



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 AM GMT

PDB ID : 3BRD
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
<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

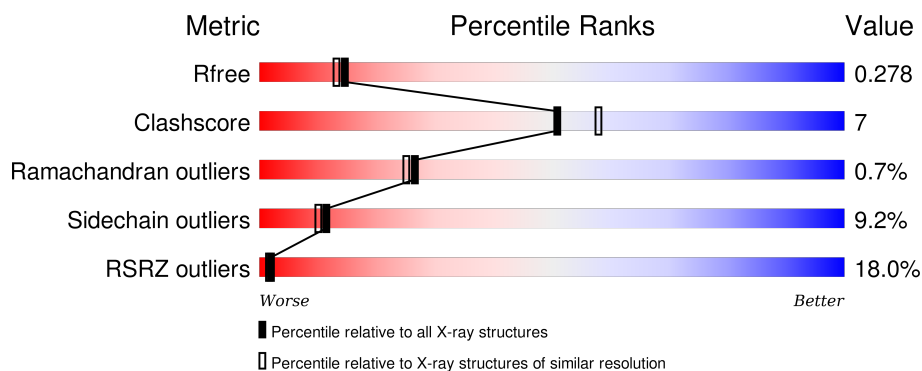
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (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 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	B	15	<div> <div>33%</div> <div>67%</div> </div>
2	C	15	<div> <div>33%</div> <div>67%</div> </div>
3	A	477	<div> <div>16%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>10%</div> </div>
4	D	29	<div> <div>34%</div> <div>38%</div> <div>10%</div> <div>•</div> <div>48%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	10	-	-	-	X
5	EDO	A	3	-	-	-	X
5	EDO	A	5	-	-	-	X
5	EDO	A	9	-	-	-	X
5	EDO	D	6	-	-	-	X

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

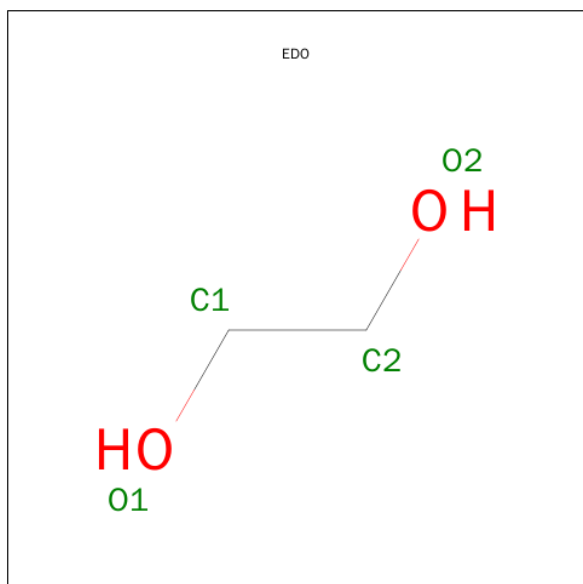
- Molecule 4 is a protein called Protein lin-12.

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 (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is water.

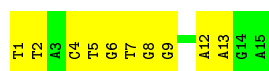
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total 98	O 98	0	0
6	B	24	Total 24	O 24	0	0
6	C	9	Total 9	O 9	0	0

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.

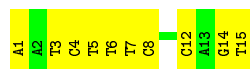
- Molecule 1: DNA (5'-D(*DTP*DTP*DAP*DCP*DTP*DGP*DTP*DGP*DGP*DGP*DAP*DAP*DAP*DGP*DA)-3')

Chain B: 



