



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 AM GMT

PDB ID : 2PZS
Title : Phi29 DNA polymerase complexed with primer-template DNA (post-translocation binary complex)
Authors : Berman, A.J.; Kamtekar, S.; Goodman, J.L.; Lazaro, J.M.; de Vega, M.; Blanco, L.; Salas, M.; Steitz, T.A.
Deposited on : 2007-05-18
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

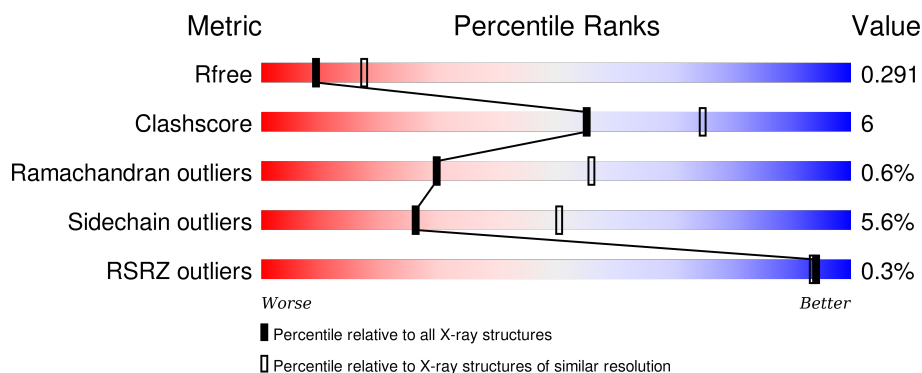
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	<div> <div>20%</div> <div>70%</div> <div>10%</div> </div>
1	X	10	<div> <div>50%</div> <div>30%</div> <div>20%</div> </div>
2	S	17	<div> <div>6%</div> <div>18%</div> <div>53%</div> <div>12%</div> <div>18%</div> </div>
2	T	17	<div> <div>6%</div> <div>12%</div> <div>18%</div> <div>71%</div> </div>
2	U	17	<div> <div>6%</div> <div>24%</div> <div>18%</div> <div>59%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Y	17	<div><div></div><div>35%</div><div>35%</div><div>12%</div><div>18%</div></div>
3	A	575	<div><div></div><div>84%</div><div>14%</div><div>• •</div></div>
3	B	575	<div><div></div><div>83%</div><div>14%</div><div>• •</div></div>
3	C	575	<div><div></div><div>83%</div><div>13%</div><div>• •</div></div>
3	D	575	<div><div></div><div>77%</div><div>19%</div><div>• •</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19783 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(GACTGCTTAC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
1	R	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 2 is a DNA chain called 5'-d(CTAACACGTAAGCAGTC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
2	T	5	Total	C	N	O	P	0	0	0
			99	48	21	26	4			
2	U	7	Total	C	N	O	P	0	0	0
			140	68	28	38	6			
2	S	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
3	B	566	Total	C	N	O	S	0	0	0
			4617	3008	743	845	21			
3	C	563	Total	C	N	O	S	0	0	0
			4596	2996	738	841	21			
3	D	564	Total	C	N	O	S	0	0	0
			4606	3003	739	843	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	ASP	ENGINEERED	UNP P03680
A	66	ALA	ASP	ENGINEERED	UNP P03680
B	12	ALA	ASP	ENGINEERED	UNP P03680
B	66	ALA	ASP	ENGINEERED	UNP P03680
C	12	ALA	ASP	ENGINEERED	UNP P03680
C	66	ALA	ASP	ENGINEERED	UNP P03680
D	12	ALA	ASP	ENGINEERED	UNP P03680
D	66	ALA	ASP	ENGINEERED	UNP P03680

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	27	Total O 27 27	0	0
4	C	19	Total O 19 19	0	0
4	D	8	Total O 8 8	0	0
4	X	2	Total O 2 2	0	0
4	Y	1	Total O 1 1	0	0

3 Residue-property plots

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

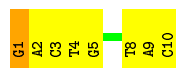
- Molecule 1: 5'-d(GACTGCTTAC)-3'

Chain X: 



- Molecule 1: 5'-d(GACTGCTTAC)-3'

Chain R: 



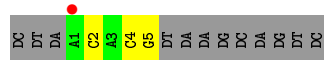
- Molecule 2: 5'-d(CTAACACGTAAGCAGTC)-3'

Chain Y: 



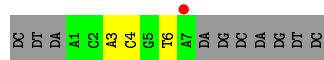
- Molecule 2: 5'-d(CTAACACGTAAGCAGTC)-3'

Chain T: 




- Molecule 2: 5'-d(CTAACACGTAAGCAGTC)-3'

Chain U: 

