



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:17 AM UTC

PDB ID : 1K8G / pdb_00001k8g
Title : Crystal Structure of the N-terminal domain of Oxytricha nova telomere end binding protein alpha subunit both uncomplexed and complexed with telomeric ssDNA
Authors : Classen, S.; Ruggles, J.A.; Schultz, S.C.
Deposited on : 2001-10-24
Resolution : 2.60 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

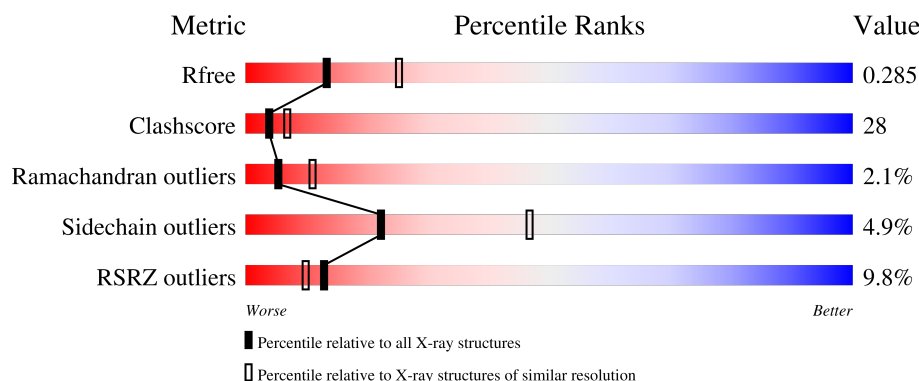
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	D	6	17% 67% 33%
1	E	6	17% 50% 33%
2	A	320	9% 45% 34% • 16%
2	B	320	8% 40% 41% 5% • 14%
2	C	320	9% 40% 41% 5% 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7040 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.

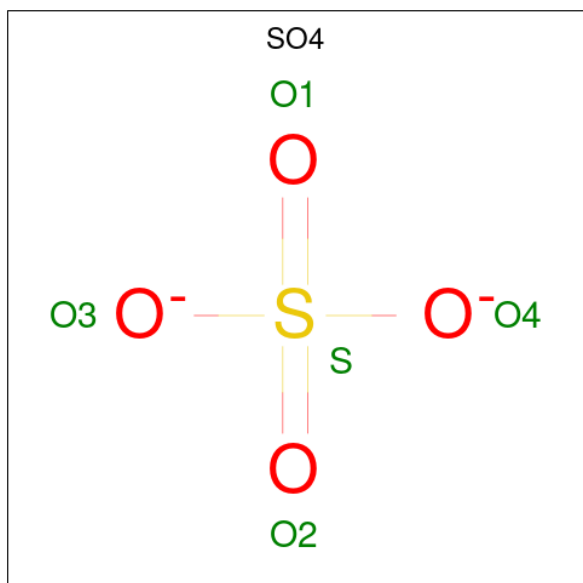
- Molecule 1 is a DNA chain called 5'-D(TP*TP*GP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	4	Total	C	N	O	P	0	0	0
			85	40	20	22	3			
1	E	4	Total	C	N	O	P	0	0	0
			85	40	20	22	3			

- Molecule 2 is a protein called Telomere-Binding Protein alpha Subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	269	Total	C	N	O	S	0	0	0
			2177	1395	367	413	2			
2	B	275	Total	C	N	O	S	0	0	0
			2231	1424	379	426	2			
2	C	278	Total	C	N	O	S	0	0	0
			2249	1435	383	429	2			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

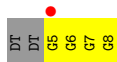
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total O 2 2	0	0
4	E	1	Total O 1 1	0	0
4	A	59	Total O 59 59	0	0
4	B	55	Total O 55 55	0	0
4	C	66	Total O 66 66	0	0

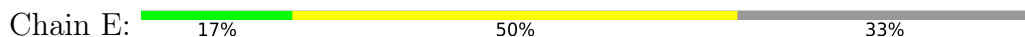
3 Residue-property plots

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.

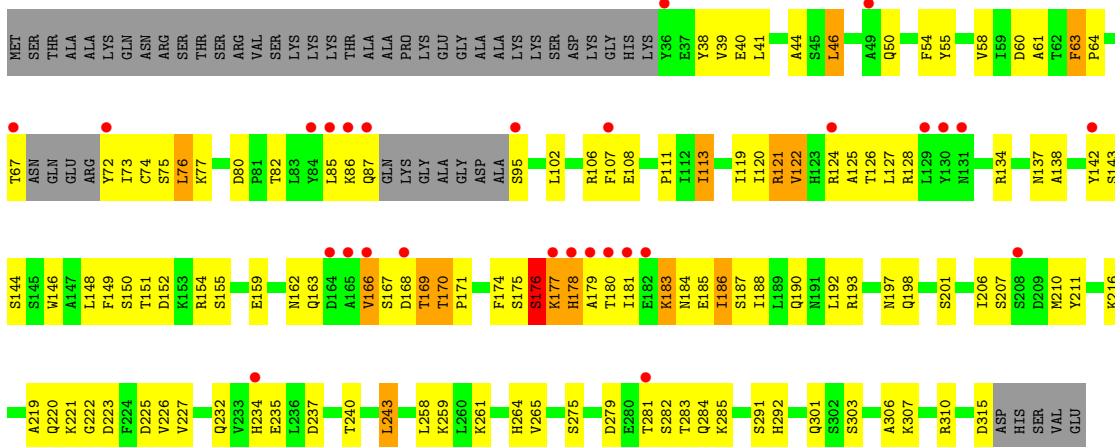
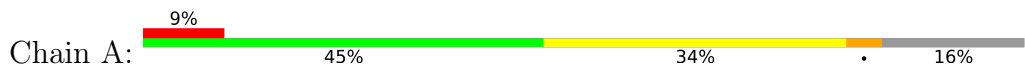
- Molecule 1: 5'-D(TP*TP*GP*GP*GP*G)-3'



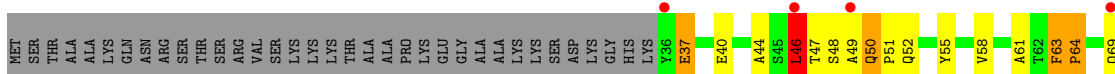
- Molecule 1: 5'-D(TP*TP*GP*GP*GP*G)-3'

