



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 AM UTC

PDB ID : 4A0B / pdb_00004a0b
Title : Structure of hsDDB1-drDDB2 bound to a 16 bp CPD-duplex (pyrimidine at D-1 position) at 3.8 Å resolution (CPD 4)
Authors : Scrima, A.; Fischer, E.S.; Iwai, S.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-08
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

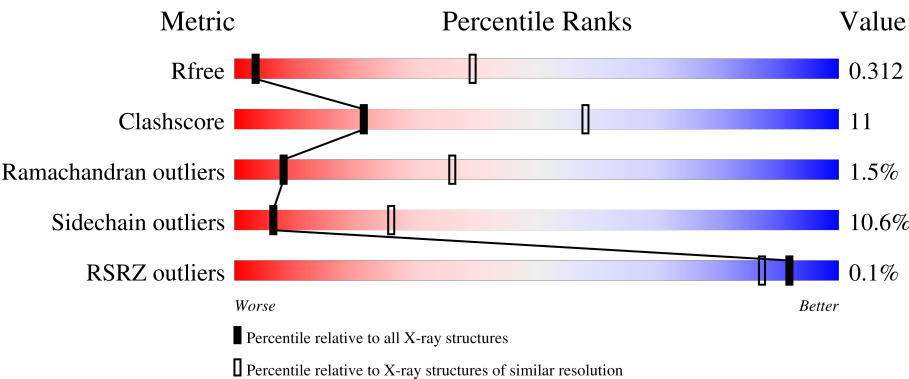
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1159	63%27%•6%
1	C	1159	65%27%•6%
2	B	382	63%26%•7%
2	D	382	65%24%••7%
3	G	15	60%27%7%7%

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Mol	Chain	Length	Quality of chain
3	I	15	 60% 20% 7% 13%
4	H	16	 6% 50% 38% 12%
4	J	16	 6% 81% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23938 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 DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1090	Total	C	N	O	S	0	0	0
			8543	5423	1443	1631	46			
1	C	1095	Total	C	N	O	S	0	0	0
			8582	5447	1449	1639	47			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	HIS	-	expression tag	UNP Q16531
A	-11	VAL	-	expression tag	UNP Q16531
A	-10	ASP	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	224	SER	GLU	engineered mutation	UNP Q16531
C	-18	MET	-	expression tag	UNP Q16531
C	-17	HIS	-	expression tag	UNP Q16531
C	-16	HIS	-	expression tag	UNP Q16531
C	-15	HIS	-	expression tag	UNP Q16531
C	-14	HIS	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP Q16531
C	-12	HIS	-	expression tag	UNP Q16531
C	-11	VAL	-	expression tag	UNP Q16531
C	-10	ASP	-	expression tag	UNP Q16531
C	-9	GLU	-	expression tag	UNP Q16531
C	-8	ASN	-	expression tag	UNP Q16531
C	-7	LEU	-	expression tag	UNP Q16531
C	-6	TYR	-	expression tag	UNP Q16531
C	-5	PHE	-	expression tag	UNP Q16531
C	-4	GLN	-	expression tag	UNP Q16531
C	-3	GLY	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531
C	224	SER	GLU	engineered mutation	UNP Q16531

- Molecule 2 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	354	Total	C	N	O	S	0	0	0
			2839	1804	498	526	11			
2	D	355	Total	C	N	O	S	0	0	0
			2843	1806	499	527	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	MET	-	expression tag	UNP Q2YDS1
B	77	HIS	-	expression tag	UNP Q2YDS1
B	78	HIS	-	expression tag	UNP Q2YDS1
B	79	HIS	-	expression tag	UNP Q2YDS1
B	80	HIS	-	expression tag	UNP Q2YDS1
B	81	HIS	-	expression tag	UNP Q2YDS1
B	82	HIS	-	expression tag	UNP Q2YDS1
B	83	ARG	-	expression tag	UNP Q2YDS1
B	84	ARG	-	expression tag	UNP Q2YDS1
B	85	LEU	-	expression tag	UNP Q2YDS1
B	86	VAL	-	expression tag	UNP Q2YDS1
B	87	PRO	-	expression tag	UNP Q2YDS1
B	88	ARG	-	expression tag	UNP Q2YDS1
B	89	GLY	-	expression tag	UNP Q2YDS1
B	90	SER	-	expression tag	UNP Q2YDS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	91	GLY	-	expression tag	UNP Q2YDS1
B	92	GLY	-	expression tag	UNP Q2YDS1
B	93	ARG	-	expression tag	UNP Q2YDS1
B	180	GLN	LEU	variant	UNP Q2YDS1
B	214	ARG	TRP	variant	UNP Q2YDS1
D	76	MET	-	expression tag	UNP Q2YDS1
D	77	HIS	-	expression tag	UNP Q2YDS1
D	78	HIS	-	expression tag	UNP Q2YDS1
D	79	HIS	-	expression tag	UNP Q2YDS1
D	80	HIS	-	expression tag	UNP Q2YDS1
D	81	HIS	-	expression tag	UNP Q2YDS1
D	82	HIS	-	expression tag	UNP Q2YDS1
D	83	ARG	-	expression tag	UNP Q2YDS1
D	84	ARG	-	expression tag	UNP Q2YDS1
D	85	LEU	-	expression tag	UNP Q2YDS1
D	86	VAL	-	expression tag	UNP Q2YDS1
D	87	PRO	-	expression tag	UNP Q2YDS1
D	88	ARG	-	expression tag	UNP Q2YDS1
D	89	GLY	-	expression tag	UNP Q2YDS1
D	90	SER	-	expression tag	UNP Q2YDS1
D	91	GLY	-	expression tag	UNP Q2YDS1
D	92	GLY	-	expression tag	UNP Q2YDS1
D	93	ARG	-	expression tag	UNP Q2YDS1
D	180	GLN	LEU	variant	UNP Q2YDS1
D	214	ARG	TRP	variant	UNP Q2YDS1

- Molecule 3 is a DNA chain called 5'-D(*DGP*GP*TP*GP*AP*AP*AP*(TTD)P*AP*GP*CP*AP*GP*DGP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	14	Total	C	N	O	P	0	0	0
			312	149	61	88	14			
3	I	13	Total	C	N	O	P	0	0	0
			290	139	56	82	13			

- Molecule 4 is a DNA chain called 5'-D(*CP*CP*TP*GP*CP*TP*CP*CP*TP*TP*TP*CP*AP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	14	Total	C	N	O	P	0	0	0
			274	133	44	84	13			

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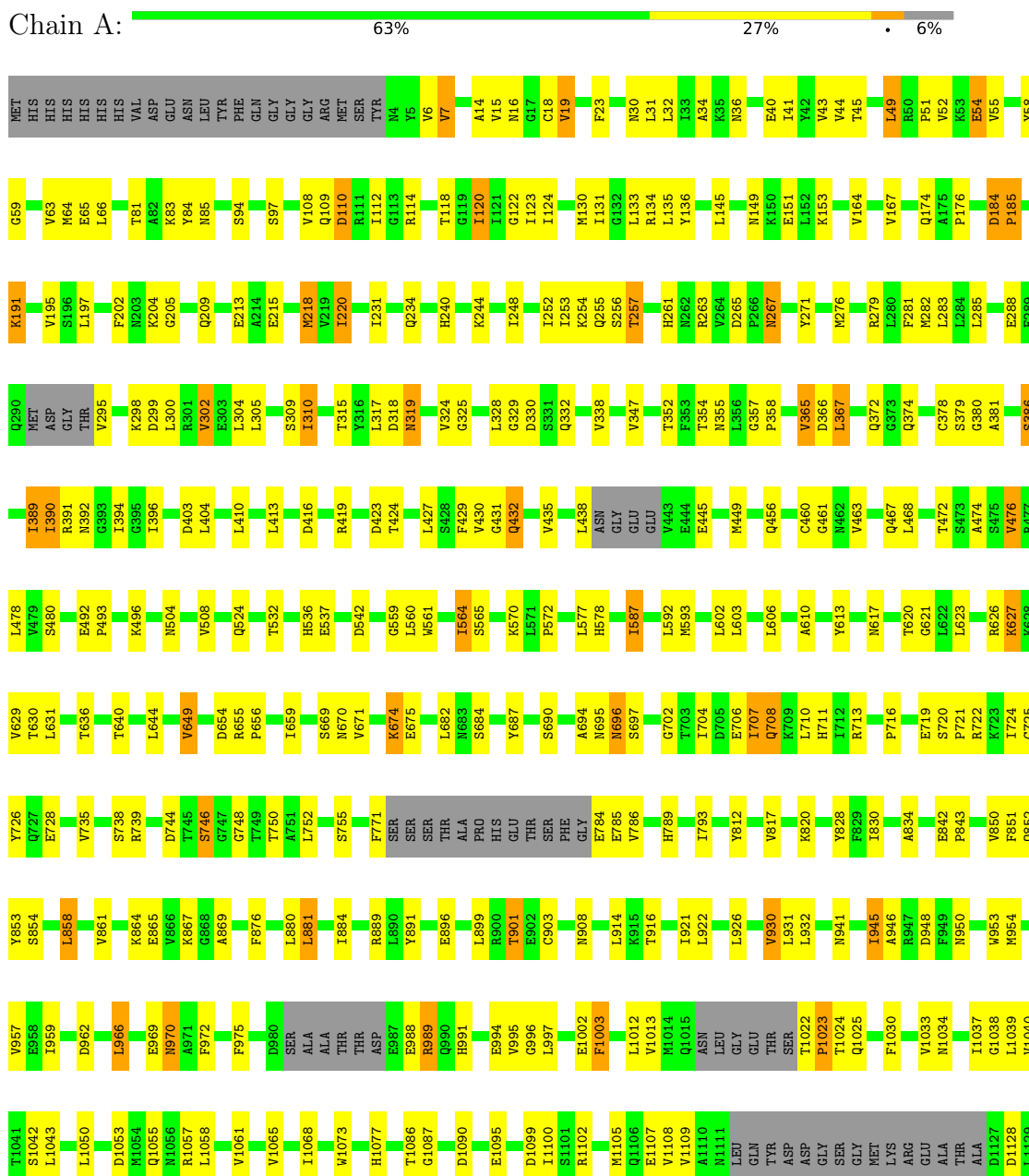
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	13	Total	C	N	O	P	0	0	0
			255	124	41	78	12			

