



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:23 AM UTC

PDB ID : 4J2X / pdb_00004j2x
Title : CSL (RBP-Jk) with corepressor KyoT2 bound to DNA
Authors : Collins, K.J.; Kovall, R.A.
Deposited on : 2013-02-05
Resolution : 2.85 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

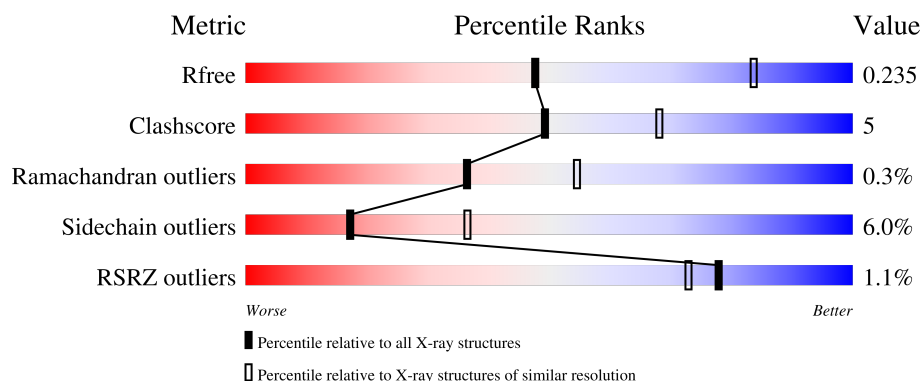
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	A	427	4% 78% 18% ..
1	C	427	78% 19% ..
2	B	28	54% 46%
2	D	28	4% 43% 7% 46% .
3	E	15	40% 47% 13%

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Mol	Chain	Length	Quality of chain
3	G	15	
4	F	15	
4	H	15	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8160 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 protein called Recombining binding protein suppressor of hairless.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	2	0
			3339	2114	573	626	26			
1	C	421	Total	C	N	O	S	0	1	0
			3349	2119	574	631	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP P31266
A	49	PRO	-	expression tag	UNP P31266
A	50	LEU	-	expression tag	UNP P31266
A	51	GLY	-	expression tag	UNP P31266
A	52	SER	-	expression tag	UNP P31266
A	115	THR	ARG	engineered mutation	UNP P31266
C	48	GLY	-	expression tag	UNP P31266
C	49	PRO	-	expression tag	UNP P31266
C	50	LEU	-	expression tag	UNP P31266
C	51	GLY	-	expression tag	UNP P31266
C	52	SER	-	expression tag	UNP P31266
C	115	THR	ARG	engineered mutation	UNP P31266

- Molecule 2 is a protein called Four and a half LIM domains protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	S	0	0	0
			121	81	20	19	1			
2	D	15	Total	C	N	O	S	0	0	0
			121	81	20	19	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	SER	-	expression tag	UNP P97447
D	183	SER	-	expression tag	UNP P97447

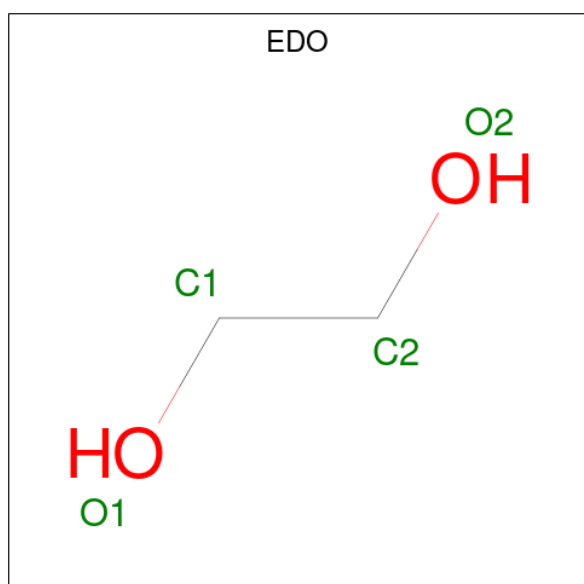
- Molecule 3 is a DNA chain called 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'.

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

- Molecule 4 is a DNA chain called 5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			
4	H	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

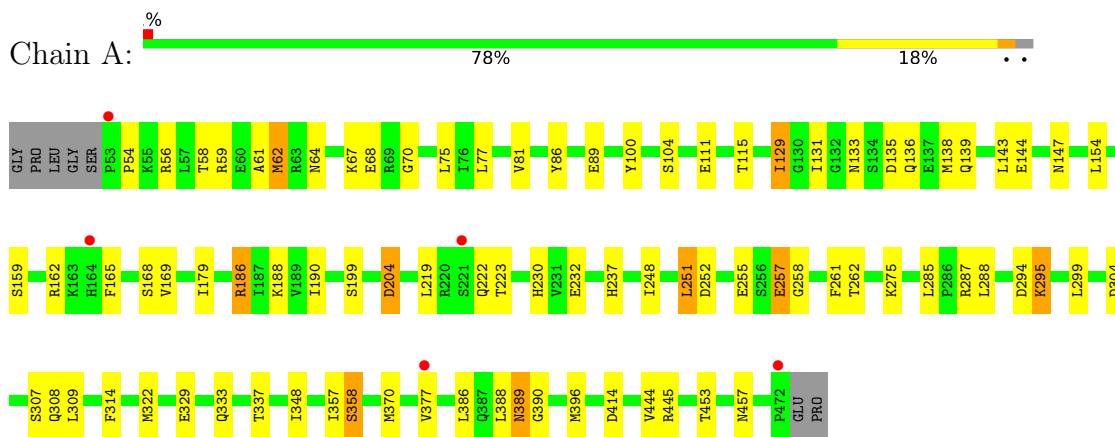
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	C	5	Total 5	O 5	0	0

