Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:27 am BST

PDB ID	:	6O4F
Title	:	Structure of ALDH7A1 mutant N167S complexed with alpha-aminoadipate
Authors	:	Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on	:	2019-02-28
Resolution	:	1.90 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:

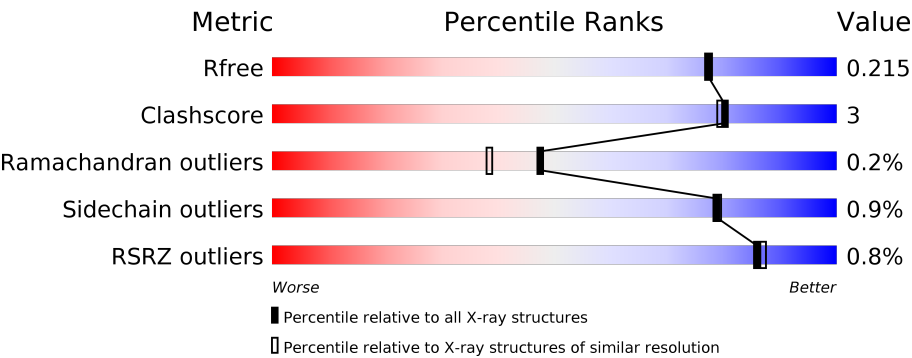|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.215
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		0.9%
RSRZ outliers		0.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	513	92% 7% •
1	B	513	% 91% 8% •
1	C	513	91% 8% •
1	D	513	% 92% 7% •
1	E	513	2% 91% 7% •
1	F	513	% 90% 8% •

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Mol	Chain	Length	Quality of chain
1	G	513	94% 5%
1	H	513	92% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32982 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total 3840	C 2442	N 665	O 716	S 17	0	1	0
1	B	508	Total 3945	C 2506	N 682	O 739	S 18	0	15	0
1	C	508	Total 3845	C 2443	N 667	O 716	S 19	0	2	0
1	D	509	Total 3941	C 2507	N 686	O 730	S 18	0	16	0
1	E	509	Total 3954	C 2514	N 686	O 737	S 17	0	14	0
1	F	508	Total 3940	C 2504	N 681	O 736	S 19	0	16	0
1	G	508	Total 3861	C 2454	N 669	O 719	S 19	0	3	0
1	H	509	Total 3853	C 2448	N 667	O 720	S 18	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	167	SER	ASN	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	167	SER	ASN	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	167	SER	ASN	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	167	SER	ASN	engineered mutation	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P49419
E	167	SER	ASN	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	167	SER	ASN	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	167	SER	ASN	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	167	SER	ASN	engineered mutation	UNP P49419

- Molecule 2 is 2-AMINOHEXANEDIOIC ACID (three-letter code: UN1) (formula: $C_6H_{11}NO_4$) (labeled as "Ligand of Interest" by author).
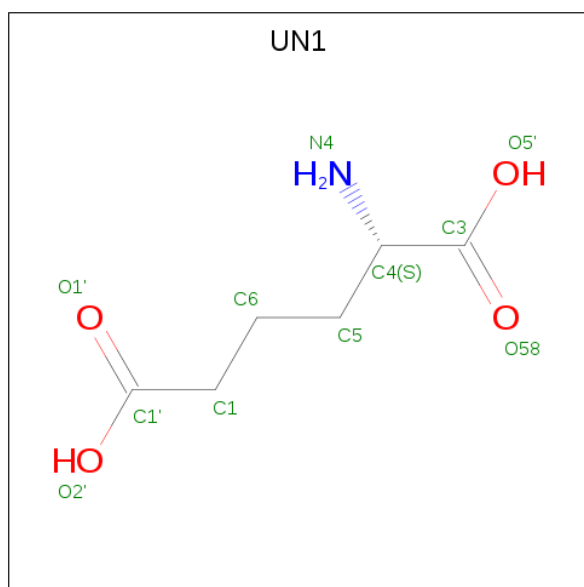
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 11	C 6	N 1	O 4	0	1
2	E	1	Total 11	C 6	N 1	O 4	0	0
2	F	1	Total 11	C 6	N 1	O 4	0	1

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	237	Total 237	O 237	0	0
4	B	219	Total 219	O 219	0	0
4	C	243	Total 243	O 243	0	0
4	D	192	Total 192	O 192	0	0
4	E	240	Total 240	O 240	0	0
4	F	204	Total 204	O 204	0	0
4	G	219	Total 219	O 219	0	0
4	H	204	Total 204	O 204	0	0

3 Residue-property plots (i)

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

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain A:

92%   7%   •

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain B:

%

91%   8%   •
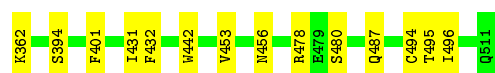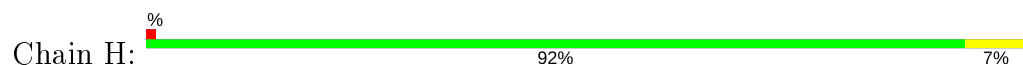
• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain C:

91%   8%   •

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain D:

%

92%   7%   •

I457 P458 E471 S480 T495 I496 N497 L502 P503 L504 A505 I508 K509 F510 Q511

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain E:

2%

91%　　　　7%

GLY HIS MET SER T3 R68 V104 E118 Y122 I136 I151 A171 I198 G230 R238 K252 R264 I276 L285 V286 V287 P288 L291 F292 A293 C302 I310 I314 A325 L354 V373 I431 F432 W442 L443 S448

N454 I457 P458 S480 R490 T495 I496 N497 L502 P503 L504 A505 Q506 G507 I508 K509 F510 Q511

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain F:

