



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:06 AM GMT

PDB ID : 2PE5
Title : Crystal Structure of the Lac Repressor bound to ONPG in repressed state
Authors : Daber, R.; Stayrook, S.E.; Rosenberg, A.; Lewis, M.
Deposited on : 2007-04-02
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

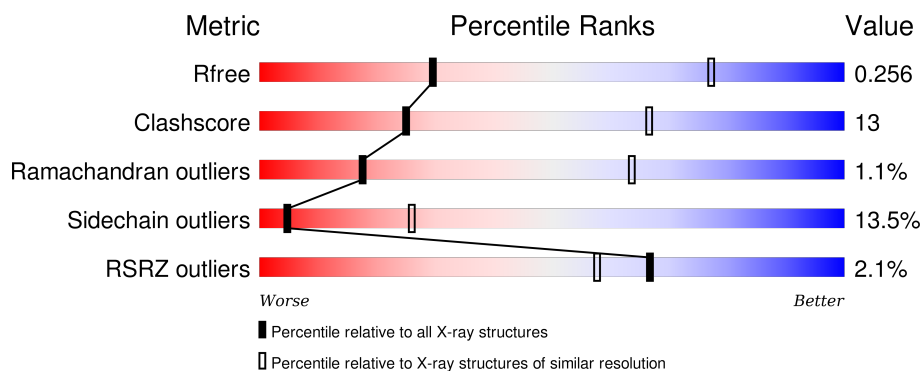
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	D	20	<div> <div>30%</div> <div>50%</div> <div>5%</div> <div>15%</div> </div>
1	E	20	<div> <div>30%</div> <div>45%</div> <div>10%</div> <div>15%</div> </div>
1	F	20	<div> <div>40%</div> <div>40%</div> <div>35%</div> <div>10%</div> <div>15%</div> </div>
2	A	330	<div> <div>2%</div> <div>64%</div> <div>31%</div> <div>• •</div> </div>
2	B	330	<div> <div>%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	330	 <div> <div>2%</div> <div>68%</div> <div>28%</div> <div>• •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8527 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 DNA (5'-D(*DAP*DAP*DTP*DTP*DGP*DTP*DGP*DAP*DGP*DCP*DGP*DCP*DTP*DCP*DAP*DCP*DAP*DAP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	17	Total	C	N	O	P	0	0	0
			348	166	62	103	17			
1	E	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			
1	F	17	Total	C	N	O	P	0	0	0
			349	166	65	101	17			

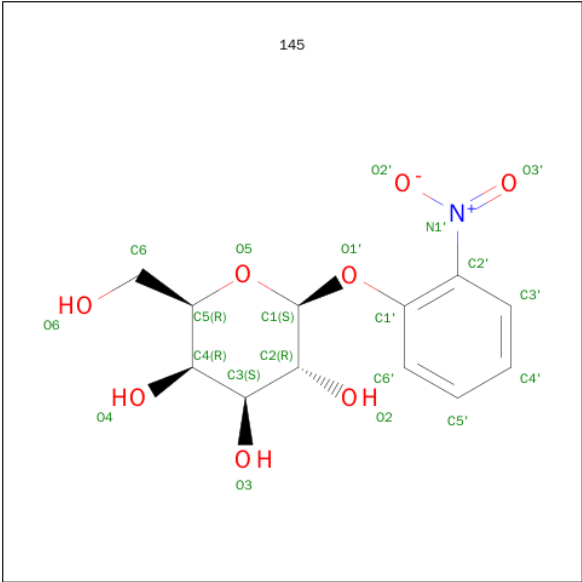
- Molecule 2 is a protein called Lactose operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	328	Total	C	N	O	S	0	0	0
			2468	1544	438	475	11			
2	B	330	Total	C	N	O	S	0	0	0
			2482	1553	440	478	11			
2	C	328	Total	C	N	O	S	0	0	0
			2468	1544	438	475	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	LEU	SER	ENGINEERED	UNP P03023
B	61	LEU	SER	ENGINEERED	UNP P03023
C	61	LEU	SER	ENGINEERED	UNP P03023

- Molecule 3 is 1-O-[O-NITROPHENYL]-BETA-D-GALACTOPYRANOSE (three-letter code: 145) (formula: C₁₂H₁₅NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	12	1	8		
3	B	1	Total	C	N	O	0	0
			21	12	1	8		
3	C	1	Total	C	N	O	0	0
			21	12	1	8		

3 Residue-property plots [i](#)

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

- Molecule 1: DNA (5'-D(*DAP*DAP*DTP*DTP*DGP*DTP*DGP*DAP*DGP*DCP*DGP*DCP*DTP*DCP*DAP*DCP*DAP*DAP*DTP*DT)-3')

Chain D: 



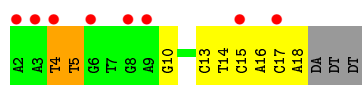
- Molecule 1: DNA (5'-D(*DAP*DAP*DTP*DTP*DGP*DTP*DGP*DAP*DGP*DCP*DGP*DCP*DTP*DCP*DAP*DCP*DAP*DAP*DTP*DT)-3')

Chain E: 



