



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:49 PM GMT

PDB ID : 4Q0D
Title : Crystal structure of TS-DHFR from *Cryptosporidium hominis* in complex with NADPH, FdUMP, methotrexate and 2-amino-4-oxo-4,7-dihydro-pyrrolo[2,3-d]pyrimidine-methyl-phenyl-L-glutamic acid.
Authors : Kumar, V.P.; Anderson, K.S.
Deposited on : 2014-04-01
Resolution : 3.45 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

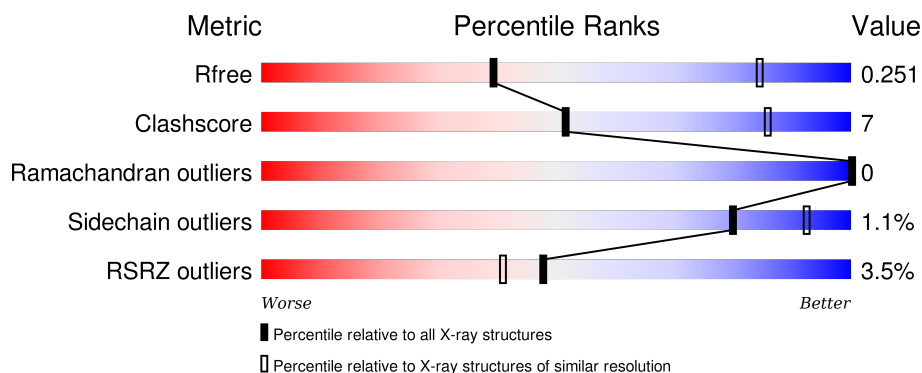
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1007 (3.54-3.34)
Clashscore	102246	1044 (3.52-3.36)
Ramachandran outliers	100387	1013 (3.52-3.36)
Sidechain outliers	100360	1014 (3.52-3.36)
RSRZ outliers	91569	1012 (3.54-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>78%</div> <div>19%</div> <div>..</div> </div>
1	B	521	<div> <div>3%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	C	521	<div> <div>5%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	D	521	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	E	521	<div> <div>2%</div> <div>78%</div> <div>19%</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
4	2XB	B	603	X	-	-	-

2 Entry composition [i](#)

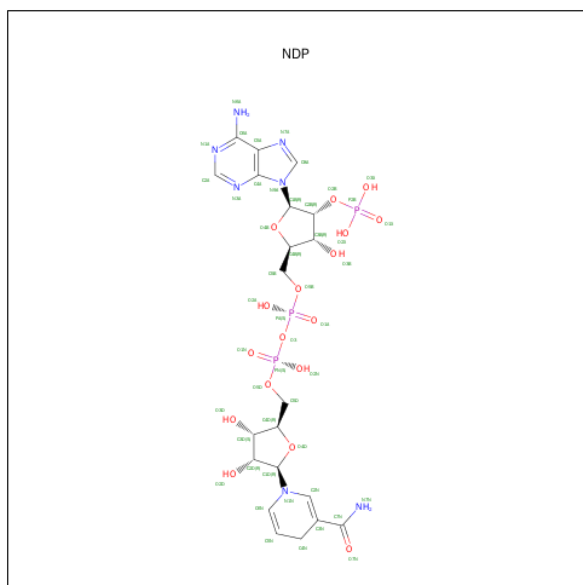
There are 5 unique types of molecules in this entry. The entry contains 21345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	508	Total	C	N	O	S	0	0	0
			4137	2644	695	776	22			
1	A	508	Total	C	N	O	S	0	0	0
			4137	2644	695	776	22			
1	B	508	Total	C	N	O	S	0	0	0
			4137	2644	695	776	22			
1	C	508	Total	C	N	O	S	0	0	0
			4137	2644	695	776	22			
1	D	508	Total	C	N	O	S	0	0	0
			4137	2644	695	776	22			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



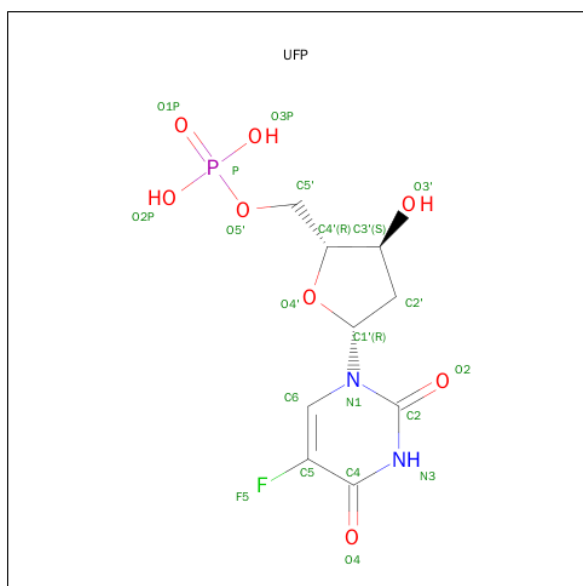
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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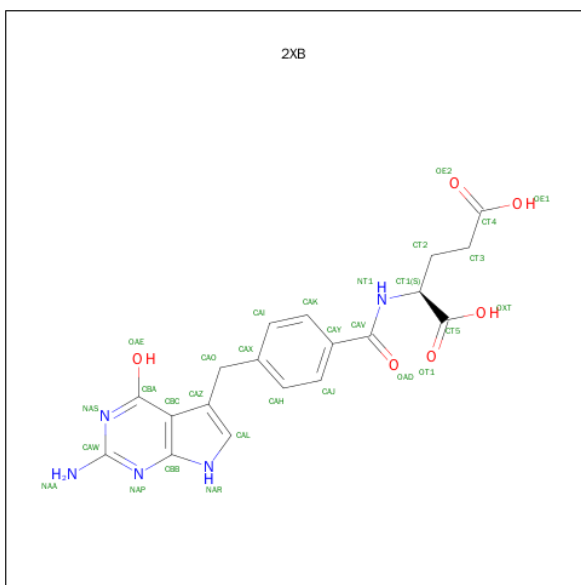
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: C₉H₁₂FN₂O₈P).



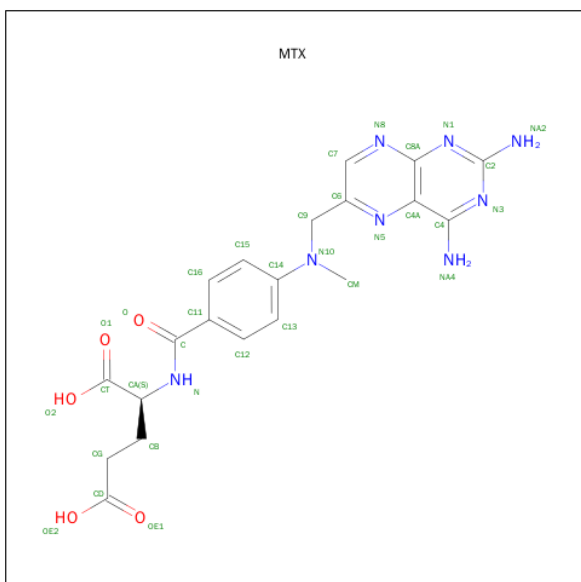
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is N-{4-[(2-AMINO-4-HYDROXY-7H-PYRROLO[2,3-D]PYRIMIDIN-5-YL)METHYL]BENZOYL}-L-GLUTAMIC ACID (three-letter code: 2XB) (formula: C₁₉H₁₉N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total 30	C 19	N 5	O 6	0	0
4	A	1	Total 30	C 19	N 5	O 6	0	0
4	B	1	Total 30	C 19	N 5	O 6	0	0
4	C	1	Total 30	C 19	N 5	O 6	0	0
4	D	1	Total 30	C 19	N 5	O 6	0	0

- Molecule 5 is METHOTREXATE (three-letter code: MTX) (formula: $\text{C}_{20}\text{H}_{22}\text{N}_8\text{O}_5$).