3 Residue-property plots

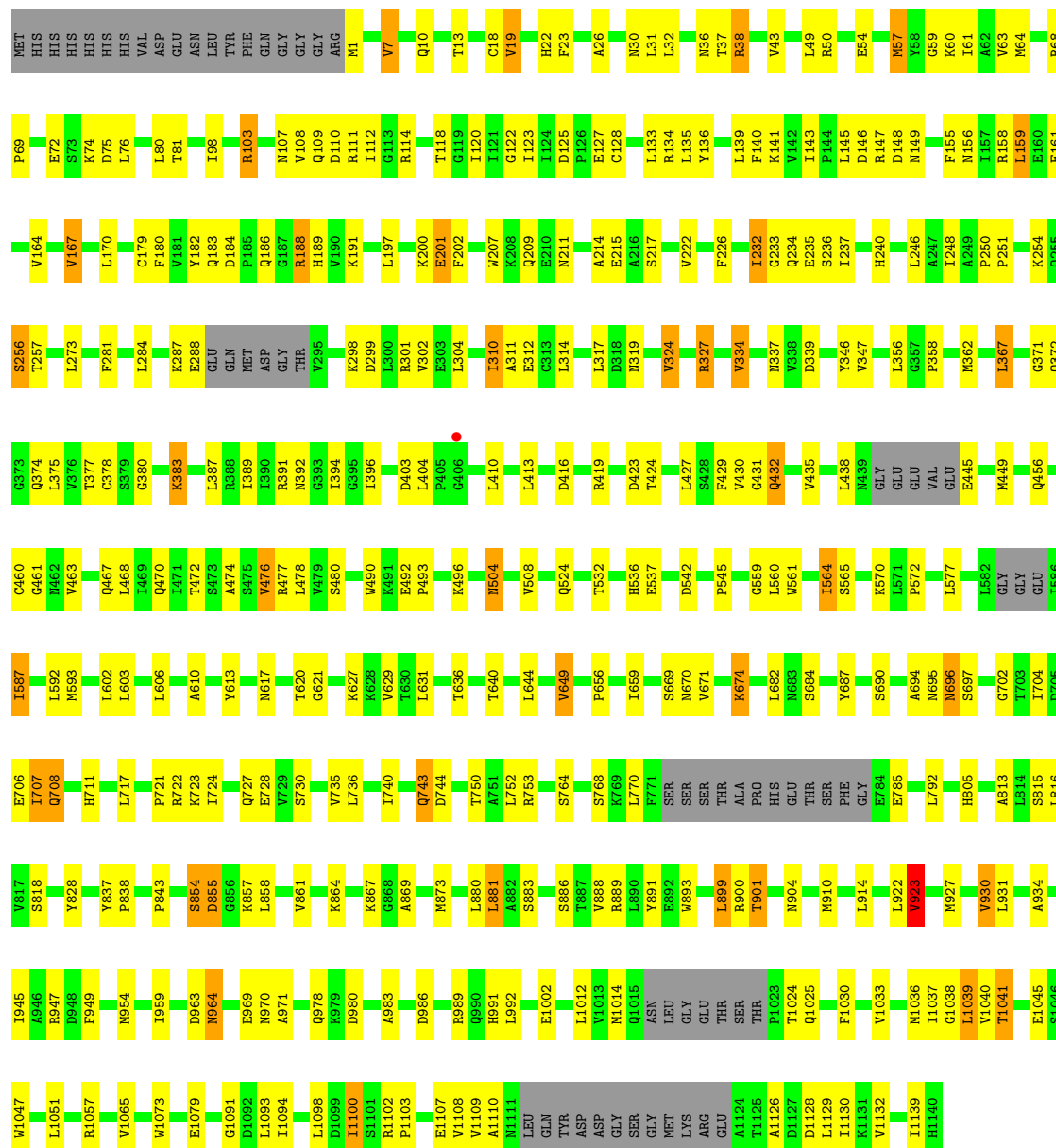
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1



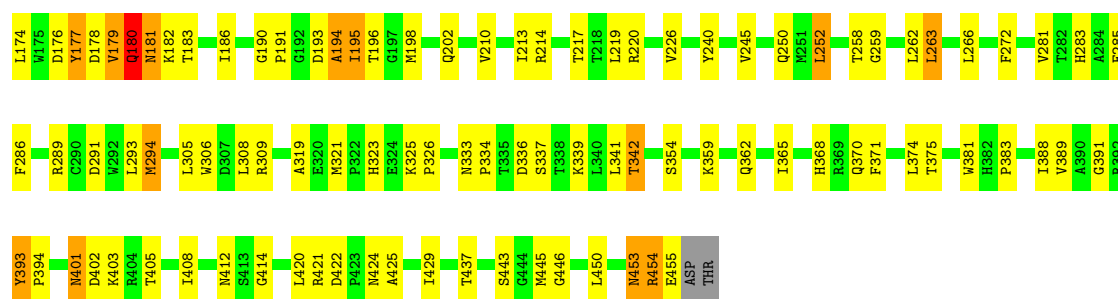


● Molecule 1: DNA DAMAGE-BINDING PROTEIN 1



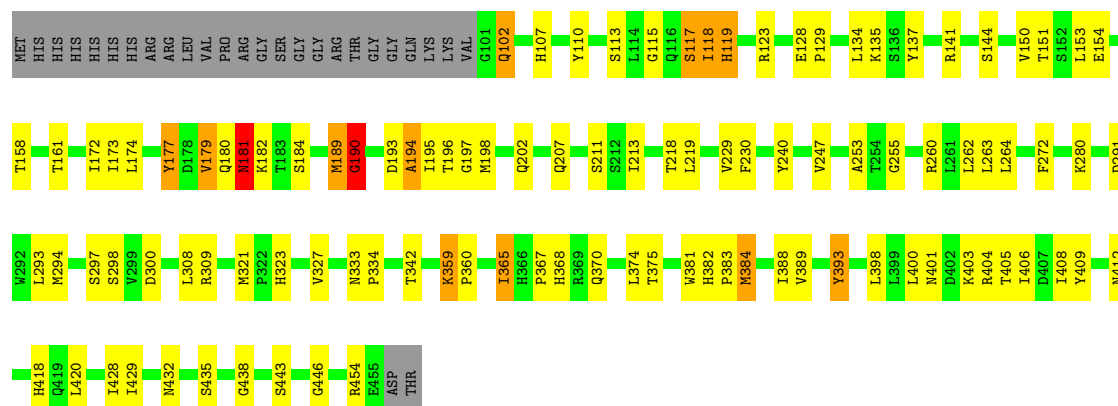
● Molecule 2: DNA DAMAGE-BINDING PROTEIN 2





• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

Chain D: 65% 24% 7%



• Molecule 3: 5'-D(*DGP*GP*TP*GP*AP*AP*AP*(TTD)P*AP*GP*CP*AP*GP*DGP)-3',

Chain G: 60% 27% 7%



• Molecule 3: 5'-D(*DGP*GP*TP*GP*AP*AP*AP*(TTD)P*AP*GP*CP*AP*GP*DGP)-3',

Chain I: 60% 20% 7% 13%



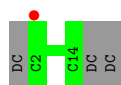
• Molecule 4: 5'-D(*CP*CP*TP*GP*CP*TP*CP*CP*TP*TP*TP*CP*AP*CP*CP*C)-3'

Chain H: 6% 50% 38% 12%



• Molecule 4: 5'-D(*CP*CP*TP*GP*CP*TP*CP*CP*TP*TP*TP*CP*AP*CP*CP*C)-3'

Chain J:  6% 81% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	113.10Å 145.90Å 224.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 3.80 47.72 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.72-3.80) 99.7 (47.72-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.243 , 0.319 0.240 , 0.312	Depositor DCC
R_{free} test set	1862 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	102.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/8697	0.79	4/11777 (0.0%)
1	C	0.48	0/8737	0.78	4/11831 (0.0%)
2	B	0.49	0/2913	0.82	0/3957
2	D	0.48	0/2917	0.83	2/3962 (0.1%)
3	G	0.22	0/306	0.76	0/470
3	I	0.20	0/281	0.67	0/431
4	H	0.25	0/304	0.92	0/465
4	J	0.22	0/283	0.79	0/433
All	All	0.47	0/24438	0.80	10/33326 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1025	GLN	N-CA-C	7.42	119.88	110.24
1	C	785	GLU	N-CA-C	6.11	119.46	110.30
2	D	190	GLY	N-CA-C	5.49	123.53	112.34
1	A	1134	GLU	N-CA-C	5.29	116.73	111.07
2	D	181	ASN	N-CA-C	5.28	117.95	111.82
1	C	234	GLN	N-CA-C	-5.25	107.42	113.88
1	C	923	VAL	N-CA-C	5.23	114.27	106.85
1	A	184	ASP	CA-C-N	5.12	126.24	119.84
1	A	184	ASP	C-N-CA	5.12	126.24	119.84
1	A	1139	ILE	N-CA-C	-5.03	108.39	113.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8543	0	8538	193	0
1	C	8582	0	8588	183	0
2	B	2839	0	2785	64	0
2	D	2843	0	2788	72	0
3	G	312	0	171	8	0
3	I	290	0	160	4	0
4	H	274	0	160	6	0
4	J	255	0	149	0	0
All	All	23938	0	23339	515	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 11.