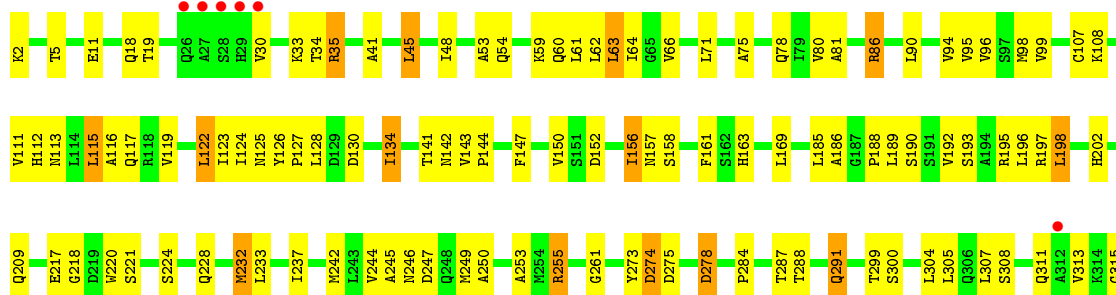
- Molecule 1: DNA (5'-D(*DAP*DAP*DTP*DTP*DGP*DTP*DGP*DAP*DGP*DCP*DGP*DCP*DTP*DCP*DAP*DCP*DAP*DAP*DTP*DT)-3')

Chain F: 



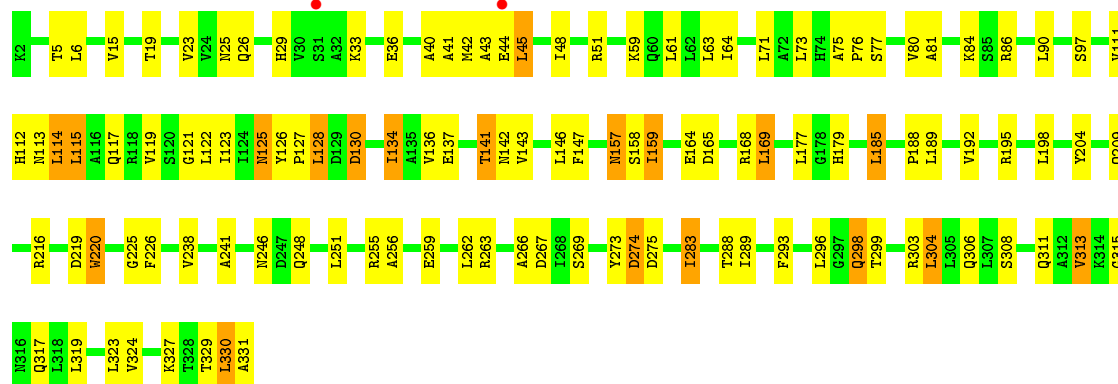
- Molecule 2: Lactose operon repressor

Chain A: 

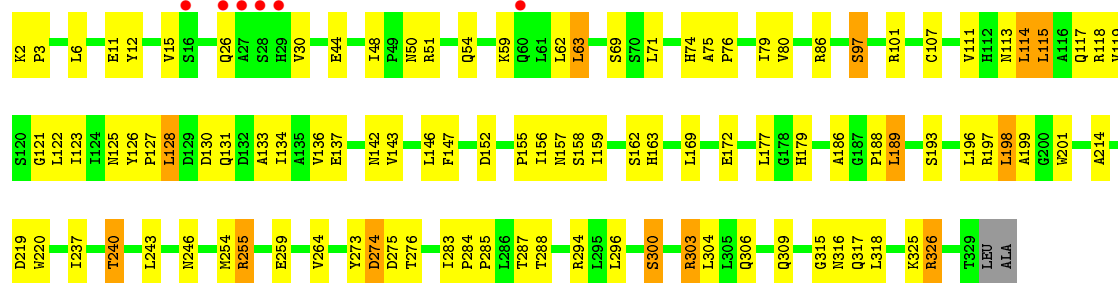




• Molecule 2: Lactose operon repressor



• Molecule 2: Lactose operon repressor



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	253.08Å 253.08Å 203.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.50 19.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-3.50) 99.9 (19.98-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.287 0.217 , 0.256	Depositor DCC
R_{free} test set	1581 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31298 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8527	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 145

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	0.88	0/389	1.84	14/598 (2.3%)
1	E	0.90	0/391	2.13	22/601 (3.7%)
1	F	0.87	0/391	2.00	22/601 (3.7%)
2	A	0.45	0/2502	0.64	0/3401
2	B	0.45	0/2516	0.65	0/3419
2	C	0.45	0/2502	0.62	0/3401
All	All	0.53	0/8691	0.97	58/12021 (0.5%)

