Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 08:45 PM UTC

PDB ID	:	9IEX / pdb_00009iex
Title	:	Human Deoxyhypusine Synthase Fragment Screening Campaign - VT0155 follow-up ligand DMP7
Authors	:	Wilk, P.; Wator-Wilk, E.; Grudnik, P.
Deposited on	:	2025-02-15
Resolution	:	1.95 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:

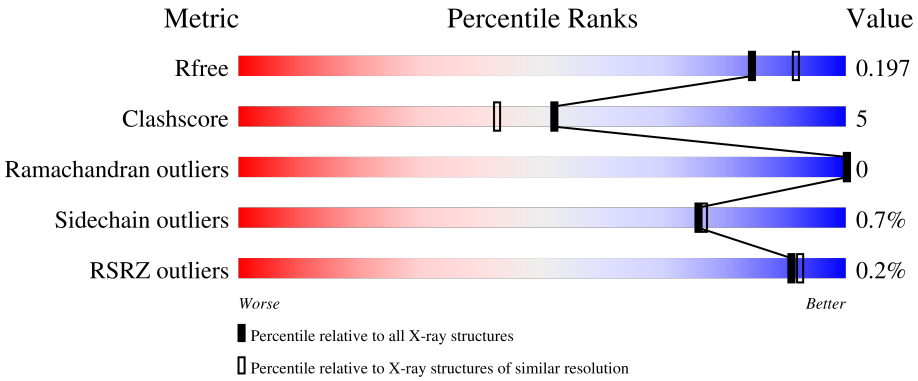
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 <=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	397	70% 9% • 20%
1	C	397	69% 11% 20%
2	B	397	73% 10% • 17%
2	D	397	% 73% 10% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10945 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 Deoxyhypusine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	10	0
			2543	1623	432	473	15			
1	C	319	Total	C	N	O	S	0	8	0
			2523	1607	432	469	15			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	GLY	-	expression tag	UNP P49366
A	371	GLY	-	expression tag	UNP P49366
A	372	VAL	-	expression tag	UNP P49366
A	373	GLU	-	expression tag	UNP P49366
A	374	GLU	-	expression tag	UNP P49366
A	375	ASP	-	expression tag	UNP P49366
A	376	LEU	-	expression tag	UNP P49366
A	377	ILE	-	expression tag	UNP P49366
A	378	LYS	-	expression tag	UNP P49366
A	379	CYS	-	expression tag	UNP P49366
A	380	LEU	-	expression tag	UNP P49366
A	381	ALA	-	expression tag	UNP P49366
A	382	PRO	-	expression tag	UNP P49366
A	383	THR	-	expression tag	UNP P49366
A	384	TYR	-	expression tag	UNP P49366
A	385	LEU	-	expression tag	UNP P49366
A	386	GLY	-	expression tag	UNP P49366
A	387	GLU	-	expression tag	UNP P49366
A	388	PHE	-	expression tag	UNP P49366
A	389	SER	-	expression tag	UNP P49366
A	390	LEU	-	expression tag	UNP P49366
A	391	ARG	-	expression tag	UNP P49366
A	392	GLY	-	expression tag	UNP P49366
A	393	LYS	-	expression tag	UNP P49366
A	394	GLU	-	expression tag	UNP P49366

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Chain	Residue	Modelled	Actual	Comment	Reference
A	395	LEU	-	expression tag	UNP P49366
A	396	ARG	-	expression tag	UNP P49366
A	397	GLU	-	expression tag	UNP P49366
C	370	GLY	-	expression tag	UNP P49366
C	371	GLY	-	expression tag	UNP P49366
C	372	VAL	-	expression tag	UNP P49366
C	373	GLU	-	expression tag	UNP P49366
C	374	GLU	-	expression tag	UNP P49366
C	375	ASP	-	expression tag	UNP P49366
C	376	LEU	-	expression tag	UNP P49366
C	377	ILE	-	expression tag	UNP P49366
C	378	LYS	-	expression tag	UNP P49366
C	379	CYS	-	expression tag	UNP P49366
C	380	LEU	-	expression tag	UNP P49366
C	381	ALA	-	expression tag	UNP P49366
C	382	PRO	-	expression tag	UNP P49366
C	383	THR	-	expression tag	UNP P49366
C	384	TYR	-	expression tag	UNP P49366
C	385	LEU	-	expression tag	UNP P49366
C	386	GLY	-	expression tag	UNP P49366
C	387	GLU	-	expression tag	UNP P49366
C	388	PHE	-	expression tag	UNP P49366
C	389	SER	-	expression tag	UNP P49366
C	390	LEU	-	expression tag	UNP P49366
C	391	ARG	-	expression tag	UNP P49366
C	392	GLY	-	expression tag	UNP P49366
C	393	LYS	-	expression tag	UNP P49366
C	394	GLU	-	expression tag	UNP P49366
C	395	LEU	-	expression tag	UNP P49366
C	396	ARG	-	expression tag	UNP P49366
C	397	GLU	-	expression tag	UNP P49366

