209:VAL:HA	1:A:274:VAL:HG11	2.00	0.43
1:C:246:VAL:O	1:C:250:LEU:HB2	2.17	0.43
1:A:212:LEU:HA	1:A:212:LEU:HD23	1.71	0.43
1:A:56:MET:CE	1:B:157:PHE:HD1	2.32	0.43
1:B:130:LEU:O	1:B:133:ILE:HB	2.18	0.43
1:B:206:PRO:HG2	1:B:207:ILE:HD12	2.00	0.43
1:B:84:LYS:HD3	1:B:412:VAL:HG13	2.01	0.43
1:C:77:ARG:HD3	1:C:416:GLU:HG2	2.01	0.43
1:B:154:THR:O	1:B:155:ILE:C	2.61	0.43
1:B:247:TYR:OH	1:B:312:ASP:OD2	2.35	0.43
1:A:77:ARG:HD3	1:A:416:GLU:HG2	2.00	0.42
1:A:160:ILE:CG2	1:C:197:ILE:HG21	2.48	0.42
1:B:248:PHE:HE2	1:B:262:ILE:HD11	1.83	0.42
1:A:129:PRO:O	1:A:131:VAL:N	2.51	0.42
1:A:285:THR:HG22	1:A:406:LEU:HD21	2.02	0.42
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.72	0.42
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.71	0.42
1:C:275:THR:C	1:C:277:SER:H	2.27	0.42
1:A:215:TYR:O	1:A:219:GLU:HB2	2.20	0.42
1:A:85:ILE:HG21	1:A:302:THR:HG22	2.01	0.42
1:A:141:ASN:HA	1:A:142:PRO:HD3	1.77	0.42
1:C:188:ASN:O	1:C:192:GLU:HB2	2.20	0.42
1:C:74:SER:CB	1:C:75:PRO:HD3	2.49	0.42
1:C:129:PRO:O	1:C:131:VAL:N	2.52	0.42
1:C:259:ILE:H	1:C:259:ILE:HG13	1.66	0.42
1:C:303:LEU:HD21	1:C:406:LEU:HD23	2.01	0.42
1:A:66:LEU:HD21	1:A:159:ILE:HG13	2.02	0.42
1:A:130:LEU:O	1:A:133:ILE:HB	2.20	0.42
1:A:228:LEU:HD21	1:A:385:MET:HG2	2.01	0.42
1:A:386:ILE:HD13	1:A:386:ILE:HA	1.76	0.42
1:B:310:ASN:HB3	1:B:405:ASP:OD1	2.19	0.42
1:C:78:LEU:HA	1:C:81:VAL:HG12	2.02	0.42
1:A:21:ILE:HD13	1:A:21:ILE:HA	1.91	0.42
1:B:85:ILE:HG21	1:B:302:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.78	0.42
1:B:382:ALA:HA	1:B:385:MET:HE2	2.02	0.41
1:C:27:GLY:O	1:C:218:ALA:HB2	2.19	0.41
1:A:247:TYR:O	1:A:248:PHE:C	2.63	0.41
1:B:373:PRO:C	1:B:375:THR:H	2.27	0.41
1:A:89:TYR:O	1:A:92:THR:OG1	2.35	0.41
1:B:179:SER:O	1:B:182:THR:HB	2.20	0.41
1:C:54:LEU:O	1:C:58:VAL:HG23	2.20	0.41
1:A:43:VAL:C	1:A:45:PRO:HD2	2.45	0.41
1:A:294:ILE:HG22	1:A:295:SER:H	1.85	0.41
1:A:399:MET:HB3	1:A:399:MET:HE2	1.65	0.41
1:B:105:ARG:HD3	1:B:323:PHE:HE2	1.85	0.41
1:C:81:VAL:HG23	1:C:412:VAL:CG1	2.51	0.41
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.93	0.41
1:A:44:LYS:N	1:A:45:PRO:CD	2.84	0.41
1:A:301:PHE:CD2	1:A:301:PHE:C	2.99	0.41
1:A:338:GLN:HB2	1:A:341:ILE:HD12	2.01	0.41
1:B:74:SER:CB	1:B:75:PRO:HD3	2.51	0.41
1:B:78:LEU:HA	1:B:81:VAL:HG12	2.02	0.41
1:B:393:LEU:HB2	1:B:397:ARG:HH21	1.86	0.41
1:C:90:LEU:HD13	1:C:90:LEU:HA	1.86	0.41
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.69	0.41
1:A:393:LEU:O	1:A:397:ARG:HB3	2.21	0.41
1:A:28:LEU:HD13	1:A:217:MET:HG3	2.03	0.41
1:A:204:TYR:C	1:A:206:PRO:HD2	2.46	0.41
1:B:212:LEU:HD12	1:B:274:VAL:HG12	2.03	0.41
1:C:28:LEU:N	1:C:217:MET:HB3	2.36	0.41
1:C:44:LYS:N	1:C:45:PRO:CD	2.83	0.41
1:A:58:VAL:O	1:A:62:VAL:HG23	2.21	0.41
1:C:28:LEU:HD13	1:C:217:MET:HG3	2.02	0.41
1:A:190:LEU:O	1:A:191:ALA:C	2.63	0.41
1:C:191:ALA:O	1:C:195:TYR:CD1	2.74	0.41
1:A:69:GLY:O	1:A:297:GLY:HA2	2.21	0.40
1:A:321:CYS:O	1:A:322:THR:C	2.63	0.40
1:B:376:ASP:HA	1:B:377:PRO:HD3	1.93	0.40
1:C:341:ILE:O	1:C:342:VAL:C	2.65	0.40
1:A:212:LEU:HD12	1:A:274:VAL:HG12	2.02	0.40
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.80	0.40
1:B:21:ILE:HD13	1:B:21:ILE:HA	1.95	0.40
1:B:213:ILE:O	1:B:217:MET:HB2	2.22	0.40
1:C:294:ILE:HG22	1:C:295:SER:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:THR:C	1:A:277:SER:H	2.29	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	396/422 (94%)	309 (78%)	71 (18%)	16 (4%)	2	15
1	B	392/422 (93%)	319 (81%)	60 (15%)	13 (3%)	3	19
1	C	397/422 (94%)	317 (80%)	66 (17%)	14 (4%)	3	18
All	All	1185/1266 (94%)	945 (80%)	197 (17%)	43 (4%)	2	17

