



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:14 PM GMT

PDB ID : 4KY8  
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, methotrexate, FdUMP and 4-((2-amino-6-methyl-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl)thio)-2-chlorophenyl)-L-glutamic acid  
Authors : Kumar, V.P.; Anderson, K.S.  
Deposited on : 2013-05-28  
Resolution : 3.08 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

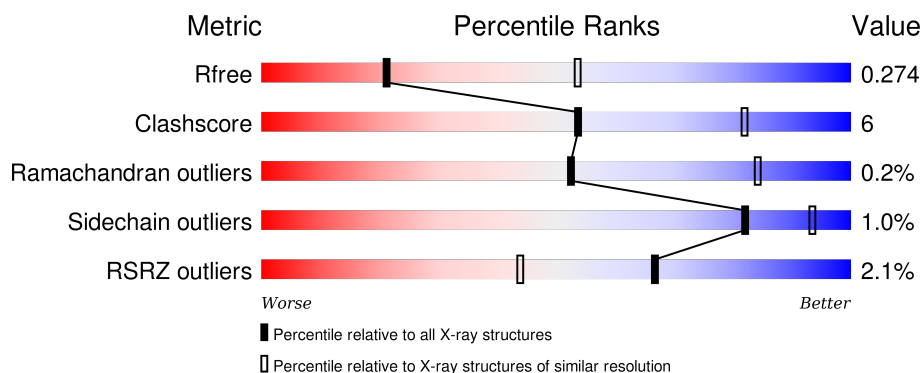
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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))
$R_{free}$	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	521	<div> <div>2%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	B	521	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	C	521	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	D	521	<div> <div>%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	E	521	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	1UF	B	604	-	-	-	X

## 2 Entry composition [i](#)

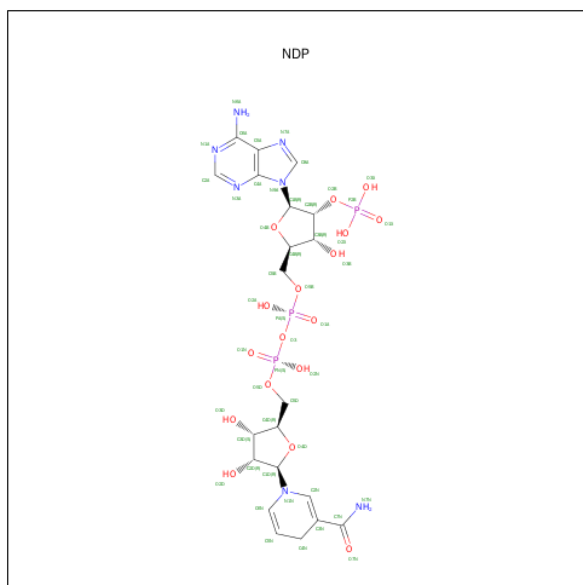
There are 5 unique types of molecules in this entry. The entry contains 21240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional thymidylate synthase-dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	B	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	C	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	D	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			
1	E	505	Total	C	N	O	S	0	0	0
			4114	2630	691	771	22			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



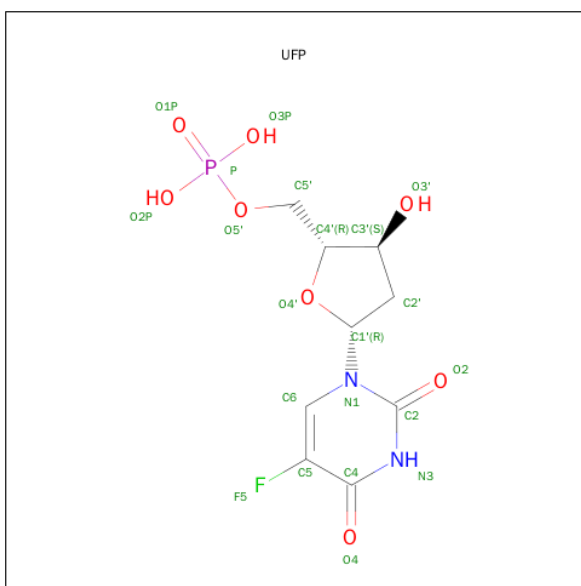
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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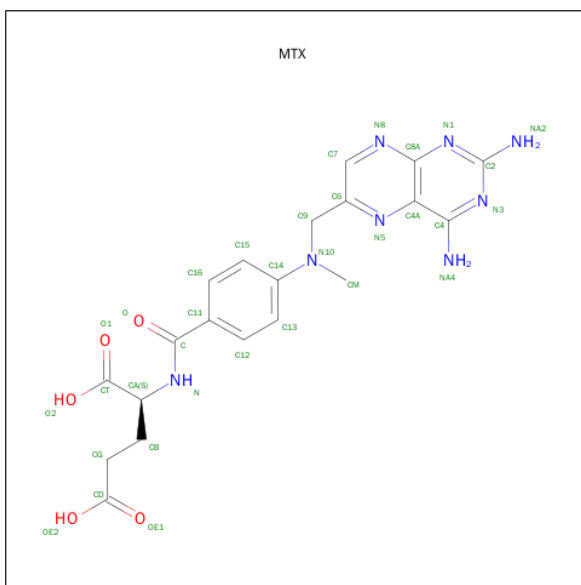
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: C<sub>9</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>8</sub>P).



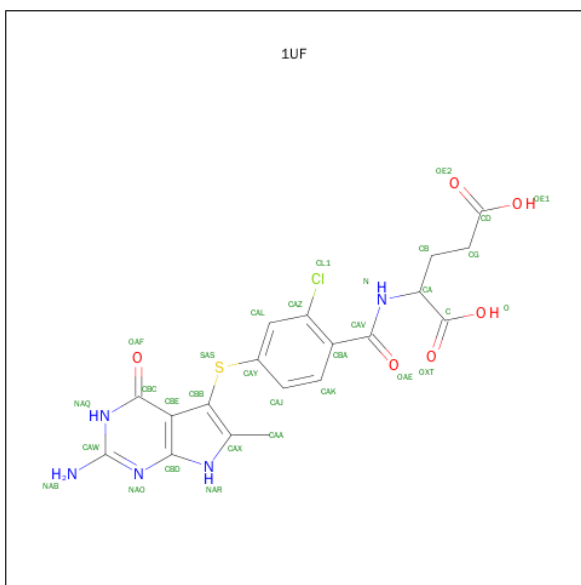
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 33	C 20	N 8	O 5	0	0
4	B	1	Total 33	C 20	N 8	O 5	0	0
4	C	1	Total 33	C 20	N 8	O 5	0	0
4	D	1	Total 33	C 20	N 8	O 5	0	0
4	E	1	Total 33	C 20	N 8	O 5	0	0

- Molecule 5 is N-{4-[(2-AMINO-6-METHYL-4-OXO-4,7-DIHYDRO-3H-PYRROLO[2,3-D]PYRIMIDIN-5-YL)SULFANYL]-2-CHLOROBENZOYL}-L-GLUTAMIC ACID (three-letter code: 1UF) (formula:  $C_{19}H_{18}ClN_5O_6S$ ).