- Molecule 2 is a protein called Deoxyhypusine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	13	0
			2629	1672	444	498	15			
2	D	329	Total	C	N	O	S	0	14	0
			2641	1678	452	496	15			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	275	UNK	CYS	conflict	UNP P49366
B	370	GLY	-	expression tag	UNP P49366
B	371	GLY	-	expression tag	UNP P49366
B	372	VAL	-	expression tag	UNP P49366
B	373	GLU	-	expression tag	UNP P49366
B	374	GLU	-	expression tag	UNP P49366
B	375	ASP	-	expression tag	UNP P49366
B	376	LEU	-	expression tag	UNP P49366
B	377	ILE	-	expression tag	UNP P49366
B	378	LYS	-	expression tag	UNP P49366
B	379	CYS	-	expression tag	UNP P49366
B	380	LEU	-	expression tag	UNP P49366
B	381	ALA	-	expression tag	UNP P49366
B	382	PRO	-	expression tag	UNP P49366
B	383	THR	-	expression tag	UNP P49366
B	384	TYR	-	expression tag	UNP P49366
B	385	LEU	-	expression tag	UNP P49366
B	386	GLY	-	expression tag	UNP P49366
B	387	GLU	-	expression tag	UNP P49366
B	388	PHE	-	expression tag	UNP P49366
B	389	SER	-	expression tag	UNP P49366
B	390	LEU	-	expression tag	UNP P49366
B	391	ARG	-	expression tag	UNP P49366
B	392	GLY	-	expression tag	UNP P49366
B	393	LYS	-	expression tag	UNP P49366
B	394	GLU	-	expression tag	UNP P49366
B	395	LEU	-	expression tag	UNP P49366
B	396	ARG	-	expression tag	UNP P49366
B	397	GLU	-	expression tag	UNP P49366
D	275	UNK	CYS	conflict	UNP P49366
D	370	GLY	-	expression tag	UNP P49366
D	371	GLY	-	expression tag	UNP P49366
D	372	VAL	-	expression tag	UNP P49366
D	373	GLU	-	expression tag	UNP P49366
D	374	GLU	-	expression tag	UNP P49366
D	375	ASP	-	expression tag	UNP P49366
D	376	LEU	-	expression tag	UNP P49366
D	377	ILE	-	expression tag	UNP P49366
D	378	LYS	-	expression tag	UNP P49366
D	379	CYS	-	expression tag	UNP P49366
D	380	LEU	-	expression tag	UNP P49366
D	381	ALA	-	expression tag	UNP P49366
D	382	PRO	-	expression tag	UNP P49366

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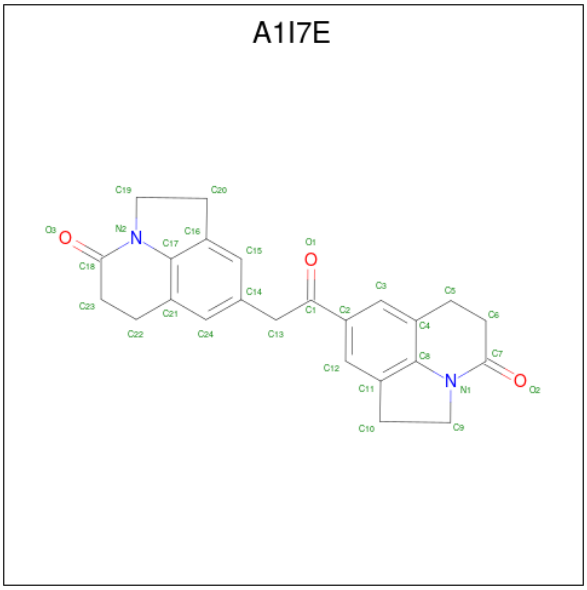
Chain	Residue	Modelled	Actual	Comment	Reference
D	383	THR	-	expression tag	UNP P49366
D	384	TYR	-	expression tag	UNP P49366
D	385	LEU	-	expression tag	UNP P49366
D	386	GLY	-	expression tag	UNP P49366
D	387	GLU	-	expression tag	UNP P49366
D	388	PHE	-	expression tag	UNP P49366
D	389	SER	-	expression tag	UNP P49366
D	390	LEU	-	expression tag	UNP P49366
D	391	ARG	-	expression tag	UNP P49366
D	392	GLY	-	expression tag	UNP P49366
D	393	LYS	-	expression tag	UNP P49366
D	394	GLU	-	expression tag	UNP P49366
D	395	LEU	-	expression tag	UNP P49366
D	396	ARG	-	expression tag	UNP P49366
D	397	GLU	-	expression tag	UNP P49366

- Molecule 3 is 6-[2-oxidanylidene-2-(11-oxidanylidene-1-azatricyclo[6.3.1.0^{4,12}]dodeca-4(12),5,7-trien-6-yl)ethyl]-1-azatricyclo[6.3.1.0^{4,12}]dodeca-4,6,8(12)-trien-11-one (CCD ID: A1I7E) (formula: $C_{24}H_{22}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 29 24 2 3	0	0
3	B	1	Total C N O 29 24 2 3	0	0

- Molecule 4 is water.