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	B	72	SER
1	B	115	LEU
1	C	72	SER
1	C	114	HIS
1	C	335	VAL
1	A	71	ALA
1	A	114	HIS
1	A	115	LEU
1	A	334	THR
1	A	335	VAL
1	B	71	ALA
1	B	114	HIS
1	B	334	THR
1	B	335	VAL
1	C	71	ALA

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Mol	Chain	Res	Type
1	C	334	THR
1	C	77	ARG
1	C	218	ALA
1	A	77	ARG
1	A	222	VAL
1	B	77	ARG
1	C	116	ALA
1	C	120	GLN
1	C	222	VAL
1	A	78	LEU
1	A	110	GLY
1	B	222	VAL
1	C	130	LEU
1	A	218	ALA
1	B	78	LEU
1	B	110	GLY
1	B	132	HIS
1	B	218	ALA
1	A	243	ILE
1	C	110	GLY
1	A	119	GLY
1	C	243	ILE
1	A	74	SER
1	C	74	SER
1	A	44	LYS
1	A	282	LEU
1	B	74	SER

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	277/330 (84%)	230 (83%)	47 (17%)	2	10
1	B	274/330 (83%)	224 (82%)	50 (18%)	2	8
1	C	276/330 (84%)	227 (82%)	49 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	827/990 (84%)	681 (82%)	146 (18%)	2 8

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	72	SER
1	A	78	LEU
1	A	90	LEU
1	A	97	VAL
1	A	99	LEU
1	A	102	ILE
1	A	105	ARG
1	A	106	LEU
1	A	115	LEU
1	A	120	GLN
1	A	140	THR
1	A	151	VAL
1	A	152	LEU
1	A	154	THR
1	A	160	ILE
1	A	166	THR
1	A	179	SER
1	A	192	GLU
1	A	198	VAL
1	A	202	MET
1	A	203	GLN
1	A	213	ILE
1	A	217	MET
1	A	219	GLU
1	A	245	LEU
1	A	253	ILE
1	A	256	ILE
1	A	259	ILE
1	A	270	LEU
1	A	279	SER
1	A	284	VAL
1	A	285	THR
1	A	288	VAL
1	A	305	LEU
1	A	308	THR
1	A	311	MET