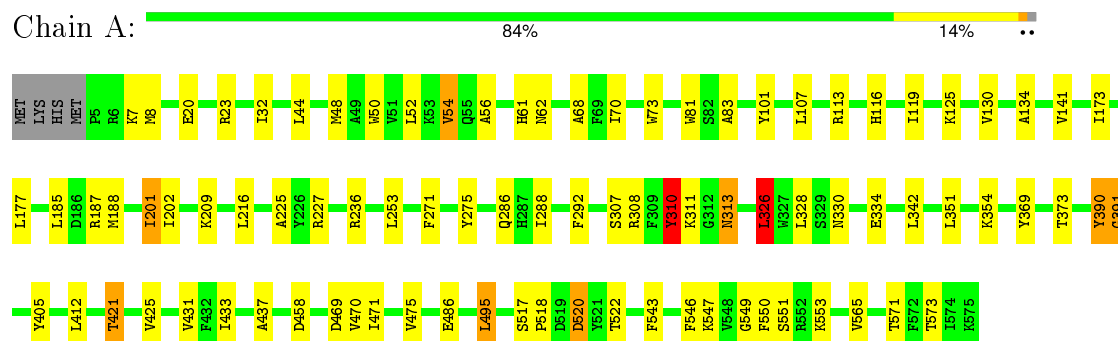


- Molecule 2: 5'-d(CTAACACGTAAGCAGTC)-3'

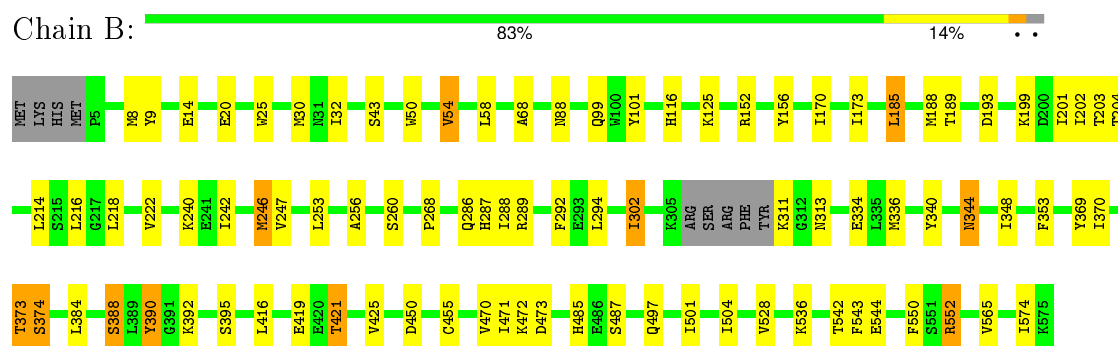
Chain S: 