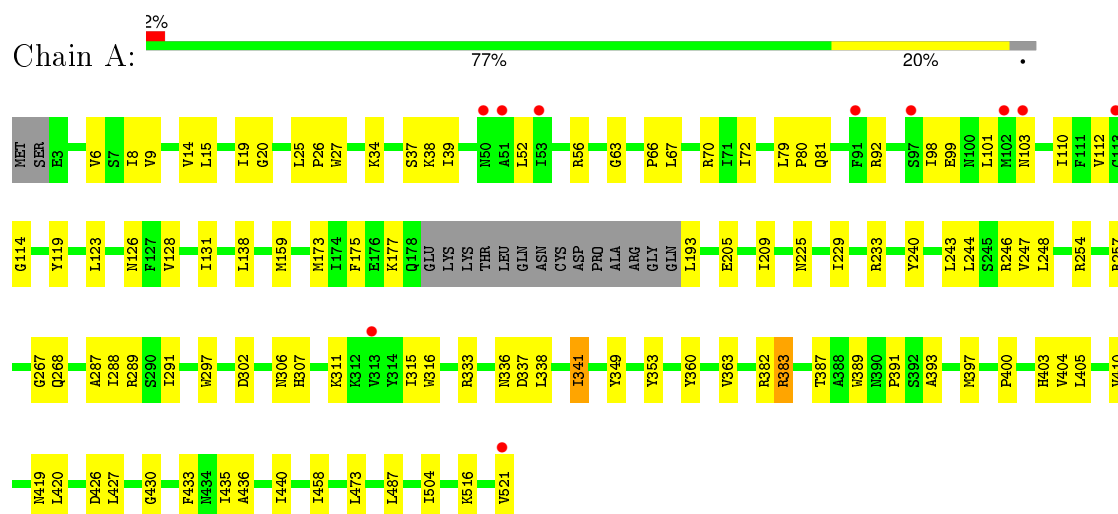


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	B	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	C	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	D	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0
5	E	1	Total 32	C 19	Cl 1	N 5	O 6	S 1	0	0

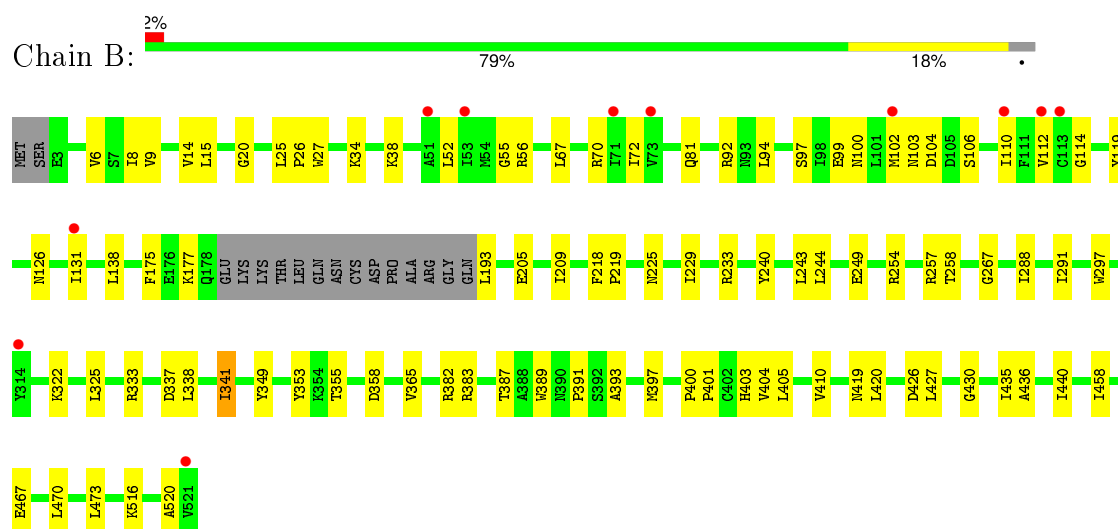
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

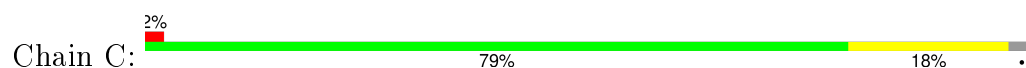
- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



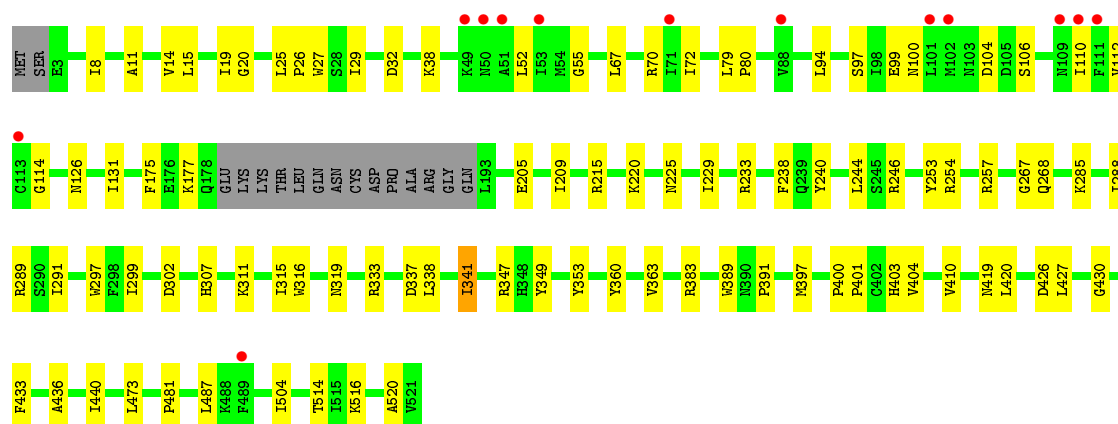
- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



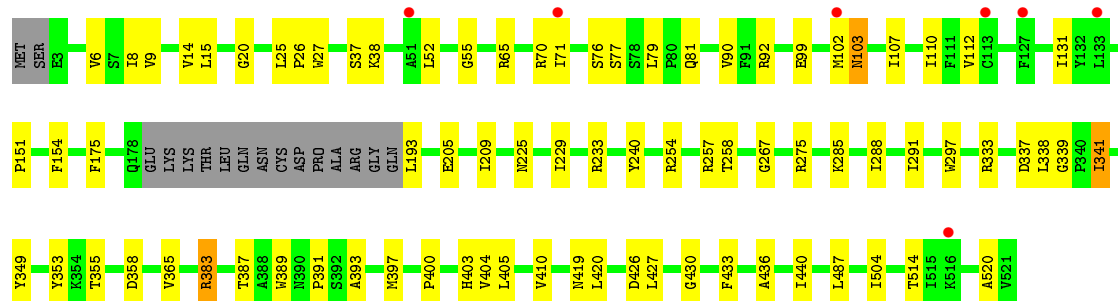
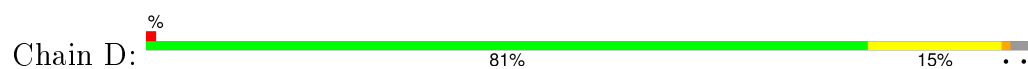
- Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



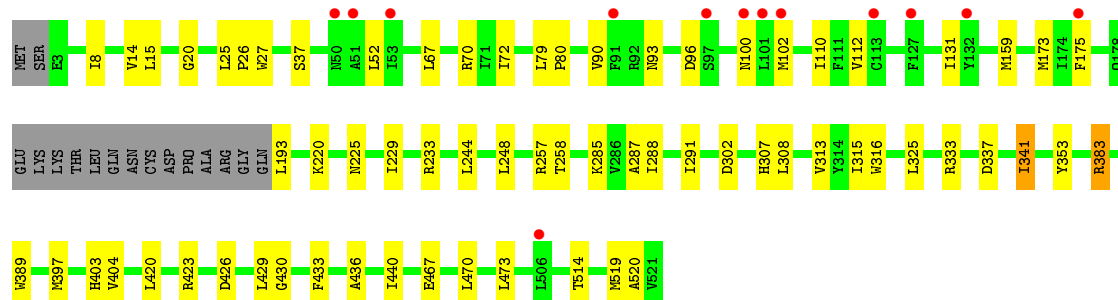
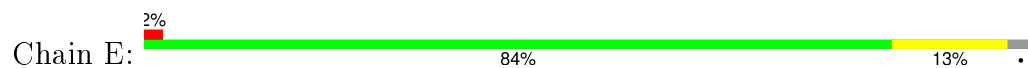




• Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



• Molecule 1: Bifunctional thymidylate synthase-dihydrofolate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.16Å 115.67Å 218.77Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	48.12 – 3.08 49.13 – 3.08	Depositor EDS
% Data completeness (in resolution range)	71.2 (48.12-3.08) 71.3 (49.13-3.08)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.232 , 0.266 0.249 , 0.274	Depositor DCC
$R_{free}$ test set	1961 reflections (2.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.1	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 21.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 70100 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	21240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UFP, NDP, MTX, 1UF