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Mol	Chain	Res	Type
1	A	314	THR
1	A	339	LEU
1	A	340	THR
1	A	343	LEU
1	A	347	LEU
1	A	372	LEU
1	A	386	ILE
1	A	387	LEU
1	A	389	ILE
1	A	397	ARG
1	B	54	LEU
1	B	61	ILE
1	B	72	SER
1	B	78	LEU
1	B	81	VAL
1	B	90	LEU
1	B	97	VAL
1	B	99	LEU
1	B	102	ILE
1	B	105	ARG
1	B	106	LEU
1	B	131	VAL
1	B	140	THR
1	B	151	VAL
1	B	152	LEU
1	B	154	THR
1	B	166	THR
1	B	179	SER
1	B	192	GLU
1	B	197	ILE
1	B	198	VAL
1	B	202	MET
1	B	203	GLN
1	B	213	ILE
1	B	217	MET
1	B	219	GLU
1	B	245	LEU
1	B	250	LEU
1	B	253	ILE
1	B	256	ILE
1	B	259	ILE
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	279	SER
1	B	284	VAL
1	B	285	THR
1	B	288	VAL
1	B	308	THR
1	B	309	ILE
1	B	311	MET
1	B	314	THR
1	B	334	THR
1	B	339	LEU
1	B	340	THR
1	B	343	LEU
1	B	347	LEU
1	B	372	LEU
1	B	386	ILE
1	B	387	LEU
1	B	389	ILE
1	B	397	ARG
1	C	54	LEU
1	C	72	SER
1	C	78	LEU
1	C	90	LEU
1	C	97	VAL
1	C	99	LEU
1	C	102	ILE
1	C	105	ARG
1	C	106	LEU
1	C	131	VAL
1	C	140	THR
1	C	151	VAL
1	C	152	LEU
1	C	154	THR
1	C	160	ILE
1	C	166	THR
1	C	179	SER
1	C	192	GLU
1	C	197	ILE
1	C	198	VAL
1	C	202	MET
1	C	203	GLN
1	C	213	ILE
1	C	217	MET

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Mol	Chain	Res	Type
1	C	219	GLU
1	C	245	LEU
1	C	253	ILE
1	C	256	ILE
1	C	259	ILE
1	C	270	LEU
1	C	279	SER
1	C	284	VAL
1	C	285	THR
1	C	288	VAL
1	C	305	LEU
1	C	308	THR
1	C	309	ILE
1	C	311	MET
1	C	314	THR
1	C	339	LEU
1	C	340	THR
1	C	343	LEU
1	C	347	LEU
1	C	372	LEU
1	C	378	ASN
1	C	386	ILE
1	C	387	LEU
1	C	389	ILE
1	C	397	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	327	ASN
1	B	40	HIS
1	B	150	GLN
1	B	327	ASN
1	C	40	HIS
1	C	327	ASN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	ASP	A	426	-	7,8,8	1.11	0	6,10,10	1.08	1 (16%)
4	PLM	C	425	-	15,16,17	0.65	0	14,15,17	0.42	0
4	PLM	B	425	-	15,16,17	0.47	0	14,15,17	0.52	0
4	PLM	A	428	-	15,16,17	0.53	0	14,15,17	0.47	0
3	ASP	A	425	-	7,8,8	1.44	2 (28%)	6,10,10	1.08	1 (16%)
3	ASP	A	427	-	7,8,8	1.24	1 (14%)	6,10,10	1.41	1 (16%)

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	ASP	A	426	-	-	2/8/8/8	-
4	PLM	C	425	-	-	11/14/14/15	-
4	PLM	B	425	-	-	11/14/14/15	-
4	PLM	A	428	-	-	11/14/14/15	-
3	ASP	A	425	-	-	4/8/8/8	-
3	ASP	A	427	-	-	3/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	425	ASP	OXT-C	-2.79	1.21	1.30
3	A	427	ASP	OXT-C	-2.43	1.22	1.30
3	A	425	ASP	OD2-CG	-2.26	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	427	ASP	OXT-C-O	-2.83	117.65	124.08
3	A	425	ASP	OXT-C-O	-2.24	119.00	124.08
3	A	426	ASP	OXT-C-O	-2.20	119.08	124.08

