



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:42 PM UTC

PDB ID : 3BRD / pdb_00003brd
Title : CSL (Lag-1) bound to DNA with Lin-12 RAM peptide, P212121
Authors : Wilson, J.J.; Kovall, R.A.
Deposited on : 2007-12-21
Resolution : 2.21 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

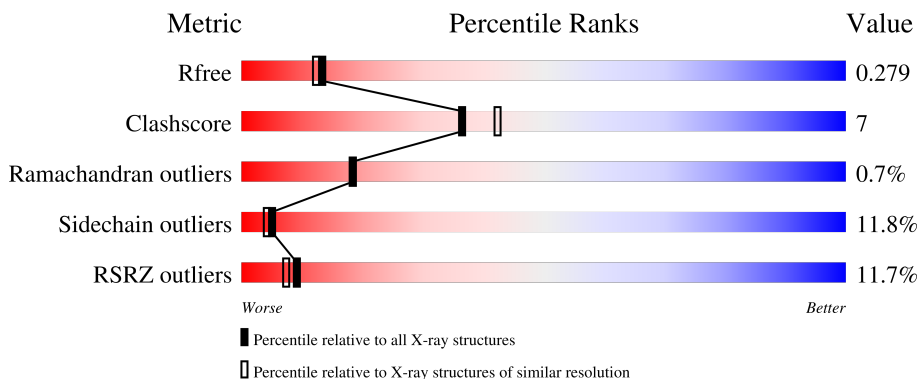
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	477	
4	D	29	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4328 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	427	Total	C	N	O	S	0	4	0
			3423	2174	592	639	18			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

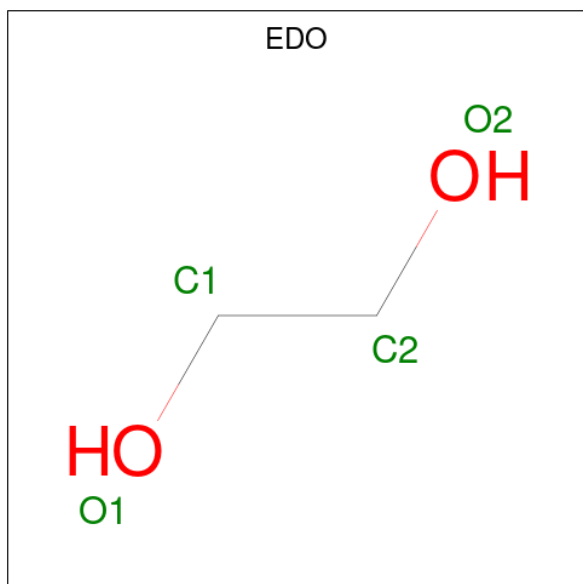
- Molecule 4 is a protein called Protein lin-12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	S	0	0	0
			125	78	24	20	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	929	SER	-	expression tag	UNP P14585

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

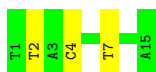
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	24	Total 24	O 24	0	0
6	C	9	Total 9	O 9	0	0
6	A	98	Total 98	O 98	0	0

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.

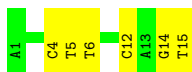
- Molecule 1: DNA (5'-D(*DTP*DTP*DAP*DCP*DTP*DGP*DTP*DGP*DGP*DGP*DAP*DAP*DAP*DGP*DA)-3')

Chain B: 