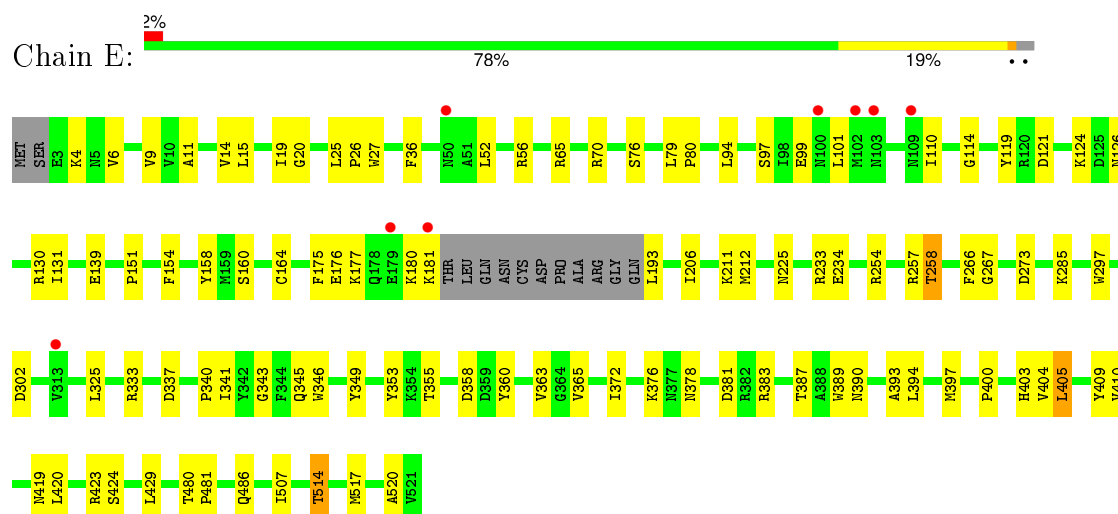


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total 33	C 20	N 8	O 5	0	0
5	A	1	Total 33	C 20	N 8	O 5	0	0
5	B	1	Total 33	C 20	N 8	O 5	0	0
5	C	1	Total 33	C 20	N 8	O 5	0	0
5	D	1	Total 33	C 20	N 8	O 5	0	0

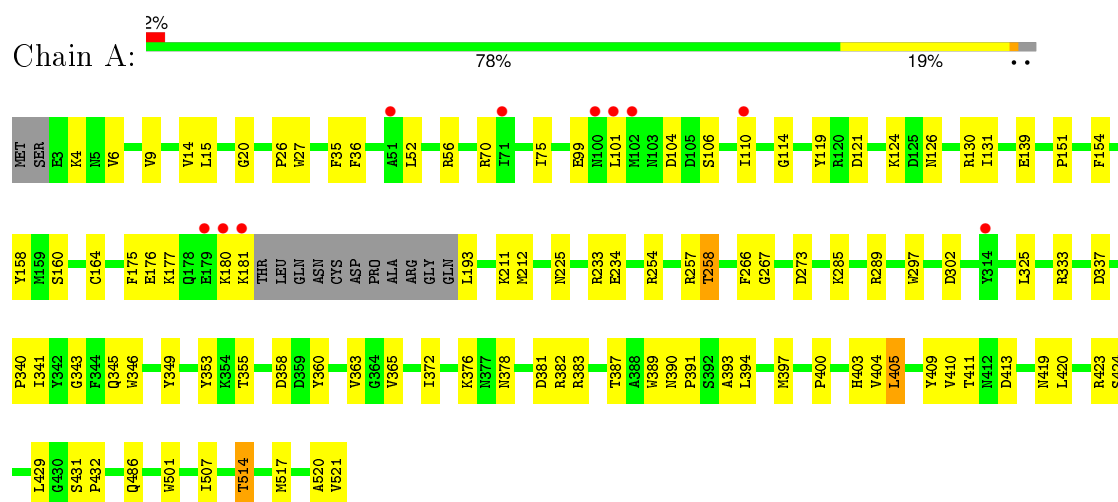
3 Residue-property plots

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.

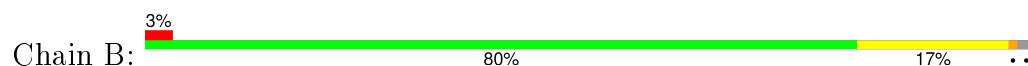
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

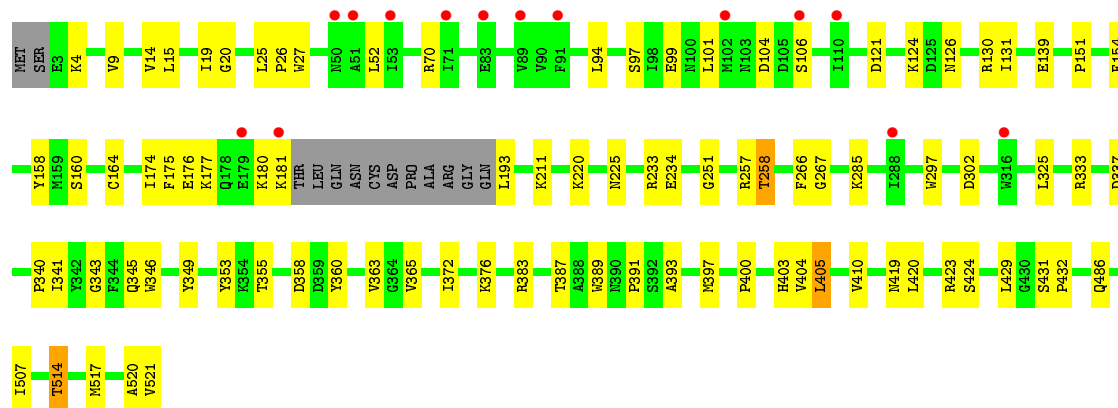


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

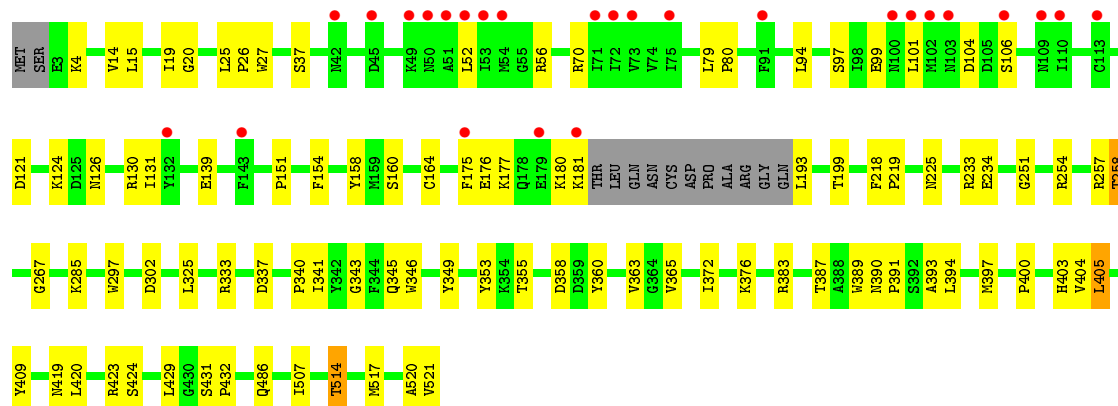
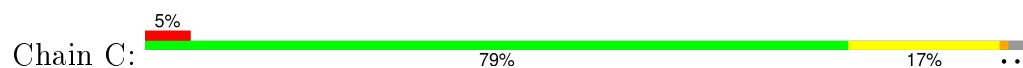


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

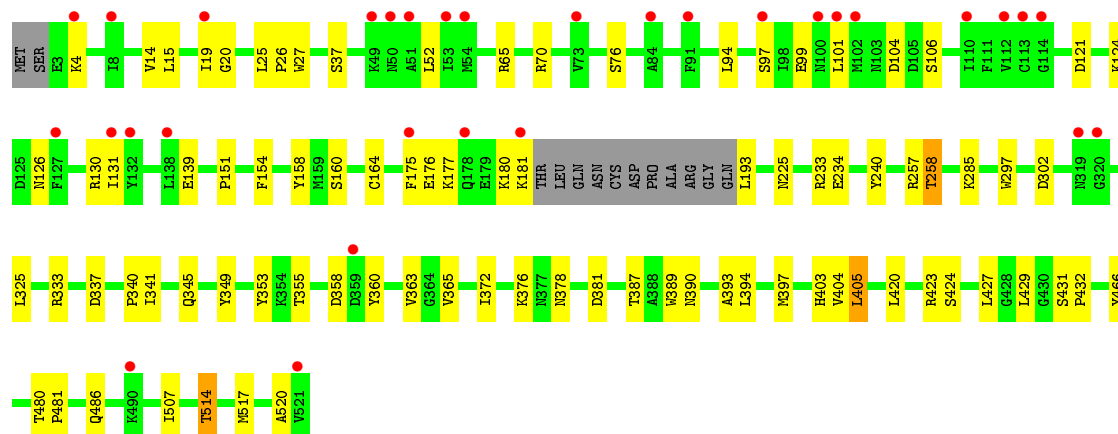
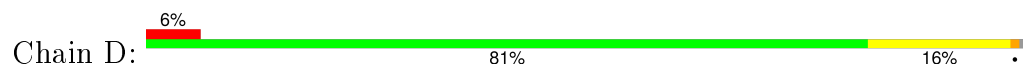




- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: Bifunctional dihydrofolate reductase-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	213.61Å 115.03Å 217.64Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	48.94 – 3.45 48.94 – 3.45	Depositor EDS
% Data completeness (in resolution range)	90.2 (48.94-3.45) 83.6 (48.94-3.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.217 , 0.242 0.237 , 0.251	Depositor DCC
R_{free} test set	2024 reflections (3.59%)	DCC
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 62864 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21345	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.375 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, 2XB

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	0.22	0/4232	0.40	0/5718
1	B	0.22	0/4232	0.40	0/5718
1	C	0.22	0/4232	0.40	0/5718
1	D	0.22	0/4232	0.40	0/5718
1	E	0.22	0/4232	0.40	0/5718
All	All	0.22	0/21160	0.40	0/28590

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	4137	0	4070	70	0
1	B	4137	0	4070	60	0
1	C	4137	0	4070	63	0
1	D	4137	0	4070	50	0
1	E	4137	0	4070	71	0
2	A	48	0	26	2	0
2	B	48	0	26	1	0
2	C	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	26	2	0
2	E	48	0	26	3	0
3	A	21	0	10	0	0
3	B	21	0	10	2	0
3	C	21	0	10	1	0
3	D	21	0	10	2	0
3	E	21	0	10	2	0
4	A	30	0	17	1	0
4	B	30	0	17	0	0
4	C	30	0	17	0	0
4	D	30	0	16	0	0
4	E	30	0	17	0	0
5	A	33	0	20	4	0
5	B	33	0	20	4	0
5	C	33	0	20	2	0
5	D	33	0	20	2	0
5	E	33	0	20	5	0
All	All	21345	0	20714	285	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 7.

