



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:50 pm BST

PDB ID : 5WKP
Title : Crystal Structure of the Human mitochondrial Cysteine Desulfurase in complex with ISD11 and Iron-Sulfur Cluster Scaffold Protein ISCU1, and E. coli ACP1 protein at 3.15Å
Authors : Boniecki, M.T.; Cygler, M.
Deposited on : 2017-07-25
Resolution : 3.15 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

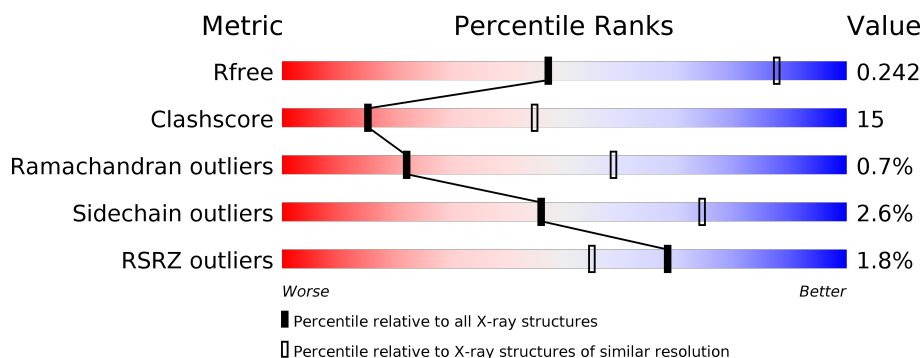
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	406	
1	E	406	
2	B	91	
2	F	91	
3	C	77	
3	G	77	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	150	<div><div></div><div>13%</div><div>54%</div><div>24%</div><div>•</div><div>21%</div></div>
4	H	150	<div><div></div><div>43%</div><div>38%</div><div>•</div><div>16%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9898 atoms, of which 12 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2926	1853	503	552	18			
1	E	398	Total	C	N	O	S	0	0	0
			3001	1893	519	570	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	initiating methionine	UNP Q9Y697
A	53	GLY	-	expression tag	UNP Q9Y697
A	54	SER	-	expression tag	UNP Q9Y697
A	55	SER	-	expression tag	UNP Q9Y697
E	52	MET	-	initiating methionine	UNP Q9Y697
E	53	GLY	-	expression tag	UNP Q9Y697
E	54	SER	-	expression tag	UNP Q9Y697
E	55	SER	-	expression tag	UNP Q9Y697

- Molecule 2 is a protein called LYR motif-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			633	401	117	114	1			
2	F	82	Total	C	N	O	S	0	0	0
			660	418	122	119	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	SER	variant	UNP Q9HD34
F	11	ALA	SER	variant	UNP Q9HD34

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	72	Total 454	C 288	N 76	O 89	S 1	0	0	0
3	G	71	Total 506	C 320	N 78	O 107	S 1	0	0	0

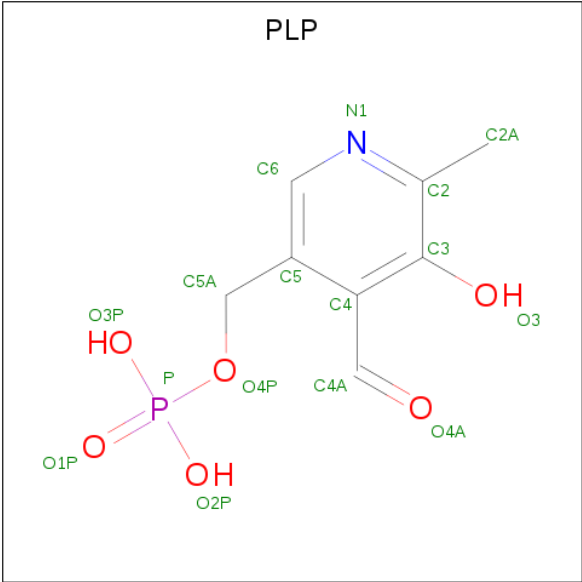
- Molecule 4 is a protein called Iron-sulfur cluster assembly enzyme ISCU, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	118	Total 699	C 434	N 125	O 137	S 3	0	0	0
4	H	126	Total 909	C 572	N 154	O 178	S 5	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

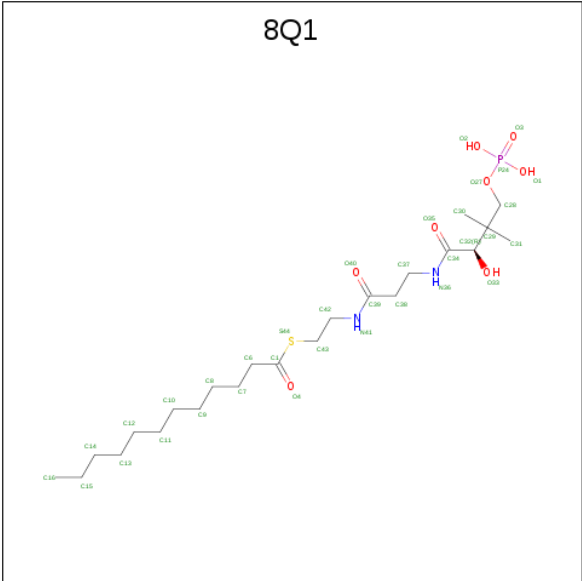
Chain	Residue	Modelled	Actual	Comment	Reference
D	115	ILE	MET	engineered mutation	UNP Q9H1K1
D	143	LEU	-	expression tag	UNP Q9H1K1
D	144	GLU	-	expression tag	UNP Q9H1K1
D	145	HIS	-	expression tag	UNP Q9H1K1
D	146	HIS	-	expression tag	UNP Q9H1K1
D	147	HIS	-	expression tag	UNP Q9H1K1
D	148	HIS	-	expression tag	UNP Q9H1K1
D	149	HIS	-	expression tag	UNP Q9H1K1
D	150	HIS	-	expression tag	UNP Q9H1K1
H	115	ILE	MET	engineered mutation	UNP Q9H1K1
H	143	LEU	-	expression tag	UNP Q9H1K1
H	144	GLU	-	expression tag	UNP Q9H1K1
H	145	HIS	-	expression tag	UNP Q9H1K1
H	146	HIS	-	expression tag	UNP Q9H1K1
H	147	HIS	-	expression tag	UNP Q9H1K1
H	148	HIS	-	expression tag	UNP Q9H1K1
H	149	HIS	-	expression tag	UNP Q9H1K1
H	150	HIS	-	expression tag	UNP Q9H1K1

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			21	8	6	1	5	1		
5	E	1	Total	C	H	N	O	P	0	0
			21	8	6	1	5	1		

