Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:53 PM GMT

PDB ID	:	4Q0E
Title	:	Crystal structure of TS-DHFR from Cryptosporidium hominis in complex with NADPH, FdUMP 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	:	2.78 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

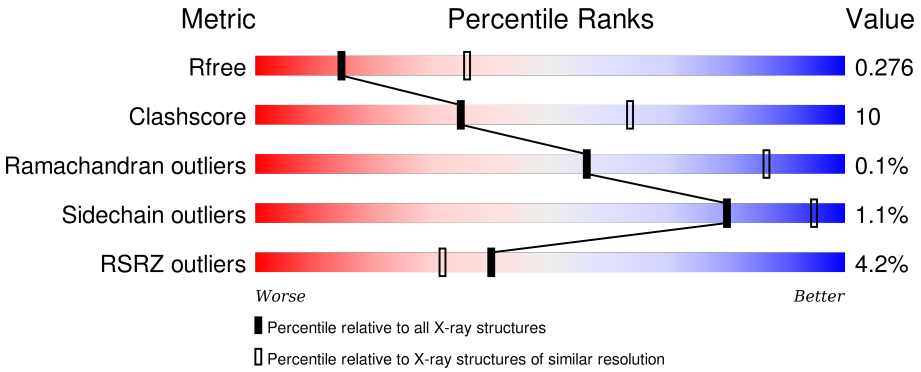
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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 <=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	% 74% 22%
1	B	521	6% 78% 18%
1	C	521	4% 75% 21%
1	D	521	3% 77% 19%
1	E	521	7% 79% 17%

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	A	604	X	-	-	-
4	2XB	B	604	X	-	-	-
4	2XB	C	604	X	-	-	-
4	2XB	D	604	X	-	-	-
4	2XB	E	604	X	-	-	-

2 Entry composition

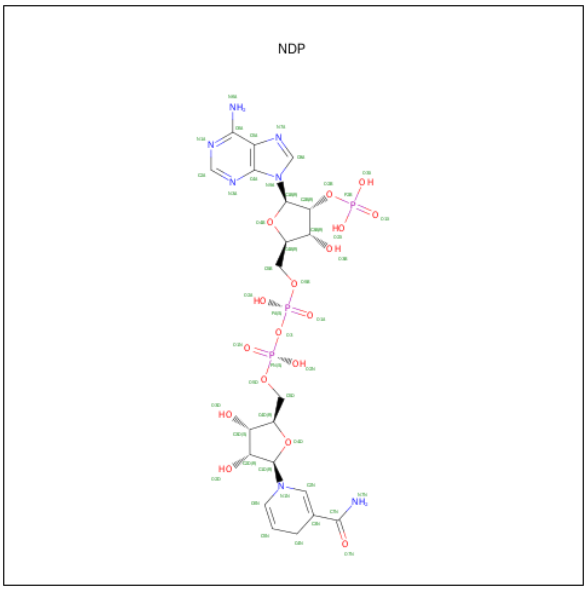
There are 5 unique types of molecules in this entry. The entry contains 21154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			
1	B	505	Total	C	N	O	S	0	0	0
			4095	2619	689	765	22			
1	C	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			
1	D	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	22			
1	E	505	Total	C	N	O	S	0	0	0
			4099	2621	689	767	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	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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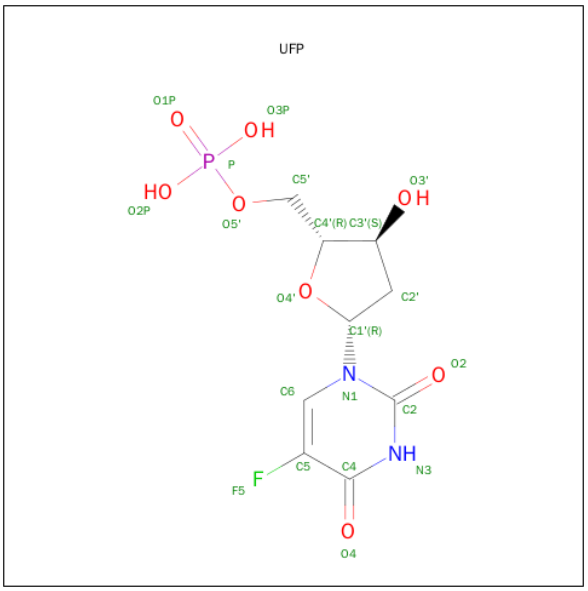
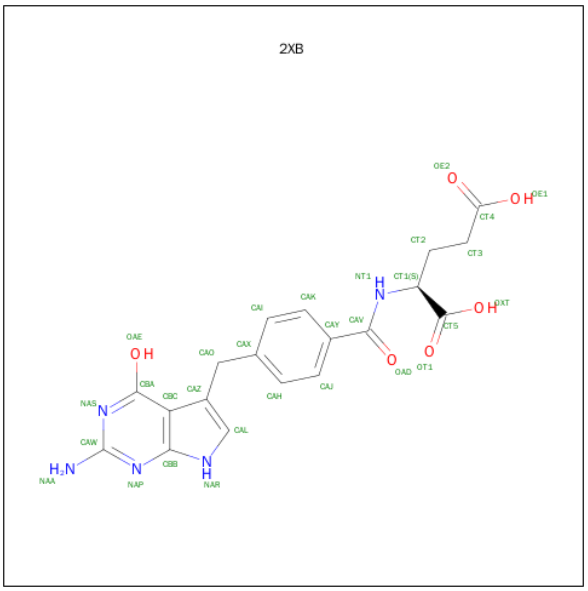
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



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

- 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: $C_{19}H_{19}N_5O_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	2	Total O 2 2	0	0

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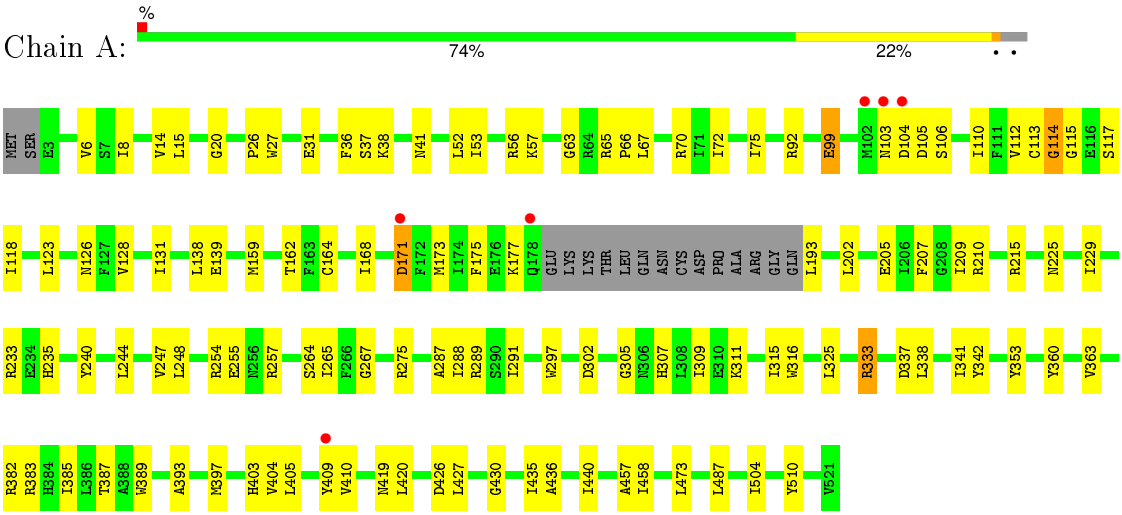
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	6	Total O 6 6	0	0
5	D	1	Total O 1 1	0	0
5	E	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

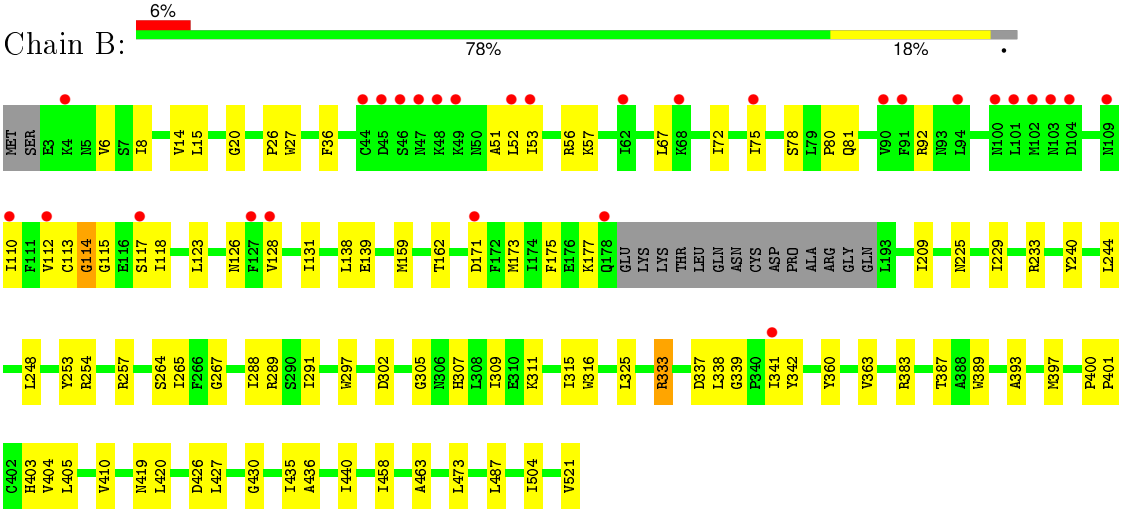
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:



