



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:43 PM EDT

PDB ID : 3H9K / pdb_00003h9k
Title : Structures of Thymidylate Synthase R163K with Substrates and Inhibitors
Show Subunit Asymmetry
Authors : Gibson, L.M.; Lovelace, L.L.; Lebioda, L.
Deposited on : 2009-04-30
Resolution : 2.65 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

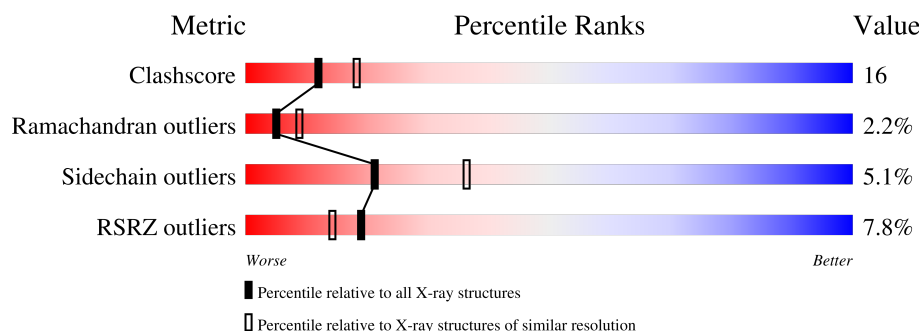
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	313	2% 68% 20% • 10%
1	B	313	4% 64% 24% • 10%
1	C	313	4% 60% 27% • 10%
1	D	313	20% 45% 37% 6% 11%
1	E	313	5% 63% 24% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11468 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.

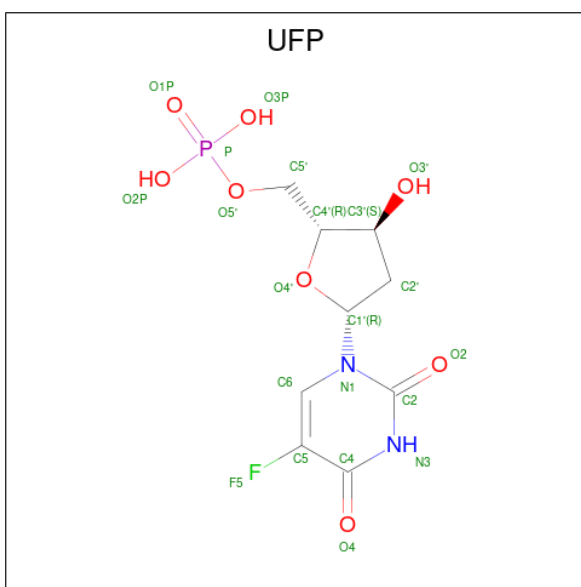
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	B	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	C	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	D	280	Total	C	N	O	S	0	0	0
			2261	1446	394	410	11			
1	E	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			

There are 5 discrepancies between the modelled and reference sequences:

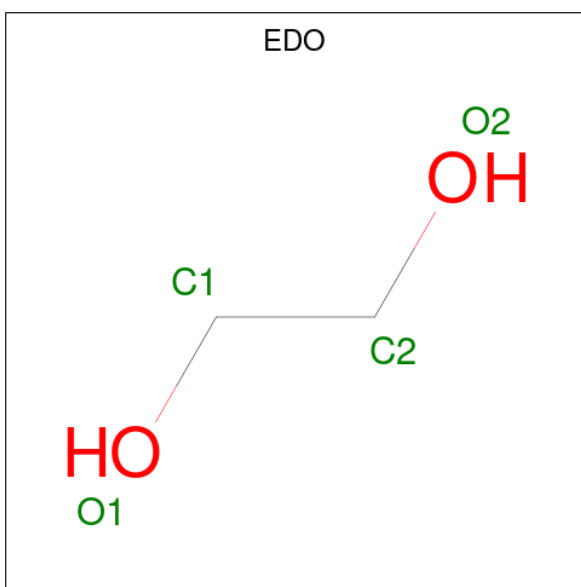
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LYS	ARG	engineered mutation	UNP P04818
B	163	LYS	ARG	engineered mutation	UNP P04818
C	163	LYS	ARG	engineered mutation	UNP P04818
D	163	LYS	ARG	engineered mutation	UNP P04818
E	163	LYS	ARG	engineered mutation	UNP P04818

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: C₉H₁₂FN₂O₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
2	B	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		
2	D	1	Total	C	F	N	O	P	0	0
			21	9	1	2	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



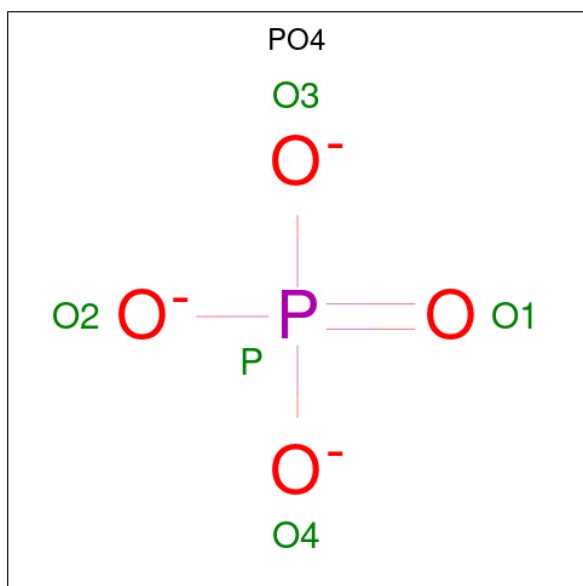
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			4	2 2		

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

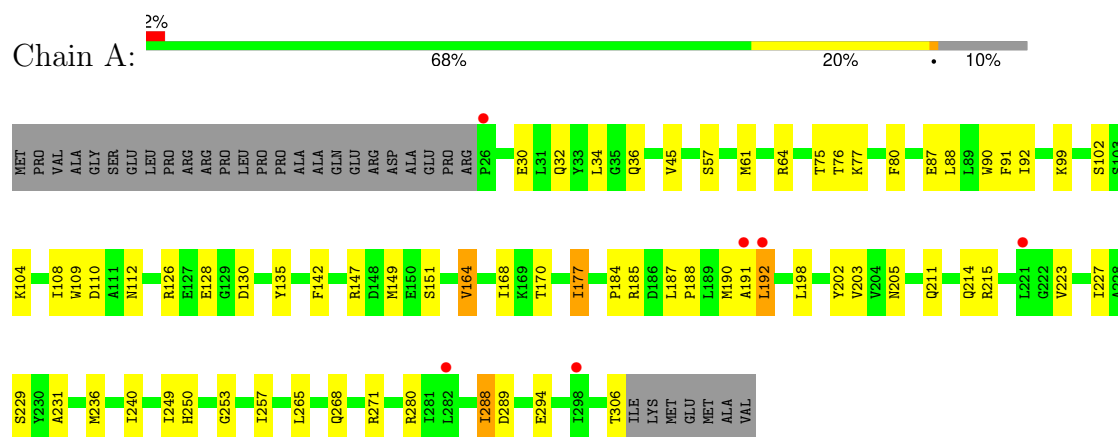
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	10	Total	O	0	0
			10	10		
5	C	12	Total	O	0	0
			12	12		
5	D	6	Total	O	0	0
			6	6		
5	E	14	Total	O	0	0
			14	14		

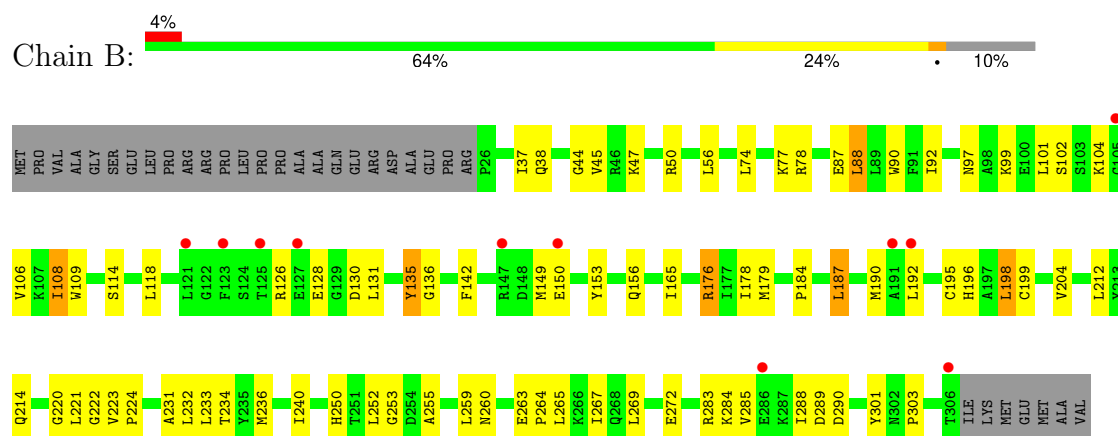
3 Residue-property plots [i](#)

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.

