



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:23 PM UTC

PDB ID : 6O4F / pdb_00006o4f
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 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

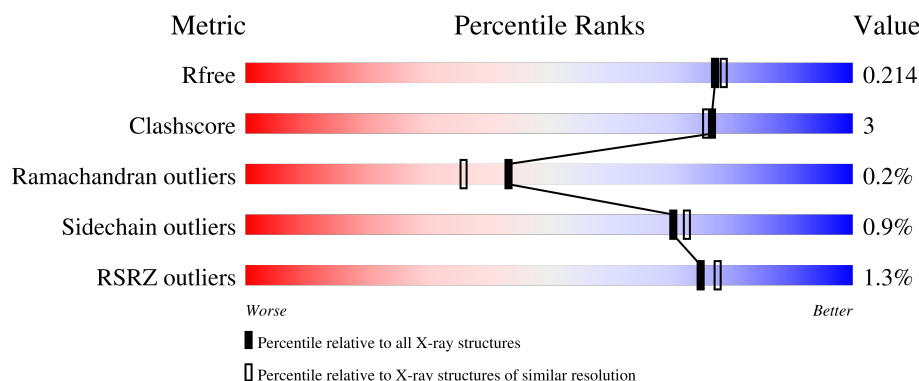
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	513	
1	B	513	
1	C	513	
1	D	513	
1	E	513	

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Mol	Chain	Length	Quality of chain
1	F	513	2% 90% 8%
1	G	513	93% 6%
1	H	513	% 91% 8%

2 Entry composition

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

There are 24 discrepancies between the modelled and reference sequences:

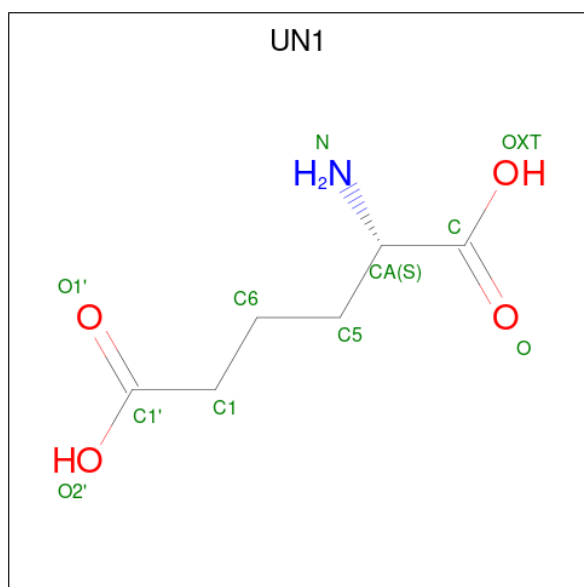
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	167	SER	ASN	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	167	SER	ASN	engineered mutation	UNP P49419
C	-1	GLY	-	expression 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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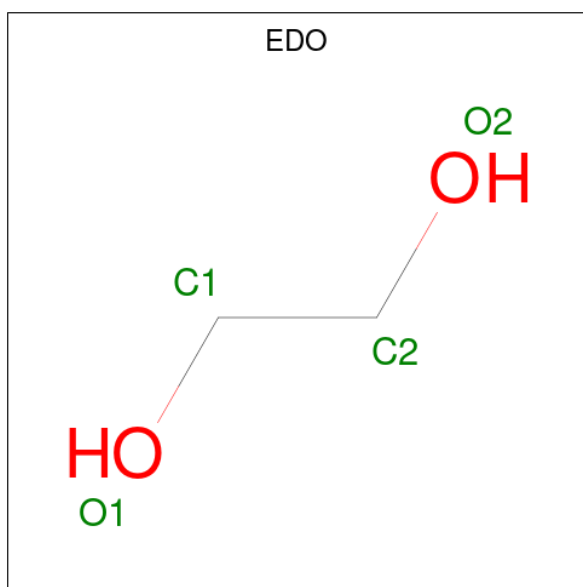
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P49419
E	167	SER	ASN	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	167	SER	ASN	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression 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 (CCD ID: UN1) (formula: $C_6H_{11}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			11	6	1	4		
2	E	1	Total	C	N	O	0	0
			11	6	1	4		
2	F	1	Total	C	N	O	0	1
			11	6	1	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

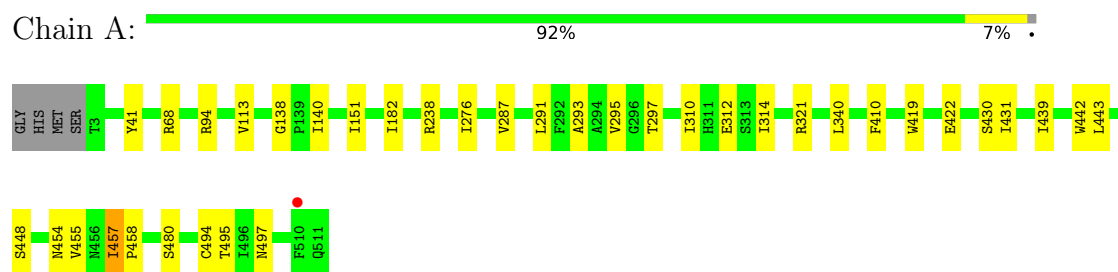
- Molecule 4 is water.