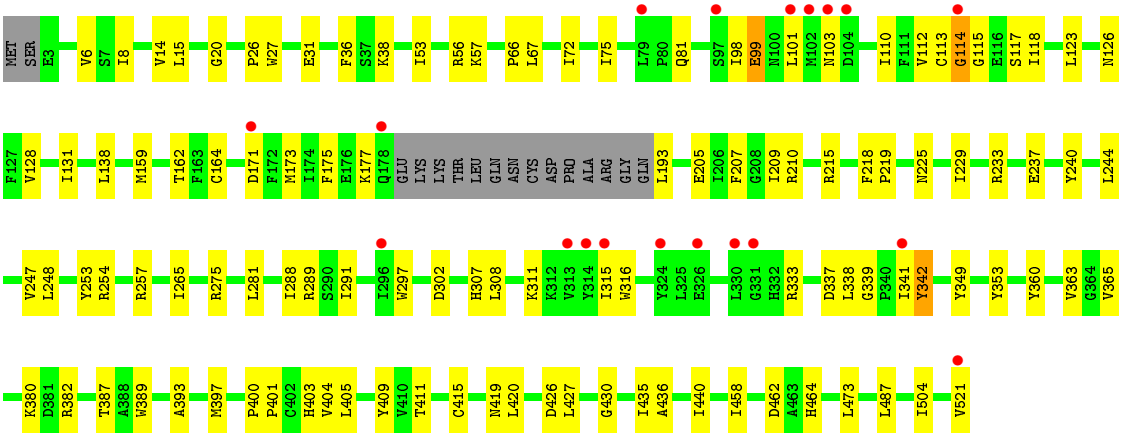
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:



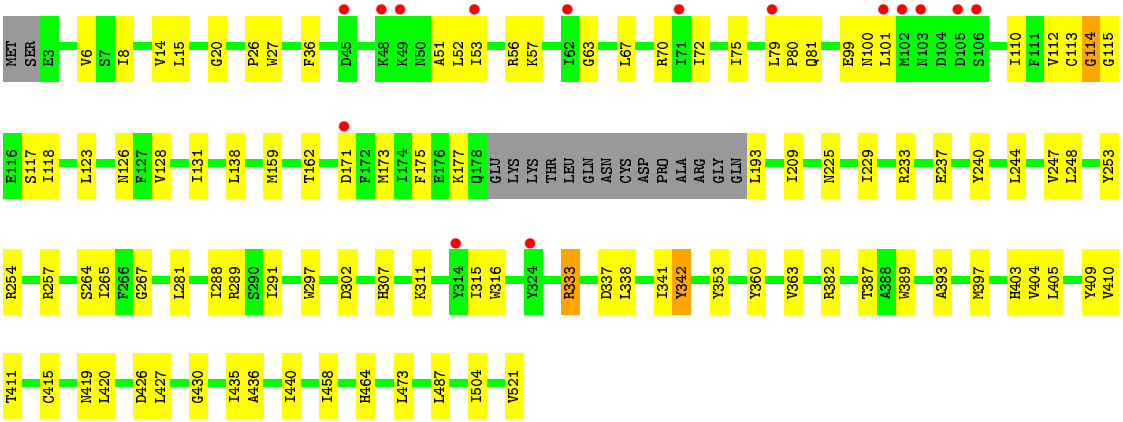
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain C:



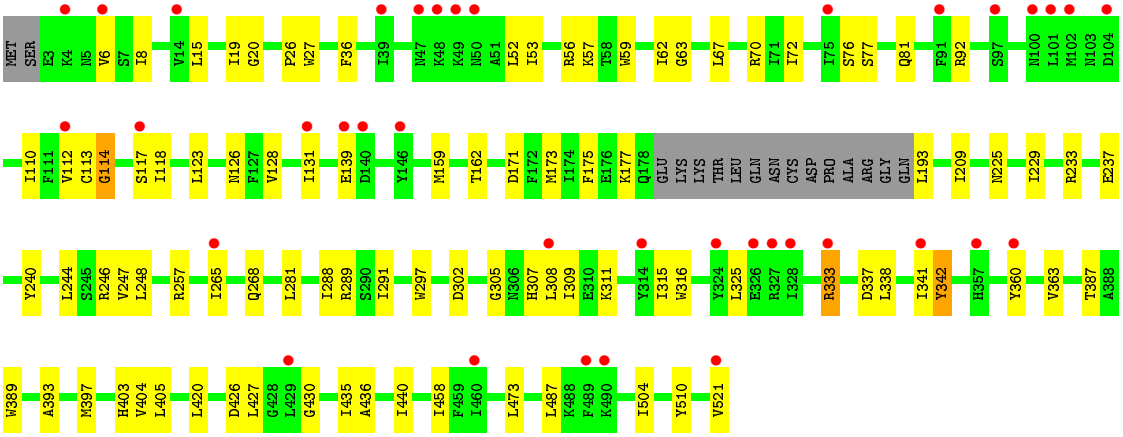
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D:



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.63Å 115.54Å 217.97Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	48.05 – 2.78 48.05 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.05-2.78) 89.0 (48.05-2.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.255 , 0.270 0.265 , 0.276	Depositor DCC
R_{free} test set	2017 reflections (1.73%)	DCC
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 124124 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21154	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UFP, NDP, 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	0.34	1/4194 (0.0%)	0.45	1/5671 (0.0%)
1	B	0.31	1/4190 (0.0%)	0.45	2/5666 (0.0%)
1	C	0.33	1/4194 (0.0%)	0.44	1/5671 (0.0%)
1	D	0.30	1/4194 (0.0%)	0.43	1/5671 (0.0%)
1	E	0.27	1/4194 (0.0%)	0.43	1/5671 (0.0%)
All	All	0.31	5/20966 (0.0%)	0.44	6/28350 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	GLY	C-N	5.30	1.42	1.33
1	A	114	GLY	C-N	5.30	1.42	1.33
1	E	114	GLY	C-N	5.29	1.42	1.33
1	C	114	GLY	C-N	5.29	1.42	1.33
1	B	114	GLY	C-N	5.25	1.42	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	114	GLY	C-N-CA	-6.53	108.58	122.30
1	E	114	GLY	C-N-CA	-6.52	108.61	122.30
1	A	114	GLY	C-N-CA	-6.50	108.66	122.30
1	B	114	GLY	C-N-CA	-6.48	108.69	122.30
1	D	114	GLY	C-N-CA	-6.47	108.72	122.30
1	B	410	VAL	O-C-N	-5.72	113.55	122.70

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	4099	0	4021	100	0
1	B	4095	0	4017	76	0
1	C	4099	0	4021	92	0
1	D	4099	0	4021	83	0
1	E	4099	0	4021	77	0
2	A	48	0	26	12	0
2	B	48	0	26	12	0
2	C	48	0	26	12	0
2	D	48	0	26	12	0
2	E	48	0	26	9	0
3	A	21	0	10	3	0
3	B	21	0	10	3	0
3	C	21	0	10	4	0
3	D	21	0	10	4	0
3	E	21	0	10	2	0
4	A	60	0	34	6	0
4	B	60	0	34	6	0
4	C	60	0	34	6	0
4	D	60	0	34	6	0
4	E	60	0	34	5	0
5	A	8	0	0	2	0
5	B	2	0	0	0	0
5	C	6	0	0	1	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
All	All	21154	0	20451	410	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 10.