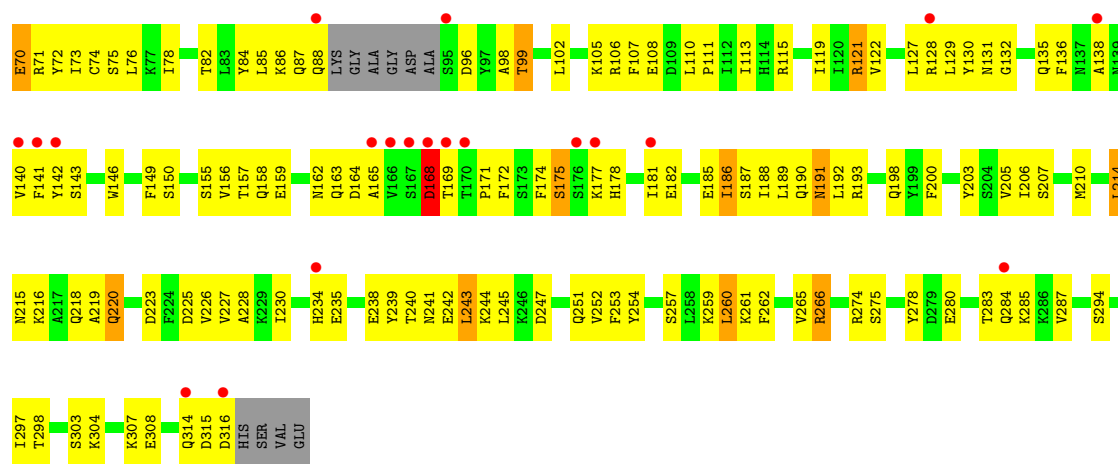


- Molecule 2: Telomere-Binding Protein alpha Subunit

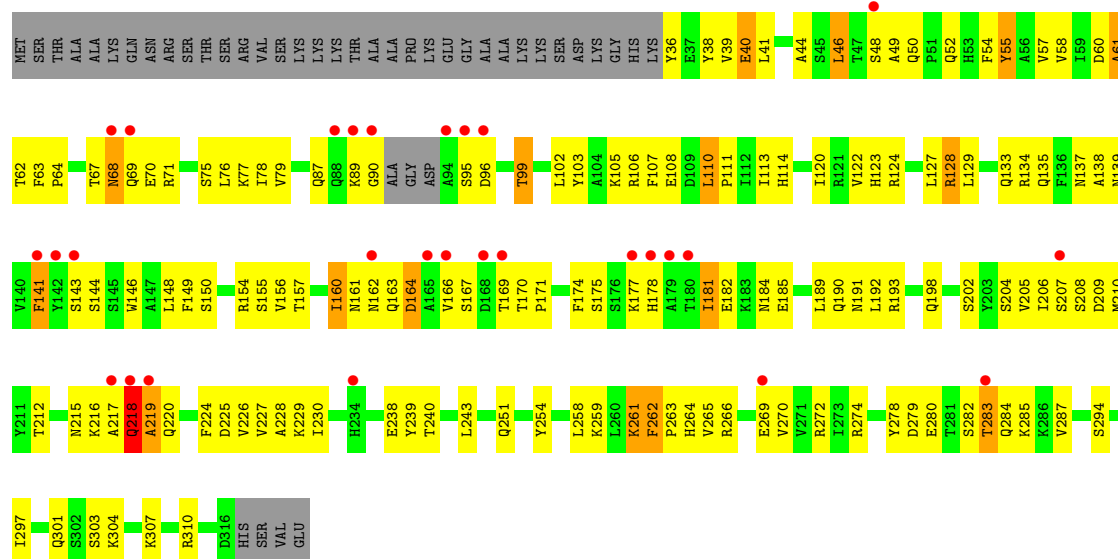


- Molecule 2: Telomere-Binding Protein alpha Subunit





● Molecule 2: Telomere-Binding Protein alpha Subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.18Å 121.18Å 137.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.60) 99.7 (30.00-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.285 0.245 , 0.285	Depositor DCC
R_{free} test set	3583 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7040	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	D	0.33	0/96	0.77	0/148
1	E	0.42	0/96	0.65	0/148
2	A	0.58	0/2221	1.13	18/3008 (0.6%)
2	B	0.58	0/2276	1.07	16/3083 (0.5%)
2	C	0.59	0/2294	1.11	21/3106 (0.7%)
All	All	0.58	0/6983	1.09	55/9493 (0.6%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	169	THR	N-CA-C	-10.38	98.79	114.16
2	B	69	GLN	OE1-CD-NE2	-9.73	112.86	122.60
2	B	50	GLN	OE1-CD-NE2	-9.37	113.23	122.60
2	A	163	GLN	OE1-CD-NE2	-9.29	113.31	122.60
2	C	218	GLN	OE1-CD-NE2	-9.26	113.34	122.60
2	C	301	GLN	OE1-CD-NE2	-9.15	113.45	122.60
2	B	50	GLN	N-CA-C	8.65	119.55	109.60
2	A	46	LEU	N-CA-C	-7.54	103.65	112.92
2	C	262	PHE	CA-C-N	7.50	127.53	119.28
2	C	262	PHE	C-N-CA	7.50	127.53	119.28
2	B	168	ASP	N-CA-C	-7.26	103.99	112.92
2	C	297	ILE	N-CA-C	7.22	118.28	108.17
2	B	69	GLN	CG-CD-NE2	6.90	126.75	116.40
2	C	301	GLN	CG-CD-NE2	6.78	126.58	116.40
2	A	223	ASP	N-CA-C	6.74	120.26	110.28
2	B	69	GLN	N-CA-C	6.59	121.03	113.19
2	B	287	VAL	N-CA-C	6.52	117.23	108.11
2	A	168	ASP	CA-C-N	6.51	131.31	120.70
2	A	168	ASP	C-N-CA	6.51	131.31	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	163	GLN	CG-CD-NE2	6.37	125.95	116.40
2	B	46	LEU	N-CA-C	-6.28	105.20	112.92
2	B	50	GLN	CG-CD-NE2	6.26	125.79	116.40
2	C	218	GLN	CG-CD-NE2	6.26	125.78	116.40
2	B	63	PHE	CA-C-N	-6.05	113.71	119.76
2	B	63	PHE	C-N-CA	-6.05	113.71	119.76
2	C	259	LYS	N-CA-C	6.03	117.86	111.28
2	C	46	LEU	N-CA-C	-5.95	106.02	113.28
2	A	63	PHE	N-CA-C	-5.63	101.95	110.39
2	B	172	PHE	N-CA-C	-5.53	106.53	113.28
2	C	160	ILE	CB-CA-C	-5.52	104.79	112.02
2	C	61	ALA	N-CA-C	5.48	116.85	108.52
2	B	214	LEU	N-CA-C	5.46	117.23	111.28
2	C	141	PHE	N-CA-C	-5.44	106.49	113.23
2	A	183	LYS	N-CA-C	5.41	117.17	111.28
2	C	155	SER	N-CA-C	-5.39	103.27	110.55
2	C	110	LEU	CA-C-N	5.35	126.18	120.13
2	C	110	LEU	C-N-CA	5.35	126.18	120.13
2	B	162	ASN	N-CA-C	5.33	119.08	112.58
2	A	63	PHE	CA-C-N	-5.32	114.44	119.76
2	A	63	PHE	C-N-CA	-5.32	114.44	119.76
2	A	144	SER	N-CA-C	5.29	117.55	110.35
2	B	64	PRO	N-CA-C	-5.20	103.02	111.19
2	A	170	THR	CA-C-N	5.20	125.11	119.76
2	A	170	THR	C-N-CA	5.20	125.11	119.76
2	B	175	SER	N-CA-C	5.15	116.70	111.14
2	C	40	GLU	N-CA-C	-5.14	102.87	110.48
2	A	177	LYS	N-CA-C	-5.13	107.53	112.97
2	A	222	GLY	CA-C-N	5.13	128.15	120.87
2	A	222	GLY	C-N-CA	5.13	128.15	120.87
2	C	304	LYS	N-CA-C	-5.11	105.79	111.36
2	A	50	GLN	N-CA-C	5.08	117.00	110.39
2	C	55	TYR	N-CA-C	-5.03	101.95	109.95
2	C	78	ILE	N-CA-C	5.03	115.72	108.48
2	C	261	LYS	N-CA-C	-5.02	107.29	113.41
2	C	240	THR	N-CA-C	5.01	117.42	109.50