- Molecule 6 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



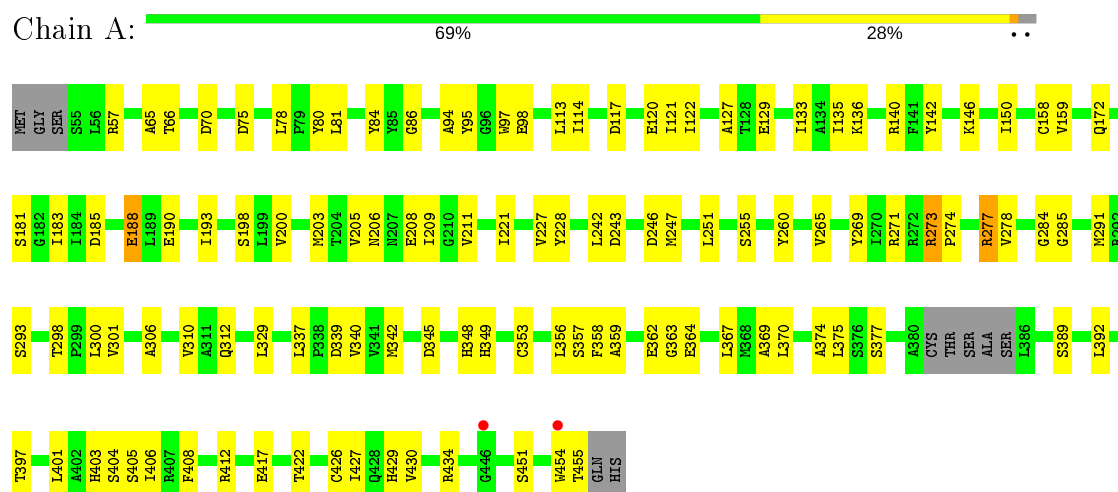
Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	G	1	Total	C	N	O	P	S	0	0
			34	23	2	7	1	1		

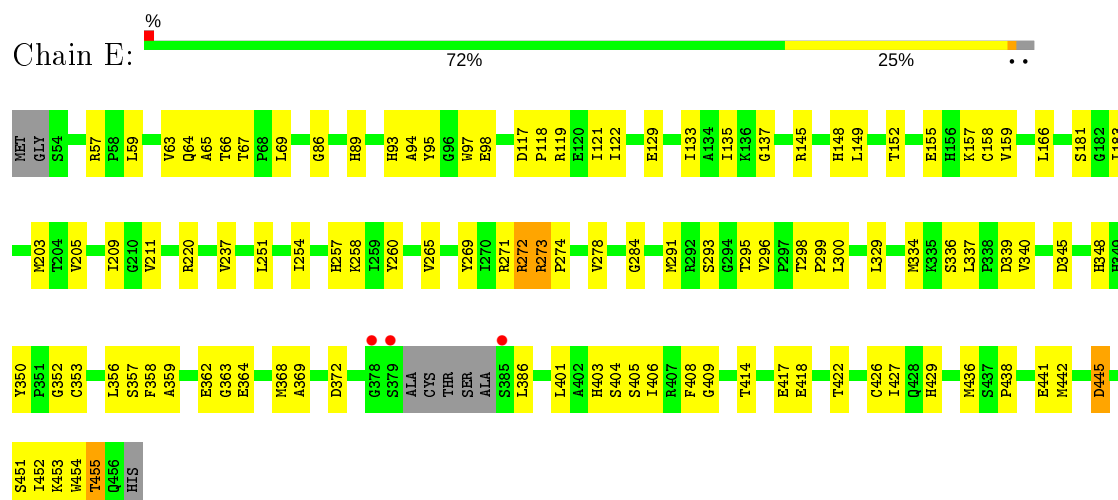
3 Residue-property plots

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: Cysteine desulfurase, mitochondrial



• Molecule 1: Cysteine desulfurase, mitochondrial

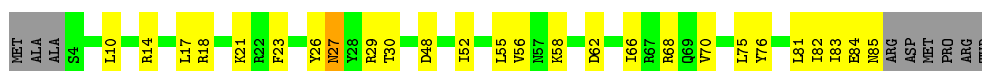


• Molecule 2: LYR motif-containing protein 4





- Molecule 2: LYR motif-containing protein 4



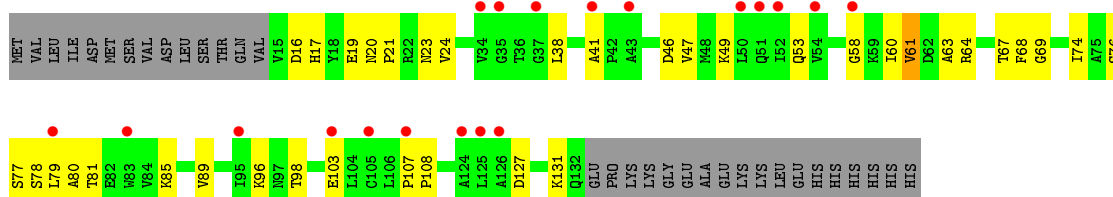
- Molecule 3: Acyl carrier protein



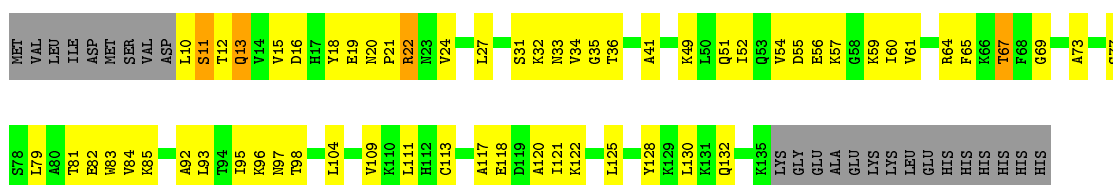
- Molecule 3: Acyl carrier protein



- Molecule 4: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



- Molecule 4: Iron-sulfur cluster assembly enzyme ISCU, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.36Å 123.29Å 151.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.15 49.39 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.39-3.15) 99.8 (49.39-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.186 , 0.242 0.188 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (6.15%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9898	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8Q1, PLP

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	0.27	0/2982	0.44	0/4060
1	E	0.27	0/3057	0.45	0/4148
2	B	0.25	0/641	0.39	0/868
2	F	0.25	0/668	0.38	0/899
3	C	0.23	0/456	0.39	0/626
3	G	0.25	0/509	0.41	0/694
4	D	0.24	0/706	0.43	0/975
4	H	0.24	0/921	0.45	0/1252
All	All	0.26	0/9940	0.43	0/13522

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2926	0	2807	81	0
1	E	3001	0	2914	82	0
2	B	633	0	609	17	0
2	F	660	0	659	23	0
3	C	454	0	368	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	506	0	464	24	0
4	D	699	0	521	26	0
4	H	909	0	904	51	0
5	A	15	6	7	1	0
5	E	15	6	7	0	0
6	C	34	0	0	1	0
6	G	34	0	0	2	0
All	All	9886	12	9260	288	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 15.