All (410) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:GLU:HB2	1:E:510:TYR:CE1	1.44	1.51
1:E:139:GLU:HB2	1:E:510:TYR:CZ	1.68	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ARG:CZ	1:D:409:TYR:OH	1.93	1.15
1:E:139:GLU:CB	1:E:510:TYR:CE1	2.28	1.15
1:B:254:ARG:NE	1:D:409:TYR:OH	1.95	0.98
1:B:254:ARG:HD2	1:B:264:SER:HB3	1.49	0.92
1:C:162:THR:HA	1:C:171:ASP:OD1	1.70	0.90
1:A:56:ARG:H	2:A:601:NDP:H4B	1.39	0.87
1:E:15:LEU:HD12	1:E:139:GLU:HG3	1.56	0.87
1:B:56:ARG:H	2:B:601:NDP:H4B	1.39	0.86
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.38	0.86
1:D:56:ARG:H	2:D:601:NDP:H4B	1.40	0.85
1:B:254:ARG:CZ	1:D:409:TYR:CZ	2.59	0.84
1:D:52:LEU:HD11	1:D:70:ARG:HD2	1.58	0.83
1:E:15:LEU:HB2	1:E:139:GLU:OE2	1.80	0.81
1:B:36:PHE:CE2	4:B:604:2XB:H9	2.17	0.80
1:E:36:PHE:CE2	4:E:604:2XB:H9	2.17	0.80
1:E:247:VAL:HA	1:E:265:ILE:HD12	1.64	0.78
1:B:254:ARG:HD2	1:B:264:SER:CB	2.13	0.78
1:A:36:PHE:CE2	4:A:604:2XB:H9	2.18	0.78
1:A:14:VAL:HG13	1:A:15:LEU:HG	1.65	0.78
1:E:113:CYS:O	4:E:604:2XB:H17	1.84	0.77
1:A:15:LEU:HD11	1:A:510:TYR:HB3	1.65	0.77
1:C:36:PHE:CE2	4:C:604:2XB:H9	2.19	0.77
1:B:113:CYS:O	4:B:604:2XB:H17	1.85	0.77
1:C:56:ARG:H	2:C:601:NDP:H4B	1.50	0.77
1:D:36:PHE:CE2	4:D:604:2XB:H9	2.20	0.76
1:A:409:TYR:OH	1:C:254:ARG:CZ	2.34	0.76
1:D:113:CYS:O	4:D:604:2XB:H17	1.87	0.75
1:A:56:ARG:N	2:A:601:NDP:H4B	2.02	0.74
1:C:113:CYS:O	4:C:604:2XB:H17	1.87	0.74
1:A:113:CYS:O	4:A:604:2XB:H17	1.88	0.74
1:C:56:ARG:N	2:C:601:NDP:H4B	2.03	0.73
1:B:56:ARG:N	2:B:601:NDP:H4B	2.02	0.73
1:B:57:LYS:HG3	2:B:601:NDP:H51A	1.72	0.71
1:D:56:ARG:N	2:D:601:NDP:H4B	2.03	0.71
1:D:57:LYS:HG3	2:D:601:NDP:H51A	1.72	0.71
1:A:57:LYS:HG3	2:A:601:NDP:H51A	1.72	0.71
1:D:333:ARG:HG2	1:D:333:ARG:NH1	1.99	0.70
1:C:57:LYS:HG3	2:C:601:NDP:H51A	1.71	0.70
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.76	0.68
1:B:8:ILE:HG12	1:B:112:VAL:HB	1.76	0.68
1:B:56:ARG:HB3	2:B:601:NDP:O3B	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.75	0.68
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.76	0.68
1:A:56:ARG:HB3	2:A:601:NDP:O3B	1.94	0.67
1:E:139:GLU:CB	1:E:510:TYR:CZ	2.63	0.67
1:D:411:THR:OG1	1:D:415:CYS:HB2	1.93	0.67
1:C:56:ARG:HB3	2:C:601:NDP:O3B	1.95	0.67
2:C:601:NDP:H42N	4:C:604:2XB:CAL	2.24	0.67
1:B:162:THR:HA	1:B:171:ASP:OD1	1.95	0.67
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.76	0.67
1:D:247:VAL:HG22	1:D:265:ILE:HG12	1.75	0.67
1:E:59:TRP:CE3	1:E:62:ILE:HD11	2.29	0.67
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.76	0.67
1:A:52:LEU:HD11	1:A:70:ARG:HD2	1.77	0.67
1:D:162:THR:HA	1:D:171:ASP:OD1	1.95	0.67
2:D:601:NDP:H42N	4:D:604:2XB:CAL	2.24	0.66
1:D:56:ARG:HB3	2:D:601:NDP:O3B	1.95	0.66
2:A:601:NDP:H42N	4:A:604:2XB:CAL	2.25	0.66
1:A:205:GLU:OE1	1:C:38:LYS:NZ	2.29	0.66
2:D:601:NDP:H42N	4:D:604:2XB:CAZ	2.26	0.65
1:E:247:VAL:HA	1:E:265:ILE:CD1	2.26	0.65
1:D:253:TYR:HB3	1:E:63:GLY:HA2	1.78	0.65
1:C:253:TYR:HB3	1:D:63:GLY:HA2	1.76	0.65
2:C:601:NDP:H42N	4:C:604:2XB:CAZ	2.26	0.65
1:E:162:THR:HA	1:E:171:ASP:OD1	1.95	0.65
1:A:63:GLY:HA2	1:B:253:TYR:HB3	1.77	0.65
1:E:257:ARG:NE	3:E:602:UFP:O2P	2.28	0.65
2:A:601:NDP:H42N	4:A:604:2XB:CAZ	2.27	0.65
1:D:333:ARG:CG	1:D:333:ARG:HH11	2.08	0.65
1:D:244:LEU:HD11	1:D:473:LEU:HD13	1.79	0.65
1:B:244:LEU:HD11	1:B:473:LEU:HD13	1.79	0.65
1:A:244:LEU:HD11	1:A:473:LEU:HD13	1.79	0.65
2:B:601:NDP:H42N	4:B:604:2XB:CAL	2.27	0.64
1:C:289:ARG:NH2	1:C:311:LYS:O	2.31	0.64
1:C:229:ILE:HG22	1:C:233:ARG:HG2	1.80	0.64
1:D:289:ARG:NH2	1:D:311:LYS:O	2.31	0.64
1:A:289:ARG:NH2	1:A:311:LYS:O	2.31	0.64
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.63	0.64
1:B:289:ARG:NH2	1:B:311:LYS:O	2.31	0.64
1:E:289:ARG:NH2	1:E:311:LYS:O	2.31	0.64
1:E:333:ARG:HG2	1:E:333:ARG:NH1	2.10	0.64
1:E:229:ILE:HG22	1:E:233:ARG:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:LEU:HD11	1:E:473:LEU:HD13	1.79	0.64
2:B:601:NDP:H42N	4:B:604:2XB:CAZ	2.28	0.63
1:B:333:ARG:NH1	1:B:333:ARG:HG2	2.12	0.63
1:C:244:LEU:HD11	1:C:473:LEU:HD13	1.79	0.63
1:D:53:ILE:O	1:D:113:CYS:HB2	1.99	0.63
1:D:229:ILE:HG22	1:D:233:ARG:HG2	1.80	0.63
1:D:51:ALA:C	1:D:52:LEU:HD23	2.19	0.63
1:A:410:VAL:O	1:C:254:ARG:NH2	2.25	0.63
1:C:257:ARG:NE	3:C:602:UFP:O2P	2.30	0.62
1:C:247:VAL:HG22	1:C:265:ILE:HG12	1.79	0.62
1:B:229:ILE:HG22	1:B:233:ARG:HG2	1.80	0.62
1:B:225:ASN:O	1:B:233:ARG:NH2	2.33	0.62
1:A:275:ARG:HD2	1:C:215:ARG:NH1	2.14	0.62
1:A:409:TYR:OH	1:C:254:ARG:NE	2.33	0.62
1:A:225:ASN:O	1:A:233:ARG:NH2	2.33	0.62
1:C:225:ASN:O	1:C:233:ARG:NH2	2.33	0.62
1:B:254:ARG:NH1	1:D:409:TYR:CE1	2.68	0.62
1:A:53:ILE:O	1:A:113:CYS:HB2	1.99	0.62
1:B:53:ILE:O	1:B:113:CYS:HB2	2.00	0.62
1:A:229:ILE:HG22	1:A:233:ARG:HG2	1.80	0.61
3:B:602:UFP:O1P	1:D:382:ARG:NE	2.32	0.61
1:E:53:ILE:O	1:E:113:CYS:HB2	2.00	0.61
1:D:225:ASN:O	1:D:233:ARG:NH2	2.33	0.61
1:B:333:ARG:HH11	1:B:333:ARG:CG	2.12	0.61
1:E:225:ASN:O	1:E:233:ARG:NH2	2.33	0.61
1:C:53:ILE:O	1:C:113:CYS:HB2	1.99	0.61
1:E:139:GLU:N	1:E:510:TYR:OH	2.33	0.61
1:A:56:ARG:H	2:A:601:NDP:C4B	2.12	0.61
1:E:15:LEU:CD1	1:E:139:GLU:HG3	2.29	0.60
1:A:409:TYR:CZ	1:C:254:ARG:CZ	2.84	0.60
1:B:56:ARG:H	2:B:601:NDP:C4B	2.12	0.60
1:C:99:GLU:CD	1:C:103:ASN:HD21	2.05	0.60
1:A:104:ASP:O	1:A:106:SER:N	2.35	0.59
1:A:104:ASP:C	1:A:106:SER:H	2.03	0.59
3:A:602:UFP:O1P	1:C:382:ARG:NE	2.35	0.59
1:B:254:ARG:NH1	1:D:409:TYR:CZ	2.71	0.59
1:E:15:LEU:HD12	1:E:139:GLU:CG	2.31	0.59
1:D:56:ARG:H	2:D:601:NDP:C4B	2.13	0.59
1:D:117:SER:OG	2:D:601:NDP:O1A	2.21	0.58
1:A:403:HIS:HB2	1:A:420:LEU:HD11	1.85	0.58
1:E:333:ARG:HH11	1:E:333:ARG:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ASN:OD1	1:C:177:LYS:NZ	2.36	0.58
1:C:98:ILE:HG22	1:C:101:LEU:HD13	1.86	0.58
1:C:409:TYR:HA	5:C:706:HOH:O	2.02	0.58
1:A:75:ILE:O	2:A:601:NDP:H1B	2.04	0.57
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.85	0.57
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.86	0.57
1:C:117:SER:OG	2:C:601:NDP:O1A	2.21	0.57
1:E:333:ARG:HH11	1:E:333:ARG:CG	2.17	0.57
1:A:117:SER:OG	2:A:601:NDP:O1A	2.22	0.57
1:B:75:ILE:O	2:B:601:NDP:H1B	2.04	0.57
1:E:126:ASN:OD1	1:E:177:LYS:NZ	2.36	0.57
1:A:126:ASN:OD1	1:A:177:LYS:NZ	2.36	0.57
1:D:114:GLY:O	1:D:118:ILE:HB	2.05	0.57
1:C:56:ARG:HB3	2:C:601:NDP:H4B	1.87	0.56
1:D:75:ILE:O	2:D:601:NDP:H1B	2.05	0.56
1:C:114:GLY:O	1:C:118:ILE:HB	2.06	0.56
1:D:56:ARG:HB3	2:D:601:NDP:H4B	1.87	0.56
1:C:98:ILE:CG2	1:C:101:LEU:HD13	2.35	0.56
1:C:75:ILE:O	2:C:601:NDP:H1B	2.05	0.56
1:A:56:ARG:HB3	2:A:601:NDP:H4B	1.88	0.56