All (515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HG2	1:A:54:GLU:HG3	1.44	0.97
1:A:864:LYS:HG3	1:A:899:LEU:HB2	1.51	0.93
1:A:204:LYS:HG2	1:A:205:GLY:H	1.33	0.91
1:C:391:ARG:HH21	1:C:711:HIS:HD2	1.18	0.90
2:D:102:GLN:HG3	2:D:107:HIS:HB3	1.54	0.89
1:A:972:PHE:HD1	1:A:1003:PHE:HB3	1.39	0.87
1:C:843:PRO:HG2	1:C:869:ALA:HB2	1.57	0.85
1:A:655:ARG:HD3	1:A:1138:ARG:NH1	1.92	0.84
1:C:362:MET:HE3	1:C:375:LEU:HD11	1.60	0.83
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.61	0.82
1:A:151:GLU:HB2	1:A:153:LYS:HD2	1.59	0.82
1:C:889:ARG:HE	1:C:904:ASN:HD21	1.25	0.82
2:B:128:GLU:HG3	2:B:129:PRO:HD3	1.62	0.81
2:D:128:GLU:HG3	2:D:129:PRO:HD3	1.63	0.80
1:A:392:ASN:HB2	1:A:1012:LEU:HB3	1.63	0.80
2:B:161:THR:O	2:B:176:ASP:HB2	1.80	0.80
1:C:964:ASN:HB3	1:C:978:GLN:HG2	1.62	0.80
1:C:837:TYR:HB3	1:C:838:PRO:HD2	1.65	0.77
1:C:59:GLY:HA2	1:C:1073:TRP:CZ3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HB2	1:A:305:LEU:HD11	1.65	0.76
2:D:263:LEU:HB3	2:D:272:PHE:HB3	1.67	0.75
1:A:19:VAL:HG23	1:A:64:MET:HE3	1.69	0.74
2:B:339:LYS:HE3	2:B:412:ASN:HD21	1.53	0.74
1:C:391:ARG:HH21	1:C:711:HIS:CD2	2.04	0.73
1:A:1022:THR:N	1:A:1023:PRO:HD3	2.01	0.73
1:A:63:VAL:HG11	1:A:122:GLY:HA3	1.70	0.73
2:D:177:TYR:HD1	2:D:177:TYR:H	1.37	0.73
1:C:146:ASP:HB2	1:C:149:ASN:HB2	1.71	0.73
1:C:394:ILE:HD12	1:C:670:ASN:O	1.91	0.71
2:B:323:HIS:NE2	2:B:342:THR:HG21	2.06	0.71
2:D:150:VAL:HG12	2:D:446:GLY:O	1.92	0.70
1:C:170:LEU:HD11	1:C:179:CYS:HB2	1.73	0.70
1:A:996:GLY:HA2	1:A:1087:GLY:HA3	1.74	0.70
2:B:134:LEU:HA	2:B:137:TYR:CD1	2.27	0.70
1:A:655:ARG:HD3	1:A:1138:ARG:HH11	1.53	0.69
1:A:972:PHE:CD1	1:A:1003:PHE:HB3	2.25	0.69
1:C:1102:ARG:HG3	1:C:1103:PRO:HD3	1.73	0.69
2:B:214:ARG:HD3	3:G:9:TTD:H5A2	1.75	0.69
1:A:1033:VAL:HG11	2:B:115:GLY:HA3	1.74	0.69
1:A:394:ILE:HD12	1:A:670:ASN:O	1.93	0.68
1:A:631:LEU:HD23	1:A:1138:ARG:HH22	1.58	0.68
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.76	0.68
1:A:903:CYS:SG	1:A:941:ASN:HA	2.34	0.68
2:D:323:HIS:NE2	2:D:342:THR:HG21	2.08	0.67
2:D:207:GLN:HB3	2:D:219:LEU:HD21	1.77	0.67
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.77	0.66
1:A:81:THR:HG22	1:A:83:LYS:H	1.58	0.66
1:C:857:LYS:HG3	1:C:858:LEU:H	1.61	0.66
2:B:119:HIS:C	2:B:119:HIS:ND1	2.54	0.65
1:A:930:VAL:HG13	1:A:954:MET:HE3	1.79	0.65
1:A:1003:PHE:HZ	2:B:112:SER:O	1.79	0.65
1:C:31:LEU:HD23	1:C:49:LEU:HD21	1.79	0.65
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.31	0.65
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.79	0.65
2:D:119:HIS:ND1	2:D:119:HIS:C	2.55	0.65
2:D:174:LEU:HB3	2:D:184:SER:HB3	1.78	0.65
1:C:1047:TRP:HZ3	1:C:1132:VAL:HG13	1.63	0.64
1:C:22:HIS:HB3	1:C:26:ALA:HA	1.77	0.64
1:A:191:LYS:HG2	1:A:209:GLN:HG3	1.79	0.64
1:A:570:LYS:HG2	1:A:572:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:HG3	2:D:129:PRO:CD	2.28	0.63
1:C:358:PRO:HD2	1:C:380:GLY:HA2	1.81	0.63
1:C:922:LEU:HD22	1:C:959:ILE:HG13	1.81	0.63
1:C:63:VAL:HG11	1:C:122:GLY:HA3	1.81	0.63
1:C:656:PRO:HB2	1:C:671:VAL:HB	1.79	0.62
1:A:726:TYR:HE2	1:A:728:GLU:HG2	1.63	0.62
1:C:19:VAL:HG23	1:C:64:MET:HE3	1.82	0.62
2:D:253:ALA:CB	2:D:294:MET:HE1	2.28	0.62
1:C:423:ASP:HA	1:C:438:LEU:HD12	1.81	0.62
2:B:305:LEU:HD12	2:B:319:ALA:HB3	1.81	0.62
1:A:234:GLN:HG3	1:A:257:THR:HG22	1.80	0.62
1:A:204:LYS:HG2	1:A:205:GLY:N	2.12	0.62
1:A:423:ASP:HA	1:A:438:LEU:HD12	1.81	0.62
2:D:123:ARG:HD3	2:D:384:MET:O	2.00	0.62
1:A:577:LEU:HD23	1:A:621:GLY:HA3	1.82	0.61
1:C:577:LEU:HD23	1:C:621:GLY:HA3	1.83	0.61
2:D:151:THR:HA	2:D:375:THR:HG21	1.83	0.61
1:A:59:GLY:HA2	1:A:1073:TRP:NE1	2.15	0.61
2:D:181:ASN:HD22	2:D:182:LYS:N	1.99	0.61
1:C:112:ILE:HD12	2:D:293:LEU:HD13	1.83	0.61
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.83	0.60
2:D:134:LEU:HA	2:D:137:TYR:CD1	2.36	0.60
1:A:771:PHE:HZ	1:A:865:GLU:HG3	1.65	0.60
2:B:194:ALA:HB3	2:B:213:ILE:HD12	1.83	0.60
1:A:492:GLU:HG2	1:A:493:PRO:HD2	1.83	0.60
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.83	0.60
1:C:492:GLU:HG2	1:C:493:PRO:HD2	1.83	0.60
3:G:6:DA:H1'	3:G:7:DA:H5'	1.84	0.60
1:C:7:VAL:HG13	1:C:1091:GLY:HA3	1.84	0.60
2:B:150:VAL:HG12	2:B:446:GLY:O	2.02	0.60
1:A:726:TYR:CE2	1:A:728:GLU:HG2	2.37	0.59
1:C:690:SER:HA	1:C:702:GLY:O	2.02	0.59
2:D:119:HIS:C	2:D:119:HIS:HD1	2.10	0.59
1:A:14:ALA:HB3	1:A:1034:ASN:HD22	1.67	0.59
1:A:706:GLU:OE1	1:A:711:HIS:HB2	2.02	0.59
1:A:298:LYS:HD3	1:A:299:ASP:HB2	1.84	0.59
1:C:883:SER:HB2	1:C:914:LEU:HD11	1.85	0.59
2:D:102:GLN:HG3	2:D:107:HIS:CB	2.30	0.59
1:A:1003:PHE:CZ	2:B:112:SER:O	2.55	0.59
1:C:334:VAL:HG21	1:C:347:VAL:HG12	1.85	0.59
2:B:323:HIS:HE2	2:B:342:THR:HG21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PRO:O	1:A:379:SER:HA	2.03	0.58
1:A:682:LEU:HB2	1:A:690:SER:O	2.03	0.58
1:C:273:LEU:HB2	1:C:281:PHE:HB2	1.85	0.58
1:C:723:LYS:HB2	1:C:736:LEU:HD12	1.83	0.58
1:A:649:VAL:HG13	1:A:659:ILE:HB	1.84	0.58
1:A:690:SER:HA	1:A:702:GLY:O	2.03	0.58
1:A:1095:GLU:HG2	1:A:1137:THR:HG22	1.85	0.58
1:C:374:GLN:HE22	1:C:391:ARG:HA	1.69	0.58
1:A:84:TYR:HB3	1:A:108:VAL:HG23	1.87	0.57
1:C:1079:GLU:OE2	2:D:123:ARG:NH2	2.36	0.57
1:C:570:LYS:HG2	1:C:572:PRO:HD2	1.86	0.57
2:D:194:ALA:HB3	2:D:213:ILE:HD12	1.86	0.57
2:D:179:VAL:HB	2:D:181:ASN:ND2	2.19	0.57
2:B:129:PRO:HA	2:B:132:ARG:HH11	1.69	0.57
1:C:649:VAL:HG13	1:C:659:ILE:HB	1.86	0.57
1:C:682:LEU:HB2	1:C:690:SER:O	2.05	0.57
2:B:325:LYS:HB3	2:B:326:PRO:HD2	1.86	0.57
1:C:161:GLU:OE2	1:C:191:LYS:HE3	2.05	0.56
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.86	0.56
1:A:828:TYR:HE1	1:A:861:VAL:HG21	1.69	0.56
1:A:954:MET:HE1	1:A:975:PHE:HZ	1.70	0.56
1:C:1051:LEU:HD22	1:C:1094:ILE:HD13	1.87	0.56
1:C:930:VAL:HG22	1:C:954:MET:HE2	1.88	0.56
2:B:193:ASP:HA	2:B:214:ARG:HB3	1.88	0.56
1:C:201:GLU:HG3	1:C:202:PHE:N	2.21	0.56
1:A:954:MET:HE1	1:A:975:PHE:CZ	2.40	0.56
1:A:630:THR:HG21	1:A:1130:ILE:CG1	2.36	0.56
1:C:334:VAL:HG21	1:C:347:VAL:CG1	2.35	0.56
1:A:1061:VAL:HG11	1:A:1108:VAL:CG1	2.36	0.55
1:C:23:PHE:H	1:C:30:ASN:ND2	2.04	0.55
1:C:949:PHE:CZ	1:C:991:HIS:HA	2.41	0.55
2:B:240:TYR:HE1	2:B:262:LEU:HD13	1.70	0.55
2:D:406:ILE:HD11	2:D:429:ILE:HG21	1.88	0.55
1:C:394:ILE:HA	1:C:706:GLU:HG3	1.87	0.55
2:D:141:ARG:HD2	2:D:177:TYR:HB2	1.88	0.55
1:A:467:GLN:HG2	1:A:480:SER:HA	1.89	0.55
1:A:876:PHE:HD1	1:A:916:THR:HG1	1.53	0.55
2:B:453:ASN:HD22	2:B:454:ARG:N	2.05	0.55
1:A:328:LEU:HD23	1:A:381:ALA:HB3	1.89	0.55
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.42	0.55
1:C:391:ARG:NH2	1:C:711:HIS:HD2	1.96	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ILE:HA	1:A:706:GLU:HG3	1.89	0.54
2:B:286:PHE:HE2	2:B:308:LEU:HD21	1.72	0.54
1:C:857:LYS:HG3	1:C:858:LEU:N	2.21	0.54
3:G:6:DA:H2''	3:G:7:DA:OP2	2.08	0.54
1:A:881:LEU:HD13	1:A:914:LEU:HD23	1.88	0.54
1:C:110:ASP:HB2	1:C:136:TYR:CE1	2.43	0.54
1:C:182:TYR:OH	1:C:209:GLN:OE1	2.23	0.53
1:A:329:GLY:HA2	1:A:355:ASN:HB3	1.90	0.53
1:A:670:ASN:HD21	1:A:1138:ARG:HD3	1.74	0.53
1:A:834:ALA:HB2	1:A:869:ALA:HA	1.90	0.53
1:A:309:SER:HB3	1:A:332:GLN:HG2	1.89	0.53
2:B:151:THR:HA	2:B:375:THR:HG21	1.89	0.53
1:C:120:ILE:HG23	1:C:135:LEU:HD23	1.90	0.53
2:D:297:SER:HB2	2:D:327:VAL:HG12	1.90	0.53
1:C:10:GLN:HB3	1:C:1037:ILE:H	1.73	0.53
1:C:232:ILE:HG12	1:C:237:ILE:CD1	2.39	0.53
3:G:3:DG:N2	4:H:14:DC:O2	2.42	0.53
2:D:173:ILE:HG13	2:D:184:SER:O	2.08	0.53
1:C:889:ARG:HE	1:C:904:ASN:ND2	2.01	0.53
2:D:161:THR:HA	2:D:177:TYR:CE1	2.44	0.53
1:C:854:SER:O	1:C:855:ASP:HB3	2.08	0.53
1:A:204:LYS:CG	1:A:205:GLY:H	2.10	0.52
1:A:267:ASN:OD1	1:A:267:ASN:N	2.41	0.52
1:A:830:ILE:HG12	1:A:850:VAL:HG13	1.91	0.52
1:C:888:VAL:HG21	1:C:923:VAL:HG11	1.92	0.52
1:A:921:ILE:O	1:A:932:LEU:HD12	2.08	0.52
1:C:492:GLU:OE1	1:C:496:LYS:HB2	2.10	0.52
1:C:1041:THR:HG21	1:C:1139:ILE:HD12	1.90	0.52