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	428	PLM	O2-C1-C2-C3
4	B	425	PLM	O2-C1-C2-C3
4	C	425	PLM	O2-C1-C2-C3
4	B	425	PLM	CB-CC-CD-CE
4	C	425	PLM	C2-C3-C4-C5
4	C	425	PLM	CB-CC-CD-CE
4	A	428	PLM	C2-C3-C4-C5
4	A	428	PLM	CB-CC-CD-CE
4	B	425	PLM	CA-CB-CC-CD
4	C	425	PLM	CA-CB-CC-CD
4	B	425	PLM	C2-C3-C4-C5
4	A	428	PLM	C9-CA-CB-CC
4	A	428	PLM	C8-C9-CA-CB
4	A	428	PLM	CA-CB-CC-CD
4	C	425	PLM	C8-C9-CA-CB
4	C	425	PLM	C9-CA-CB-CC
4	B	425	PLM	C9-CA-CB-CC
3	A	425	ASP	C-CA-CB-CG
4	B	425	PLM	C8-C9-CA-CB
4	B	425	PLM	C4-C5-C6-C7
4	A	428	PLM	C4-C5-C6-C7
4	C	425	PLM	C4-C5-C6-C7
3	A	425	ASP	N-CA-CB-CG
3	A	426	ASP	N-CA-CB-CG
3	A	427	ASP	N-CA-CB-CG
4	C	425	PLM	C3-C4-C5-C6