All (288) 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:181:SER:HB2	1:A:345:ASP:HB2	1.39	0.99
1:E:209:ILE:HG13	1:E:211:VAL:HG23	1.49	0.94
1:A:209:ILE:HG13	1:A:211:VAL:HG23	1.54	0.90
4:H:97:ASN:N	4:H:118:GLU:OE1	2.08	0.87
1:A:277:ARG:HB3	1:A:277:ARG:HH21	1.42	0.84
1:A:208:GLU:OE1	1:A:389:SER:OG	1.97	0.83
1:E:337:LEU:HD11	1:E:427:ILE:HA	1.61	0.83
1:A:377:SER:OG	1:A:405:SER:O	1.97	0.81
3:C:19:GLN:O	3:C:22:VAL:HG22	1.82	0.80
2:F:14:ARG:HG2	2:F:18:ARG:HH21	1.47	0.80
6:C:301:8Q1:O40	6:C:301:8Q1:N36	2.14	0.79
3:G:52:THR:HG22	3:G:53:GLU:H	1.49	0.78
3:G:10:ILE:HD11	3:G:49:GLU:CB	2.15	0.77
4:H:92:ALA:O	4:H:95:ILE:HG12	1.85	0.77
3:G:24:ASN:HB3	3:G:66:GLN:OE1	1.84	0.76
1:E:271:ARG:HD3	1:E:274:PRO:HD2	1.66	0.76
1:A:271:ARG:HD3	1:A:274:PRO:HD2	1.70	0.74
4:H:60:ILE:HD12	4:H:84:VAL:HG22	1.70	0.74
4:H:32:LYS:O	4:H:132:GLN:NE2	2.20	0.74
1:A:127:ALA:HB2	1:A:255:SER:HB2	1.69	0.73
3:G:15:LEU:HD22	3:G:34:ALA:HB2	1.71	0.73
1:E:135:ILE:HD11	1:E:159:VAL:HG13	1.70	0.73
1:E:181:SER:HB2	1:E:345:ASP:HB2	1.72	0.72
1:E:454:TRP:O	1:E:455:THR:HG23	1.90	0.72
1:E:362:GLU:OE1	1:E:364:GLU:N	2.23	0.72
1:A:300:LEU:HD11	1:E:300:LEU:HD11	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLU:OE1	1:A:364:GLU:N	2.22	0.71
4:H:95:ILE:HG13	4:H:121:ILE:HD13	1.73	0.71
1:E:451:SER:O	1:E:453:LYS:N	2.22	0.69
3:C:14:GLN:HG2	3:C:42:LEU:HD13	1.73	0.69
1:A:135:ILE:HD11	1:A:159:VAL:HG13	1.74	0.69
1:E:441:GLU:OE2	4:H:49:LYS:NZ	2.23	0.69
6:G:301:8Q1:O33	6:G:301:8Q1:O27	2.08	0.68
4:D:127:ASP:O	4:D:131:LYS:N	2.26	0.68
4:D:38:LEU:HD23	4:D:49:LYS:HB2	1.75	0.68
1:A:277:ARG:HB3	1:A:277:ARG:NH2	2.09	0.68
2:B:17:LEU:O	2:B:21:LYS:HG2	1.93	0.68
1:E:273:ARG:CB	1:E:274:PRO:HD3	2.26	0.66
1:E:438:PRO:O	1:E:442:MET:HG3	1.94	0.66
1:A:158:CYS:HA	1:E:284:GLY:HA2	1.77	0.65
2:B:27:ASN:N	2:B:27:ASN:OD1	2.28	0.65
1:E:237:VAL:HG21	1:E:254:ILE:HG12	1.77	0.65
4:H:67:THR:HG21	4:H:77:SER:OG	1.96	0.65
1:A:273:ARG:CB	1:A:274:PRO:HD3	2.27	0.65
1:A:363:GLY:N	1:A:403:HIS:O	2.32	0.63
4:H:16:ASP:O	4:H:20:ASN:HB3	1.97	0.63
3:G:54:ILE:HG12	3:G:71:TYR:CE2	2.34	0.63
1:E:135:ILE:CD1	1:E:159:VAL:HG13	2.29	0.62
1:A:337:LEU:HD21	1:A:427:ILE:HG23	1.80	0.62
3:G:10:ILE:HD11	3:G:49:GLU:HB2	1.80	0.62
4:H:60:ILE:CD1	4:H:84:VAL:HG22	2.29	0.62
1:A:454:TRP:HB3	4:D:41:ALA:HB2	1.83	0.61
1:A:86:GLY:HA3	1:A:95:TYR:O	2.00	0.61
2:F:14:ARG:NH2	3:G:47:GLU:OE2	2.33	0.61
1:E:356:LEU:O	1:E:405:SER:HA	2.01	0.61
1:A:306:ALA:O	1:A:310:VAL:HG23	2.01	0.61
1:E:265:VAL:HB	1:E:300:LEU:HB3	1.82	0.61
1:A:362:GLU:HG3	4:D:69:GLY:HA2	1.83	0.60
2:B:68:ARG:HG2	2:F:75:LEU:HD22	1.81	0.60
3:C:54:ILE:HG22	3:C:59:ALA:HB2	1.82	0.60
1:A:356:LEU:O	1:A:405:SER:HA	2.02	0.60
1:E:362:GLU:HG3	4:H:69:GLY:HA2	1.84	0.60
4:D:79:LEU:HD11	4:D:103:GLU:CG	2.31	0.60
1:E:417:GLU:HB3	2:F:83:ILE:HD11	1.83	0.60
3:C:23:THR:OG1	3:C:26:ALA:HB2	2.01	0.59
2:F:10:LEU:HD11	6:G:301:8Q1:C28	2.32	0.59
1:A:285:GLY:HA2	1:E:157:LYS:HG2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:12:THR:HG23	4:H:13:GLN:HE21	1.67	0.59
2:B:23:PHE:O	2:B:29:ARG:NH1	2.35	0.59
1:A:260:TYR:OH	1:A:412:ARG:N	2.35	0.59
4:D:23:ASN:O	4:D:64:ARG:HA	2.02	0.59
2:F:52:ILE:O	2:F:56:VAL:HG23	2.03	0.59
3:G:54:ILE:HG22	3:G:59:ALA:HB2	1.85	0.59
1:E:334:MET:HG2	1:E:340:VAL:HG13	1.85	0.58
4:H:11:SER:O	4:H:15:VAL:HG23	2.03	0.58
1:A:251:LEU:HA	1:A:269:TYR:O	2.03	0.58
2:B:14:ARG:O	3:C:44:MET:HE1	2.03	0.58
1:A:136:LYS:O	1:A:140:ARG:HG3	2.03	0.57
1:A:183:ILE:HD11	1:A:348:HIS:HB2	1.86	0.57
4:H:20:ASN:N	4:H:21:PRO:HD3	2.18	0.57
1:E:369:ALA:HB1	1:E:429:HIS:CD2	2.39	0.57
1:A:135:ILE:CD1	1:A:159:VAL:HG13	2.34	0.57
1:E:148:HIS:C	1:E:149:LEU:HD12	2.24	0.57
1:A:358:PHE:O	1:A:404:SER:HB3	2.05	0.57
3:C:18:LYS:O	3:C:21:GLU:HG2	2.05	0.57
4:H:13:GLN:H	4:H:13:GLN:HE21	1.53	0.57
1:A:265:VAL:HB	1:A:300:LEU:HB3	1.87	0.57
4:H:93:LEU:O	4:H:122:LYS:HE2	2.05	0.56
3:C:22:VAL:O	3:C:22:VAL:HG23	2.05	0.56
1:E:273:ARG:CB	1:E:274:PRO:CD	2.83	0.56
1:E:363:GLY:N	1:E:403:HIS:O	2.38	0.56
4:H:93:LEU:HD23	4:H:125:LEU:HD12	1.86	0.56
1:A:392:LEU:HD11	1:A:405:SER:OG	2.05	0.56
1:E:336:SER:O	1:E:337:LEU:HD23	2.04	0.56
1:A:94:ALA:O	1:A:98:GLU:HG2	2.06	0.56
1:E:137:GLY:HA3	1:E:278:VAL:HG13	1.86	0.56
1:A:284:GLY:HA2	1:E:158:CYS:HA	1.88	0.56
1:E:334:MET:HG2	1:E:340:VAL:CG1	2.36	0.56
1:A:374:ALA:HB1	1:E:93:HIS:CD2	2.41	0.56
4:H:31:SER:O	4:H:32:LYS:HB3	2.06	0.56
3:G:11:ILE:HD13	3:G:28:PHE:HE1	1.71	0.55
4:D:41:ALA:N	4:D:47:VAL:HG22	2.22	0.55
1:E:94:ALA:O	1:E:98:GLU:HG2	2.06	0.55
1:E:441:GLU:O	1:E:445:ASP:HB2	2.06	0.55
1:A:273:ARG:CB	1:A:274:PRO:CD	2.84	0.55
1:A:430:VAL:O	1:A:434:ARG:HG3	2.07	0.55
2:B:66:ILE:O	2:B:70:VAL:HG23	2.07	0.55
1:A:129:GLU:O	1:A:133:ILE:HG13	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:ILE:HD11	1:E:408:PHE:CZ	2.41	0.54
1:A:454:TRP:HZ3	4:D:38:LEU:HD11	1.71	0.54
3:C:59:ALA:HA	3:C:62:ILE:HD13	1.89	0.54
2:F:26:TYR:O	2:F:30:THR:HG23	2.07	0.54
1:A:278:VAL:HG12	1:A:291:MET:HE1	1.89	0.53
1:E:298:THR:HB	1:E:299:PRO:HD3	1.89	0.53
1:E:64:GLN:NE2	1:E:353:CYS:HB2	2.23	0.53
1:E:86:GLY:HA3	1:E:95:TYR:O	2.08	0.53
1:E:357:SER:HA	1:E:404:SER:O	2.08	0.53
1:E:89:HIS:CE1	1:E:296:VAL:HG23	2.43	0.53
4:H:73:ALA:HA	4:H:113:CYS:HB3	1.89	0.53
1:E:220:ARG:HB3	1:E:220:ARG:NH1	2.23	0.53
2:F:18:ARG:HG3	3:G:44:MET:HE3	1.90	0.53
4:H:22:ARG:HG3	4:H:82:GLU:OE1	2.08	0.52
4:D:21:PRO:HB2	4:D:24:VAL:HG23	1.89	0.52
1:A:243:ASP:HB3	1:A:246:ASP:HB2	1.91	0.52
1:A:337:LEU:HD11	1:A:427:ILE:HA	1.92	0.52
1:E:337:LEU:HD21	1:E:427:ILE:HG23	1.91	0.52
1:A:342:MET:HA	1:A:356:LEU:HD23	1.91	0.52
1:E:257:HIS:CE1	1:E:258:LYS:HE3	2.45	0.51
4:H:55:ASP:N	4:H:59:LYS:O	2.36	0.51
2:B:75:LEU:HD22	2:F:68:ARG:HG2	1.92	0.51
4:H:13:GLN:HG3	4:H:104:LEU:HA	1.91	0.51
1:E:386:LEU:CD2	4:H:109:VAL:HG13	2.40	0.51
1:A:114:ILE:HD11	1:A:121:ILE:HD11	1.92	0.51
1:A:422:THR:O	1:A:426:CYS:HB2	2.11	0.51
4:D:107:PRO:HB2	4:D:108:PRO:HD2	1.92	0.51
1:E:63:VAL:HG22	1:E:409:GLY:HA3	1.92	0.51
1:A:374:ALA:HB1	1:E:93:HIS:CG	2.45	0.51
1:A:120:GLU:OE1	1:A:271:ARG:HA	2.11	0.50
1:A:94:ALA:HA	1:A:97:TRP:CE3	2.47	0.50
1:E:358:PHE:O	1:E:404:SER:HB3	2.11	0.50
1:A:242:LEU:HA	1:A:247:MET:HE3	1.92	0.50
2:B:26:TYR:O	2:B:30:THR:HG23	2.11	0.50
4:D:77:SER:O	4:D:81:THR:HG23	2.12	0.50
1:E:340:VAL:O	1:E:340:VAL:HG13	2.12	0.50
2:F:10:LEU:HD21	3:G:36:SER:HB2	1.92	0.50
1:E:368:MET:CE	4:H:10:LEU:HD21	2.41	0.50
1:A:454:TRP:O	1:A:455:THR:HB	2.13	0.49
4:D:19:GLU:OE1	4:D:19:GLU:HA	2.12	0.49
4:H:130:LEU:O	4:H:130:LEU:HD22	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:19:GLU:HA	4:H:19:GLU:OE1	2.12	0.49
4:H:36:THR:HG1	4:H:51:GLN:HE21	1.58	0.49
1:A:121:ILE:C	1:A:122:ILE:HD12	2.33	0.49
1:A:340:VAL:HG13	1:A:340:VAL:O	2.13	0.49
1:E:251:LEU:HA	1:E:269:TYR:O	2.12	0.49
1:A:242:LEU:HA	1:A:247:MET:CE	2.43	0.48
2:B:12:LEU:HD21	2:B:59:ALA:HB3	1.95	0.48
1:E:220:ARG:CZ	1:E:220:ARG:HB3	2.44	0.48
1:E:94:ALA:HA	1:E:97:TRP:CE3	2.48	0.48
1:A:127:ALA:CB	1:A:255:SER:HB2	2.41	0.48
1:A:298:THR:HA	1:A:301:VAL:HG22	1.95	0.48
4:D:21:PRO:HB2	4:D:24:VAL:CG2	2.44	0.48
1:E:129:GLU:O	1:E:133:ILE:HG13	2.13	0.47
1:A:357:SER:HA	1:A:404:SER:O	2.14	0.47
3:C:65:VAL:O	3:C:69:ILE:HG13	2.14	0.47
4:D:76:SER:O	4:D:80:ALA:HB2	2.14	0.47
4:H:60:ILE:HB	4:H:85:LYS:O	2.14	0.47
3:C:68:ALA:O	3:C:72:ILE:HD13	2.14	0.47
1:A:417:GLU:CB	2:B:83:ILE:HD11	2.44	0.47
4:D:38:LEU:HD23	4:D:49:LYS:CB	2.43	0.47
1:E:369:ALA:HB1	1:E:429:HIS:CG	2.50	0.47
1:E:183:ILE:HD11	1:E:348:HIS:HB2	1.95	0.47
1:E:59:LEU:HD21	2:F:83:ILE:HB	1.96	0.47
3:G:50:PHE:CD1	3:G:72:ILE:HD13	2.49	0.47
4:H:79:LEU:HD11	4:H:83:TRP:CE2	2.50	0.47
1:A:80:TYR:CD1	1:A:84:TYR:HB2	2.51	0.46
2:B:26:TYR:CD2	2:B:81:LEU:HD12	2.50	0.46
1:A:367:LEU:CD2	1:A:375:LEU:HB2	2.46	0.46
1:E:152:THR:OG1	1:E:155:GLU:HG2	2.16	0.46
4:H:95:ILE:HG13	4:H:121:ILE:CD1	2.44	0.46
4:H:20:ASN:N	4:H:21:PRO:CD	2.78	0.46
4:D:53:GLN:CB	4:D:61:VAL:HG22	2.45	0.46
4:D:67:THR:HG21	4:D:74:ILE:HA	1.98	0.46
2:F:17:LEU:O	2:F:21:LYS:HG3	2.16	0.46
1:E:155:GLU:OE2	1:E:203:MET:HG2	2.16	0.46
4:H:32:LYS:HG3	4:H:32:LYS:O	2.15	0.46
1:A:206:ASN:OD1	1:A:209:ILE:HG12	2.16	0.45
1:E:386:LEU:HD22	4:H:109:VAL:HG13	1.98	0.45
4:H:52:ILE:HD11	4:H:125:LEU:HD23	1.98	0.45
4:H:54:VAL:HB	4:H:128:TYR:CE1	2.52	0.45
1:E:67:THR:HB	1:E:260:TYR:CD1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ASP:HB3	1:E:359:ALA:CB	2.46	0.45
3:G:22:VAL:HG12	3:G:22:VAL:O	2.16	0.45
1:E:369:ALA:HB2	4:H:18:TYR:OH	2.17	0.45
4:H:60:ILE:O	4:H:85:LYS:O	2.35	0.45
1:A:65:ALA:O	1:A:66:THR:HB	2.16	0.45
1:A:113:LEU:HD13	1:A:312:GLN:HB2	1.99	0.45
1:A:370:LEU:HD13	1:A:375:LEU:CD1	2.47	0.45
4:D:20:ASN:N	4:D:21:PRO:HD3	2.32	0.45
4:D:46:ASP:HA	4:D:68:PHE:O	2.17	0.45
2:F:27:ASN:OD1	2:F:27:ASN:N	2.31	0.45
4:H:34:VAL:HA	4:H:52:ILE:O	2.17	0.45
2:F:84:GLU:O	2:F:85:ASN:HB2	2.16	0.44
4:H:65:PHE:HB3	4:H:81:THR:HG21	1.98	0.44
1:A:98:GLU:CD	1:E:57:ARG:HH12	2.21	0.44
2:F:55:LEU:O	2:F:58:LYS:HG2	2.18	0.44
1:A:300:LEU:HD11	1:E:300:LEU:CD1	2.45	0.44
1:A:329:LEU:HD23	1:A:329:LEU:C	2.37	0.44
4:H:31:SER:C	4:H:33:ASN:H	2.19	0.44
1:E:278:VAL:HB	1:E:291:MET:HE3	2.00	0.44
1:E:422:THR:O	1:E:426:CYS:HB2	2.17	0.44
1:E:121:ILE:C	1:E:122:ILE:HD12	2.38	0.44
1:E:65:ALA:O	1:E:66:THR:HB	2.17	0.44
2:F:18:ARG:HA	3:G:44:MET:HE1	2.00	0.44
4:H:31:SER:HB3	4:H:34:VAL:HG23	1.99	0.44
1:A:57:ARG:HH12	1:E:98:GLU:CD	2.21	0.44
3:G:10:ILE:HG22	3:G:11:ILE:N	2.32	0.44
3:G:4:GLU:OE1	3:G:4:GLU:HA	2.17	0.44
2:B:84:GLU:O	2:B:85:ASN:HB2	2.17	0.44
1:E:339:ASP:HB3	1:E:359:ALA:HB3	1.98	0.44
1:A:185:ASP:HB3	1:A:188:GLU:HB2	1.99	0.43
4:D:58:GLY:O	4:D:89:VAL:HG23	2.18	0.43
1:E:350:TYR:CE2	1:E:352:GLY:HA3	2.53	0.43
1:A:117:ASP:HB3	1:A:120:GLU:HG3	2.00	0.43
1:A:78:LEU:HD23	1:A:81:LEU:HD12	2.00	0.43
4:H:130:LEU:O	4:H:130:LEU:HD13	2.18	0.43
4:H:27:LEU:HD21	4:H:64:ARG:HG2	2.00	0.43
2:B:52:ILE:O	2:B:56:VAL:HG23	2.18	0.43
2:B:63:LEU:HD21	2:B:67:ARG:NH2	2.33	0.43
1:E:372:ASP:HB3	2:F:82:ILE:HD12	2.01	0.43
3:G:4:GLU:OE2	3:G:73:ASN:ND2	2.51	0.43
1:A:142:TYR:CZ	1:A:228:TYR:HE2	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:501:PLP:O3P	1:E:295:THR:HB	2.19	0.43
1:E:358:PHE:N	1:E:404:SER:O	2.50	0.43
1:E:436:MET:HG2	4:H:24:VAL:HG11	2.01	0.43
3:G:11:ILE:HD13	3:G:28:PHE:CE1	2.53	0.43
4:H:52:ILE:CD1	4:H:125:LEU:HD23	2.49	0.43
3:C:28:PHE:HE2	3:C:62:ILE:HG22	1.84	0.43
4:D:17:HIS:HB3	4:D:78:SER:CB	2.49	0.43
1:E:203:MET:HE2	1:E:205:VAL:O	2.18	0.43
2:F:48:ASP:O	2:F:52:ILE:HG13	2.18	0.43
1:A:203:MET:HE2	1:A:205:VAL:O	2.19	0.43
1:E:414:THR:HA	1:E:418:GLU:OE1	2.18	0.43
4:H:35:GLY:O	4:H:51:GLN:HA	2.19	0.42
2:B:32:ALA:O	2:B:36:ILE:HG13	2.19	0.42
4:D:23:ASN:CB	4:D:63:ALA:O	2.67	0.42
4:H:31:SER:CB	4:H:34:VAL:HG23	2.49	0.42
1:A:75:ASP:OD1	2:F:76:TYR:OH	2.15	0.42
1:A:406:ILE:HD11	1:A:408:PHE:CZ	2.54	0.42
1:E:329:LEU:HD23	1:E:329:LEU:C	2.40	0.42
1:A:339:ASP:HB3	1:A:359:ALA:CB	2.50	0.42
2:B:41:ARG:NH2	3:C:38:ASP:OD1	2.52	0.42
3:G:52:THR:HG22	3:G:53:GLU:N	2.26	0.42
1:A:150:ILE:HD11	1:A:193:ILE:HA	2.00	0.42
1:A:369:ALA:HB1	1:A:429:HIS:CG	2.54	0.42
1:A:70:ASP:OD2	1:A:412:ARG:NH2	2.53	0.42
1:E:357:SER:HB3	1:E:401:LEU:HD22	2.02	0.42
3:G:10:ILE:O	3:G:13:GLU:HG2	2.18	0.42
4:D:16:ASP:O	4:D:20:ASN:HB3	2.20	0.42
1:E:284:GLY:HA3	1:E:293:SER:HB3	2.02	0.42
1:A:190:GLU:HG2	1:A:221:ILE:HG23	2.01	0.42
1:A:278:VAL:CG1	1:A:291:MET:HE1	2.50	0.42
1:A:349:HIS:NE2	1:A:353:CYS:O	2.53	0.42
3:G:11:ILE:HG23	3:G:15:LEU:HD12	2.02	0.42
3:C:8:LYS:O	3:C:19:GLN:HG2	2.21	0.41
1:E:454:TRP:HB3	4:H:41:ALA:HB2	2.02	0.41
4:D:63:ALA:O	4:D:64:ARG:HD3	2.20	0.41
2:F:62:ASP:O	2:F:66:ILE:HG13	2.21	0.41
4:H:65:PHE:CE1	4:H:67:THR:HG23	2.54	0.41
4:H:56:GLU:HG3	4:H:57:LYS:HG3	2.01	0.41
1:E:166:LEU:HD23	1:E:166:LEU:HA	1.88	0.41
3:G:62:ILE:O	3:G:62:ILE:HG22	2.20	0.41
4:D:38:LEU:O	4:D:38:LEU:HD13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:10:ILE:HD11	3:G:49:GLU:HB3	1.97	0.41
2:B:22:ARG:HB2	2:B:70:VAL:HG11	2.02	0.41
3:G:50:PHE:CG	3:G:72:ILE:HD13	2.56	0.41
1:A:200:VAL:HG23	1:A:227:VAL:HG11	2.03	0.41
4:H:117:ALA:O	4:H:120:ALA:HB3	2.21	0.41
1:A:146:LYS:CB	1:A:198:SER:HB3	2.51	0.41
3:C:65:VAL:HG12	3:C:69:ILE:CD1	2.51	0.41
1:E:119:ARG:HD2	1:E:272:ARG:HH11	1.86	0.41
2:F:23:PHE:HB2	2:F:29:ARG:HB2	2.03	0.41
4:D:60:ILE:O	4:D:85:LYS:O	2.39	0.40
2:F:66:ILE:O	2:F:70:VAL:HG23	2.21	0.40
4:H:27:LEU:HD21	4:H:64:ARG:CG	2.51	0.40
3:C:65:VAL:HG12	3:C:69:ILE:HD11	2.03	0.40
2:F:26:TYR:CD2	2:F:81:LEU:HD12	2.56	0.40
1:A:284:GLY:HA3	1:A:293:SER:HB3	2.02	0.40
1:E:117:ASP:OD1	1:E:118:PRO:HD2	2.21	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	392/406 (97%)	375 (96%)	15 (4%)	2 (0%)	29	65
1	E	394/406 (97%)	378 (96%)	14 (4%)	2 (0%)	29	65
2	B	79/91 (87%)	74 (94%)	5 (6%)	0	100	100
2	F	80/91 (88%)	76 (95%)	4 (5%)	0	100	100
3	C	70/77 (91%)	63 (90%)	6 (9%)	1 (1%)	11	43
3	G	69/77 (90%)	62 (90%)	5 (7%)	2 (3%)	4	25
4	D	116/150 (77%)	104 (90%)	11 (10%)	1 (1%)	17	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	124/150 (83%)	111 (90%)	12 (10%)	1 (1%)	19	55
All	All	1324/1448 (91%)	1243 (94%)	72 (5%)	9 (1%)	22	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	E	273	ARG
1	E	452	ILE
1	A	451	SER
3	C	62	ILE
4	D	96	LYS
3	G	4	GLU
3	G	62	ILE
4	H	96	LYS