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

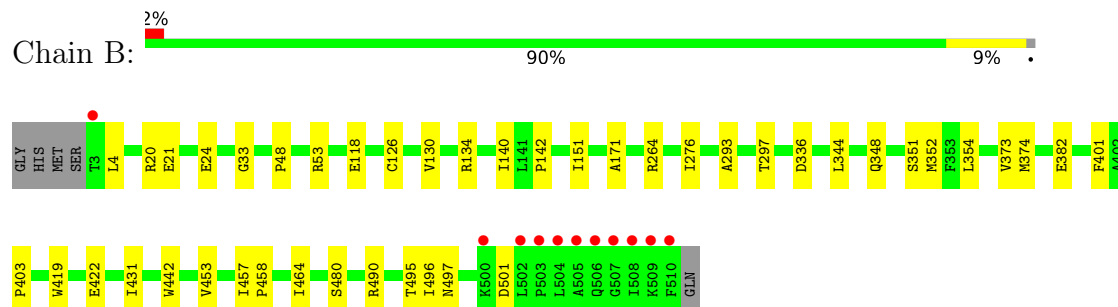
3 Residue-property plots

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.

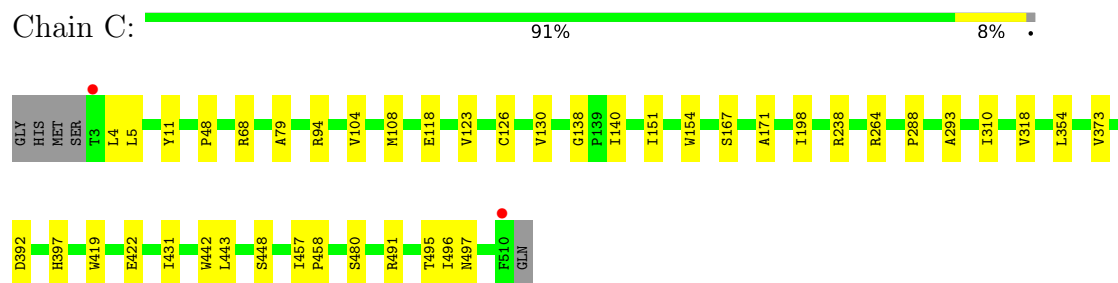
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



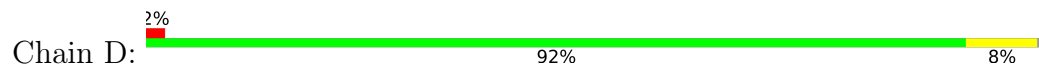
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

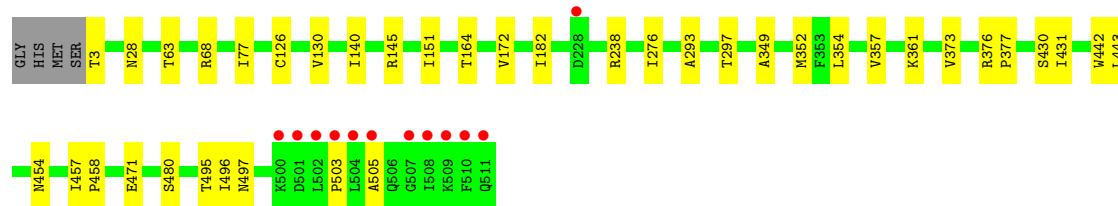


- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

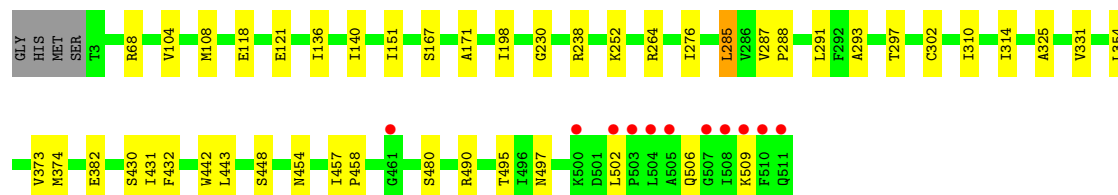
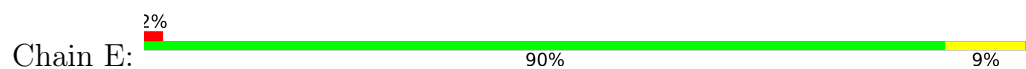


- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

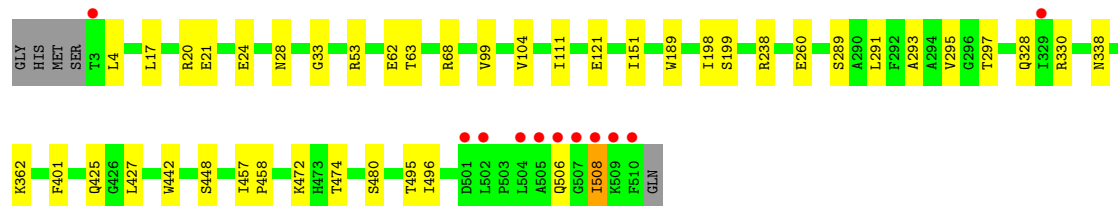
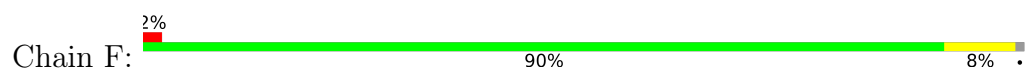




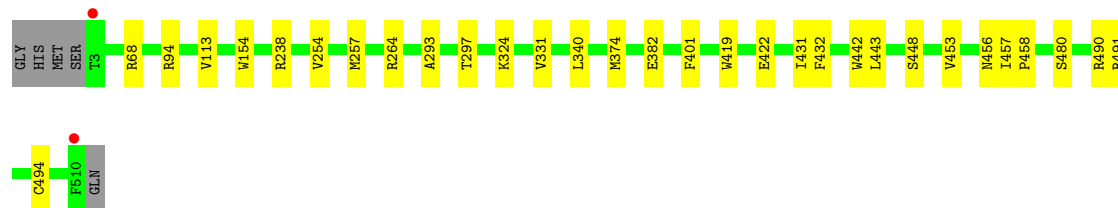
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



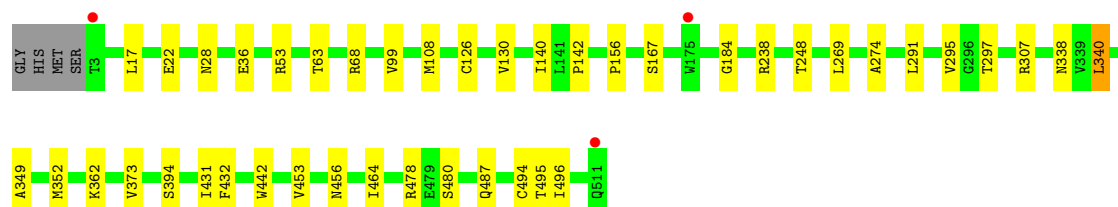
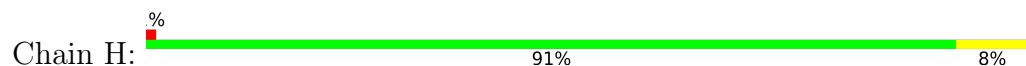
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.173 , 0.218 0.169 , 0.214	Depositor DCC
R_{free} test set	14081 reflections (4.78%)	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)	0.35 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: EDO, UN1

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	0.31	0/3922	0.50	0/5325
1	B	0.29	0/4035	0.48	0/5475
1	C	0.30	0/3931	0.49	0/5335
1	D	0.26	0/4032	0.46	0/5473
1	E	0.29	0/4038	0.48	0/5479
1	F	0.29	0/4035	0.48	0/5476
1	G	0.29	0/3950	0.48	0/5358
1	H	0.27	0/3936	0.46	0/5341
All	All	0.29	0/31879	0.48	0/43262