1:A:382:ARG:NE	3:C:602:UFP:O1P	2.39	0.56
1:B:114:GLY:O	1:B:118:ILE:HB	2.06	0.56
1:B:288:ILE:HD11	1:B:440:ILE:HD11	1.88	0.55
1:A:114:GLY:O	1:A:118:ILE:HB	2.06	0.55
1:E:288:ILE:HD11	1:E:440:ILE:HD11	1.89	0.55
1:C:247:VAL:HG22	1:C:265:ILE:CD1	2.37	0.55
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.88	0.55
1:B:56:ARG:HB3	2:B:601:NDP:H4B	1.87	0.55
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.88	0.54
1:D:126:ASN:OD1	1:D:177:LYS:NZ	2.36	0.54
1:C:240:TYR:OH	1:C:427:LEU:O	2.25	0.54
1:A:267:GLY:HA2	1:C:419:ASN:HD21	1.72	0.54
1:E:114:GLY:O	1:E:118:ILE:HB	2.06	0.54
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.89	0.54
1:D:302:ASP:OD2	1:D:307:HIS:ND1	2.40	0.54
1:B:419:ASN:HD21	1:D:267:GLY:HA2	1.73	0.54
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.90	0.53
1:B:56:ARG:CB	2:B:601:NDP:H4B	2.39	0.53
1:B:240:TYR:OH	1:B:427:LEU:O	2.25	0.53
1:B:267:GLY:HA2	1:D:419:ASN:HD21	1.74	0.53
1:A:99:GLU:O	1:A:103:ASN:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:ASP:OD2	1:E:307:HIS:ND1	2.40	0.53
1:A:240:TYR:OH	1:A:427:LEU:O	2.25	0.53
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.90	0.53
1:A:257:ARG:NE	3:A:602:UFP:O2P	2.41	0.53
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.90	0.53
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.41	0.53
1:D:56:ARG:CB	2:D:601:NDP:H4B	2.39	0.53
1:C:56:ARG:CB	2:C:601:NDP:H4B	2.39	0.53
1:B:126:ASN:OD1	1:B:177:LYS:NZ	2.36	0.53
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.90	0.52
1:A:56:ARG:CB	2:A:601:NDP:H4B	2.39	0.52
1:A:409:TYR:CE1	1:C:254:ARG:NH1	2.78	0.52
1:D:247:VAL:HG22	1:D:265:ILE:CD1	2.39	0.52
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.92	0.52
1:A:207:PHE:CE1	1:C:31:GLU:HG2	2.45	0.52
1:E:240:TYR:OH	1:E:427:LEU:O	2.25	0.52
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.90	0.52
1:A:382:ARG:HG2	1:C:462:ASP:OD2	2.10	0.52
1:C:56:ARG:H	2:C:601:NDP:C4B	2.21	0.52
1:D:99:GLU:O	1:D:101:LEU:N	2.43	0.52
1:A:275:ARG:HD2	1:C:215:ARG:CZ	2.40	0.51
1:A:210:ARG:NH2	1:C:164:CYS:O	2.43	0.51
1:E:77:SER:HB3	2:E:601:NDP:H2A	1.92	0.51
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.92	0.51
4:D:604:2XB:H2	4:D:604:2XB:OXT	2.10	0.51
1:B:257:ARG:HH11	3:B:602:UFP:H5'2	1.76	0.51
1:C:302:ASP:OD2	1:C:307:HIS:ND1	2.41	0.51
1:C:411:THR:OG1	1:C:415:CYS:HB2	2.11	0.51
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.46	0.51
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.46	0.51
1:D:123:LEU:HD23	1:D:128:VAL:HG11	1.93	0.51
4:E:604:2XB:H2	4:E:604:2XB:OXT	2.10	0.51
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.92	0.51
1:B:123:LEU:HD23	1:B:128:VAL:HG11	1.93	0.51
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.46	0.50
4:B:604:2XB:H2	4:B:604:2XB:OXT	2.10	0.50
1:E:257:ARG:HH11	3:E:602:UFP:H5'2	1.75	0.50
1:A:342:TYR:CD2	1:A:403:HIS:CE1	2.99	0.50
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.46	0.50
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.92	0.50
4:C:604:2XB:OXT	4:C:604:2XB:H2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:NH1	1:C:275:ARG:HD2	2.26	0.50
4:A:604:2XB:OXT	4:A:604:2XB:H2	2.10	0.50
1:E:56:ARG:HB3	2:E:601:NDP:H4B	1.94	0.50
1:E:123:LEU:HD23	1:E:128:VAL:HG11	1.93	0.50
1:D:240:TYR:OH	1:D:427:LEU:O	2.25	0.50
1:B:138:LEU:O	1:B:139:GLU:HG2	2.12	0.50
1:C:337:ASP:OD1	1:C:353:TYR:OH	2.24	0.50
1:A:342:TYR:CE2	1:A:403:HIS:CE1	3.00	0.50
1:B:302:ASP:OD2	1:B:307:HIS:ND1	2.40	0.50
1:A:123:LEU:HD23	1:A:128:VAL:HG11	1.93	0.50
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.92	0.50
1:D:247:VAL:HG22	1:D:265:ILE:CG1	2.41	0.49
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.94	0.49
1:A:138:LEU:O	1:A:139:GLU:HG2	2.12	0.49
1:A:31:GLU:HG2	1:C:207:PHE:CE1	2.48	0.49
1:A:409:TYR:CZ	1:C:254:ARG:NH1	2.80	0.49
1:E:6:VAL:HG22	1:E:110:ILE:HB	1.95	0.49
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.46	0.49
1:E:342:TYR:CD2	1:E:403:HIS:CE1	3.00	0.49
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.28	0.49
1:B:36:PHE:CE2	4:B:604:2XB:CAK	2.94	0.48
1:C:247:VAL:HG22	1:C:265:ILE:CG1	2.42	0.48
1:A:247:VAL:HG22	1:A:265:ILE:HG12	1.95	0.48
1:E:333:ARG:HA	1:E:333:ARG:HD3	1.66	0.48
1:A:104:ASP:C	1:A:106:SER:N	2.67	0.48
1:A:6:VAL:HG22	1:A:110:ILE:HB	1.96	0.48
1:D:257:ARG:NE	3:D:602:UFP:O2P	2.45	0.48
1:D:6:VAL:HG22	1:D:110:ILE:HB	1.95	0.48
1:E:297:TRP:HH2	1:E:338:LEU:HD12	1.79	0.48
1:A:297:TRP:HH2	1:A:338:LEU:HD12	1.79	0.48
1:D:257:ARG:NH2	1:D:521:VAL:OXT	2.42	0.48
1:E:36:PHE:CE2	4:E:604:2XB:CAK	2.94	0.48
1:E:56:ARG:NH1	2:E:601:NDP:O1X	2.47	0.48
1:A:99:GLU:HB2	1:A:103:ASN:HD21	1.78	0.48
1:A:247:VAL:HG22	1:A:265:ILE:CD1	2.44	0.48
1:B:297:TRP:HH2	1:B:338:LEU:HD12	1.79	0.48
1:C:6:VAL:HG22	1:C:110:ILE:HB	1.95	0.48
1:C:123:LEU:HD23	1:C:128:VAL:HG11	1.93	0.48
1:C:115:GLY:HA2	2:C:601:NDP:O2A	2.14	0.48
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.79	0.47
1:A:115:GLY:HA2	2:A:601:NDP:O2A	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ASP:OD1	1:A:353:TYR:OH	2.24	0.47
1:B:6:VAL:HG22	1:B:110:ILE:HB	1.95	0.47
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.97	0.47
1:D:403:HIS:HB2	1:D:420:LEU:HD11	1.97	0.47
1:E:67:LEU:HG	1:E:72:ILE:HD11	1.97	0.47
1:B:257:ARG:NE	3:B:602:UFP:O2P	2.47	0.47
1:A:255:GLU:HG2	1:C:380:LYS:HD2	1.97	0.47
1:C:339:GLY:O	1:C:341:ILE:N	2.44	0.46
1:E:52:LEU:HD11	1:E:70:ARG:HD2	1.97	0.46
1:D:115:GLY:HA2	2:D:601:NDP:O2A	2.15	0.46
1:E:20:GLY:HA2	1:E:26:PRO:HD3	1.97	0.46
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.97	0.46
1:B:115:GLY:HA2	2:B:601:NDP:O2A	2.14	0.46
1:A:37:SER:O	1:A:41:ASN:ND2	2.48	0.46
1:E:325:LEU:HD13	1:E:333:ARG:HB3	1.97	0.46
1:D:387:THR:HB	1:D:405:LEU:HD12	1.98	0.46
1:C:67:LEU:HG	1:C:72:ILE:HD11	1.97	0.46
1:C:297:TRP:CH2	1:C:341:ILE:HD11	2.51	0.46
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.98	0.46
1:E:92:ARG:HA	1:E:92:ARG:HD3	1.64	0.46
1:E:257:ARG:NH2	1:E:521:VAL:OXT	2.42	0.46
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.98	0.46
1:C:403:HIS:HB2	1:C:420:LEU:HD11	1.97	0.46
1:B:67:LEU:HG	1:B:72:ILE:HD11	1.97	0.46
1:A:164:CYS:O	1:C:210:ARG:NH2	2.49	0.46
1:B:117:SER:OG	2:B:601:NDP:O1A	2.24	0.46
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.98	0.46
1:B:387:THR:HB	1:B:405:LEU:HD12	1.98	0.46
1:A:215:ARG:CZ	1:C:275:ARG:HD2	2.46	0.46
1:D:14:VAL:HG13	1:D:15:LEU:HG	1.98	0.46
1:D:67:LEU:HG	1:D:72:ILE:HD11	1.97	0.46
1:C:341:ILE:O	1:C:342:TYR:C	2.53	0.45