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	D	85	0	46	7	0
1	E	85	0	46	7	0
2	A	2177	0	2164	124	0
2	B	2231	0	2210	138	0
2	C	2249	0	2231	126	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
4	A	59	0	0	1	0
4	B	55	0	0	7	0
4	C	66	0	0	3	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
All	All	7040	0	6697	384	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 28.

All (384) 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)
2:C:169:THR:HG21	2:C:181:ILE:HG12	1.29	1.08
2:A:85:LEU:HD13	2:A:95:SER:HA	1.42	1.02
2:B:141:PHE:HD2	2:B:142:TYR:HD2	1.09	1.01
2:A:169:THR:HG23	2:A:181:ILE:HD11	1.45	0.98
2:A:206:ILE:HA	2:A:210:MET:CE	1.94	0.98
2:C:206:ILE:HA	2:C:210:MET:HE2	1.45	0.96
2:C:154:ARG:NH1	2:C:162:ASN:HA	1.80	0.96
2:B:207:SER:H	2:B:210:MET:HE2	1.32	0.95
2:B:87:GLN:O	2:B:88:GLN:HG2	1.66	0.94
2:C:58:VAL:HG11	2:C:113:ILE:HD13	1.48	0.94
2:C:283:THR:HG23	2:C:284:GLN:H	1.38	0.88
2:B:141:PHE:HD2	2:B:142:TYR:CD2	1.91	0.87
2:A:169:THR:CG2	2:A:181:ILE:HD11	2.03	0.87
2:A:279:ASP:OD1	2:A:281:THR:HG22	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:ARG:HH12	2:C:162:ASN:HA	1.36	0.86
2:A:176:SER:CB	2:A:179:ALA:HB2	2.07	0.83
2:C:181:ILE:HD12	2:C:185:GLU:OE1	1.79	0.83
2:C:218:GLN:HG3	2:C:278:TYR:CE2	2.14	0.82
2:B:71:ARG:NH1	2:B:105:LYS:HE2	1.94	0.82
2:A:176:SER:OG	2:A:179:ALA:HB2	1.80	0.82
2:A:121:ARG:HH12	2:A:181:ILE:CG2	1.93	0.82
2:B:141:PHE:CD2	2:B:142:TYR:HD2	1.97	0.82
2:A:206:ILE:HA	2:A:210:MET:HE2	1.62	0.81
2:C:105:LYS:HE3	2:C:141:PHE:HB2	1.63	0.80
2:B:85:LEU:HD13	2:B:96:ASP:OD2	1.81	0.80
2:B:158:GLN:HG2	2:B:163:GLN:HE21	1.46	0.80
2:A:121:ARG:HH12	2:A:181:ILE:HG22	1.47	0.80
2:A:207:SER:H	2:A:210:MET:HE2	1.47	0.80
2:A:124:ARG:HD3	2:A:143:SER:O	1.83	0.79
2:A:180:THR:HG22	2:A:181:ILE:N	1.96	0.79
1:E:6:DG:H3'	1:E:7:DG:C5'	2.13	0.79
2:B:70:GLU:O	2:B:71:ARG:HD3	1.82	0.79
2:C:102:LEU:HD23	2:C:138:ALA:HB3	1.65	0.78
2:B:230:ILE:HD13	2:B:265:VAL:HG13	1.66	0.78
2:A:180:THR:HG22	2:A:181:ILE:H	1.48	0.78
2:B:61:ALA:CB	2:B:76:LEU:HD22	2.14	0.78
2:A:75:SER:C	2:A:76:LEU:HD23	2.10	0.76
2:C:230:ILE:HD13	2:C:265:VAL:HG13	1.68	0.74
2:A:181:ILE:HB	2:A:185:GLU:OE1	1.87	0.73
2:C:67:THR:OG1	2:C:71:ARG:HB3	1.89	0.73
2:C:169:THR:CG2	2:C:181:ILE:HG12	2.14	0.73
2:B:61:ALA:HB2	2:B:76:LEU:HD22	1.69	0.72
2:B:266:ARG:HH11	2:B:266:ARG:HG2	1.54	0.72
2:A:197:ASN:O	2:A:201:SER:HB3	1.90	0.71
2:A:154:ARG:NH1	2:A:162:ASN:HA	2.05	0.71
1:D:5:DG:N3	1:D:5:DG:H2'	2.06	0.70
2:C:128:ARG:NH1	2:C:135:GLN:OE1	2.23	0.70
2:A:225:ASP:H	2:B:87:GLN:HE22	1.38	0.70
1:D:6:DG:H3'	1:D:7:DG:C5'	2.21	0.70
2:C:61:ALA:CB	2:C:76:LEU:HD22	2.22	0.70
2:A:243:LEU:HD11	2:A:265:VAL:HG11	1.74	0.69
2:B:216:LYS:HG2	2:C:202:SER:HB2	1.74	0.69
2:B:70:GLU:C	2:B:71:ARG:HD3	2.17	0.69
2:B:169:THR:HG22	2:B:169:THR:O	1.92	0.68
2:B:71:ARG:HH12	2:B:105:LYS:HE2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:PRO:HG3	2:C:146:TRP:CD2	2.28	0.68
2:A:85:LEU:HB2	2:A:95:SER:HB2	1.76	0.68
2:A:154:ARG:HH12	2:A:162:ASN:HA	1.59	0.68
2:A:85:LEU:HB2	2:A:95:SER:CB	2.23	0.68
2:C:160:ILE:HG12	2:C:266:ARG:HH21	1.59	0.67
2:B:130:TYR:O	2:B:131:ASN:OD1	2.12	0.67
2:B:304:LYS:HE3	2:B:308:GLU:OE2	1.95	0.67
2:C:189:LEU:HD21	2:C:193:ARG:NH2	2.10	0.66
2:C:279:ASP:HB3	2:C:282:SER:HB2	1.75	0.66
2:B:243:LEU:HD11	2:B:265:VAL:HG11	1.77	0.66
2:C:206:ILE:HA	2:C:210:MET:CE	2.21	0.65
2:B:105:LYS:HD2	2:B:141:PHE:CE1	2.31	0.65
2:A:185:GLU:O	2:A:186:ILE:C	2.40	0.65
2:A:87:GLN:HE22	2:C:225:ASP:H	1.44	0.65