All (285) 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:20:GLY:HA2	1:C:26:PRO:HD3	1.67	0.77
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.67	0.77
1:E:20:GLY:HA2	1:E:26:PRO:HD3	1.67	0.76
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.67	0.76
1:E:400:PRO:HG2	1:A:383:ARG:HE	1.50	0.76
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.67	0.76
1:D:25:LEU:HD11	5:D:604:MTX:H7	1.68	0.75
1:D:37:SER:HB2	5:D:604:MTX:HB1	1.68	0.73
1:B:258:THR:HG21	1:B:520:ALA:HB1	1.72	0.72
1:A:258:THR:HG21	1:A:520:ALA:HB1	1.72	0.72
1:B:121:ASP:HA	1:B:124:LYS:HB3	1.73	0.71
1:B:383:ARG:HE	1:C:400:PRO:HG2	1.55	0.71
1:D:258:THR:HG21	1:D:520:ALA:HB1	1.72	0.71
1:A:121:ASP:HA	1:A:124:LYS:HB3	1.73	0.70
1:E:387:THR:HB	1:E:405:LEU:HD12	1.74	0.70
1:E:383:ARG:HE	1:A:400:PRO:HG2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASP:HA	1:C:124:LYS:HB3	1.73	0.70
1:B:225:ASN:O	1:B:233:ARG:NH2	2.25	0.70
1:C:258:THR:HG21	1:C:520:ALA:HB1	1.73	0.69
1:C:387:THR:HB	1:C:405:LEU:HD12	1.74	0.69
1:D:225:ASN:O	1:D:233:ARG:NH2	2.25	0.69
1:D:121:ASP:HA	1:D:124:LYS:HB3	1.73	0.69
1:D:387:THR:HB	1:D:405:LEU:HD12	1.73	0.69
1:E:121:ASP:HA	1:E:124:LYS:HB3	1.73	0.69
1:C:25:LEU:HD11	5:C:604:MTX:H7	1.75	0.69
1:A:387:THR:HB	1:A:405:LEU:HD12	1.74	0.69
1:E:225:ASN:O	1:E:233:ARG:NH2	2.25	0.69
1:C:225:ASN:O	1:C:233:ARG:NH2	2.26	0.69
1:E:258:THR:HG21	1:E:520:ALA:HB1	1.73	0.69
1:B:387:THR:HB	1:B:405:LEU:HD12	1.74	0.68
1:A:225:ASN:O	1:A:233:ARG:NH2	2.26	0.68
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.78	0.66
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.78	0.66
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.78	0.66
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.78	0.65
1:E:419:ASN:HD21	1:A:267:GLY:HA2	1.61	0.64
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.78	0.64
1:E:56:ARG:NH1	2:E:601:NDP:O1X	2.31	0.64
1:B:267:GLY:HA2	1:C:419:ASN:HD21	1.64	0.63
3:E:602:UFP:O1P	1:A:382:ARG:NE	2.31	0.63
1:B:400:PRO:HG2	1:C:383:ARG:HE	1.63	0.63
1:B:257:ARG:NE	3:B:602:UFP:O2P	2.30	0.63
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.83	0.61
1:C:52:LEU:HD11	1:C:70:ARG:HD2	1.82	0.61
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.34	0.60
1:B:52:LEU:HD11	1:B:70:ARG:HD2	1.83	0.60
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.82	0.60
1:D:257:ARG:NE	3:D:602:UFP:O2P	2.32	0.60
1:E:130:ARG:NH1	1:E:176:GLU:OE2	2.35	0.60
1:E:234:GLU:OE1	1:A:211:LYS:NZ	2.35	0.59
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.83	0.59
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.85	0.59
1:D:130:ARG:NH1	1:D:176:GLU:OE2	2.36	0.58
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.85	0.58
1:C:130:ARG:NH1	1:C:176:GLU:OE2	2.36	0.58
1:B:130:ARG:NH1	1:B:176:GLU:OE2	2.36	0.58
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LYS:NZ	1:A:234:GLU:OE1	2.37	0.57
1:C:56:ARG:NH1	2:C:601:NDP:O1X	2.38	0.57
1:C:37:SER:HB2	5:C:604:MTX:HB1	1.86	0.57
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.85	0.56
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.86	0.56
1:A:9:VAL:O	5:A:604:MTX:NA4	2.38	0.56
1:B:25:LEU:HD11	5:B:604:MTX:H7	1.87	0.55
1:E:267:GLY:HA2	1:A:419:ASN:HD21	1.72	0.55
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.43	0.54
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.89	0.54
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.89	0.54
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.90	0.54
1:E:19:ILE:O	2:E:601:NDP:H2N	2.08	0.54
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.89	0.54
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.43	0.54
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.43	0.54
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.89	0.54
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.43	0.53
1:B:14:VAL:HG13	1:B:15:LEU:HG	1.90	0.53
1:B:4:LYS:HG2	1:B:101:LEU:HD23	1.91	0.53
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.89	0.53
1:D:126:ASN:OD1	1:D:177:LYS:NZ	2.35	0.53
1:E:4:LYS:HG2	1:E:101:LEU:HD23	1.91	0.53
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.89	0.53
1:E:9:VAL:O	5:E:604:MTX:NA4	2.42	0.53
1:D:4:LYS:HG2	1:D:101:LEU:HD23	1.91	0.52
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.44	0.52
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.90	0.52
1:D:466:TYR:HH	3:D:602:UFP:HO3'	1.56	0.52
1:C:349:TYR:HB3	1:C:365:VAL:HB	1.92	0.52
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.91	0.52
1:E:409:TYR:HB2	1:A:266:PHE:CE1	2.45	0.52
1:C:4:LYS:HG2	1:C:101:LEU:HD23	1.91	0.52
1:E:349:TYR:HB3	1:E:365:VAL:HB	1.92	0.52
1:B:349:TYR:HB3	1:B:365:VAL:HB	1.92	0.51
1:B:391:PRO:HD2	1:C:349:TYR:CE2	2.45	0.51
1:A:4:LYS:HG2	1:A:101:LEU:HD23	1.91	0.51
1:C:19:ILE:O	2:C:601:NDP:H2N	2.11	0.51
1:A:349:TYR:HB3	1:A:365:VAL:HB	1.92	0.50
1:E:254:ARG:NH2	1:A:410:VAL:O	2.43	0.50
1:C:158:TYR:OH	1:C:234:GLU:OE2	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:TYR:HB3	1:D:365:VAL:HB	1.92	0.50
1:E:266:PHE:CE1	1:A:409:TYR:HB2	2.47	0.49
1:A:158:TYR:OH	1:A:234:GLU:OE2	2.22	0.49
1:E:65:ARG:NH1	1:C:251:GLY:O	2.44	0.49
1:C:337:ASP:OD1	1:C:353:TYR:OH	2.29	0.49
1:B:360:TYR:O	1:B:363:VAL:HG12	2.13	0.49
1:B:9:VAL:O	5:B:604:MTX:NA4	2.45	0.48
1:A:337:ASP:OD1	1:A:353:TYR:OH	2.30	0.48
1:E:257:ARG:NE	3:E:602:UFP:O2P	2.43	0.48
1:D:355:THR:OG1	1:D:358:ASP:OD2	2.29	0.48
1:D:360:TYR:O	1:D:363:VAL:HG12	2.14	0.48
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.35	0.48
1:E:76:SER:OG	2:E:601:NDP:O2X	2.24	0.48
1:B:419:ASN:HD21	1:C:267:GLY:HA2	1.78	0.48
1:C:325:LEU:HD23	1:C:333:ARG:HB3	1.96	0.48
1:D:325:LEU:HD23	1:D:333:ARG:HB3	1.96	0.48
1:B:337:ASP:OD1	1:B:353:TYR:OH	2.30	0.48
1:E:325:LEU:HD23	1:E:333:ARG:HB3	1.96	0.47
1:C:360:TYR:O	1:C:363:VAL:HG12	2.13	0.47
1:E:360:TYR:O	1:E:363:VAL:HG12	2.14	0.47
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.49	0.47
1:E:400:PRO:HG2	1:A:383:ARG:NE	2.24	0.47
1:A:56:ARG:HD3	2:A:601:NDP:O2X	2.14	0.47
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.49	0.47
1:B:325:LEU:HD23	1:B:333:ARG:HB3	1.96	0.47
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.49	0.47
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.49	0.47
1:E:337:ASP:OD1	1:E:353:TYR:OH	2.30	0.47
1:A:360:TYR:O	1:A:363:VAL:HG12	2.14	0.47
1:A:325:LEU:HD23	1:A:333:ARG:HB3	1.96	0.47
1:B:355:THR:OG1	1:B:358:ASP:OD2	2.29	0.47
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.49	0.46
1:B:285:LYS:HB3	1:B:514:THR:HB	1.97	0.46
1:D:19:ILE:O	2:D:601:NDP:H2N	2.15	0.46
1:E:285:LYS:HB3	1:E:514:THR:HB	1.97	0.46
1:C:285:LYS:HB3	1:C:514:THR:HB	1.97	0.46
1:D:337:ASP:OD1	1:D:353:TYR:OH	2.30	0.46
1:B:486:GLN:HB2	1:B:507:ILE:HB	1.98	0.46
1:D:285:LYS:HB3	1:D:514:THR:HB	1.97	0.46
1:E:372:ILE:HG22	1:E:376:LYS:HE2	1.98	0.46
1:C:372:ILE:HG22	1:C:376:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:VAL:O	1:A:254:ARG:NH2	2.49	0.46
1:D:15:LEU:HD12	1:D:139:GLU:HG3	1.98	0.46
1:D:240:TYR:OH	1:D:427:LEU:O	2.30	0.46
1:A:75:ILE:O	2:A:601:NDP:H1B	2.16	0.45