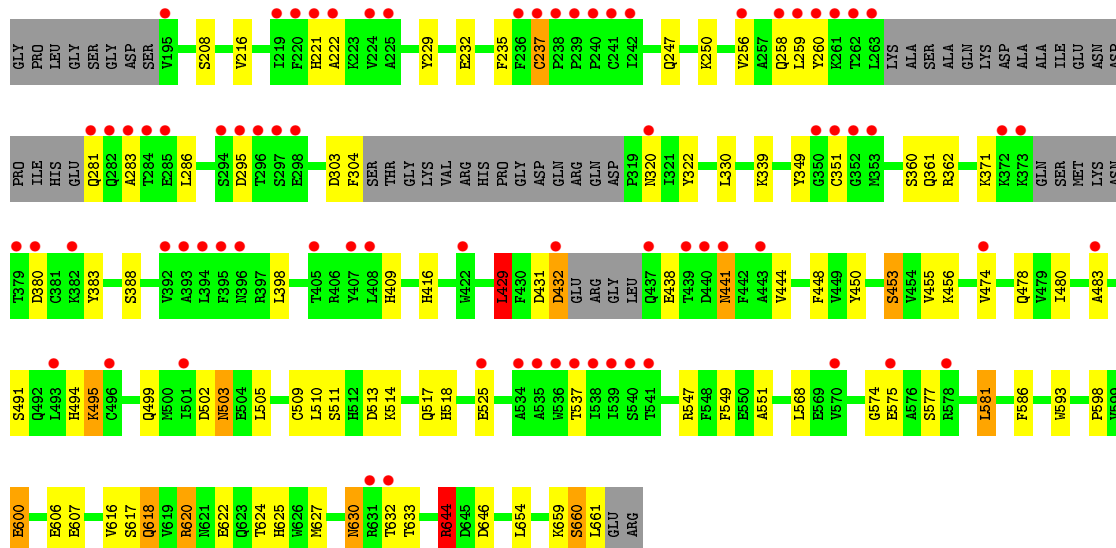
- Molecule 2: DNA (5'-D(*DAP*DAP*DTP*DCP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DAP*DGP*DT)-3')

Chain C: 

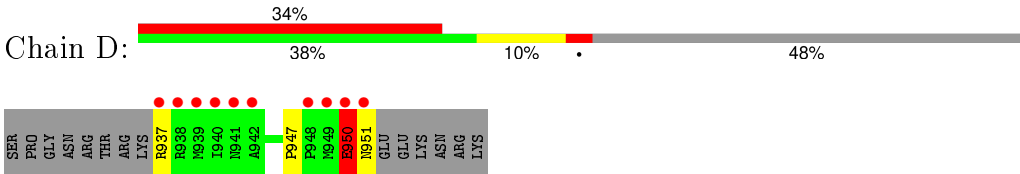


- Molecule 3: Lin-12 and glp-1 phenotype protein 1, isoform a

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 39.86 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.87-2.21) 94.4 (39.86-2.21)	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 0.251 , 0.278	Depositor DCC
R_{free} test set	1818 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 36498 reflections (0.008%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.27	0/350	1.94	11/540 (2.0%)
2	C	1.54	4/332 (1.2%)	2.03	9/509 (1.8%)
3	A	0.77	2/3512 (0.1%)	0.79	5/4743 (0.1%)
4	D	4.54	4/128 (3.1%)	1.17	2/172 (1.2%)
All	All	1.19	10/4322 (0.2%)	1.11	27/5964 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	950	GLU	CD-OE1	40.63	1.70	1.25
4	D	950	GLU	CD-OE2	26.51	1.54	1.25
3	A	237	CYS	CB-SG	-11.32	1.63	1.82
4	D	951	ASN	CG-OD1	10.63	1.47	1.24
4	D	951	ASN	CG-ND2	8.05	1.52	1.32
2	C	1	DA	C2'-C1'	7.71	1.60	1.52
3	A	509	CYS	CB-SG	-6.83	1.70	1.82
2	C	1	DA	O4'-C1'	6.54	1.50	1.42
2	C	1	DA	C5'-C4'	6.02	1.57	1.51
2	C	1	DA	C4'-O4'	5.32	1.50	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	12	DC	O4'-C1'-N1	-9.80	101.14	108.00
4	D	950	GLU	CG-CD-OE2	-7.70	102.90	118.30
1	B	2	DT	O4'-C1'-N1	-7.49	102.76	108.00
1	B	12	DA	O4'-C1'-N9	-7.18	102.97	108.00
1	B	7	DT	C6-C5-C7	-6.95	118.73	122.90
1	B	4	DC	P-O3'-C3'	6.86	127.94	119.70
2	C	6	DT	O4'-C1'-N1	-6.62	103.37	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	950	GLU	OE1-CD-OE2	6.36	130.93	123.30
1	B	7	DT	C4-C5-C7	6.35	122.81	119.00
1	B	8	DG	C8-N9-C4	-6.15	103.94	106.40
2	C	12	DC	N1-C1'-C2'	6.01	124.03	112.60
2	C	1	DA	O4'-C1'-N9	-5.90	103.87	108.00
1	B	5	DT	O4'-C1'-N1	-5.83	103.92	108.00
1	B	13	DA	O5'-P-OP2	-5.68	100.59	105.70
2	C	1	DA	C8-N9-C4	-5.65	103.54	105.80
3	A	620	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	9	DG	O5'-P-OP2	-5.55	100.71	105.70
2	C	7	DT	C4'-C3'-C2'	5.28	107.85	103.10
2	C	8	DC	P-O3'-C3'	5.25	126.01	119.70
1	B	1	DT	N3-C4-O4	5.18	123.00	119.90
3	A	620	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	C	3	DT	O5'-P-OP2	-5.17	101.05	105.70
2	C	1	DA	P-O3'-C3'	5.15	125.89	119.70
3	A	581	LEU	CA-CB-CG	5.12	127.09	115.30
3	A	429	LEU	CA-CB-CG	5.12	127.06	115.30
3	A	644	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	6	DG	C5-C6-N1	5.04	114.02	111.50