1:D:6:DG:H3'	1:D:7:DG:H5''	1.79	0.64
2:C:156:VAL:HG13	2:C:157:THR:N	2.12	0.64
2:B:206:ILE:HA	2:B:210:MET:CE	2.27	0.64
2:B:257:SER:HB2	2:B:262:PHE:HD1	1.62	0.64
2:C:207:SER:HB3	2:C:210:MET:HG3	1.80	0.64
2:B:99:THR:HG21	4:B:343:HOH:O	1.97	0.64
2:C:166:VAL:HB	2:C:170:THR:HG21	1.79	0.64
2:B:191:ASN:N	2:B:191:ASN:HD22	1.95	0.63
2:B:155:SER:HB3	2:B:158:GLN:HG3	1.80	0.63
2:C:61:ALA:HB1	2:C:76:LEU:HD22	1.80	0.63
2:A:102:LEU:HD23	2:A:138:ALA:HB3	1.81	0.63
2:A:149:PHE:CZ	2:A:171:PRO:HG3	2.34	0.63
2:A:180:THR:CG2	2:A:181:ILE:H	2.11	0.62
2:B:72:TYR:CE2	2:B:107:PHE:HB2	2.34	0.62
2:C:160:ILE:HG23	2:C:266:ARG:NH2	2.15	0.62
2:B:168:ASP:O	2:B:193:ARG:NH2	2.31	0.62
2:C:111:PRO:HG3	2:C:146:TRP:CE2	2.34	0.62
2:A:206:ILE:HA	2:A:210:MET:HE3	1.81	0.61
2:B:177:LYS:O	2:B:178:HIS:HD2	1.84	0.61
2:B:207:SER:N	2:B:210:MET:HE2	2.11	0.61
2:C:204:SER:O	2:C:206:ILE:N	2.34	0.60
2:C:238:GLU:HB2	2:C:239:TYR:CE1	2.36	0.60
2:A:180:THR:CG2	2:A:181:ILE:N	2.64	0.60
2:A:221:LYS:HG2	4:B:340:HOH:O	2.01	0.60
2:A:177:LYS:O	2:A:178:HIS:HB2	2.02	0.59
2:A:282:SER:HB2	2:A:285:LYS:O	2.01	0.59
2:B:37:GLU:O	2:B:37:GLU:HG2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:226:VAL:HG12	2:C:227:VAL:N	2.17	0.59
2:B:40:GLU:OE1	2:B:82:THR:HG21	2.02	0.59
2:B:61:ALA:HB1	2:B:76:LEU:HD22	1.84	0.59
2:C:215:ASN:OD1	2:C:216:LYS:HG3	2.02	0.59
2:B:78:ILE:HG13	2:B:98:ALA:HB3	1.85	0.59
2:B:111:PRO:HG3	2:B:146:TRP:CD2	2.38	0.59
2:C:48:SER:C	2:C:50:GLN:H	2.11	0.59
1:E:6:DG:H3'	1:E:7:DG:H5''	1.84	0.59
2:A:186:ILE:O	2:A:190:GLN:HG2	2.03	0.59
2:C:217:ALA:HB1	2:C:224:PHE:CZ	2.38	0.59
2:A:142:TYR:HD2	2:A:143:SER:HG	1.51	0.58
2:A:207:SER:N	2:A:210:MET:HE2	2.15	0.58
2:A:226:VAL:HG12	2:A:227:VAL:N	2.18	0.58
2:A:150:SER:O	2:A:193:ARG:NH1	2.36	0.58
2:C:70:GLU:O	2:C:105:LYS:HA	2.03	0.58
2:C:243:LEU:HD11	2:C:265:VAL:HG11	1.85	0.58
2:B:146:TRP:CE2	2:B:175:SER:HB3	2.39	0.57
2:C:212:THR:HG21	2:C:220:GLN:HE21	1.68	0.57
2:C:64:PRO:HB2	2:C:107:PHE:CE1	2.40	0.57
1:D:6:DG:N2	2:A:128:ARG:NH2	2.52	0.57
2:A:185:GLU:O	2:A:188:ILE:N	2.37	0.57
2:A:146:TRP:NE1	2:A:175:SER:HB3	2.20	0.57
2:C:129:LEU:HD12	2:C:133:GLN:O	2.05	0.57
2:A:74:CYS:SG	2:A:76:LEU:HD21	2.45	0.57
2:C:190:GLN:OE1	2:C:190:GLN:HA	2.04	0.57
2:B:235:GLU:HG3	4:B:327:HOH:O	2.04	0.57
2:A:177:LYS:O	2:A:178:HIS:CB	2.53	0.56
2:A:225:ASP:H	2:B:87:GLN:NE2	2.03	0.56
2:A:185:GLU:O	2:A:187:SER:N	2.39	0.56
2:A:60:ASP:HB3	2:A:77:LYS:HB2	1.88	0.56
2:A:85:LEU:HB2	2:A:95:SER:HA	1.88	0.56
2:A:85:LEU:CD1	2:A:95:SER:HA	2.25	0.56
2:B:46:LEU:HD22	2:B:127:LEU:CD2	2.36	0.56
2:B:216:LYS:O	2:B:220:GLN:OE1	2.24	0.56
2:A:167:SER:O	2:A:170:THR:HB	2.07	0.55
2:B:274:ARG:O	2:B:275:SER:HB3	2.06	0.55
2:C:44:ALA:HB1	2:C:52:GLN:OE1	2.06	0.55
2:C:114:HIS:HB2	2:C:156:VAL:HG11	1.87	0.55
2:C:61:ALA:HB2	2:C:76:LEU:HD22	1.88	0.55
2:B:102:LEU:HD23	2:B:138:ALA:HB3	1.87	0.55
2:C:206:ILE:CA	2:C:210:MET:HE2	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:PHE:CD2	2:B:142:TYR:CD2	2.82	0.55
2:B:181:ILE:HG13	2:B:181:ILE:O	2.07	0.54
2:C:177:LYS:O	2:C:178:HIS:CG	2.60	0.54
2:C:207:SER:HB3	2:C:210:MET:CG	2.38	0.54
2:A:72:TYR:HE2	2:A:107:PHE:CE1	2.25	0.54
2:C:239:TYR:O	2:C:258:LEU:HD12	2.08	0.54
2:A:206:ILE:CA	2:A:210:MET:HE2	2.36	0.54
2:A:58:VAL:HG11	2:A:113:ILE:HG12	1.90	0.53
2:C:156:VAL:HG13	2:C:157:THR:H	1.73	0.53
2:C:149:PHE:CE2	2:C:169:THR:O	2.60	0.53
2:A:121:ARG:HH12	2:A:181:ILE:HG21	1.74	0.53
2:B:280:GLU:OE1	2:B:280:GLU:HA	2.09	0.53
2:C:99:THR:HG21	4:C:373:HOH:O	2.09	0.53
2:A:124:ARG:HD3	2:A:143:SER:C	2.33	0.53