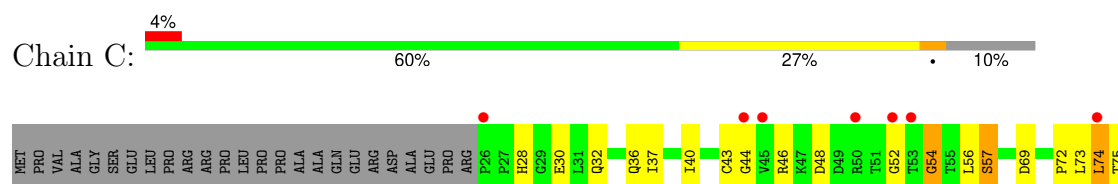
• Molecule 1: Thymidylate synthase

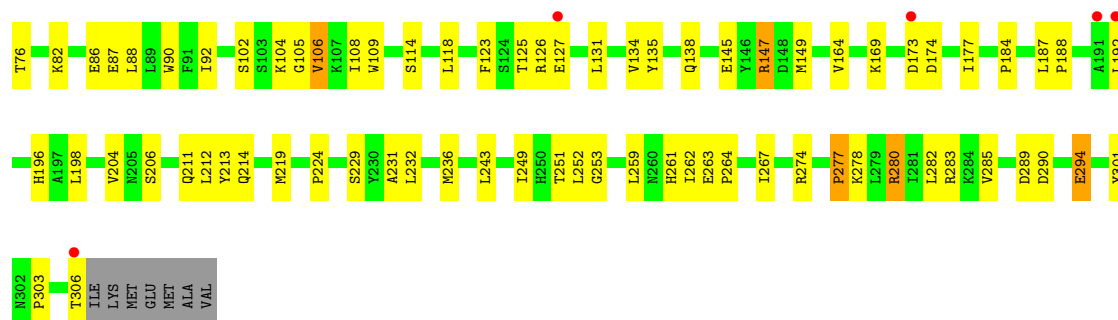


• Molecule 1: Thymidylate synthase

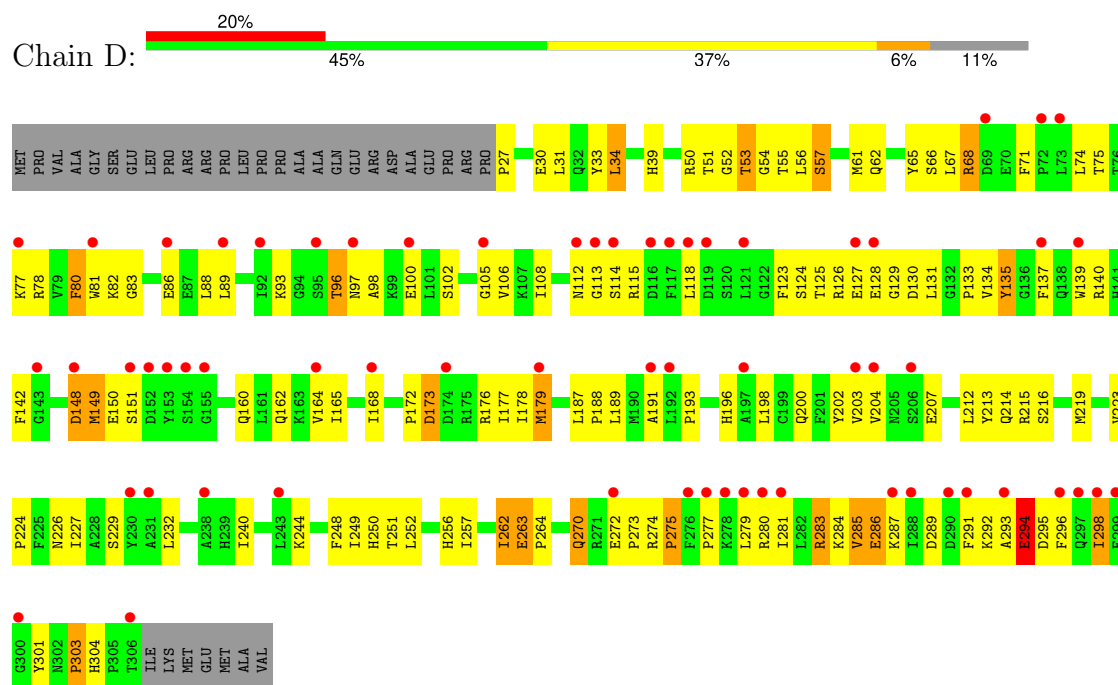


• Molecule 1: Thymidylate synthase

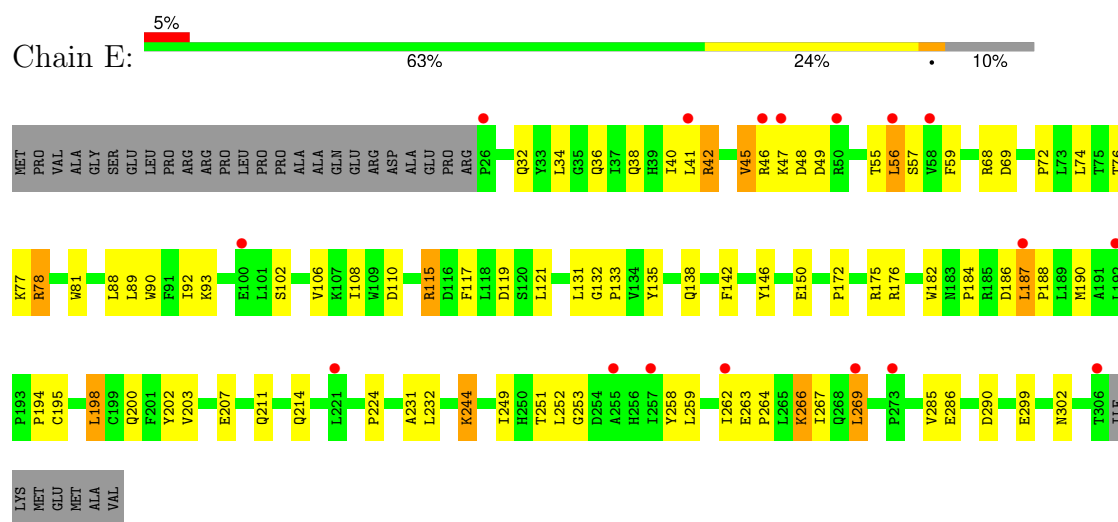




• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.28Å 122.19Å 99.83Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-2.65) 94.0 (50.00-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.260 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11468	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, EDO, UFP