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	294/346 (85%)	289 (98%)	5 (2%)	60	82
1	E	310/346 (90%)	305 (98%)	5 (2%)	62	83
2	B	59/80 (74%)	58 (98%)	1 (2%)	60	82
2	F	65/80 (81%)	64 (98%)	1 (2%)	65	84
3	C	29/66 (44%)	29 (100%)	0	100	100
3	G	49/66 (74%)	46 (94%)	3 (6%)	18	50
4	D	38/126 (30%)	36 (95%)	2 (5%)	22	55
4	H	95/126 (75%)	88 (93%)	7 (7%)	13	43
All	All	939/1236 (76%)	915 (97%)	24 (3%)	46	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	188	GLU
1	A	277	ARG
1	A	397	THR
1	A	401	LEU
2	B	27	ASN
4	D	61	VAL
4	D	98	THR
1	E	69	LEU
1	E	145	ARG
1	E	272	ARG
1	E	445	ASP
1	E	455	THR
2	F	27	ASN
3	G	3	ILE
3	G	4	GLU
3	G	9	LYS
4	H	11	SER
4	H	13	GLN
4	H	22	ARG
4	H	61	VAL
4	H	67	THR
4	H	98	THR
4	H	111	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
4	H	13	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	$\# Z > 2$
5	PLP	E	501	1	15,15,16	1.55	3 (20%)	20,22,23	1.12	2 (10%)
6	8Q1	C	301	3	27,33,34	1.82	6 (22%)	32,40,43	1.75	7 (21%)
5	PLP	A	501	1	15,15,16	1.54	3 (20%)	20,22,23	1.09	2 (10%)
6	8Q1	G	301	3	27,33,34	1.77	6 (22%)	32,40,43	1.79	7 (21%)