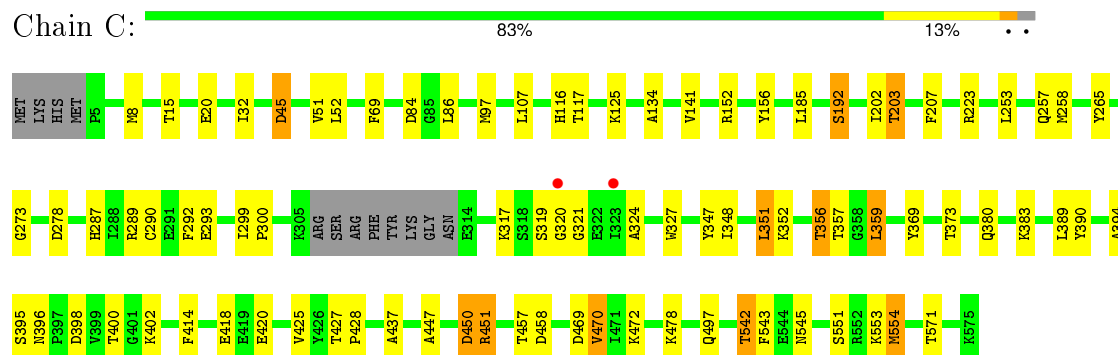
• Molecule 3: DNA polymerase



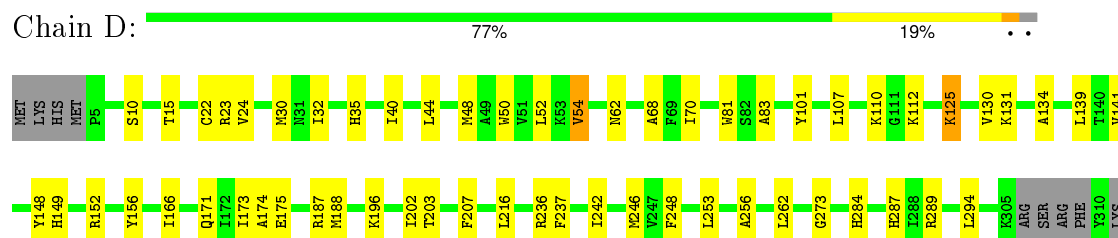
• Molecule 3: DNA polymerase

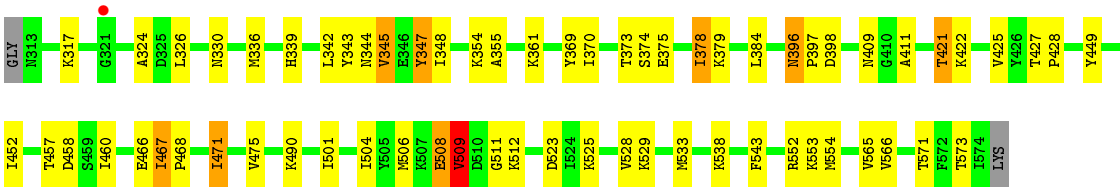


• Molecule 3: DNA polymerase



• Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.63Å 146.29Å 115.05Å 90.00° 117.93° 90.00°	Depositor
Resolution (Å)	45.22 – 2.60 45.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.22-2.60) 98.3 (45.21-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.219 , 0.275 0.236 , 0.291	Depositor DCC
R_{free} test set	9704 reflections (10.15%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , -5.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 95622 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	19783	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	R	1.29	0/223	1.87	8/342 (2.3%)
1	X	0.96	0/223	1.69	7/342 (2.0%)
2	S	1.38	0/319	1.59	6/490 (1.2%)
2	T	1.47	0/111	1.84	2/169 (1.2%)
2	U	1.61	1/157 (0.6%)	1.76	4/240 (1.7%)
2	Y	1.12	0/319	1.82	9/490 (1.8%)
3	A	0.57	0/4788	0.63	1/6459 (0.0%)
3	B	0.56	1/4734 (0.0%)	0.61	0/6386
3	C	0.53	0/4713	0.58	0/6359
3	D	0.52	0/4723	0.61	1/6374 (0.0%)
All	All	0.63	2/20310 (0.0%)	0.76	38/27651 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	3
3	D	1	3
All	All	1	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	455	CYS	CB-SG	-5.59	1.72	1.81
2	U	6	DT	C1'-N1	5.59	1.56	1.49

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	4	DA	O4'-C4'-C3'	-13.62	97.83	106.00
2	U	6	DT	O4'-C1'-N1	10.58	115.41	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	1	DG	P-O3'-C3'	9.13	130.66	119.70
2	Y	7	DC	O4'-C1'-N1	9.04	114.33	108.00
2	S	6	DA	O4'-C1'-N9	-8.65	101.94	108.00
1	X	6	DC	O4'-C4'-C3'	-8.31	101.01	106.00
2	S	15	DG	O4'-C1'-N9	8.11	113.68	108.00
2	Y	11	DA	O4'-C1'-N9	7.73	113.41	108.00
1	X	10	DC	O4'-C1'-N1	7.65	113.35	108.00
2	U	6	DT	O4'-C1'-C2'	-7.54	99.87	105.90
1	R	5	DG	O4'-C1'-N9	7.48	113.23	108.00
2	Y	4	DA	C4'-C3'-C2'	-7.00	96.80	103.10
1	X	1	DG	P-O3'-C3'	7.00	128.09	119.70
2	S	11	DA	O4'-C1'-N9	6.93	112.85	108.00
2	S	17	DC	O4'-C1'-N1	6.90	112.83	108.00
3	D	467	ILE	N-CA-C	-6.86	92.48	111.00
1	R	1	DG	C5-C6-O6	-6.71	124.57	128.60
2	T	5	DG	C8-N9-C4	-6.36	103.86	106.40
2	Y	6	DA	O4'-C1'-N9	-6.14	103.70	108.00
2	T	2	DC	O4'-C1'-N1	6.05	112.24	108.00
1	R	10	DC	O4'-C1'-N1	6.03	112.22	108.00
1	X	6	DC	C4'-C3'-C2'	-5.96	97.74	103.10
2	Y	4	DA	O4'-C1'-N9	5.82	112.07	108.00
2	Y	12	DG	O4'-C1'-N9	5.75	112.02	108.00
1	X	7	DT	N3-C4-O4	5.74	123.35	119.90
2	U	4	DC	O4'-C1'-N1	5.72	112.01	108.00
1	X	10	DC	C1'-O4'-C4'	-5.42	104.69	110.10
1	R	1	DG	O4'-C1'-N9	-5.41	104.22	108.00
3	A	326	LEU	CA-CB-CG	5.27	127.41	115.30
1	R	2	DA	O4'-C1'-N9	5.24	111.67	108.00
1	X	5	DG	C1'-O4'-C4'	-5.23	104.87	110.10
1	R	8	DT	C4-C5-C7	5.19	122.11	119.00
2	Y	7	DC	C4'-C3'-C2'	-5.18	98.44	103.10
2	S	12	DG	O4'-C1'-N9	5.13	111.59	108.00
1	R	4	DT	O4'-C1'-N1	5.12	111.58	108.00
2	S	8	DG	N1-C6-O6	-5.11	116.83	119.90
2	Y	7	DC	P-O3'-C3'	5.06	125.77	119.70
2	U	6	DT	C1'-O4'-C4'	-5.01	105.09	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	346	GLU	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	310	TYR	Peptide
3	A	391	GLY	Peptide
3	A	520	ASP	Peptide
3	D	344	ASN	Peptide
3	D	466	GLU	Peptide
3	D	509	VAL	Peptide