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	0.56	0/2328	0.95	4/3150 (0.1%)
1	B	0.50	0/2328	0.89	5/3150 (0.2%)
1	C	0.52	0/2328	0.93	3/3150 (0.1%)
1	D	0.45	0/2320	0.87	3/3138 (0.1%)
1	E	0.49	0/2328	0.86	3/3150 (0.1%)
All	All	0.50	0/11632	0.90	18/15738 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	ALA	N-CA-C	-8.56	102.03	111.36
1	A	231	ALA	N-CA-C	-8.05	102.58	111.36
1	B	253	GLY	N-CA-C	-7.77	103.14	110.21
1	A	253	GLY	N-CA-C	-7.36	103.51	110.21
1	C	253	GLY	N-CA-C	-6.53	104.27	110.21
1	B	234	THR	N-CA-C	-6.30	104.04	111.03
1	C	57	SER	N-CA-C	6.00	119.50	109.95
1	E	195	CYS	N-CA-C	-5.87	106.12	113.28
1	B	178	ILE	N-CA-C	5.84	117.16	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	SER	N-CA-C	5.82	118.03	109.24
1	B	37	ILE	N-CA-C	-5.68	104.83	110.62
1	A	57	SER	N-CA-C	5.66	118.62	109.40
1	D	96	THR	N-CA-C	-5.56	105.81	112.59
1	A	170	THR	N-CA-C	5.51	117.37	111.36
1	B	231	ALA	N-CA-C	-5.47	105.40	111.36
1	D	52	GLY	N-CA-C	-5.42	107.76	115.30
1	E	231	ALA	N-CA-C	-5.38	105.58	111.82
1	E	57	SER	N-CA-C	5.26	118.22	110.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	213	TYR	Sidechain
1	E	202	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	2268	0	2235	56	0
1	B	2268	0	2235	64	0
1	C	2268	0	2235	70	0
1	D	2261	0	2228	121	0
1	E	2268	0	2235	62	0
2	A	21	0	10	1	0
2	B	21	0	10	0	0
2	D	21	0	10	2	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	12	0	0	0	0
5	B	10	0	0	0	0
5	C	12	0	0	1	0
5	D	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	14	0	0	0	0
All	All	11468	0	11210	355	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (355) 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:C:263:GLU:HG2	1:C:264:PRO:HD3	1.39	1.05
1:C:280:ARG:HH11	1:C:280:ARG:HB3	1.29	0.94
1:B:165:ILE:HD12	1:B:240:ILE:HD11	1.50	0.92
1:C:88:LEU:HD23	1:C:236:MET:HE3	1.52	0.92
1:A:130:ASP:HB2	1:A:149:MET:HE2	1.52	0.92
1:D:298:ILE:H	1:D:298:ILE:HD12	1.34	0.91
1:D:123:PHE:HB3	1:D:126:ARG:HD2	1.61	0.82
1:A:271:ARG:HH22	1:A:306:THR:HB	1.45	0.81
1:B:50:ARG:HH11	1:B:50:ARG:HB2	1.47	0.80
1:E:55:THR:HG22	1:E:258:TYR:HA	1.63	0.80
1:C:88:LEU:HD23	1:C:236:MET:CE	2.14	0.77
1:D:160:GLN:O	1:D:164:VAL:HG23	1.85	0.77
1:D:33:TYR:HD1	1:D:34:LEU:HD12	1.49	0.77
1:D:204:VAL:HG21	1:E:45:VAL:HG21	1.68	0.75
1:C:263:GLU:CG	1:C:264:PRO:HD3	2.16	0.74
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.69	0.74
1:C:294:GLU:H	1:C:294:GLU:CD	1.95	0.73
1:D:280:ARG:NH1	1:D:280:ARG:HB3	2.04	0.73
1:D:279:LEU:HD11	1:D:296:PHE:HB3	1.71	0.73
1:C:285:VAL:HG13	1:C:290:ASP:HB2	1.69	0.73
1:D:270:GLN:HE21	1:D:270:GLN:HA	1.54	0.73
1:A:168:ILE:HD13	1:A:177:ILE:HD13	1.70	0.72
1:C:102:SER:HA	1:C:106:VAL:O	1.90	0.72
1:D:214:GLN:HB3	1:D:252:LEU:HD23	1.70	0.72
1:D:53:THR:HG22	1:D:54:GLY:N	2.03	0.71
1:A:32:GLN:NE2	1:A:64:ARG:H	1.88	0.70
1:E:36:GLN:O	1:E:40:ILE:HG12	1.93	0.69
1:E:259:LEU:HA	1:E:262:ILE:HG12	1.76	0.68
1:B:153:TYR:HA	1:B:156:GLN:NE2	2.09	0.68
1:B:88:LEU:HD12	1:B:232:LEU:HD23	1.76	0.67
1:D:139:TRP:CG	1:D:179:MET:HE1	2.30	0.66
1:C:263:GLU:HG2	1:C:264:PRO:CD	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:HIS:HB3	1:C:212:LEU:HD11	1.77	0.66
1:D:285:VAL:HG12	1:D:286:GLU:H	1.61	0.65
1:A:91:PHE:CE1	1:A:135:TYR:HB2	2.31	0.65
1:C:174:ASP:HB3	1:C:177:ILE:HD11	1.79	0.65
1:D:298:ILE:HD12	1:D:298:ILE:N	2.10	0.65
1:A:147:ARG:HB3	1:A:151:SER:OG	1.98	0.64
1:D:115:ARG:NH2	1:D:127:GLU:HA	2.12	0.63
1:D:74:LEU:HD22	1:D:74:LEU:H	1.64	0.63
1:B:252:LEU:HD13	1:B:255:ALA:HB2	1.81	0.62
1:A:187:LEU:HB2	1:A:188:PRO:HD3	1.80	0.62
1:B:223:VAL:HG13	1:B:250:HIS:HE1	1.64	0.62
1:B:196:HIS:HB3	1:B:212:LEU:HD11	1.82	0.62
1:D:200:GLN:HE22	1:E:253:GLY:HA3	1.65	0.62
2:D:565:UFP:H5'2	1:E:175:ARG:HH21	1.65	0.61
1:B:50:ARG:HB2	1:B:50:ARG:NH1	2.15	0.61
1:E:102:SER:HA	1:E:106:VAL:O	2.00	0.61
1:E:88:LEU:O	1:E:92:ILE:HG12	2.01	0.61
1:C:214:GLN:HB3	1:C:252:LEU:HD23	1.82	0.61
1:B:214:GLN:HB3	1:B:252:LEU:HD23	1.83	0.60
1:D:57:SER:HB3	1:D:256:HIS:HB3	1.82	0.60
1:A:87:GLU:O	1:A:90:TRP:HB3	2.00	0.60
1:A:102:SER:HB2	1:A:110:ASP:OD1	2.02	0.60
1:A:257:ILE:HD13	1:A:265:LEU:HD13	1.83	0.60
1:B:88:LEU:O	1:B:92:ILE:HG12	2.02	0.60
1:B:285:VAL:HG13	1:B:290:ASP:HB2	1.83	0.60
1:D:112:ASN:HB3	1:D:191:ALA:HB1	1.84	0.60
1:C:48:ASP:HA	1:C:54:GLY:HA2	1.83	0.60
1:A:30:GLU:OE1	1:A:76:THR:HG23	2.02	0.59
1:C:277:PRO:HG2	1:C:301:TYR:CD1	2.37	0.59
1:A:192:LEU:O	1:A:192:LEU:HD22	2.02	0.59
1:D:62:GLN:HA	1:D:250:HIS:O	2.03	0.59
2:A:400:UFP:O2P	1:B:176:ARG:NH2	2.35	0.58
1:B:285:VAL:CG1	1:B:290:ASP:HB2	2.33	0.58
1:D:81:TRP:NE1	1:D:298:ILE:HD11	2.18	0.58
1:B:78:ARG:HE	1:B:303:PRO:HG2	1.68	0.58
1:C:108:ILE:HG13	1:C:109:TRP:CD1	2.39	0.58
1:C:277:PRO:HG3	1:C:301:TYR:HA	1.85	0.58
1:C:74:LEU:HD12	1:C:224:PRO:HB3	1.85	0.58
1:D:294:GLU:CD	1:D:294:GLU:H	2.11	0.58
1:C:232:LEU:HG	1:C:236:MET:HE3	1.86	0.58
1:E:182:TRP:CZ2	1:E:187:LEU:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HG2	1:B:130:ASP:HB3	1.85	0.57
1:B:198:LEU:HD12	1:B:198:LEU:C	2.29	0.57
1:E:214:GLN:HB3	1:E:252:LEU:HD23	1.87	0.57
1:C:127:GLU:HB2	1:C:149:MET:HE2	1.86	0.57
1:D:88:LEU:HD23	1:D:232:LEU:HD23	1.84	0.57
1:D:98:ALA:HB3	1:D:129:GLY:HA2	1.86	0.57
1:A:99:LYS:NZ	1:A:128:GLU:HG3	2.18	0.57
1:E:198:LEU:C	1:E:198:LEU:HD12	2.30	0.57
1:E:266:LYS:NZ	1:E:266:LYS:HB3	2.20	0.57
1:C:108:ILE:HG13	1:C:109:TRP:HD1	1.69	0.56
1:D:80:PHE:CE1	1:D:82:LYS:HB3	2.40	0.56
1:C:173:ASP:HB2	5:C:315:HOH:O	2.05	0.56
1:D:68:ARG:HD2	1:D:207:GLU:OE1	2.05	0.56
1:D:207:GLU:HA	1:D:244:LYS:O	2.05	0.56
1:C:187:LEU:N	1:C:188:PRO:HD2	2.20	0.56
1:A:294:GLU:CD	1:A:294:GLU:H	2.14	0.56
1:B:301:TYR:CZ	1:B:303:PRO:HG3	2.40	0.56
1:A:202:TYR:CE1	1:B:47:LYS:HE3	2.41	0.56
1:A:88:LEU:O	1:A:92:ILE:HG12	2.06	0.56
1:C:277:PRO:HG2	1:C:301:TYR:HD1	1.71	0.56
1:A:192:LEU:N	1:A:192:LEU:HD13	2.20	0.55
1:D:39:HIS:HD2	1:D:61:MET:HE3	1.71	0.55