1:B:14:VAL:HG13	1:B:15:LEU:HG	1.99	0.45
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.98	0.45
1:A:325:LEU:HD13	1:A:333:ARG:HB3	1.99	0.45
1:A:387:THR:HB	1:A:405:LEU:HD12	1.98	0.45
1:C:387:THR:HB	1:C:405:LEU:HD12	1.98	0.45
1:A:341:ILE:O	1:A:342:TYR:C	2.54	0.45
1:B:297:TRP:CH2	1:B:341:ILE:HD11	2.51	0.45
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.98	0.45
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:HA	1:A:171:ASP:OD1	2.17	0.45
1:D:333:ARG:HA	1:D:333:ARG:HD3	1.68	0.45
1:D:337:ASP:OD1	1:D:353:TYR:OH	2.24	0.45
1:D:52:LEU:HD23	1:D:52:LEU:N	2.30	0.45
1:C:36:PHE:CE2	4:C:604:2XB:CAK	2.98	0.45
1:B:257:ARG:NH2	1:B:521:VAL:OXT	2.42	0.45
1:C:20:GLY:HA2	1:C:26:PRO:HD3	1.98	0.45
1:E:403:HIS:HB2	1:E:420:LEU:HD11	1.97	0.45
1:D:342:TYR:CD2	1:D:403:HIS:CE1	3.05	0.45
1:C:14:VAL:HG13	1:C:15:LEU:HG	1.99	0.45
1:E:387:THR:HB	1:E:405:LEU:HD12	1.98	0.45
1:D:20:GLY:HA2	1:D:26:PRO:HD3	1.98	0.45
1:B:265:ILE:HG13	1:B:463:ALA:HB3	1.98	0.45
1:E:159:MET:HA	1:E:173:MET:HG2	2.00	0.44
1:B:254:ARG:NH2	1:D:410:VAL:O	2.42	0.44
1:C:257:ARG:HH11	3:C:602:UFP:H5'2	1.82	0.44
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.98	0.44
1:B:159:MET:HA	1:B:173:MET:HG2	2.00	0.44
1:A:63:GLY:O	1:A:65:ARG:HG3	2.17	0.44
2:E:601:NDP:H6N	2:E:601:NDP:H52N	1.99	0.44
1:B:325:LEU:HD13	1:B:333:ARG:HB3	1.99	0.44
1:A:92:ARG:HD3	1:A:92:ARG:HA	1.64	0.44
1:B:487:LEU:HD11	1:B:504:ILE:HG23	2.00	0.44
1:A:159:MET:HA	1:A:173:MET:HG2	2.00	0.44
1:A:487:LEU:HD11	1:A:504:ILE:HG23	2.00	0.44
1:C:257:ARG:NH2	1:C:521:VAL:OXT	2.42	0.43
1:E:487:LEU:HD11	1:E:504:ILE:HG23	2.00	0.43
1:C:487:LEU:HD11	1:C:504:ILE:HG23	2.00	0.43
1:D:159:MET:HA	1:D:173:MET:HG2	1.99	0.43
1:B:254:ARG:NH2	1:D:409:TYR:CZ	2.86	0.43
1:E:57:LYS:HB2	2:E:601:NDP:O3	2.19	0.43
1:A:244:LEU:O	1:A:248:LEU:HB2	2.19	0.43
1:C:338:LEU:N	1:C:338:LEU:CD1	2.82	0.43
1:B:244:LEU:O	1:B:248:LEU:HB2	2.19	0.43
1:E:76:SER:HA	2:E:601:NDP:H1B	2.00	0.43
1:E:81:GLN:OE1	1:E:92:ARG:NH2	2.51	0.43
1:C:159:MET:HA	1:C:173:MET:HG2	2.00	0.43
1:B:51:ALA:C	1:B:52:LEU:HD23	2.39	0.43
1:D:487:LEU:HD11	1:D:504:ILE:HG23	2.00	0.43
1:A:36:PHE:CE2	4:A:604:2XB:CAK	2.96	0.43
1:E:19:ILE:HB	2:E:601:NDP:N7N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ARG:HH11	3:D:602:UFP:H5'2	1.84	0.43
1:E:246:ARG:NH1	1:E:268:GLN:OE1	2.38	0.43
1:E:117:SER:OG	2:E:601:NDP:O1A	2.34	0.43
1:A:287:ALA:HB1	5:A:706:HOH:O	2.19	0.43
1:E:308:LEU:HD12	1:E:308:LEU:HA	1.91	0.42
1:C:393:ALA:O	1:C:397:MET:HG3	2.19	0.42
1:D:244:LEU:O	1:D:248:LEU:HB2	2.19	0.42
1:C:435:ILE:HG12	1:C:458:ILE:HD12	2.02	0.42
1:D:435:ILE:HG12	1:D:458:ILE:HD12	2.01	0.42
1:D:36:PHE:CE2	4:D:604:2XB:CAK	2.98	0.42
1:A:305:GLY:CA	5:A:708:HOH:O	2.66	0.42
1:B:333:ARG:HD3	1:B:333:ARG:HA	1.71	0.42
1:E:244:LEU:O	1:E:248:LEU:HB2	2.19	0.42
1:A:297:TRP:CH2	1:A:341:ILE:HD11	2.55	0.42
1:E:15:LEU:CB	1:E:139:GLU:OE2	2.61	0.42
1:B:393:ALA:O	1:B:397:MET:HG3	2.19	0.42
1:D:254:ARG:HD2	1:D:264:SER:HB3	2.02	0.42
1:B:78:SER:O	1:B:80:PRO:HD3	2.19	0.42
1:D:393:ALA:O	1:D:397:MET:HG3	2.19	0.42
1:E:139:GLU:CB	1:E:510:TYR:CD1	2.98	0.42
1:B:339:GLY:O	1:B:341:ILE:N	2.43	0.42
1:E:393:ALA:O	1:E:397:MET:HG3	2.19	0.42
1:B:81:GLN:NE2	1:B:92:ARG:HH21	2.17	0.42
1:A:257:ARG:HH11	3:A:602:UFP:H5'2	1.84	0.42
1:E:297:TRP:CH2	1:E:341:ILE:HD11	2.55	0.42
1:A:393:ALA:O	1:A:397:MET:HG3	2.19	0.42
1:C:244:LEU:O	1:C:248:LEU:HB2	2.19	0.41
1:A:333:ARG:HD3	1:A:333:ARG:HA	1.69	0.41
1:A:333:ARG:HG3	1:A:337:ASP:HB3	2.01	0.41
1:E:435:ILE:HG12	1:E:458:ILE:HD12	2.01	0.41
1:D:464:HIS:CE1	3:D:602:UFP:HO3'	2.38	0.41
1:E:426:ASP:HB3	1:E:430:GLY:H	1.85	0.41
1:B:360:TYR:O	1:B:363:VAL:HG22	2.20	0.41
1:E:360:TYR:O	1:E:363:VAL:HG22	2.20	0.41
1:A:435:ILE:HG12	1:A:458:ILE:HD12	2.02	0.41
1:C:400:PRO:HA	1:C:401:PRO:HD3	1.92	0.41
1:D:360:TYR:O	1:D:363:VAL:HG22	2.20	0.41
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.92	0.41
1:B:315:ILE:HG13	1:B:316:TRP:CD1	2.56	0.41
1:A:426:ASP:HB3	1:A:430:GLY:H	1.85	0.41
1:A:138:LEU:HD11	1:A:168:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:TRP:CH2	1:D:341:ILE:HD11	2.55	0.41
1:D:341:ILE:O	1:D:342:TYR:C	2.57	0.41
1:A:171:ASP:OD2	1:A:235:HIS:HD2	2.03	0.41
1:E:315:ILE:HG13	1:E:316:TRP:CD1	2.56	0.41
1:D:426:ASP:HB3	1:D:430:GLY:H	1.85	0.41
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.56	0.41
2:E:601:NDP:H42N	4:E:604:2XB:CAO	2.51	0.41
1:D:79:LEU:HA	1:D:80:PRO:HD3	1.85	0.41
1:D:315:ILE:HG13	1:D:316:TRP:CD1	2.56	0.41
1:A:383:ARG:O	1:A:385:ILE:N	2.54	0.41
1:C:360:TYR:O	1:C:363:VAL:HG22	2.20	0.41
1:E:139:GLU:N	1:E:510:TYR:CZ	2.89	0.41
1:C:464:HIS:CE1	3:C:602:UFP:HO3'	2.39	0.41
1:C:338:LEU:HD23	1:C:341:ILE:HD13	2.03	0.41
1:B:426:ASP:HB3	1:B:430:GLY:H	1.86	0.41
1:C:426:ASP:HB3	1:C:430:GLY:H	1.85	0.41
1:B:435:ILE:HG12	1:B:458:ILE:HD12	2.01	0.41
1:A:254:ARG:HD2	1:A:264:SER:HB3	2.03	0.41
1:A:360:TYR:O	1:A:363:VAL:HG22	2.20	0.41
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.56	0.41
1:A:38:LYS:NZ	1:C:205:GLU:OE1	2.54	0.41
1:C:66:PRO:HA	1:C:72:ILE:HD12	2.04	0.40
1:C:237:GLU:HG3	1:C:281:LEU:HD22	2.03	0.40
1:A:341:ILE:O	1:A:342:TYR:O	2.40	0.40
1:A:305:GLY:O	1:A:309:ILE:HG13	2.22	0.40
1:B:305:GLY:O	1:B:309:ILE:HG13	2.22	0.40
1:A:66:PRO:HA	1:A:72:ILE:HD12	2.04	0.40
1:E:305:GLY:O	1:E:309:ILE:HG13	2.22	0.40
1:E:126:ASN:HD21	1:E:177:LYS:HE3	1.86	0.40
1:D:464:HIS:CE1	3:D:602:UFP:O3'	2.74	0.40
1:C:349:TYR:HB3	1:C:365:VAL:HB	2.04	0.40
1:D:237:GLU:HG3	1:D:281:LEU:HD22	2.03	0.40
1:E:237:GLU:HG3	1:E:281:LEU:HD22	2.03	0.40
1:C:218:PHE:HA	1:C:219:PRO:HD3	1.95	0.40
1:E:139:GLU:CG	1:E:510:TYR:CD1	3.05	0.40
1:B:254:ARG:CD	1:D:409:TYR:OH	2.68	0.40
1:A:202:LEU:HD13	1:C:38:LYS:HB3	2.03	0.40
1:C:126:ASN:HD21	1:C:177:LYS:HE3	1.86	0.40
1:C:308:LEU:HA	1:C:308:LEU:HD12	1.91	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	501/521 (96%)	473 (94%)	27 (5%)	1 (0%)	52 84
1	B	501/521 (96%)	472 (94%)	29 (6%)	0	100 100
1	C	501/521 (96%)	473 (94%)	28 (6%)	0	100 100
1	D	501/521 (96%)	469 (94%)	31 (6%)	1 (0%)	52 84
1	E	501/521 (96%)	474 (95%)	27 (5%)	0	100 100
All	All	2505/2605 (96%)	2361 (94%)	142 (6%)	2 (0%)	56 87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	D	100	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/470 (96%)	447 (99%)	5 (1%)	80 95
1	B	451/470 (96%)	447 (99%)	4 (1%)	84 96
1	C	452/470 (96%)	446 (99%)	6 (1%)	76 93
1	D	452/470 (96%)	446 (99%)	6 (1%)	76 93
1	E	452/470 (96%)	448 (99%)	4 (1%)	84 96
All	All	2259/2350 (96%)	2234 (99%)	25 (1%)	80 95