1:C:340:PRO:HB2	1:C:345:GLN:HE21	1.81	0.45
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.99	0.45
1:B:372:ILE:HG22	1:B:376:LYS:HE2	1.98	0.45
1:D:340:PRO:HB2	1:D:345:GLN:HE21	1.81	0.45
1:B:383:ARG:NE	1:C:400:PRO:HG2	2.28	0.45
1:D:372:ILE:HG22	1:D:376:LYS:HE2	1.98	0.45
1:A:9:VAL:HG12	5:A:604:MTX:N3	2.32	0.45
1:E:15:LEU:HD12	1:E:139:GLU:HG3	1.99	0.45
1:A:372:ILE:HG22	1:A:376:LYS:HE2	1.97	0.45
1:D:158:TYR:OH	1:D:234:GLU:OE2	2.22	0.45
1:D:486:GLN:HB2	1:D:507:ILE:HB	1.98	0.45
1:B:9:VAL:HG12	5:B:604:MTX:N3	2.30	0.45
1:C:15:LEU:HD12	1:C:139:GLU:HG3	1.99	0.45
1:A:355:THR:OG1	1:A:358:ASP:OD2	2.29	0.45
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.99	0.45
1:B:174:ILE:HD11	1:C:199:THR:HG21	1.99	0.45
3:B:602:UFP:O3P	1:C:383:ARG:NH2	2.50	0.45
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.99	0.45
1:B:160:SER:HA	1:B:234:GLU:HB3	1.99	0.45
1:A:340:PRO:HB2	1:A:345:GLN:HE21	1.82	0.45
1:D:160:SER:HA	1:D:234:GLU:HB3	1.99	0.45
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.99	0.44
1:E:486:GLN:HB2	1:E:507:ILE:HB	1.98	0.44
1:A:104:ASP:OD1	1:A:106:SER:OG	2.33	0.44
1:A:285:LYS:HB3	1:A:514:THR:HB	1.98	0.44
1:E:70:ARG:HH22	5:E:604:MTX:CT	2.29	0.44
1:E:160:SER:HA	1:E:234:GLU:HB3	1.99	0.44
1:A:486:GLN:HB2	1:A:507:ILE:HB	1.98	0.44
1:A:160:SER:HA	1:A:234:GLU:HB3	1.99	0.44
1:B:15:LEU:HD12	1:B:139:GLU:HG3	2.00	0.44
1:A:15:LEU:HD12	1:A:139:GLU:HG3	1.99	0.44
1:D:104:ASP:OD1	1:D:106:SER:OG	2.33	0.44
1:B:349:TYR:CE2	1:C:391:PRO:HD2	2.52	0.44
1:C:257:ARG:NH2	1:C:521:VAL:OXT	2.44	0.44
1:C:486:GLN:HB2	1:C:507:ILE:HB	1.98	0.44
1:B:340:PRO:HB2	1:B:345:GLN:HE21	1.81	0.44
1:A:70:ARG:HH22	5:A:604:MTX:CT	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:CYS:HB2	1:E:486:GLN:NE2	2.33	0.44
1:E:349:TYR:CE2	1:A:391:PRO:HD2	2.53	0.44
1:B:19:ILE:O	2:B:601:NDP:H2N	2.18	0.44
1:C:104:ASP:OD1	1:C:106:SER:OG	2.33	0.44
1:C:393:ALA:O	1:C:397:MET:HG3	2.18	0.44
1:E:340:PRO:HB2	1:E:345:GLN:HE21	1.82	0.43
1:E:11:ALA:HB2	5:E:604:MTX:NA2	2.33	0.43
1:D:393:ALA:O	1:D:397:MET:HG3	2.18	0.43
1:D:180:LYS:HG3	1:D:181:LYS:H	1.83	0.43
1:B:393:ALA:O	1:B:397:MET:HG3	2.18	0.43
1:D:423:ARG:HG3	1:D:424:SER:N	2.34	0.43
1:A:393:ALA:O	1:A:397:MET:HG3	2.18	0.43
1:C:180:LYS:HG3	1:C:181:LYS:H	1.83	0.43
1:E:423:ARG:HG3	1:E:424:SER:N	2.34	0.43
1:E:180:LYS:HG3	1:E:181:LYS:H	1.83	0.43
1:B:410:VAL:O	1:C:254:ARG:NH2	2.49	0.43
1:E:158:TYR:OH	1:E:234:GLU:OE2	2.23	0.43
1:E:126:ASN:OD1	1:E:177:LYS:NZ	2.35	0.43
1:C:218:PHE:HA	1:C:219:PRO:HD3	1.92	0.43
1:C:160:SER:HA	1:C:234:GLU:HB3	1.99	0.43
1:A:180:LYS:HG3	1:A:181:LYS:H	1.83	0.43
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.99	0.43
1:B:158:TYR:OH	1:B:234:GLU:OE2	2.23	0.43
1:C:164:CYS:HB2	1:C:486:GLN:NE2	2.34	0.43
1:E:393:ALA:O	1:E:397:MET:HG3	2.19	0.43
1:A:257:ARG:NH2	1:A:521:VAL:OXT	2.44	0.43
1:E:25:LEU:HD11	5:E:604:MTX:H7	2.00	0.43
1:E:355:THR:OG1	1:E:358:ASP:OD2	2.29	0.43
1:B:70:ARG:HH22	5:B:604:MTX:CT	2.30	0.43
1:C:423:ARG:HG3	1:C:424:SER:N	2.34	0.43
1:B:180:LYS:HG3	1:B:181:LYS:H	1.83	0.43
1:B:94:LEU:O	1:B:97:SER:OG	2.25	0.43
1:C:355:THR:O	1:C:360:TYR:OH	2.33	0.42
1:D:164:CYS:HB2	1:D:486:GLN:NE2	2.33	0.42
1:C:94:LEU:O	1:C:97:SER:OG	2.26	0.42
1:E:343:GLY:HA2	1:E:346:TRP:HB2	2.01	0.42
1:A:164:CYS:HB2	1:A:486:GLN:NE2	2.33	0.42
1:A:341:ILE:HG22	1:A:397:MET:HE2	2.01	0.42
1:A:36:PHE:CE2	5:A:604:MTX:H16	2.54	0.42
1:B:341:ILE:HG22	1:B:397:MET:HE2	2.02	0.42
1:E:480:THR:HA	1:E:481:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HD21	1:A:517:MET:HB2	2.02	0.42
1:E:212:MET:SD	1:A:273:ASP:HB2	2.59	0.42
1:C:429:LEU:HD21	1:C:517:MET:HB2	2.02	0.42
1:B:164:CYS:HB2	1:B:486:GLN:NE2	2.34	0.42
1:C:343:GLY:HA2	1:C:346:TRP:HB2	2.02	0.42
1:C:355:THR:OG1	1:C:358:ASP:OD2	2.30	0.42
1:E:341:ILE:HG22	1:E:397:MET:HE2	2.02	0.42
1:A:423:ARG:HG3	1:A:424:SER:N	2.34	0.42
1:E:36:PHE:CE2	5:E:604:MTX:H16	2.55	0.42
1:E:79:LEU:HA	1:E:80:PRO:HD3	1.89	0.42
1:B:211:LYS:NZ	1:C:234:GLU:OE1	2.52	0.42
1:C:257:ARG:NE	3:C:602:UFP:O2P	2.42	0.42
1:B:343:GLY:HA2	1:B:346:TRP:HB2	2.02	0.42
1:A:343:GLY:HA2	1:A:346:TRP:HB2	2.02	0.42
1:A:4:LYS:H	1:A:101:LEU:HD22	1.85	0.41
1:E:206:ILE:HD11	1:A:35:PHE:HA	2.01	0.41
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.35	0.41
1:D:480:THR:HA	1:D:481:PRO:HD3	1.90	0.41
1:D:151:PRO:HG2	1:D:154:PHE:CD1	2.56	0.41
1:C:126:ASN:OD1	1:C:177:LYS:NZ	2.35	0.41
1:B:4:LYS:H	1:B:101:LEU:HD22	1.86	0.41
1:D:76:SER:OG	2:D:601:NDP:O2X	2.25	0.41
1:D:429:LEU:HD21	1:D:517:MET:HB2	2.02	0.41
1:A:151:PRO:HG2	1:A:154:PHE:CD1	2.56	0.41
1:E:151:PRO:HG2	1:E:154:PHE:CD1	2.56	0.41
1:D:94:LEU:O	1:D:97:SER:OG	2.26	0.41
1:A:378:ASN:ND2	1:A:381:ASP:HB2	2.36	0.41
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.89	0.41
1:C:341:ILE:HG22	1:C:397:MET:HE2	2.02	0.41
1:B:266:PHE:CE1	1:C:409:TYR:HB2	2.55	0.41
1:A:520:ALA:O	4:A:603:2XB:NAA	2.54	0.41
1:B:220:LYS:HB2	1:B:220:LYS:HE3	1.93	0.41
1:A:431:SER:HB3	1:A:432:PRO:HD3	2.03	0.41
1:E:4:LYS:H	1:E:101:LEU:HD22	1.86	0.41
1:D:341:ILE:HG22	1:D:397:MET:HE2	2.01	0.41
1:C:151:PRO:HG2	1:C:154:PHE:CD1	2.56	0.41
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.56	0.41
1:A:6:VAL:HG22	1:A:110:ILE:HB	2.03	0.41
1:E:94:LEU:O	1:E:97:SER:OG	2.26	0.41
1:A:411:THR:OG1	1:A:413:ASP:OD1	2.26	0.41
1:D:431:SER:HB3	1:D:432:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:LEU:HD21	1:E:517:MET:HB2	2.02	0.41
1:E:273:ASP:HB2	1:A:212:MET:SD	2.61	0.41
1:B:423:ARG:HG3	1:B:424:SER:N	2.34	0.41
1:E:383:ARG:NE	1:A:400:PRO:HG2	2.30	0.41
1:E:390:ASN:O	1:E:394:LEU:HG	2.21	0.41
1:B:104:ASP:OD1	1:B:106:SER:OG	2.33	0.41
1:E:341:ILE:HA	1:E:397:MET:HE2	2.03	0.40
1:A:390:ASN:O	1:A:394:LEU:HG	2.21	0.40
1:C:390:ASN:O	1:C:394:LEU:HG	2.21	0.40
1:D:4:LYS:H	1:D:101:LEU:HD22	1.86	0.40
1:B:431:SER:HB3	1:B:432:PRO:HD3	2.02	0.40
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.36	0.40
1:E:6:VAL:HG22	1:E:110:ILE:HB	2.04	0.40
1:B:429:LEU:HD21	1:B:517:MET:HB2	2.02	0.40
1:C:4:LYS:H	1:C:101:LEU:HD22	1.86	0.40
1:B:151:PRO:HG2	1:B:154:PHE:CD1	2.55	0.40
1:E:114:GLY:HA3	1:E:119:TYR:CE1	2.56	0.40
1:C:431:SER:HB3	1:C:432:PRO:HD3	2.03	0.40
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.44	0.40
1:B:251:GLY:O	1:D:65:ARG:NH1	2.53	0.40
1:A:114:GLY:HA3	1:A:119:TYR:CE1	2.56	0.40
1:D:390:ASN:O	1:D:394:LEU:HG	2.21	0.40
1:E:378:ASN:ND2	1:E:381:ASP:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	504/521 (97%)	483 (96%)	21 (4%)	0	100	100
1	B	504/521 (97%)	483 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	504/521 (97%)	483 (96%)	21 (4%)	0	100	100
1	D	504/521 (97%)	483 (96%)	21 (4%)	0	100	100
1	E	504/521 (97%)	482 (96%)	22 (4%)	0	100	100
All	All	2520/2605 (97%)	2414 (96%)	106 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	458/470 (97%)	453 (99%)	5 (1%)	80	92
1	B	458/470 (97%)	453 (99%)	5 (1%)	80	92
1	C	458/470 (97%)	453 (99%)	5 (1%)	80	92
1	D	458/470 (97%)	453 (99%)	5 (1%)	80	92
1	E	458/470 (97%)	453 (99%)	5 (1%)	80	92
All	All	2290/2350 (97%)	2265 (99%)	25 (1%)	80	92