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	0.21	0/4209	0.37	0/5688
1	B	0.21	0/4209	0.37	0/5688
1	C	0.21	0/4209	0.37	0/5688
1	D	0.21	0/4209	0.37	0/5688
1	E	0.21	0/4209	0.37	0/5688
All	All	0.21	0/21045	0.37	0/28440

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	4114	0	4049	73	0
1	B	4114	0	4049	63	0
1	C	4114	0	4049	60	0
1	D	4114	0	4049	55	0
1	E	4114	0	4049	40	1
2	A	48	0	26	4	0
2	B	48	0	26	4	0
2	C	48	0	26	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	26	4	0
2	E	48	0	26	1	0
3	A	21	0	10	2	0
3	B	21	0	10	3	0
3	C	21	0	10	2	0
3	D	21	0	10	1	0
3	E	21	0	10	2	1
4	A	33	0	20	5	0
4	B	33	0	20	3	0
4	C	33	0	20	2	0
4	D	33	0	20	3	0
4	E	33	0	20	2	0
5	A	32	0	16	4	0
5	B	32	0	16	0	0
5	C	32	0	16	3	0
5	D	32	0	16	1	0
5	E	32	0	16	6	0
All	All	21240	0	20605	270	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 6.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:NH1	3:B:602:UFP:O3P	2.05	0.89
3:C:602:UFP:O3P	1:D:383:ARG:NH1	2.21	0.73
1:C:244:LEU:HD11	1:C:473:LEU:HD13	1.72	0.71
1:E:257:ARG:NE	3:E:602:UFP:O2P	2.19	0.71
1:C:383:ARG:HE	1:D:400:PRO:HG2	1.54	0.71
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.72	0.69
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.75	0.68
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.75	0.68
1:B:8:ILE:HG12	1:B:112:VAL:HB	1.76	0.68
1:E:25:LEU:HD11	4:E:603:MTX:H7	1.76	0.68
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.77	0.67
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.76	0.67
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.75	0.67
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.77	0.67
1:E:37:SER:HB2	4:E:603:MTX:HB1	1.75	0.67
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PRO:HG2	1:B:383:ARG:HE	1.60	0.66
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.78	0.66
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.78	0.65
1:A:244:LEU:HD11	1:A:473:LEU:HD13	1.78	0.65
1:C:410:VAL:O	1:D:254:ARG:NH2	2.25	0.64
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.80	0.64
1:A:289:ARG:NH2	1:A:311:LYS:O	2.31	0.64
1:C:257:ARG:NE	3:C:602:UFP:O2P	2.26	0.64
1:B:244:LEU:HD11	1:B:473:LEU:HD13	1.77	0.64
1:A:349:TYR:HH	1:B:349:TYR:HH	1.42	0.64
1:C:349:TYR:HH	1:D:349:TYR:HH	1.44	0.64
1:D:79:LEU:HD22	1:D:90:VAL:HG21	1.80	0.64
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.80	0.63
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.81	0.63
1:C:289:ARG:NH2	1:C:311:LYS:O	2.32	0.63
1:D:257:ARG:NE	3:D:602:UFP:O2P	2.29	0.62
1:E:244:LEU:HD11	1:E:473:LEU:HD13	1.81	0.62
1:A:225:ASN:O	1:A:233:ARG:NH2	2.33	0.62
1:C:285:LYS:HB3	1:C:514:THR:HG22	1.83	0.61
1:A:99:GLU:HB3	1:A:103:ASN:HD21	1.63	0.61
1:A:229:ILE:HG22	1:A:233:ARG:HG2	1.80	0.61
1:B:229:ILE:HG22	1:B:233:ARG:HG2	1.82	0.61
1:D:285:LYS:HB3	1:D:514:THR:HG22	1.82	0.61
1:B:258:THR:HG21	1:B:520:ALA:HB1	1.83	0.60
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.83	0.60
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.82	0.60
1:A:419:ASN:HD21	1:B:267:GLY:HA2	1.67	0.59
1:D:225:ASN:O	1:D:233:ARG:NH2	2.35	0.59
1:E:229:ILE:HG22	1:E:233:ARG:HG2	1.83	0.59
1:B:225:ASN:O	1:B:233:ARG:NH2	2.35	0.59
1:E:225:ASN:O	1:E:233:ARG:NH2	2.35	0.59
1:C:520:ALA:O	5:C:604:1UF:NAB	2.36	0.59
1:E:288:ILE:HD11	1:E:440:ILE:HD11	1.83	0.59
1:C:229:ILE:HG22	1:C:233:ARG:HG2	1.84	0.58
1:C:225:ASN:O	1:C:233:ARG:NH2	2.37	0.58
1:D:25:LEU:HD11	4:D:603:MTX:H7	1.86	0.58
1:B:349:TYR:HB3	1:B:365:VAL:HB	1.85	0.58
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.85	0.57
1:C:246:ARG:NH1	1:C:268:GLN:OE1	2.36	0.57
1:E:258:THR:HG21	1:E:520:ALA:HB1	1.87	0.57
1:C:419:ASN:HD21	1:D:267:GLY:HA2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:GLN:OE1	1:D:92:ARG:NH2	2.37	0.57
1:C:267:GLY:HA2	1:D:419:ASN:HD21	1.69	0.57
1:E:285:LYS:HB3	1:E:514:THR:HG22	1.86	0.56
1:D:229:ILE:HG22	1:D:233:ARG:HG2	1.86	0.56
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.37	0.56
1:E:79:LEU:HD22	1:E:90:VAL:HG21	1.88	0.56
1:B:322:LYS:NZ	1:B:333:ARG:O	2.38	0.55
1:C:205:GLU:OE1	1:D:38:LYS:NZ	2.32	0.54
1:D:349:TYR:HB3	1:D:365:VAL:HB	1.89	0.54
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.89	0.54
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.89	0.54
1:B:288:ILE:HD11	1:B:440:ILE:HD11	1.89	0.54
1:A:37:SER:HB2	4:A:603:MTX:HB1	1.88	0.54
1:A:81:GLN:OE1	1:A:92:ARG:NH2	2.40	0.54
1:A:123:LEU:HD23	1:A:128:VAL:HG11	1.90	0.53
1:C:25:LEU:HD11	4:C:603:MTX:H7	1.90	0.53
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.89	0.53
1:B:325:LEU:HD23	1:B:333:ARG:HB3	1.89	0.53
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.89	0.53
1:B:6:VAL:HG22	1:B:110:ILE:HB	1.91	0.53
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.90	0.53
1:D:99:GLU:O	1:D:103:ASN:ND2	2.41	0.53
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.90	0.53
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.44	0.53
1:A:240:TYR:OH	1:A:427:LEU:O	2.25	0.53
1:C:38:LYS:NZ	1:D:205:GLU:OE1	2.32	0.52
1:D:426:ASP:HB3	1:D:430:GLY:H	1.74	0.52
1:B:99:GLU:HB2	1:B:103:ASN:HD21	1.75	0.52
1:A:25:LEU:HD11	4:A:603:MTX:H7	1.90	0.52
1:C:240:TYR:OH	1:C:427:LEU:O	2.24	0.52
1:E:429:LEU:HD13	5:E:604:1UF:CL1	2.47	0.52
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.92	0.52
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.91	0.51
1:C:254:ARG:NH2	1:D:410:VAL:O	2.28	0.51
1:B:114:GLY:HA3	2:B:601:NDP:H5N	1.92	0.51
1:C:104:ASP:OD1	1:C:106:SER:OG	2.24	0.51
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.43	0.51
1:A:6:VAL:HG22	1:A:110:ILE:HB	1.93	0.51
1:B:467:GLU:HA	1:B:470:LEU:HD23	1.91	0.51
1:B:81:GLN:OE1	1:B:92:ARG:NH2	2.42	0.50
1:E:433:PHE:CZ	5:E:604:1UF:H10	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASP:OD1	1:B:106:SER:OG	2.21	0.50
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.92	0.50
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.47	0.50
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.47	0.50
1:D:341:ILE:HG22	1:D:397:MET:HE3	1.94	0.49
1:A:246:ARG:NH1	1:A:268:GLN:OE1	2.37	0.49
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.93	0.49
1:B:55:GLY:HA3	2:B:601:NDP:H52A	1.93	0.49
1:D:355:THR:OG1	1:D:358:ASP:OD2	2.24	0.49
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.44	0.49
5:E:604:1UF:H2	5:E:604:1UF:CAV	2.43	0.49
1:D:76:SER:HA	2:D:601:NDP:H1B	1.95	0.49
1:A:433:PHE:CE1	5:A:604:1UF:H10	2.47	0.49
1:D:71:ILE:HD12	1:D:107:ILE:HD11	1.92	0.49
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.46	0.49
1:B:25:LEU:HD11	4:B:603:MTX:H7	1.94	0.49
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.94	0.49
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.95	0.48
1:E:467:GLU:HA	1:E:470:LEU:HD23	1.95	0.48
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.94	0.48
1:E:341:ILE:HG22	1:E:397:MET:HE3	1.94	0.48
1:A:114:GLY:HA3	2:A:601:NDP:H5N	1.94	0.48
1:A:267:GLY:HA2	1:B:419:ASN:HD21	1.78	0.48
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.48	0.48
1:A:254:ARG:NH2	1:B:410:VAL:O	2.27	0.48
1:C:11:ALA:O	2:C:601:NDP:N7N	2.46	0.48