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	R	200	0	115	2	2
1	X	200	0	115	1	0
2	S	284	0	158	5	2
2	T	99	0	57	2	0
2	U	140	0	80	1	0
2	Y	284	0	158	4	0
3	A	4668	0	4676	54	0
3	B	4617	0	4626	48	0
3	C	4596	0	4604	57	0
3	D	4606	0	4605	78	0
4	A	32	0	0	1	0
4	B	27	0	0	0	0
4	C	19	0	0	0	0
4	D	8	0	0	0	0
4	X	2	0	0	0	0
4	Y	1	0	0	0	0
All	All	19783	0	19194	243	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (243) 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)
3:D:30:MET:HE2	3:D:171:GLN:HA	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:PHE:CB	3:C:293:GLU:HA	1.83	1.04
3:A:101:TYR:HB3	3:A:188:MET:HE3	1.45	0.98
3:B:101:TYR:HB3	3:B:188:MET:HE3	1.47	0.94
3:C:292:PHE:HB3	3:C:293:GLU:HA	1.50	0.90
3:C:292:PHE:HB2	3:C:293:GLU:HA	1.55	0.85
3:D:52:LEU:O	3:D:107:LEU:HD11	1.81	0.78
3:A:130:VAL:HG22	3:A:173:ILE:HD11	1.66	0.78
3:A:253:LEU:HD21	3:A:437:ALA:HB1	1.69	0.75
3:B:216:LEU:HD11	3:B:421:THR:HG21	1.69	0.74
3:C:202:ILE:O	3:C:203:THR:HB	1.85	0.74
3:A:553:LYS:HG3	3:A:571:THR:HG22	1.71	0.73
3:B:216:LEU:CD1	3:B:421:THR:HG21	2.19	0.73
2:Y:7:DC:H2"	3:A:391:GLY:O	1.88	0.73
3:D:130:VAL:HG22	3:D:173:ILE:HD11	1.71	0.72
2:S:13:DC:H5"	3:D:573:THR:O	1.91	0.71
3:D:468:PRO:O	3:D:471:ILE:HG22	1.92	0.69
3:B:101:TYR:HB3	3:B:188:MET:CE	2.23	0.68
3:D:125:LYS:HE3	3:D:187:ARG:O	1.94	0.68
3:A:44:LEU:HD11	3:A:48:MET:CE	2.24	0.68
3:C:396:ASN:HD21	3:C:398:ASP:HB3	1.58	0.67
3:D:273:GLY:HA2	3:D:347:TYR:O	1.94	0.66
3:A:101:TYR:HB3	3:A:188:MET:CE	2.23	0.66
3:D:378:ILE:C	3:D:378:ILE:HD13	2.15	0.66
3:C:292:PHE:CB	3:C:293:GLU:CA	2.68	0.65
3:D:30:MET:HE2	3:D:171:GLN:CA	2.21	0.65
2:S:16:DT:C4	2:S:17:DC:N4	2.64	0.65
3:D:396:ASN:HD22	3:D:398:ASP:H	1.45	0.64
2:T:4:DC:OP2	3:B:392:LYS:NZ	2.30	0.64
3:A:44:LEU:HD11	3:A:48:MET:HE1	1.79	0.63
3:C:380:GLN:HE22	3:C:383:LYS:NZ	1.96	0.63
3:D:533:MET:CE	3:D:538:LYS:HA	2.29	0.62
3:C:447:ALA:HB1	3:C:470:VAL:HG11	1.79	0.62
3:A:125:LYS:NZ	3:A:185:LEU:O	2.32	0.62
3:D:553:LYS:HG3	3:D:571:THR:HG22	1.81	0.61
3:C:356:THR:HG23	3:C:359:LEU:HD12	1.83	0.61
3:B:50:TRP:O	3:B:54:VAL:HG22	2.01	0.60
3:A:44:LEU:CD1	3:A:48:MET:CE	2.79	0.60
3:C:292:PHE:HB2	3:C:293:GLU:CA	2.28	0.60
3:D:374:SER:OG	3:D:378:ILE:HD12	2.02	0.60
3:D:506:MET:HE3	3:D:525:LYS:HE3	1.83	0.60
3:D:287:HIS:CD2	3:D:348:ILE:HD12	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:SER:HB2	3:D:32:ILE:HD11	1.85	0.59
3:A:292:PHE:HB3	3:A:342:LEU:HD23	1.85	0.59
3:B:370:ILE:O	3:B:374:SER:OG	2.20	0.58
3:B:289:ARG:NH1	3:B:348:ILE:HD11	2.19	0.58
3:D:509:VAL:CG2	3:D:509:VAL:O	2.50	0.58
3:D:48:MET:HE1	3:D:70:ILE:HG23	1.85	0.58
3:D:508:GLU:O	3:D:509:VAL:HG12	2.03	0.57
3:A:551:SER:HB2	3:A:573:THR:HG23	1.86	0.57
3:D:343:TYR:O	3:D:345:VAL:HB	2.03	0.57
3:B:344:ASN:HD22	3:B:344:ASN:N	2.03	0.57