1:C:1047:TRP:CZ3	1:C:1132:VAL:HG13	2.45	0.52
1:C:837:TYR:HB3	1:C:838:PRO:CD	2.39	0.52
3:G:9:TTD:H5R1	3:G:11:DA:C8	2.44	0.52
1:A:7:VAL:HG23	1:A:1039:LEU:HB3	1.92	0.52
1:C:68:ARG:HB2	1:C:75:ASP:OD1	2.10	0.52
1:C:188:ARG:HD2	1:C:215:GLU:H	1.74	0.52
1:C:387:LEU:HG	1:C:717:LEU:HD11	1.90	0.52
2:D:403:LYS:HB3	2:D:405:THR:HG23	1.92	0.52
2:B:339:LYS:HE3	2:B:412:ASN:ND2	2.22	0.52
4:H:7:DC:C2'	4:H:8:DC:H5'	2.39	0.52
1:C:467:GLN:HG2	1:C:480:SER:HA	1.92	0.52
1:C:706:GLU:C	1:C:708:GLN:H	2.18	0.52
2:D:181:ASN:HD22	2:D:182:LYS:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1061:VAL:HG11	1:A:1108:VAL:HG12	1.91	0.51
2:B:119:HIS:C	2:B:119:HIS:HD1	2.16	0.51
1:C:38:ARG:HG3	1:C:54:GLU:OE2	2.10	0.51
2:D:197:GLY:N	2:D:211:SER:OG	2.40	0.51
1:A:404:LEU:HD21	1:A:427:LEU:HD13	1.93	0.51
1:C:934:ALA:HB2	1:C:945:ILE:HD11	1.92	0.51
2:B:250:GLN:HA	2:B:266:LEU:HD12	1.92	0.51
1:C:404:LEU:HD21	1:C:427:LEU:HD13	1.92	0.51
2:B:178:ASP:C	2:B:180:GLN:H	2.19	0.51
1:C:476:VAL:HG21	1:C:508:VAL:HG11	1.93	0.51
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.92	0.51
1:A:472:THR:HG23	1:A:474:ALA:H	1.76	0.51
1:A:1025:GLN:HB3	1:A:1042:SER:HB2	1.92	0.51
1:A:476:VAL:HG21	1:A:508:VAL:HG11	1.93	0.50
1:A:492:GLU:OE1	1:A:496:LYS:HB2	2.10	0.50
1:A:950:ASN:HB2	1:A:994:GLU:OE2	2.11	0.50
1:C:298:LYS:HD3	1:C:299:ASP:HB2	1.93	0.50
2:D:323:HIS:HE2	2:D:342:THR:HG21	1.76	0.50
1:A:134:ARG:HH11	1:A:164:VAL:HB	1.75	0.50
1:C:394:ILE:HD11	1:C:669:SER:HB3	1.92	0.50
1:A:744:ASP:HB2	1:A:750:THR:OG1	2.12	0.50
1:C:429:PHE:HB2	1:C:432:GLN:HB2	1.94	0.50
1:C:460:CYS:SG	1:C:461:GLY:N	2.84	0.50
1:A:130:MET:HE3	1:A:176:PRO:HG2	1.92	0.50
1:A:988:GLU:HA	1:A:991:HIS:CD2	2.47	0.50
1:C:31:LEU:HD13	1:C:317:LEU:HD21	1.92	0.50
1:C:413:LEU:HD11	1:C:468:LEU:HG	1.94	0.50
2:D:388:ILE:O	2:D:408:ILE:HA	2.12	0.50
1:C:232:ILE:HG12	1:C:237:ILE:HD12	1.93	0.50
1:C:288:GLU:OE1	1:C:298:LYS:HG3	2.12	0.50
1:A:724:ILE:HG13	1:A:735:VAL:HG22	1.92	0.50
1:C:828:TYR:CE1	1:C:861:VAL:HG21	2.47	0.50
2:D:161:THR:HA	2:D:177:TYR:OH	2.12	0.50
1:C:617:ASN:HB2	1:C:620:THR:OG1	2.12	0.50
2:D:240:TYR:HE1	2:D:262:LEU:HD13	1.77	0.50
1:A:58:TYR:HB2	1:A:1068:ILE:HB	1.93	0.49
1:A:631:LEU:HD23	1:A:1138:ARG:NH2	2.25	0.49
1:A:365:VAL:HG12	1:A:367:LEU:HG	1.94	0.49
1:A:81:THR:HB	1:A:85:ASN:H	1.77	0.49
1:A:460:CYS:SG	1:A:461:GLY:N	2.85	0.49
2:D:230:PHE:HB3	2:D:264:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:HG23	1:A:261:HIS:CE1	2.46	0.49
1:A:394:ILE:HD11	1:A:669:SER:HB3	1.93	0.49
1:A:630:THR:HG21	1:A:1130:ILE:HG13	1.93	0.49
2:B:170:GLY:HA2	2:B:195:ILE:HD12	1.94	0.49
1:C:927:MET:HE2	2:D:384:MET:HG2	1.93	0.49
1:A:830:ILE:HG23	1:A:850:VAL:HG22	1.95	0.49
1:C:914:LEU:HG	1:C:923:VAL:HG12	1.93	0.49
1:A:15:VAL:HG11	1:A:325:GLY:HA3	1.92	0.49
2:B:263:LEU:CB	2:B:272:PHE:HB3	2.43	0.49
1:C:537:GLU:HB2	1:C:561:TRP:HB2	1.95	0.49
1:C:843:PRO:CG	1:C:869:ALA:HB2	2.36	0.49
1:A:285:LEU:HG	1:A:300:LEU:HD21	1.94	0.49
2:B:259:GLY:HA2	2:B:281:VAL:HG23	1.95	0.49
1:A:429:PHE:HB2	1:A:432:GLN:HB2	1.95	0.48
1:C:374:GLN:NE2	1:C:391:ARG:HA	2.27	0.48
2:B:286:PHE:CE2	2:B:308:LEU:HD21	2.48	0.48
1:A:413:LEU:HD11	1:A:468:LEU:HG	1.96	0.48
1:C:226:PHE:HZ	1:C:287:LYS:HE2	1.78	0.48
1:C:923:VAL:HG23	1:C:931:LEU:HB3	1.95	0.48
1:A:537:GLU:HB2	1:A:561:TRP:HB2	1.95	0.48
1:C:140:PHE:HB2	1:C:159:LEU:HD12	1.95	0.48
1:A:997:LEU:N	1:A:1086:THR:O	2.45	0.48
2:B:333:ASN:HB3	2:B:381:TRP:CE2	2.48	0.48
1:C:10:GLN:HG2	1:C:356:LEU:HD12	1.95	0.48
1:C:18:CYS:HA	1:C:32:LEU:O	2.13	0.48
1:C:764:SER:HG	1:C:805:HIS:HD1	1.61	0.48
1:A:416:ASP:HB2	1:A:419:ARG:HB3	1.96	0.48
2:B:393:TYR:C	2:B:393:TYR:HD1	2.22	0.48
1:C:107:ASN:OD1	1:C:109:GLN:HG2	2.13	0.48
1:C:214:ALA:O	1:C:215:GLU:HB2	2.14	0.48
1:C:969:GLU:OE1	1:C:971:ALA:HB3	2.13	0.48
1:A:410:LEU:HD11	1:A:694:ALA:HB3	1.95	0.48
2:B:388:ILE:O	2:B:408:ILE:HA	2.14	0.48
1:C:410:LEU:HD11	1:C:694:ALA:HB3	1.95	0.48
1:A:1024:THR:HG21	1:A:1139:ILE:HD13	1.95	0.48
1:A:1095:GLU:HG2	1:A:1137:THR:CG2	2.43	0.48
2:B:128:GLU:HG3	2:B:129:PRO:CD	2.39	0.48
1:C:7:VAL:HG23	1:C:1039:LEU:HB3	1.96	0.47
1:A:134:ARG:NH1	1:A:164:VAL:HB	2.29	0.47
1:A:195:VAL:HG22	1:A:202:PHE:HE1	1.79	0.47
2:D:172:ILE:HD11	2:D:195:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HB2	1:C:136:TYR:CD1	2.48	0.47
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.60	0.47
2:B:393:TYR:C	2:B:393:TYR:CD1	2.92	0.47
1:C:472:THR:HG23	1:C:474:ALA:H	1.78	0.47
2:D:297:SER:HB2	2:D:327:VAL:CG1	2.45	0.47
2:D:333:ASN:HB3	2:D:381:TRP:CE2	2.49	0.47
1:A:252:ILE:HG22	1:A:281:PHE:HE1	1.79	0.47
1:C:235:GLU:HG2	1:C:254:LYS:HG3	1.96	0.47
1:C:378:CYS:HB3	1:C:721:PRO:HB2	1.97	0.47
1:C:922:LEU:CD2	1:C:959:ILE:HG13	2.45	0.47
1:A:378:CYS:HB3	1:A:721:PRO:HG2	1.97	0.47
1:A:389:ILE:HD12	1:A:713:ARG:HB3	1.97	0.47
1:A:1053:ASP:O	1:A:1057:ARG:HG3	2.15	0.47
1:C:256:SER:HB3	1:C:257:THR:H	1.61	0.47
1:C:587:ILE:HD13	1:C:587:ILE:H	1.80	0.47
2:D:367:PRO:HB2	2:D:393:TYR:O	2.15	0.47
1:C:167:VAL:HG13	1:C:180:PHE:HB3	1.97	0.47
1:C:312:GLU:HG3	1:C:327:ARG:HD3	1.97	0.47
1:A:606:LEU:HD12	1:A:610:ALA:HB3	1.97	0.47
1:A:722:ARG:NH1	1:A:738:SER:OG	2.48	0.47
1:C:57:MET:HG3	1:C:61:ILE:HD11	1.96	0.47
1:C:139:LEU:HB3	1:C:156:ASN:HD22	1.80	0.47
1:C:764:SER:OG	1:C:805:HIS:ND1	2.47	0.47
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.16	0.46
2:B:341:LEU:HD21	2:B:388:ILE:HG23	1.97	0.46
2:D:393:TYR:C	2:D:393:TYR:HD1	2.24	0.46
1:A:391:ARG:HB3	1:A:711:HIS:HB3	1.97	0.46
1:A:631:LEU:HD12	1:A:636:THR:HG21	1.97	0.46
1:A:706:GLU:C	1:A:708:GLN:H	2.23	0.46
1:A:889:ARG:HD3	1:A:901:THR:HB	1.97	0.46
3:I:2:DG:H2"	3:I:3:DG:C8	2.50	0.46
1:A:627:LYS:HE3	1:A:1105:MET:HE2	1.97	0.46
2:D:393:TYR:C	2:D:393:TYR:CD1	2.93	0.46
1:A:536:HIS:HB2	1:A:560:LEU:HB3	1.98	0.46
1:C:964:ASN:HB3	1:C:978:GLN:CG	2.40	0.46
2:D:117:SER:O	2:D:119:HIS:N	2.48	0.46
2:D:135:LYS:HG2	2:D:418:HIS:CE1	2.51	0.46
2:D:404:ARG:NH1	2:D:428:ILE:HG13	2.30	0.46
1:C:207:TRP:CH2	1:C:240:HIS:HB2	2.50	0.46
1:C:310:ILE:HG23	1:C:383:LYS:HE3	1.98	0.46
2:B:391:GLY:HA3	2:B:429:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:GLN:HE21	1:C:374:GLN:HA	1.79	0.46
1:C:431:GLY:HA2	1:C:456:GLN:HB2	1.97	0.46
2:D:388:ILE:HB	2:D:409:TYR:HB2	1.98	0.46
3:G:9:TTD:O2	3:G:9:TTD:O4'	2.33	0.46
1:A:282:MET:O	1:A:302:VAL:HA	2.16	0.46
1:A:431:GLY:HA2	1:A:456:GLN:HB2	1.98	0.46
1:A:966:LEU:HD11	1:A:1040:VAL:HG21	1.98	0.46
1:C:631:LEU:HD12	1:C:636:THR:HG21	1.98	0.46
4:H:6:DT:H1'	4:H:7:DC:H5'	1.98	0.46
3:I:9:TTD:H6	3:I:9:TTD:H2''	1.76	0.46
1:C:986:ASP:HA	1:C:989:ARG:HG2	1.98	0.45
2:D:255:GLY:HA2	2:D:260:ARG:O	2.16	0.45
2:B:240:TYR:CE1	2:B:262:LEU:HD13	2.51	0.45
2:B:245:VAL:HG12	2:B:252:LEU:HB2	1.97	0.45
1:C:114:ARG:HH12	2:D:412:ASN:HD21	1.63	0.45
1:C:592:LEU:HD21	1:C:640:THR:HG23	1.98	0.45
1:C:603:LEU:HD23	1:C:613:TYR:HB3	1.99	0.45
1:C:1033:VAL:HG11	2:D:115:GLY:HA3	1.98	0.45
1:A:114:ARG:NE	2:B:336:ASP:OD2	2.47	0.45
1:C:60:LYS:O	1:C:81:THR:HA	2.16	0.45
1:C:372:GLN:CG	1:C:374:GLN:HG2	2.46	0.45
1:C:606:LEU:HD12	1:C:610:ALA:HB3	1.98	0.45
1:A:184:ASP:CB	1:A:185:PRO:HD2	2.37	0.45
1:C:467:GLN:HE22	1:C:524:GLN:H	1.64	0.45
1:A:43:VAL:HG22	1:A:52:VAL:HG22	1.98	0.45
1:C:383:LYS:HG2	1:C:753:ARG:NH1	2.31	0.45
1:C:536:HIS:HB2	1:C:560:LEU:HB3	1.97	0.45
1:A:16:ASN:HB3	1:A:34:ALA:O	2.16	0.45
2:B:153:LEU:HD12	2:B:165:VAL:HG22	1.99	0.45
2:B:334:PRO:HG2	2:B:383:PRO:HA	1.99	0.45
4:H:12:DC:H2''	4:H:13:DA:OP2	2.15	0.45
1:A:617:ASN:HB2	1:A:620:THR:OG1	2.17	0.45
1:A:626:ARG:H	1:A:1102:ARG:HB2	1.81	0.45
3:I:3:DG:H2''	3:I:4:DT:H71	1.99	0.45
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.98	0.44
1:A:603:LEU:HD23	1:A:613:TYR:HB3	1.99	0.44
1:A:989:ARG:HA	1:A:989:ARG:NE	2.32	0.44
2:D:218:THR:HG22	2:D:229:VAL:HA	1.99	0.44
2:D:435:SER:O	2:D:438:GLY:N	2.50	0.44