%

90%　　　　8%

GLY HIS MET SER T3 L4 A12 L17 R20 E21 E24 N28 G33 R53 T63 R68 V99 V104 M108 I111 E121 I151 W189 I198 S199 R238 E260 S289 A290 L291 F292 A293 A294 V295 G296 T297 N320 Q328

I329 R330 N338 K362 F401 Q425 G426 L427 W442 S448 I457 P458 K472 H473 T474 S480 T495 I496 P503 L504 A505 I508 K509 F510 GLN

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain G:

94%　　　　5%

GLY HIS MET SER T3 R68 R94 V113 W154 R238 R264 A293 T297 K324 L340 F401 W419 E422 I431 F432 W442 L443 S448 V453 N456 I457 P458 S480 R490 R491 C494 F510 GLN

• Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain H:

%

92%　　　　7%

GLY HIS MET SER T3 P9 A12 L17 E22 N28 E36 R53 T63 R68 V99 C126 V130 I140 L141 P142 P156 G184 R238 T248 L269 A274 L291 V295 G296 T297 R307 N338 V339 L340 M352

K362 S394 F401 I431 F432 W442 V453 N456 R478 E479 S480 Q487 C494 T495 I496 Q511

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.68Å 158.56Å 156.83Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	48.79 – 1.90 48.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.79-1.90) 96.4 (48.79-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.85 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.173 , 0.218 0.169 , 0.215	Depositor DCC
R_{free} test set	14081 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.9	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32982	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4295e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UN1, EDO

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	0.39	0/3922	0.54	0/5325
1	B	4.15	2/4035 (0.0%)	0.67	6/5475 (0.1%)
1	C	0.38	0/3931	0.54	0/5335
1	D	3.70	2/4032 (0.0%)	0.65	4/5473 (0.1%)
1	E	4.50	2/4038 (0.0%)	0.64	4/5479 (0.1%)
1	F	3.85	2/4035 (0.0%)	0.65	6/5476 (0.1%)
1	G	0.37	0/3950	0.54	0/5358
1	H	0.35	0/3936	0.52	0/5341
All	All	2.90	8/31879 (0.0%)	0.60	20/43262 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	504[A]	LEU	CB-CG	201.34	7.36	1.52
1	E	504[B]	LEU	CB-CG	201.34	7.36	1.52
1	B	504[A]	LEU	CB-CG	185.78	6.91	1.52
1	B	504[B]	LEU	CB-CG	185.78	6.91	1.52
1	F	504[A]	LEU	CB-CG	172.11	6.51	1.52
1	F	504[B]	LEU	CB-CG	172.11	6.51	1.52
1	D	504[A]	LEU	CB-CG	165.48	6.32	1.52
1	D	504[B]	LEU	CB-CG	165.48	6.32	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	504[A]	LEU	CB-CG-CD1	-18.83	78.98	111.00
1	B	504[B]	LEU	CB-CG-CD1	-18.83	78.98	111.00
1	D	504[A]	LEU	CB-CG-CD1	-17.07	81.98	111.00
1	D	504[B]	LEU	CB-CG-CD1	-17.07	81.98	111.00
1	F	504[A]	LEU	CB-CG-CD1	-16.56	82.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	504[B]	LEU	CB-CG-CD1	-16.56	82.85	111.00
1	E	504[A]	LEU	CB-CG-CD1	-13.32	88.36	111.00
1	E	504[B]	LEU	CB-CG-CD1	-13.32	88.36	111.00
1	E	504[A]	LEU	CA-CB-CG	-11.42	89.04	115.30
1	E	504[B]	LEU	CA-CB-CG	-11.42	89.04	115.30
1	D	504[A]	LEU	CB-CG-CD2	9.28	126.78	111.00
1	D	504[B]	LEU	CB-CG-CD2	9.28	126.78	111.00
1	F	504[A]	LEU	CB-CG-CD2	8.88	126.09	111.00
1	F	504[B]	LEU	CB-CG-CD2	8.88	126.09	111.00
1	B	504[A]	LEU	CB-CG-CD2	6.71	122.41	111.00
1	B	504[B]	LEU	CB-CG-CD2	6.71	122.41	111.00
1	B	504[A]	LEU	CA-CB-CG	-6.51	100.34	115.30
1	B	504[B]	LEU	CA-CB-CG	-6.51	100.34	115.30
1	F	504[A]	LEU	CA-CB-CG	-5.73	102.12	115.30
1	F	504[B]	LEU	CA-CB-CG	-5.73	102.12	115.30

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	3840	0	3817	25	0
1	B	3945	0	3912	32	0
1	C	3845	0	3824	30	0
1	D	3941	0	3901	26	0
1	E	3954	0	3931	29	0
1	F	3940	0	3897	30	0
1	G	3861	0	3860	15	0
1	H	3853	0	3827	19	0
2	B	11	0	9	0	0
2	E	11	0	9	2	0
2	F	11	0	9	0	0
3	B	4	0	6	0	0
3	E	4	0	6	1	0
3	F	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	237	0	0	2	0
4	B	219	0	0	3	0
4	C	243	0	0	0	0
4	D	192	0	0	0	0
4	E	240	0	0	1	0
4	F	204	0	0	3	0
4	G	219	0	0	2	0
4	H	204	0	0	0	0
All	All	32982	0	31014	165	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 3.