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
2	B	1	1

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	15	DC	O4'-C4'-C3'	-12.40	98.56	106.00
1	E	15	DC	O3'-P-O5'	-12.00	81.20	104.00
1	D	7	DT	O3'-P-O5'	-11.78	81.61	104.00
1	E	4	DT	P-O3'-C3'	10.98	132.88	119.70
1	F	4	DT	O3'-P-O5'	-10.35	84.34	104.00
1	F	17	DC	O3'-P-O5'	-10.32	84.39	104.00
1	E	17	DC	O3'-P-O5'	-10.28	84.48	104.00
1	E	4	DT	OP2-P-O3'	-10.09	83.01	105.20
1	F	15	DC	OP1-P-O3'	-9.60	84.09	105.20
1	E	17	DC	OP1-P-O3'	-9.34	84.64	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	15	DC	O4'-C4'-C3'	-8.82	100.71	106.00
1	E	15	DC	OP1-P-O3'	-8.80	85.84	105.20
1	F	15	DC	O3'-P-O5'	-8.51	87.83	104.00
1	F	17	DC	OP2-P-O3'	-8.31	86.91	105.20
1	F	4	DT	OP1-P-O3'	-8.31	86.92	105.20
1	F	10	DG	O4'-C1'-N9	8.23	113.76	108.00
1	F	4	DT	OP2-P-O3'	-8.16	87.25	105.20
1	E	4	DT	O3'-P-O5'	-8.11	88.58	104.00
1	F	15	DC	OP2-P-O3'	-8.11	87.36	105.20
1	D	13	DC	O4'-C1'-N1	8.07	113.65	108.00
1	F	17	DC	OP1-P-O3'	-8.05	87.48	105.20
1	D	8	DG	O5'-P-OP2	7.97	120.26	110.70
1	E	4	DT	OP1-P-O3'	-7.89	87.84	105.20
1	D	7	DT	OP2-P-O3'	-7.53	88.63	105.20
1	F	18	DA	O4'-C4'-C3'	-7.46	101.52	104.50
1	D	15	DC	O4'-C1'-N1	7.40	113.18	108.00
1	D	15	DC	P-O3'-C3'	7.30	128.46	119.70
1	D	7	DT	OP1-P-O3'	-7.24	89.28	105.20
1	E	17	DC	OP2-P-O3'	-7.04	89.72	105.20
1	F	17	DC	P-O3'-C3'	6.71	127.75	119.70
1	E	15	DC	OP2-P-O3'	-6.57	90.75	105.20
1	E	16	DA	O4'-C1'-N9	6.49	112.55	108.00
1	D	15	DC	C4'-C3'-C2'	-6.49	97.26	103.10
1	E	12	DG	O4'-C1'-N9	6.36	112.45	108.00
1	D	16	DA	O4'-C1'-N9	6.15	112.31	108.00
1	E	5	DT	O5'-P-OP1	6.03	117.94	110.70
1	F	5	DT	OP1-P-OP2	6.01	128.62	119.60
1	E	15	DC	O4'-C1'-N1	5.86	112.10	108.00
1	D	10	DG	O4'-C1'-N9	5.85	112.09	108.00
1	E	16	DA	O5'-P-OP2	5.76	117.61	110.70
1	D	17	DC	O4'-C4'-C3'	-5.62	102.25	104.50
1	F	17	DC	O4'-C1'-C2'	-5.53	101.47	105.90
1	E	16	DA	O4'-C1'-C2'	-5.52	101.48	105.90
1	E	8	DG	C4'-C3'-C2'	-5.49	98.16	103.10
1	D	7	DT	P-O3'-C3'	5.48	126.27	119.70
1	F	18	DA	O4'-C1'-N9	5.45	111.82	108.00
1	F	15	DC	P-O3'-C3'	5.31	126.07	119.70
1	F	17	DC	O4'-C1'-N1	5.29	111.70	108.00
1	F	5	DT	O5'-P-OP1	5.28	117.03	110.70
1	E	4	DT	O4'-C1'-N1	5.27	111.69	108.00
1	E	5	DT	OP1-P-OP2	5.26	127.50	119.60
1	F	16	DA	OP1-P-OP2	5.25	127.48	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	DT	P-O3'-C3'	5.21	125.95	119.70
1	F	5	DT	O4'-C1'-N1	5.17	111.62	108.00
1	F	16	DA	O5'-P-OP2	5.16	116.89	110.70
1	E	17	DC	P-O3'-C3'	5.15	125.88	119.70
1	D	21	DT	O4'-C1'-N1	5.02	111.51	108.00
1	E	18	DA	O5'-P-OP1	5.01	116.71	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	44	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	42	MET	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	D	348	0	193	4	0
1	E	349	0	192	7	0
1	F	349	0	192	2	0
2	A	2468	0	2518	70	0
2	B	2482	0	2534	80	0
2	C	2468	0	2518	64	0
3	A	21	0	15	5	0
3	B	21	0	15	4	0
3	C	21	0	15	4	0
All	All	8527	0	8192	212	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 13.