1:C:114:GLY:HA3	2:C:601:NDP:H5N	1.96	0.48
1:A:287:ALA:HB3	5:A:604:1UF:H3	1.96	0.48
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.96	0.48
1:B:240:TYR:OH	1:B:427:LEU:O	2.28	0.47
1:E:433:PHE:CE2	5:E:604:1UF:H10	2.48	0.47
1:C:319:ASN:OD1	5:C:604:1UF:NAR	2.45	0.47
1:D:37:SER:HB2	4:D:603:MTX:HB1	1.97	0.47
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.80	0.47
1:A:341:ILE:HA	1:A:397:MET:HE3	1.96	0.47
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.96	0.47
1:C:383:ARG:HH22	1:D:257:ARG:HD3	1.80	0.47
2:A:601:NDP:H42N	4:A:603:MTX:C6	2.44	0.47
1:C:19:ILE:O	2:C:601:NDP:H2N	2.15	0.47
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.97	0.47
1:D:258:THR:HG21	1:D:520:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:HD3	1:B:383:ARG:HH22	1.80	0.46
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.97	0.46
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.80	0.46
1:E:423:ARG:NH2	3:E:602:UFP:O3P	2.49	0.46
2:B:601:NDP:H8A	2:B:601:NDP:H51A	1.97	0.46
1:E:519:MET:HB2	5:E:604:1UF:CL1	2.52	0.46
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.97	0.46
1:D:77:SER:HB3	2:D:601:NDP:H2A	1.97	0.46
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.98	0.46
1:C:299:ILE:O	1:C:347:ARG:NH1	2.45	0.46
1:C:55:GLY:HA3	2:C:601:NDP:H52A	1.97	0.46
1:B:100:ASN:HB2	1:B:110:ILE:HD11	1.98	0.46
1:A:410:VAL:O	1:B:254:ARG:NH2	2.29	0.46
1:D:387:THR:HB	1:D:405:LEU:HD12	1.98	0.45
3:A:602:UFP:O1P	1:B:382:ARG:NE	2.50	0.45
1:C:433:PHE:CZ	5:C:604:1UF:H10	2.51	0.45
1:C:383:ARG:NE	1:D:400:PRO:HG2	2.27	0.45
5:A:604:1UF:H2	5:A:604:1UF:CAV	2.46	0.45
1:C:426:ASP:HB3	1:C:430:GLY:H	1.82	0.45
1:E:93:ASN:ND2	1:E:96:ASP:H	2.14	0.45
1:B:341:ILE:HG22	1:B:397:MET:HE3	1.99	0.45
1:A:257:ARG:NE	3:A:602:UFP:O2P	2.44	0.45
1:E:426:ASP:HB3	1:E:430:GLY:H	1.82	0.44
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.98	0.44
1:C:126:ASN:OD1	1:C:177:LYS:NZ	2.50	0.44
1:E:308:LEU:HG	1:E:313:VAL:HB	1.99	0.44
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.98	0.44
1:E:100:ASN:HB2	1:E:110:ILE:HD11	1.99	0.44
1:E:20:GLY:HA2	1:E:26:PRO:HD3	2.00	0.44
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.98	0.44
1:C:100:ASN:HB2	1:C:110:ILE:HD11	1.99	0.44
2:D:601:NDP:H6N	2:D:601:NDP:H52N	2.00	0.44
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.99	0.44
1:C:67:LEU:HG	1:C:72:ILE:HD11	2.00	0.44
1:D:240:TYR:OH	1:D:427:LEU:O	2.29	0.44
1:A:79:LEU:HA	1:A:80:PRO:HD3	1.86	0.44
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.98	0.44
1:B:243:LEU:HG	1:B:427:LEU:HD21	2.00	0.44
1:B:14:VAL:HG13	1:B:15:LEU:HG	2.00	0.44
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.89	0.44
1:A:244:LEU:O	1:A:248:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ALA:O	1:B:397:MET:HG3	2.18	0.44
1:C:341:ILE:HA	1:C:397:MET:HE3	2.00	0.44
2:E:601:NDP:H6N	2:E:601:NDP:H52N	1.98	0.44
1:D:487:LEU:HD11	1:D:504:ILE:HG23	2.00	0.44
1:A:114:GLY:HA2	1:A:119:TYR:CZ	2.53	0.43
1:A:159:MET:HA	1:A:173:MET:HG2	2.00	0.43
1:B:9:VAL:O	4:B:603:MTX:NA4	2.51	0.43
1:E:287:ALA:HB3	5:E:604:1UF:H3	1.99	0.43
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.83	0.43
1:A:487:LEU:HD11	1:A:504:ILE:HG23	2.00	0.43
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.90	0.43
1:D:337:ASP:OD1	1:D:353:TYR:OH	2.24	0.43
1:A:9:VAL:HG12	4:A:603:MTX:N3	2.33	0.43
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.48	0.43
1:C:94:LEU:O	1:C:97:SER:OG	2.30	0.43
1:A:387:THR:HB	1:A:405:LEU:HD12	2.00	0.43
1:A:205:GLU:OE1	1:B:38:LYS:NZ	2.29	0.43
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.99	0.43
1:B:9:VAL:HG12	4:B:603:MTX:N3	2.34	0.43
1:A:243:LEU:O	1:A:247:VAL:HG12	2.19	0.43
1:A:56:ARG:NH1	2:A:601:NDP:O1X	2.52	0.43
1:B:67:LEU:HG	1:B:72:ILE:HD11	2.00	0.43
1:B:291:ILE:HD13	1:B:436:ALA:HB3	2.01	0.42
1:A:38:LYS:NZ	1:B:205:GLU:OE1	2.32	0.42
1:B:94:LEU:O	1:B:97:SER:OG	2.30	0.42
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.55	0.42
1:D:6:VAL:HG22	1:D:110:ILE:HB	2.01	0.42
1:B:337:ASP:OD1	1:B:353:TYR:OH	2.31	0.42
1:E:79:LEU:HA	1:E:80:PRO:HD3	1.92	0.42
1:D:14:VAL:HG13	1:D:15:LEU:HG	2.01	0.42
1:A:435:ILE:HG12	1:A:458:ILE:HD12	2.00	0.42
1:B:20:GLY:HA2	1:B:26:PRO:HD3	2.00	0.42
1:A:393:ALA:O	1:A:397:MET:HG3	2.19	0.42
1:A:34:LYS:O	1:A:38:LYS:HG3	2.20	0.42
1:B:249:GLU:O	1:D:65:ARG:NH2	2.53	0.42
1:A:400:PRO:HG2	1:B:383:ARG:NE	2.29	0.42
1:B:218:PHE:CD1	1:B:219:PRO:HD2	2.55	0.42
1:C:215:ARG:NH1	1:D:275:ARG:HD2	2.34	0.42
1:A:433:PHE:CZ	5:A:604:1UF:H10	2.54	0.42
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.85	0.42
1:A:19:ILE:O	2:A:601:NDP:H2N	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:THR:OG1	1:B:358:ASP:OD2	2.27	0.42
1:E:159:MET:HA	1:E:173:MET:HG2	2.01	0.42
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.55	0.41
1:A:9:VAL:O	4:A:603:MTX:NA4	2.53	0.41
1:B:426:ASP:HB3	1:B:430:GLY:H	1.84	0.41
1:C:131:ILE:HB	1:C:175:PHE:HB2	2.01	0.41
1:C:337:ASP:OD1	1:C:353:TYR:OH	2.26	0.41
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.55	0.41
1:E:67:LEU:HG	1:E:72:ILE:HD11	2.03	0.41
1:E:337:ASP:OD1	1:E:353:TYR:OH	2.26	0.41
1:D:55:GLY:HA3	2:D:601:NDP:H52A	2.03	0.41
1:C:360:TYR:O	1:C:363:VAL:HG22	2.21	0.41
1:D:393:ALA:O	1:D:397:MET:HG3	2.21	0.41
1:A:426:ASP:HB3	1:A:430:GLY:H	1.86	0.41
1:A:337:ASP:OD1	1:A:353:TYR:OH	2.23	0.41
1:B:34:LYS:O	1:B:38:LYS:HG3	2.20	0.41
1:D:433:PHE:CZ	5:D:604:1UF:H10	2.56	0.41
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.55	0.41
1:C:487:LEU:HD11	1:C:504:ILE:HG23	2.03	0.41
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.49	0.41
1:A:349:TYR:OH	1:B:349:TYR:OH	2.31	0.41
1:A:66:PRO:HA	1:A:72:ILE:HD12	2.03	0.41
1:A:341:ILE:HG22	1:A:397:MET:HE3	2.03	0.41
1:A:98:ILE:HG22	1:A:101:LEU:HG	2.03	0.41
1:B:387:THR:HB	1:B:405:LEU:HD12	2.02	0.41
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.56	0.41
1:C:238:PHE:CE1	1:C:481:PRO:HG2	2.56	0.41
1:A:257:ARG:NH2	1:A:521:VAL:OXT	2.43	0.41
1:E:244:LEU:O	1:E:248:LEU:HB2	2.20	0.41
2:C:601:NDP:H42N	4:C:603:MTX:C6	2.51	0.41
1:D:9:VAL:HG12	4:D:603:MTX:N3	2.35	0.40
1:E:325:LEU:HD12	1:E:325:LEU:HA	1.90	0.40
1:A:360:TYR:O	1:A:363:VAL:HG22	2.21	0.40
1:B:435:ILE:HG12	1:B:458:ILE:HD12	2.04	0.40
1:C:29:ILE:HG22	1:C:32:ASP:H	1.85	0.40
1:C:400:PRO:HA	1:C:401:PRO:HD3	1.91	0.40
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.56	0.40
1:B:56:ARG:H	2:B:601:NDP:C4B	2.34	0.40
1:A:63:GLY:HA2	1:C:253:TYR:HB3	2.03	0.40
1:E:403:HIS:HB2	1:E:420:LEU:HD11	2.02	0.40
1:A:39:ILE:HA	1:A:39:ILE:HD12	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.56	0.40
1:A:306:ASN:ND2	1:A:336:ASN:HB2	2.37	0.40
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.86	0.40
1:A:382:ARG:NE	3:B:602:UFP:O1P	2.54	0.40
1:B:257:ARG:NE	3:B:602:UFP:O2P	2.45	0.40
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.56	0.40
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.57	0.40
1:C:341:ILE:HG22	1:C:397:MET:HE3	2.03	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:E:383:ARG:NH1	3:E:602:UFP:O3P[2_859]	2.06	0.14