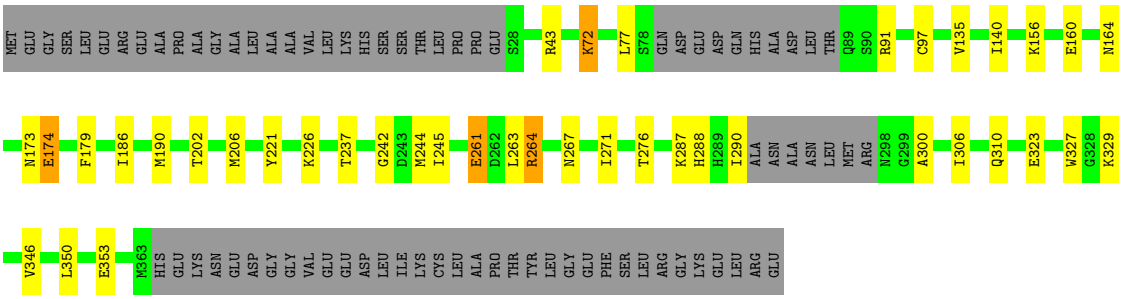
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	145	Total O 145 145	0	0
4	B	147	Total O 147 147	0	0
4	C	137	Total O 137 137	0	0
4	D	122	Total O 122 122	0	0

3 Residue-property plots (i)

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

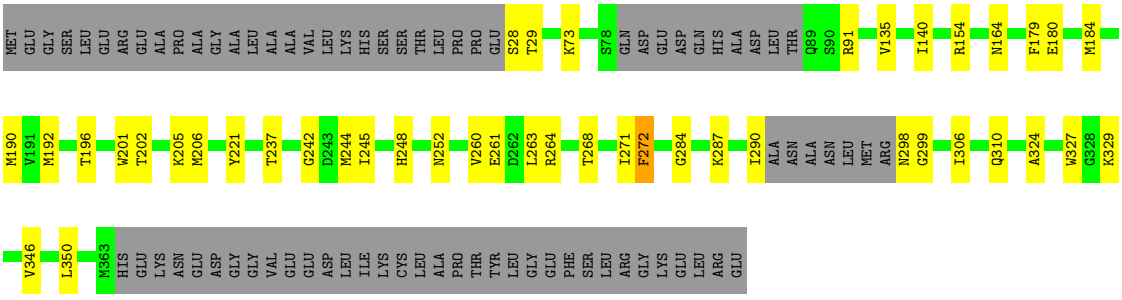
• Molecule 1: Deoxyhypusine synthase

Chain A:



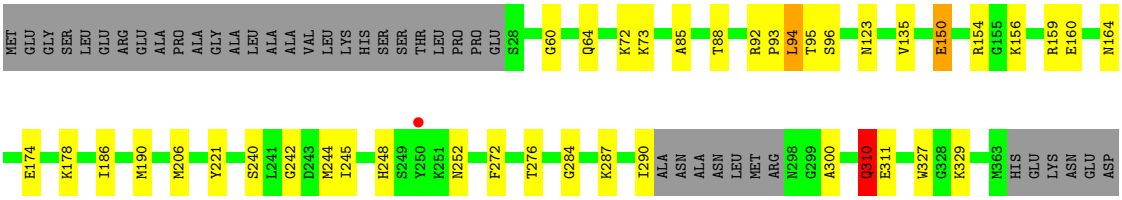
• Molecule 1: Deoxyhypusine synthase

Chain C:



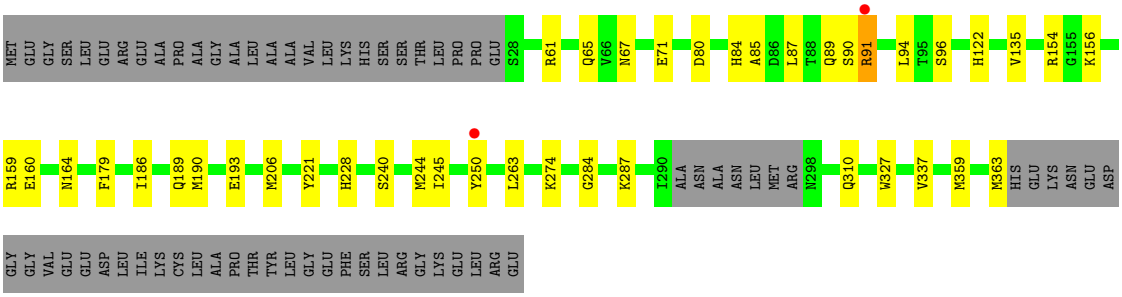
• Molecule 2: Deoxyhypusine synthase

Chain B:



• Molecule 2: Deoxyhypusine synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	104.32Å 104.32Å 159.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.58 – 1.95 49.58 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.58-1.95) 88.8 (49.58-1.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.64 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.174 , 0.197 0.175 , 0.197	Depositor DCC
R_{free} test set	2100 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.479 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10945	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSS, A1I7E