All (212) 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:A:126:TYR:CD1	2:A:127:PRO:HD2	2.10	0.86
2:B:63:LEU:HD22	2:B:119:VAL:HG12	1.62	0.81
2:B:44:GLU:O	2:B:45:LEU:HG	1.81	0.80
2:C:126:TYR:CD2	2:C:127:PRO:HD2	2.17	0.79
2:C:71:LEU:HD21	2:C:80:VAL:HG21	1.66	0.77
2:B:263:ARG:HG2	2:B:267:ASP:OD2	1.85	0.77
2:B:41:ALA:O	2:B:45:LEU:HD12	1.85	0.76
2:B:130:ASP:O	2:B:134:ILE:HG13	1.86	0.76
2:C:79:ILE:HD12	2:C:296:LEU:HD23	1.67	0.75
2:C:79:ILE:CD1	2:C:296:LEU:HD23	2.17	0.75
2:B:330:LEU:HD23	2:B:330:LEU:H	1.51	0.75
2:C:54:GLN:HE21	2:C:59:LYS:HD2	1.53	0.73
2:C:273:TYR:O	2:C:274:ASP:HB2	1.89	0.73
2:B:293:PHE:HE2	3:B:902:145:H5'	1.53	0.72
2:C:296:LEU:O	2:C:300:SER:HB2	1.91	0.70
2:A:193:SER:O	2:A:197:ARG:HG3	1.92	0.69
2:A:123:ILE:HD13	2:A:300:SER:HB3	1.74	0.69
2:A:150:VAL:HG21	2:A:156:ILE:HD11	1.74	0.68
2:B:25:ASN:HD21	2:B:59:LYS:HE2	1.61	0.66
2:B:71:LEU:HD21	2:B:80:VAL:HG21	1.78	0.66
2:A:237:ILE:H	2:A:237:ILE:HD12	1.61	0.65
1:F:13:DC:OP2	2:C:6:LEU:HB2	1.97	0.65
2:A:157:ASN:HA	2:A:315:GLY:O	1.97	0.64
2:B:293:PHE:HE2	3:B:902:145:C5'	2.11	0.64
2:A:71:LEU:HD12	2:A:98:MET:CE	2.28	0.63
2:C:123:ILE:HG13	2:C:304:LEU:CD1	2.28	0.63
2:B:246:ASN:HA	2:B:273:TYR:O	1.98	0.63
2:B:40:ALA:O	2:B:43:ALA:O	2.17	0.63
2:C:63:LEU:HD13	2:C:119:VAL:HG12	1.81	0.63
2:A:273:TYR:O	2:A:274:ASP:HB2	1.99	0.63
2:C:130:ASP:O	2:C:134:ILE:HG12	2.00	0.62
2:B:263:ARG:HG3	2:B:266:ALA:HB3	1.82	0.62
2:C:273:TYR:O	2:C:274:ASP:CB	2.47	0.61
2:C:255:ARG:HD3	2:C:259:GLU:OE1	2.01	0.61
2:A:30:VAL:HA	2:A:35:ARG:HH22	1.66	0.60
2:B:44:GLU:CD	2:B:44:GLU:O	2.39	0.60
2:B:266:ALA:HA	2:B:331:ALA:O	2.01	0.60
2:B:327:LYS:HA	2:B:330:LEU:HD21	1.83	0.59
2:C:133:ALA:HB1	2:C:156:ILE:HD11	1.84	0.59
2:B:119:VAL:HG21	2:B:122:LEU:HD21	1.83	0.59
2:B:219:ASP:O	2:B:220:TRP:HB2	2.01	0.59
2:C:123:ILE:HG13	2:C:304:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PHE:CE2	3:B:902:145:H5'	2.38	0.57
2:A:284:PRO:HG2	2:A:328:THR:HG22	1.87	0.57
2:C:134:ILE:HD11	2:C:155:PRO:HG2	1.86	0.57
2:A:71:LEU:HD21	2:A:80:VAL:HG21	1.87	0.57
2:A:122:LEU:N	2:A:122:LEU:HD23	2.20	0.56
2:A:71:LEU:HD12	2:A:98:MET:HE1	1.86	0.56
2:B:157:ASN:ND2	2:B:157:ASN:H	2.03	0.56
2:B:157:ASN:HA	2:B:315:GLY:O	2.05	0.56
2:A:245:ALA:HB3	2:A:249:MET:CE	2.36	0.56
2:A:198:LEU:HD22	2:A:202:HIS:CE1	2.41	0.56
2:A:111:VAL:HG13	2:A:122:LEU:HD11	1.86	0.56
2:A:95:VAL:HG21	2:A:117:GLN:OE1	2.06	0.55
2:A:273:TYR:O	2:A:274:ASP:CB	2.54	0.55
2:A:246:ASN:HA	2:A:273:TYR:O	2.06	0.55
2:C:121:GLY:HA3	2:C:304:LEU:HD21	1.88	0.54
1:D:11:DC:N4	1:E:11:DC:N4	2.55	0.54
2:B:255:ARG:HH11	2:B:259:GLU:CD	2.10	0.54
2:C:75:ALA:O	2:C:79:ILE:HG12	2.08	0.54
2:A:66:VAL:HG22	2:A:123:ILE:HB	1.91	0.53
2:A:107:CYS:O	2:A:111:VAL:HG23	2.08	0.53
2:B:5:THR:HG22	2:B:6:LEU:N	2.24	0.53
2:B:141:THR:O	2:B:142:ASN:HB2	2.09	0.53
2:B:275:ASP:HA	2:B:288:THR:HG21	1.90	0.52
2:C:157:ASN:HA	2:C:315:GLY:O	2.09	0.52
1:E:14:DT:H2''	1:E:15:DC:C6	2.45	0.52
2:B:298:GLN:HE21	2:B:299:THR:N	2.07	0.52
2:A:96:VAL:HG13	2:B:84:LYS:NZ	2.25	0.52
1:E:12:DG:H1'	2:A:53:ALA:HB1	1.90	0.52
2:A:287:THR:HG23	2:A:326:ARG:H	1.74	0.52
2:A:197:ARG:HH22	3:A:901:145:C1'	2.23	0.52
2:B:269:SER:HB3	2:B:329:THR:HA	1.92	0.52