## 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	501/521 (96%)	472 (94%)	28 (6%)	1 (0%)	52	84
1	B	501/521 (96%)	471 (94%)	29 (6%)	1 (0%)	52	84
1	C	501/521 (96%)	472 (94%)	28 (6%)	1 (0%)	52	84
1	D	501/521 (96%)	472 (94%)	28 (6%)	1 (0%)	52	84
1	E	501/521 (96%)	474 (95%)	26 (5%)	1 (0%)	52	84
All	All	2505/2605 (96%)	2361 (94%)	139 (6%)	5 (0%)	52	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	341	ILE

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Mol	Chain	Res	Type
1	C	341	ILE
1	D	341	ILE
1	A	341	ILE
1	E	341	ILE

### 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	456/470 (97%)	451 (99%)	5 (1%)	80	93
1	B	456/470 (97%)	451 (99%)	5 (1%)	80	93
1	C	456/470 (97%)	452 (99%)	4 (1%)	84	94
1	D	456/470 (97%)	451 (99%)	5 (1%)	80	93
1	E	456/470 (97%)	452 (99%)	4 (1%)	84	94
All	All	2280/2350 (97%)	2257 (99%)	23 (1%)	82	93

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	193	LEU
1	A	209	ILE
1	A	383	ARG
1	A	516	LYS
1	B	102	MET
1	B	138	LEU
1	B	193	LEU
1	B	209	ILE
1	B	516	LYS
1	C	99	GLU
1	C	209	ILE
1	C	220	LYS
1	C	516	LYS
1	D	102	MET

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Mol	Chain	Res	Type
1	D	103	ASN
1	D	193	LEU
1	D	209	ILE
1	D	383	ARG
1	E	102	MET
1	E	193	LEU
1	E	220	LYS
1	E	383	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	GLN
1	A	103	ASN
1	B	5	ASN
1	B	24	GLN
1	B	100	ASN
1	B	103	ASN
1	C	5	ASN
1	C	24	GLN
1	C	100	ASN
1	C	103	ASN
1	D	24	GLN
1	D	100	ASN
1	D	103	ASN
1	D	422	GLN
1	E	5	ASN
1	E	24	GLN
1	E	93	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

20 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	NDP	A	601	-	42,52,52	1.88	10 (23%)	55,80,80	1.63	6 (10%)
3	UFP	A	602	-	18,22,22	1.23	1 (5%)	21,33,33	1.76	2 (9%)
4	MTX	A	603	-	27,35,35	1.74	6 (22%)	30,49,49	1.53	7 (23%)
5	1UF	A	604	-	26,34,34	2.38	8 (30%)	24,49,49	2.38	7 (29%)
2	NDP	B	601	-	42,52,52	1.89	10 (23%)	55,80,80	1.59	6 (10%)
3	UFP	B	602	-	18,22,22	1.24	1 (5%)	21,33,33	1.79	3 (14%)
4	MTX	B	603	-	27,35,35	1.74	6 (22%)	30,49,49	1.54	6 (20%)
5	1UF	B	604	-	26,34,34	2.38	7 (26%)	24,49,49	2.36	9 (37%)
2	NDP	C	601	-	42,52,52	1.88	10 (23%)	55,80,80	1.60	5 (9%)
3	UFP	C	602	-	18,22,22	1.23	1 (5%)	21,33,33	1.77	2 (9%)
4	MTX	C	603	-	27,35,35	1.74	6 (22%)	30,49,49	1.53	7 (23%)
5	1UF	C	604	-	26,34,34	2.39	8 (30%)	24,49,49	2.29	7 (29%)
2	NDP	D	601	-	42,52,52	1.88	10 (23%)	55,80,80	1.60	5 (9%)
3	UFP	D	602	-	18,22,22	1.22	1 (5%)	21,33,33	1.78	3 (14%)
4	MTX	D	603	-	27,35,35	1.74	6 (22%)	30,49,49	1.53	7 (23%)
5	1UF	D	604	-	26,34,34	2.37	7 (26%)	24,49,49	2.36	9 (37%)
2	NDP	E	601	-	42,52,52	1.88	10 (23%)	55,80,80	1.65	7 (12%)
3	UFP	E	602	-	18,22,22	1.22	1 (5%)	21,33,33	1.78	2 (9%)
4	MTX	E	603	-	27,35,35	1.74	6 (22%)	30,49,49	1.53	7 (23%)
5	1UF	E	604	-	26,34,34	2.38	8 (30%)	24,49,49	2.38	8 (33%)

