



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:19 PM UTC

PDB ID : 3BRF / pdb_00003brf
Title : CSL (Lag-1) bound to DNA with Lin-12 RAM peptide, C2221
Authors : Wilson, J.J.; Kovall, R.A.
Deposited on : 2007-12-21
Resolution : 2.47 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

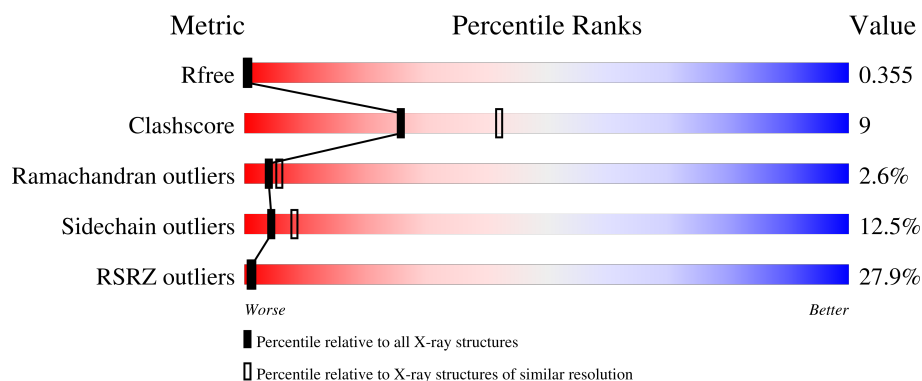
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	B	15	
2	C	15	
3	A	478	
4	D	14	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4179 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(*DTP*DTP*DAP*DCP*DTP*DGP*DTP*DG*GP*DGP*DGP*DAP*DAP*DAP*DGP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			

- Molecule 2 is a DNA chain called DNA (5'-D(*DAP*DAP*DTP*DCP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DAP*DGP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			298	145	50	89	14			

- Molecule 3 is a protein called Lin-12 and glp-1 phenotype protein 1, isoform a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	423	Total	C	N	O	S	0	2	0
			3383	2149	583	633	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	SER	-	expression tag	UNP Q9TYY1
A	187	GLY	-	expression tag	UNP Q9TYY1
A	188	PRO	-	expression tag	UNP Q9TYY1
A	189	LEU	-	expression tag	UNP Q9TYY1
A	190	GLY	-	expression tag	UNP Q9TYY1
A	191	SER	-	expression tag	UNP Q9TYY1

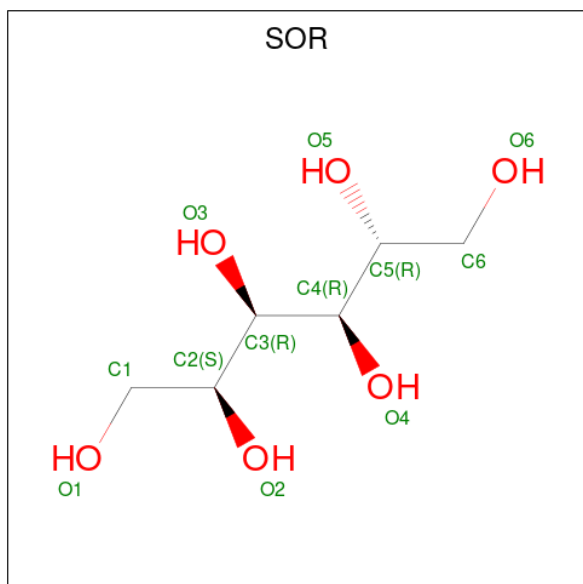
- Molecule 4 is a protein called Protein lin-12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	13	Total	C	N	O	S	0	0	0
			106	68	18	17	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	937	SER	-	expression tag	UNP P14585

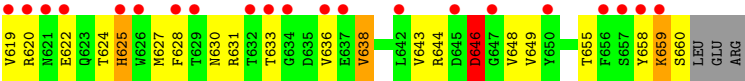
- Molecule 5 is sorbitol (CCD ID: SOR) (formula: $C_6H_{14}O_6$).