2:A:98:MET:HE1	2:B:81:ALA:HA	1.92	0.51
2:B:126:TYR:HD1	2:B:128:LEU:HD13	1.75	0.51
2:C:146:LEU:HD21	2:C:159:ILE:HD12	1.93	0.51
2:A:75:ALA:HB2	3:A:901:145:H2	1.92	0.51
2:A:232:MET:HG3	2:A:233:LEU:N	2.25	0.51
2:A:62:LEU:HG	2:A:305:LEU:HD11	1.93	0.51
2:B:168:ARG:HG3	2:B:204:TYR:CE2	2.45	0.50
2:B:306:GLN:HE21	2:B:313:VAL:HG21	1.76	0.50
2:C:133:ALA:HB1	2:C:156:ILE:CD1	2.42	0.50
2:B:188:PRO:HD2	2:B:220:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:VAL:HG21	2:B:122:LEU:CD2	2.42	0.50
2:A:188:PRO:HD2	2:A:220:TRP:CE2	2.45	0.50
2:A:30:VAL:HA	2:A:35:ARG:NH2	2.26	0.50
2:B:128:LEU:HD23	2:B:147:PHE:HE2	1.77	0.50
2:A:64:ILE:HB	2:A:94:VAL:HG22	1.94	0.50
2:A:63:LEU:HD13	2:A:119:VAL:HA	1.94	0.50
2:A:218:GLY:HA3	2:A:249:MET:SD	2.52	0.49
1:D:9:DA:C2'	1:D:10:DG:H5'	2.41	0.49
2:C:128:LEU:HD23	2:C:147:PHE:HE2	1.77	0.49
2:A:224:SER:O	2:A:228:GLN:HB2	2.12	0.49
2:A:130:ASP:O	2:A:134:ILE:HG12	2.13	0.49
2:B:147:PHE:O	2:B:158:SER:HA	2.12	0.49
2:B:125:ASN:C	2:B:125:ASN:HD22	2.16	0.49
2:A:147:PHE:O	2:A:158:SER:HA	2.13	0.49
2:B:25:ASN:ND2	2:B:59:LYS:HE2	2.25	0.49
2:C:111:VAL:HG21	2:C:136:VAL:HG13	1.94	0.48
2:A:275:ASP:HA	2:A:288:THR:HG21	1.95	0.48
2:A:48:ILE:HG23	2:B:112:HIS:NE2	2.28	0.48
2:B:130:ASP:O	2:B:134:ILE:CG1	2.60	0.48
2:C:254:MET:HG2	2:C:264:VAL:HG11	1.94	0.48
2:A:71:LEU:HD12	2:A:98:MET:HE2	1.93	0.48
2:B:179:HIS:CE1	2:B:241:ALA:HB2	2.48	0.48
2:C:201:TRP:CD1	2:C:243:LEU:HD13	2.48	0.47
2:C:179:HIS:ND1	2:C:240:THR:HB	2.28	0.47
2:B:275:ASP:OD2	2:B:324:VAL:HG21	2.14	0.47
2:B:238:VAL:O	2:B:238:VAL:HG23	2.14	0.47
2:C:158:SER:OG	2:C:316:ASN:ND2	2.47	0.47
2:C:26:GLN:HG3	2:C:30:VAL:HG21	1.96	0.47
2:C:123:ILE:HG13	2:C:304:LEU:HD13	1.96	0.47
2:B:5:THR:HG22	2:B:6:LEU:H	1.80	0.47
2:C:303:ARG:HA	2:C:306:GLN:HE21	1.80	0.47
2:C:303:ARG:HA	2:C:306:GLN:NE2	2.30	0.47
2:A:185:LEU:HB3	2:A:244:VAL:HG13	1.97	0.47
2:C:51:ARG:HA	2:C:54:GLN:HG2	1.96	0.47
2:C:79:ILE:HD11	2:C:296:LEU:HD23	1.92	0.47
2:B:296:LEU:CD2	3:B:902:145:H4'	2.45	0.47
2:B:288:THR:OG1	2:B:289:ILE:N	2.48	0.47
2:A:152:ASP:N	2:A:152:ASP:OD2	2.47	0.47
2:A:147:PHE:CD1	2:A:156:ILE:HG13	2.50	0.46
2:B:121:GLY:HA3	2:B:304:LEU:HD21	1.97	0.46
2:C:285:PRO:HB2	2:C:326:ARG:HG2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:VAL:HG21	2:C:122:LEU:CD2	2.45	0.46
2:B:248:GLN:O	2:B:251:LEU:HB3	2.16	0.46
2:B:75:ALA:N	2:B:76:PRO:HD2	2.31	0.46
2:C:162:SER:HA	2:C:318:LEU:HD23	1.97	0.46
2:C:275:ASP:HA	2:C:288:THR:HG21	1.97	0.46
2:C:193:SER:HA	2:C:196:LEU:HD12	1.96	0.46
2:A:192:VAL:HG22	2:A:195:ARG:NH2	2.31	0.46
2:C:274:ASP:OD2	3:C:903:145:O3	2.31	0.45
2:A:186:ALA:HB2	2:A:198:LEU:HG	1.98	0.45
2:C:115:LEU:HA	2:C:115:LEU:HD13	1.75	0.45
2:B:114:LEU:HD23	2:B:122:LEU:HD22	1.97	0.45
2:C:188:PRO:HD2	2:C:220:TRP:CE2	2.51	0.45
2:B:219:ASP:O	2:B:220:TRP:CB	2.65	0.45
2:A:107:CYS:HB2	2:A:126:TYR:CD2	2.52	0.45
1:E:15:DC:N4	2:A:18:GLN:OE1	2.46	0.45
2:C:134:ILE:CD1	2:C:155:PRO:HG2	2.46	0.45
2:A:78:GLN:O	2:A:81:ALA:HB3	2.17	0.45
1:F:4:DT:H2"	1:F:5:DT:C6	2.51	0.45
2:A:221:SER:O	2:A:249:MET:HG2	2.17	0.45
2:A:197:ARG:HH22	3:A:901:145:C6'	2.29	0.44
2:A:144:PRO:HG2	2:A:308:SER:HA	1.98	0.44