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	0.52	4/2604 (0.2%)	0.71	6/3522 (0.2%)
1	C	0.43	0/2574	0.60	4/3482 (0.1%)
2	B	0.46	4/2687 (0.1%)	0.63	7/3636 (0.2%)
2	D	0.53	4/2702 (0.1%)	0.64	6/3655 (0.2%)
All	All	0.49	12/10567 (0.1%)	0.65	23/14295 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	250[A]	TYR	CA-C	9.78	1.66	1.52
2	D	250[B]	TYR	CA-C	9.78	1.66	1.52
2	D	250[A]	TYR	N-CA	7.72	1.56	1.46
2	D	250[B]	TYR	N-CA	7.72	1.56	1.46
1	A	261[A]	GLU	CA-C	7.62	1.62	1.52
1	A	261[B]	GLU	CA-C	7.62	1.62	1.52
2	B	150[A]	GLU	CA-C	7.08	1.61	1.52
2	B	150[B]	GLU	CA-C	7.08	1.61	1.52
2	B	310[A]	GLN	CA-C	6.94	1.61	1.52
2	B	310[B]	GLN	CA-C	6.94	1.61	1.52
1	A	264[A]	ARG	CA-C	6.26	1.60	1.52
1	A	264[B]	ARG	CA-C	6.26	1.60	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264[A]	ARG	CA-C-O	11.77	132.89	120.42
1	A	264[B]	ARG	CA-C-O	11.77	132.89	120.42
2	B	94	LEU	CA-CB-CG	11.57	156.80	116.30
1	A	329	LYS	CB-CG-CD	-10.61	86.91	111.30
2	D	91[A]	ARG	CA-C-O	9.81	130.94	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	91[B]	ARG	CA-C-O	9.81	130.94	120.55
2	D	250[A]	TYR	CA-C-O	-8.49	110.82	120.24
2	D	250[B]	TYR	CA-C-O	-8.49	110.82	120.24
1	A	261[A]	GLU	CA-C-O	7.91	128.81	120.42
1	A	261[B]	GLU	CA-C-O	7.91	128.81	120.42
1	C	28	SER	CA-C-N	-7.40	110.97	121.99
1	C	28	SER	C-N-CA	-7.40	110.97	121.99
1	C	271	ILE	N-CA-C	7.01	117.78	110.62
2	D	91[A]	ARG	N-CA-C	6.52	118.39	111.28
2	D	91[B]	ARG	N-CA-C	6.52	118.39	111.28
2	B	93	PRO	CA-C-N	-6.18	109.78	121.66
2	B	93	PRO	C-N-CA	-6.18	109.78	121.66
2	B	94	LEU	N-CA-CB	5.91	118.54	110.38
2	B	94	LEU	CB-CA-C	-5.22	100.06	111.71
1	A	329	LYS	CG-CD-CE	5.12	123.07	111.30
2	B	310[A]	GLN	CA-C-O	5.11	126.79	120.92
2	B	310[B]	GLN	CA-C-O	5.11	126.79	120.92
1	C	29	THR	CA-CB-CG2	-5.00	101.99	110.50

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	2543	0	2534	27	1
1	C	2523	0	2514	30	0
2	B	2629	0	2600	30	0
2	D	2641	0	2620	29	1
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	145	0	0	1	0
4	B	147	0	0	5	0
4	C	137	0	0	1	0
4	D	122	0	0	2	0
All	All	10945	0	10268	106	1

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 5.