1:A:120:ILE:H	1:A:120:ILE:HG13	1.55	0.44
1:A:869:ALA:O	1:A:884:ILE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:LEU:HB2	1:A:959:ILE:HD11	1.99	0.44
1:C:127:GLU:O	1:C:128:CYS:HB2	2.18	0.44
1:A:94:SER:HB3	1:A:97:SER:HB2	2.00	0.44
1:C:424:THR:HG23	1:C:435:VAL:HG13	2.00	0.44
1:A:84:TYR:HB2	1:A:109:GLN:HB3	2.00	0.44
1:A:631:LEU:CD2	1:A:1138:ARG:HH22	2.27	0.44
1:A:684:SER:HB3	1:A:687:TYR:HB2	1.98	0.44
1:C:69:PRO:HG2	1:C:76:LEU:HD12	1.99	0.44
1:C:470:GLN:OE1	1:C:477:ARG:HD3	2.17	0.44
1:A:19:VAL:HG11	1:A:66:LEU:H	1.81	0.44
1:A:213:GLU:HG2	1:A:215:GLU:H	1.82	0.44
1:C:80:LEU:HD22	1:C:133:LEU:HD11	1.99	0.44
1:C:889:ARG:NE	1:C:904:ASN:HD21	2.04	0.44
1:C:1079:GLU:HG2	1:C:1079:GLU:O	2.18	0.44
1:A:357:GLY:HA2	1:A:358:PRO:C	2.43	0.44
1:A:390:ILE:HD12	1:A:1037:ILE:HD11	2.00	0.44
1:A:424:THR:HG23	1:A:435:VAL:HG13	1.98	0.44
1:C:1057:ARG:HH12	1:C:1110:ALA:HB3	1.82	0.44
1:C:1102:ARG:HG3	1:C:1103:PRO:CD	2.45	0.44
1:A:309:SER:CB	1:A:332:GLN:HG2	2.48	0.44
1:A:926:LEU:HD21	2:B:126:LEU:HD11	1.99	0.44
2:B:403:LYS:HB3	2:B:405:THR:HG23	1.99	0.44
1:C:416:ASP:HB2	1:C:419:ARG:HB3	1.99	0.44
2:D:179:VAL:HB	2:D:181:ASN:HD21	1.83	0.44
1:A:746:SER:C	1:A:748:GLY:H	2.25	0.44
1:A:1128:ASP:HA	1:A:1130:ILE:HG22	1.99	0.44
2:B:161:THR:O	2:B:176:ASP:CB	2.60	0.44
1:C:184:ASP:C	1:C:186:GLN:H	2.26	0.44
1:C:893:TRP:HE3	1:C:899:LEU:HD13	1.83	0.44
1:C:992:LEU:HD23	1:C:992:LEU:HA	1.91	0.44
1:A:255:GLN:H	1:A:255:GLN:HG2	1.58	0.43
1:A:324:VAL:HB	1:A:332:GLN:HB2	1.99	0.43
1:C:72:GLU:OE1	1:C:103:ARG:NH2	2.51	0.43
1:C:684:SER:HB3	1:C:687:TYR:HB2	1.99	0.43
2:D:298:SER:HB3	2:D:300:ASP:OD1	2.18	0.43
1:A:23:PHE:H	1:A:30:ASN:ND2	2.16	0.43
1:A:828:TYR:CE1	1:A:861:VAL:HG21	2.52	0.43
1:C:392:ASN:CB	1:C:1012:LEU:HB3	2.48	0.43
2:D:365:ILE:HG23	2:D:398:LEU:HD21	2.00	0.43
2:D:382:HIS:CG	2:D:383:PRO:HD2	2.54	0.43
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:ILE:HG13	1:C:735:VAL:HG22	2.01	0.43
2:D:161:THR:CA	2:D:177:TYR:CE1	3.01	0.43
1:C:374:GLN:HE22	1:C:391:ARG:CA	2.30	0.43
1:A:31:LEU:HD13	1:A:317:LEU:HD21	2.00	0.43
1:C:108:VAL:HG11	1:C:143:ILE:HD11	1.99	0.43
2:D:177:TYR:CD1	2:D:177:TYR:N	2.73	0.43
3:G:9:TTD:H2"	3:G:9:TTD:H6	1.95	0.43
2:D:432:ASN:OD1	2:D:443:SER:OG	2.32	0.43
1:A:1022:THR:N	1:A:1023:PRO:CD	2.78	0.43
2:B:333:ASN:HA	2:B:334:PRO:HD3	1.89	0.43
2:B:362:GLN:HG2	2:B:414:GLY:HA3	2.00	0.43
1:C:371:GLY:O	1:C:1014:MET:HG2	2.18	0.43
1:C:736:LEU:HD22	1:C:813:ALA:HB1	2.01	0.43
2:D:110:TYR:O	2:D:113:SER:HB3	2.19	0.43
2:D:359:LYS:HA	2:D:360:PRO:HD3	1.91	0.43
1:A:592:LEU:HD21	1:A:640:THR:HG23	2.00	0.43
1:A:695:ASN:C	1:A:697:SER:H	2.26	0.43
1:A:889:ARG:HD2	1:A:891:TYR:CE2	2.53	0.43
1:C:197:LEU:HD23	1:C:197:LEU:H	1.83	0.43
1:C:644:LEU:HB3	1:C:707:ILE:HD13	2.01	0.43
1:C:768:SER:C	1:C:770:LEU:H	2.27	0.43
1:C:843:PRO:HG2	1:C:869:ALA:CB	2.37	0.43
1:C:334:VAL:CG2	1:C:347:VAL:HG12	2.48	0.42
1:C:889:ARG:HD3	1:C:901:THR:HB	1.99	0.42
2:D:117:SER:C	2:D:119:HIS:N	2.77	0.42
1:C:183:GLN:NE2	1:C:188:ARG:HH21	2.16	0.42
1:C:1030:PHE:HE2	1:C:1040:VAL:HG23	1.85	0.42
1:A:112:ILE:HG23	2:B:354:SER:HB2	2.02	0.42
1:A:310:ILE:HG21	1:A:328:LEU:HD13	2.01	0.42
1:A:644:LEU:HB3	1:A:707:ILE:HD13	2.00	0.42
1:A:719:GLU:HG2	1:A:755:SER:HB2	2.01	0.42
2:B:294:MET:HB3	2:B:306:TRP:HB2	2.01	0.42
1:C:59:GLY:HA2	1:C:1073:TRP:CE3	2.53	0.42
1:C:695:ASN:C	1:C:697:SER:H	2.27	0.42
1:A:49:LEU:N	1:A:49:LEU:HD12	2.35	0.42
1:A:467:GLN:HE22	1:A:524:GLN:H	1.65	0.42
1:A:593:MET:HB3	1:A:602:LEU:HD23	2.01	0.42
1:C:337:ASN:O	1:C:346:TYR:HB3	2.19	0.42
1:C:392:ASN:HB3	1:C:1012:LEU:HB3	2.00	0.42
1:C:743:GLN:HG2	1:C:744:ASP:O	2.19	0.42
2:D:154:GLU:HG3	2:D:198:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:CD1	1:A:1037:ILE:HD11	2.50	0.42
2:B:193:ASP:O	2:B:213:ILE:HB	2.20	0.42
1:A:234:GLN:HG3	1:A:257:THR:CG2	2.46	0.42
1:A:587:ILE:HD13	1:A:587:ILE:H	1.84	0.42
1:A:876:PHE:HD1	1:A:916:THR:OG1	2.02	0.42
2:B:210:VAL:O	2:B:217:THR:HA	2.19	0.42
1:C:232:ILE:CG2	1:C:233:GLY:N	2.82	0.42
1:C:727:GLN:HE21	1:C:730:SER:HB2	1.83	0.42
2:D:161:THR:C	2:D:177:TYR:HE1	2.27	0.42
1:A:793:ILE:HG21	1:A:853:TYR:CD1	2.54	0.42
1:C:374:GLN:NE2	1:C:391:ARG:HG3	2.35	0.42
1:A:255:GLN:HG3	1:A:279:ARG:HH12	1.85	0.42
2:B:161:THR:HA	2:B:177:TYR:OH	2.19	0.42
2:B:422:ASP:OD2	2:B:424:ASN:HB2	2.19	0.42
1:C:38:ARG:HD2	1:C:38:ARG:HA	1.85	0.42
1:C:284:LEU:HD22	1:C:301:ARG:HH21	1.84	0.42
1:A:842:GLU:HG2	1:A:843:PRO:HD2	2.00	0.42
2:B:148:ARG:HD3	3:G:9:TTD:OP1	2.20	0.42
2:B:161:THR:HA	2:B:177:TYR:CZ	2.54	0.42
1:C:250:PRO:HA	1:C:251:PRO:HD3	1.88	0.42
1:C:593:MET:HB3	1:C:602:LEU:HD23	2.02	0.42
2:D:128:GLU:N	2:D:129:PRO:HD2	2.35	0.42
1:C:542:ASP:OD2	1:C:593:MET:HG2	2.20	0.42
1:C:695:ASN:OD1	1:C:695:ASN:N	2.48	0.42
1:C:559:GLY:HA2	1:C:565:SER:O	2.21	0.41
1:C:708:GLN:OE1	1:C:708:GLN:HA	2.20	0.41
2:D:280:LYS:O	2:D:298:SER:HA	2.19	0.41
2:D:406:ILE:HG13	2:D:429:ILE:HD13	2.02	0.41
1:A:234:GLN:HE21	1:A:257:THR:HG23	1.85	0.41
1:A:578:HIS:CE1	1:A:623:LEU:H	2.38	0.41
1:A:880:LEU:HB3	1:A:891:TYR:HB2	2.02	0.41
1:C:880:LEU:O	1:C:891:TYR:N	2.52	0.41
2:D:161:THR:HA	2:D:177:TYR:CZ	2.55	0.41
1:A:654:ASP:HA	1:A:675:GLU:HA	2.03	0.41
1:A:953:TRP:O	1:A:970:ASN:HB2	2.21	0.41
2:D:153:LEU:O	2:D:154:GLU:HG2	2.20	0.41
1:A:288:GLU:HB2	1:A:298:LYS:HB2	2.02	0.41
1:C:188:ARG:HD2	1:C:215:GLU:N	2.33	0.41
1:C:1030:PHE:CZ	1:C:1038:GLY:HA3	2.55	0.41
1:A:908:ASN:HD21	1:A:931:LEU:HD13	1.84	0.41
2:D:189:MET:HG3	2:D:190:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLU:HB2	1:A:124:ILE:HD12	2.02	0.41
1:A:708:GLN:OE1	1:A:708:GLN:HA	2.21	0.41
2:B:283:HIS:NE2	2:B:285:GLU:HB2	2.36	0.41
2:B:394:PRO:HB3	2:B:402:ASP:HB3	2.02	0.41
4:H:7:DC:H2'	4:H:8:DC:H5'	2.03	0.41
1:A:789:HIS:CD2	1:A:812:TYR:HA	2.56	0.41
1:A:970:ASN:HD22	1:A:970:ASN:HA	1.68	0.41
1:C:311:ALA:HB2	1:C:324:VAL:HG12	2.02	0.41
1:A:218:MET:HG2	1:A:261:HIS:CD2	2.56	0.41
1:A:930:VAL:HG23	1:A:948:ASP:HB3	2.02	0.41
1:C:362:MET:HB3	1:C:377:THR:HG22	2.03	0.41
2:D:189:MET:O	2:D:193:ASP:HB2	2.21	0.41
1:A:23:PHE:H	1:A:30:ASN:HD22	1.68	0.41
1:A:108:VAL:O	1:A:109:GLN:C	2.64	0.41
1:A:851:PHE:HB3	1:A:858:LEU:HD21	2.02	0.41
1:A:945:ILE:HG22	1:A:946:ALA:N	2.36	0.41
2:B:289:ARG:HD3	2:B:337:SER:HB2	2.03	0.41
2:B:371:PHE:HE1	4:H:8:DC:O2	2.03	0.41
1:C:43:VAL:HG23	1:C:50:ARG:HB2	2.03	0.41
1:C:134:ARG:NH1	1:C:164:VAL:HB	2.35	0.41
1:C:504:ASN:HD22	1:C:545:PRO:HD3	1.86	0.41
1:C:881:LEU:HD13	1:C:914:LEU:CD2	2.51	0.41
1:C:983:ALA:HB3	1:C:989:ARG:HE	1.86	0.41
3:I:3:DG:H2''	3:I:4:DT:C7	2.51	0.41
1:A:988:GLU:O	1:A:991:HIS:HB2	2.21	0.41
2:B:425:ALA:HB1	2:B:445:MET:SD	2.61	0.41
1:C:358:PRO:HD2	1:C:380:GLY:CA	2.50	0.41
1:C:881:LEU:CD1	1:C:914:LEU:HD23	2.51	0.41
1:A:386:SER:HB3	1:A:716:PRO:HA	2.03	0.40
1:A:542:ASP:OD2	1:A:593:MET:HG2	2.20	0.40
1:A:559:GLY:HA2	1:A:565:SER:O	2.22	0.40
1:A:719:GLU:OE1	1:A:739:ARG:HB3	2.21	0.40
1:C:727:GLN:HG3	1:C:818:SER:OG	2.21	0.40
2:B:180:GLN:HB3	2:B:181:ASN:H	1.68	0.40
2:B:220:ARG:HD2	2:B:226:VAL:HG22	2.02	0.40
1:C:155:PHE:CD2	1:C:200:LYS:HG2	2.56	0.40
2:D:207:GLN:HB3	2:D:219:LEU:CD2	2.50	0.40
1:A:988:GLU:HA	1:A:991:HIS:HD2	1.85	0.40
2:B:401:ASN:HD22	2:B:401:ASN:HA	1.57	0.40
1:C:476:VAL:HG13	1:C:490:TRP:HB3	2.03	0.40
2:D:161:THR:C	2:D:177:TYR:CE1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:ASN:HA	2:D:334:PRO:HD3	1.85	0.40
1:A:231:ILE:HD13	1:A:240:HIS:CD2	2.57	0.40
1:A:390:ILE:HG22	1:A:710:LEU:HD12	2.02	0.40
1:C:10:GLN:O	1:C:1036:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1076/1159 (93%)	960 (89%)	100 (9%)	16 (2%)	8	36
1	C	1081/1159 (93%)	953 (88%)	114 (10%)	14 (1%)	9	38
2	B	352/382 (92%)	307 (87%)	36 (10%)	9 (3%)	4	27
2	D	353/382 (92%)	318 (90%)	30 (8%)	5 (1%)	9	37
All	All	2862/3082 (93%)	2538 (89%)	280 (10%)	44 (2%)	8	36