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	3840	0	3817	26	0
1	B	3945	0	3912	34	0
1	C	3845	0	3824	31	0
1	D	3941	0	3901	27	0
1	E	3954	0	3931	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3940	0	3897	31	0
1	G	3861	0	3860	18	0
1	H	3853	0	3827	21	0
2	B	11	0	4	0	0
2	E	11	0	4	2	0
2	F	11	0	4	0	0
3	B	4	0	6	0	0
3	E	4	0	6	1	0
3	F	4	0	6	0	0
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	30999	180	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 (180) 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:B:348:GLN:HG2	1:B:352:MET:HE2	1.74	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:331:VAL:HG21	1:G:374:MET:HE1	1.88	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:E:331:VAL:HG21	1:E:374:MET:HE1	1.88	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: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:N	4:E:702:HOH:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:108:MET:HE3	1:C:167:SER:HA	1.96	0.47
1:F:442:TRP:CH2	1:F:448:SER:HB2	2.50	0.47
1:B:457:ILE:HD12	4:B:707:HOH:O	2.15	0.47
1:C:442:TRP:CH2	1:C:448:SER:HB2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ALA:HA	1:H:352:MET:HE2	1.99	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:E:121:GLU:HG2	1:F:506[B]:GLN:CD	2.43	0.44
1:H:108:MET:HE3	1:H:167:SER:HA	2.00	0.44
1:D:276:ILE:HB	1:D:431:ILE:HG22	2.00	0.44
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:374:MET:HE3	1:E:382:GLU:HA	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:108:MET:HE3	1:E:167:SER:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:374:MET:HE3	1:G:382:GLU:HA	2.02	0.42
1:A:41:TYR:CZ	1:F:362:LYS:HG2	2.55	0.42
1:G:254:VAL:HA	1:G:257:MET:HE3	2.01	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:D:430:SER:OG	1:D:457:ILE:O	2.32	0.42
1:E:136:ILE:O	1:H:142:PRO:HD3	2.20	0.42
1:F:68:ARG:HD2	1:F:238:ARG:HB3	2.01	0.42
1:F:111:ILE:HB	4:F:735:HOH:O	2.19	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:B:374:MET:HE3	1:B:382:GLU:HA	2.02	0.41
1:C:293:ALA:HB2	1:C:458:PRO:HB2	2.01	0.41
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:D:349:ALA:HA	1:D:352:MET:HE2	2.03	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:A:430:SER:OG	1:A:457:ILE:O	2.34	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:G:419:TRP:O	1:G:422:GLU:HG2	2.21	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:E:430:SER:OG	1:E:457:ILE:O	2.31	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%)	43	36
1	B	520/513 (101%)	502 (96%)	17 (3%)	1 (0%)	43	36
1	C	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	43	36
1	D	522/513 (102%)	504 (97%)	17 (3%)	1 (0%)	43	36
1	E	520/513 (101%)	503 (97%)	16 (3%)	1 (0%)	43	36
1	F	521/513 (102%)	504 (97%)	16 (3%)	1 (0%)	43	36
1	G	509/513 (99%)	496 (97%)	12 (2%)	1 (0%)	43	36
1	H	508/513 (99%)	487 (96%)	20 (4%)	1 (0%)	43	36
All	All	4116/4104 (100%)	3979 (97%)	129 (3%)	8 (0%)	43	36

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%)	393 (99%)	4 (1%)	68	70
1	B	410/410 (100%)	405 (99%)	5 (1%)	63	63
1	C	399/410 (97%)	399 (100%)	0	100	100
1	D	404/410 (98%)	400 (99%)	4 (1%)	68	70
1	E	410/410 (100%)	407 (99%)	3 (1%)	76	78
1	F	408/410 (100%)	403 (99%)	5 (1%)	63	63
1	G	404/410 (98%)	401 (99%)	3 (1%)	76	78
1	H	399/410 (97%)	392 (98%)	7 (2%)	51	50
All	All	3231/3280 (98%)	3200 (99%)	31 (1%)	70	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	297	THR
1	A	340	LEU
1	A	457	ILE
1	B	297	THR
1	B	401	PHE
1	B	464	ILE
1	B	501[A]	ASP
1	B	501[B]	ASP
1	D	3	THR
1	D	77	ILE
1	D	182	ILE
1	D	297	THR
1	E	140	ILE
1	E	285	LEU
1	E	297	THR
1	F	62	GLU
1	F	297	THR
1	F	401	PHE
1	F	508[A]	ILE
1	F	508[B]	ILE
1	G	297	THR
1	G	340	LEU
1	G	401	PHE

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Mol	Chain	Res	Type
1	H	36	GLU
1	H	297	THR
1	H	340	LEU
1	H	362	LYS
1	H	373	VAL
1	H	394	SER
1	H	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	155	ASN
1	A	249	GLN
1	A	338	ASN
1	A	412	ASN
1	B	46	ASN
1	B	88	GLN
1	B	98	GLN
1	B	155	ASN
1	B	213	ASN
1	B	259	GLN
1	C	120	GLN
1	C	155	ASN
1	D	46	ASN
1	D	88	GLN
1	D	120	GLN
1	D	155	ASN
1	D	213	ASN
1	D	379	ASN
1	E	54	GLN
1	E	155	ASN
1	F	54	GLN
1	F	88	GLN
1	F	120	GLN
1	F	155	ASN
1	F	213	ASN
1	F	249	GLN
1	G	46	ASN
1	G	98	GLN
1	G	120	GLN
1	G	155	ASN

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Mol	Chain	Res	Type
1	G	259	GLN
1	H	46	ASN
1	H	153	GLN
1	H	155	ASN
1	H	379	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	UN1	F	601[B]	-	9,10,10	1.06	0	9,12,12	1.27	0
3	EDO	B	602	-	3,3,3	0.45	0	2,2,2	0.44	0
2	UN1	E	601	-	9,10,10	0.95	0	9,12,12	1.47	3 (33%)
3	EDO	F	602	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	E	602	-	3,3,3	0.48	0	2,2,2	0.15	0
2	UN1	B	601[A]	-	9,10,10	1.09	0	9,12,12	1.33	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	UN1	O2'-C1'-C1	2.35	121.44	114.00
2	B	601[A]	UN1	OXT-C-O	-2.33	118.79	124.08
2	E	601	UN1	C5-C6-C1	-2.12	107.61	113.26
2	E	601	UN1	OXT-C-O	-2.06	119.41	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	UN1	OXT-C-CA-N
2	B	601[A]	UN1	O-C-CA-N
2	B	601[A]	UN1	OXT-C-CA-N
3	E	602	EDO	O1-C1-C2-O2
2	F	601[B]	UN1	OXT-C-CA-N