3:C:134:ALA:HB1	3:C:141:VAL:HB	1.86	0.56
3:B:214:LEU:HD21	3:B:268:PRO:CD	2.36	0.56
3:D:202:ILE:O	3:D:203:THR:OG1	2.16	0.56
3:B:152:ARG:HD3	3:B:156:TYR:CE2	2.41	0.56
3:D:369:TYR:CZ	3:D:373:THR:HG21	2.41	0.56
3:A:7:LYS:O	3:A:56:ALA:HB1	2.06	0.55
3:D:32:ILE:HD12	3:D:174:ALA:HA	1.89	0.55
3:A:225:ALA:O	3:A:431:VAL:HG13	2.07	0.55
3:B:8:MET:HB3	3:B:32:ILE:HD12	1.87	0.55
3:C:542:THR:HG22	3:C:545:ASN:CG	2.27	0.55
3:D:471:ILE:O	3:D:475:VAL:HG23	2.06	0.55
3:D:468:PRO:HB2	3:D:471:ILE:HG22	1.89	0.54
3:A:70:ILE:HD13	3:A:119:ILE:HD12	1.89	0.54
3:B:302:ILE:HG21	3:B:336:MET:CE	2.37	0.54
3:A:253:LEU:HD22	3:A:458:ASP:HB3	1.90	0.54
3:D:253:LEU:HD22	3:D:458:ASP:HB3	1.89	0.54
3:C:15:THR:HG21	3:C:69:PHE:CE1	2.42	0.54
2:U:3:DA:OP1	3:C:192:SER:OG	2.21	0.54
3:D:374:SER:OG	3:D:378:ILE:HG23	2.08	0.54
3:D:81:TRP:CH2	3:D:83:ALA:HB2	2.43	0.54
3:A:48:MET:HG2	3:A:73:TRP:CD2	2.43	0.53
3:A:310:TYR:HA	3:A:311:LYS:HB2	1.91	0.53
3:D:30:MET:CE	3:D:171:GLN:HG3	2.39	0.53
3:A:48:MET:HG2	3:A:73:TRP:CE3	2.44	0.53
3:C:8:MET:HB3	3:C:32:ILE:HD12	1.90	0.52
3:D:48:MET:CE	3:D:70:ILE:HG23	2.39	0.52
3:A:130:VAL:CG2	3:A:173:ILE:HD11	2.39	0.52
3:B:292:PHE:CD1	3:B:302:ILE:HD11	2.45	0.52
3:A:326:LEU:N	3:A:326:LEU:HD23	2.25	0.52
3:D:533:MET:HE3	3:D:538:LYS:HG2	1.91	0.52
3:D:40:ILE:HD13	3:D:166:ILE:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:384:LEU:O	3:B:388:SER:OG	2.27	0.51
3:D:30:MET:HE1	3:D:171:GLN:HG3	1.92	0.51
3:D:533:MET:CE	3:D:538:LYS:HG2	2.41	0.51
3:D:504:ILE:CG2	3:D:506:MET:HE2	2.41	0.51
3:A:390:TYR:HB2	3:A:433:ILE:HD13	1.93	0.51
2:Y:4:DA:H2'	2:Y:4:DA:N3	2.24	0.51
3:C:369:TYR:CZ	3:C:373:THR:HG21	2.46	0.51
3:C:289:ARG:O	3:C:290:CYS:HB3	2.11	0.51
3:D:284:HIS:CE1	3:D:330:ASN:HB3	2.45	0.51
3:D:248:PHE:HB2	3:D:460:ILE:HG13	1.93	0.51
3:D:533:MET:HE1	3:D:538:LYS:HA	1.92	0.51
3:B:268:PRO:HB3	3:B:353:PHE:CE2	2.46	0.51
3:C:400:THR:HG23	3:C:418:GLU:O	2.11	0.51
3:D:509:VAL:O	3:D:509:VAL:HG23	2.11	0.50
3:B:292:PHE:CE1	3:B:302:ILE:HD11	2.47	0.50
3:A:134:ALA:HB1	3:A:141:VAL:HB	1.93	0.50
3:C:51:VAL:HG13	3:C:117:THR:HG21	1.94	0.50
3:A:173:ILE:HD12	4:A:597:HOH:O	2.12	0.50
2:Y:14:DA:H5''	3:A:571:THR:O	2.11	0.50
3:D:501:ILE:HG22	3:D:528:VAL:HG22	1.92	0.50
3:C:265:TYR:CD2	3:C:356:THR:HG22	2.47	0.50
3:B:216:LEU:HD13	3:B:421:THR:HG21	1.93	0.49
3:C:152:ARG:HD3	3:C:156:TYR:CE2	2.47	0.49
3:D:237:PHE:HD2	3:D:242:ILE:HG21	1.77	0.49
3:A:495:LEU:HD22	3:A:546:PHE:CE2	2.47	0.49
2:S:8:DG:H2'	2:S:9:DT:C6	2.46	0.49
3:B:313:ASN:O	3:B:497:GLN:NE2	2.39	0.49
3:D:345:VAL:O	3:D:345:VAL:HG22	2.13	0.49
3:D:508:GLU:O	3:D:509:VAL:CG1	2.61	0.48
3:A:8:MET:HB3	3:A:32:ILE:HD12	1.95	0.48
3:B:9:TYR:HB2	3:B:58:LEU:HD22	1.94	0.48
3:D:50:TRP:O	3:D:54:VAL:HG22	2.14	0.48
3:D:506:MET:HE3	3:D:525:LYS:CE	2.44	0.48
3:C:289:ARG:HA	3:C:324:ALA:O	2.13	0.48