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	ILE
2	B	183	THR
2	B	194	ALA
1	C	707	ILE
1	C	855	ASP
1	A	674	LYS
1	A	707	ILE
1	A	854	SER
1	A	945	ILE
2	B	179	VAL
2	B	190	GLY

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Mol	Chain	Res	Type
1	C	674	LYS
2	D	118	ILE
2	D	190	GLY
2	D	194	ALA
2	D	368	HIS
1	A	367	LEU
2	B	180	GLN
1	C	36	ASN
1	C	367	LEU
2	D	117	SER
1	A	185	PRO
1	A	319	ASN
1	A	696	ASN
2	B	117	SER
1	C	696	ASN
1	C	1128	ASP
1	A	36	ASN
1	A	51	PRO
1	A	330	ASP
1	A	504	ASN
2	B	191	PRO
1	C	111	ARG
1	C	463	VAL
1	C	504	ASN
1	C	963	ASP
1	C	1100	ILE
1	C	1126	ALA
1	A	463	VAL
1	A	1109	VAL
2	B	368	HIS
1	A	1023	PRO
1	A	564	ILE
1	C	564	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	957/1015 (94%)	852 (89%)	105 (11%)	6	24
1	C	962/1015 (95%)	862 (90%)	100 (10%)	7	26
2	B	313/335 (93%)	276 (88%)	37 (12%)	5	22
2	D	313/335 (93%)	285 (91%)	28 (9%)	9	32
All	All	2545/2700 (94%)	2275 (89%)	270 (11%)	6	26