All (165) 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:293:ALA:HB2	1:E:458:PRO:HB3	1.61	0.82
1:F:293:ALA:HB2	1:F:458:PRO:HB3	1.63	0.80
1:G:293:ALA:HB2	1:G:458:PRO:HB3	1.65	0.77
1:D:293:ALA:HB2	1:D:458:PRO:HB3	1.65	0.77
1:B:151:ILE:HB	1:C:140:ILE:HD11	1.68	0.74
1:A:293:ALA:HB2	1:A:458:PRO:HB3	1.72	0.72
1:E:291:LEU:HD22	1:E:325:ALA:HB1	1.75	0.69
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.77	0.67
1:E:230:GLY:HA3	3:E:602:EDO:H21	1.77	0.66
1:A:94:ARG:NH1	4:A:601:HOH:O	2.31	0.64
1:G:68:ARG:HD2	1:G:238:ARG:HB3	1.82	0.62
1:B:24:GLU:HG3	1:B:53:ARG:HH21	1.66	0.61
1:A:457:ILE:HD11	1:B:495:THR:HB	1.82	0.61
1:E:285:LEU:HD22	1:E:432:PHE:HE2	1.66	0.60
1:A:276:ILE:HB	1:A:431:ILE:HG22	1.83	0.60
1:E:264:ARG:HH22	1:E:490:ARG:HA	1.65	0.60
1:B:118:GLU:HG3	1:B:171:ALA:HB2	1.83	0.59
1:F:20:ARG:NH2	1:F:24:GLU:OE2	2.25	0.59
1:E:118:GLU:HG3	1:E:171:ALA:HB2	1.85	0.58
1:C:68:ARG:HD2	1:C:238:ARG:HB3	1.85	0.58
1:D:376[A]:ARG:NH1	1:D:377:PRO:O	2.37	0.58
1:E:151:ILE:HB	1:H:140:ILE:HD11	1.86	0.58
1:A:443:LEU:HD13	1:B:151:ILE:HD11	1.86	0.57
1:G:264:ARG:HH22	1:G:490:ARG:HA	1.70	0.57
1:F:33:GLY:O	1:F:53:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:ARG:HD2	1:H:238:ARG:HB3	1.87	0.57
1:C:443:LEU:HD13	1:D:151:ILE:HD11	1.87	0.56
1:C:5:LEU:HD22	1:C:11:TYR:CE2	2.41	0.56
1:B:33:GLY:O	1:B:53:ARG:NH1	2.39	0.56
1:E:104:VAL:HA	1:E:198:ILE:HD11	1.87	0.56
1:C:293:ALA:HB2	1:C:458:PRO:CB	2.36	0.55
1:G:443:LEU:HD11	1:H:496:ILE:HD11	1.88	0.55
1:G:94:ARG:NH1	4:G:604:HOH:O	2.41	0.54
1:B:140:ILE:CD1	1:C:151:ILE:HG23	2.38	0.54
1:C:118:GLU:HG3	1:C:171:ALA:HB2	1.90	0.54
1:C:293:ALA:HB2	1:C:458:PRO:HB3	1.89	0.54
1:E:497:ASN:HB2	1:F:457:ILE:HG23	1.89	0.54
1:C:457:ILE:HD11	1:D:495:THR:HB	1.89	0.54
1:D:376[A]:ARG:HG3	1:D:376[A]:ARG:HH11	1.72	0.53
1:A:140:ILE:HD11	1:D:151:ILE:HB	1.90	0.53
1:C:496:ILE:HD11	1:D:443:LEU:HD11	1.90	0.53
1:B:354:LEU:HD21	1:B:373:VAL:HG23	1.90	0.53
1:A:140:ILE:HG23	1:A:151:ILE:HG22	1.90	0.53
1:C:264:ARG:NH1	1:D:471:GLU:OE1	2.43	0.52
1:C:495:THR:HB	1:D:457:ILE:HD11	1.90	0.52
1:E:454:ASN:HB3	1:E:457:ILE:HG13	1.91	0.52
1:D:374:MET:HE3	1:D:382:GLU:HA	1.91	0.52
1:C:443:LEU:HD11	1:D:496:ILE:HD11	1.90	0.52
1:E:68:ARG:HD2	1:E:238:ARG:HB3	1.92	0.52
1:A:439:ILE:HG23	1:A:455:VAL:HG21	1.93	0.51
1:B:351:SER:HB2	1:E:354:LEU:HD12	1.91	0.51
1:E:506[B]:GLN:HG2	1:F:121:GLU:HG3	1.93	0.51
1:C:126:CYS:O	1:C:130:VAL:HG23	2.11	0.51
1:F:20:ARG:NH1	4:F:702:HOH:O	2.43	0.51
2:E:601:UN1:N4	4:E:702:HOH:O	2.35	0.50
1:A:454:ASN:HB3	1:A:457:ILE:HG13	1.94	0.50
1:C:457:ILE:HG23	1:D:497:ASN:HB2	1.94	0.50
1:E:457:ILE:HD11	1:F:495:THR:HB	1.93	0.50
1:A:140:ILE:CD1	1:D:151:ILE:HB	2.42	0.50
1:E:495:THR:HB	1:F:457:ILE:HD11	1.94	0.50
1:A:287:VAL:HG21	1:A:321:ARG:HD2	1.94	0.49
1:B:20:ARG:NH2	1:B:24:GLU:OE2	2.44	0.49
1:A:138:GLY:O	1:D:140:ILE:HG22	2.12	0.49
1:H:291:LEU:O	1:H:295:VAL:HG22	2.12	0.49
1:A:497:ASN:HB2	1:B:457:ILE:HG23	1.94	0.49
1:B:293:ALA:HB2	1:B:458:PRO:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502[B]:LEU:HD11	1:F:289:SER:OG	2.13	0.49
1:B:276:ILE:HB	1:B:431:ILE:HG22	1.95	0.49
1:B:142:PRO:HB2	1:C:79:ALA:HB3	1.95	0.48
1:C:431:ILE:HG23	1:C:442:TRP:CE2	2.48	0.48
1:F:17:LEU:HD21	1:F:99:VAL:HG13	1.95	0.48
1:G:453:VAL:O	1:H:494:CYS:HA	2.14	0.48
1:C:104:VAL:HA	1:C:198:ILE:HD11	1.94	0.48
1:F:293:ALA:HB2	1:F:458:PRO:CB	2.38	0.48
1:E:354:LEU:HD21	1:E:373:VAL:HG23	1.95	0.48
1:B:431:ILE:HG23	1:B:442:TRP:CE2	2.49	0.48
1:C:94:ARG:HG3	1:C:123:VAL:HG11	1.95	0.48
1:F:68:ARG:NH2	4:F:701:HOH:O	2.33	0.48
1:H:22:GLU:HG2	1:H:53:ARG:HE	1.79	0.47
1:F:442:TRP:CH2	1:F:448:SER:HB2	2.50	0.47
1:C:442:TRP:CH2	1:C:448:SER:HB2	2.50	0.47
1:B:457:ILE:HD12	4:B:707:HOH:O	2.15	0.47
1:D:354:LEU:HD21	1:D:373:VAL:HG23	1.97	0.47
1:D:454:ASN:HB3	1:D:457:ILE:HG13	1.97	0.47
1:B:134:ARG:HG3	4:B:852:HOH:O	2.15	0.47
1:B:419:TRP:O	1:B:422:GLU:HG2	2.15	0.47
1:A:442:TRP:CH2	1:A:448:SER:HB2	2.50	0.47
1:E:276:ILE:HB	1:E:431:ILE:HG22	1.97	0.46
1:E:443:LEU:HD11	1:F:496:ILE:HD11	1.97	0.46
1:D:164:THR:HG22	1:D:172:VAL:HG12	1.96	0.46
1:C:392:ASP:HA	1:C:397:HIS:NE2	2.30	0.46
1:B:4:LEU:HD12	1:B:21:GLU:HG3	1.96	0.46
1:D:28:ASN:HB3	1:D:63:THR:HG23	1.98	0.46
1:B:126:CYS:O	1:B:130:VAL:HG23	2.15	0.46