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	NDP	A	601	-	-	0/30/77/77	0/5/5/5
3	UFP	A	602	-	-	0/6/22/22	0/2/2/2
4	MTX	A	603	-	-	0/19/25/25	0/3/3/3
5	1UF	A	604	-	-	0/13/21/21	0/3/3/3
2	NDP	B	601	-	-	0/30/77/77	0/5/5/5
3	UFP	B	602	-	-	0/6/22/22	0/2/2/2
4	MTX	B	603	-	-	0/19/25/25	0/3/3/3
5	1UF	B	604	-	-	1/13/21/21	0/3/3/3
2	NDP	C	601	-	-	0/30/77/77	0/5/5/5
3	UFP	C	602	-	-	0/6/22/22	0/2/2/2
4	MTX	C	603	-	-	0/19/25/25	0/3/3/3
5	1UF	C	604	-	-	0/13/21/21	0/3/3/3
2	NDP	D	601	-	-	0/30/77/77	0/5/5/5
3	UFP	D	602	-	-	0/6/22/22	0/2/2/2
4	MTX	D	603	-	-	0/19/25/25	0/3/3/3
5	1UF	D	604	-	-	0/13/21/21	0/3/3/3
2	NDP	E	601	-	-	0/30/77/77	0/5/5/5
3	UFP	E	602	-	-	0/6/22/22	0/2/2/2
4	MTX	E	603	-	-	0/19/25/25	0/3/3/3
5	1UF	E	604	-	-	0/13/21/21	0/3/3/3

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NDP	C4N-C5N	-3.95	1.40	1.49
2	E	601	NDP	C4N-C5N	-3.92	1.40	1.49
2	C	601	NDP	C4N-C5N	-3.91	1.40	1.49
2	A	601	NDP	C4N-C5N	-3.90	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.89	1.40	1.49
2	B	601	NDP	C2D-C3D	-3.83	1.43	1.53
2	A	601	NDP	C2D-C3D	-3.82	1.43	1.53
2	E	601	NDP	C2D-C3D	-3.82	1.43	1.53
2	C	601	NDP	C2D-C3D	-3.81	1.43	1.53
2	D	601	NDP	C2D-C3D	-3.79	1.43	1.53
2	D	601	NDP	C3B-C2B	-3.78	1.44	1.53
2	A	601	NDP	C3B-C2B	-3.76	1.44	1.53
2	C	601	NDP	C3B-C2B	-3.73	1.44	1.53
2	B	601	NDP	C3B-C2B	-3.73	1.44	1.53
2	E	601	NDP	C3B-C2B	-3.64	1.44	1.53
4	D	603	MTX	CB-CA	-2.60	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	1UF	CB-CA	-2.59	1.49	1.53
5	A	604	1UF	CB-CA	-2.58	1.49	1.53
4	B	603	MTX	CB-CA	-2.55	1.49	1.53
4	C	603	MTX	CB-CA	-2.54	1.49	1.53
4	E	603	MTX	CB-CA	-2.53	1.49	1.53
5	B	604	1UF	CB-CA	-2.53	1.49	1.53
4	A	603	MTX	CB-CA	-2.52	1.49	1.53
5	D	604	1UF	CB-CA	-2.49	1.49	1.53
5	E	604	1UF	CB-CA	-2.49	1.49	1.53
2	E	601	NDP	C3B-C4B	-2.35	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.32	1.46	1.53
2	B	601	NDP	C3B-C4B	-2.31	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.31	1.46	1.53
2	D	601	NDP	C3B-C4B	-2.27	1.46	1.53
2	B	601	NDP	C3D-C4D	-2.25	1.46	1.53
2	C	601	NDP	C3D-C4D	-2.22	1.47	1.53
2	D	601	NDP	C3D-C4D	-2.21	1.47	1.53
2	E	601	NDP	C3D-C4D	-2.16	1.47	1.53
2	A	601	NDP	C3D-C4D	-2.12	1.47	1.53
5	E	604	1UF	CA-N	-2.08	1.43	1.46
5	A	604	1UF	CA-N	-2.04	1.43	1.46
5	C	604	1UF	CA-N	-2.00	1.43	1.46
4	C	603	MTX	C14-N10	2.19	1.45	1.39
4	A	603	MTX	C14-N10	2.20	1.45	1.39
4	B	603	MTX	C14-N10	2.21	1.46	1.39
4	D	603	MTX	C14-N10	2.22	1.46	1.39
4	E	603	MTX	C14-N10	2.23	1.46	1.39
2	A	601	NDP	C4A-N3A	2.28	1.39	1.35
4	E	603	MTX	C7-N8	2.29	1.35	1.31
2	B	601	NDP	C4A-N3A	2.32	1.39	1.35
4	C	603	MTX	C7-N8	2.34	1.35	1.31
4	A	603	MTX	C7-N8	2.34	1.35	1.31
2	D	601	NDP	C4A-N3A	2.34	1.39	1.35
4	B	603	MTX	C7-N8	2.35	1.35	1.31
4	D	603	MTX	C7-N8	2.36	1.35	1.31
2	C	601	NDP	C4A-N3A	2.36	1.39	1.35
2	E	601	NDP	C4A-N3A	2.41	1.39	1.35
2	C	601	NDP	C2N-C3N	2.50	1.40	1.34
2	B	601	NDP	C2N-C3N	2.50	1.40	1.34
2	A	601	NDP	C2N-C3N	2.50	1.40	1.34
2	D	601	NDP	C2N-C3N	2.50	1.40	1.34
2	E	601	NDP	C2N-C3N	2.51	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	UFP	C4-C5	2.67	1.41	1.38
4	D	603	MTX	C4-NA4	2.68	1.43	1.34
4	A	603	MTX	C4-NA4	2.70	1.43	1.34
4	E	603	MTX	C4-NA4	2.71	1.43	1.34
3	E	602	UFP	C4-C5	2.71	1.41	1.38
4	C	603	MTX	C4-NA4	2.71	1.43	1.34
4	B	603	MTX	C4-NA4	2.73	1.43	1.34
3	C	602	UFP	C4-C5	2.74	1.41	1.38
3	A	602	UFP	C4-C5	2.79	1.42	1.38
3	B	602	UFP	C4-C5	2.84	1.42	1.38
2	A	601	NDP	C6N-C5N	3.23	1.39	1.33
2	B	601	NDP	C6N-C5N	3.25	1.39	1.33
2	D	601	NDP	C6N-C5N	3.26	1.39	1.33
2	C	601	NDP	C6N-C5N	3.28	1.39	1.33
2	E	601	NDP	C6N-C5N	3.30	1.39	1.33
5	E	604	1UF	CBD-NAR	3.32	1.41	1.34
5	A	604	1UF	CBD-NAR	3.33	1.41	1.34
5	D	604	1UF	CBD-NAR	3.34	1.41	1.34
5	B	604	1UF	CBD-NAR	3.38	1.41	1.34
5	C	604	1UF	CBD-NAR	3.42	1.41	1.34
5	E	604	1UF	CBC-NAQ	3.63	1.39	1.33
5	C	604	1UF	CBC-NAQ	3.64	1.39	1.33
5	A	604	1UF	CBC-NAQ	3.64	1.39	1.33
5	B	604	1UF	CBC-NAQ	3.65	1.39	1.33
5	D	604	1UF	CBC-NAQ	3.68	1.39	1.33
2	A	601	NDP	C7N-N7N	3.68	1.44	1.33
2	C	601	NDP	C7N-N7N	3.72	1.44	1.33
2	D	601	NDP	C7N-N7N	3.72	1.44	1.33
2	E	601	NDP	C7N-N7N	3.72	1.44	1.33
2	B	601	NDP	C7N-N7N	3.72	1.44	1.33
5	E	604	1UF	CAV-N	4.17	1.43	1.34
5	A	604	1UF	CAV-N	4.21	1.43	1.34
5	C	604	1UF	CAV-N	4.27	1.43	1.34
5	D	604	1UF	CAV-N	4.34	1.44	1.34
5	B	604	1UF	CAV-N	4.46	1.44	1.34
2	A	601	NDP	C6A-N6A	4.51	1.48	1.34
2	B	601	NDP	C6A-N6A	4.52	1.48	1.34
2	C	601	NDP	C6A-N6A	4.52	1.48	1.34
5	D	604	1UF	CAW-NAB	4.54	1.43	1.34
2	E	601	NDP	C6A-N6A	4.56	1.49	1.34
2	D	601	NDP	C6A-N6A	4.56	1.49	1.34
5	B	604	1UF	CAW-NAB	4.56	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	604	1UF	CAW-NAB	4.58	1.43	1.34
5	C	604	1UF	CAW-NAB	4.60	1.43	1.34
5	A	604	1UF	CAW-NAB	4.61	1.43	1.34
4	D	603	MTX	C-N	4.82	1.45	1.34
4	B	603	MTX	C-N	4.90	1.45	1.34
4	A	603	MTX	C-N	4.90	1.45	1.34
4	B	603	MTX	C2-NA2	4.94	1.44	1.34
4	E	603	MTX	C-N	4.94	1.45	1.34
4	C	603	MTX	C-N	4.95	1.45	1.34
4	E	603	MTX	C2-NA2	4.95	1.44	1.34
4	C	603	MTX	C2-NA2	4.95	1.44	1.34
4	A	603	MTX	C2-NA2	4.97	1.44	1.34
4	D	603	MTX	C2-NA2	4.97	1.44	1.34
5	A	604	1UF	OAF-CBC	5.49	1.37	1.24
5	C	604	1UF	OAF-CBC	5.49	1.37	1.24
5	B	604	1UF	OAF-CBC	5.50	1.37	1.24
5	D	604	1UF	OAF-CBC	5.51	1.37	1.24
5	E	604	1UF	OAF-CBC	5.52	1.37	1.24
5	B	604	1UF	CAW-NAQ	5.85	1.45	1.35
5	D	604	1UF	CAW-NAQ	5.87	1.45	1.35
5	A	604	1UF	CAW-NAQ	5.88	1.45	1.35
5	C	604	1UF	CAW-NAQ	5.90	1.45	1.35
5	E	604	1UF	CAW-NAQ	5.93	1.45	1.35