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	53	0
4	D	125	0	124	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	9	0	0	0	0
All	All	4328	0	3902	56	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 (56) 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:CD	4:D:950:GLU:OE1	1.70	1.30
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	0.73
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:250:LYS:HE2	3:A:322:TYR:HE1	1.66	0.60
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:600:GLU:H	3:A:600:GLU:CD	2.07	0.58
3:A:517:GLN:HG3	4:D:947:PRO:HB2	1.88	0.56
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:568:LEU:HD22	3:A:581:LEU:HD22	1.93	0.49
3:A:659:LYS:C	3:A:660:SER:O	2.46	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:518:HIS:HA	4:D:950:GLU:OE1	2.14	0.48
3:A:448:PHE:O	5:A:10:EDO:C1	2.62	0.48
3:A:495:LYS:NZ	6:A:681:HOH:O	2.44	0.47
3:A:549:PHE:CE2	3:A:551:ALA:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:525:GLU:CD	3:A:525:GLU:N	2.66	0.45
3:A:229:TYR:O	3:A:232:GLU:HG2	2.17	0.44
3:A:441:ASN:N	3:A:441:ASN:OD1	2.47	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:600:GLU:HG2	6:A:747:HOH:O	2.18	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: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
3:A:503:ASN:HD22	3:A:503:ASN:C	2.23	0.42
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:630:ASN:ND2	3:A:632:THR:H	2.19	0.40
3:A:444:VAL:O	4:D:937:ARG:HA	2.22	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 [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	421/477 (88%)	408 (97%)	11 (3%)	2 (0%)	34 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	13/29 (45%)	12 (92%)	0	1 (8%)	1	0
All	All	434/506 (86%)	420 (97%)	11 (2%)	3 (1%)	26	25

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%)	344 (90%)	36 (10%)	11	9
4	D	14/27 (52%)	14 (100%)	0	100	100
All	All	394/443 (89%)	358 (91%)	36 (9%)	11	10

All (36) 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	295	ASP
3	A	320	ASN
3	A	339	LYS
3	A	371	LYS
3	A	380	ASP
3	A	398	LEU
3	A	429	LEU

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Mol	Chain	Res	Type
3	A	432	ASP
3	A	441	ASN
3	A	453	SER
3	A	455	VAL
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	503	ASN
3	A	511	SER
3	A	514	LYS
3	A	575	GLU
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	630	ASN
3	A	644	ARG
3	A	654	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
3	A	258	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 carbohydrates 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	1	-	3,3,3	0.53	0	2,2,2	0.49	0
5	EDO	A	10	-	3,3,3	0.41	0	2,2,2	0.34	0
5	EDO	A	2	-	3,3,3	0.71	0	2,2,2	0.27	0
5	EDO	A	3	-	3,3,3	0.48	0	2,2,2	0.63	0
5	EDO	A	4	-	3,3,3	0.42	0	2,2,2	0.69	0
5	EDO	A	5	-	3,3,3	0.80	0	2,2,2	0.51	0
5	EDO	A	8	-	3,3,3	0.55	0	2,2,2	0.31	0
5	EDO	A	9	-	3,3,3	0.45	0	2,2,2	0.41	0
5	EDO	C	16	-	3,3,3	0.61	0	2,2,2	0.24	0
5	EDO	D	6	-	3,3,3	0.56	0	2,2,2	0.22	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	1	-	-	0/1/1/1	0/0/0/0
5	EDO	A	10	-	-	0/1/1/1	0/0/0/0
5	EDO	A	2	-	-	0/1/1/1	0/0/0/0
5	EDO	A	3	-	-	0/1/1/1	0/0/0/0
5	EDO	A	4	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	5	-	-	0/1/1/1	0/0/0/0
5	EDO	A	8	-	-	0/1/1/1	0/0/0/0
5	EDO	A	9	-	-	0/1/1/1	0/0/0/0
5	EDO	C	16	-	-	0/1/1/1	0/0/0/0
5	EDO	D	6	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.05	0	100 100	42, 45, 48, 49	0
2	C	15/15 (100%)	-0.27	0	100 100	39, 42, 49, 51	0
3	A	427/477 (89%)	0.89	75 (17%)	2 2	31, 41, 61, 74	0
4	D	15/29 (51%)	2.60	10 (66%)	0 0	22, 28, 37, 38	0
All	All	472/536 (88%)	0.88	85 (18%)	2 1	22, 41, 60, 74	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	483	ALA	11.6
3	A	263	LEU	9.1
3	A	260	TYR	6.5
3	A	379	THR	6.3
4	D	951	ASN	5.9
4	D	949	MET	5.7
3	A	281	GLN	5.2
3	A	353	MET	4.8
3	A	578	ARG	4.7
3	A	350	GLY	4.7
3	A	393	ALA	4.6
4	D	937	ARG	4.6
3	A	238	PRO	4.6
3	A	222	ALA	4.5
3	A	394	LEU	4.1
3	A	537	THR	3.9
3	A	493	LEU	3.9
4	D	940	ILE	3.9
3	A	282	GLN	3.9
3	A	539	ILE	3.8
3	A	439	THR	3.8