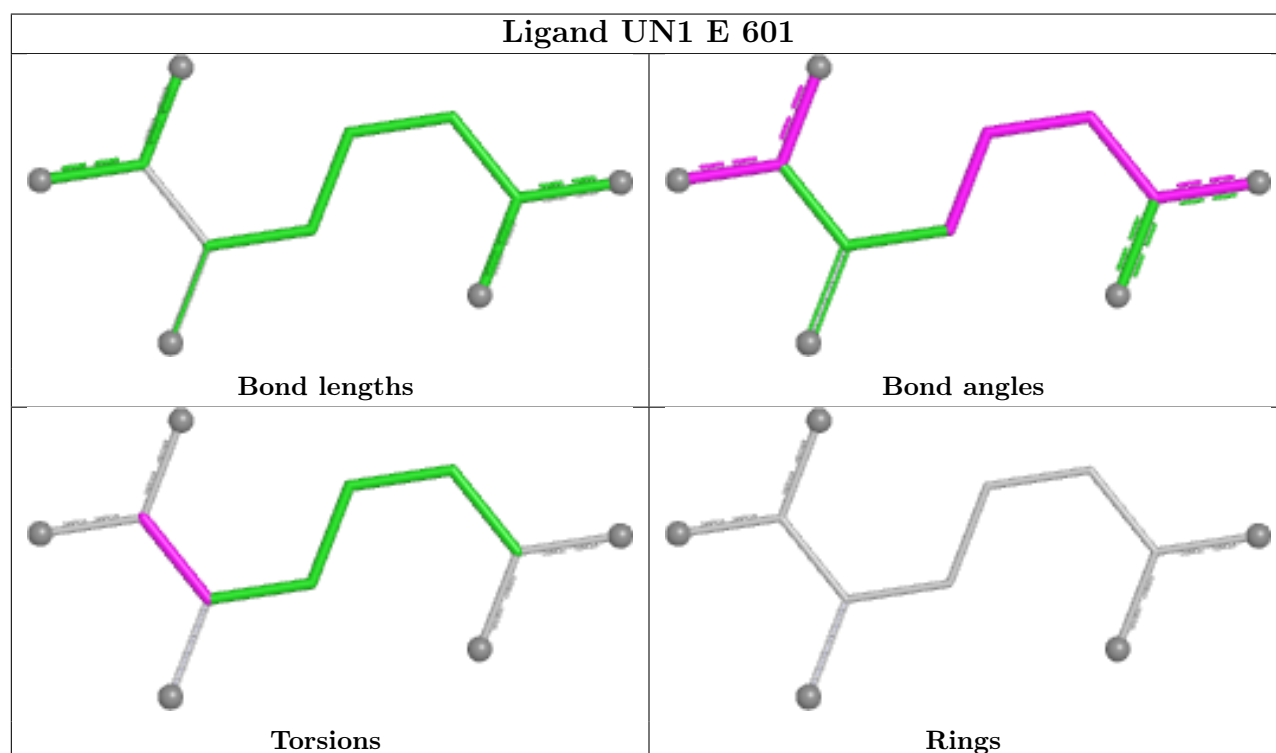
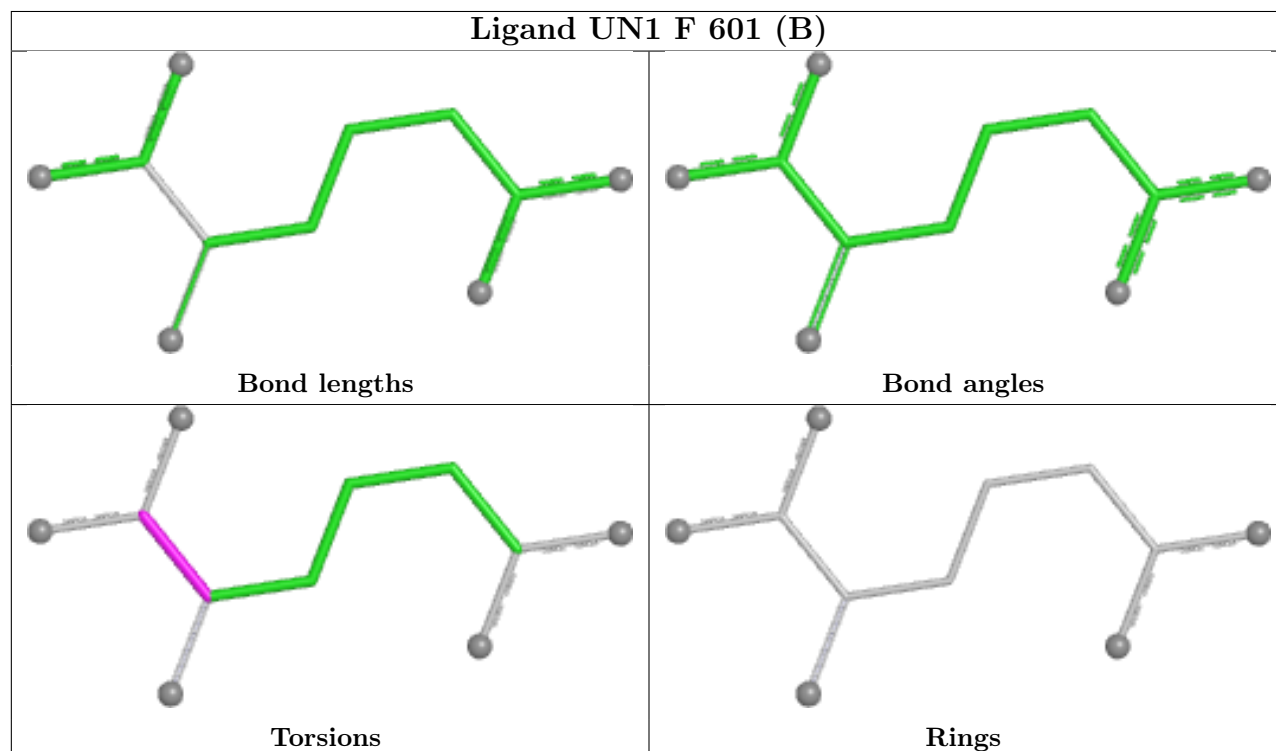
There are no ring outliers.