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NDP	N3A-C2A-N1A	-8.53	122.36	128.89
2	C	601	NDP	N3A-C2A-N1A	-8.52	122.37	128.89
2	E	601	NDP	N3A-C2A-N1A	-8.50	122.39	128.89
2	B	601	NDP	N3A-C2A-N1A	-8.43	122.44	128.89
2	A	601	NDP	N3A-C2A-N1A	-8.37	122.48	128.89
5	D	604	1UF	NAO-CAW-NAQ	-6.07	118.20	127.44
5	B	604	1UF	NAO-CAW-NAQ	-6.06	118.21	127.44
5	E	604	1UF	NAO-CAW-NAQ	-6.06	118.22	127.44
5	A	604	1UF	NAO-CAW-NAQ	-6.04	118.24	127.44
5	C	604	1UF	NAO-CAW-NAQ	-6.02	118.28	127.44
5	A	604	1UF	CBE-CBC-NAQ	-5.90	119.72	124.19
5	C	604	1UF	CBE-CBC-NAQ	-5.86	119.75	124.19
5	B	604	1UF	CBE-CBC-NAQ	-5.82	119.78	124.19
5	D	604	1UF	CBE-CBC-NAQ	-5.80	119.80	124.19
5	E	604	1UF	CBE-CBC-NAQ	-5.79	119.81	124.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NDP	PN-O3-PA	-4.40	120.37	132.73
2	E	601	NDP	PN-O3-PA	-4.17	121.03	132.73
2	B	601	NDP	PN-O3-PA	-3.96	121.59	132.73
2	C	601	NDP	PN-O3-PA	-3.78	122.11	132.73
2	D	601	NDP	PN-O3-PA	-3.72	122.29	132.73
4	D	603	MTX	N1-C2-N3	-3.35	122.35	127.44
4	A	603	MTX	N1-C2-N3	-3.34	122.35	127.44
4	E	603	MTX	N1-C2-N3	-3.33	122.38	127.44
4	B	603	MTX	N1-C2-N3	-3.31	122.41	127.44
4	C	603	MTX	N1-C2-N3	-3.30	122.42	127.44
3	C	602	UFP	C5-C4-N3	-2.93	119.07	122.34
3	A	602	UFP	C5-C4-N3	-2.89	119.12	122.34
3	E	602	UFP	C5-C4-N3	-2.88	119.13	122.34
3	B	602	UFP	C5-C4-N3	-2.86	119.15	122.34
3	D	602	UFP	C5-C4-N3	-2.86	119.15	122.34
2	A	601	NDP	C4A-C5A-N7A	-2.72	106.97	109.48
2	E	601	NDP	C4A-C5A-N7A	-2.71	106.99	109.48
2	B	601	NDP	C4A-C5A-N7A	-2.66	107.03	109.48
2	D	601	NDP	C4A-C5A-N7A	-2.63	107.06	109.48
2	C	601	NDP	C4A-C5A-N7A	-2.63	107.06	109.48
5	B	604	1UF	CAZ-CBA-CAV	-2.27	119.50	122.70
5	B	604	1UF	CAL-CAZ-CBA	-2.23	120.10	121.59
5	E	604	1UF	CAL-CAZ-CBA	-2.15	120.15	121.59
5	C	604	1UF	CAL-CAZ-CBA	-2.13	120.17	121.59
5	A	604	1UF	CAL-CAZ-CBA	-2.09	120.20	121.59
5	D	604	1UF	CAZ-CBA-CAV	-2.08	119.77	122.70
5	D	604	1UF	CAL-CAZ-CBA	-2.08	120.20	121.59
3	B	602	UFP	O4'-C1'-N1	2.04	111.25	107.72
4	A	603	MTX	C6-C9-N10	2.06	117.36	113.78
2	A	601	NDP	O5D-C5D-C4D	2.08	116.77	109.12
2	B	601	NDP	O3-PN-O5D	2.08	108.46	102.94
2	B	601	NDP	O5B-C5B-C4B	2.11	116.88	109.12
4	E	603	MTX	CM-N10-C9	2.11	119.95	114.23
5	D	604	1UF	CAK-CBA-CAZ	2.12	120.32	117.77
5	E	604	1UF	CAK-CBA-CAZ	2.12	120.32	117.77
2	B	601	NDP	O5D-C5D-C4D	2.12	116.95	109.12
2	E	601	NDP	O5B-C5B-C4B	2.13	116.96	109.12
5	C	604	1UF	NAB-CAW-NAQ	2.14	120.74	117.20
5	B	604	1UF	NAB-CAW-NAQ	2.14	120.74	117.20
4	D	603	MTX	CM-N10-C9	2.14	120.03	114.23
4	B	603	MTX	CM-N10-C9	2.14	120.03	114.23
4	A	603	MTX	CM-N10-C9	2.15	120.07	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	1UF	NAB-CAW-NAQ	2.16	120.77	117.20
4	C	603	MTX	CM-N10-C9	2.16	120.08	114.23
2	C	601	NDP	O5D-C5D-C4D	2.17	117.13	109.12
5	A	604	1UF	NAB-CAW-NAQ	2.19	120.82	117.20
2	D	601	NDP	O5D-C5D-C4D	2.20	117.25	109.12
3	D	602	UFP	O4'-C1'-N1	2.21	111.53	107.72
5	E	604	1UF	NAB-CAW-NAQ	2.21	120.85	117.20
2	D	601	NDP	O3-PN-O5D	2.22	108.82	102.94
2	E	601	NDP	O5D-C5D-C4D	2.24	117.36	109.12
2	A	601	NDP	O3-PN-O5D	2.24	108.88	102.94
2	E	601	NDP	O3-PA-O5B	2.26	108.92	102.94
2	C	601	NDP	O3-PN-O5D	2.26	108.94	102.94
4	D	603	MTX	C6-C9-N10	2.30	117.77	113.78
4	C	603	MTX	CG-CB-CA	2.30	117.66	112.99
2	A	601	NDP	O3-PA-O5B	2.32	109.10	102.94
5	B	604	1UF	CAK-CBA-CAZ	2.35	120.59	117.77
2	E	601	NDP	O3-PN-O5D	2.35	109.17	102.94
4	E	603	MTX	CG-CB-CA	2.35	117.77	112.99
4	A	603	MTX	CG-CB-CA	2.38	117.83	112.99
4	C	603	MTX	C6-C9-N10	2.45	118.04	113.78
4	E	603	MTX	N8-C8A-N1	2.55	119.79	116.14
4	D	603	MTX	CG-CB-CA	2.59	118.24	112.99
4	D	603	MTX	C11-C-N	2.60	121.56	116.93
4	E	603	MTX	C11-C-N	2.60	121.57	116.93
4	E	603	MTX	C6-C9-N10	2.62	118.34	113.78
4	C	603	MTX	C11-C-N	2.63	121.61	116.93
4	A	603	MTX	C11-C-N	2.65	121.64	116.93
4	B	603	MTX	CG-CB-CA	2.66	118.40	112.99
4	C	603	MTX	N8-C8A-N1	2.67	119.96	116.14
4	D	603	MTX	N8-C8A-N1	2.69	119.98	116.14
5	C	604	1UF	CBC-NAQ-CAW	2.72	119.71	115.94
5	E	604	1UF	CBC-NAQ-CAW	2.73	119.72	115.94
5	D	604	1UF	CBC-NAQ-CAW	2.73	119.73	115.94
5	B	604	1UF	CBC-NAQ-CAW	2.74	119.75	115.94
4	B	603	MTX	N8-C8A-N1	2.76	120.08	116.14
5	D	604	1UF	CAY-SAS-CBB	2.76	109.32	101.96
5	A	604	1UF	CBC-NAQ-CAW	2.78	119.80	115.94
4	B	603	MTX	C11-C-N	2.79	121.90	116.93
4	A	603	MTX	N8-C8A-N1	2.79	120.14	116.14
5	B	604	1UF	CAY-SAS-CBB	2.82	109.47	101.96
5	C	604	1UF	CAY-SAS-CBB	2.85	109.57	101.96
5	A	604	1UF	CAY-SAS-CBB	3.13	110.32	101.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	604	1UF	CAY-SAS-CBB	3.15	110.36	101.96
4	E	603	MTX	C7-N8-C8A	3.34	120.86	116.93
4	D	603	MTX	C7-N8-C8A	3.36	120.88	116.93
5	C	604	1UF	CG-CB-CA	3.37	119.84	112.99
4	B	603	MTX	C7-N8-C8A	3.39	120.93	116.93
4	A	603	MTX	C7-N8-C8A	3.41	120.94	116.93
4	C	603	MTX	C7-N8-C8A	3.46	121.01	116.93
5	B	604	1UF	CG-CB-CA	3.88	120.87	112.99
5	A	604	1UF	CG-CB-CA	4.15	121.41	112.99
5	E	604	1UF	CG-CB-CA	4.16	121.43	112.99
5	D	604	1UF	CG-CB-CA	4.59	122.31	112.99
3	D	602	UFP	C4-N3-C2	6.54	120.90	115.25
3	C	602	UFP	C4-N3-C2	6.55	120.91	115.25
3	A	602	UFP	C4-N3-C2	6.56	120.91	115.25
3	B	602	UFP	C4-N3-C2	6.56	120.91	115.25
3	E	602	UFP	C4-N3-C2	6.65	120.99	115.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	604	1UF	CB-CA-N-CAV