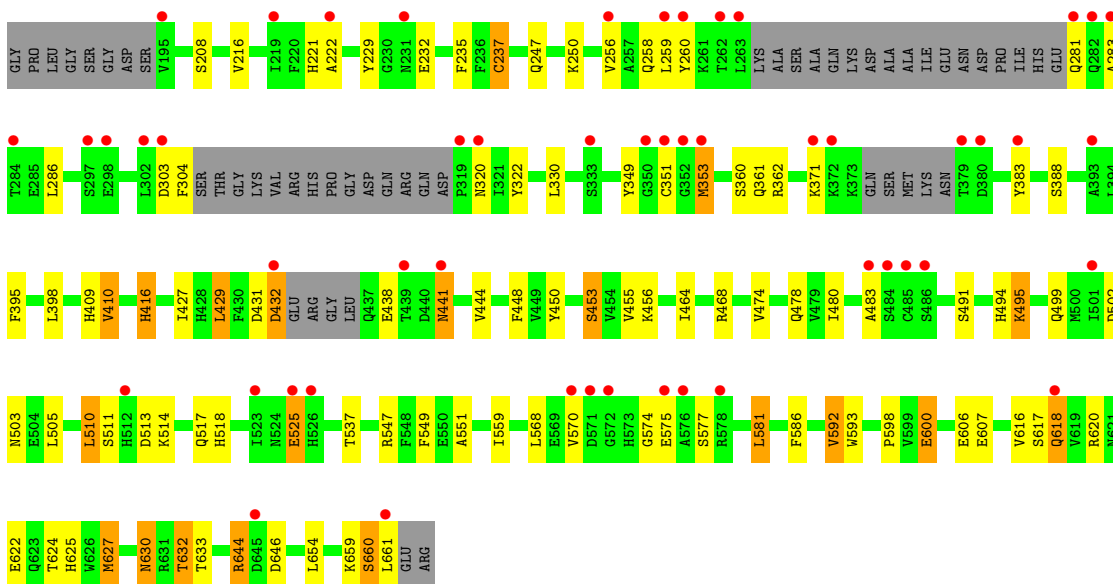
- Molecule 2: DNA (5'-D(*DAP*DAP*DTP*DCP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DAP*DGP*DT)-3')

Chain C: 

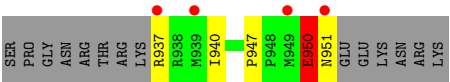
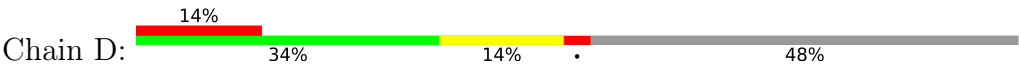


- Molecule 3: Lin-12 and glp-1 phenotype protein 1, isoform a

Chain A: 



- Molecule 4: Protein lin-12



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.15Å 98.87Å 126.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 2.21 39.87 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.87-2.21) 94.6 (39.87-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3.0020	Depositor
R, R_{free}	0.208 , 0.257 0.253 , 0.279	Depositor DCC
R_{free} test set	1819 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4328	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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: EDO

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	0.56	0/350	1.33	3/540 (0.6%)
2	C	0.74	0/332	1.48	3/509 (0.6%)
3	A	0.89	3/3512 (0.1%)	0.98	3/4743 (0.1%)
4	D	3.08	6/128 (4.7%)	1.36	2/172 (1.2%)
All	All	0.99	9/4322 (0.2%)	1.08	11/5964 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	950	GLU	CD-OE1	23.68	1.70	1.25
4	D	950	GLU	CD-OE2	15.51	1.54	1.25
4	D	951	ASN	CG-OD1	12.51	1.47	1.23
4	D	951	ASN	CG-ND2	9.39	1.52	1.33
4	D	950	GLU	C-O	6.93	1.32	1.24
4	D	950	GLU	C-N	6.54	1.42	1.33
3	A	592	VAL	CA-CB	5.58	1.61	1.54
3	A	237	CYS	CB-SG	-5.53	1.63	1.81
3	A	427	ILE	CA-CB	5.03	1.60	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	12	DC	N1-C1'-C2'	7.02	124.03	113.50
4	D	951	ASN	OD1-CG-ND2	6.91	129.51	122.60
4	D	950	GLU	CG-CD-OE2	-6.74	102.90	118.40
3	A	237	CYS	CB-CA-C	-5.77	102.48	110.16
2	C	12	DC	C4'-C3'-O3'	-5.72	101.43	110.00
2	C	6	DT	N1-C1'-C2'	5.43	121.65	113.50
3	A	395	PHE	N-CA-C	5.19	117.70	109.50
1	B	4	DC	P-O3'-C3'	5.16	127.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	DT	N1-C1'-C2'	5.08	121.12	113.50
3	A	410	VAL	N-CA-CB	5.08	117.08	110.99
1	B	7	DT	N1-C1'-C2'	5.06	121.09	113.50

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	B	311	0	171	0	0
2	C	298	0	172	2	0
3	A	3423	0	3375	55	0
4	D	125	0	124	6	0
5	A	32	0	48	2	0
5	C	4	0	6	0	0
5	D	4	0	6	0	0
6	A	98	0	0	2	0
6	B	24	0	0	0	0
6	C	9	0	0	0	0
All	All	4328	0	3902	58	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 7.