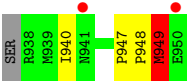
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	7	Total	O	0	0
			7	7		
6	C	11	Total	O	0	0
			11	11		
6	A	39	Total	O	0	0
			39	39		



● Molecule 4: Protein lin-12



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	62.94Å 95.97Å 223.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.28 – 2.47 28.28 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.28-2.47) 99.2 (28.28-2.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.3.0020	Depositor
R, R_{free}	0.230 , 0.277 0.314 , 0.355	Depositor DCC
R_{free} test set	1255 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4179	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: SOR

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	B	0.51	0/350	1.28	2/540 (0.4%)
2	C	0.51	0/332	1.21	1/509 (0.2%)
3	A	0.66	1/3463 (0.0%)	0.88	4/4675 (0.1%)
4	D	0.51	0/109	0.90	1/147 (0.7%)
All	All	0.64	1/4254 (0.0%)	0.96	8/5871 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	644	ARG	CZ-NH1	6.55	1.42	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	THR	N-CA-C	-7.56	97.13	108.99
3	A	638	VAL	N-CA-C	6.70	115.20	107.89
3	A	431	ASP	N-CA-C	6.18	114.68	108.75
4	D	949	MET	N-CA-C	5.73	118.60	107.71
1	B	13	DA	N9-C1'-C2'	5.56	121.83	113.50
3	A	402	THR	N-CA-C	-5.10	99.94	110.80
2	C	3	DT	N1-C1'-C2'	5.07	121.10	113.50
1	B	5	DT	O4'-C1'-N1	-5.01	100.89	108.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	401	GLN	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	B	311	0	171	4	0
2	C	298	0	172	3	0
3	A	3383	0	3329	69	0
4	D	106	0	105	2	0
5	A	24	0	28	5	0
6	A	39	0	0	1	0
6	B	7	0	0	0	0
6	C	11	0	0	0	0
All	All	4179	0	3805	75	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 9.