2:A:197:ASN:O	2:A:201:SER:CB	2.57	0.53
2:B:206:ILE:HA	2:B:210:MET:HE3	1.89	0.53
2:C:68:ASN:C	2:C:68:ASN:OD1	2.52	0.53
2:B:70:GLU:O	2:B:105:LYS:HA	2.09	0.53
2:B:155:SER:O	2:B:159:GLU:HG2	2.09	0.53
2:B:234:HIS:HB3	2:B:242:GLU:HB3	1.89	0.53
2:C:167:SER:O	2:C:170:THR:HG22	2.09	0.53
2:B:297:ILE:HG22	2:B:298:THR:O	2.09	0.52
2:C:60:ASP:HB3	2:C:77:LYS:HB2	1.91	0.52
2:A:63:PHE:CD2	2:A:64:PRO:HD2	2.44	0.52
2:B:218:GLN:HB2	4:B:351:HOH:O	2.08	0.52
2:B:129:LEU:HD21	2:B:132:GLY:CA	2.40	0.52
2:B:186:ILE:O	2:B:190:GLN:HB2	2.09	0.52
2:B:73:ILE:HG22	2:B:74:CYS:N	2.23	0.52
2:A:152:ASP:OD2	2:A:301:GLN:HG3	2.09	0.52
2:A:207:SER:HB3	2:A:210:MET:HG3	1.92	0.52
2:B:149:PHE:CZ	2:B:171:PRO:HG3	2.44	0.52
2:C:207:SER:H	2:C:210:MET:HE2	1.73	0.52
2:A:126:THR:CG2	2:A:137:ASN:HB2	2.40	0.52
2:B:87:GLN:O	2:B:88:GLN:CG	2.50	0.52
2:B:129:LEU:HD21	2:B:132:GLY:HA2	1.92	0.52
2:C:218:GLN:O	2:C:220:GLN:N	2.42	0.51
2:C:160:ILE:HG23	2:C:266:ARG:HH22	1.75	0.51
2:A:176:SER:HB2	2:A:179:ALA:HB2	1.89	0.51
2:B:266:ARG:HG2	2:B:266:ARG:NH1	2.22	0.51
2:C:103:TYR:HE1	2:C:137:ASN:HD22	1.57	0.51
2:A:226:VAL:CG1	2:A:227:VAL:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:VAL:HG12	2:B:140:VAL:O	2.11	0.51
2:C:124:ARG:NH1	2:C:124:ARG:HG3	2.25	0.51
2:B:219:ALA:HB2	2:C:198:GLN:HB3	1.92	0.51
2:C:124:ARG:HG3	2:C:124:ARG:HH11	1.75	0.51
2:C:254:TYR:CE1	2:C:285:LYS:HE3	2.45	0.51
2:C:261:LYS:C	2:C:263:PRO:HD3	2.35	0.51
2:A:85:LEU:HB2	2:A:95:SER:CA	2.41	0.50
2:B:261:LYS:HE2	2:B:262:PHE:CZ	2.46	0.50
2:A:166:VAL:HG12	2:A:167:SER:N	2.25	0.50
2:A:174:PHE:CE1	2:A:178:HIS:HA	2.46	0.50
2:B:215:ASN:HA	2:B:251:GLN:HG3	1.94	0.50
2:C:68:ASN:ND2	2:C:71:ARG:HB2	2.27	0.50
2:B:230:ILE:CD1	2:B:265:VAL:HG13	2.40	0.50
2:B:259:LYS:HD2	4:B:327:HOH:O	2.11	0.50
1:D:8:DG:O6	2:A:275:SER:HB2	2.11	0.50
2:B:44:ALA:HA	2:B:52:GLN:HE22	1.77	0.50
2:C:228:ALA:O	2:C:270:VAL:HA	2.10	0.50
2:B:218:GLN:HG3	2:B:278:TYR:CE1	2.47	0.50
2:A:146:TRP:CE2	2:A:175:SER:HB3	2.47	0.49
2:B:58:VAL:HG11	2:B:113:ILE:HG12	1.94	0.49
2:C:307:LYS:HG2	2:C:310:ARG:NH2	2.26	0.49
2:C:239:TYR:CD1	2:C:239:TYR:N	2.79	0.49
1:E:5:DG:H4'	2:B:73:ILE:HD11	1.93	0.49
2:B:257:SER:HA	4:B:328:HOH:O	2.12	0.49
2:C:36:TYR:HB3	2:C:38:TYR:CE1	2.47	0.49
2:B:228:ALA:HB2	2:B:247:ASP:HB3	1.94	0.49
2:C:181:ILE:O	2:C:181:ILE:HG23	2.12	0.49
2:A:75:SER:O	2:A:76:LEU:HD23	2.12	0.49
2:B:46:LEU:HD22	2:B:127:LEU:HD23	1.93	0.49
2:B:164:ASP:OD1	2:B:165:ALA:N	2.46	0.49
2:C:75:SER:C	2:C:76:LEU:HD23	2.38	0.49
2:A:67:THR:HG21	2:A:73:ILE:HD12	1.95	0.49
2:A:61:ALA:CB	2:A:76:LEU:HD22	2.43	0.49
2:A:183:LYS:C	2:A:185:GLU:N	2.69	0.49
2:B:189:LEU:HD21	2:B:193:ARG:NH2	2.28	0.48
2:C:123:HIS:HB3	2:C:124:ARG:NH1	2.28	0.48
1:D:7:DG:H1	2:A:225:ASP:CG	2.21	0.48
2:A:119:ILE:HD13	2:A:192:LEU:HD23	1.94	0.48
2:C:282:SER:OG	2:C:285:LYS:O	2.30	0.48
2:B:64:PRO:HG3	2:B:111:PRO:O	2.13	0.48
2:B:119:ILE:CG2	2:B:192:LEU:HD23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ASP:O	2:C:89:LYS:NZ	2.45	0.48
2:B:146:TRP:NE1	2:B:175:SER:HB3	2.28	0.48
2:B:158:GLN:HG2	2:B:163:GLN:NE2	2.21	0.48
2:C:46:LEU:HD23	2:C:127:LEU:HG	1.95	0.48
2:C:184:ASN:OD1	2:C:185:GLU:N	2.46	0.48
2:C:303:SER:O	2:C:307:LYS:HG3	2.14	0.48
2:C:264:HIS:O	2:C:266:ARG:HG2	2.12	0.48
2:A:119:ILE:CG2	2:A:120:ILE:N	2.77	0.48
2:C:62:THR:HG22	2:C:274:ARG:NH1	2.29	0.48
2:C:229:LYS:HA	2:C:269:GLU:O	2.14	0.48
2:B:283:THR:HG23	2:B:283:THR:O	2.14	0.47
2:B:63:PHE:CD2	2:B:261:LYS:HE3	2.50	0.47
2:B:168:ASP:OD1	2:B:168:ASP:N	2.36	0.47