3:B:199:LYS:HG2	3:B:204:THR:HG22	1.94	0.48
3:D:378:ILE:O	3:D:378:ILE:HD13	2.13	0.48
3:D:504:ILE:HG21	3:D:506:MET:CE	2.44	0.48
3:D:101:TYR:HB3	3:D:188:MET:HE3	1.95	0.48
3:D:262:LEU:HG	3:D:355:ALA:HB1	1.95	0.48
3:C:287:HIS:ND1	3:C:327:TRP:CE2	2.82	0.48
3:D:449:TYR:O	3:D:452:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:390:TYR:CD1	3:B:390:TYR:C	2.86	0.48
3:C:134:ALA:CB	3:C:141:VAL:HB	2.44	0.47
3:B:542:THR:HG21	3:C:554:MET:HE3	1.96	0.47
3:C:497:GLN:H	3:C:497:GLN:CD	2.18	0.47
2:S:4:DA:N3	2:S:4:DA:H2'	2.30	0.47
3:A:405:TYR:O	3:A:412:LEU:HD12	2.14	0.47
3:D:50:TRP:CZ2	3:D:54:VAL:HG11	2.50	0.47
3:B:125:LYS:NZ	3:B:193:ASP:OD2	2.46	0.47
3:A:216:LEU:HD11	3:A:421:THR:HG21	1.97	0.47
3:D:202:ILE:HD11	3:D:207:PHE:HD1	1.79	0.47
3:D:336:MET:HE3	3:D:342:LEU:HD21	1.97	0.47
3:B:247:VAL:HB	3:B:487:SER:HB3	1.97	0.47
3:A:68:ALA:CB	3:A:565:VAL:HG23	2.45	0.46
3:C:258:MET:CE	3:C:389:LEU:HD23	2.45	0.46
3:D:202:ILE:HD11	3:D:207:PHE:CD1	2.51	0.46
3:D:40:ILE:HD13	3:D:166:ILE:HG22	1.97	0.46
3:D:294:LEU:HD12	3:D:339:HIS:O	2.16	0.46
2:T:4:DC:OP2	3:B:189:THR:OG1	2.31	0.46
3:D:253:LEU:O	3:D:256:ALA:HB3	2.16	0.46
3:B:550:PHE:HB3	3:B:574:ILE:HD12	1.98	0.46
2:Y:8:DG:H3'	2:Y:9:DT:H72	1.97	0.46
3:C:278:ASP:OD2	3:C:352:LYS:NZ	2.41	0.46
3:A:141:VAL:HG13	3:A:141:VAL:O	2.16	0.46
3:C:319:SER:O	3:C:321:GLY:N	2.49	0.46
3:A:326:LEU:N	3:A:326:LEU:CD2	2.80	0.46
3:D:427:THR:N	3:D:428:PRO:CD	2.79	0.46
3:C:402:LYS:HE3	3:C:414:PHE:CG	2.51	0.46
3:C:542:THR:HG22	3:C:545:ASN:H	1.81	0.45
3:A:471:ILE:CG2	3:A:475:VAL:HG23	2.45	0.45
3:D:30:MET:HE3	3:D:35:HIS:CD2	2.51	0.45
3:A:495:LEU:HD21	3:A:547:LYS:HA	1.99	0.45
3:A:50:TRP:O	3:A:54:VAL:HG22	2.16	0.45
3:D:68:ALA:CB	3:D:565:VAL:HG23	2.47	0.45
3:D:125:LYS:CE	3:D:187:ARG:O	2.64	0.45
3:B:302:ILE:HG21	3:B:336:MET:HE3	1.98	0.45
3:C:202:ILE:HD11	3:C:207:PHE:HD1	1.82	0.45
3:B:501:ILE:HG22	3:B:528:VAL:HG22	1.99	0.45
3:A:549:GLY:O	3:A:550:PHE:C	2.55	0.44
3:D:396:ASN:ND2	3:D:397:PRO:HD2	2.32	0.44
3:A:134:ALA:CB	3:A:141:VAL:HB	2.48	0.44
3:D:152:ARG:HD3	3:D:156:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:286:GLN:HG3	3:B:288:ILE:HG23	2.00	0.44
3:C:253:LEU:HD22	3:C:458:ASP:HB3	1.99	0.44
3:D:471:ILE:HD13	3:D:475:VAL:CG2	2.47	0.44
3:A:330:ASN:ND2	3:A:334:GLU:OE2	2.38	0.44
3:D:370:ILE:HG23	3:D:378:ILE:HD11	1.99	0.44
3:A:313:ASN:H	3:A:313:ASN:HD22	1.64	0.44
3:D:15:THR:HG22	3:D:24:VAL:HG22	2.00	0.44
3:A:61:HIS:CD2	3:A:130:VAL:HG23	2.53	0.43
3:C:450:ASP:HB3	3:C:451:ARG:HG2	1.99	0.43
3:C:52:LEU:O	3:C:107:LEU:HD11	2.16	0.43
3:D:139:LEU:HD22	3:D:175:GLU:OE1	2.18	0.43
3:C:292:PHE:N	3:C:292:PHE:CD2	2.86	0.43
3:A:125:LYS:HE3	3:A:187:ARG:O	2.17	0.43
3:C:141:VAL:HG13	3:C:141:VAL:O	2.18	0.43
3:B:99:GLN:HE21	3:B:99:GLN:HA	1.81	0.43
3:C:553:LYS:HA	3:C:571:THR:HA	1.99	0.43