1:D:142:PHE:CE2	1:E:184:PRO:HD2	2.42	0.55
1:A:168:ILE:HG23	1:A:203:VAL:HG21	1.88	0.55
1:B:264:PRO:O	1:B:267:ILE:HG13	2.07	0.55
1:B:301:TYR:O	1:B:303:PRO:HD3	2.06	0.55
1:D:89:LEU:O	1:D:93:LYS:HG3	2.06	0.55
1:E:285:VAL:CG1	1:E:290:ASP:HB2	2.37	0.55
1:B:267:ILE:HD12	1:B:267:ILE:C	2.32	0.55
1:D:123:PHE:HB3	1:D:126:ARG:CD	2.36	0.55
1:A:271:ARG:NH2	1:A:306:THR:HB	2.20	0.54
1:B:109:TRP:CZ3	1:B:192:LEU:HD21	2.42	0.54
1:D:97:ASN:OD1	1:D:149:MET:HG3	2.07	0.54
1:C:123:PHE:HB3	1:C:126:ARG:HG3	1.88	0.54
1:E:249:ILE:HD12	1:E:249:ILE:N	2.22	0.54
1:A:280:ARG:HG2	1:A:280:ARG:HH11	1.72	0.54
1:D:178:ILE:HG12	1:D:200:GLN:HG3	1.89	0.54
1:B:236:MET:HE2	1:B:288:ILE:HD11	1.89	0.54
1:C:280:ARG:HB3	1:C:280:ARG:NH1	2.10	0.54
1:E:32:GLN:O	1:E:36:GLN:HG3	2.08	0.54
1:E:285:VAL:HG13	1:E:290:ASP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:N	1:B:192:LEU:HD23	2.23	0.54
1:E:74:LEU:HD12	1:E:224:PRO:HB3	1.90	0.54
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.89	0.54
1:E:133:PRO:HD3	1:E:146:TYR:CD2	2.42	0.54
1:D:74:LEU:H	1:D:74:LEU:CD2	2.20	0.54
1:B:223:VAL:HG13	1:B:250:HIS:CE1	2.42	0.53
1:C:30:GLU:HG3	1:C:74:LEU:HD22	1.90	0.53
1:D:65:TYR:CE2	1:D:227:ILE:HD13	2.43	0.53
1:D:298:ILE:H	1:D:298:ILE:CD1	2.12	0.53
1:E:41:LEU:HA	1:E:56:LEU:HD23	1.89	0.53
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.72	0.53
1:D:291:PHE:C	1:D:292:LYS:HD2	2.34	0.53
1:E:106:VAL:HG12	1:E:108:ILE:HG12	1.89	0.53
1:C:86:GLU:HB2	1:C:106:VAL:HG21	1.90	0.53
1:C:88:LEU:O	1:C:92:ILE:HG13	2.09	0.53
1:C:206:SER:HA	1:C:243:LEU:HD22	1.89	0.53
1:D:56:LEU:HD22	1:D:262:ILE:HD11	1.90	0.53
1:E:38:GLN:HB3	1:E:269:LEU:HD11	1.91	0.53
1:E:46:ARG:NH1	1:E:259:LEU:HD11	2.24	0.53
1:D:280:ARG:HB3	1:D:280:ARG:HH11	1.70	0.53
1:B:283:ARG:HG2	1:B:284:LYS:H	1.73	0.53
1:C:261:HIS:C	1:C:264:PRO:HD2	2.33	0.53
1:D:196:HIS:HB3	1:D:212:LEU:HD11	1.90	0.52
1:D:223:VAL:HB	1:D:224:PRO:HD3	1.91	0.52
1:E:187:LEU:N	1:E:188:PRO:HD2	2.24	0.52
1:E:38:GLN:HG3	1:E:42:ARG:HH11	1.73	0.52
1:E:117:PHE:CE1	1:E:121:LEU:HD11	2.45	0.52
1:A:198:LEU:C	1:A:198:LEU:HD12	2.35	0.52
1:D:67:LEU:HD11	1:D:248:PHE:HB2	1.92	0.52
1:C:204:VAL:O	1:C:204:VAL:HG13	2.09	0.52
1:B:265:LEU:O	1:B:269:LEU:HD23	2.10	0.52
1:C:198:LEU:C	1:C:198:LEU:HD12	2.34	0.52
1:D:34:LEU:CD1	1:D:34:LEU:H	2.22	0.52
1:E:81:TRP:HH2	1:E:232:LEU:HD13	1.75	0.52
1:C:123:PHE:HB3	1:C:126:ARG:CG	2.40	0.51
1:D:66:SER:C	1:D:67:LEU:HD23	2.36	0.51
1:E:88:LEU:CD2	1:E:232:LEU:HD23	2.41	0.51
1:A:271:ARG:HH12	1:A:306:THR:HG21	1.74	0.51
1:C:44:GLY:HA2	1:C:57:SER:O	2.11	0.51
1:C:249:ILE:HD12	1:C:249:ILE:N	2.26	0.51
1:E:90:TRP:HH2	1:E:131:LEU:CD1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD11	1:B:128:GLU:HA	1.93	0.51
1:E:172:PRO:O	1:E:203:VAL:HB	2.11	0.51
1:C:36:GLN:O	1:C:40:ILE:HG13	2.11	0.50
1:D:286:GLU:HG2	1:D:287:LYS:HG3	1.93	0.50
1:D:106:VAL:CG1	1:D:108:ILE:HG12	2.41	0.50
1:D:176:ARG:HG3	1:D:176:ARG:HH11	1.75	0.50
1:B:135:TYR:O	1:B:136:GLY:C	2.55	0.50
1:D:78:ARG:HG2	1:D:303:PRO:HG2	1.92	0.50
1:D:293:ALA:C	1:D:295:ASP:H	2.19	0.50
1:E:89:LEU:O	1:E:93:LYS:HG3	2.12	0.50
1:E:263:GLU:N	1:E:264:PRO:HD2	2.27	0.50
1:D:74:LEU:HD22	1:D:74:LEU:N	2.25	0.50
1:B:114:SER:O	1:B:118:LEU:HG	2.12	0.50
1:D:113:GLY:O	1:D:128:GLU:HG3	2.11	0.50
1:B:97:ASN:HD21	1:B:99:LYS:HB2	1.77	0.50
1:B:301:TYR:CE1	1:B:303:PRO:HG3	2.47	0.50
1:C:48:ASP:HB3	1:C:52:GLY:HA2	1.93	0.50
1:C:211:GLN:NE2	1:C:251:THR:OG1	2.45	0.49
1:A:236:MET:HE2	1:A:288:ILE:HD11	1.94	0.49
1:C:294:GLU:CD	1:C:294:GLU:N	2.67	0.49
1:D:115:ARG:CD	1:D:128:GLU:HB2	2.43	0.49
1:B:87:GLU:O	1:B:90:TRP:HB3	2.13	0.49
1:D:75:THR:HG21	1:D:274:ARG:O	2.12	0.49
1:E:102:SER:HB3	1:E:110:ASP:OD2	2.13	0.49
1:B:108:ILE:HG13	1:B:109:TRP:HD1	1.78	0.49
1:D:164:VAL:HG21	1:D:179:MET:HG3	1.95	0.49
1:C:114:SER:O	1:C:118:LEU:HG	2.12	0.49
1:E:259:LEU:HA	1:E:262:ILE:CG1	2.43	0.49
1:D:71:PHE:CE2	1:D:279:LEU:HD22	2.49	0.48
1:D:251:THR:HG21	1:E:251:THR:HG21	1.95	0.48
1:D:96:THR:HG21	1:D:137:PHE:HB2	1.95	0.48
1:D:249:ILE:N	1:D:249:ILE:HD12	2.28	0.48
1:A:187:LEU:HD23	1:A:190:MET:CE	2.44	0.48
1:D:82:LYS:HE3	1:D:105:GLY:HA3	1.94	0.48
1:A:205:ASN:HD21	1:B:45:VAL:HG11	1.78	0.48
1:C:82:LYS:NZ	1:C:105:GLY:HA3	2.28	0.48
1:D:55:THR:HB	1:D:257:ILE:O	2.14	0.48
1:A:271:ARG:HH22	1:A:306:THR:CB	2.22	0.47
1:B:106:VAL:HG12	1:B:108:ILE:HG12	1.96	0.47
1:D:270:GLN:HE21	1:D:270:GLN:CA	2.26	0.47
1:E:138:GLN:OE1	1:E:138:GLN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ARG:NH2	1:E:176:ARG:NH1	2.61	0.47
1:D:130:ASP:N	1:D:149:MET:HE3	2.29	0.47
1:A:102:SER:C	1:A:104:LYS:H	2.22	0.47
1:D:51:THR:O	1:D:51:THR:HG22	2.14	0.47
1:A:126:ARG:HD3	1:A:130:ASP:CG	2.40	0.47
1:C:277:PRO:CG	1:C:301:TYR:HD1	2.26	0.47
1:E:68:ARG:HE	1:E:207:GLU:CD	2.23	0.47
1:A:108:ILE:HG13	1:A:109:TRP:CD1	2.50	0.47
1:C:263:GLU:O	1:C:267:ILE:HG13	2.15	0.47
1:E:133:PRO:O	1:E:190:MET:HE2	2.13	0.47
1:B:187:LEU:HA	1:B:190:MET:HE3	1.97	0.47
1:C:32:GLN:O	1:C:36:GLN:HG3	2.14	0.47
1:C:40:ILE:HD12	1:C:219:MET:HG3	1.97	0.47
1:D:106:VAL:HG12	1:D:108:ILE:HG12	1.95	0.47
1:D:114:SER:O	1:D:118:LEU:HG	2.14	0.47
1:D:149:MET:HG2	1:D:150:GLU:N	2.30	0.47
1:D:187:LEU:HB3	1:D:188:PRO:HD3	1.97	0.47
1:A:164:VAL:O	1:A:168:ILE:HG12	2.15	0.47
1:C:147:ARG:HH12	1:E:302:ASN:ND2	2.12	0.47
1:E:207:GLU:HA	1:E:244:LYS:O	2.15	0.47
1:C:69:ASP:O	1:C:278:LYS:HE2	2.15	0.47
1:E:267:ILE:HD12	1:E:267:ILE:H	1.79	0.47
1:C:109:TRP:CE3	1:C:131:LEU:HD13	2.49	0.46
1:C:147:ARG:HH12	1:E:302:ASN:CG	2.23	0.46
1:E:190:MET:SD	1:E:194:PRO:HD3	2.55	0.46
1:B:149:MET:HG3	1:B:150:GLU:HG2	1.97	0.46
1:D:301:TYR:C	1:D:303:PRO:HD3	2.40	0.46
1:B:50:ARG:HH11	1:B:50:ARG:CB	2.24	0.46
1:C:28:HIS:HD2	1:C:30:GLU:HB3	1.80	0.46
1:D:301:TYR:CZ	1:D:303:PRO:HG3	2.50	0.46
1:A:187:LEU:HD23	1:A:190:MET:HE3	1.98	0.46
1:A:192:LEU:N	1:A:192:LEU:CD1	2.79	0.46
1:D:274:ARG:NH1	1:D:303:PRO:O	2.48	0.46