2:B:207:SER:HB2	2:B:210:MET:HG3	1.96	0.47
2:C:106:ARG:CZ	2:C:108:GLU:OE2	2.61	0.47
2:C:48:SER:O	2:C:50:GLN:N	2.42	0.47
2:C:206:ILE:HD13	2:C:210:MET:CE	2.45	0.47
2:A:225:ASP:N	2:B:87:GLN:HE22	2.08	0.47
2:A:306:ALA:O	2:A:310:ARG:HG3	2.14	0.47
2:B:105:LYS:CD	2:B:141:PHE:CE1	2.98	0.47
2:C:283:THR:HG23	2:C:284:GLN:N	2.17	0.47
2:A:73:ILE:CG2	2:A:74:CYS:N	2.77	0.47
2:B:185:GLU:O	2:B:186:ILE:C	2.58	0.47
2:C:48:SER:C	2:C:50:GLN:N	2.73	0.47
2:B:75:SER:C	2:B:76:LEU:HD23	2.40	0.47
2:B:185:GLU:O	2:B:188:ILE:N	2.48	0.47
2:C:39:VAL:HG23	4:C:343:HOH:O	2.15	0.47
2:C:63:PHE:HB2	2:C:294:SER:O	2.15	0.47
2:C:75:SER:O	2:C:76:LEU:HD23	2.13	0.47
2:C:265:VAL:O	2:C:266:ARG:HD3	2.14	0.47
2:B:200:PHE:CZ	2:B:205:VAL:HG11	2.50	0.47
2:A:119:ILE:HG22	2:A:120:ILE:N	2.29	0.47
2:C:207:SER:C	2:C:209:ASP:H	2.23	0.47
2:B:55:TYR:HB3	2:B:192:LEU:HD22	1.97	0.46
2:C:207:SER:O	2:C:209:ASP:N	2.49	0.46
1:E:6:DG:H3'	1:E:7:DG:H5'	1.97	0.46
2:A:86:LYS:O	2:A:87:GLN:C	2.58	0.46
2:A:169:THR:O	2:A:169:THR:HG22	2.14	0.46
2:A:206:ILE:HD13	2:A:210:MET:CE	2.46	0.46
2:B:218:GLN:HG3	2:B:278:TYR:CZ	2.51	0.46
2:C:39:VAL:HG12	2:C:40:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:80:ASP:OD1	2:A:80:ASP:C	2.58	0.46
2:A:142:TYR:CD2	2:A:143:SER:N	2.83	0.46
2:B:314:GLN:HA	2:B:314:GLN:OE1	2.16	0.46
2:A:198:GLN:HB3	2:C:219:ALA:HB2	1.97	0.46
2:B:315:ASP:OD1	2:B:316:ASP:N	2.49	0.46
2:C:164:ASP:OD1	2:C:164:ASP:N	2.49	0.46
2:B:127:LEU:HD13	2:B:136:PHE:CE2	2.51	0.46
2:A:41:LEU:O	2:A:134:ARG:NH1	2.48	0.46
2:A:61:ALA:HB1	2:A:76:LEU:HD22	1.98	0.46
2:A:216:LYS:O	2:A:220:GLN:HG2	2.16	0.45
2:A:219:ALA:HB2	2:B:198:GLN:HB3	1.98	0.45
2:B:64:PRO:HB3	2:B:110:LEU:HB2	1.98	0.45
2:B:284:GLN:O	2:B:284:GLN:HG2	2.16	0.45
2:C:46:LEU:HD23	2:C:127:LEU:CD2	2.46	0.45
2:C:146:TRP:CE2	2:C:175:SER:HB3	2.52	0.45
2:A:46:LEU:HD22	2:A:127:LEU:CD2	2.46	0.45
2:A:235:GLU:OE2	2:A:259:LYS:NZ	2.50	0.45
2:C:218:GLN:HG3	2:C:278:TYR:CD2	2.50	0.45
2:A:39:VAL:HG11	2:A:44:ALA:HA	1.98	0.45
2:A:95:SER:N	2:A:207:SER:HB2	2.32	0.45
2:C:89:LYS:HB2	2:C:90:GLY:H	1.66	0.45
2:B:73:ILE:CG2	2:B:74:CYS:N	2.80	0.45
2:C:156:VAL:CG1	2:C:157:THR:N	2.79	0.45
2:C:182:GLU:HA	2:C:182:GLU:OE1	2.17	0.45
2:A:55:TYR:HB3	2:A:192:LEU:HD22	2.00	0.44
2:B:72:TYR:CE1	2:B:107:PHE:N	2.86	0.44
2:C:139:ASN:HB3	2:C:141:PHE:CZ	2.52	0.44
2:A:183:LYS:C	2:A:185:GLU:H	2.26	0.44
1:E:6:DG:H5'	2:B:73:ILE:HD13	1.99	0.44
2:A:121:ARG:NH1	2:A:181:ILE:HG22	2.23	0.44
2:B:235:GLU:HA	2:B:241:ASN:ND2	2.33	0.44
2:C:146:TRP:NE1	2:C:175:SER:HB3	2.32	0.44
2:C:226:VAL:CG1	2:C:227:VAL:N	2.79	0.44
2:B:61:ALA:HB1	2:B:76:LEU:CD2	2.46	0.44
2:B:99:THR:HG22	2:B:135:GLN:HG3	1.98	0.44
2:C:54:PHE:CD1	2:C:54:PHE:C	2.95	0.44
2:B:185:GLU:O	2:B:187:SER:N	2.51	0.44
2:C:55:TYR:HB3	2:C:192:LEU:HD22	1.99	0.44
2:A:149:PHE:CE2	2:A:171:PRO:HG3	2.53	0.44
2:B:244:LYS:HG3	2:B:254:TYR:CE2	2.52	0.44
2:C:251:GLN:OE1	2:C:251:GLN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:183:LYS:O	2:A:185:GLU:N	2.51	0.44
2:B:182:GLU:OE1	2:B:182:GLU:HA	2.17	0.44
2:C:280:GLU:OE1	2:C:280:GLU:N	2.50	0.44
2:B:225:ASP:H	2:C:87:GLN:HE22	1.65	0.44
2:A:120:ILE:HG13	2:A:148:LEU:HD23	2.00	0.44
2:B:226:VAL:HG12	2:B:227:VAL:N	2.33	0.44
2:C:62:THR:CG2	2:C:274:ARG:NH1	2.81	0.43
2:C:150:SER:O	2:C:193:ARG:NH1	2.51	0.43
2:C:285:LYS:O	2:C:287:VAL:HG23	2.18	0.43
2:C:262:PHE:N	2:C:263:PRO:HD3	2.32	0.43
2:B:48:SER:C	2:B:50:GLN:H	2.26	0.43
2:B:128:ARG:HG2	2:B:129:LEU:N	2.33	0.43
2:A:283:THR:OG1	2:A:284:GLN:N	2.49	0.43