All (75) 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:A:438:GLU:HB2	3:A:439:THR:HG23	1.23	1.14
3:A:335:SER:HB3	5:A:1:SOR:O6	1.64	0.96
3:A:454:VAL:HG13	3:A:501:ILE:HD11	1.57	0.84
3:A:227:LYS:NZ	5:A:2:SOR:H11	1.93	0.83
3:A:227:LYS:HZ2	5:A:2:SOR:H11	1.47	0.75
3:A:476:LYS:O	3:A:478:GLN:N	2.24	0.71
3:A:468:ARG:HG3	3:A:501:ILE:HD13	1.77	0.67
3:A:555:VAL:HG11	3:A:646:ASP:HB3	1.76	0.66
3:A:337:LYS:O	6:A:692:HOH:O	2.15	0.64
3:A:511:SER:O	3:A:514:LYS:HG2	1.97	0.62
2:C:1:DA:H2''	2:C:2:DA:C8	2.34	0.62
3:A:594:PHE:O	3:A:638:VAL:HB	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:247:GLN:HA	3:A:247:GLN:OE1	2.03	0.59
3:A:221:HIS:CE1	3:A:360:SER:HB2	2.39	0.58
3:A:594:PHE:HD1	3:A:599:VAL:HG21	1.69	0.58
3:A:438:GLU:CB	3:A:439:THR:HG23	2.16	0.56
3:A:398:LEU:HD13	3:A:402:THR:HG23	1.86	0.56
3:A:454:VAL:CG1	3:A:501:ILE:HD11	2.35	0.55
3:A:214:GLU:OE1	3:A:547:ARG:HD2	2.06	0.55
3:A:594:PHE:CD1	3:A:599:VAL:HG21	2.42	0.54
3:A:592:VAL:HG11	3:A:611:CYS:SG	2.48	0.54
3:A:550:GLU:OE2	3:A:554:GLN:HA	2.09	0.53
3:A:227:LYS:HZ1	5:A:2:SOR:H11	1.73	0.53
3:A:255:ARG:HD3	3:A:554:GLN:HB3	1.90	0.53
3:A:499:GLN:HB3	3:A:507:TYR:CE2	2.44	0.52
3:A:353:MET:HA	3:A:353:MET:HE2	1.92	0.52
3:A:335:SER:HB3	5:A:1:SOR:HO6	1.69	0.50
3:A:630:ASN:ND2	3:A:633:THR:H	2.10	0.50
3:A:636:VAL:O	3:A:658:TYR:HB2	2.12	0.50
3:A:212:LYS:H	3:A:212:LYS:HD2	1.77	0.50
3:A:212:LYS:HD2	3:A:212:LYS:N	2.27	0.49
3:A:474:VAL:HG22	3:A:495:LYS:HB3	1.94	0.49
3:A:524:ASN:HB2	3:A:527:ARG:CB	2.42	0.49
3:A:476:LYS:C	3:A:478:GLN:H	2.21	0.48
3:A:415:PHE:HE1	3:A:464:ILE:HG22	1.79	0.48
1:B:14:DG:H1'	1:B:15:DA:H5'	1.94	0.48
3:A:475:ASP:O	3:A:476:LYS:O	2.32	0.48
3:A:524:ASN:HB3	3:A:526:HIS:H	1.79	0.48
3:A:235:PHE:HA	3:A:330:LEU:O	2.14	0.48
3:A:507:TYR:OH	3:A:528:HIS:HD2	1.97	0.48
3:A:416:HIS:HB2	3:A:513:ASP:O	2.13	0.47
3:A:217:ILE:HD12	3:A:244:LEU:CD2	2.45	0.47
3:A:221:HIS:HD2	3:A:222:ALA:O	1.97	0.47
1:B:10:DG:O6	3:A:368:LYS:NZ	2.48	0.47
2:C:13:DA:N3	3:A:401:GLN:HG2	2.29	0.47
3:A:213:TYR:HB3	3:A:549:PHE:CE1	2.51	0.46
3:A:237:CYS:HA	3:A:238:PRO:C	2.41	0.46
3:A:473:LYS:HB3	3:A:480:ILE:HG12	1.98	0.46
3:A:659:LYS:O	3:A:660:SER:C	2.58	0.46
3:A:616:VAL:O	3:A:619:VAL:HG22	2.17	0.45
3:A:564:VAL:O	3:A:583:GLY:HA3	2.16	0.45
3:A:488:GLU:HA	3:A:489:PRO:HD3	1.86	0.45
3:A:198:LEU:HD22	3:A:643:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:627:MET:HG3	3:A:628:PHE:CD1	2.52	0.45
1:B:8:DG:H5'	3:A:400:SER:HB3	1.98	0.44
3:A:370:SER:OG	3:A:372:LYS:HD3	2.18	0.44
2:C:1:DA:C2'	2:C:2:DA:C8	3.01	0.43
3:A:617:SER:HA	3:A:620:ARG:HH12	1.84	0.43
3:A:201:ASP:HA	3:A:204:ILE:HD12	2.01	0.43
3:A:593:TRP:CD1	3:A:643:VAL:HG12	2.53	0.43
3:A:613:ILE:HG13	3:A:614:PRO:HD2	2.01	0.42
3:A:624:THR:O	3:A:625:HIS:HB2	2.18	0.42
1:B:13:DA:H1'	1:B:14:DG:H5'	2.01	0.42
3:A:217:ILE:HD12	3:A:244:LEU:HD21	2.01	0.42
3:A:564:VAL:CG2	3:A:584:ARG:HE	2.33	0.42
4:D:947:PRO:HA	4:D:948:PRO:HD3	1.87	0.42
3:A:255:ARG:NH1	3:A:550:GLU:HB2	2.35	0.42
4:D:949:MET:HE2	4:D:949:MET:HB3	1.90	0.42
3:A:504:GLU:OE1	3:A:504:GLU:HA	2.19	0.41
3:A:524:ASN:HB2	3:A:527:ARG:HB3	2.02	0.41
3:A:543:LYS:NZ	3:A:545:GLU:OE1	2.54	0.41
3:A:564:VAL:HG21	3:A:584:ARG:HE	1.85	0.41
3:A:398:LEU:HD11	3:A:404:SER:O	2.20	0.41
3:A:579:VAL:HG11	3:A:594:PHE:HZ	1.86	0.41
3:A:381:CYS:O	3:A:382:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	415/478 (87%)	376 (91%)	28 (7%)	11 (3%)	4	5
4	D	11/14 (79%)	9 (82%)	2 (18%)	0	100	100
All	All	426/492 (87%)	385 (90%)	30 (7%)	11 (3%)	4	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	399	ARG
3	A	403	VAL
3	A	476	LYS
3	A	401	GLN
3	A	477	GLN
3	A	625	HIS
3	A	200	SER
3	A	552	MET
3	A	603	PHE
3	A	381	CYS
3	A	646	ASP

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	375/417 (90%)	329 (88%)	46 (12%)	4	8
4	D	12/13 (92%)	10 (83%)	2 (17%)	2	3
All	All	387/430 (90%)	339 (88%)	48 (12%)	4	8