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

Mol	Chain	Res	Type
1	A	99	GLU
1	A	171	ASP
1	A	193	LEU
1	A	209	ILE
1	A	333	ARG
1	B	209	ILE
1	B	333	ARG
1	B	342	TYR
1	B	383	ARG
1	C	81	GLN
1	C	99	GLU
1	C	138	LEU
1	C	193	LEU
1	C	209	ILE
1	C	342	TYR
1	D	81	GLN
1	D	138	LEU
1	D	193	LEU
1	D	209	ILE
1	D	333	ARG
1	D	342	TYR
1	E	193	LEU
1	E	209	ILE
1	E	333	ARG
1	E	342	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	24	GLN
1	A	384	HIS
1	B	5	ASN
1	B	24	GLN
1	C	5	ASN
1	D	5	ASN
1	D	24	GLN
1	E	5	ASN
1	E	24	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	1.86	10 (23%)	55,80,80	1.77	9 (16%)
3	UFP	A	602	-	18,22,22	1.23	1 (5%)	21,33,33	1.78	2 (9%)
4	2XB	A	603	-	26,32,32	2.09	7 (26%)	25,45,45	2.07	5 (20%)
4	2XB	A	604	-	26,32,32	2.10	7 (26%)	25,45,45	2.08	5 (20%)
2	NDP	B	601	-	42,52,52	1.86	10 (23%)	55,80,80	1.77	9 (16%)
3	UFP	B	602	-	18,22,22	1.24	1 (5%)	21,33,33	1.77	2 (9%)
4	2XB	B	603	-	26,32,32	2.08	7 (26%)	25,45,45	2.07	5 (20%)
4	2XB	B	604	-	26,32,32	2.09	7 (26%)	25,45,45	2.08	5 (20%)
2	NDP	C	601	-	42,52,52	1.86	10 (23%)	55,80,80	1.78	9 (16%)
3	UFP	C	602	-	18,22,22	1.23	1 (5%)	21,33,33	1.76	2 (9%)
4	2XB	C	603	-	26,32,32	2.09	7 (26%)	25,45,45	2.07	5 (20%)
4	2XB	C	604	-	26,32,32	2.11	7 (26%)	25,45,45	2.08	5 (20%)
2	NDP	D	601	-	42,52,52	1.87	10 (23%)	55,80,80	1.77	9 (16%)
3	UFP	D	602	-	18,22,22	1.21	1 (5%)	21,33,33	1.78	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	2XB	D	603	-	26,32,32	2.08	7 (26%)	25,45,45	2.07	5 (20%)
4	2XB	D	604	-	26,32,32	2.09	7 (26%)	25,45,45	2.08	5 (20%)
2	NDP	E	601	-	42,52,52	1.88	10 (23%)	55,80,80	1.67	7 (12%)
3	UFP	E	602	-	18,22,22	1.22	1 (5%)	21,33,33	1.80	2 (9%)
4	2XB	E	603	-	26,32,32	2.08	7 (26%)	25,45,45	2.07	5 (20%)
4	2XB	E	604	-	26,32,32	2.10	7 (26%)	25,45,45	2.07	5 (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
4	2XB	A	604	-	1/1/4/5	0/14/21/21	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	2XB	B	603	-	-	0/14/21/21	0/3/3/3
4	2XB	B	604	-	1/1/4/5	0/14/21/21	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	2XB	C	603	-	-	0/14/21/21	0/3/3/3
4	2XB	C	604	-	1/1/4/5	0/14/21/21	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	2XB	D	603	-	-	0/14/21/21	0/3/3/3
4	2XB	D	604	-	1/1/4/5	0/14/21/21	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	2XB	E	603	-	-	0/14/21/21	0/3/3/3
4	2XB	E	604	-	1/1/4/5	0/14/21/21	0/3/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C4N-C5N	-3.99	1.40	1.49
2	D	601	NDP	C4N-C5N	-3.91	1.40	1.49
2	B	601	NDP	C4N-C5N	-3.89	1.40	1.49
2	A	601	NDP	C4N-C5N	-3.87	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NDP	C2D-C3D	-3.85	1.42	1.53
2	C	601	NDP	C4N-C5N	-3.85	1.40	1.49
2	A	601	NDP	C2D-C3D	-3.63	1.43	1.53
2	B	601	NDP	C2D-C3D	-3.62	1.43	1.53
2	C	601	NDP	C2D-C3D	-3.61	1.43	1.53
2	D	601	NDP	C2D-C3D	-3.61	1.43	1.53
2	E	601	NDP	C3B-C2B	-3.59	1.44	1.53
2	A	601	NDP	C3B-C2B	-3.47	1.45	1.53
2	C	601	NDP	C3B-C2B	-3.46	1.45	1.53
2	B	601	NDP	C3B-C2B	-3.45	1.45	1.53
2	D	601	NDP	C3B-C2B	-3.45	1.45	1.53
4	E	603	2XB	CT2-CT1	-2.74	1.49	1.53
4	C	603	2XB	CT2-CT1	-2.74	1.49	1.53
4	A	603	2XB	CT2-CT1	-2.73	1.49	1.53
4	B	603	2XB	CT2-CT1	-2.70	1.49	1.53
4	A	604	2XB	CT2-CT1	-2.69	1.49	1.53
4	D	603	2XB	CT2-CT1	-2.67	1.49	1.53
4	C	604	2XB	CT2-CT1	-2.67	1.49	1.53
4	B	604	2XB	CT2-CT1	-2.66	1.49	1.53
4	E	604	2XB	CT2-CT1	-2.64	1.49	1.53
4	D	604	2XB	CT2-CT1	-2.63	1.49	1.53
4	A	603	2XB	CT1-NT1	-2.36	1.43	1.46
4	C	603	2XB	CT1-NT1	-2.34	1.43	1.46
4	B	603	2XB	CT1-NT1	-2.33	1.43	1.46
2	E	601	NDP	C3B-C4B	-2.33	1.46	1.53
4	D	603	2XB	CT1-NT1	-2.32	1.43	1.46
4	E	603	2XB	CT1-NT1	-2.31	1.43	1.46
2	D	601	NDP	C3B-C4B	-2.28	1.46	1.53
4	C	604	2XB	CT1-NT1	-2.28	1.43	1.46
2	B	601	NDP	C3B-C4B	-2.26	1.46	1.53
2	A	601	NDP	C3B-C4B	-2.25	1.46	1.53
2	C	601	NDP	C3B-C4B	-2.25	1.46	1.53
4	E	604	2XB	CT1-NT1	-2.24	1.43	1.46
4	D	604	2XB	CT1-NT1	-2.24	1.43	1.46
4	A	604	2XB	CT1-NT1	-2.21	1.43	1.46
2	E	601	NDP	C3D-C4D	-2.20	1.47	1.53
4	B	604	2XB	CT1-NT1	-2.16	1.43	1.46
2	C	601	NDP	C3D-C4D	-2.11	1.47	1.53
2	A	601	NDP	C3D-C4D	-2.08	1.47	1.53
2	B	601	NDP	C3D-C4D	-2.07	1.47	1.53
2	D	601	NDP	C3D-C4D	-2.07	1.47	1.53
4	D	604	2XB	OAE-CBA	2.02	1.37	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	2XB	OAE-CBA	2.02	1.37	1.28
4	A	604	2XB	OAE-CBA	2.03	1.37	1.28
4	D	603	2XB	OAE-CBA	2.04	1.37	1.28
4	E	604	2XB	OAE-CBA	2.05	1.37	1.28
4	C	603	2XB	OAE-CBA	2.05	1.37	1.28
4	E	603	2XB	OAE-CBA	2.05	1.37	1.28
4	B	604	2XB	OAE-CBA	2.05	1.37	1.28
4	A	603	2XB	OAE-CBA	2.05	1.38	1.28
4	B	603	2XB	OAE-CBA	2.05	1.38	1.28
2	E	601	NDP	C4A-N3A	2.29	1.39	1.35
2	A	601	NDP	C4A-N3A	2.37	1.39	1.35
2	D	601	NDP	C4A-N3A	2.37	1.39	1.35
2	B	601	NDP	C4A-N3A	2.38	1.39	1.35
2	C	601	NDP	C4A-N3A	2.39	1.39	1.35
2	E	601	NDP	C2N-C3N	2.51	1.40	1.34
2	C	601	NDP	C2N-C3N	2.54	1.40	1.34
2	B	601	NDP	C2N-C3N	2.55	1.40	1.34
2	A	601	NDP	C2N-C3N	2.55	1.40	1.34
2	D	601	NDP	C2N-C3N	2.56	1.41	1.34
3	D	602	UFP	C4-C5	2.61	1.41	1.38
3	A	602	UFP	C4-C5	2.66	1.41	1.38
3	C	602	UFP	C4-C5	2.70	1.41	1.38
3	E	602	UFP	C4-C5	2.71	1.41	1.38
3	B	602	UFP	C4-C5	2.82	1.42	1.38
2	E	601	NDP	C6N-C5N	3.30	1.39	1.33
2	A	601	NDP	C6N-C5N	3.31	1.39	1.33
2	D	601	NDP	C6N-C5N	3.32	1.39	1.33
2	B	601	NDP	C6N-C5N	3.34	1.39	1.33
2	C	601	NDP	C6N-C5N	3.34	1.39	1.33
4	D	603	2XB	CBB-NAR	3.52	1.41	1.34
4	B	603	2XB	CBB-NAR	3.53	1.41	1.34
4	D	604	2XB	CBB-NAR	3.54	1.41	1.34
4	E	603	2XB	CBB-NAR	3.55	1.41	1.34
4	C	604	2XB	CBB-NAR	3.55	1.41	1.34
4	A	603	2XB	CBB-NAR	3.55	1.41	1.34
4	B	604	2XB	CBB-NAR	3.56	1.41	1.34
4	C	603	2XB	CBB-NAR	3.57	1.41	1.34
4	A	604	2XB	CBB-NAR	3.58	1.41	1.34
4	E	604	2XB	CBB-NAR	3.58	1.41	1.34
2	B	601	NDP	C7N-N7N	3.74	1.44	1.33
2	A	601	NDP	C7N-N7N	3.75	1.44	1.33
2	D	601	NDP	C7N-N7N	3.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NDP	C7N-N7N	3.75	1.44	1.33
2	E	601	NDP	C7N-N7N	3.76	1.44	1.33
4	B	603	2XB	CAV-NT1	4.07	1.43	1.34
4	D	603	2XB	CAV-NT1	4.08	1.43	1.34
4	E	603	2XB	CAV-NT1	4.08	1.43	1.34
4	A	603	2XB	CAV-NT1	4.09	1.43	1.34
4	B	604	2XB	CAV-NT1	4.10	1.43	1.34
4	A	604	2XB	CAV-NT1	4.11	1.43	1.34
4	E	604	2XB	CAV-NT1	4.11	1.43	1.34
4	C	604	2XB	CAV-NT1	4.12	1.43	1.34
4	D	604	2XB	CAV-NT1	4.12	1.43	1.34
4	C	603	2XB	CAV-NT1	4.12	1.43	1.34
4	D	603	2XB	CAW-NAA	4.48	1.43	1.34
2	E	601	NDP	C6A-N6A	4.50	1.48	1.34
4	B	603	2XB	CAW-NAA	4.51	1.43	1.34
4	A	603	2XB	CAW-NAA	4.51	1.43	1.34
4	E	603	2XB	CAW-NAA	4.52	1.43	1.34
2	C	601	NDP	C6A-N6A	4.53	1.48	1.34
4	C	603	2XB	CAW-NAA	4.53	1.43	1.34
2	A	601	NDP	C6A-N6A	4.55	1.49	1.34
2	B	601	NDP	C6A-N6A	4.56	1.49	1.34
4	E	604	2XB	CAW-NAA	4.57	1.43	1.34
2	D	601	NDP	C6A-N6A	4.58	1.49	1.34
4	B	604	2XB	CAW-NAA	4.58	1.43	1.34
4	A	604	2XB	CAW-NAA	4.59	1.43	1.34
4	D	604	2XB	CAW-NAA	4.60	1.43	1.34
4	C	604	2XB	CAW-NAA	4.62	1.43	1.34
4	D	603	2XB	CAW-NAS	5.85	1.45	1.35
4	B	603	2XB	CAW-NAS	5.88	1.45	1.35
4	E	603	2XB	CAW-NAS	5.89	1.45	1.35
4	A	603	2XB	CAW-NAS	5.89	1.45	1.35
4	C	603	2XB	CAW-NAS	5.89	1.45	1.35
4	D	604	2XB	CAW-NAS	5.93	1.45	1.35
4	B	604	2XB	CAW-NAS	5.95	1.46	1.35
4	E	604	2XB	CAW-NAS	5.96	1.46	1.35
4	C	604	2XB	CAW-NAS	5.98	1.46	1.35
4	A	604	2XB	CAW-NAS	5.99	1.46	1.35