1:C:285:VAL:CG1	1:C:290:ASP:HB2	2.44	0.46
1:D:82:LYS:CE	1:D:105:GLY:HA3	2.46	0.46
1:D:281:ILE:HA	1:D:295:ASP:O	2.16	0.46
1:E:244:LYS:HB2	1:E:244:LYS:NZ	2.30	0.46
1:B:135:TYR:OH	1:B:195:CYS:N	2.48	0.46
1:C:28:HIS:CD2	1:C:30:GLU:H	2.33	0.46
1:C:259:LEU:O	1:C:262:ILE:HG12	2.15	0.46
1:D:301:TYR:O	1:D:303:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:PRO:HD2	1:D:189:LEU:O	2.15	0.46
1:D:204:VAL:HG21	1:E:45:VAL:CG2	2.42	0.46
1:A:187:LEU:HA	1:A:190:MET:CE	2.45	0.46
1:C:280:ARG:HH11	1:C:280:ARG:CB	2.13	0.46
1:D:77:LYS:HD2	1:D:78:ARG:O	2.16	0.46
1:D:34:LEU:HD12	1:D:34:LEU:N	2.30	0.45
1:C:206:SER:HA	1:C:243:LEU:CD2	2.45	0.45
1:E:34:LEU:HD11	1:E:76:THR:HG21	1.98	0.45
1:A:211:GLN:HG3	1:A:249:ILE:HB	1.99	0.45
1:D:123:PHE:CB	1:D:126:ARG:HD2	2.38	0.45
1:D:124:SER:C	1:D:126:ARG:H	2.25	0.45
1:E:132:GLY:HA2	1:E:146:TYR:CE2	2.51	0.45
1:A:240:ILE:HD11	1:A:288:ILE:HA	1.98	0.45
1:B:108:ILE:HG13	1:B:109:TRP:CD1	2.52	0.45
1:B:252:LEU:HD13	1:B:255:ALA:CB	2.47	0.44
1:D:196:HIS:ND1	1:D:214:GLN:HG3	2.32	0.44
1:A:99:LYS:HZ2	1:A:128:GLU:HG3	1.82	0.44
1:D:168:ILE:HG23	1:D:203:VAL:HG21	1.99	0.44
1:A:192:LEU:HD22	1:A:192:LEU:C	2.42	0.44
1:A:187:LEU:HA	1:A:190:MET:HE2	2.00	0.44
1:B:109:TRP:CE3	1:B:131:LEU:HD13	2.52	0.44
1:C:28:HIS:CD2	1:C:30:GLU:HB3	2.52	0.44
1:C:30:GLU:OE1	1:C:76:THR:HG23	2.17	0.44
1:C:184:PRO:HA	1:C:187:LEU:HD12	1.99	0.44
1:D:66:SER:O	1:D:67:LEU:HD23	2.18	0.44
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.99	0.44
1:D:88:LEU:HD23	1:D:232:LEU:CD2	2.47	0.44
1:C:87:GLU:O	1:C:90:TRP:HB3	2.17	0.44
1:D:102:SER:HA	1:D:106:VAL:O	2.18	0.44
1:E:115:ARG:HH21	1:E:115:ARG:HB2	1.83	0.44
1:B:44:GLY:O	1:B:56:LEU:HD22	2.18	0.44
1:B:77:LYS:HD2	1:B:77:LYS:C	2.43	0.44
1:B:179:MET:HB2	1:B:199:CYS:SG	2.57	0.44
1:E:88:LEU:HD23	1:E:232:LEU:HD23	1.99	0.44
1:D:96:THR:CG2	1:D:137:PHE:HB2	2.48	0.43
1:D:215:ARG:HG3	1:D:215:ARG:HH11	1.82	0.43
1:D:39:HIS:CD2	1:D:61:MET:HE3	2.53	0.43
1:D:88:LEU:CD2	1:D:232:LEU:HD23	2.48	0.43
1:B:301:TYR:C	1:B:303:PRO:HD3	2.43	0.43
1:C:37:ILE:CD1	1:C:219:MET:HB3	2.49	0.43
1:D:27:PRO:HB2	1:D:31:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:VAL:HG12	1:D:286:GLU:N	2.30	0.43
1:E:77:LYS:HB3	1:E:78:ARG:H	1.52	0.43
1:A:205:ASN:ND2	1:B:45:VAL:HG11	2.33	0.43
1:D:164:VAL:O	1:D:168:ILE:HG13	2.18	0.43
1:D:173:ASP:HB2	1:E:47:LYS:HE3	2.00	0.43
1:B:126:ARG:CG	1:B:130:ASP:HB3	2.49	0.43
1:A:32:GLN:O	1:A:36:GLN:HG3	2.19	0.43
1:B:288:ILE:HG23	1:B:289:ASP:OD2	2.19	0.43
1:C:164:VAL:HG13	1:C:177:ILE:HG22	2.01	0.43
1:D:134:VAL:O	1:D:135:TYR:C	2.60	0.43
1:D:140:ARG:HG3	1:D:140:ARG:HH11	1.84	0.42
1:D:198:LEU:HD12	1:D:198:LEU:C	2.44	0.42
1:D:283:ARG:O	1:D:284:LYS:C	2.62	0.42
1:C:75:THR:HG21	1:C:274:ARG:O	2.19	0.42
1:D:34:LEU:HD12	1:D:34:LEU:H	1.84	0.42
1:D:301:TYR:CE1	1:D:303:PRO:HG3	2.54	0.42
1:E:302:ASN:C	1:E:302:ASN:HD22	2.26	0.42
1:B:88:LEU:HD21	1:B:233:LEU:HD13	2.01	0.42
1:E:211:GLN:HA	1:E:249:ILE:O	2.20	0.42
1:A:126:ARG:HG2	1:A:130:ASP:CB	2.44	0.42
1:A:268:GLN:HA	1:A:271:ARG:HD2	2.02	0.42
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.49	0.42
1:D:127:GLU:HB3	1:D:149:MET:HE1	2.00	0.42
1:A:30:GLU:CD	1:A:76:THR:HG23	2.45	0.42
1:A:142:PHE:CD2	1:A:142:PHE:C	2.97	0.42
1:B:198:LEU:C	1:B:198:LEU:CD1	2.92	0.42
1:B:102:SER:HA	1:B:106:VAL:O	2.19	0.42
1:D:115:ARG:HD3	1:D:128:GLU:HB2	2.02	0.42
1:D:131:LEU:O	1:D:134:VAL:HG13	2.20	0.42
1:D:177:ILE:C	1:D:178:ILE:HG13	2.45	0.42
1:A:223:VAL:O	1:A:227:ILE:HG13	2.20	0.41
1:C:134:VAL:O	1:C:135:TYR:C	2.62	0.41
1:D:34:LEU:CD1	1:D:34:LEU:N	2.83	0.41
1:A:214:GLN:OE1	1:A:250:HIS:HE1	2.03	0.41
1:B:102:SER:C	1:B:104:LYS:H	2.27	0.41
1:D:213:TYR:OH	1:E:200:GLN:NE2	2.52	0.41
1:E:198:LEU:C	1:E:198:LEU:CD1	2.94	0.41
1:B:283:ARG:HG2	1:B:284:LYS:N	2.35	0.41
1:D:86:GLU:HB3	1:D:106:VAL:HG21	2.02	0.41
1:D:162:GLN:OE1	1:D:165:ILE:HD12	2.20	0.41
1:E:186:ASP:O	1:E:190:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:HD2	1:B:142:PHE:CE2	2.55	0.41
1:D:226:ASN:O	1:D:227:ILE:C	2.64	0.41
1:D:270:GLN:HA	1:D:270:GLN:NE2	2.29	0.41
1:A:91:PHE:CD1	1:A:135:TYR:HB2	2.55	0.41
1:B:153:TYR:O	1:B:156:GLN:HB2	2.20	0.41
1:C:283:ARG:NH1	1:C:285:VAL:HG22	2.36	0.41
1:A:45:VAL:CG2	1:B:204:VAL:HG21	2.50	0.41
1:A:112:ASN:HB3	1:A:191:ALA:HB1	2.03	0.41
1:A:185:ARG:HH21	1:A:185:ARG:HG3	1.86	0.41
1:C:82:LYS:HZ3	1:C:105:GLY:HA3	1.84	0.41
1:D:148:ASP:OD1	1:D:151:SER:HB2	2.20	0.41
1:C:106:VAL:HG12	1:C:108:ILE:HG12	2.03	0.41
1:D:176:ARG:HG3	1:D:176:ARG:NH1	2.35	0.41
1:D:193:PRO:HG3	1:E:176:ARG:HD3	2.02	0.41
1:D:202:TYR:HB2	1:E:59:PHE:CD2	2.55	0.41
1:A:215:ARG:NH1	1:A:215:ARG:HG3	2.36	0.41
1:B:38:GLN:OE1	1:B:269:LEU:HD12	2.21	0.41
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.75	0.41
1:C:104:LYS:HE2	1:C:104:LYS:HB3	1.90	0.41
1:C:263:GLU:H	1:C:263:GLU:CD	2.28	0.41
1:D:30:GLU:O	1:D:34:LEU:HD13	2.21	0.41
1:D:115:ARG:HH21	1:D:127:GLU:HA	1.81	0.41
1:E:119:ASP:C	1:E:121:LEU:H	2.29	0.41
1:D:280:ARG:HB3	1:D:280:ARG:CZ	2.50	0.41
2:D:565:UFP:H5'2	1:E:175:ARG:NH2	2.34	0.41
1:A:30:GLU:O	1:A:34:LEU:HG	2.21	0.40
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.56	0.40
1:B:74:LEU:HD12	1:B:224:PRO:HB3	2.03	0.40
1:C:73:LEU:O	1:C:74:LEU:C	2.64	0.40
1:A:75:THR:C	1:A:77:LYS:H	2.29	0.40
1:D:214:GLN:HB3	1:D:252:LEU:CD2	2.44	0.40
1:E:138:GLN:O	1:E:142:PHE:HB2	2.21	0.40
1:C:102:SER:C	1:C:104:LYS:H	2.29	0.40
1:D:263:GLU:N	1:D:264:PRO:HD2	2.37	0.40
1:D:272:GLU:HA	1:D:273:PRO:HD2	1.91	0.40
1:D:286:GLU:N	1:D:286:GLU:CD	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/313 (89%)	262 (94%)	15 (5%)	2 (1%)	18	30
1	B	279/313 (89%)	250 (90%)	25 (9%)	4 (1%)	9	14
1	C	279/313 (89%)	247 (88%)	24 (9%)	8 (3%)	3	5
1	D	278/313 (89%)	234 (84%)	32 (12%)	12 (4%)	2	2
1	E	279/313 (89%)	246 (88%)	29 (10%)	4 (1%)	9	14
All	All	1394/1565 (89%)	1239 (89%)	125 (9%)	30 (2%)	5	9