1:F:189:TRP:CH2	1:F:199:SER:HA	2.51	0.46
1:B:336:ASP:HB3	4:B:890:HOH:O	2.14	0.45
1:E:291:LEU:HD21	1:F:508[A]:ILE:HD12	1.98	0.45
1:E:442:TRP:CH2	1:E:448:SER:HB2	2.51	0.45
1:A:457:ILE:HG23	1:B:497:ASN:HB2	1.98	0.45
1:G:457:ILE:HD11	1:H:495:THR:HB	1.98	0.45
1:G:442:TRP:CH2	1:G:448:SER:HB2	2.51	0.45
1:A:291:LEU:O	1:A:295:VAL:HG22	2.17	0.45
1:H:17:LEU:HD21	1:H:99:VAL:HG13	1.99	0.45
1:H:338:ASN:O	1:H:340:LEU:HD22	2.17	0.45
1:F:291:LEU:O	1:F:295:VAL:HG22	2.16	0.44
1:D:145:ARG:NH1	1:D:505[B]:ALA:HB2	2.33	0.44
1:D:276:ILE:HB	1:D:431:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HD12	1:C:138:GLY:O	2.18	0.44
1:E:252:LYS:HE2	1:F:260:GLU:O	2.18	0.44
1:F:427:LEU:HD13	1:F:474:THR:HG21	2.00	0.44
1:A:494:CYS:HA	1:B:453:VAL:O	2.18	0.44
1:A:495:THR:HB	1:B:457:ILE:HD11	1.99	0.43
1:A:443:LEU:HD11	1:B:496:ILE:HD11	2.00	0.43
1:E:310:ILE:HG22	1:E:314:ILE:HG13	1.99	0.43
1:B:4:LEU:HD23	1:B:48:PRO:HB2	1.98	0.43
1:H:432:PHE:CD2	1:H:456:ASN:HA	2.53	0.43
1:A:113:VAL:HG13	4:A:790:HOH:O	2.18	0.43
1:G:432:PHE:CD2	1:G:456:ASN:HA	2.53	0.43
1:A:419:TRP:O	1:A:422:GLU:HG2	2.19	0.43
1:B:24:GLU:HG3	1:B:53:ARG:NH2	2.33	0.43
1:C:288:PRO:HB2	1:D:503[A]:PRO:HG2	2.01	0.43
1:E:443:LEU:HD13	1:F:151:ILE:HD11	2.01	0.43
1:G:113:VAL:HG13	4:G:762:HOH:O	2.17	0.43
1:B:344:LEU:HD21	1:B:403:PRO:HD3	2.01	0.43
1:H:431:ILE:HG23	1:H:442:TRP:CE2	2.53	0.43
1:D:126:CYS:O	1:D:130:VAL:HG23	2.19	0.43
1:C:154:TRP:CH2	1:C:491:ARG:HB2	2.54	0.42
1:H:156:PRO:HG3	1:H:184:GLY:HA3	2.00	0.42
1:H:126:CYS:O	1:H:130:VAL:HG23	2.18	0.42
1:A:312:GLU:HG3	1:A:410:PHE:O	2.19	0.42
1:B:293:ALA:HB2	1:B:458:PRO:HB3	2.01	0.42
1:B:293:ALA:HB2	1:B:458:PRO:HB2	2.02	0.42
1:F:104:VAL:HA	1:F:198:ILE:HD11	2.01	0.42
1:A:41:TYR:CZ	1:F:362:LYS:HG2	2.55	0.42
1:A:310:ILE:HG22	1:A:314:ILE:HG13	2.00	0.42
1:H:274:ALA:HA	1:H:307:ARG:O	2.20	0.42
1:D:68:ARG:HD2	1:D:238:ARG:HB3	2.02	0.42
1:F:111:ILE:HB	4:F:735:HOH:O	2.19	0.42
1:F:68:ARG:HD2	1:F:238:ARG:HB3	2.01	0.42
1:E:136:ILE:O	1:H:142:PRO:HD3	2.20	0.42
1:C:4:LEU:HD23	1:C:48:PRO:HB2	2.02	0.42
1:C:419:TRP:O	1:C:422:GLU:HG2	2.20	0.41
1:E:302:CYS:SG	2:E:601:UN1:C1'	3.08	0.41
1:G:494:CYS:HA	1:H:453:VAL:O	2.19	0.41
1:G:154:TRP:CH2	1:G:491:ARG:HB2	2.55	0.41
1:C:354:LEU:HD21	1:C:373:VAL:HG13	2.03	0.41
1:E:287:VAL:HB	1:E:288:PRO:HD3	2.02	0.41
1:C:293:ALA:HB2	1:C:458:PRO:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:ASN:HB3	1:F:63:THR:HG23	2.03	0.41
1:C:497:ASN:HB2	1:D:457:ILE:HG23	2.02	0.41
1:F:4:LEU:CD1	1:F:21:GLU:HG3	2.50	0.41
1:G:431:ILE:HG23	1:G:442:TRP:CE2	2.56	0.41
1:G:419:TRP:O	1:G:422:GLU:HG2	2.21	0.41
1:C:310:ILE:HD13	1:C:318:VAL:HB	2.03	0.41
1:G:324:LYS:HB2	1:G:324:LYS:HE3	1.91	0.41
1:E:509[A]:LYS:N	1:F:328:GLN:OE1	2.44	0.41
1:H:248:THR:HA	1:H:269:LEU:HD13	2.03	0.41
1:D:431:ILE:HG23	1:D:442:TRP:CE2	2.55	0.40
1:H:478:ARG:O	1:H:487:GLN:NE2	2.47	0.40
1:B:264:ARG:HH22	1:B:490:ARG:HA	1.86	0.40
1:D:357:VAL:HG12	1:D:361:LYS:HE2	2.03	0.40
1:E:506[B]:GLN:CG	1:F:121:GLU:HG3	2.51	0.40
1:F:425:GLN:O	1:F:472:LYS:HE3	2.21	0.40
1:H:28:ASN:HB3	1:H:63:THR:HG23	2.03	0.40
1:F:330:ARG:HD3	1:F:338:ASN:O	2.21	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	508/513 (99%)	491 (97%)	16 (3%)	1 (0%)	47	38
1	B	520/513 (101%)	502 (96%)	17 (3%)	1 (0%)	47	38
1	C	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	47	38
1	D	522/513 (102%)	504 (97%)	17 (3%)	1 (0%)	47	38
1	E	520/513 (101%)	503 (97%)	16 (3%)	1 (0%)	47	38
1	F	521/513 (102%)	504 (97%)	16 (3%)	1 (0%)	47	38
1	G	509/513 (99%)	496 (97%)	12 (2%)	1 (0%)	47	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	508/513 (99%)	487 (96%)	20 (4%)	1 (0%)	47	38
All	All	4116/4104 (100%)	3979 (97%)	129 (3%)	8 (0%)	47	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	B	480	SER
1	C	480	SER
1	D	480	SER
1	E	480	SER
1	F	480	SER
1	H	480	SER
1	G	480	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/410 (97%)	394 (99%)	3 (1%)	81	82
1	B	410/410 (100%)	403 (98%)	7 (2%)	60	57
1	C	399/410 (97%)	399 (100%)	0	100	100
1	D	404/410 (98%)	398 (98%)	6 (2%)	65	62
1	E	410/410 (100%)	406 (99%)	4 (1%)	76	76
1	F	408/410 (100%)	401 (98%)	7 (2%)	60	57
1	G	404/410 (98%)	401 (99%)	3 (1%)	84	84
1	H	399/410 (97%)	394 (99%)	5 (1%)	69	68
All	All	3231/3280 (98%)	3196 (99%)	35 (1%)	78	73