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	NDP	N3A-C2A-N1A	-8.70	122.23	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NDP	N3A-C2A-N1A	-8.59	122.31	128.89
2	B	601	NDP	N3A-C2A-N1A	-8.57	122.33	128.89
2	D	601	NDP	N3A-C2A-N1A	-8.54	122.36	128.89
2	A	601	NDP	N3A-C2A-N1A	-8.52	122.37	128.89
4	B	604	2XB	NAP-CAW-NAS	-5.96	118.37	127.44
4	A	604	2XB	NAP-CAW-NAS	-5.93	118.41	127.44
4	E	604	2XB	NAP-CAW-NAS	-5.93	118.42	127.44
4	C	604	2XB	NAP-CAW-NAS	-5.92	118.42	127.44
4	D	604	2XB	NAP-CAW-NAS	-5.91	118.45	127.44
4	E	603	2XB	NAP-CAW-NAS	-5.87	118.50	127.44
4	A	603	2XB	NAP-CAW-NAS	-5.87	118.50	127.44
4	B	603	2XB	NAP-CAW-NAS	-5.87	118.50	127.44
4	C	603	2XB	NAP-CAW-NAS	-5.83	118.56	127.44
4	D	603	2XB	NAP-CAW-NAS	-5.83	118.56	127.44
4	C	603	2XB	CBC-CBA-NAS	-4.79	119.59	124.39
4	E	603	2XB	CBC-CBA-NAS	-4.78	119.60	124.39
4	D	603	2XB	CBC-CBA-NAS	-4.76	119.62	124.39
4	A	603	2XB	CBC-CBA-NAS	-4.75	119.63	124.39
4	B	603	2XB	CBC-CBA-NAS	-4.72	119.66	124.39
4	C	604	2XB	CBC-CBA-NAS	-4.65	119.73	124.39
4	D	604	2XB	CBC-CBA-NAS	-4.61	119.77	124.39
4	E	604	2XB	CBC-CBA-NAS	-4.60	119.78	124.39
4	A	604	2XB	CBC-CBA-NAS	-4.58	119.81	124.39
2	D	601	NDP	PN-O3-PA	-4.58	119.87	132.73
2	B	601	NDP	PN-O3-PA	-4.58	119.88	132.73
2	C	601	NDP	PN-O3-PA	-4.57	119.89	132.73
2	A	601	NDP	PN-O3-PA	-4.57	119.90	132.73
4	B	604	2XB	CBC-CBA-NAS	-4.56	119.83	124.39
2	E	601	NDP	PN-O3-PA	-4.19	120.95	132.73
3	A	602	UFP	C5-C4-N3	-3.00	119.00	122.34
3	D	602	UFP	C5-C4-N3	-2.96	119.04	122.34
3	C	602	UFP	C5-C4-N3	-2.93	119.08	122.34
3	B	602	UFP	C5-C4-N3	-2.92	119.08	122.34
3	E	602	UFP	C5-C4-N3	-2.92	119.08	122.34
2	A	601	NDP	C4B-O4B-C1B	-2.90	106.53	109.72
2	B	601	NDP	C4B-O4B-C1B	-2.90	106.53	109.72
2	D	601	NDP	C4B-O4B-C1B	-2.89	106.54	109.72
2	C	601	NDP	C4B-O4B-C1B	-2.89	106.54	109.72
4	B	603	2XB	CAZ-CBC-CBB	-2.88	105.75	110.09
4	D	603	2XB	CAZ-CBC-CBB	-2.87	105.77	110.09
4	E	603	2XB	CAZ-CBC-CBB	-2.86	105.77	110.09
4	A	603	2XB	CAZ-CBC-CBB	-2.84	105.81	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	603	2XB	CAZ-CBC-CBB	-2.84	105.81	110.09
2	C	601	NDP	C4A-C5A-N7A	-2.77	106.93	109.48
4	B	604	2XB	CAZ-CBC-CBB	-2.77	105.91	110.09
4	D	604	2XB	CAZ-CBC-CBB	-2.76	105.93	110.09
4	A	604	2XB	CAZ-CBC-CBB	-2.76	105.93	110.09
2	A	601	NDP	C4A-C5A-N7A	-2.76	106.94	109.48
2	B	601	NDP	C4A-C5A-N7A	-2.75	106.95	109.48
4	C	604	2XB	CAZ-CBC-CBB	-2.75	105.95	110.09
4	E	604	2XB	CAZ-CBC-CBB	-2.74	105.95	110.09
2	D	601	NDP	C4A-C5A-N7A	-2.74	106.96	109.48
2	E	601	NDP	C4A-C5A-N7A	-2.73	106.97	109.48
2	E	601	NDP	O5B-C5B-C4B	2.10	116.87	109.12
2	C	601	NDP	C3D-C2D-C1D	2.10	105.63	101.40
2	A	601	NDP	C3D-C2D-C1D	2.11	105.65	101.40
2	B	601	NDP	C3D-C2D-C1D	2.12	105.66	101.40
4	D	603	2XB	NAA-CAW-NAS	2.12	120.72	117.20
2	D	601	NDP	C3D-C2D-C1D	2.12	105.67	101.40
4	B	603	2XB	NAA-CAW-NAS	2.13	120.72	117.20
4	C	603	2XB	NAA-CAW-NAS	2.13	120.73	117.20
4	E	603	2XB	NAA-CAW-NAS	2.13	120.73	117.20
4	A	603	2XB	NAA-CAW-NAS	2.14	120.74	117.20
4	C	604	2XB	NAA-CAW-NAS	2.15	120.77	117.20
4	A	604	2XB	NAA-CAW-NAS	2.16	120.78	117.20
4	E	604	2XB	NAA-CAW-NAS	2.16	120.78	117.20
4	D	604	2XB	NAA-CAW-NAS	2.16	120.78	117.20
2	C	601	NDP	O5B-C5B-C4B	2.17	117.10	109.12
2	A	601	NDP	O5B-C5B-C4B	2.17	117.13	109.12
2	B	601	NDP	O5B-C5B-C4B	2.18	117.15	109.12
2	D	601	NDP	O5B-C5B-C4B	2.18	117.17	109.12
4	B	604	2XB	NAA-CAW-NAS	2.19	120.83	117.20
2	E	601	NDP	O5D-C5D-C4D	2.25	117.42	109.12
2	E	601	NDP	O3-PA-O5B	2.27	108.95	102.94
2	D	601	NDP	O5D-C5D-C4D	2.27	117.50	109.12
2	A	601	NDP	O5D-C5D-C4D	2.28	117.52	109.12
2	B	601	NDP	O5D-C5D-C4D	2.28	117.52	109.12
2	C	601	NDP	O5D-C5D-C4D	2.29	117.55	109.12
2	E	601	NDP	O3-PN-O5D	2.33	109.11	102.94
2	C	601	NDP	O3-PN-O5D	2.36	109.20	102.94
2	A	601	NDP	O3-PN-O5D	2.37	109.22	102.94
2	B	601	NDP	O3-PN-O5D	2.37	109.24	102.94
2	D	601	NDP	O3-PN-O5D	2.38	109.25	102.94
2	B	601	NDP	O3-PA-O5B	2.47	109.48	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NDP	O3-PA-O5B	2.47	109.49	102.94
2	D	601	NDP	O3-PA-O5B	2.47	109.50	102.94
2	A	601	NDP	O3-PA-O5B	2.48	109.50	102.94
4	B	603	2XB	CT3-CT2-CT1	3.12	119.33	112.99
4	E	603	2XB	CT3-CT2-CT1	3.13	119.35	112.99
4	D	603	2XB	CT3-CT2-CT1	3.13	119.35	112.99
4	C	603	2XB	CT3-CT2-CT1	3.14	119.36	112.99
4	A	603	2XB	CT3-CT2-CT1	3.15	119.39	112.99
4	E	604	2XB	CT3-CT2-CT1	3.19	119.46	112.99
4	B	604	2XB	CT3-CT2-CT1	3.19	119.47	112.99
4	D	604	2XB	CT3-CT2-CT1	3.20	119.49	112.99
4	C	604	2XB	CT3-CT2-CT1	3.20	119.50	112.99
4	A	604	2XB	CT3-CT2-CT1	3.21	119.50	112.99
3	B	602	UFP	C4-N3-C2	6.58	120.94	115.25
3	C	602	UFP	C4-N3-C2	6.66	121.00	115.25
3	D	602	UFP	C4-N3-C2	6.69	121.03	115.25
3	A	602	UFP	C4-N3-C2	6.71	121.05	115.25
3	E	602	UFP	C4-N3-C2	6.79	121.12	115.25