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	53	THR
1	D	68	ARG
1	B	135	TYR
1	B	222	GLY
1	C	46	ARG
1	C	54	GLY
1	D	173	ASP
1	E	45	VAL
1	C	282	LEU
1	D	80	PHE
1	D	125	THR
1	D	172	PRO
1	D	275	PRO
1	D	283	ARG
1	D	294	GLU
1	B	108	ILE
1	C	43	CYS
1	E	42	ARG
1	E	135	TYR
1	A	80	PHE
1	D	135	TYR

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Mol	Chain	Res	Type
1	A	177	ILE
1	C	74	LEU
1	D	303	PRO
1	B	220	GLY
1	C	72	PRO
1	C	303	PRO
1	D	277	PRO
1	E	72	PRO
1	C	277	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/271 (90%)	239 (98%)	6 (2%)	43	65
1	B	245/271 (90%)	235 (96%)	10 (4%)	27	46
1	C	245/271 (90%)	232 (95%)	13 (5%)	20	35
1	D	244/271 (90%)	225 (92%)	19 (8%)	11	20
1	E	245/271 (90%)	231 (94%)	14 (6%)	18	32
All	All	1224/1355 (90%)	1162 (95%)	62 (5%)	21	36

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MET
1	A	164	VAL
1	A	192	LEU
1	A	229	SER
1	A	288	ILE
1	A	289	ASP
1	B	88	LEU
1	B	101	LEU
1	B	176	ARG
1	B	187	LEU

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Mol	Chain	Res	Type
1	B	198	LEU
1	B	221	LEU
1	B	259	LEU
1	B	260	ASN
1	B	263	GLU
1	B	272	GLU
1	C	56	LEU
1	C	106	VAL
1	C	125	THR
1	C	138	GLN
1	C	145	GLU
1	C	147	ARG
1	C	169	LYS
1	C	192	LEU
1	C	229	SER
1	C	280	ARG
1	C	289	ASP
1	C	294	GLU
1	C	306	THR
1	D	34	LEU
1	D	100	GLU
1	D	148	ASP
1	D	149	MET
1	D	179	MET
1	D	216	SER
1	D	219	MET
1	D	229	SER
1	D	240	ILE
1	D	262	ILE
1	D	263	GLU
1	D	270	GLN
1	D	275	PRO
1	D	285	VAL
1	D	286	GLU
1	D	289	ASP
1	D	294	GLU
1	D	298	ILE
1	D	304	HIS
1	E	48	ASP
1	E	49	ASP
1	E	56	LEU
1	E	69	ASP

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Mol	Chain	Res	Type
1	E	78	ARG
1	E	115	ARG
1	E	150	GLU
1	E	187	LEU
1	E	198	LEU
1	E	244	LYS
1	E	266	LYS
1	E	269	LEU
1	E	286	GLU
1	E	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	62	GLN
1	A	141	HIS
1	A	156	GLN
1	A	196	HIS
1	A	205	ASN
1	A	211	GLN
1	A	250	HIS
1	A	268	GLN
1	A	302	ASN
1	B	62	GLN
1	B	112	ASN
1	B	141	HIS
1	B	211	GLN
1	B	268	GLN
1	B	270	GLN
1	B	302	ASN
1	C	28	HIS
1	C	38	GLN
1	C	112	ASN
1	C	141	HIS
1	C	156	GLN
1	C	200	GLN
1	C	211	GLN
1	C	302	ASN
1	D	39	HIS
1	D	62	GLN
1	D	97	ASN

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Mol	Chain	Res	Type
1	D	171	ASN
1	D	200	GLN
1	D	270	GLN
1	E	32	GLN
1	E	36	GLN
1	E	62	GLN
1	E	112	ASN
1	E	141	HIS
1	E	171	ASN
1	E	200	GLN
1	E	268	GLN
1	E	297	GLN
1	E	302	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	PO4	C	365	-	4,4,4	1.69	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UFP	B	400	-	22,22,22	1.22	2 (9%)	32,33,33	2.64	9 (28%)
2	UFP	D	565	-	22,22,22	1.20	2 (9%)	32,33,33	2.90	10 (31%)
3	EDO	A	401	-	3,3,3	0.53	0	2,2,2	0.15	0
4	PO4	D	616	-	4,4,4	1.67	0	6,6,6	0.47	0
2	UFP	A	400	-	22,22,22	1.16	2 (9%)	32,33,33	2.83	10 (31%)
3	EDO	B	401	-	3,3,3	0.49	0	2,2,2	0.01	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	UFP	B	400	-	-	2/10/22/22	0/2/2/2
2	UFP	D	565	-	-	2/10/22/22	0/2/2/2
3	EDO	A	401	-	-	1/1/1/1	-
2	UFP	A	400	-	-	4/10/22/22	0/2/2/2
3	EDO	B	401	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	UFP	P-O1P	3.30	1.60	1.50
2	A	400	UFP	P-O1P	2.89	1.59	1.50
2	D	565	UFP	C6-C5	2.82	1.37	1.33
2	B	400	UFP	C6-C5	2.72	1.37	1.33
2	A	400	UFP	C6-C5	2.72	1.37	1.33
2	D	565	UFP	P-O1P	2.57	1.58	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	UFP	C5-C4-N3	7.93	119.89	112.64
2	D	565	UFP	O4-C4-C5	-7.90	118.96	125.69
2	A	400	UFP	C5-C4-N3	7.53	119.53	112.64
2	D	565	UFP	C5-C4-N3	7.32	119.33	112.64
2	A	400	UFP	O4-C4-C5	-7.24	119.53	125.69
2	B	400	UFP	O4-C4-C5	-6.58	120.09	125.69
2	D	565	UFP	F5-C5-C4	5.17	121.00	116.47
2	D	565	UFP	C6-C5-C4	-5.13	117.89	122.57
2	A	400	UFP	F5-C5-C4	4.99	120.84	116.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	UFP	F5-C5-C4	4.84	120.71	116.47
2	B	400	UFP	C4-N3-C2	-4.79	121.06	127.34
2	A	400	UFP	C6-C5-C4	-4.63	118.34	122.57
2	A	400	UFP	C4-N3-C2	-4.62	121.29	127.34
2	D	565	UFP	C4-N3-C2	-4.42	121.54	127.34
2	B	400	UFP	C6-C5-C4	-4.37	118.58	122.57
2	A	400	UFP	C4'-O4'-C1'	-4.29	99.32	109.51
2	D	565	UFP	C4'-O4'-C1'	-4.21	99.52	109.51
2	D	565	UFP	N3-C2-N1	4.02	120.13	114.89
2	A	400	UFP	N3-C2-N1	3.89	119.96	114.89
2	D	565	UFP	O4'-C1'-N1	3.88	114.76	107.86
2	B	400	UFP	N3-C2-N1	3.53	119.49	114.89
2	A	400	UFP	O4'-C1'-N1	3.48	114.04	107.86
2	B	400	UFP	C4'-O4'-C1'	-3.43	101.35	109.51
2	A	400	UFP	C1'-N1-C2	2.78	123.10	117.66
2	D	565	UFP	C1'-N1-C2	2.67	122.88	117.66
2	B	400	UFP	O4'-C1'-N1	2.55	112.39	107.86
2	D	565	UFP	C1'-N1-C6	-2.35	116.79	120.74
2	A	400	UFP	C1'-N1-C6	-2.28	116.91	120.74
2	B	400	UFP	C1'-N1-C2	2.16	121.88	117.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	UFP	O4'-C1'-N1-C6
2	B	400	UFP	O4'-C1'-N1-C2
2	D	565	UFP	O4'-C1'-N1-C2
2	D	565	UFP	O4'-C1'-N1-C6
3	A	401	EDO	O1-C1-C2-O2
3	B	401	EDO	O1-C1-C2-O2
2	A	400	UFP	O4'-C1'-N1-C6
2	A	400	UFP	C2'-C1'-N1-C2
2	A	400	UFP	O4'-C1'-N1-C2
2	A	400	UFP	C2'-C1'-N1-C6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