All (58) 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)
4:D:950:GLU:OE1	4:D:950:GLU:CD	1.70	1.34
3:A:303:ASP:OD2	3:A:304:PHE:N	1.95	1.00
3:A:525:GLU:H	3:A:525:GLU:CD	1.91	0.78
3:A:495:LYS:CE	3:A:537:THR:OG1	2.39	0.71
3:A:448:PHE:O	5:A:10:EDO:H11	1.97	0.64
3:A:600:GLU:H	3:A:600:GLU:CD	2.07	0.62
3:A:250:LYS:HE2	3:A:322:TYR:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:431:ASP:O	3:A:432:ASP:HB2	2.03	0.59
3:A:518:HIS:ND1	4:D:950:GLU:OE1	2.34	0.58
3:A:221:HIS:CE1	3:A:360:SER:HB2	2.39	0.58
3:A:517:GLN:HG3	4:D:947:PRO:HB2	1.88	0.56
3:A:659:LYS:C	3:A:660:SER:O	2.46	0.54
3:A:431:ASP:O	3:A:432:ASP:CB	2.54	0.54
3:A:630:ASN:ND2	3:A:633:THR:H	2.05	0.54
3:A:438:GLU:OE2	3:A:456:LYS:NZ	2.36	0.53
3:A:388:SER:HB2	3:A:429:LEU:HD22	1.91	0.53
3:A:260:TYR:HH	3:A:281:GLN:N	2.06	0.53
3:A:283:ALA:HB1	3:A:351:CYS:HB3	1.89	0.52
3:A:586:PHE:O	3:A:606:GLU:HG2	2.10	0.52
3:A:495:LYS:HE2	3:A:537:THR:OG1	2.11	0.51
3:A:221:HIS:HD2	3:A:222:ALA:O	1.93	0.51
3:A:409:HIS:ND1	3:A:416:HIS:HE1	2.07	0.51
3:A:491:SER:HB3	3:A:494:HIS:CE1	2.48	0.49
3:A:525:GLU:CD	3:A:525:GLU:N	2.66	0.49
3:A:568:LEU:HD22	3:A:581:LEU:HD22	1.93	0.49
3:A:510:LEU:HD11	3:A:513:ASP:H	1.78	0.49
2:C:4:DC:H2'	2:C:5:DT:H72	1.95	0.48
3:A:495:LYS:HE3	3:A:537:THR:OG1	2.13	0.48
3:A:624:THR:O	3:A:627:MET:HG2	2.14	0.48
3:A:448:PHE:O	5:A:10:EDO:C1	2.62	0.48
3:A:518:HIS:HA	4:D:950:GLU:OE1	2.14	0.48
3:A:503:ASN:HD22	3:A:503:ASN:C	2.23	0.47
3:A:549:PHE:CE2	3:A:551:ALA:HA	2.50	0.47
3:A:216:VAL:HG22	3:A:547:ARG:HG2	1.96	0.46
3:A:503:ASN:HD22	3:A:505:LEU:H	1.63	0.46
3:A:229:TYR:O	3:A:232:GLU:HG2	2.17	0.44
3:A:441:ASN:OD1	3:A:441:ASN:N	2.47	0.44
3:A:353:MET:HE2	3:A:353:MET:HB2	1.90	0.44
3:A:644:ARG:HD2	3:A:646:ASP:OD1	2.17	0.44
3:A:568:LEU:CD2	3:A:581:LEU:HD22	2.48	0.44
3:A:431:ASP:O	3:A:432:ASP:OD2	2.36	0.43
3:A:256:VAL:HG21	3:A:349:TYR:CE1	2.54	0.43
3:A:450:TYR:O	3:A:453:SER:HB2	2.18	0.43
3:A:600:GLU:HG2	6:A:747:HOH:O	2.18	0.43
3:A:221:HIS:HE1	3:A:361:GLN:H	1.65	0.43
3:A:235:PHE:HA	3:A:330:LEU:O	2.18	0.43
3:A:362[A]:ARG:NE	3:A:383:TYR:OH	2.46	0.43
3:A:660:SER:O	3:A:661:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:495:LYS:NZ	6:A:681:HOH:O	2.44	0.42
3:A:518:HIS:HD1	4:D:950:GLU:CD	2.27	0.41
3:A:503:ASN:ND2	3:A:505:LEU:H	2.17	0.41
3:A:618:GLN:HE21	3:A:618:GLN:HB3	1.62	0.41
3:A:574:GLY:O	3:A:577:SER:OG	2.37	0.41
3:A:444:VAL:O	4:D:937:ARG:HA	2.22	0.40
3:A:630:ASN:ND2	3:A:632:THR:H	2.19	0.40
3:A:593:TRP:CE2	3:A:598:PRO:HB3	2.56	0.40
2:C:14:DG:H2''	2:C:15:DT:H5'	2.02	0.40
3:A:620:ARG:HG3	3:A:625:HIS:HA	2.04	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	421/477 (88%)	408 (97%)	11 (3%)	2 (0%)	24	26
4	D	13/29 (45%)	12 (92%)	0	1 (8%)	1	0
All	All	434/506 (86%)	420 (97%)	11 (2%)	3 (1%)	18	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	660	SER
4	D	950	GLU
3	A	483	ALA