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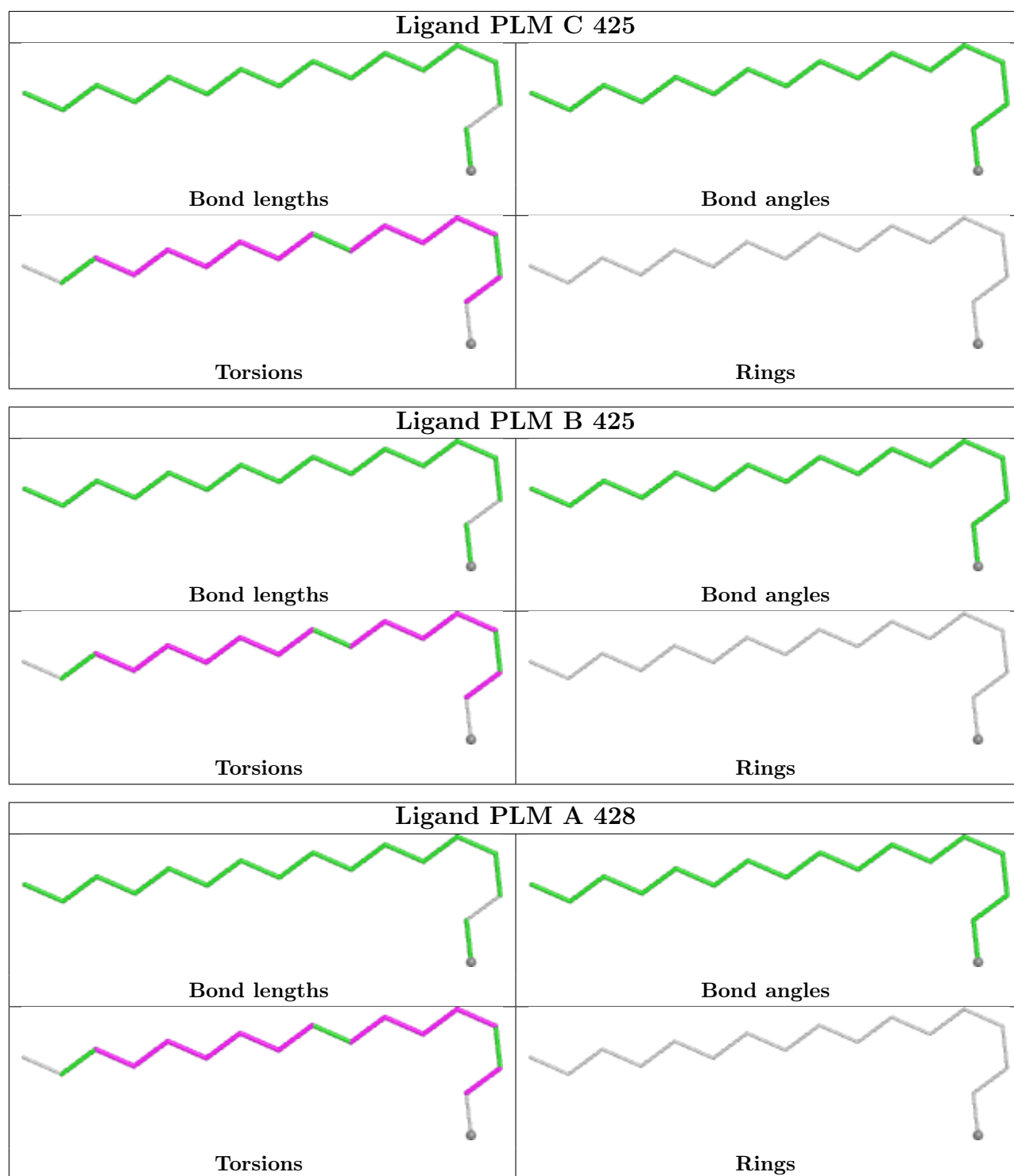
Mol	Chain	Res	Type	Atoms
4	A	428	PLM	C3-C4-C5-C6
4	A	428	PLM	C5-C6-C7-C8
4	B	425	PLM	C3-C4-C5-C6
4	C	425	PLM	C5-C6-C7-C8
4	A	428	PLM	CC-CD-CE-CF
4	B	425	PLM	C5-C6-C7-C8
4	C	425	PLM	CC-CD-CE-CF
4	B	425	PLM	C7-C8-C9-CA
4	C	425	PLM	C7-C8-C9-CA
4	B	425	PLM	CC-CD-CE-CF
4	A	428	PLM	C7-C8-C9-CA
3	A	426	ASP	C-CA-CB-CG
3	A	427	ASP	C-CA-CB-CG
3	A	427	ASP	OXT-C-CA-N
3	A	425	ASP	O-C-CA-N
3	A	425	ASP	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	426	ASP	2	0
3	A	425	ASP	3	0
3	A	427	ASP	3	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 ⓘ