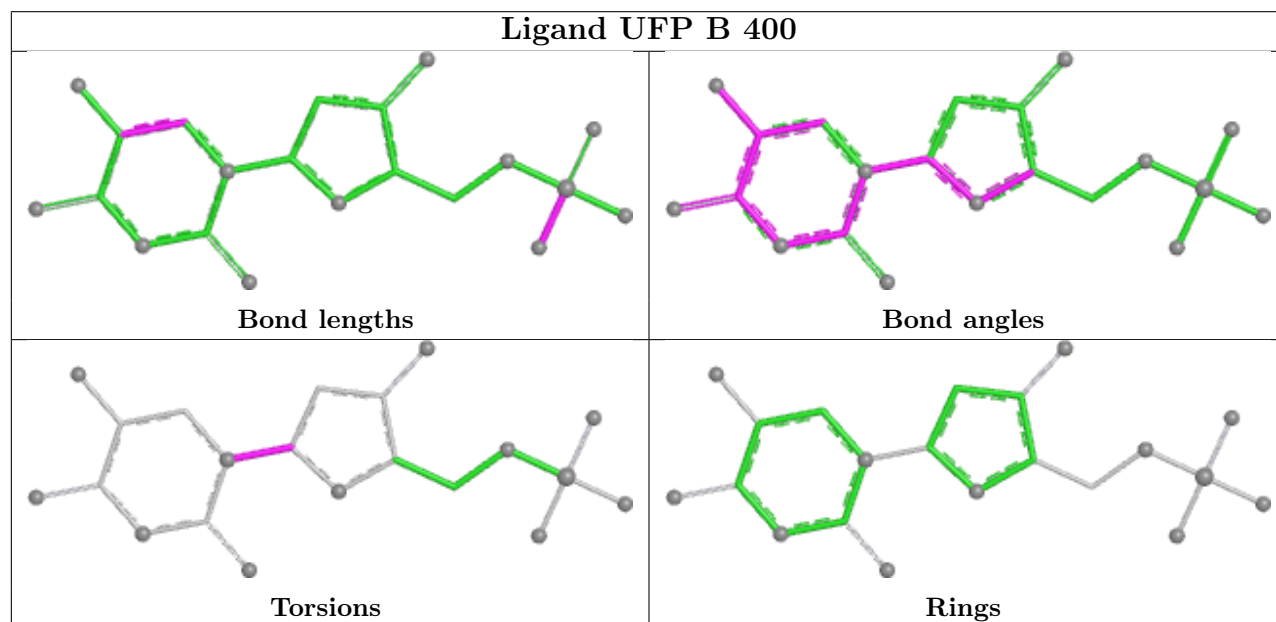
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	565	UFP	2	0

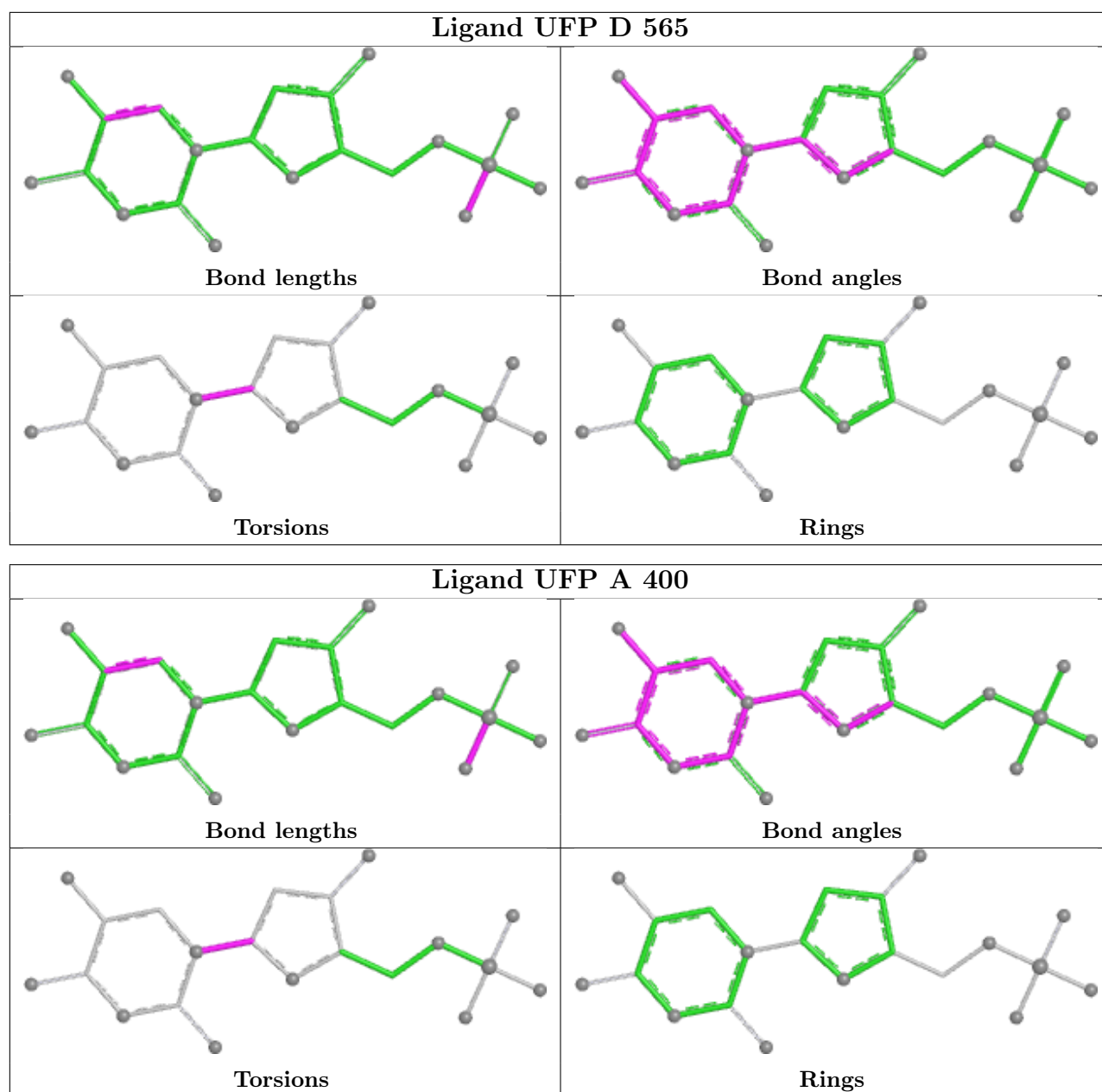
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	UFP	1	0

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	281/313 (89%)	0.10	6 (2%) 63 57	28, 47, 71, 83	0
1	B	281/313 (89%)	0.46	11 (3%) 43 35	27, 58, 93, 105	0
1	C	281/313 (89%)	0.30	12 (4%) 40 32	30, 54, 84, 106	0
1	D	280/313 (89%)	1.30	63 (22%) 2 1	36, 80, 109, 128	0
1	E	281/313 (89%)	0.65	17 (6%) 27 21	30, 64, 107, 129	0
All	All	1404/1565 (89%)	0.56	109 (7%) 19 14	27, 58, 101, 129	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	297	GLN	4.7
1	E	255	ALA	4.4
1	B	191	ALA	3.8
1	B	150	GLU	3.8
1	D	154	SER	3.8
1	D	114	SER	3.6
1	D	206	SER	3.5
1	E	26	PRO	3.5
1	D	152	ASP	3.4
1	D	139	TRP	3.4
1	D	192	LEU	3.3
1	D	105	GLY	3.3
1	D	153	TYR	3.2
1	E	306	THR	3.1
1	D	288	ILE	3.1
1	D	137	PHE	3.1
1	E	262	ILE	3.1
1	D	296	PHE	3.1
1	D	191	ALA	3.0
1	D	293	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	45	VAL	3.0
1	A	26	PRO	2.9
1	C	173	ASP	2.9
1	C	44	GLY	2.9
1	D	238	ALA	2.9
1	D	174	ASP	2.9
1	D	119	ASP	2.9
1	D	306	THR	2.9
1	D	298	ILE	2.8
1	E	56	LEU	2.8
1	E	58	VAL	2.8
1	D	168	ILE	2.8
1	E	47	LYS	2.8
1	D	128	GLU	2.8
1	D	164	VAL	2.8
1	D	77	LYS	2.7
1	D	72	PRO	2.7
1	A	192	LEU	2.7
1	D	121	LEU	2.7
1	E	187	LEU	2.7
1	D	81	TRP	2.7
1	D	118	LEU	2.7
1	B	123	PHE	2.6
1	B	306	THR	2.6
1	C	127	GLU	2.6
1	D	143	GLY	2.6
1	D	155	GLY	2.6
1	E	192	LEU	2.5
1	D	276	PHE	2.5
1	D	69	ASP	2.5
1	D	100	GLU	2.5
1	D	127	GLU	2.5
1	D	73	LEU	2.5
1	E	50	ARG	2.5
1	D	117	PHE	2.5
1	D	291	PHE	2.5
1	B	127	GLU	2.4
1	C	192	LEU	2.4
1	D	272	GLU	2.4
1	D	148	ASP	2.4
1	C	306	THR	2.4
1	D	290	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	278	LYS	2.4
1	A	191	ALA	2.4
1	E	257	ILE	2.3
1	B	125	THR	2.3
1	C	26	PRO	2.3
1	C	191	ALA	2.3
1	D	179	MET	2.3
1	D	151	SER	2.3
1	A	221	LEU	2.3
1	D	89	LEU	2.3
1	E	41	LEU	2.3
1	E	221	LEU	2.3
1	D	92	ILE	2.2
1	D	97	ASN	2.2
1	D	231	ALA	2.2
1	D	230	TYR	2.2
1	D	197	ALA	2.2
1	B	147	ARG	2.2
1	D	112	ASN	2.2
1	D	277	PRO	2.2
1	D	243	LEU	2.2
1	D	279	LEU	2.2
1	B	192	LEU	2.1
1	D	113	GLY	2.1
1	D	204	VAL	2.1
1	D	86	GLU	2.1
1	D	287	LYS	2.1
1	A	282	LEU	2.1
1	C	52	GLY	2.1
1	E	46	ARG	2.1
1	D	300	GLY	2.1
1	D	116	ASP	2.1
1	B	286	GLU	2.1
1	D	299	GLU	2.1
1	E	273	PRO	2.1
1	C	74	LEU	2.1
1	B	105	GLY	2.1
1	D	281	ILE	2.1
1	C	50	ARG	2.0
1	E	100	GLU	2.0
1	C	53	THR	2.0
1	B	121	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	269	LEU	2.0
1	A	298	ILE	2.0
1	D	280	ARG	2.0
1	D	95	SER	2.0
1	D	203	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