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	VAL
1	A	18	CYS
1	A	19	VAL
1	A	32	LEU
1	A	41	ILE
1	A	44	VAL
1	A	45	THR
1	A	49	LEU
1	A	54	GLU
1	A	55	VAL
1	A	110	ASP
1	A	118	THR
1	A	120	ILE
1	A	123	ILE
1	A	149	ASN
1	A	167	VAL
1	A	174	GLN
1	A	191	LYS
1	A	197	LEU
1	A	218	MET
1	A	220	ILE
1	A	244	LYS
1	A	248	ILE
1	A	253	ILE
1	A	254	LYS
1	A	256	SER
1	A	257	THR
1	A	263	ARG
1	A	265	ASP
1	A	267	ASN
1	A	276	MET
1	A	295	VAL

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Mol	Chain	Res	Type
1	A	302	VAL
1	A	304	LEU
1	A	310	ILE
1	A	315	THR
1	A	318	ASP
1	A	319	ASN
1	A	338	VAL
1	A	347	VAL
1	A	352	THR
1	A	354	THR
1	A	365	VAL
1	A	366	ASP
1	A	372	GLN
1	A	374	GLN
1	A	386	SER
1	A	389	ILE
1	A	390	ILE
1	A	396	ILE
1	A	403	ASP
1	A	430	VAL
1	A	432	GLN
1	A	445	GLU
1	A	449	MET
1	A	476	VAL
1	A	478	LEU
1	A	532	THR
1	A	564	ILE
1	A	587	ILE
1	A	627	LYS
1	A	629	VAL
1	A	649	VAL
1	A	674	LYS
1	A	696	ASN
1	A	704	ILE
1	A	708	GLN
1	A	720	SER
1	A	725	CYS
1	A	746	SER
1	A	752	LEU
1	A	784	GLU
1	A	785	GLU
1	A	786	VAL

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Mol	Chain	Res	Type
1	A	817	VAL
1	A	820	LYS
1	A	852	GLN
1	A	858	LEU
1	A	867	LYS
1	A	881	LEU
1	A	896	GLU
1	A	901	THR
1	A	930	VAL
1	A	957	VAL
1	A	962	ASP
1	A	966	LEU
1	A	969	GLU
1	A	970	ASN
1	A	989	ARG
1	A	995	VAL
1	A	1002	GLU
1	A	1003	PHE
1	A	1013	VAL
1	A	1043	LEU
1	A	1050	LEU
1	A	1058	LEU
1	A	1065	VAL
1	A	1077	HIS
1	A	1099	ASP
1	A	1100	ILE
1	A	1107	GLU
1	A	1130	ILE
1	A	1131	LYS
1	A	1140	HIS
2	B	102	GLN
2	B	118	ILE
2	B	119	HIS
2	B	174	LEU
2	B	177	TYR
2	B	179	VAL
2	B	180	GLN
2	B	181	ASN
2	B	182	LYS
2	B	186	ILE
2	B	195	ILE
2	B	196	THR

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Mol	Chain	Res	Type
2	B	198	MET
2	B	202	GLN
2	B	219	LEU
2	B	252	LEU
2	B	258	THR
2	B	263	LEU
2	B	291	ASP
2	B	293	LEU
2	B	294	MET
2	B	309	ARG
2	B	321	MET
2	B	342	THR
2	B	359	LYS
2	B	365	ILE
2	B	370	GLN
2	B	374	LEU
2	B	389	VAL
2	B	393	TYR
2	B	401	ASN
2	B	420	LEU
2	B	421	ARG
2	B	437	THR
2	B	453	ASN
2	B	454	ARG
2	B	455	GLU
1	C	1	MET
1	C	7	VAL
1	C	13	THR
1	C	19	VAL
1	C	37	THR
1	C	38	ARG
1	C	57	MET
1	C	74	LYS
1	C	98	ILE
1	C	103	ARG
1	C	118	THR
1	C	123	ILE
1	C	125	ASP
1	C	141	LYS
1	C	145	LEU
1	C	147	ARG
1	C	148	ASP

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Mol	Chain	Res	Type
1	C	158	ARG
1	C	159	LEU
1	C	167	VAL
1	C	188	ARG
1	C	189	HIS
1	C	201	GLU
1	C	211	ASN
1	C	217	SER
1	C	222	VAL
1	C	232	ILE
1	C	236	SER
1	C	246	LEU
1	C	248	ILE
1	C	256	SER
1	C	302	VAL
1	C	304	LEU
1	C	310	ILE
1	C	314	LEU
1	C	319	ASN
1	C	324	VAL
1	C	327	ARG
1	C	334	VAL
1	C	339	ASP
1	C	367	LEU
1	C	383	LYS
1	C	389	ILE
1	C	396	ILE
1	C	403	ASP
1	C	430	VAL
1	C	432	GLN
1	C	445	GLU
1	C	449	MET
1	C	476	VAL
1	C	478	LEU
1	C	532	THR
1	C	564	ILE
1	C	587	ILE
1	C	627	LYS
1	C	629	VAL
1	C	649	VAL
1	C	674	LYS
1	C	696	ASN

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Mol	Chain	Res	Type
1	C	704	ILE
1	C	708	GLN
1	C	722	ARG
1	C	728	GLU
1	C	740	ILE
1	C	743	GLN
1	C	750	THR
1	C	752	LEU
1	C	792	LEU
1	C	815	SER
1	C	816	LEU
1	C	854	SER
1	C	864	LYS
1	C	867	LYS
1	C	873	MET
1	C	881	LEU
1	C	886	SER
1	C	899	LEU
1	C	900	ARG
1	C	901	THR
1	C	910	MET
1	C	923	VAL
1	C	930	VAL
1	C	947	ARG
1	C	964	ASN
1	C	970	ASN
1	C	980	ASP
1	C	1002	GLU
1	C	1024	THR
1	C	1039	LEU
1	C	1041	THR
1	C	1045	GLU
1	C	1065	VAL
1	C	1093	LEU
1	C	1098	LEU
1	C	1100	ILE
1	C	1107	GLU
1	C	1108	VAL
1	C	1109	VAL
1	C	1129	LEU
1	C	1130	ILE
2	D	102	GLN