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	400/422 (94%)	0.53	53 (13%) 7 6	98, 126, 170, 185	0
1	B	396/422 (93%)	1.06	84 (21%) 2 2	100, 133, 176, 188	0
1	C	401/422 (95%)	0.94	75 (18%) 3 3	106, 134, 178, 189	0
All	All	1197/1266 (94%)	0.84	212 (17%) 4 3	98, 132, 176, 189	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	ALA	13.2
1	B	354	GLY	12.4
1	C	308	THR	12.2
1	C	354	GLY	11.0
1	C	279	SER	10.0
1	B	355	VAL	9.7
1	B	267	ASP	9.5
1	B	352	THR	9.0
1	B	362	MET	8.9
1	B	33	TYR	8.1
1	C	370	VAL	8.0
1	C	167	TYR	7.9
1	A	355	VAL	7.6
1	C	353	ALA	7.6
1	C	309	ILE	7.3
1	C	203	GLN	7.3
1	C	371	GLY	7.2
1	B	291	GLU	6.9
1	A	45	PRO	6.8
1	A	143	PHE	6.7
1	B	199	ASN	6.7
1	B	333	LEU	6.6
1	B	318	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	358	ALA	6.5
1	C	307	ALA	6.1
1	A	46	PHE	6.0
1	B	287	ARG	5.7
1	C	350	ILE	5.7
1	B	292	MET	5.6
1	B	34	GLY	5.6
1	B	348	ALA	5.5
1	C	311	MET	5.5
1	C	220	GLN	5.4
1	B	359	GLY	5.4
1	C	120	GLN	5.4
1	C	355	VAL	5.3
1	A	291	GLU	5.2
1	B	254	TYR	5.2
1	A	354	GLY	5.2
1	B	351	GLY	5.1
1	B	347	LEU	5.1
1	B	349	SER	4.7
1	B	314	THR	4.7
1	A	279	SER	4.7
1	C	278	SER	4.7
1	B	37	HIS	4.5
1	B	167	TYR	4.5
1	A	356	PRO	4.5
1	C	95	PHE	4.5
1	B	143	PHE	4.4
1	C	369	SER	4.3
1	B	311	MET	4.3
1	C	388	GLY	4.3
1	C	351	GLY	4.3
1	B	198	VAL	4.3
1	B	313	GLY	4.2
1	B	323	PHE	4.2
1	A	116	ALA	4.2
1	B	117	VAL	4.1
1	A	371	GLY	4.1
1	C	247	TYR	4.0
1	C	119	GLY	3.9
1	B	350	ILE	3.9
1	A	413	ALA	3.9
1	C	44	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	202	MET	3.8
1	B	332	HIS	3.8
1	B	277	SER	3.8
1	C	118	GLY	3.8
1	A	375	THR	3.8
1	C	121	GLN	3.7
1	C	223	HIS	3.7
1	B	35	TYR	3.7
1	A	150	GLN	3.7
1	B	246	VAL	3.6
1	C	168	LEU	3.6
1	A	293	GLY	3.6
1	C	91	LEU	3.6
1	C	93	SER	3.6
1	B	284	VAL	3.5
1	A	368	HIS	3.5
1	C	164	ALA	3.5
1	B	74	SER	3.5
1	C	352	THR	3.4
1	A	339	LEU	3.4
1	B	253	ILE	3.3
1	C	123	GLN	3.3
1	A	117	VAL	3.3
1	C	96	ALA	3.3
1	A	245	LEU	3.2
1	B	66	LEU	3.2
1	A	280	GLY	3.2
1	C	386	ILE	3.2
1	B	20	LEU	3.2
1	A	42	TYR	3.2
1	C	170	ASN	3.2
1	A	146	LEU	3.1
1	A	329	LEU	3.1
1	B	293	GLY	3.1
1	C	212	LEU	3.1
1	A	373	PRO	3.1
1	B	278	SER	3.1
1	B	300	SER	3.1
1	A	43	VAL	3.1
1	B	170	ASN	3.1
1	C	269	MET	3.0
1	B	116	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	338	GLN	3.0
1	C	122	PHE	3.0
1	A	148	ASN	3.0
1	C	159	ILE	3.0
1	B	245	LEU	2.9
1	C	392	ILE	2.9
1	A	181	GLU	2.9
1	C	271	THR	2.9
1	B	169	MET	2.9
1	B	64	ALA	2.9
1	B	288	VAL	2.8
1	A	353	ALA	2.8
1	C	389	ILE	2.8
1	A	336	GLY	2.8
1	C	283	PRO	2.8
1	B	268	ALA	2.7
1	A	377	PRO	2.7
1	C	300	SER	2.7
1	A	120	GLN	2.7
1	C	321	CYS	2.7
1	B	247	TYR	2.7
1	B	21	ILE	2.7
1	B	368	HIS	2.6
1	C	48	ASP	2.6
1	A	63	PHE	2.6
1	A	142	PRO	2.6
1	A	170	ASN	2.6
1	C	12	VAL	2.6
1	C	117	VAL	2.6
1	B	42	TYR	2.6
1	C	368	HIS	2.6
1	C	226	GLY	2.6
1	A	309	ILE	2.6
1	A	167	TYR	2.6
1	C	204	TYR	2.6
1	C	65	SER	2.6
1	A	41	THR	2.6
1	A	324	PHE	2.5
1	C	363	LEU	2.5
1	B	175	LYS	2.5
1	C	186	ALA	2.5
1	C	291	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	305	LEU	2.5
1	C	315	ALA	2.5
1	C	378	ASN	2.5
1	A	184	LEU	2.5
1	A	372	LEU	2.5
1	C	151	VAL	2.5
1	B	305	LEU	2.5
1	C	280	GLY	2.5
1	B	249	VAL	2.5
1	C	303	LEU	2.4
1	B	150	GLN	2.4
1	B	75	PRO	2.4
1	C	306	GLY	2.4
1	B	271	THR	2.4
1	B	63	PHE	2.4
1	B	387	LEU	2.4
1	A	298	ILE	2.3
1	B	416	GLU	2.3
1	C	304	PRO	2.3
1	A	74	SER	2.3
1	A	308	THR	2.3
1	B	40	HIS	2.3
1	C	13	LEU	2.3
1	C	312	ASP	2.3
1	B	99	LEU	2.2
1	A	77	ARG	2.2
1	B	279	SER	2.2
1	B	118	GLY	2.2
1	B	356	PRO	2.2
1	A	44	LYS	2.2
1	C	252	LYS	2.2
1	C	249	VAL	2.2
1	A	113	ILE	2.2
1	B	411	ILE	2.2
1	C	364	ALA	2.2
1	B	32	HIS	2.2
1	A	320	VAL	2.2
1	A	369	SER	2.2
1	C	57	LEU	2.2
1	B	111	ALA	2.2
1	B	384	ALA	2.2
1	C	139	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	CYS	2.2
1	C	152	LEU	2.1
1	B	378	ASN	2.1
1	B	207	ILE	2.1
1	C	163	ILE	2.1
1	B	203	GLN	2.1
1	B	45	PRO	2.1
1	B	304	PRO	2.1
1	A	70	ALA	2.1
1	B	388	GLY	2.1
1	A	416	GLU	2.1
1	B	65	SER	2.1
1	B	335	VAL	2.1
1	C	391	ALA	2.1
1	B	155	ILE	2.0
1	B	361	ILE	2.0
1	A	268	ALA	2.0
1	C	61	ILE	2.0
1	C	195	TYR	2.0
1	A	122	PHE	2.0
1	A	266	LYS	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.