3:A:52:LEU:O	3:A:107:LEU:HD21	2.18	0.43
3:D:22:CYS:SG	3:D:566:VAL:HG23	2.58	0.43
3:D:134:ALA:HB1	3:D:141:VAL:HB	2.01	0.43
3:D:44:LEU:HD11	3:D:48:MET:HE2	2.01	0.43
3:B:68:ALA:CB	3:B:565:VAL:HG23	2.48	0.43
3:C:447:ALA:HB1	3:C:470:VAL:CG1	2.46	0.43
3:B:14:GLU:HG2	3:B:25:TRP:CZ2	2.54	0.43
3:B:30:MET:HB2	3:B:170:ILE:HD12	2.01	0.43
3:A:517:SER:HB2	3:A:518:PRO:HD2	2.01	0.43
3:A:70:ILE:HD13	3:A:119:ILE:CD1	2.49	0.42
3:C:45:ASP:N	3:C:45:ASP:OD1	2.51	0.42
3:C:542:THR:CG2	3:C:545:ASN:H	2.32	0.42
3:D:289:ARG:HA	3:D:324:ALA:O	2.19	0.42
3:B:369:TYR:O	3:B:373:THR:HB	2.18	0.42
3:D:370:ILE:CG2	3:D:378:ILE:HD11	2.50	0.42
3:C:351:LEU:N	3:C:351:LEU:HD12	2.35	0.42
3:C:223:ARG:NH2	3:C:394:ALA:O	2.52	0.42
3:B:185:LEU:N	3:B:185:LEU:CD1	2.83	0.42
3:A:471:ILE:HG22	3:A:475:VAL:HG23	2.00	0.42
3:B:246:MET:HE2	3:B:485:HIS:NE2	2.35	0.42
3:A:286:GLN:HG3	3:A:288:ILE:HG23	2.01	0.42
3:A:253:LEU:CD2	3:A:437:ALA:HB1	2.44	0.42
3:B:487:SER:OG	3:B:504:ILE:HD12	2.20	0.42
3:A:271:PHE:CZ	3:A:275:TYR:HB2	2.55	0.42
3:A:227:ARG:HH21	3:A:328:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:O	3:C:107:LEU:CD1	2.67	0.42
3:B:294:LEU:HA	3:B:340:TYR:CD2	2.55	0.42
3:D:504:ILE:CG2	3:D:506:MET:CE	2.98	0.42
3:A:81:TRP:CH2	3:A:83:ALA:HB2	2.54	0.42
3:C:394:ALA:O	3:C:395:SER:C	2.56	0.41
3:B:470:VAL:HG13	3:B:471:ILE:HG23	2.00	0.41
1:R:9:DA:C2	2:S:10:DA:C2	3.08	0.41
3:D:409:ASN:O	3:D:411:ALA:N	2.51	0.41
3:C:287:HIS:CD2	3:C:348:ILE:HD12	2.55	0.41
3:B:202:ILE:C	3:B:203:THR:HG23	2.40	0.41
3:A:68:ALA:HB3	3:A:565:VAL:HG23	2.03	0.41
3:C:253:LEU:HD21	3:C:437:ALA:HB1	2.02	0.41
3:C:289:ARG:HG3	3:C:348:ILE:HD11	2.01	0.41
3:D:101:TYR:HB3	3:D:188:MET:CE	2.50	0.41
3:C:273:GLY:HA2	3:C:347:TYR:O	2.20	0.41
3:C:299:ILE:CG2	3:C:300:PRO:HD2	2.50	0.41
3:B:253:LEU:O	3:B:256:ALA:HB3	2.19	0.41
3:A:369:TYR:CZ	3:A:373:THR:HG21	2.56	0.41
3:B:287:HIS:CE1	3:B:348:ILE:HD13	2.56	0.41
3:B:552:ARG:NH1	3:C:553:LYS:HB3	2.35	0.41
3:D:384:LEU:HD12	3:D:384:LEU:HA	1.94	0.41
3:C:427:THR:N	3:C:428:PRO:CD	2.83	0.41
3:C:293:GLU:HB3	3:C:317:LYS:O	2.21	0.41
3:C:356:THR:OG1	3:C:357:THR:N	2.54	0.41
3:C:253:LEU:O	3:C:257:GLN:HG2	2.20	0.41
3:C:97:MET:HE2	3:C:97:MET:N	2.36	0.41
1:X:6:DC:H2'	1:X:7:DT:C6	2.55	0.41
3:B:202:ILE:O	3:B:203:THR:HG23	2.21	0.41
3:A:201:ILE:HG22	3:A:202:ILE:HG23	2.03	0.41
1:R:3:DC:H2'	1:R:3:DC:O2	2.21	0.41
3:A:130:VAL:HG22	3:A:173:ILE:CD1	2.45	0.40
3:B:50:TRP:CE2	3:B:54:VAL:HG11	2.56	0.40
3:D:141:VAL:HG13	3:D:141:VAL:O	2.21	0.40
3:B:25:TRP:CE2	3:B:152:ARG:NE	2.89	0.40
3:D:421:THR:HG23	3:D:422:LYS:N	2.36	0.40
3:C:380:GLN:NE2	3:C:383:LYS:CE	2.85	0.40
3:B:218:LEU:O	3:B:222:VAL:HG23	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1:DG:O6	2:S:17:DC:N3[2_453]	2.15	0.05
1:R:1:DG:O6	2:S:17:DC:N4[2_453]	2.17	0.03