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Mol	Chain	Res	Type
2	D	118	ILE
2	D	119	HIS
2	D	144	SER
2	D	158	THR
2	D	177	TYR
2	D	179	VAL
2	D	180	GLN
2	D	181	ASN
2	D	189	MET
2	D	196	THR
2	D	202	GLN
2	D	247	VAL
2	D	291	ASP
2	D	308	LEU
2	D	309	ARG
2	D	321	MET
2	D	359	LYS
2	D	365	ILE
2	D	370	GLN
2	D	374	LEU
2	D	384	MET
2	D	389	VAL
2	D	393	TYR
2	D	400	LEU
2	D	401	ASN
2	D	420	LEU
2	D	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	30	ASN
1	A	105	HIS
1	A	149	ASN
1	A	209	GLN
1	A	234	GLN
1	A	240	HIS
1	A	241	ASN
1	A	261	HIS
1	A	262	ASN
1	A	455	GLN

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Mol	Chain	Res	Type
1	A	456	GLN
1	A	467	GLN
1	A	507	GLN
1	A	520	GLN
1	A	524	GLN
1	A	528	GLN
1	A	550	ASN
1	A	648	ASN
1	A	670	ASN
1	A	672	ASN
1	A	727	GLN
1	A	796	GLN
1	A	806	GLN
1	A	904	ASN
1	A	907	ASN
1	A	908	ASN
1	A	970	ASN
1	A	991	HIS
1	A	1034	ASN
1	A	1056	ASN
1	A	1140	HIS
2	B	127	GLN
2	B	140	HIS
2	B	269	HIS
2	B	370	GLN
2	B	373	HIS
2	B	401	ASN
2	B	412	ASN
2	B	419	GLN
2	B	453	ASN
1	C	30	ASN
1	C	105	HIS
1	C	183	GLN
1	C	186	GLN
1	C	240	HIS
1	C	241	ASN
1	C	255	GLN
1	C	261	HIS
1	C	319	ASN
1	C	374	GLN
1	C	455	GLN
1	C	456	GLN

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Mol	Chain	Res	Type
1	C	465	HIS
1	C	467	GLN
1	C	507	GLN
1	C	520	GLN
1	C	524	GLN
1	C	528	GLN
1	C	550	ASN
1	C	648	ASN
1	C	670	ASN
1	C	672	ASN
1	C	711	HIS
1	C	727	GLN
1	C	731	GLN
1	C	743	GLN
1	C	796	GLN
1	C	845	GLN
1	C	904	ASN
1	C	907	ASN
1	C	908	ASN
1	C	973	ASN
1	C	1034	ASN
1	C	1070	HIS
1	C	1111	ASN
2	D	102	GLN
2	D	121	GLN
2	D	140	HIS
2	D	181	ASN
2	D	201	ASN
2	D	370	GLN
2	D	373	HIS
2	D	401	ASN
2	D	412	ASN
2	D	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TTD	I	9	3	42,45,46	1.60	8 (19%)	61,74,77	2.74	16 (26%)
3	TTD	G	9	3	42,45,46	1.68	8 (19%)	61,74,77	2.45	17 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTD	I	9	3	-	13/22/109/110	0/5/6/6
3	TTD	G	9	3	-	19/22/109/110	0/5/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	9	TTD	C1'-N1	4.63	1.51	1.45
3	G	9	TTD	C1R-N1T	4.56	1.51	1.45
3	I	9	TTD	C1R-N1T	4.14	1.51	1.45
3	I	9	TTD	C1'-N1	4.13	1.51	1.45
3	G	9	TTD	C2-N1	3.82	1.43	1.36
3	I	9	TTD	C2-N1	3.46	1.43	1.36
3	G	9	TTD	C6-N1	3.43	1.51	1.46
3	G	9	TTD	O4'-C1'	2.93	1.48	1.42
3	I	9	TTD	C2T-N1T	2.91	1.42	1.36
3	I	9	TTD	C6-N1	2.88	1.51	1.46
3	I	9	TTD	C6T-N1T	2.86	1.51	1.46
3	G	9	TTD	C2T-N1T	2.49	1.41	1.36
3	I	9	TTD	O4'-C1'	2.46	1.47	1.42
3	G	9	TTD	C6T-N1T	2.32	1.50	1.46
3	G	9	TTD	C5T-C4T	2.01	1.54	1.51
3	I	9	TTD	C5T-C4T	2.01	1.54	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	9	TTD	O4R-C1R-N1T	13.54	124.69	108.65
3	G	9	TTD	O4R-C1R-N1T	8.05	118.19	108.65
3	I	9	TTD	C5T-C4T-N3T	6.90	121.88	116.09
3	I	9	TTD	C5-C4-N3	6.67	121.69	116.09
3	G	9	TTD	N3-C2-N1	6.47	123.56	116.78
3	G	9	TTD	C5-C4-N3	5.99	121.12	116.09
3	G	9	TTD	C5T-C4T-N3T	5.93	121.07	116.09
3	I	9	TTD	N3-C2-N1	5.53	122.57	116.78
3	G	9	TTD	N3T-C2T-N1T	5.34	122.37	116.78
3	I	9	TTD	N3T-C2T-N1T	5.06	122.08	116.78
3	G	9	TTD	C2R-C1R-N1T	4.86	122.15	115.59
3	G	9	TTD	C4-N3-C2	-3.78	120.97	126.67
3	I	9	TTD	C4'-O4R-C1R	-3.56	101.04	109.51
3	I	9	TTD	C4T-N3T-C2T	-3.54	121.34	126.67
3	G	9	TTD	O4R-C1R-C2R	-3.45	99.80	106.25
3	I	9	TTD	C4-N3-C2	-3.43	121.50	126.67
3	G	9	TTD	C4T-N3T-C2T	-3.27	121.73	126.67
3	G	9	TTD	O4-C4-C5	-3.17	119.76	122.71
3	G	9	TTD	O2-C2-N3	-3.13	115.71	121.49
3	G	9	TTD	C4'-O4R-C1R	-3.10	102.16	109.51
3	I	9	TTD	C2R-C1R-N1T	-3.04	111.48	115.59
3	G	9	TTD	O2T-C2T-N1T	-2.87	119.14	123.44
3	I	9	TTD	O4-C4-C5	-2.87	120.04	122.71
3	I	9	TTD	O4T-C4T-C5T	-2.77	120.13	122.71
3	I	9	TTD	O2-C2-N3	-2.68	116.55	121.49
3	I	9	TTD	C5-C5T-C6T	2.64	91.45	88.36
3	G	9	TTD	C5-C5T-C6T	2.43	91.20	88.36
3	G	9	TTD	O4T-C4T-C5T	-2.37	120.50	122.71
3	G	9	TTD	C5-C6-N1	-2.31	112.59	115.65
3	G	9	TTD	O4R-C4'-C5R	2.26	116.58	109.33
3	I	9	TTD	O4R-C1R-C2R	-2.25	102.03	106.25
3	I	9	TTD	O2T-C2T-N1T	-2.19	120.15	123.44
3	I	9	TTD	O2T-C2T-N3T	-2.06	117.69	121.49

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	9	TTD	C3R-O3R-PB-O4P
3	G	9	TTD	C3R-O3R-PB-O5R
3	G	9	TTD	O4'-C1'-N1-C2
3	G	9	TTD	C5R-O5R-PB-O3R
3	G	9	TTD	C5R-O5R-PB-O5P

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Mol	Chain	Res	Type	Atoms
3	G	9	TTD	O4R-C4'-C5R-O5R
3	I	9	TTD	C2'-C3R-O3R-PB
3	I	9	TTD	O4'-C1'-N1-C2
3	I	9	TTD	C5R-O5R-PB-O5P
3	I	9	TTD	O4R-C4'-C5R-O5R
3	G	9	TTD	C3'-C4'-C5R-O5R
3	G	9	TTD	O4'-C1'-N1-C6
3	I	9	TTD	O4'-C1'-N1-C6
3	G	9	TTD	O4'-C4R-C5'-O5'
3	I	9	TTD	C3'-C4'-C5R-O5R
3	G	9	TTD	C2R-C1R-N1T-C6T
3	I	9	TTD	O4'-C4R-C5'-O5'
3	G	9	TTD	C2R-C1R-N1T-C2T
3	I	9	TTD	C3R-C4R-C5'-O5'
3	I	9	TTD	C2'-C1'-N1-C6
3	G	9	TTD	O4R-C1R-N1T-C6T
3	G	9	TTD	C3R-C4R-C5'-O5'
3	G	9	TTD	O4R-C1R-N1T-C2T
3	G	9	TTD	C2'-C1'-N1-C6
3	G	9	TTD	C2'-C3R-O3R-PB
3	G	9	TTD	C4R-C5'-O5'-P
3	I	9	TTD	C4R-C5'-O5'-P
3	I	9	TTD	O4R-C1R-N1T-C6T
3	I	9	TTD	C2R-C1R-N1T-C6T
3	G	9	TTD	C4'-C5R-O5R-PB
3	I	9	TTD	C2'-C1'-N1-C2
3	G	9	TTD	C3R-O3R-PB-O5P

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	9	TTD	1	0
3	G	9	TTD	5	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1090/1159 (94%)	-0.42	0 100 100	68, 109, 228, 265	0
1	C	1095/1159 (94%)	-0.45	1 (0%) 92 87	70, 106, 215, 247	0
2	B	354/382 (92%)	-0.56	0 100 100	77, 98, 132, 144	0
2	D	355/382 (92%)	-0.49	0 100 100	74, 103, 147, 175	0
3	G	13/15 (86%)	-0.01	0 100 100	128, 164, 217, 229	0
3	I	12/15 (80%)	0.34	0 100 100	167, 206, 232, 286	0
4	H	14/16 (87%)	0.34	1 (7%) 22 19	131, 154, 223, 232	0
4	J	13/16 (81%)	0.79	1 (7%) 19 18	196, 230, 337, 374	0
All	All	2946/3144 (93%)	-0.44	3 (0%) 92 87	68, 106, 219, 374	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	2	DC	2.4
1	C	406	GLY	2.2
4	J	2	DC	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TTD	I	9	40/41	0.86	0.09	164,193,226,236	0
3	TTD	G	9	40/41	0.93	0.08	128,141,161,167	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.