2:C:54:GLN:O	2:C:59:LYS:HB2	2.18	0.44
2:C:188:PRO:HD3	2:C:219:ASP:HA	2.00	0.44
2:B:97:SER:HB2	2:B:114:LEU:HD13	1.99	0.44
2:A:247:ASP:O	2:A:250:ALA:HB3	2.18	0.44
2:A:197:ARG:NH2	3:A:901:145:C6'	2.81	0.44
2:B:255:ARG:HD3	2:B:259:GLU:OE1	2.18	0.44
2:C:107:CYS:HB2	2:C:126:TYR:CD1	2.53	0.43
2:A:189:LEU:HB2	2:A:217:GLU:OE2	2.18	0.43
2:C:287:THR:HG23	2:C:325:LYS:HA	2.00	0.43
2:B:165:ASP:OD1	2:B:168:ARG:NH1	2.51	0.43
2:C:163:HIS:CE1	2:C:196:LEU:HB3	2.54	0.43
2:B:273:TYR:O	2:B:274:ASP:CB	2.67	0.43
2:C:113:ASN:O	2:C:117:GLN:HG3	2.19	0.43
2:A:163:HIS:CG	2:A:196:LEU:HB3	2.53	0.43
2:A:161:PHE:CG	2:A:291:GLN:HG2	2.53	0.43
2:C:219:ASP:O	2:C:220:TRP:HB2	2.19	0.43
2:B:19:THR:O	2:B:23:VAL:HG23	2.18	0.43
2:C:75:ALA:N	2:C:76:PRO:HD2	2.34	0.43
2:A:250:ALA:O	2:A:253:ALA:HB3	2.18	0.43
2:C:186:ALA:HB2	2:C:198:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:ILE:HD11	2:B:303:ARG:HD3	2.00	0.42
2:A:255:ARG:HA	2:B:283:ILE:HD12	2.00	0.42
2:B:97:SER:HB2	2:B:114:LEU:CD1	2.49	0.42
2:B:123:ILE:HG13	2:B:304:LEU:HD13	2.00	0.42
2:C:97:SER:HB2	2:C:114:LEU:CD1	2.50	0.42
1:D:19:DA:H61	1:E:3:DA:H61	1.67	0.42
2:C:79:ILE:HD12	2:C:296:LEU:CD2	2.44	0.42
2:A:278:ASP:OD1	2:A:278:ASP:N	2.52	0.42
2:C:283:ILE:HA	2:C:284:PRO:HA	1.88	0.42
2:A:116:ALA:HB1	2:B:51:ARG:HG3	2.02	0.42
2:B:111:VAL:HG21	2:B:136:VAL:HG13	2.02	0.42
2:B:157:ASN:HB3	2:B:315:GLY:H	1.85	0.42
2:B:126:TYR:CG	2:B:127:PRO:HD2	2.55	0.42
2:A:111:VAL:O	2:A:115:LEU:HD22	2.19	0.42
2:B:192:VAL:HG22	2:B:195:ARG:NH2	2.35	0.42
2:C:152:ASP:HA	2:C:316:ASN:ND2	2.35	0.42
2:C:189:LEU:HD12	2:C:189:LEU:HA	1.84	0.42
2:A:86:ARG:HH11	2:A:90:LEU:HD21	1.84	0.42
2:C:214:ALA:HB2	2:C:237:ILE:HG21	2.01	0.42
1:D:19:DA:N6	1:E:3:DA:H61	2.18	0.41
2:A:48:ILE:HG12	2:B:112:HIS:CD2	2.55	0.41
2:B:73:LEU:HB2	2:B:76:PRO:HG3	2.02	0.41
2:C:197:ARG:HH22	3:C:903:145:C6'	2.33	0.41
2:A:41:ALA:O	2:A:45:LEU:HD12	2.21	0.41
2:B:64:ILE:HG23	2:B:304:LEU:HD22	2.02	0.41
2:A:143:VAL:HA	2:A:144:PRO:HD3	1.94	0.41
2:C:197:ARG:HH22	3:C:903:145:C1'	2.33	0.41
2:C:74:HIS:NE2	2:C:276:THR:HG22	2.35	0.41
2:A:98:MET:HE3	2:B:84:LYS:CB	2.50	0.41
2:B:226:PHE:CD1	2:B:256:ALA:HB2	2.56	0.41
2:A:112:HIS:NE2	2:B:48:ILE:HG23	2.36	0.41
1:E:12:DG:H5''	2:A:5:THR:HG23	2.01	0.41
2:B:179:HIS:ND1	2:B:241:ALA:HB2	2.36	0.41
2:C:2:LYS:N	2:C:3:PRO:HD2	2.36	0.41
2:B:273:TYR:O	2:B:274:ASP:HB2	2.21	0.40
2:B:165:ASP:O	2:B:169:LEU:HD22	2.21	0.40
2:A:274:ASP:OD2	3:A:901:145:O3	2.28	0.40
2:B:126:TYR:HD1	2:B:128:LEU:CD1	2.34	0.40
2:B:146:LEU:HA	2:B:146:LEU:HD12	1.81	0.40
2:C:134:ILE:HD11	2:C:155:PRO:CG	2.52	0.40
2:B:185:LEU:HD21	2:B:225:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:HB2	2:B:76:PRO:CG	2.51	0.40
2:C:115:LEU:O	2:C:118:ARG:NH1	2.55	0.40
2:A:54:GLN:HB3	2:A:59:LYS:HD3	2.03	0.40
2:B:111:VAL:O	2:B:115:LEU:HD22	2.21	0.40
2:B:111:VAL:HG13	2:B:122:LEU:CD1	2.51	0.40
2:C:246:ASN:HB2	3:C:903:145:O3	2.21	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	326/330 (99%)	286 (88%)	37 (11%)	3 (1%)	21	68
2	B	328/330 (99%)	294 (90%)	30 (9%)	4 (1%)	16	61
2	C	326/330 (99%)	285 (87%)	37 (11%)	4 (1%)	16	61
All	All	980/990 (99%)	865 (88%)	104 (11%)	11 (1%)	17	63