2:B:105:LYS:HG3	2:B:141:PHE:CD1	2.54	0.43
2:B:214:LEU:HD13	2:B:253:PHE:CD1	2.54	0.43
2:C:207:SER:C	2:C:209:ASP:N	2.74	0.43
2:B:46:LEU:CD2	2:B:127:LEU:HD21	2.49	0.43
2:B:129:LEU:HD23	2:B:132:GLY:H	1.84	0.43
2:C:61:ALA:HB1	2:C:76:LEU:CD2	2.46	0.43
2:A:211:TYR:CD2	2:A:211:TYR:N	2.87	0.43
2:A:38:TYR:CZ	2:A:185:GLU:OE2	2.72	0.43
2:B:260:LEU:HD12	2:B:260:LEU:HA	1.71	0.42
2:B:259:LYS:NZ	4:B:327:HOH:O	2.53	0.42
2:A:216:LYS:HD3	2:B:203:TYR:CZ	2.55	0.42
2:B:48:SER:O	2:B:50:GLN:N	2.52	0.42
2:B:50:GLN:HA	2:B:51:PRO:HD3	1.77	0.42
2:B:119:ILE:HG23	2:B:192:LEU:HD23	2.02	0.42
2:B:129:LEU:CD2	2:B:132:GLY:H	2.32	0.42
2:B:146:TRP:CZ3	2:B:174:PHE:HA	2.54	0.42
2:C:39:VAL:HG12	2:C:40:GLU:N	2.35	0.42
1:E:6:DG:C3'	1:E:7:DG:C5'	2.91	0.42
2:B:102:LEU:CD2	2:B:138:ALA:HB3	2.50	0.42
2:B:115:ARG:HB2	2:B:156:VAL:HG21	2.02	0.42
2:C:254:TYR:CZ	2:C:285:LYS:HE3	2.54	0.42
2:A:151:THR:HA	2:A:193:ARG:HD3	2.02	0.42
2:C:217:ALA:O	2:C:218:GLN:C	2.62	0.42
2:A:54:PHE:O	2:A:121:ARG:HA	2.20	0.42
2:A:72:TYR:CD1	2:A:72:TYR:N	2.87	0.42
2:A:169:THR:HG22	2:A:181:ILE:HD11	1.93	0.42
2:B:245:LEU:O	2:B:252:VAL:HA	2.20	0.42
2:B:297:ILE:HG22	2:B:298:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:122:VAL:CG2	2:A:125:ALA:HB2	2.50	0.41
2:A:170:THR:HA	2:A:171:PRO:HD3	1.79	0.41
2:C:57:VAL:HB	2:C:79:VAL:HG23	2.02	0.41
2:C:161:ASN:HB2	2:C:163:GLN:HG3	2.02	0.41
2:A:206:ILE:CD1	2:A:210:MET:HE3	2.49	0.41
2:B:87:GLN:C	2:B:88:GLN:HG2	2.39	0.41
2:B:157:THR:O	2:B:157:THR:HG22	2.19	0.41
2:C:189:LEU:CD2	2:C:193:ARG:NH2	2.79	0.41
2:C:279:ASP:O	2:C:282:SER:HB2	2.20	0.41
2:A:237:ASP:OD1	2:A:237:ASP:N	2.54	0.41
2:B:63:PHE:HB2	2:B:294:SER:O	2.20	0.41
2:A:177:LYS:O	2:A:178:HIS:CG	2.73	0.41
2:A:264:HIS:ND1	2:A:264:HIS:N	2.67	0.41
2:A:40:GLU:OE1	2:A:82:THR:HG21	2.20	0.41
2:B:106:ARG:CZ	2:B:108:GLU:OE2	2.69	0.41
2:A:111:PRO:HG3	2:A:146:TRP:CD2	2.56	0.41
2:A:167:SER:O	2:A:170:THR:CB	2.69	0.41
2:C:39:VAL:HG21	4:C:360:HOH:O	2.21	0.41
2:C:41:LEU:O	2:C:134:ARG:NH1	2.53	0.41
2:C:149:PHE:CZ	2:C:171:PRO:HG3	2.55	0.41
2:A:155:SER:O	2:A:159:GLU:HG2	2.20	0.41
2:A:291:SER:OG	2:A:292:HIS:N	2.54	0.41
2:B:111:PRO:HG3	2:B:146:TRP:CE2	2.56	0.41
2:B:185:GLU:C	2:B:187:SER:N	2.77	0.41
2:A:106:ARG:HB2	2:A:108:GLU:OE1	2.21	0.40
2:A:126:THR:HG22	2:A:137:ASN:HB2	2.01	0.40
2:A:303:SER:O	2:A:307:LYS:HG3	2.21	0.40
2:B:121:ARG:O	2:B:121:ARG:HG3	2.22	0.40
2:C:110:LEU:HA	2:C:111:PRO:HD3	1.78	0.40
2:C:120:ILE:HG13	2:C:148:LEU:HD23	2.04	0.40
2:A:72:TYR:HE2	2:A:107:PHE:CD1	2.39	0.40
2:A:76:LEU:HD23	2:A:76:LEU:N	2.34	0.40
2:A:232:GLN:HG3	2:A:234:HIS:CD2	2.55	0.40
2:B:158:GLN:OE1	2:B:165:ALA:HA	2.22	0.40
2:B:238:GLU:HG3	2:B:239:TYR:CD1	2.57	0.40
2:C:64:PRO:HB2	2:C:107:PHE:CD1	2.56	0.40
2:B:84:TYR:CE2	2:B:86:LYS:HE3	2.56	0.40
2:C:169:THR:O	2:C:170:THR:C	2.62	0.40
1:D:6:DG:H5'	2:A:73:ILE:HD13	2.03	0.40
2:A:258:LEU:HB2	4:A:337:HOH:O	2.21	0.40
2:B:303:SER:O	2:B:307:LYS:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:DG:H1	2:B:225:ASP:CG	2.30	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	
2	A	263/320 (82%)	245 (93%)	13 (5%)	5 (2%)	6	13
2	B	271/320 (85%)	245 (90%)	22 (8%)	4 (2%)	8	18
2	C	274/320 (86%)	242 (88%)	24 (9%)	8 (3%)	3	6
All	All	808/960 (84%)	732 (91%)	59 (7%)	17 (2%)	5	11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	166	VAL
2	A	176	SER
2	A	178	HIS
2	C	219	ALA
2	A	186	ILE
2	C	208	SER
2	C	283	THR
2	B	49	ALA
2	C	69	GLN
2	C	144	SER
2	C	218	GLN
2	B	70	GLU
2	C	49	ALA
2	A	184	ASN
2	B	186	ILE
2	B	143	SER