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	LEU
1	A	297	THR
1	A	401	PHE
1	B	122	TYR
1	B	297	THR
1	B	401	PHE
1	B	501[A]	ASP
1	B	501[B]	ASP
1	B	504[A]	LEU
1	B	504[B]	LEU
1	D	3	THR
1	D	108	MET
1	D	182	ILE
1	D	297	THR
1	D	504[A]	LEU
1	D	504[B]	LEU
1	E	122	TYR
1	E	285	LEU
1	E	504[A]	LEU
1	E	504[B]	LEU
1	F	108	MET
1	F	297	THR
1	F	401	PHE
1	F	504[A]	LEU
1	F	504[B]	LEU
1	F	508[A]	ILE
1	F	508[B]	ILE
1	G	297	THR
1	G	340	LEU
1	G	401	PHE
1	H	36	GLU
1	H	297	THR
1	H	362	LYS
1	H	394	SER
1	H	401	PHE

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	249	GLN
1	F	249	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	#$|Z| > 2$
3	EDO	F	602	-	3,3,3	0.47	0	2,2,2	0.37	0
2	UN1	F	601[B]	-	3,10,10	0.34	0	2,12,12	1.22	0
2	UN1	E	601	-	3,10,10	0.42	0	2,12,12	1.64	1 (50%)
3	EDO	E	602	-	3,3,3	0.52	0	2,2,2	0.10	0
2	UN1	B	601[A]	-	3,10,10	0.43	0	2,12,12	1.30	0
3	EDO	B	602	-	3,3,3	0.48	0	2,2,2	0.41	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	EDO	F	602	-	-	0/1/1/1	-
2	UN1	F	601[B]	-	-	0/4/10/10	-
2	UN1	E	601	-	-	0/4/10/10	-
3	EDO	E	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UN1	B	601[A]	-	-	0/4/10/10	-
3	EDO	B	602	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	UN1	C5-C6-C1	-2.29	107.61	112.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	602	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	UN1	2	0
3	E	602	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand UN1 F 601 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand UN1 E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand UN1 B 601 (A)