All (106) 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)
2:D:85:ALA:HB1	2:D:94:LEU:HD21	1.56	0.85
1:A:72:LYS:HG2	1:A:97:CYS:HB2	1.59	0.84
2:B:92:ARG:NH1	2:B:123:ASN:OD1	2.15	0.78
1:A:261[B]:GLU:OE1	1:A:264[B]:ARG:NH2	2.25	0.69
2:B:287:LYS:NZ	4:B:503:HOH:O	2.31	0.64
2:D:154[B]:ARG:H	2:D:154[B]:ARG:NE	1.96	0.64
2:B:85:ALA:HB1	2:B:94:LEU:CD1	2.27	0.63
2:B:88:THR:HG23	2:B:272:PHE:HB2	1.79	0.63
1:C:261[A]:GLU:HG3	1:C:264[A]:ARG:NH1	2.14	0.61
2:B:240:SER:O	2:B:244:MET:HG2	2.01	0.61
2:D:310[B]:GLN:H	2:D:310[B]:GLN:CD	2.09	0.61
1:C:180:GLU:HB2	1:C:244:MET:HE2	1.82	0.60
1:A:267:ASN:O	1:A:271:ILE:HG12	2.01	0.59
1:C:290:ILE:HD11	2:D:244:MET:HE2	1.85	0.59
2:D:186:ILE:O	2:D:190:MET:HG3	2.03	0.59
2:B:310[A]:GLN:NE2	4:B:501:HOH:O	2.16	0.58
1:A:244:MET:HE3	2:B:290:ILE:HD11	1.85	0.57
2:B:284:GLY:O	2:B:287:LYS:HE2	2.03	0.57
2:D:359:MET:HE2	2:D:363:MET:HE3	1.86	0.57
2:B:156:LYS:NZ	2:B:160:GLU:OE2	2.32	0.57
1:C:91:ARG:HD2	1:C:91:ARG:O	2.03	0.57
2:D:284:GLY:O	2:D:287:LYS:HE2	2.04	0.56
1:C:261[A]:GLU:HG3	1:C:264[A]:ARG:HH12	1.69	0.56
1:C:272:PHE:HD1	1:C:272:PHE:N	2.04	0.55
2:B:159[A]:ARG:HH11	2:B:159[A]:ARG:HG2	1.70	0.55
1:C:192:MET:HE2	1:C:196:THR:CG2	2.36	0.55
1:C:272:PHE:N	1:C:272:PHE:CD1	2.73	0.55
2:D:206:MET:HE1	2:D:245:ILE:HD11	1.88	0.54
2:B:206:MET:HE1	2:B:245:ILE:HD11	1.89	0.54
1:A:174[A]:GLU:H	1:A:174[A]:GLU:CD	2.15	0.54
1:A:288:HIS:HE1	1:A:323:GLU:OE1	1.91	0.54
2:B:329:LYS:NZ	4:B:505:HOH:O	2.38	0.54
1:C:260:VAL:O	1:C:263:LEU:HB2	2.08	0.54
2:D:67:ASN:O	2:D:71:GLU:HG2	2.09	0.53
2:D:85:ALA:CB	2:D:94:LEU:HD21	2.35	0.53
2:B:135:VAL:HA	2:B:221:TYR:CE2	2.45	0.52
2:B:94:LEU:HD13	2:B:95:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:GLN:HE21	2:D:89:GLN:HA	1.77	0.50
1:C:190:MET:HG2	1:C:201:TRP:CZ2	2.47	0.49
1:C:284:GLY:O	1:C:287:LYS:HE2	2.13	0.49
2:D:159[A]:ARG:HG2	2:D:159[A]:ARG:HH11	1.76	0.49
1:A:91:ARG:O	1:A:91:ARG:HG2	2.13	0.49
1:C:192:MET:HE2	1:C:196:THR:HG21	1.94	0.49
1:A:287:LYS:NZ	4:A:506:HOH:O	2.44	0.49
2:D:135:VAL:HA	2:D:221:TYR:CE2	2.48	0.49
2:B:190:MET:HE1	2:B:206:MET:HG3	1.94	0.49
2:D:240:SER:O	2:D:244:MET:HG2	2.13	0.49
2:D:179:PHE:HD2	2:D:244:MET:HE3	1.77	0.48
1:C:237:THR:O	1:C:242:GLY:HA3	2.14	0.48
2:D:65:GLN:HG3	2:D:337:VAL:HG23	1.94	0.48
1:C:205:LYS:NZ	1:C:261[A]:GLU:OE2	2.46	0.48
1:A:91:ARG:HG2	1:A:91:ARG:HH11	1.78	0.48
1:C:202:THR:HG21	1:C:261[A]:GLU:HB3	1.96	0.48
2:B:60:GLY:O	2:B:64:GLN:HG3	2.14	0.47
1:C:180:GLU:HG3	1:C:184:MET:HE2	1.97	0.47
1:A:263:LEU:HD21	2:B:242:GLY:O	2.14	0.47
1:C:164:ASN:HB3	2:D:327:TRP:CE2	2.50	0.46
1:A:310[B]:GLN:NE2	1:C:310[B]:GLN:HB3	2.30	0.46
2:B:311:GLU:OE1	4:B:502:HOH:O	2.20	0.46
1:C:135:VAL:HA	1:C:221:TYR:CE2	2.51	0.46
2:B:154:ARG:HA	2:B:154:ARG:HD2	1.62	0.45
1:A:135:VAL:HA	1:A:221:TYR:CE2	2.50	0.45
1:C:73:LYS:NZ	4:C:405:HOH:O	2.48	0.45
2:B:85:ALA:HB1	2:B:94:LEU:HD11	1.99	0.45
1:A:237:THR:O	1:A:242:GLY:HA3	2.17	0.45
2:B:73:LYS:NZ	4:B:508:HOH:O	2.49	0.45
2:D:156:LYS:NZ	2:D:160:GLU:OE2	2.46	0.45
1:A:186:ILE:O	1:A:190:MET:HG3	2.18	0.44
2:B:88:THR:CG2	2:B:272:PHE:HB2	2.47	0.44
1:A:244:MET:HE3	2:B:290:ILE:CD1	2.48	0.44
1:A:140:ILE:HG12	1:A:179:PHE:HB2	2.00	0.44
2:D:85:ALA:HB1	2:D:94:LEU:CD2	2.37	0.44
1:A:290:ILE:HD12	1:A:290:ILE:HA	1.80	0.44
1:C:324:ALA:HB1	1:C:329:LYS:HB3	1.99	0.44
1:A:43:ARG:NH1	1:A:353:GLU:OE1	2.50	0.43
1:A:164:ASN:HB3	2:B:327:TRP:CE2	2.52	0.43
1:C:327:TRP:CE2	2:D:164:ASN:HB3	2.53	0.43
2:D:189:GLN:O	2:D:193:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LYS:O	2:B:96:SER:HB2	2.18	0.43
2:D:84:HIS:O	2:D:87:LEU:HD12	2.18	0.43
2:B:174:GLU:HG3	2:B:178:LYS:HE3	2.00	0.43
1:C:298:ASN:HB3	1:C:299:GLY:H	1.69	0.43
1:A:206:MET:HE1	1:A:245:ILE:HD11	1.99	0.43
1:C:206:MET:HE1	1:C:245:ILE:HD11	2.01	0.43
2:D:154[A]:ARG:HA	2:D:154[A]:ARG:HD2	1.73	0.43
2:B:248:HIS:CE1	2:B:252:ASN:HB3	2.54	0.42
1:A:276:THR:OG1	1:A:300:ALA:HA	2.19	0.42
1:C:140:ILE:HG12	1:C:179:PHE:HB2	2.01	0.42
2:D:287:LYS:NZ	4:D:410:HOH:O	2.52	0.42
1:A:164:ASN:HD21	1:A:173:ASN:ND2	2.17	0.42
1:C:154:ARG:HA	1:C:154:ARG:HD2	1.79	0.42
1:A:156:LYS:O	1:A:160:GLU:HG3	2.20	0.42
1:A:202:THR:HG21	1:A:261[A]:GLU:HB3	2.01	0.41
2:B:276:THR:OG1	2:B:300:ALA:HA	2.19	0.41
1:A:306:ILE:HD11	1:A:350:LEU:HD22	2.02	0.41
1:A:77:LEU:HD23	1:A:77:LEU:H	1.86	0.41
1:C:237:THR:HB	2:D:263:LEU:HD21	2.02	0.41
1:C:306:ILE:HD11	1:C:350:LEU:HD22	2.02	0.41
2:D:91[A]:ARG:HD2	2:D:228:HIS:CE1	2.56	0.41
2:D:96:SER:HA	2:D:274:LYS:HD3	2.02	0.41
1:C:248:HIS:CE1	1:C:252:ASN:HB3	2.56	0.40
1:A:327:TRP:CE2	2:B:164:ASN:HB3	2.56	0.40
2:D:61[B]:ARG:NH1	4:D:414:HOH:O	2.55	0.40
2:D:122:HIS:ND1	2:D:359:MET:HE1	2.37	0.40
2:B:186:ILE:O	2:B:190:MET:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:NZ	2:D:80:ASP:OD2[2_564]	2.18	0.02