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	2XB	CT1
4	E	604	2XB	CT1
4	C	604	2XB	CT1
4	A	604	2XB	CT1
4	B	604	2XB	CT1

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NDP	12	0
3	A	602	UFP	3	0
4	A	604	2XB	6	0
2	B	601	NDP	12	0
3	B	602	UFP	3	0
4	B	604	2XB	6	0
2	C	601	NDP	12	0
3	C	602	UFP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	604	2XB	6	0
2	D	601	NDP	12	0
3	D	602	UFP	4	0
4	D	604	2XB	6	0
2	E	601	NDP	9	0
3	E	602	UFP	2	0
4	E	604	2XB	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	505/521 (96%)	0.23	6 (1%) 81 75	31, 47, 79, 160	0
1	B	505/521 (96%)	0.36	29 (5%) 27 20	32, 57, 103, 166	0
1	C	505/521 (96%)	0.39	19 (3%) 44 36	32, 52, 91, 175	0
1	D	505/521 (96%)	0.34	15 (2%) 54 46	31, 61, 98, 198	0
1	E	505/521 (96%)	0.70	37 (7%) 18 12	47, 79, 122, 188	0
All	All	2525/2605 (96%)	0.40	106 (4%) 40 32	31, 59, 108, 198	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	MET	6.4
1	A	102	MET	5.6
1	E	102	MET	4.3
1	A	104	ASP	4.3
1	C	521	VAL	4.2
1	A	103	ASN	4.1
1	C	324	TYR	3.7
1	E	328	ILE	3.7
1	C	331	GLY	3.6
1	E	324	TYR	3.6
1	C	102	MET	3.5
1	E	139	GLU	3.5
1	B	94	LEU	3.4
1	B	101	LEU	3.3
1	B	103	ASN	3.3
1	B	53	ILE	3.3
1	B	47	ASN	3.3
1	B	102	MET	3.2
1	C	103	ASN	3.2
1	B	104	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	49	LYS	3.2
1	E	333	ARG	3.1
1	B	127	PHE	3.1
1	E	4	LYS	3.0
1	E	341	ILE	3.0
1	E	360	TYR	3.0
1	E	140	ASP	3.0
1	B	117	SER	2.9
1	E	314	TYR	2.9
1	C	341	ILE	2.9
1	A	171	ASP	2.9
1	E	97	SER	2.9
1	E	101	LEU	2.9
1	B	4	LYS	2.9
1	E	48	LYS	2.8
1	E	49	LYS	2.8
1	C	314	TYR	2.8
1	C	326	GLU	2.8
1	B	91	PHE	2.8
1	E	6	VAL	2.7
1	B	45	ASP	2.7
1	A	178	GLN	2.7
1	D	71	ILE	2.7
1	E	14	VAL	2.7
1	E	489	PHE	2.7
1	C	330	LEU	2.7
1	A	409	TYR	2.7
1	D	103	ASN	2.7
1	E	327	ARG	2.7
1	C	171	ASP	2.7
1	E	521	VAL	2.7
1	B	171	ASP	2.6
1	C	97	SER	2.6
1	D	101	LEU	2.6
1	B	75	ILE	2.6
1	E	117	SER	2.6
1	E	100	ASN	2.5
1	C	101	LEU	2.5
1	E	47	ASN	2.5
1	D	48	LYS	2.5
1	B	112	VAL	2.5
1	E	265	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	104	ASP	2.4
1	B	110	ILE	2.4
1	B	178	GLN	2.4
1	C	296	ILE	2.4
1	E	357	HIS	2.4
1	B	109	ASN	2.4
1	B	46	SER	2.3
1	D	49	LYS	2.3
1	D	106	SER	2.3
1	B	62	ILE	2.3
1	D	171	ASP	2.3
1	D	79	LEU	2.3
1	E	131	ILE	2.3
1	C	79	LEU	2.3
1	B	100	ASN	2.3
1	E	104	ASP	2.3
1	B	128	VAL	2.3
1	E	50	ASN	2.2
1	C	315	ILE	2.2
1	D	53	ILE	2.2
1	E	146	TYR	2.2
1	E	112	VAL	2.2
1	D	324	TYR	2.2
1	D	314	TYR	2.2
1	E	326	GLU	2.2
1	B	341	ILE	2.1
1	C	178	GLN	2.1
1	E	490	LYS	2.1
1	E	429	LEU	2.1
1	D	105	ASP	2.1
1	E	39	ILE	2.1
1	E	75	ILE	2.1
1	E	91	PHE	2.1
1	B	48	LYS	2.1
1	E	460	ILE	2.1
1	B	52	LEU	2.0
1	B	90	VAL	2.0
1	D	62	ILE	2.0
1	C	313	VAL	2.0
1	C	114	GLY	2.0
1	B	68	LYS	2.0
1	E	308	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	44	CYS	2.0
1	D	45	ASP	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	2XB	B	604	30/30	0.81	0.28	1.78	60,66,87,89	0
4	2XB	B	603	30/30	0.88	0.24	1.64	61,69,83,89	0
4	2XB	D	603	30/30	0.86	0.25	1.24	71,79,93,99	0
4	2XB	A	603	30/30	0.87	0.24	1.13	47,55,69,75	0
4	2XB	D	604	30/30	0.87	0.25	1.09	51,57,78,80	0
3	UFP	C	602	21/21	0.92	0.23	0.80	57,66,74,92	0
4	2XB	C	603	30/30	0.85	0.26	0.77	61,69,83,89	0
4	2XB	E	604	30/30	0.85	0.24	0.72	65,72,93,95	0
4	2XB	E	603	30/30	0.83	0.26	0.71	87,95,109,115	0
4	2XB	C	604	30/30	0.87	0.22	0.50	44,50,71,73	0
3	UFP	B	602	21/21	0.93	0.20	0.31	54,64,71,90	0
2	NDP	D	601	48/48	0.85	0.22	0.29	62,73,77,82	0
3	UFP	A	602	21/21	0.92	0.20	0.26	41,50,58,76	0
2	NDP	B	601	48/48	0.85	0.23	0.04	79,90,94,99	0
4	2XB	A	604	30/30	0.89	0.21	-0.02	37,44,64,67	0
2	NDP	C	601	48/48	0.92	0.19	-0.12	45,56,60,65	0
2	NDP	A	601	48/48	0.93	0.17	-0.29	47,58,62,68	0
2	NDP	E	601	48/48	0.91	0.19	-0.57	69,80,84,90	0
3	UFP	D	602	21/21	0.96	0.17	-0.64	60,70,78,96	0
3	UFP	E	602	21/21	0.90	0.19	-0.80	80,89,97,115	0

6.5 Other polymers (i)

There are no such residues in this entry.