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	380/416 (91%)	335 (88%)	45 (12%)	5	4
4	D	14/27 (52%)	13 (93%)	1 (7%)	13	14
All	All	394/443 (89%)	348 (88%)	46 (12%)	5	4

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	208	SER
3	A	237	CYS
3	A	247	GLN
3	A	258	GLN
3	A	259	LEU
3	A	286	LEU
3	A	320	ASN
3	A	353	MET
3	A	371	LYS
3	A	398	LEU
3	A	410	VAL
3	A	416	HIS
3	A	429	LEU
3	A	432	ASP
3	A	441	ASN
3	A	453	SER
3	A	455	VAL
3	A	464	ILE
3	A	468	ARG
3	A	474	VAL
3	A	478	GLN
3	A	480	ILE
3	A	495	LYS
3	A	499	GLN
3	A	502	ASP
3	A	510	LEU
3	A	511	SER

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Mol	Chain	Res	Type
3	A	514	LYS
3	A	525	GLU
3	A	559	ILE
3	A	570	VAL
3	A	575	GLU
3	A	581	LEU
3	A	592	VAL
3	A	600	GLU
3	A	607	GLU
3	A	616	VAL
3	A	617	SER
3	A	618	GLN
3	A	622	GLU
3	A	627	MET
3	A	630	ASN
3	A	632	THR
3	A	644	ARG
3	A	654	LEU
4	D	940	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	196	GLN
3	A	221	HIS
3	A	258	GLN
3	A	281	GLN
3	A	361	GLN
3	A	396	ASN
3	A	416	HIS
3	A	503	ASN
3	A	529	GLN
3	A	554	GLN
3	A	618	GLN
3	A	630	ASN

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](#)

10 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	EDO	A	4	-	3,3,3	0.38	0	2,2,2	0.64	0
5	EDO	A	5	-	3,3,3	0.77	0	2,2,2	0.50	0
5	EDO	A	2	-	3,3,3	0.68	0	2,2,2	0.25	0
5	EDO	A	10	-	3,3,3	0.37	0	2,2,2	0.30	0
5	EDO	A	8	-	3,3,3	0.51	0	2,2,2	0.27	0
5	EDO	A	3	-	3,3,3	0.43	0	2,2,2	0.57	0
5	EDO	A	1	-	3,3,3	0.49	0	2,2,2	0.44	0
5	EDO	C	16	-	3,3,3	0.56	0	2,2,2	0.21	0
5	EDO	D	6	-	3,3,3	0.51	0	2,2,2	0.19	0
5	EDO	A	9	-	3,3,3	0.41	0	2,2,2	0.36	0