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	318/397 (80%)	314 (99%)	4 (1%)	0	100	100
1	C	315/397 (79%)	312 (99%)	3 (1%)	0	100	100
2	B	330/397 (83%)	327 (99%)	3 (1%)	0	100	100
2	D	331/397 (83%)	328 (99%)	3 (1%)	0	100	100
All	All	1294/1588 (82%)	1281 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	275/332 (83%)	271 (98%)	4 (2%)	57	54
1	C	272/332 (82%)	270 (99%)	2 (1%)	76	76
2	B	284/331 (86%)	280 (99%)	4 (1%)	59	56
2	D	285/331 (86%)	284 (100%)	1 (0%)	84	85
All	All	1116/1326 (84%)	1105 (99%)	11 (1%)	76	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	174[A]	GLU
1	A	174[B]	GLU
1	A	346	VAL
2	B	150[A]	GLU
2	B	150[B]	GLU
2	B	310[A]	GLN
2	B	310[B]	GLN

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Mol	Chain	Res	Type
1	C	272	PHE
1	C	346	VAL
2	D	90	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	189	GLN
1	A	267	ASN
1	A	288	HIS
2	B	189	GLN
2	B	228	HIS
1	C	65	GLN
1	C	195	ASN
1	C	289	HIS
1	C	357	GLN
2	D	79	GLN
2	D	89	GLN
2	D	161	ASN
2	D	228	HIS
2	D	298	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	CSS	D	177	2	4,6,7	1.15	0	2,6,8	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSS	A	177	1	4,6,7	0.94	0	2,6,8	0.27	0
1	CSS	C	177	1	4,6,7	0.92	0	2,6,8	0.46	0
2	CSS	B	177	2	4,6,7	1.14	0	2,6,8	0.51	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
2	CSS	D	177	2	-	0/1/5/7	-
1	CSS	A	177	1	-	0/1/5/7	-
1	CSS	C	177	1	-	0/1/5/7	-
2	CSS	B	177	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	A1I7E	B	401	-	34,34,34	0.48	0	48,52,52	1.73	7 (14%)
3	A1I7E	A	401	-	34,34,34	0.61	0	48,52,52	1.66	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1I7E	B	401	-	-	4/8/44/44	0/6/6/6
3	A1I7E	A	401	-	-	8/8/44/44	0/6/6/6

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	A1I7E	C8-N1-C7	-6.09	118.09	123.40
3	B	401	A1I7E	C8-N1-C7	-4.55	119.43	123.40
3	B	401	A1I7E	C5-C4-C3	4.32	128.43	119.91
3	B	401	A1I7E	C22-C21-C24	4.28	128.37	119.91
3	A	401	A1I7E	C14-C13-C1	3.83	121.99	114.42
3	A	401	A1I7E	C5-C4-C3	3.74	127.30	119.91
3	B	401	A1I7E	C14-C13-C1	3.63	121.59	114.42
3	B	401	A1I7E	C22-C21-C17	-3.61	113.42	119.47
3	B	401	A1I7E	C5-C4-C8	-3.55	113.51	119.47
3	A	401	A1I7E	C17-N2-C18	-3.06	120.73	123.40
3	A	401	A1I7E	C5-C4-C8	-2.91	114.60	119.47
3	A	401	A1I7E	C22-C21-C24	2.80	125.44	119.91
3	B	401	A1I7E	C13-C1-C2	2.48	120.22	118.22
3	A	401	A1I7E	C10-C11-C12	2.22	133.30	129.31
3	A	401	A1I7E	C20-C16-C15	2.11	133.10	129.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	A1I7E	C13-C1-C2-C3
3	A	401	A1I7E	C13-C1-C2-C12
3	A	401	A1I7E	O1-C1-C2-C3
3	A	401	A1I7E	O1-C1-C2-C12