Bond lengths

Bond angles

Torsions

Rings
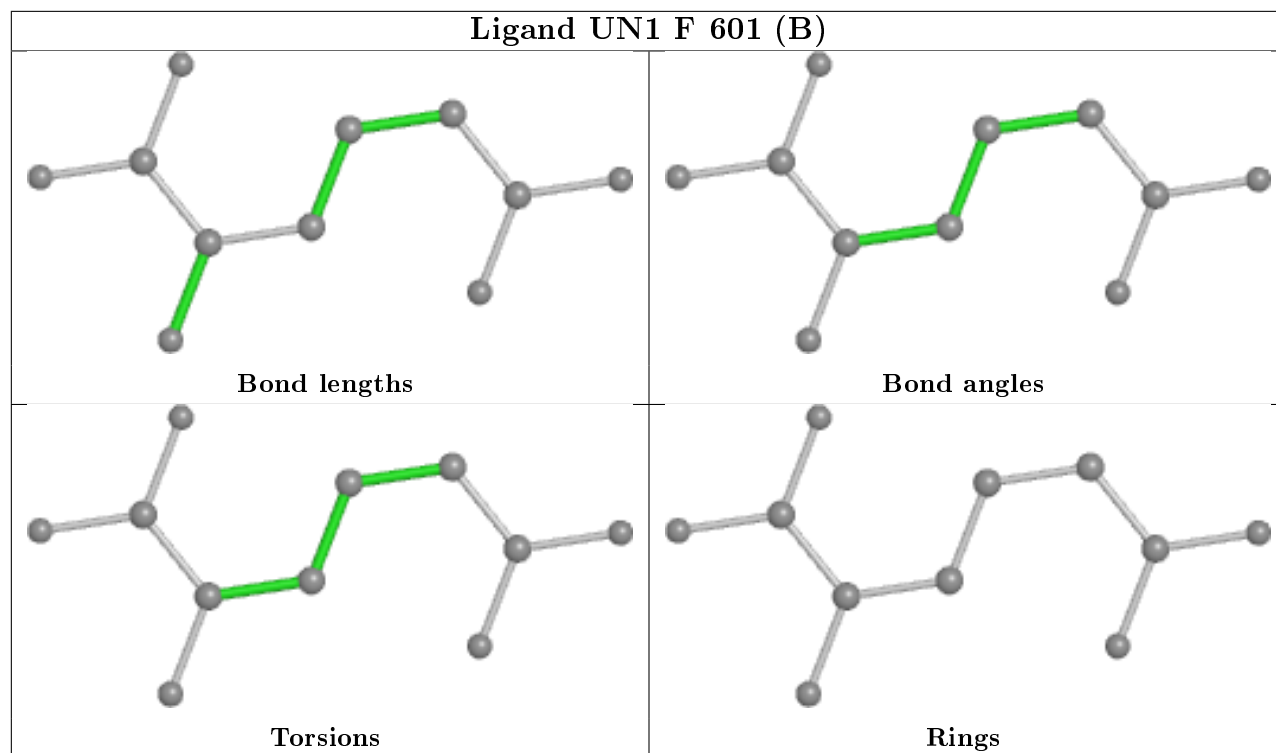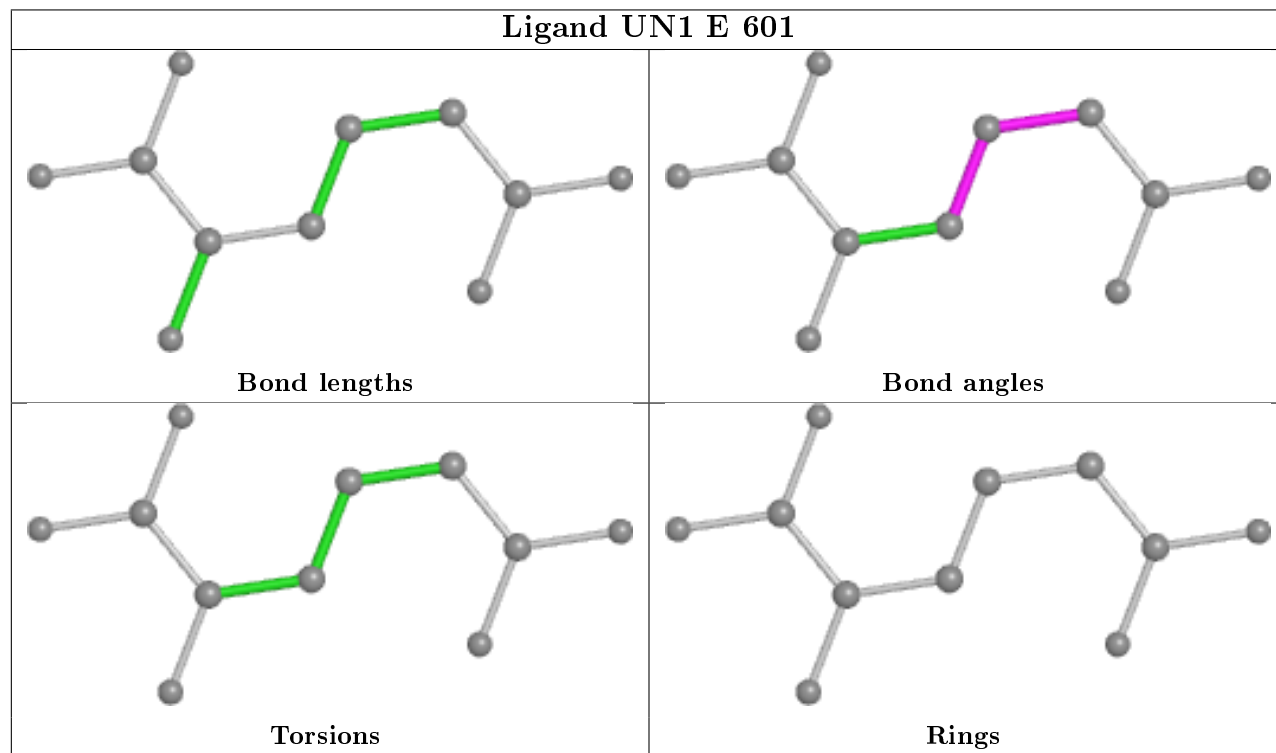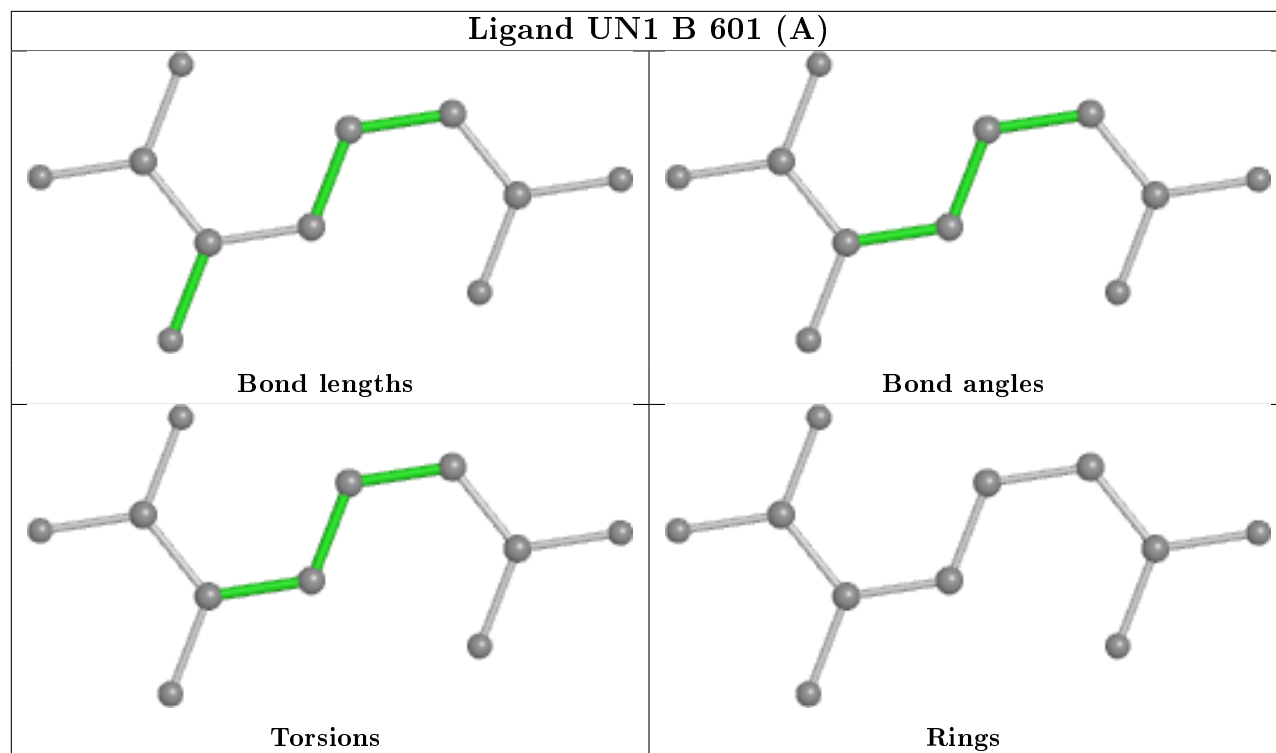
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	509/513 (99%)	-0.43	0	100	100	13, 20, 33, 52	0
1	B	508/513 (99%)	-0.38	7 (1%)	75	77	13, 21, 35, 56	1 (0%)
1	C	508/513 (99%)	-0.43	2 (0%)	92	93	13, 21, 35, 62	0
1	D	509/513 (99%)	-0.27	7 (1%)	75	77	13, 24, 40, 52	1 (0%)
1	E	509/513 (99%)	-0.39	8 (1%)	72	74	14, 21, 34, 50	1 (0%)
1	F	508/513 (99%)	-0.28	7 (1%)	75	77	14, 22, 38, 49	1 (0%)
1	G	508/513 (99%)	-0.43	0	100	100	15, 22, 36, 48	0
1	H	509/513 (99%)	-0.25	3 (0%)	89	90	15, 25, 44, 61	0