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	99	GLU
1	E	193	LEU
1	E	258	THR
1	E	405	LEU
1	E	514	THR
1	A	99	GLU
1	A	193	LEU
1	A	258	THR
1	A	405	LEU
1	A	514	THR
1	B	99	GLU
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	258	THR
1	B	405	LEU
1	B	514	THR
1	C	99	GLU
1	C	193	LEU
1	C	258	THR
1	C	405	LEU
1	C	514	THR
1	D	99	GLU
1	D	193	LEU
1	D	258	THR
1	D	405	LEU
1	D	514	THR

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

Mol	Chain	Res	Type
1	E	306	ASN
1	E	345	GLN
1	E	419	ASN
1	E	422	GLN
1	A	306	ASN
1	A	345	GLN
1	A	419	ASN
1	A	422	GLN
1	B	306	ASN
1	B	345	GLN
1	B	422	GLN
1	C	306	ASN
1	C	345	GLN
1	C	419	ASN
1	C	422	GLN
1	D	306	ASN
1	D	345	GLN
1	D	422	GLN

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	1.62	7 (12%)
3	UFP	A	602	-	18,22,22	1.24	1 (5%)	21,33,33	1.77	2 (9%)
4	2XB	A	603	-	26,32,32	2.09	6 (23%)	25,45,45	2.02	5 (20%)
5	MTX	A	604	-	27,35,35	1.76	6 (22%)	30,49,49	1.56	6 (20%)
2	NDP	B	601	-	42,52,52	1.89	10 (23%)	55,80,80	1.62	7 (12%)
3	UFP	B	602	-	18,22,22	1.22	1 (5%)	21,33,33	1.76	2 (9%)
4	2XB	B	603	-	26,32,32	2.08	5 (19%)	25,45,45	2.08	6 (24%)
5	MTX	B	604	-	27,35,35	1.72	6 (22%)	30,49,49	1.63	8 (26%)
2	NDP	C	601	-	42,52,52	1.87	10 (23%)	55,80,80	1.63	7 (12%)
3	UFP	C	602	-	18,22,22	1.23	1 (5%)	21,33,33	1.72	2 (9%)
4	2XB	C	603	-	26,32,32	2.10	7 (26%)	25,45,45	2.04	5 (20%)
5	MTX	C	604	-	27,35,35	1.73	6 (22%)	30,49,49	1.57	7 (23%)
2	NDP	D	601	-	42,52,52	1.87	10 (23%)	55,80,80	1.61	7 (12%)
3	UFP	D	602	-	18,22,22	1.23	1 (5%)	21,33,33	1.73	2 (9%)
4	2XB	D	603	-	26,32,32	2.09	6 (23%)	25,45,45	2.03	5 (20%)
5	MTX	D	604	-	27,35,35	1.74	6 (22%)	30,49,49	1.56	7 (23%)
2	NDP	E	601	-	42,52,52	1.87	10 (23%)	55,80,80	1.63	8 (14%)
3	UFP	E	602	-	18,22,22	1.24	1 (5%)	21,33,33	1.87	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2XB	E	603	-	26,32,32	2.09	7 (26%)	25,45,45	2.06	5 (20%)
5	MTX	E	604	-	27,35,35	1.74	6 (22%)	30,49,49	1.60	6 (20%)

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	2XB	A	603	-	-	0/14/21/21	0/3/3/3
5	MTX	A	604	-	-	0/19/25/25	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	2XB	B	603	-	1/1/4/5	0/14/21/21	0/3/3/3
5	MTX	B	604	-	-	0/19/25/25	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	2XB	C	603	-	-	0/14/21/21	0/3/3/3
5	MTX	C	604	-	-	0/19/25/25	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	2XB	D	603	-	-	0/14/21/21	0/3/3/3
5	MTX	D	604	-	-	0/19/25/25	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	2XB	E	603	-	-	0/14/21/21	0/3/3/3
5	MTX	E	604	-	-	0/19/25/25	0/3/3/3

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NDP	C2D-C3D	-3.94	1.42	1.53
2	A	601	NDP	C4N-C5N	-3.92	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.88	1.40	1.49
2	E	601	NDP	C4N-C5N	-3.87	1.40	1.49
2	C	601	NDP	C2D-C3D	-3.87	1.42	1.53
2	E	601	NDP	C2D-C3D	-3.87	1.42	1.53
2	B	601	NDP	C4N-C5N	-3.87	1.40	1.49
2	C	601	NDP	C4N-C5N	-3.84	1.40	1.49
2	D	601	NDP	C2D-C3D	-3.84	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NDP	C2D-C3D	-3.75	1.43	1.53
2	B	601	NDP	C3B-C2B	-3.75	1.44	1.53
2	D	601	NDP	C3B-C2B	-3.70	1.44	1.53
2	A	601	NDP	C3B-C2B	-3.69	1.44	1.53
2	E	601	NDP	C3B-C2B	-3.67	1.44	1.53
2	C	601	NDP	C3B-C2B	-3.65	1.44	1.53
4	C	603	2XB	CT2-CT1	-2.87	1.49	1.53
4	E	603	2XB	CT2-CT1	-2.73	1.49	1.53
4	B	603	2XB	CT2-CT1	-2.65	1.49	1.53
5	A	604	MTX	CB-CA	-2.64	1.49	1.53
4	A	603	2XB	CT2-CT1	-2.63	1.49	1.53
5	E	604	MTX	CB-CA	-2.62	1.49	1.53
4	D	603	2XB	CT2-CT1	-2.58	1.49	1.53
5	D	604	MTX	CB-CA	-2.53	1.49	1.53
5	B	604	MTX	CB-CA	-2.50	1.49	1.53
5	C	604	MTX	CB-CA	-2.45	1.49	1.53
4	E	603	2XB	CT1-NT1	-2.34	1.43	1.46
2	C	601	NDP	C3B-C4B	-2.33	1.46	1.53
2	B	601	NDP	C3B-C4B	-2.31	1.46	1.53
2	D	601	NDP	C3B-C4B	-2.29	1.46	1.53
2	E	601	NDP	C3B-C4B	-2.28	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.28	1.46	1.53
4	C	603	2XB	CT1-NT1	-2.19	1.43	1.46
2	C	601	NDP	C3D-C4D	-2.14	1.47	1.53
2	A	601	NDP	C3D-C4D	-2.14	1.47	1.53
2	B	601	NDP	C3D-C4D	-2.12	1.47	1.53
2	E	601	NDP	C3D-C4D	-2.12	1.47	1.53
2	D	601	NDP	C3D-C4D	-2.09	1.47	1.53
4	C	603	2XB	OAE-CBA	2.03	1.37	1.28
4	A	603	2XB	OAE-CBA	2.03	1.37	1.28
4	E	603	2XB	OAE-CBA	2.05	1.37	1.28
4	D	603	2XB	OAE-CBA	2.05	1.38	1.28
2	A	601	NDP	C4A-N3A	2.21	1.38	1.35
5	B	604	MTX	C14-N10	2.22	1.46	1.39
5	D	604	MTX	C14-N10	2.23	1.46	1.39
5	E	604	MTX	C14-N10	2.24	1.46	1.39
5	C	604	MTX	C14-N10	2.27	1.46	1.39
5	D	604	MTX	C7-N8	2.27	1.35	1.31
5	A	604	MTX	C7-N8	2.27	1.35	1.31
5	A	604	MTX	C14-N10	2.28	1.46	1.39
2	E	601	NDP	C4A-N3A	2.28	1.39	1.35
2	C	601	NDP	C4A-N3A	2.30	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	MTX	C7-N8	2.32	1.35	1.31
5	C	604	MTX	C7-N8	2.33	1.35	1.31
5	E	604	MTX	C7-N8	2.33	1.35	1.31
2	D	601	NDP	C4A-N3A	2.39	1.39	1.35
2	E	601	NDP	C2N-C3N	2.42	1.40	1.34
2	B	601	NDP	C4A-N3A	2.43	1.39	1.35
2	A	601	NDP	C2N-C3N	2.44	1.40	1.34
2	D	601	NDP	C2N-C3N	2.44	1.40	1.34
2	C	601	NDP	C2N-C3N	2.44	1.40	1.34
2	B	601	NDP	C2N-C3N	2.49	1.40	1.34
3	B	602	UFP	C4-C5	2.59	1.41	1.38
3	D	602	UFP	C4-C5	2.64	1.41	1.38
5	E	604	MTX	C4-NA4	2.70	1.43	1.34
5	B	604	MTX	C4-NA4	2.70	1.43	1.34
5	A	604	MTX	C4-NA4	2.72	1.43	1.34
3	E	602	UFP	C4-C5	2.72	1.41	1.38
5	C	604	MTX	C4-NA4	2.73	1.43	1.34
5	D	604	MTX	C4-NA4	2.75	1.43	1.34
3	C	602	UFP	C4-C5	2.77	1.42	1.38
3	A	602	UFP	C4-C5	2.83	1.42	1.38
2	A	601	NDP	C6N-C5N	3.32	1.39	1.33
2	E	601	NDP	C6N-C5N	3.33	1.39	1.33
2	D	601	NDP	C6N-C5N	3.33	1.39	1.33
2	C	601	NDP	C6N-C5N	3.36	1.39	1.33
2	B	601	NDP	C6N-C5N	3.43	1.39	1.33
4	D	603	2XB	CBB-NAR	3.48	1.41	1.34
4	B	603	2XB	CBB-NAR	3.51	1.41	1.34
4	A	603	2XB	CBB-NAR	3.53	1.41	1.34
4	E	603	2XB	CBB-NAR	3.56	1.41	1.34
4	C	603	2XB	CBB-NAR	3.57	1.41	1.34
2	D	601	NDP	C7N-N7N	3.67	1.44	1.33
2	E	601	NDP	C7N-N7N	3.68	1.44	1.33
2	C	601	NDP	C7N-N7N	3.69	1.44	1.33
2	A	601	NDP	C7N-N7N	3.70	1.44	1.33
2	B	601	NDP	C7N-N7N	3.73	1.44	1.33
4	E	603	2XB	CAV-NT1	4.10	1.43	1.34
4	C	603	2XB	CAV-NT1	4.14	1.43	1.34
4	B	603	2XB	CAV-NT1	4.23	1.43	1.34
4	D	603	2XB	CAV-NT1	4.34	1.44	1.34
4	A	603	2XB	CAV-NT1	4.38	1.44	1.34
4	E	603	2XB	CAW-NAA	4.51	1.43	1.34
2	C	601	NDP	C6A-N6A	4.53	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C6A-N6A	4.53	1.48	1.34
2	D	601	NDP	C6A-N6A	4.53	1.48	1.34
2	A	601	NDP	C6A-N6A	4.54	1.49	1.34
4	C	603	2XB	CAW-NAA	4.54	1.43	1.34
2	B	601	NDP	C6A-N6A	4.56	1.49	1.34
4	D	603	2XB	CAW-NAA	4.56	1.43	1.34
4	B	603	2XB	CAW-NAA	4.57	1.43	1.34
4	A	603	2XB	CAW-NAA	4.60	1.43	1.34
5	B	604	MTX	C-N	4.76	1.44	1.34
5	E	604	MTX	C-N	4.78	1.45	1.34
5	C	604	MTX	C-N	4.88	1.45	1.34
5	A	604	MTX	C-N	4.88	1.45	1.34
5	D	604	MTX	C-N	4.90	1.45	1.34
5	C	604	MTX	C2-NA2	4.95	1.44	1.34
5	D	604	MTX	C2-NA2	4.98	1.44	1.34
5	B	604	MTX	C2-NA2	5.00	1.44	1.34
5	A	604	MTX	C2-NA2	5.05	1.44	1.34
5	E	604	MTX	C2-NA2	5.08	1.44	1.34
4	E	603	2XB	CAW-NAS	5.87	1.45	1.35
4	A	603	2XB	CAW-NAS	5.88	1.45	1.35
4	B	603	2XB	CAW-NAS	5.90	1.45	1.35
4	C	603	2XB	CAW-NAS	5.93	1.45	1.35
4	D	603	2XB	CAW-NAS	6.00	1.46	1.35