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
5	PLP	E	501	1	-	1/6/6/8	0/1/1/1
6	8Q1	C	301	3	-	15/38/40/41	-
5	PLP	A	501	1	-	2/6/6/8	0/1/1/1
6	8Q1	G	301	3	-	7/38/40/41	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	8Q1	C39-N41	5.44	1.45	1.33
6	G	301	8Q1	C34-N36	5.42	1.45	1.33
6	C	301	8Q1	C34-N36	5.35	1.45	1.33
6	G	301	8Q1	C39-N41	5.14	1.45	1.33
5	E	501	PLP	C5-C4	-3.86	1.36	1.40
5	A	501	PLP	C5-C4	-3.86	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	8Q1	C1-S44	2.60	1.82	1.76
6	C	301	8Q1	C6-C1	2.51	1.53	1.50
6	G	301	8Q1	C1-S44	2.40	1.81	1.76
5	E	501	PLP	C3-C2	-2.33	1.38	1.40
6	G	301	8Q1	C6-C1	2.30	1.53	1.50
6	G	301	8Q1	O35-C34	-2.26	1.18	1.23
5	E	501	PLP	C3-C4	-2.25	1.35	1.40
6	G	301	8Q1	O40-C39	-2.21	1.18	1.23
6	C	301	8Q1	O40-C39	-2.19	1.18	1.23
6	C	301	8Q1	O35-C34	-2.17	1.19	1.23
5	A	501	PLP	C3-C4	-2.03	1.35	1.40
5	A	501	PLP	C3-C2	-2.00	1.38	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	301	8Q1	C6-C1-S44	6.36	120.86	113.46
6	C	301	8Q1	C6-C1-S44	5.71	120.10	113.46
6	C	301	8Q1	C38-C39-N41	3.45	122.24	116.42
6	C	301	8Q1	O4-C1-C6	-3.38	120.00	123.99
6	G	301	8Q1	O4-C1-C6	-3.37	120.02	123.99
6	C	301	8Q1	C38-C37-N36	-3.05	105.74	111.90
5	E	501	PLP	C6-C5-C4	2.95	120.48	118.16
6	G	301	8Q1	C37-C38-C39	2.86	117.11	112.36
6	C	301	8Q1	C43-S44-C1	2.75	110.43	101.87
6	G	301	8Q1	O4-C1-S44	-2.69	119.12	122.61
6	C	301	8Q1	C42-N41-C39	-2.56	118.09	122.84
5	A	501	PLP	C6-C5-C4	2.45	120.09	118.16
6	G	301	8Q1	C42-N41-C39	-2.44	118.31	122.84
5	E	501	PLP	C5-C6-N1	-2.38	119.86	123.82
6	G	301	8Q1	C38-C39-N41	2.35	120.37	116.42
5	A	501	PLP	C5-C6-N1	-2.15	120.23	123.82
6	C	301	8Q1	O4-C1-S44	-2.10	119.89	122.61
6	G	301	8Q1	C37-N36-C34	-2.03	118.97	122.59