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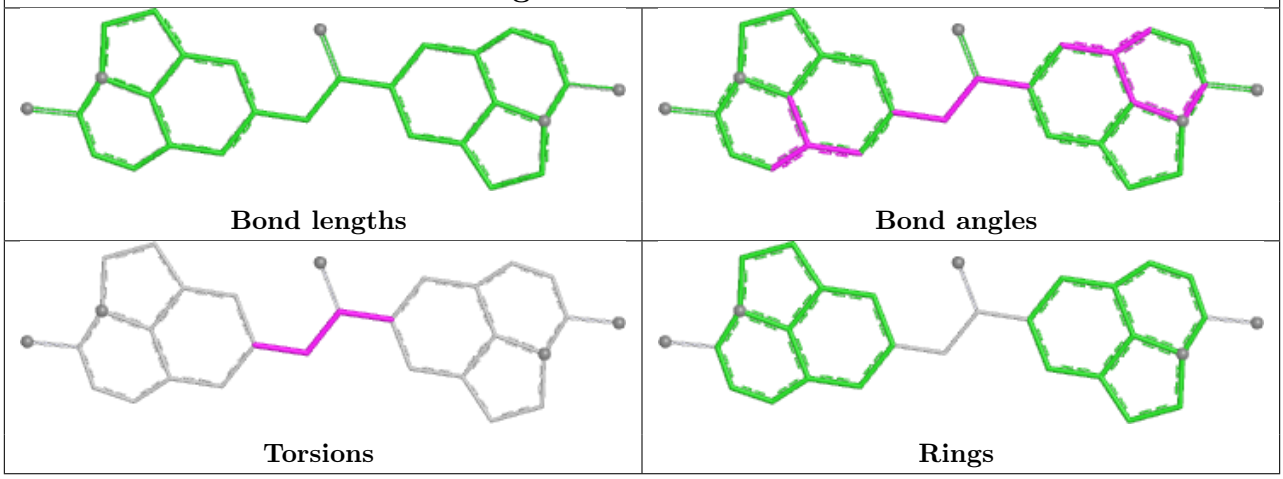
Mol	Chain	Res	Type	Atoms
3	A	401	A1I7E	C2-C1-C13-C14
3	A	401	A1I7E	O1-C1-C13-C14
3	B	401	A1I7E	C2-C1-C13-C14
3	B	401	A1I7E	O1-C1-C13-C14
3	A	401	A1I7E	C1-C13-C14-C24
3	A	401	A1I7E	C1-C13-C14-C15
3	B	401	A1I7E	C1-C13-C14-C15
3	B	401	A1I7E	C13-C1-C2-C12

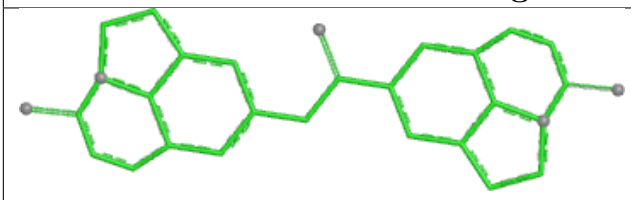
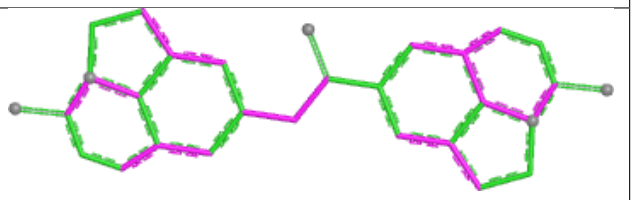
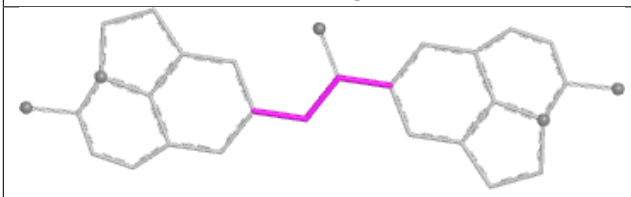
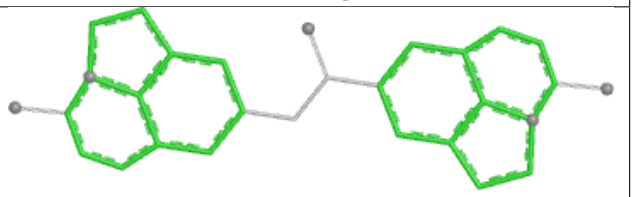
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A1I7E B 401



Ligand A1I7E A 401	
 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

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, 95^{th} 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	318/397 (80%)	-1.02	0	100	100	23, 47, 83, 140	6 (1%)
1	C	318/397 (80%)	-1.03	0	100	100	32, 47, 85, 137	3 (0%)
2	B	327/397 (82%)	-0.99	1 (0%)	90	92	30, 49, 88, 144	7 (2%)
2	D	327/397 (82%)	-1.02	2 (0%)	85	89	24, 49, 85, 157	8 (2%)
All	All	1290/1588 (81%)	-1.02	3 (0%)	91	92	23, 48, 85, 157	24 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	250[A]	TYR	3.7
2	B	250[A]	TYR	2.8
2	D	91[A]	ARG	2.0