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NDP	N3A-C2A-N1A	-8.51	122.38	128.89
2	D	601	NDP	N3A-C2A-N1A	-8.40	122.47	128.89
2	C	601	NDP	N3A-C2A-N1A	-8.37	122.48	128.89
2	E	601	NDP	N3A-C2A-N1A	-8.17	122.64	128.89
2	A	601	NDP	N3A-C2A-N1A	-8.15	122.66	128.89
4	B	603	2XB	NAP-CAW-NAS	-6.09	118.16	127.44
4	C	603	2XB	NAP-CAW-NAS	-5.94	118.40	127.44
4	D	603	2XB	NAP-CAW-NAS	-5.91	118.44	127.44
4	A	603	2XB	NAP-CAW-NAS	-5.84	118.55	127.44
4	E	603	2XB	NAP-CAW-NAS	-5.84	118.55	127.44
4	E	603	2XB	CBC-CBA-NAS	-4.75	119.63	124.39
4	C	603	2XB	CBC-CBA-NAS	-4.70	119.69	124.39
4	D	603	2XB	CBC-CBA-NAS	-4.66	119.72	124.39
4	A	603	2XB	CBC-CBA-NAS	-4.57	119.81	124.39
2	E	601	NDP	PN-O3-PA	-4.41	120.36	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	2XB	CBC-CBA-NAS	-4.26	120.12	124.39
2	C	601	NDP	PN-O3-PA	-4.18	120.98	132.73
2	A	601	NDP	PN-O3-PA	-4.02	121.45	132.73
2	B	601	NDP	PN-O3-PA	-3.97	121.59	132.73
2	D	601	NDP	PN-O3-PA	-3.88	121.83	132.73
5	E	604	MTX	N1-C2-N3	-3.52	122.09	127.44
5	B	604	MTX	N1-C2-N3	-3.46	122.17	127.44
5	D	604	MTX	N1-C2-N3	-3.45	122.19	127.44
5	A	604	MTX	N1-C2-N3	-3.41	122.25	127.44
5	C	604	MTX	N1-C2-N3	-3.37	122.31	127.44
3	E	602	UFP	C5-C4-N3	-3.12	118.87	122.34
3	C	602	UFP	C5-C4-N3	-2.96	119.04	122.34
3	A	602	UFP	C5-C4-N3	-2.94	119.07	122.34
3	B	602	UFP	C5-C4-N3	-2.93	119.08	122.34
4	C	603	2XB	CAZ-CBC-CBB	-2.92	105.69	110.09
3	D	602	UFP	C5-C4-N3	-2.87	119.15	122.34
4	E	603	2XB	CAZ-CBC-CBB	-2.86	105.78	110.09
4	A	603	2XB	CAZ-CBC-CBB	-2.82	105.84	110.09
4	D	603	2XB	CAZ-CBC-CBB	-2.79	105.89	110.09
4	B	603	2XB	CAZ-CBC-CBB	-2.78	105.89	110.09
2	C	601	NDP	C4A-C5A-N7A	-2.77	106.93	109.48
2	A	601	NDP	C4A-C5A-N7A	-2.72	106.97	109.48
2	B	601	NDP	C4A-C5A-N7A	-2.69	107.00	109.48
2	D	601	NDP	C4A-C5A-N7A	-2.69	107.01	109.48
2	E	601	NDP	C4A-C5A-N7A	-2.60	107.08	109.48
5	B	604	MTX	O-C-N	-2.07	118.71	122.44
5	A	604	MTX	O-C-N	-2.05	118.73	122.44
2	E	601	NDP	O5D-C5D-C4D	2.03	116.62	109.12
4	A	603	2XB	NAA-CAW-NAS	2.10	120.67	117.20
4	B	603	2XB	CAY-CAV-NT1	2.10	120.67	116.93
2	B	601	NDP	O5B-C5B-C4B	2.10	116.88	109.12
4	E	603	2XB	NAA-CAW-NAS	2.13	120.73	117.20
5	E	604	MTX	CM-N10-C9	2.15	120.06	114.23
5	B	604	MTX	CM-N10-C9	2.15	120.07	114.23
2	B	601	NDP	O3-PA-O5B	2.19	108.74	102.94
5	C	604	MTX	CM-N10-C9	2.19	120.16	114.23
4	B	603	2XB	NAA-CAW-NAS	2.21	120.85	117.20
5	D	604	MTX	CM-N10-C9	2.21	120.21	114.23
4	D	603	2XB	NAA-CAW-NAS	2.21	120.86	117.20
2	E	601	NDP	O5B-C5B-C4B	2.27	117.47	109.12
2	A	601	NDP	O3-PN-O5D	2.27	108.95	102.94
2	C	601	NDP	O3-PN-O5D	2.28	108.97	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NDP	O3-PN-O5D	2.28	108.98	102.94
2	C	601	NDP	O3-PA-O5B	2.28	108.99	102.94
2	C	601	NDP	O5D-C5D-C4D	2.28	117.54	109.12
2	A	601	NDP	O5D-C5D-C4D	2.29	117.56	109.12
2	A	601	NDP	O5B-C5B-C4B	2.30	117.58	109.12
5	D	604	MTX	CG-CB-CA	2.30	117.66	112.99
2	D	601	NDP	O3-PA-O5B	2.30	109.04	102.94
5	D	604	MTX	C11-C-N	2.30	121.03	116.93
2	B	601	NDP	O5D-C5D-C4D	2.31	117.64	109.12
2	D	601	NDP	O5D-C5D-C4D	2.32	117.68	109.12
4	C	603	2XB	NAA-CAW-NAS	2.33	121.05	117.20
2	E	601	NDP	O3-PA-O5B	2.35	109.17	102.94
2	D	601	NDP	O5B-C5B-C4B	2.35	117.79	109.12
2	C	601	NDP	O5B-C5B-C4B	2.36	117.81	109.12
2	E	601	NDP	O3-PN-O5D	2.36	109.20	102.94
5	B	604	MTX	C6-C9-N10	2.38	117.91	113.78
5	C	604	MTX	CG-CB-CA	2.40	117.86	112.99
2	E	601	NDP	O4D-C1D-N1N	2.43	113.20	108.07
5	D	604	MTX	N8-C8A-N1	2.51	119.73	116.14
5	C	604	MTX	C11-C-N	2.55	121.46	116.93
3	E	602	UFP	O4'-C1'-N1	2.55	112.13	107.72
2	D	601	NDP	O3-PN-O5D	2.55	109.71	102.94
2	A	601	NDP	O3-PA-O5B	2.61	109.85	102.94
5	B	604	MTX	N8-C8A-N1	2.61	119.87	116.14
5	C	604	MTX	N8-C8A-N1	2.65	119.93	116.14
5	A	604	MTX	N8-C8A-N1	2.66	119.95	116.14
5	E	604	MTX	N8-C8A-N1	2.72	120.04	116.14
4	C	603	2XB	CT3-CT2-CT1	2.73	118.54	112.99
5	B	604	MTX	CG-CB-CA	2.82	118.71	112.99
5	C	604	MTX	C6-C9-N10	2.88	118.79	113.78
5	E	604	MTX	C11-C-N	2.95	122.18	116.93
5	D	604	MTX	C6-C9-N10	2.99	118.98	113.78
5	A	604	MTX	C11-C-N	3.00	122.27	116.93
5	B	604	MTX	C11-C-N	3.14	122.52	116.93
4	E	603	2XB	CT3-CT2-CT1	3.14	119.38	112.99
5	E	604	MTX	CG-CB-CA	3.20	119.49	112.99
5	A	604	MTX	C7-N8-C8A	3.27	120.79	116.93
5	A	604	MTX	CG-CB-CA	3.29	119.68	112.99
4	A	603	2XB	CT3-CT2-CT1	3.39	119.88	112.99
4	D	603	2XB	CT3-CT2-CT1	3.43	119.96	112.99
5	D	604	MTX	C7-N8-C8A	3.44	120.99	116.93
5	E	604	MTX	C7-N8-C8A	3.48	121.03	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	2XB	CT3-CT2-CT1	3.49	120.08	112.99
5	B	604	MTX	C7-N8-C8A	3.51	121.07	116.93
5	C	604	MTX	C7-N8-C8A	3.56	121.13	116.93
3	D	602	UFP	C4-N3-C2	6.64	120.99	115.25
3	C	602	UFP	C4-N3-C2	6.65	121.00	115.25
3	A	602	UFP	C4-N3-C2	6.68	121.02	115.25
3	B	602	UFP	C4-N3-C2	6.77	121.10	115.25
3	E	602	UFP	C4-N3-C2	6.83	121.15	115.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	603	2XB	CT1