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	EDO	A	4	-	-	1/1/1/1	-
5	EDO	A	5	-	-	0/1/1/1	-
5	EDO	A	2	-	-	1/1/1/1	-
5	EDO	A	10	-	-	0/1/1/1	-
5	EDO	A	8	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	3	-	-	0/1/1/1	-
5	EDO	A	1	-	-	1/1/1/1	-
5	EDO	C	16	-	-	1/1/1/1	-
5	EDO	D	6	-	-	0/1/1/1	-
5	EDO	A	9	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	16	EDO	O1-C1-C2-O2
5	A	1	EDO	O1-C1-C2-O2
5	A	2	EDO	O1-C1-C2-O2
5	A	9	EDO	O1-C1-C2-O2
5	A	4	EDO	O1-C1-C2-O2
5	A	8	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	10	EDO	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%)	0.74	0	100 100	42, 45, 48, 49	0
2	C	15/15 (100%)	0.55	0	100 100	39, 42, 49, 51	0
3	A	427/477 (89%)	0.94	51 (11%)	9 7	22, 41, 61, 74	4 (0%)
4	D	15/29 (51%)	1.33	4 (26%)	1 1	22, 28, 37, 38	0
All	All	472/536 (88%)	0.94	55 (11%)	9 7	22, 41, 60, 74	4 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	483	ALA	7.4
3	A	263	LEU	4.9
3	A	578	ARG	4.7
3	A	195	VAL	4.4
3	A	439	THR	4.3
3	A	575	GLU	4.2
3	A	260	TYR	3.9
3	A	571	ASP	3.8
3	A	353	MET	3.7
3	A	525	GLU	3.6
3	A	432	ASP	3.6
3	A	379	THR	3.4
3	A	350	GLY	3.4
3	A	485	CYS	3.4
3	A	372	LYS	3.3
3	A	259	LEU	3.2
3	A	441	ASN	3.1
3	A	281	GLN	3.1
3	A	526	HIS	3.0
3	A	319	PRO	3.0
3	A	298	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	380	ASP	2.8
3	A	576	ALA	2.7
3	A	231	ASN	2.7
3	A	256	VAL	2.7
3	A	352	GLY	2.6
3	A	383	TYR	2.6
3	A	501	ILE	2.6
3	A	645	ASP	2.6
4	D	949	MET	2.5
3	A	297	SER	2.5
3	A	283	ALA	2.5
3	A	523	ILE	2.5
3	A	320	ASN	2.5
3	A	351	CYS	2.4
3	A	484	SER	2.4
3	A	284	THR	2.4
3	A	333	SER	2.4
3	A	570	VAL	2.4
3	A	661	LEU	2.4
3	A	222	ALA	2.3
3	A	282	GLN	2.3
3	A	371	LYS	2.3
4	D	939	MET	2.3
3	A	219	ILE	2.3
3	A	618	GLN	2.2
3	A	303	ASP	2.2
3	A	572	GLY	2.1
4	D	951	ASN	2.1
3	A	486	SER	2.1
3	A	302	LEU	2.1
3	A	262	THR	2.0
4	D	937	ARG	2.0
3	A	393	ALA	2.0
3	A	512	HIS	2.0

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

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	EDO	A	2	4/4	0.64	0.27	64,66,67,67	0
5	EDO	A	5	4/4	0.75	0.20	45,52,54,54	0
5	EDO	D	6	4/4	0.77	0.21	77,78,78,78	0
5	EDO	A	3	4/4	0.78	0.24	80,81,82,82	0
5	EDO	A	8	4/4	0.79	0.19	80,81,81,81	0
5	EDO	A	9	4/4	0.80	0.32	63,64,64,65	0
5	EDO	A	10	4/4	0.85	0.15	56,57,57,58	0
5	EDO	A	1	4/4	0.86	0.18	51,53,55,56	0
5	EDO	C	16	4/4	0.86	0.28	71,73,74,75	0
5	EDO	A	4	4/4	0.87	0.18	56,56,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.