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Mol	Chain	Res	Type
2	C	205	VAL

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	
2	A	240/281 (85%)	231 (96%)	9 (4%)	29	56
2	B	246/281 (88%)	231 (94%)	15 (6%)	17	37
2	C	247/281 (88%)	235 (95%)	12 (5%)	22	47
All	All	733/843 (87%)	697 (95%)	36 (5%)	22	47

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	76	LEU
2	A	113	ILE
2	A	121	ARG
2	A	122	VAL
2	A	176	SER
2	A	240	THR
2	A	243	LEU
2	A	261	LYS
2	A	315	ASP
2	B	37	GLU
2	B	46	LEU
2	B	47	THR
2	B	99	THR
2	B	121	ARG
2	B	122	VAL
2	B	150	SER
2	B	168	ASP
2	B	191	ASN
2	B	220	GLN
2	B	240	THR
2	B	243	LEU

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Mol	Chain	Res	Type
2	B	260	LEU
2	B	266	ARG
2	B	285	LYS
2	C	68	ASN
2	C	95	SER
2	C	96	ASP
2	C	99	THR
2	C	122	VAL
2	C	128	ARG
2	C	143	SER
2	C	164	ASP
2	C	174	PHE
2	C	181	ILE
2	C	191	ASN
2	C	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	52	GLN
2	A	87	GLN
2	A	215	ASN
2	A	220	GLN
2	A	232	GLN
2	A	241	ASN
2	B	52	GLN
2	B	137	ASN
2	B	162	ASN
2	B	163	GLN
2	B	178	HIS
2	B	191	ASN
2	B	234	HIS
2	B	241	ASN
2	B	251	GLN
2	C	137	ASN
2	C	292	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	SO4	C	322	-	4,4,4	0.41	0	6,6,6	0.22	0
3	SO4	B	321	-	4,4,4	0.34	0	6,6,6	0.23	0
3	SO4	B	322	-	4,4,4	0.42	0	6,6,6	0.13	0
3	SO4	A	321	-	4,4,4	0.32	0	6,6,6	0.20	0
3	SO4	C	321	-	4,4,4	0.36	0	6,6,6	0.27	0
3	SO4	A	322	-	4,4,4	0.36	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	4/6 (66%)	0.77	1 (25%) 2 1	48, 54, 60, 72	0
1	E	4/6 (66%)	0.99	0 100 100	53, 58, 69, 75	0
2	A	269/320 (84%)	0.50	28 (10%) 11 9	22, 41, 68, 81	0
2	B	275/320 (85%)	0.59	24 (8%) 16 12	20, 44, 71, 79	0
2	C	278/320 (86%)	0.56	28 (10%) 12 9	23, 44, 69, 74	0
All	All	830/972 (85%)	0.55	81 (9%) 13 10	20, 44, 70, 81	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	94	ALA	5.1
2	C	169	THR	4.6
2	A	86	LYS	4.6
2	C	217	ALA	4.6
2	B	142	TYR	4.6
2	C	180	THR	4.2
2	A	85	LEU	4.1
2	B	36	TYR	4.1
2	B	166	VAL	4.0
2	A	142	TYR	3.8
2	B	141	PHE	3.7
2	B	88	GLN	3.5
2	A	234	HIS	3.5
2	B	168	ASP	3.4
2	C	166	VAL	3.4
2	B	316	ASP	3.4
2	A	124	ARG	3.4
2	A	95	SER	3.3
2	A	107	PHE	3.2
2	C	141	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	168	ASP	3.0
2	B	69	GLN	3.0
2	A	87	GLN	2.9
2	B	46	LEU	2.9
2	A	178	HIS	2.9
2	B	284	GLN	2.9
2	A	177	LYS	2.9
1	D	5	DG	2.8
2	C	234	HIS	2.8
2	B	181	ILE	2.8
2	C	96	ASP	2.8
2	B	165	ALA	2.8
2	A	129	LEU	2.7
2	A	180	THR	2.6
2	B	49	ALA	2.6
2	C	165	ALA	2.6
2	A	72	TYR	2.6
2	A	165	ALA	2.6
2	C	90	GLY	2.5
2	A	67	THR	2.5
2	A	36	TYR	2.5
2	C	218	GLN	2.5
2	C	68	ASN	2.5
2	C	168	ASP	2.5
2	C	177	LYS	2.4
2	B	234	HIS	2.4
2	B	128	ARG	2.4
2	B	177	LYS	2.4
2	A	179	ALA	2.4
2	B	176	SER	2.3
2	C	162	ASN	2.3
2	C	89	LYS	2.3
2	C	179	ALA	2.3
2	A	281	THR	2.3
2	A	84	TYR	2.3
2	A	181	ILE	2.2
2	C	283	THR	2.2
2	C	88	GLN	2.2
2	A	49	ALA	2.2
2	C	269	GLU	2.2
2	A	164	ASP	2.2
2	B	167	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	207	SER	2.2
2	B	95	SER	2.2
2	C	48	SER	2.2
2	C	143	SER	2.2
2	A	182	GLU	2.1
2	A	131	ASN	2.1
2	C	178	HIS	2.1
2	C	95	SER	2.1
2	B	138	ALA	2.1
2	A	130	TYR	2.1
2	B	170	THR	2.1
2	C	69	GLN	2.1
2	A	166	VAL	2.1
2	B	140	VAL	2.1
2	B	169	THR	2.0
2	C	219	ALA	2.0
2	A	208	SER	2.0
2	B	314	GLN	2.0
2	C	142	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	322	5/5	0.84	0.12	81,82,83,85	0
3	SO4	B	322	5/5	0.86	0.12	92,93,94,95	0
3	SO4	C	322	5/5	0.89	0.13	66,66,67,68	0
3	SO4	B	321	5/5	0.92	0.12	58,59,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	321	5/5	0.93	0.12	71,73,74,75	0
3	SO4	C	321	5/5	0.94	0.08	71,72,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.