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	274	ASP
2	B	274	ASP
2	C	274	ASP
2	A	311	GLN
2	B	29	HIS
2	C	50	ASN
2	B	45	LEU
2	B	220	TRP
2	C	199	ALA
2	A	261	GLY
2	C	15	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	268/269 (100%)	230 (86%)	38 (14%)	4	24
2	B	269/269 (100%)	229 (85%)	40 (15%)	4	22
2	C	268/269 (100%)	237 (88%)	31 (12%)	7	33
All	All	805/807 (100%)	696 (86%)	109 (14%)	5	26

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	LYS
2	A	11	GLU
2	A	19	THR
2	A	33	LYS
2	A	34	THR
2	A	35	ARG
2	A	45	LEU
2	A	60	GLN
2	A	61	LEU
2	A	63	LEU
2	A	86	ARG
2	A	99	VAL
2	A	108	LYS
2	A	113	ASN
2	A	115	LEU
2	A	122	LEU
2	A	124	ILE
2	A	125	ASN
2	A	128	LEU
2	A	134	ILE
2	A	141	THR
2	A	142	ASN
2	A	156	ILE
2	A	169	LEU
2	A	190	SER
2	A	198	LEU

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Mol	Chain	Res	Type
2	A	209	GLN
2	A	232	MET
2	A	242	MET
2	A	255	ARG
2	A	278	ASP
2	A	291	GLN
2	A	299	THR
2	A	304	LEU
2	A	307	LEU
2	A	313	VAL
2	A	319	LEU
2	A	322	SER
2	B	15	VAL
2	B	26	GLN
2	B	33	LYS
2	B	36	GLU
2	B	61	LEU
2	B	77	SER
2	B	86	ARG
2	B	90	LEU
2	B	113	ASN
2	B	114	LEU
2	B	115	LEU
2	B	117	GLN
2	B	125	ASN
2	B	128	LEU
2	B	130	ASP
2	B	134	ILE
2	B	137	GLU
2	B	141	THR
2	B	143	VAL
2	B	157	ASN
2	B	159	ILE
2	B	164	GLU
2	B	169	LEU
2	B	177	LEU
2	B	185	LEU
2	B	189	LEU
2	B	198	LEU
2	B	209	GLN
2	B	216	ARG
2	B	262	LEU