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Mol	Chain	Res	Type	RSRZ
4	D	939	MET	3.8
3	A	575	GLU	3.7
3	A	352	GLY	3.7
3	A	219	ILE	3.6
3	A	224	VAL	3.5
3	A	395	PHE	3.5
3	A	241	CYS	3.5
3	A	538	ILE	3.5
3	A	372	LYS	3.4
3	A	380	ASP	3.4
3	A	541	THR	3.4
3	A	437	GLN	3.3
3	A	237	CYS	3.3
3	A	262	THR	3.2
3	A	392	VAL	3.2
3	A	239	PRO	3.2
3	A	351	CYS	3.1
3	A	220	PHE	3.1
3	A	407	TYR	3.1
3	A	298	GLU	3.0
3	A	225	ALA	3.0
3	A	295	ASP	3.0
3	A	285	GLU	3.0
3	A	261	LYS	3.0
3	A	284	THR	3.0
3	A	240	PRO	2.9
3	A	405	THR	2.9
3	A	422	TRP	2.9
3	A	540	SER	2.9
3	A	221	HIS	2.8
4	D	938	ARG	2.8
3	A	236	PHE	2.7
3	A	283	ALA	2.7
3	A	441	ASN	2.7
3	A	297	SER	2.6
4	D	950	GLU	2.6
3	A	294	SER	2.5
3	A	195	VAL	2.5
3	A	631[A]	ARG	2.5
3	A	535	ALA	2.5
3	A	536	TRP	2.5
3	A	501	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	443	ALA	2.5
3	A	474	VAL	2.4
3	A	396	ASN	2.4
3	A	525	GLU	2.4
3	A	382	LYS	2.3
3	A	258	GLN	2.3
3	A	256	VAL	2.3
4	D	941	ASN	2.3
3	A	408	LEU	2.3
3	A	296	THR	2.2
3	A	570	VAL	2.2
3	A	496	CYS	2.2
3	A	440	ASP	2.2
3	A	320	ASN	2.2
4	D	948	PRO	2.2
3	A	259	LEU	2.2
3	A	242	ILE	2.1
3	A	373	LYS	2.1
3	A	632	THR	2.1
4	D	942	ALA	2.1
3	A	534	ALA	2.0
3	A	432	ASP	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 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(\AA^2)	Q<0.9
5	EDO	A	9	4/4	0.80	0.51	18.75	63,64,64,65	0
5	EDO	A	3	4/4	0.79	0.31	4.23	80,81,82,82	0
5	EDO	D	6	4/4	0.87	0.38	3.19	77,78,78,78	0
5	EDO	A	10	4/4	0.94	0.19	2.05	56,57,57,58	0
5	EDO	A	5	4/4	0.77	0.26	2.04	45,52,54,54	0
5	EDO	C	16	4/4	0.72	0.24	1.61	71,73,74,75	0
5	EDO	A	2	4/4	0.44	0.31	0.87	64,66,67,67	0
5	EDO	A	4	4/4	0.92	0.24	0.63	56,56,58,59	0
5	EDO	A	1	4/4	0.78	0.22	0.18	51,53,55,56	0
5	EDO	A	8	4/4	0.67	0.28	-	80,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.