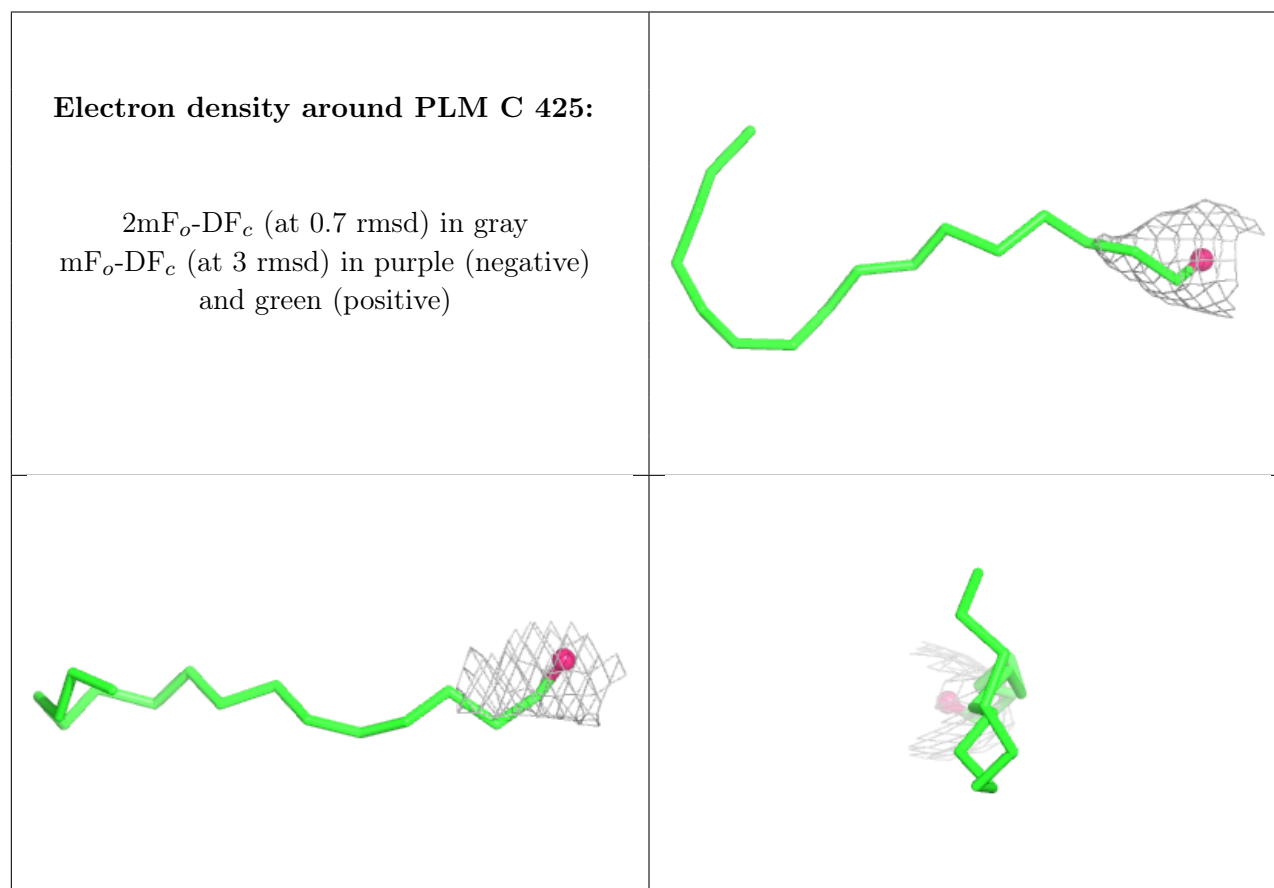
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLM	C	425	17/18	0.74	0.42	149,152,157,157	0
3	ASP	A	425	9/9	0.85	0.12	111,113,114,114	0