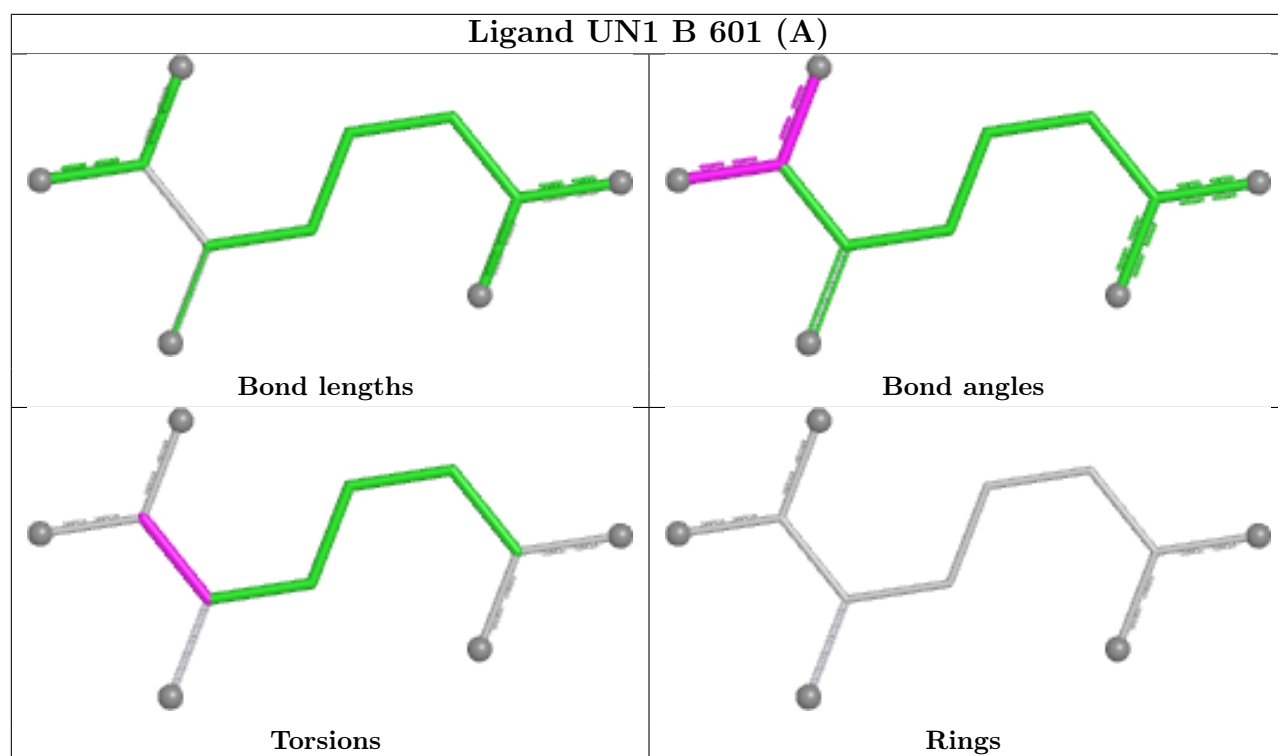
2 monomers are involved in 3 short contacts:

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 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	509/513 (99%)	-0.52	1 (0%) 91 92	10, 20, 33, 52	1 (0%)
1	B	508/513 (99%)	-0.41	11 (2%) 62 66	9, 21, 35, 56	15 (2%)
1	C	508/513 (99%)	-0.47	2 (0%) 88 90	10, 21, 35, 62	2 (0%)
1	D	509/513 (99%)	-0.28	12 (2%) 59 63	9, 23, 40, 52	16 (3%)
1	E	509/513 (99%)	-0.41	11 (2%) 62 66	12, 20, 33, 49	14 (2%)
1	F	508/513 (99%)	-0.35	11 (2%) 62 66	11, 21, 38, 49	16 (3%)
1	G	508/513 (99%)	-0.42	2 (0%) 88 90	12, 22, 36, 48	3 (0%)
1	H	509/513 (99%)	-0.30	3 (0%) 85 87	12, 25, 44, 61	1 (0%)
All	All	4068/4104 (99%)	-0.40	53 (1%) 75 78	9, 22, 38, 62	68 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	511[A]	GLN	6.5
1	D	511[A]	GLN	6.0
1	E	508[A]	ILE	5.6
1	F	508[A]	ILE	5.3
1	B	508[A]	ILE	5.1
1	D	508[A]	ILE	5.1
1	E	502[A]	LEU	5.0
1	D	505[A]	ALA	4.9
1	B	510[A]	PHE	4.9
1	E	510[A]	PHE	4.8
1	D	502[A]	LEU	4.8
1	D	509[A]	LYS	4.7
1	D	510[A]	PHE	4.5
1	B	502[A]	LEU	4.4
1	F	510[A]	PHE	4.4
1	E	504[A]	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	504[A]	LEU	4.2
1	E	503[A]	PRO	4.2
1	E	507[A]	GLY	4.1
1	F	505[A]	ALA	4.0
1	C	510	PHE	3.9
1	B	505[A]	ALA	3.5
1	E	505[A]	ALA	3.5
1	D	507[A]	GLY	3.5
1	F	507[A]	GLY	3.3
1	B	509[A]	LYS	3.2
1	E	500[A]	LYS	3.1
1	E	509[A]	LYS	3.0
1	F	504[A]	LEU	2.9
1	F	501[A]	ASP	2.8
1	F	329	ILE	2.8
1	H	175	TRP	2.7
1	B	504[A]	LEU	2.6
1	F	502[A]	LEU	2.6
1	B	500[A]	LYS	2.5
1	D	503[A]	PRO	2.5
1	D	501[A]	ASP	2.4
1	F	506[A]	GLN	2.4
1	F	3	THR	2.3
1	H	511	GLN	2.3
1	B	507[A]	GLY	2.3
1	D	228	ASP	2.3
1	B	3	THR	2.3
1	A	510	PHE	2.2
1	D	500[A]	LYS	2.2
1	B	503[A]	PRO	2.2
1	B	506[A]	GLN	2.1
1	C	3	THR	2.1
1	F	509[A]	LYS	2.1
1	E	461	GLY	2.1
1	G	510	PHE	2.0
1	G	3	THR	2.0
1	H	3	THR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

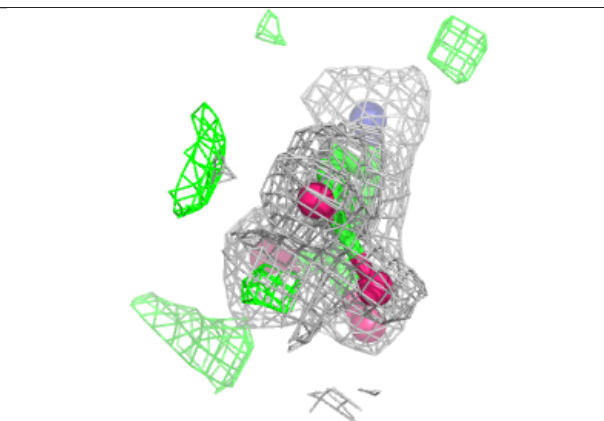
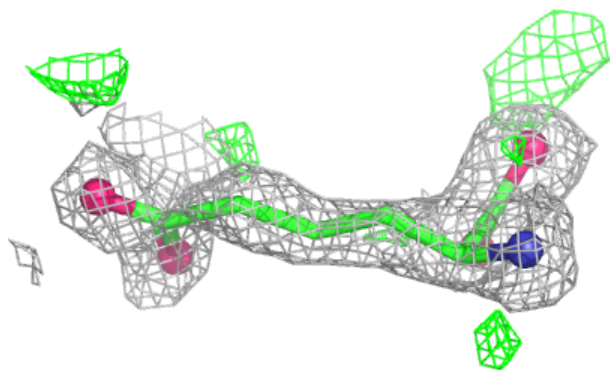
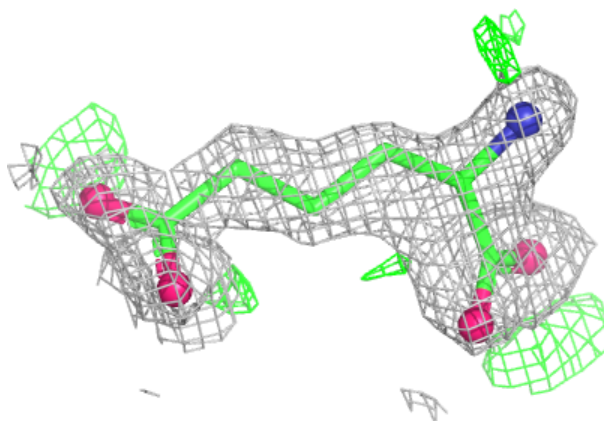
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UN1	F	601[B]	11/11	0.85	0.13	16,23,26,29	11
2	UN1	E	601	11/11	0.86	0.15	23,38,62,62	11
2	UN1	B	601[A]	11/11	0.89	0.12	23,29,40,42	11
3	EDO	E	602	4/4	0.94	0.08	31,32,34,39	0
3	EDO	F	602	4/4	0.94	0.08	24,28,28,29	0
3	EDO	B	602	4/4	0.96	0.07	21,28,30,34	0