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

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, 95^{th} 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
1	CSS	A	177	7/8	0.99	0.04	46,48,59,75	0
2	CSS	B	177	7/8	0.99	0.05	60,65,78,98	0
1	CSS	C	177	7/8	0.99	0.04	46,50,63,80	0
2	CSS	D	177	7/8	0.99	0.05	61,65,74,108	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

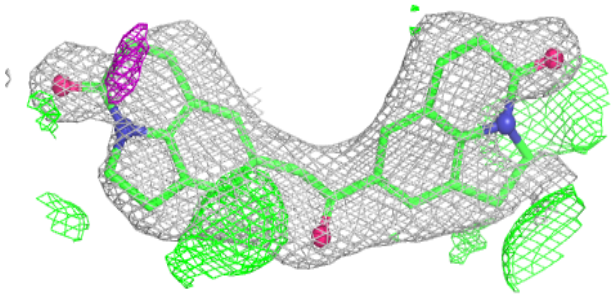
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

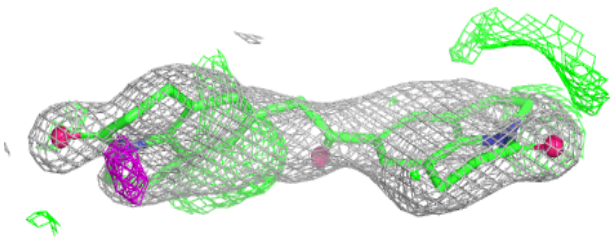
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1I7E	A	401	29/29	0.97	0.09	40,58,67,70	29
3	A1I7E	B	401	29/29	0.97	0.08	41,55,61,73	29

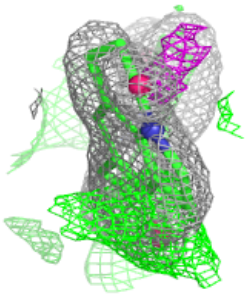
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1I7E A 401:

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

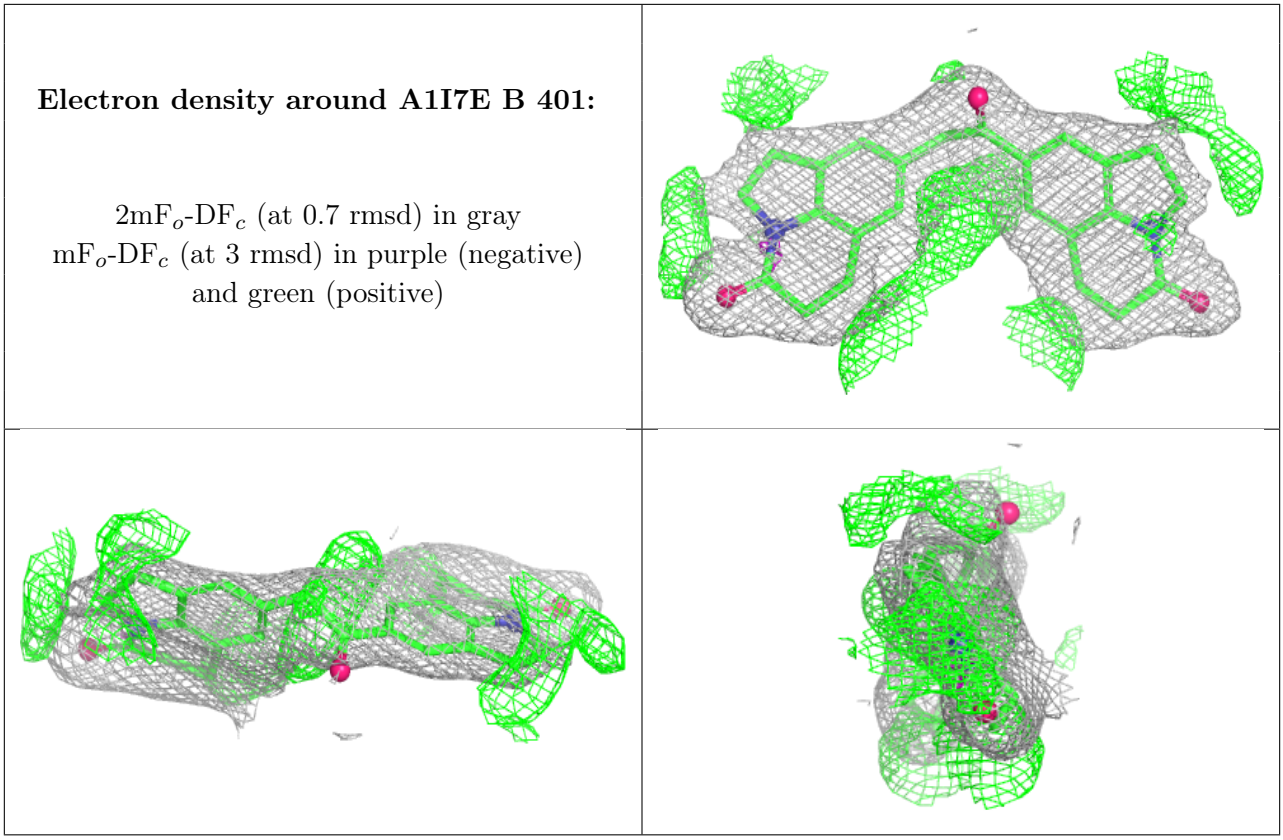






Electron density around A1I7E B 401:

$2mF_o$-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.