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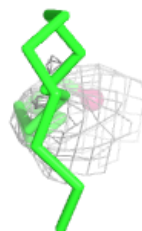
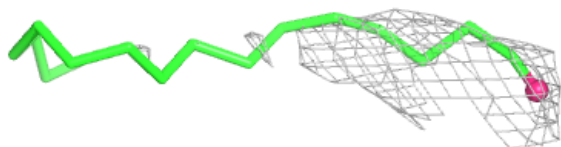
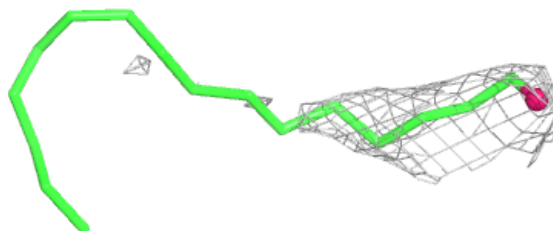
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PLM	B	425	17/18	0.86	0.38	150,152,157,157	0
2	NA	C	423	1/1	0.86	0.31	78,78,78,78	0
3	ASP	A	427	9/9	0.87	0.11	121,123,123,123	0
3	ASP	A	426	9/9	0.90	0.12	124,125,126,126	0
2	NA	B	423	1/1	0.91	0.15	65,65,65,65	0
2	NA	C	424	1/1	0.92	0.37	90,90,90,90	0
2	NA	A	424	1/1	0.92	0.21	84,84,84,84	0
4	PLM	A	428	17/18	0.93	0.23	151,154,160,160	0
2	NA	B	424	1/1	0.97	0.14	118,118,118,118	0
2	NA	A	423	1/1	0.99	0.07	57,57,57,57	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.

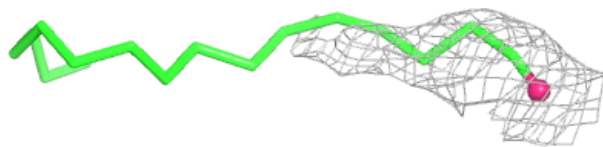
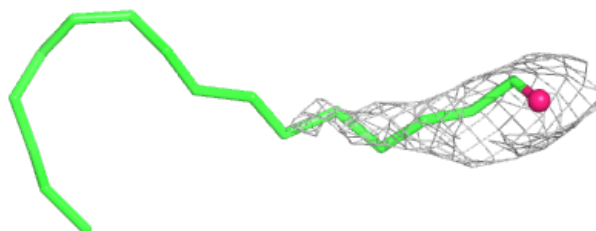


Electron density around PLM B 425:

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

**Electron density around PLM A 428:**

$2mF_o-DF_c$ (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.