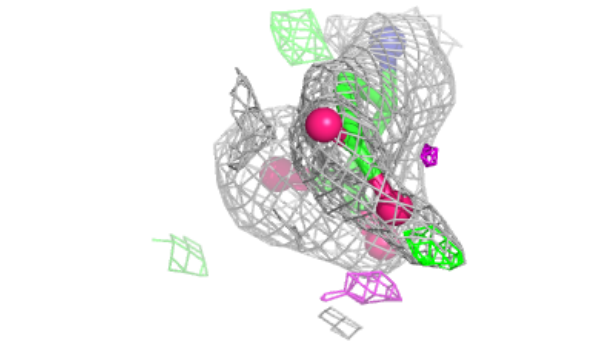
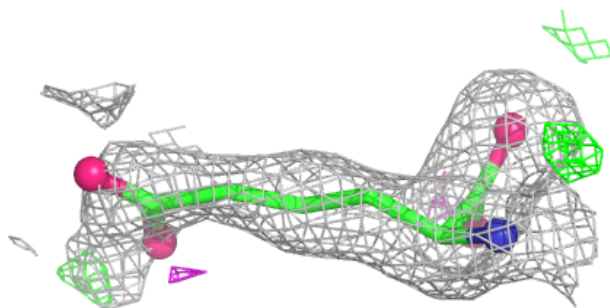
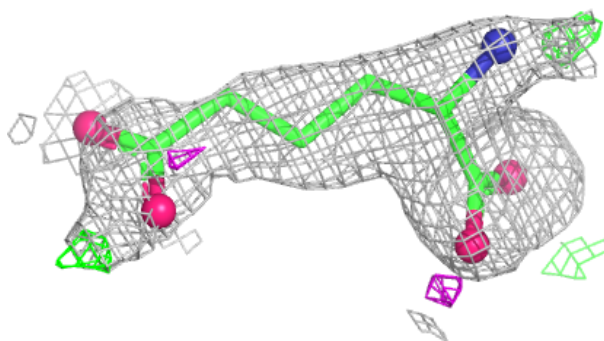
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UN1 F 601 (B):

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

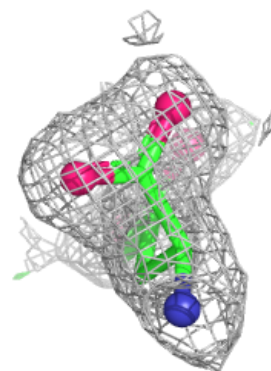
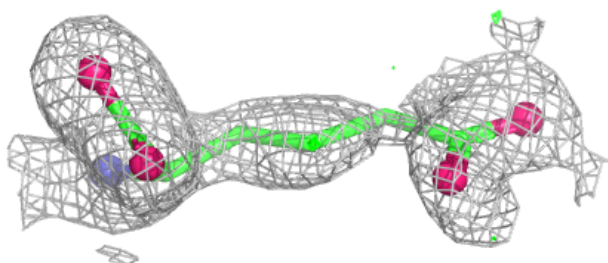
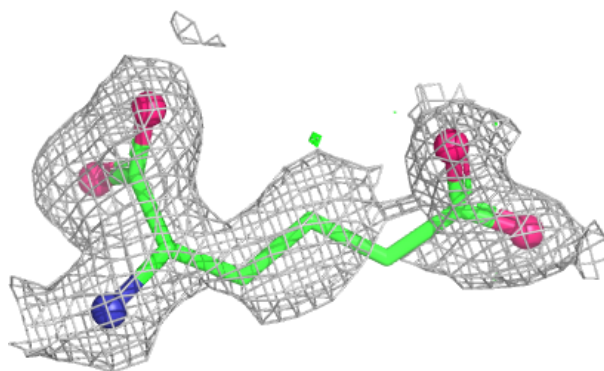
**Electron density around UN1 E 601:**

$2mF_o-DF_c$ (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.