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	301	8Q1	O4-C1-S44-C43
6	C	301	8Q1	C6-C1-S44-C43
6	C	301	8Q1	C28-C29-C32-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	301	8Q1	C28-C29-C32-O33
6	C	301	8Q1	C30-C29-C32-C34
6	C	301	8Q1	C31-C29-C32-C34
6	C	301	8Q1	C31-C29-C32-O33
6	C	301	8Q1	O33-C32-C34-N36
6	C	301	8Q1	N36-C37-C38-C39
6	C	301	8Q1	C42-C43-S44-C1
6	G	301	8Q1	O27-C28-C29-C30
6	G	301	8Q1	O27-C28-C29-C31
6	G	301	8Q1	O27-C28-C29-C32
6	C	301	8Q1	O33-C32-C34-O35
5	A	501	PLP	C5A-O4P-P-O1P
6	C	301	8Q1	C11-C10-C9-C8
6	C	301	8Q1	C30-C29-C32-O33
6	C	301	8Q1	C10-C11-C12-C13
6	G	301	8Q1	C10-C11-C12-C13
6	G	301	8Q1	C9-C10-C11-C12
6	G	301	8Q1	C38-C37-N36-C34
6	G	301	8Q1	C42-C43-S44-C1
5	A	501	PLP	C5A-O4P-P-O2P
5	E	501	PLP	C5A-O4P-P-O1P
6	C	301	8Q1	C9-C10-C11-C12