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	201	ASP
3	A	212	LYS
3	A	224	VAL
3	A	258	GLN
3	A	260	TYR
3	A	262	THR
3	A	295	ASP
3	A	298	GLU
3	A	301	GLN
3	A	333	SER
3	A	353	MET
3	A	372	LYS

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Mol	Chain	Res	Type
3	A	375	SER
3	A	398	LEU
3	A	399	ARG
3	A	403	VAL
3	A	410	VAL
3	A	416	HIS
3	A	429	LEU
3	A	433	GLU
3	A	439	THR
3	A	445	ARG
3	A	455	VAL
3	A	461	VAL
3	A	474	VAL
3	A	501	ILE
3	A	508	LEU
3	A	510	LEU
3	A	514	LYS
3	A	527	ARG
3	A	543	LYS
3	A	554	GLN
3	A	559	ILE
3	A	564	VAL
3	A	592	VAL
3	A	599	VAL
3	A	601	THR
3	A	607	GLU
3	A	611	CYS
3	A	622	GLU
3	A	631	ARG
3	A	646	ASP
3	A	648	VAL
3	A	649	VAL
3	A	655	THR
3	A	659	LYS
4	D	940	ILE
4	D	949	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
3	A	374	GLN

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Mol	Chain	Res	Type
3	A	396	ASN
3	A	416	HIS
3	A	428	HIS
3	A	441	ASN
3	A	503	ASN
3	A	517	GLN
3	A	524	ASN
3	A	528	HIS
3	A	554	GLN
3	A	557	ASN
3	A	582	HIS
3	A	623	GLN

5.3.3 RNA [i](#)

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](#)

2 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	$\# Z > 2$
5	SOR	A	2	-	11,11,11	0.47	0	14,14,14	1.40	4 (28%)
5	SOR	A	1	-	11,11,11	0.35	0	14,14,14	1.57	2 (14%)

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
5	SOR	A	2	-	-	11/16/16/16	-
5	SOR	A	1	-	-	10/16/16/16	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	SOR	O6-C6-C5	-3.71	103.36	111.16
5	A	1	SOR	O5-C5-C4	3.36	117.12	109.25
5	A	2	SOR	C2-C3-C4	-2.50	108.63	112.48
5	A	2	SOR	O4-C4-C5	2.48	114.57	108.93
5	A	2	SOR	C5-C4-C3	-2.21	109.08	112.48
5	A	2	SOR	O3-C3-C2	2.07	113.62	108.93