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 35 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	508/521 (97%)	0.18	10 (1%) 68 63	28, 68, 105, 187	0
1	B	508/521 (97%)	0.23	14 (2%) 56 50	51, 79, 115, 202	0
1	C	508/521 (97%)	0.24	26 (5%) 32 27	42, 77, 126, 187	0
1	D	508/521 (97%)	0.52	31 (6%) 25 22	63, 104, 144, 188	0
1	E	508/521 (97%)	0.09	8 (1%) 74 69	27, 63, 100, 190	0
All	All	2540/2605 (97%)	0.25	89 (3%) 48 41	27, 77, 130, 202	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	102	MET	4.8
1	C	181	LYS	4.6
1	A	179	GLU	4.5
1	C	101	LEU	3.9
1	A	102	MET	3.9
1	C	50	ASN	3.9
1	B	102	MET	3.8
1	C	53	ILE	3.6
1	D	53	ILE	3.5
1	C	109	ASN	3.3
1	A	51	ALA	3.3
1	D	51	ALA	3.3
1	C	51	ALA	3.3
1	D	102	MET	3.2
1	D	50	ASN	3.2
1	C	179	GLU	3.2
1	E	181	LYS	3.1
1	C	102	MET	3.1
1	C	49	LYS	3.1
1	D	319	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	110	ILE	2.9
1	D	127	PHE	2.8
1	B	71	ILE	2.8
1	B	181	LYS	2.8
1	D	114	GLY	2.8
1	E	179	GLU	2.7
1	E	103	ASN	2.7
1	C	45	ASP	2.7
1	C	113	CYS	2.7
1	D	131	ILE	2.7
1	D	113	CYS	2.6
1	B	179	GLU	2.6
1	B	50	ASN	2.6
1	D	19	ILE	2.6
1	B	53	ILE	2.5
1	A	71	ILE	2.5
1	A	181	LYS	2.5
1	D	175	PHE	2.5
1	B	51	ALA	2.5
1	C	71	ILE	2.5
1	D	91	PHE	2.4
1	C	73	VAL	2.4
1	A	314	TYR	2.4
1	D	138	LEU	2.4
1	C	100	ASN	2.4
1	D	101	LEU	2.4
1	B	106	SER	2.4
1	D	73	VAL	2.4
1	D	132	TYR	2.4
1	B	83	GLU	2.4
1	D	100	ASN	2.3
1	D	320	GLY	2.3
1	E	50	ASN	2.3
1	C	42	ASN	2.3
1	D	178	GLN	2.3
1	B	89	VAL	2.3
1	C	72	ILE	2.3
1	C	75	ILE	2.3
1	E	100	ASN	2.3
1	D	84	ALA	2.3
1	D	112	VAL	2.3
1	D	521	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASN	2.2
1	D	359	ASP	2.2
1	B	91	PHE	2.2
1	C	143	PHE	2.2
1	D	490	LYS	2.2
1	C	52	LEU	2.2
1	B	288	ILE	2.2
1	D	49	LYS	2.2
1	C	103	ASN	2.2
1	C	175	PHE	2.2
1	E	109	ASN	2.1
1	D	97	SER	2.1
1	C	132	TYR	2.1
1	E	313	VAL	2.1
1	D	110	ILE	2.1
1	D	54	MET	2.1
1	D	4	LYS	2.1
1	D	8	ILE	2.1
1	A	101	LEU	2.1
1	C	91	PHE	2.1
1	C	54	MET	2.1
1	A	180	LYS	2.1
1	B	110	ILE	2.0
1	B	316	TRP	2.0
1	C	106	SER	2.0
1	A	110	ILE	2.0
1	D	181	LYS	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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	2XB	E	603	30/30	0.90	0.36	1.97	55,63,77,83	0
4	2XB	A	603	30/30	0.86	0.35	1.63	69,77,91,97	0
5	MTX	D	604	33/33	0.84	0.38	1.58	93,100,110,115	0
4	2XB	B	603	30/30	0.85	0.38	1.23	80,88,102,108	0
4	2XB	C	603	30/30	0.88	0.31	0.87	60,68,82,88	0
5	MTX	B	604	33/33	0.89	0.27	0.72	64,72,86,91	0
5	MTX	C	604	33/33	0.87	0.31	0.60	79,88,95,99	0
4	2XB	D	603	30/30	0.85	0.38	0.58	108,116,130,135	0
5	MTX	E	604	33/33	0.89	0.25	0.57	54,61,81,84	0
5	MTX	A	604	33/33	0.91	0.24	0.13	55,63,68,70	0
3	UFP	E	602	21/21	0.91	0.23	0.06	60,70,78,96	0
3	UFP	C	602	21/21	0.94	0.22	0.02	66,75,83,101	0
3	UFP	B	602	21/21	0.91	0.22	-0.14	78,87,95,113	0
3	UFP	A	602	21/21	0.92	0.22	-0.26	65,75,83,101	0
2	NDP	D	601	48/48	0.92	0.21	-0.77	88,99,103,108	0
2	NDP	A	601	48/48	0.93	0.18	-0.90	54,66,70,75	0
2	NDP	C	601	48/48	0.92	0.21	-0.99	97,108,112,117	0
3	UFP	D	602	21/21	0.91	0.18	-1.07	108,118,125,144	0
2	NDP	E	601	48/48	0.95	0.16	-1.14	59,70,74,80	0
2	NDP	B	601	48/48	0.94	0.17	-1.19	75,86,90,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.