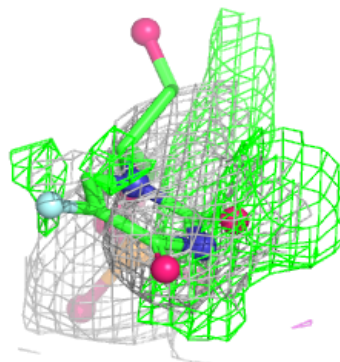
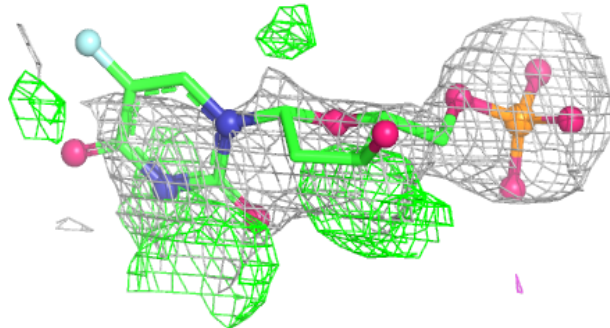
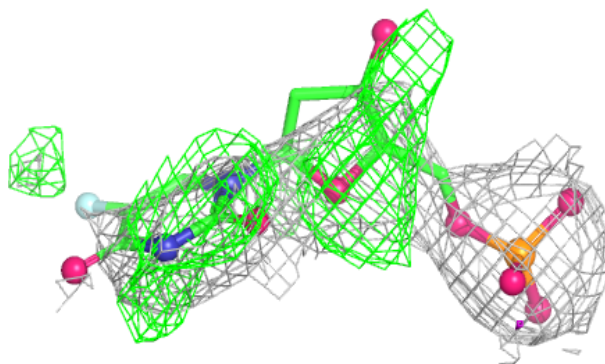
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	401	4/4	0.81	0.20	73,78,80,83	0
2	UFP	B	400	21/21	0.86	0.31	71,86,88,89	17
3	EDO	A	401	4/4	0.87	0.18	76,80,80,81	0
2	UFP	D	565	21/21	0.88	0.23	55,90,99,102	17
4	PO4	D	616	5/5	0.89	0.10	97,97,98,99	0
4	PO4	C	365	5/5	0.90	0.17	99,100,101,102	0
2	UFP	A	400	21/21	0.90	0.18	52,90,106,111	0

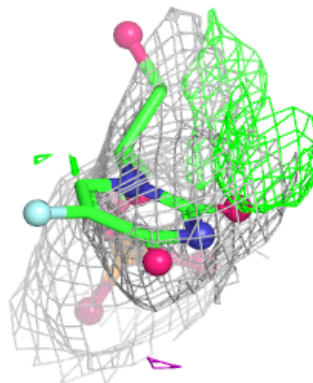
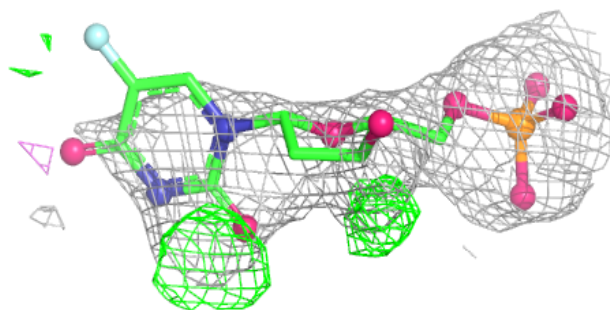
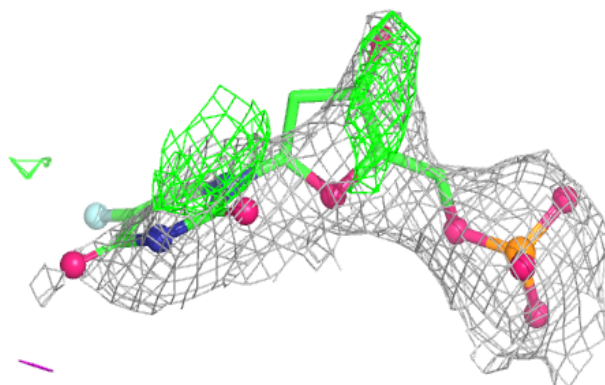
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

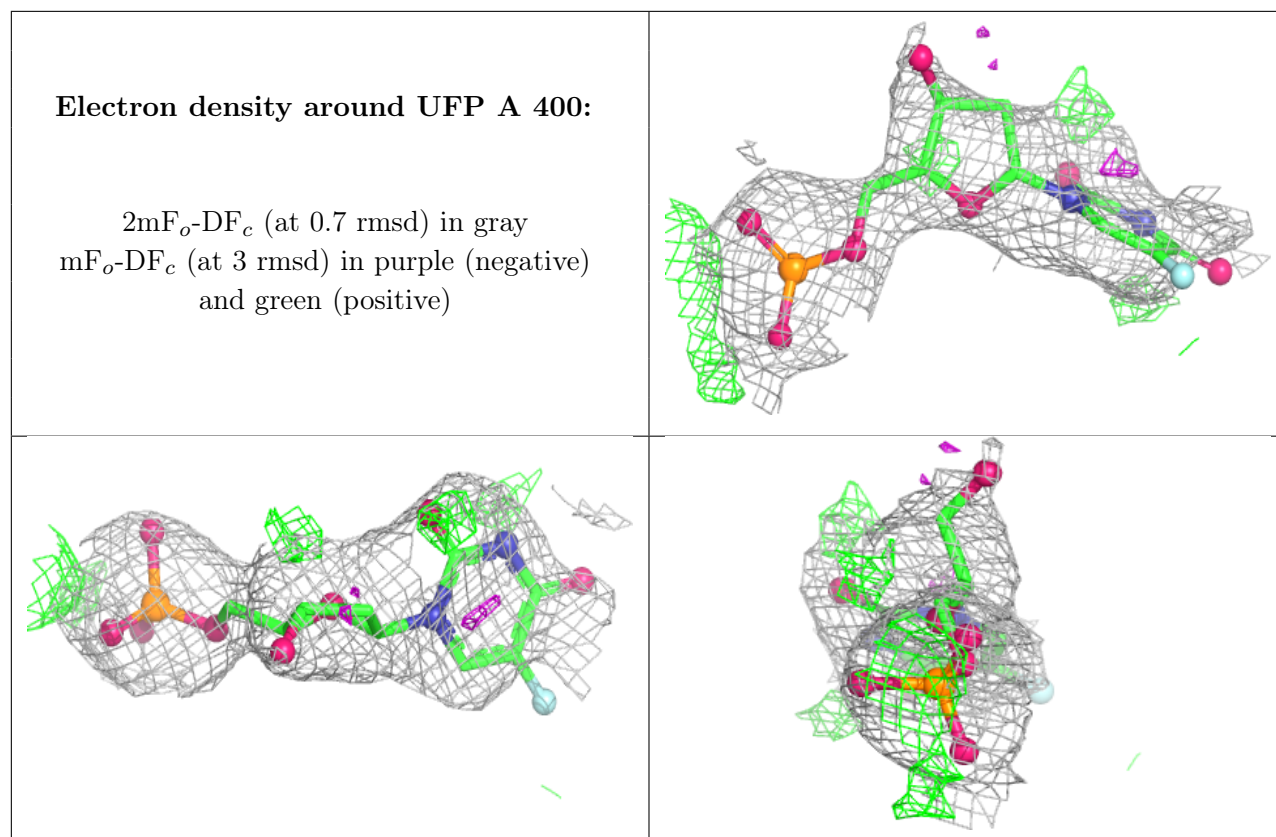
Electron density around UFP B 400:

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

**Electron density around UFP D 565:**

$2mF_o-DF_c$ (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.