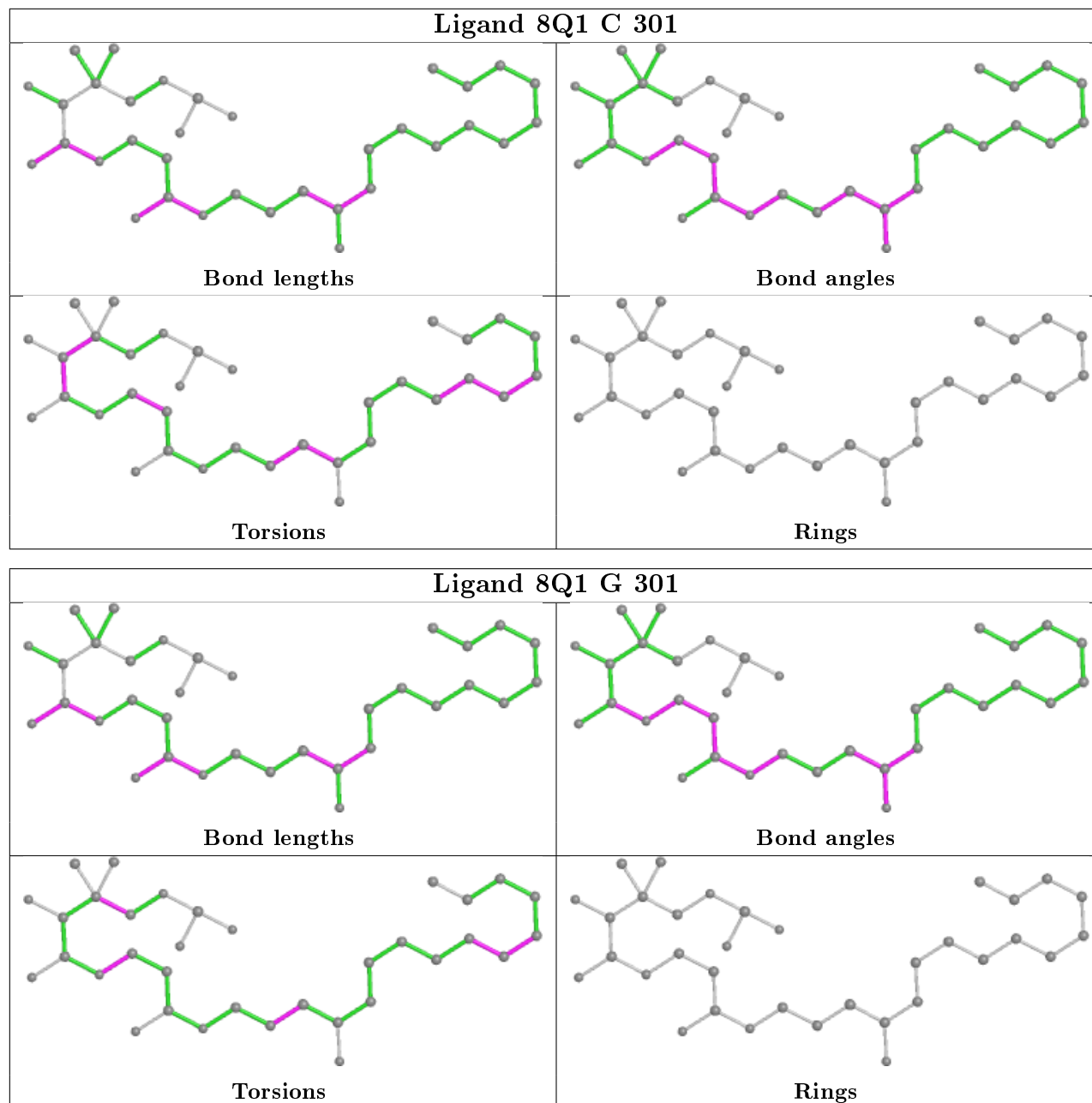
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	8Q1	1	0
5	A	501	PLP	1	0
6	G	301	8Q1	2	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	396/406 (97%)	-0.22	2 (0%) 91 86	46, 73, 140, 207	0
1	E	398/406 (98%)	-0.30	3 (0%) 86 78	45, 71, 118, 177	0
2	B	81/91 (89%)	-0.29	0 100 100	67, 92, 121, 156	0
2	F	82/91 (90%)	-0.43	0 100 100	55, 77, 107, 130	0
3	C	72/77 (93%)	0.21	0 100 100	92, 134, 162, 171	0
3	G	71/77 (92%)	-0.25	0 100 100	67, 92, 128, 154	0
4	D	118/150 (78%)	0.90	19 (16%) 1 1	126, 161, 187, 202	0
4	H	126/150 (84%)	-0.19	0 100 100	66, 88, 127, 147	0
All	All	1344/1448 (92%)	-0.14	24 (1%) 68 55	45, 81, 164, 207	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	34	VAL	5.1
1	E	378	GLY	3.9
4	D	41	ALA	3.6
4	D	37	GLY	3.6
4	D	50	LEU	3.4
1	A	446	GLY	3.1
1	E	379	SER	2.8
4	D	58	GLY	2.8
1	A	454	TRP	2.6
4	D	95	ILE	2.6
4	D	52	ILE	2.5
4	D	126	ALA	2.5
4	D	83	TRP	2.5
4	D	105	CYS	2.4
1	E	385	SER	2.4
4	D	35	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	79	LEU	2.3
4	D	107	PRO	2.3
4	D	103	GLU	2.3
4	D	43	ALA	2.2
4	D	124	ALA	2.2
4	D	125	LEU	2.1
4	D	51	GLN	2.1
4	D	54	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