All	All	4068/4104 (99%)	-0.36	34 (0%)	86	87	13, 22, 38, 62	4 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	508[A]	ILE	5.5
1	E	504[A]	LEU	5.3
1	F	508[A]	ILE	4.5
1	E	502[A]	LEU	4.2
1	B	505[A]	ALA	4.2
1	E	503[A]	PRO	4.1
1	F	505[A]	ALA	3.9
1	D	504[A]	LEU	3.9
1	B	508[A]	ILE	3.8
1	D	505[A]	ALA	3.8
1	E	505[A]	ALA	3.8
1	B	504[A]	LEU	3.4
1	D	508[A]	ILE	3.4
1	B	503[A]	PRO	2.8
1	E	510[A]	PHE	2.7
1	B	502[A]	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	507[A]	GLY	2.6
1	B	510[A]	PHE	2.6
1	F	504[A]	LEU	2.5
1	D	503[A]	PRO	2.5
1	C	507	GLY	2.4
1	D	502[A]	LEU	2.4
1	D	510[A]	PHE	2.4
1	H	352	MET	2.4
1	C	510	PHE	2.3
1	D	329	ILE	2.2
1	B	506[A]	GLN	2.2
1	H	12	ALA	2.2
1	F	320	ASN	2.1
1	F	12	ALA	2.1
1	F	503[A]	PRO	2.1
1	H	9	PRO	2.1
1	E	509[A]	LYS	2.1
1	F	510[A]	PHE	2.1