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Mol	Chain	Res	Type
2	B	283	ILE
2	B	298	GLN
2	B	304	LEU
2	B	308	SER
2	B	311	GLN
2	B	313	VAL
2	B	317	GLN
2	B	319	LEU
2	B	323	LEU
2	B	330	LEU
2	C	11	GLU
2	C	12	TYR
2	C	44	GLU
2	C	48	ILE
2	C	62	LEU
2	C	63	LEU
2	C	69	SER
2	C	86	ARG
2	C	97	SER
2	C	101	ARG
2	C	114	LEU
2	C	115	LEU
2	C	125	ASN
2	C	128	LEU
2	C	131	GLN
2	C	137	GLU
2	C	142	ASN
2	C	143	VAL
2	C	169	LEU
2	C	172	GLU
2	C	177	LEU
2	C	189	LEU
2	C	198	LEU
2	C	240	THR
2	C	255	ARG
2	C	294	ARG
2	C	300	SER
2	C	303	ARG
2	C	309	GLN
2	C	317	GLN
2	C	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	78	GLN
2	A	113	ASN
2	A	125	ASN
2	A	153	GLN
2	A	209	GLN
2	A	291	GLN
2	A	311	GLN
2	B	25	ASN
2	B	46	ASN
2	B	89	GLN
2	B	113	ASN
2	B	125	ASN
2	B	153	GLN
2	B	157	ASN
2	B	227	GLN
2	B	231	GLN
2	B	298	GLN
2	B	306	GLN
2	C	26	GLN
2	C	54	GLN
2	C	89	GLN
2	C	125	ASN
2	C	153	GLN
2	C	202	HIS
2	C	306	GLN
2	C	316	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

3 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	145	A	901	-	20,22,22	2.21	1 (5%)	26,31,31	2.11	4 (15%)
3	145	B	902	-	20,22,22	2.28	2 (10%)	26,31,31	2.40	9 (34%)
3	145	C	903	-	20,22,22	2.27	1 (5%)	26,31,31	2.19	3 (11%)

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	145	A	901	-	-	0/9/30/30	0/2/2/2
3	145	B	902	-	-	0/9/30/30	0/2/2/2
3	145	C	903	-	-	0/9/30/30	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	145	O1'-C1	2.75	1.45	1.41
3	A	901	145	O3'-N1'	9.60	1.41	1.22
3	B	902	145	O3'-N1'	9.63	1.41	1.22
3	C	903	145	O3'-N1'	9.84	1.42	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	145	O1'-C1'-C6'	-9.77	97.99	123.93
3	A	901	145	O1'-C1'-C6'	-7.37	104.37	123.93
3	B	902	145	O1'-C1'-C6'	-5.93	108.17	123.93
3	B	902	145	O5-C1-O1'	-4.62	96.05	108.39
3	A	901	145	O5-C1-O1'	-4.21	97.14	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	145	O5-C1-O1'	-2.87	100.73	108.39
3	B	902	145	O5-C1-C2	-2.78	104.57	110.28
3	A	901	145	C6-C5-C4	-2.47	106.93	113.02
3	B	902	145	C6-C5-C4	-2.46	106.96	113.02
3	B	902	145	C6'-C1'-C2'	-2.20	112.93	118.51
3	B	902	145	C4'-C3'-C2'	2.06	122.11	118.63
3	B	902	145	C1'-O1'-C1	2.28	122.21	117.96
3	C	903	145	O5-C5-C4	2.39	114.17	109.68
3	B	902	145	C5'-C6'-C1'	3.25	125.80	119.79
3	A	901	145	O1'-C1-C2	4.10	113.79	107.12
3	B	902	145	O1'-C1-C2	6.28	117.34	107.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	145	5	0
3	B	902	145	4	0
3	C	903	145	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	17/20 (85%)	0.24	0 100 100	61, 98, 117, 119	0
1	E	17/20 (85%)	0.22	0 100 100	57, 90, 133, 135	0
1	F	17/20 (85%)	1.76	8 (47%) 0 0	119, 165, 205, 209	0
2	A	328/330 (99%)	-0.40	6 (1%) 71 62	23, 40, 113, 126	0
2	B	330/330 (100%)	-0.53	2 (0%) 90 85	14, 30, 81, 97	0
2	C	328/330 (99%)	-0.39	6 (1%) 71 62	15, 30, 150, 155	0
All	All	1037/1050 (98%)	-0.38	22 (2%) 67 58	14, 35, 136, 209	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	DA	4.5
2	A	27	ALA	4.0
2	A	28	SER	3.5
1	F	17	DC	3.4
2	C	29	HIS	3.3
2	A	30	VAL	3.3
2	C	28	SER	3.3
2	C	27	ALA	3.2
1	F	8	DG	3.0
2	A	312	ALA	2.8
2	B	31	SER	2.6
1	F	9	DA	2.6
2	A	26	GLN	2.5
2	C	16	SER	2.5
2	C	26	GLN	2.4
1	F	4	DT	2.4
1	F	6	DG	2.4
2	C	60	GLN	2.4
2	A	29	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	15	DC	2.1
2	B	44	GLU	2.1
1	F	3	DA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	145	C	903	21/21	0.95	0.16	-0.15	10,15,23,23	0
3	145	B	902	21/21	0.96	0.15	-0.37	6,10,15,15	0
3	145	A	901	21/21	0.97	0.14	-0.60	15,17,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.