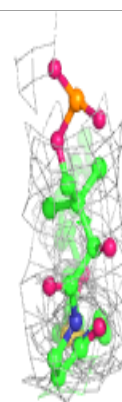
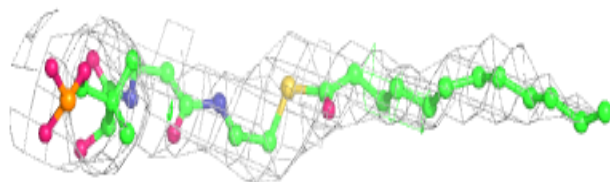
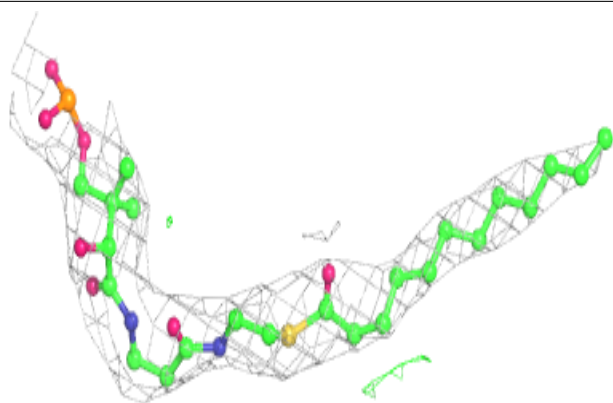
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	8Q1	C	301	34/35	0.94	0.28	59,96,119,122	0
6	8Q1	G	301	34/35	0.94	0.28	68,89,95,101	0
5	PLP	A	501	15/16	0.95	0.27	71,85,96,96	0
5	PLP	E	501	15/16	0.96	0.20	50,63,82,89	0

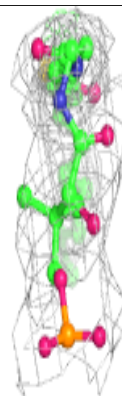
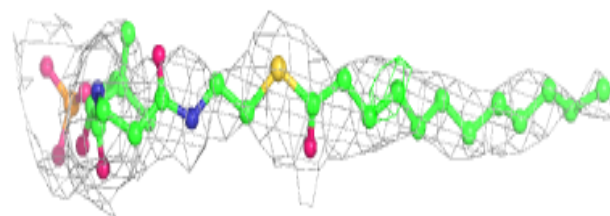
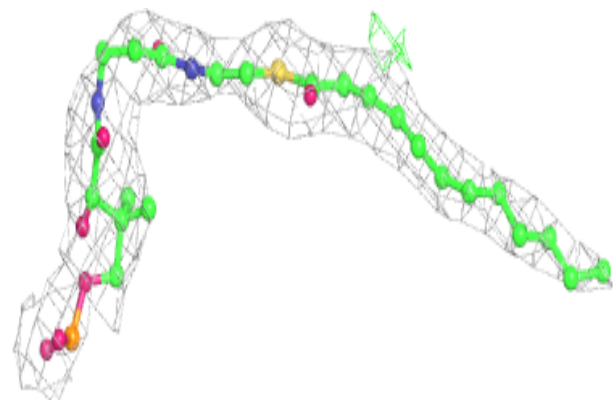
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8Q1 C 301:

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

**Electron density around 8Q1 G 301:**

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



6.5 Other polymers

There are no such residues in this entry.