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	SOR	C2-C3-C4-C5
5	A	1	SOR	C2-C3-C4-O4
5	A	1	SOR	O3-C3-C4-C5
5	A	1	SOR	C3-C4-C5-C6
5	A	1	SOR	C3-C4-C5-O5
5	A	1	SOR	O4-C4-C5-O5
5	A	2	SOR	C1-C2-C3-O3
5	A	2	SOR	O2-C2-C3-C4
5	A	2	SOR	O2-C2-C3-O3
5	A	2	SOR	O4-C4-C5-C6
5	A	1	SOR	O1-C1-C2-O2
5	A	2	SOR	O4-C4-C5-O5
5	A	2	SOR	C3-C4-C5-O5
5	A	1	SOR	O4-C4-C5-C6
5	A	2	SOR	C1-C2-C3-C4
5	A	2	SOR	C3-C4-C5-C6
5	A	1	SOR	O3-C3-C4-O4
5	A	2	SOR	C2-C3-C4-C5
5	A	1	SOR	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	2	SOR	O3-C3-C4-C5
5	A	2	SOR	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	SOR	3	0
5	A	1	SOR	2	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	B	15/15 (100%)	1.88	5 (33%) 1 1	36, 40, 46, 48	0
2	C	15/15 (100%)	2.40	11 (73%) 0 0	36, 40, 46, 47	0
3	A	423/478 (88%)	1.53	112 (26%) 1 1	23, 40, 50, 58	2 (0%)
4	D	13/14 (92%)	1.27	2 (15%) 5 4	41, 44, 46, 48	0
All	All	466/522 (89%)	1.56	130 (27%) 1 1	23, 40, 49, 58	2 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	572	GLY	6.4
3	A	399	ARG	6.1
3	A	571	ASP	5.8
3	A	626	TRP	4.4
3	A	260	TYR	4.4
2	C	1	DA	3.9
3	A	570	VAL	3.8
3	A	590	LEU	3.8
3	A	262	THR	3.7
3	A	629	THR	3.7
3	A	258	GLN	3.7
3	A	575	GLU	3.6
3	A	402	THR	3.6
3	A	198	LEU	3.6
3	A	610	HIS	3.5
3	A	637	GLU	3.5
3	A	600	GLU	3.4
3	A	656	PHE	3.3
3	A	403	VAL	3.3
3	A	362[A]	ARG	3.3
3	A	344	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	461	VAL	3.3
3	A	588	PRO	3.2
2	C	14	DG	3.2
3	A	632	THR	3.2
3	A	333	SER	3.2
3	A	577	SER	3.2
3	A	615	PRO	3.2
3	A	201	ASP	3.1
3	A	580	GLU	3.1
3	A	574	GLY	3.1
3	A	634	GLY	3.1
3	A	401	GLN	3.1
3	A	319	PRO	3.1
3	A	608	SER	3.1
3	A	620	ARG	3.1
3	A	208	SER	3.0
1	B	1	DT	3.0
1	B	13	DA	3.0
3	A	597	THR	3.0
3	A	207	LEU	2.9
3	A	438	GLU	2.9
3	A	596	ALA	2.9
3	A	658	TYR	2.9
2	C	2	DA	2.9
3	A	554	GLN	2.9
3	A	568	LEU	2.9
3	A	400	SER	2.9
3	A	611	CYS	2.9
3	A	380	ASP	2.9
1	B	14	DG	2.8
3	A	213	TYR	2.8
3	A	605	SER	2.8
3	A	625	HIS	2.8
3	A	353	MET	2.8
3	A	284	THR	2.7
3	A	480	ILE	2.7
3	A	619	VAL	2.7
3	A	578	ARG	2.7
2	C	4	DC	2.7
3	A	593	TRP	2.7
2	C	8	DC	2.6
3	A	633	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	645	ASP	2.6
3	A	650	TYR	2.6
3	A	560	SER	2.5
3	A	549	PHE	2.5
3	A	551	ALA	2.5
3	A	576	ALA	2.5
3	A	234	ARG	2.5
3	A	381	CYS	2.5
1	B	12	DA	2.5
3	A	579	VAL	2.5
3	A	621	ASN	2.4
3	A	636	VAL	2.4
3	A	230	GLY	2.4
3	A	293	GLY	2.4
3	A	389	GLY	2.4
3	A	594	PHE	2.4
3	A	332	ILE	2.4
3	A	573	HIS	2.4
2	C	11	DA	2.4
3	A	622	GLU	2.4
3	A	200	SER	2.4
3	A	199	THR	2.3
3	A	329	THR	2.3
3	A	202	ARG	2.3
3	A	351	CYS	2.3
2	C	3	DT	2.3
3	A	204	ILE	2.3
2	C	5	DT	2.3
3	A	614	PRO	2.3
2	C	7	DT	2.3
3	A	612	SER	2.3
3	A	617	SER	2.3
2	C	13	DA	2.3
3	A	604	ARG	2.2
3	A	618	GLN	2.2
3	A	642	LEU	2.2
3	A	569	GLU	2.2
3	A	474	VAL	2.2
3	A	363	ILE	2.2
4	D	950	GLU	2.2
1	B	3	DA	2.2
2	C	10	DC	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	443	ALA	2.2
3	A	483	ALA	2.2
3	A	371	LYS	2.1
3	A	224	VAL	2.1
3	A	555	VAL	2.1
3	A	553	GLY	2.1
3	A	229	TYR	2.1
3	A	392	VAL	2.1
3	A	222	ALA	2.1
3	A	591	LYS	2.1
3	A	659	LYS	2.1
3	A	485[A]	CYS	2.1
3	A	497	ALA	2.1
3	A	331	TYR	2.1
4	D	941	ASN	2.0
3	A	232	GLU	2.0
3	A	246	GLY	2.0
3	A	647	GLY	2.0
3	A	238	PRO	2.0
3	A	657	SER	2.0
3	A	582	HIS	2.0
3	A	628	PHE	2.0
3	A	411	GLU	2.0
3	A	366	ILE	2.0
3	A	536	TRP	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
5	SOR	A	2	12/12	0.72	0.21	57,64,71,71	0
5	SOR	A	1	12/12	0.89	0.14	19,23,26,27	12

6.5 Other polymers [i](#)

There are no such residues in this entry.