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(Å^2)	Q<0.9
2	UN1	F	601[B]	11/11	0.80	0.31	16,23,26,29	11
2	UN1	E	601	11/11	0.85	0.20	23,38,62,62	11
2	UN1	B	601[A]	11/11	0.89	0.19	23,29,40,42	11
3	EDO	E	602	4/4	0.95	0.11	31,32,34,39	0
3	EDO	F	602	4/4	0.96	0.14	24,28,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	602	4/4	0.96	0.10	21,28,30,34	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 UN1 F 601 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
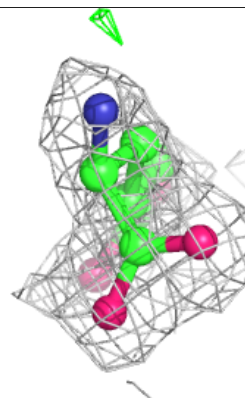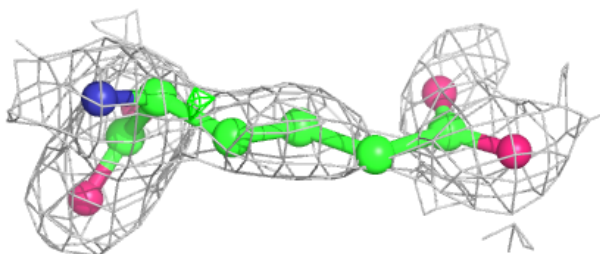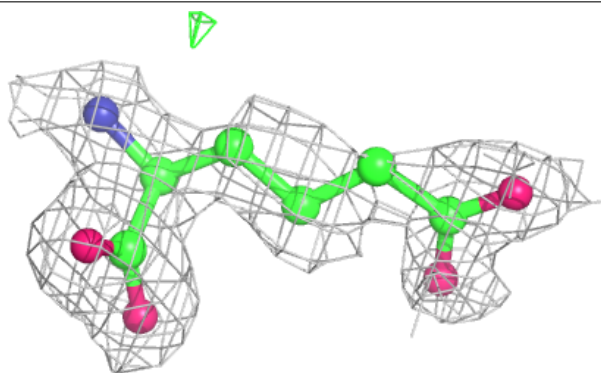and green (positive)
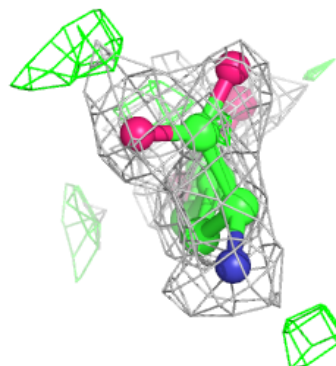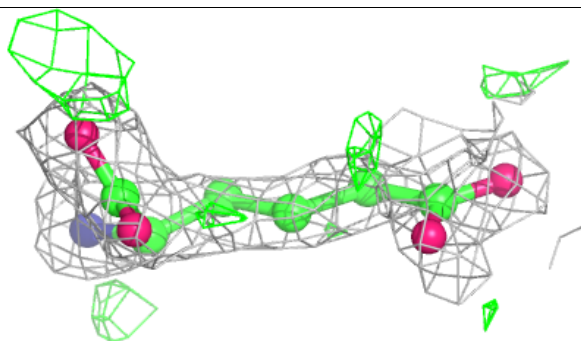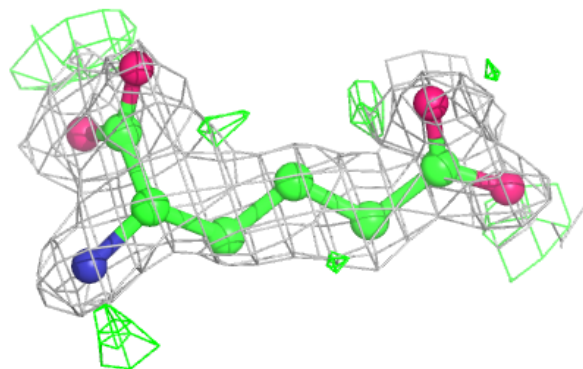
Electron density around UN1 E 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
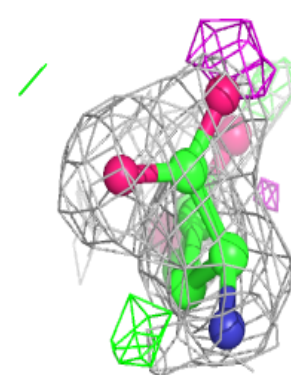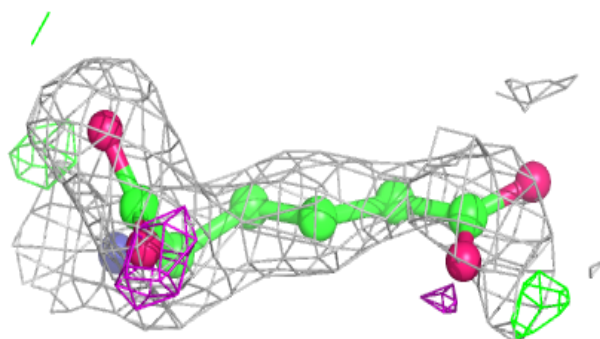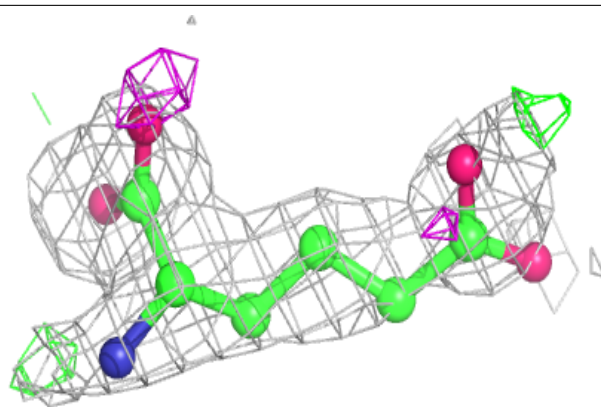
Electron density around UN1 B 601 (A):

$2mF_o-DF_c$ (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.