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	
3	A	569/575 (99%)	537 (94%)	30 (5%)	2 (0%)	39	65
3	B	562/575 (98%)	538 (96%)	23 (4%)	1 (0%)	52	77
3	C	559/575 (97%)	526 (94%)	28 (5%)	5 (1%)	21	42
3	D	559/575 (97%)	527 (94%)	27 (5%)	5 (1%)	21	42
All	All	2249/2300 (98%)	2128 (95%)	108 (5%)	13 (1%)	30	56

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	345	VAL
3	A	425	VAL
3	C	320	GLY
3	A	62	ASN
3	D	62	ASN
3	C	457	THR
3	B	425	VAL
3	C	450	ASP
3	C	203	THR
3	C	425	VAL
3	D	425	VAL
3	D	509	VAL
3	D	511	GLY

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	
3	A	502/506 (99%)	477 (95%)	25 (5%)	30	56
3	B	497/506 (98%)	466 (94%)	31 (6%)	23	45
3	C	495/506 (98%)	473 (96%)	22 (4%)	35	63
3	D	496/506 (98%)	463 (93%)	33 (7%)	20	40
All	All	1990/2024 (98%)	1879 (94%)	111 (6%)	26	50

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	GLU
3	A	23	ARG
3	A	54	VAL
3	A	113	ARG
3	A	116	HIS
3	A	177	LEU
3	A	201	ILE
3	A	209	LYS
3	A	236	ARG
3	A	307	SER
3	A	308	ARG
3	A	310	TYR
3	A	313	ASN
3	A	326	LEU
3	A	351	LEU
3	A	354	LYS
3	A	390	TYR
3	A	421	THR
3	A	469	ASP
3	A	470	VAL
3	A	486	GLU
3	A	495	LEU
3	A	520	ASP
3	A	522	THR

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Mol	Chain	Res	Type
3	A	543	PHE
3	B	20	GLU
3	B	43	SER
3	B	54	VAL
3	B	88	ASN
3	B	116	HIS
3	B	173	ILE
3	B	185	LEU
3	B	201	ILE
3	B	240	LYS
3	B	242	ILE
3	B	246	MET
3	B	260	SER
3	B	302	ILE
3	B	311	LYS
3	B	334	GLU
3	B	344	ASN
3	B	373	THR
3	B	374	SER
3	B	388	SER
3	B	390	TYR
3	B	395	SER
3	B	416	LEU
3	B	419	GLU
3	B	421	THR
3	B	450	ASP
3	B	472	LYS
3	B	473	ASP
3	B	536	LYS
3	B	543	PHE
3	B	544	GLU
3	B	552	ARG
3	C	20	GLU
3	C	45	ASP
3	C	84	ASP
3	C	86	LEU
3	C	116	HIS
3	C	125	LYS
3	C	185	LEU
3	C	192	SER
3	C	351	LEU
3	C	356	THR

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Mol	Chain	Res	Type
3	C	359	LEU
3	C	390	TYR
3	C	420	GLU
3	C	451	ARG
3	C	469	ASP
3	C	470	VAL
3	C	472	LYS
3	C	478	LYS
3	C	542	THR
3	C	543	PHE
3	C	551	SER
3	C	554	MET
3	D	23	ARG
3	D	54	VAL
3	D	110	LYS
3	D	112	LYS
3	D	125	LYS
3	D	131	LYS
3	D	148	TYR
3	D	149	HIS
3	D	196	LYS
3	D	216	LEU
3	D	236	ARG
3	D	246	MET
3	D	317	LYS
3	D	326	LEU
3	D	347	TYR
3	D	354	LYS
3	D	361	LYS
3	D	375	GLU
3	D	378	ILE
3	D	379	LYS
3	D	396	ASN
3	D	421	THR
3	D	457	THR
3	D	467	ILE
3	D	471	ILE
3	D	490	LYS
3	D	508	GLU
3	D	512	LYS
3	D	523	ASP
3	D	529	LYS

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Mol	Chain	Res	Type
3	D	543	PHE
3	D	552	ARG
3	D	554	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	183	GLN
3	A	303	GLN
3	A	313	ASN
3	A	497	GLN
3	B	99	GLN
3	B	330	ASN
3	B	344	ASN
3	B	380	GLN
3	C	183	GLN
3	C	380	GLN
3	C	396	ASN
3	D	35	HIS
3	D	171	GLN
3	D	284	HIS
3	D	396	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	R	10/10 (100%)	-0.21	0 100 100	34, 45, 50, 53	0
1	X	10/10 (100%)	-1.08	0 100 100	21, 27, 30, 30	0
2	S	14/17 (82%)	-0.15	1 (7%) 19 13	28, 36, 53, 56	0
2	T	5/17 (29%)	0.14	1 (20%) 1 1	26, 32, 38, 57	0
2	U	7/17 (41%)	0.32	1 (14%) 4 2	26, 37, 55, 64	0
2	Y	14/17 (82%)	-0.67	0 100 100	20, 26, 42, 56	0
3	A	571/575 (99%)	-0.46	0 100 100	15, 25, 32, 43	2 (0%)
3	B	566/575 (98%)	-0.46	0 100 100	18, 25, 32, 41	0
3	C	563/575 (97%)	-0.40	2 (0%) 93 91	16, 25, 31, 39	0
3	D	564/575 (98%)	-0.36	1 (0%) 95 95	9, 25, 31, 41	0
All	All	2324/2388 (97%)	-0.42	6 (0%) 94 93	9, 25, 32, 64	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	323	ILE	2.7
2	S	4	DA	2.5
3	D	321	GLY	2.5
3	C	320	GLY	2.3
2	T	1	DA	2.2
2	U	7	DA	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.