There are no ring outliers.

19 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NDP	4	0
3	A	602	UFP	2	0
4	A	603	MTX	5	0
5	A	604	1UF	4	0
2	B	601	NDP	4	0
3	B	602	UFP	3	0
4	B	603	MTX	3	0
2	C	601	NDP	5	0
3	C	602	UFP	2	0
4	C	603	MTX	2	0
5	C	604	1UF	3	0
2	D	601	NDP	4	0
3	D	602	UFP	1	0
4	D	603	MTX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	604	1UF	1	0
2	E	601	NDP	1	0
3	E	602	UFP	2	1
4	E	603	MTX	2	0
5	E	604	1UF	6	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	505/521 (96%)	-0.06	10 (1%) 68 46	43, 70, 109, 201	0
1	B	505/521 (96%)	0.07	11 (2%) 65 42	45, 75, 112, 188	0
1	C	505/521 (96%)	0.00	13 (2%) 59 35	40, 83, 124, 205	0
1	D	505/521 (96%)	-0.03	7 (1%) 78 59	52, 85, 127, 194	0
1	E	505/521 (96%)	0.14	13 (2%) 59 35	62, 105, 146, 186	0
All	All	2525/2605 (96%)	0.02	54 (2%) 67 44	40, 83, 132, 205	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	50	ASN	4.6
1	E	113	CYS	4.5
1	B	51	ALA	4.0
1	C	113	CYS	3.8
1	E	102	MET	3.8
1	C	110	ILE	3.5
1	E	101	LEU	3.2
1	B	113	CYS	3.1
1	E	50	ASN	3.1
1	A	51	ALA	3.0
1	B	521	VAL	2.9
1	A	102	MET	2.9
1	C	102	MET	2.8
1	A	521	VAL	2.8
1	B	71	ILE	2.8
1	B	112	VAL	2.7
1	E	132	TYR	2.6
1	A	50	ASN	2.6
1	B	102	MET	2.6
1	C	53	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	97	SER	2.5
1	E	91	PHE	2.5
1	C	51	ALA	2.5
1	B	314	TYR	2.4
1	B	53	ILE	2.4
1	D	516	LYS	2.4
1	C	111	PHE	2.4
1	D	127	PHE	2.4
1	A	113	CYS	2.3
1	C	49	LYS	2.3
1	D	113	CYS	2.3
1	E	175	PHE	2.3
1	E	506	LEU	2.3
1	E	100	ASN	2.2
1	E	127	PHE	2.2
1	E	53	ILE	2.2
1	A	91	PHE	2.2
1	C	109	ASN	2.2
1	A	103	ASN	2.1
1	A	313	VAL	2.1
1	B	131	ILE	2.1
1	D	71	ILE	2.1
1	C	489	PHE	2.1
1	D	102	MET	2.1
1	E	51	ALA	2.1
1	D	51	ALA	2.1
1	B	110	ILE	2.1
1	C	88	VAL	2.1
1	B	73	VAL	2.1
1	D	133	LEU	2.0
1	A	97	SER	2.0
1	A	53	ILE	2.0
1	C	71	ILE	2.0
1	C	101	LEU	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	1UF	A	604	32/32	0.89	0.37	1.48	77,85,102,112	0
5	1UF	B	604	32/32	0.81	0.43	1.41	86,94,111,121	0
5	1UF	D	604	32/32	0.82	0.35	1.14	109,117,135,145	0
4	MTX	E	603	33/33	0.85	0.35	1.06	93,101,121,123	0
4	MTX	D	603	33/33	0.82	0.29	0.95	78,85,106,108	0
5	1UF	C	604	32/32	0.86	0.30	0.69	84,92,109,119	0
5	1UF	E	604	32/32	0.78	0.34	0.36	135,143,160,170	0
4	MTX	A	603	33/33	0.86	0.25	0.21	64,71,91,94	0
4	MTX	C	603	33/33	0.84	0.26	0.21	88,95,115,118	0
4	MTX	B	603	33/33	0.85	0.27	0.13	62,69,89,91	0
3	UFP	C	602	21/21	0.91	0.23	0.07	72,82,90,108	0
3	UFP	A	602	21/21	0.90	0.22	-0.08	69,79,87,105	0
3	UFP	E	602	21/21	0.85	0.23	-0.22	112,122,129,147	0
3	UFP	B	602	21/21	0.85	0.23	-0.29	73,82,90,108	0
2	NDP	C	601	48/48	0.90	0.17	-0.39	88,100,104,109	0
3	UFP	D	602	21/21	0.89	0.20	-0.49	84,94,102,120	0
2	NDP	E	601	48/48	0.93	0.17	-0.62	92,103,107,113	0
2	NDP	D	601	48/48	0.90	0.17	-0.79	80,91,95,100	0
2	NDP	A	601	48/48	0.95	0.15	-0.83	62,74,78,83	0
2	NDP	B	601	48/48	0.93	0.17	-0.91	57,69,73,78	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.