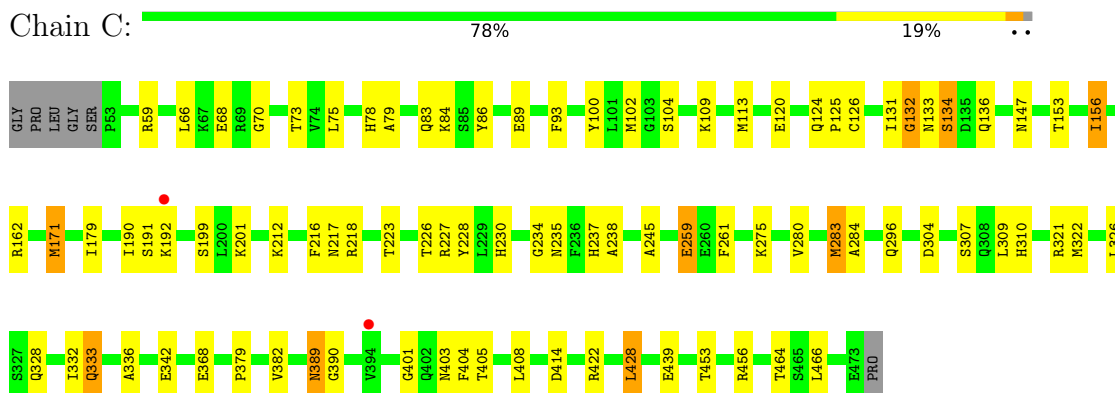
3 Residue-property plots

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: Recombining binding protein suppressor of hairless



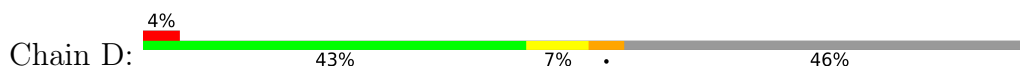
- Molecule 1: Recombining binding protein suppressor of hairless

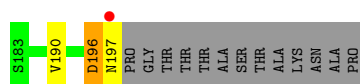


- Molecule 2: Four and a half LIM domains protein 1



- Molecule 2: Four and a half LIM domains protein 1

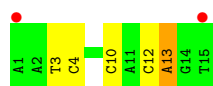




- Molecule 3: 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'



- Molecule 3: 5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3'



- Molecule 4: 5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'



- Molecule 4: 5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.16Å 97.29Å 144.10Å 90.00° 93.17° 90.00°	Depositor
Resolution (Å)	40.30 – 2.85 40.30 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.0 (40.30-2.85) 94.0 (40.30-2.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.188 , 0.231 0.189 , 0.235	Depositor DCC
R_{free} test set	1898 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8160	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	A	0.86	2/3418 (0.1%)	1.26	12/4620 (0.3%)
1	C	0.85	1/3425 (0.0%)	1.28	21/4628 (0.5%)
2	B	0.88	0/126	1.16	0/172
2	D	0.87	0/126	1.29	2/172 (1.2%)
3	E	0.43	0/332	1.54	9/509 (1.8%)
3	G	0.46	0/332	1.37	1/509 (0.2%)
4	F	0.42	0/350	1.37	6/540 (1.1%)
4	H	0.45	0/350	1.32	2/540 (0.4%)
All	All	0.80	3/8459 (0.0%)	1.29	53/11690 (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
1	C	0	1
3	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	MET	SD-CE	-9.56	1.55	1.79
1	C	171	MET	SD-CE	-7.06	1.61	1.79
1	A	59	ARG	C-N	5.00	1.40	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	GLU	CA-C-N	10.91	141.35	121.70
1	C	259	GLU	C-N-CA	10.91	141.35	121.70
4	F	1	DT	P-O3'-C3'	8.75	133.33	120.20
1	C	153	THR	N-CA-C	7.71	120.75	110.88
1	C	466	LEU	N-CA-C	7.24	121.23	110.52
1	C	404	PHE	CA-CB-CG	7.07	120.86	113.80
1	C	235	ASN	CA-CB-CG	7.00	119.60	112.60
1	C	93	PHE	CA-CB-CG	6.96	120.76	113.80
3	E	2	DA	P-O3'-C3'	6.93	130.59	120.20
1	A	389	ASN	N-CA-C	6.58	121.05	112.89
1	A	204	ASP	CA-CB-CG	6.53	119.13	112.60
4	H	11	DA	P-O3'-C3'	6.45	129.87	120.20
2	D	196	ASP	CA-C-N	6.44	133.29	121.70
2	D	196	ASP	C-N-CA	6.44	133.29	121.70
3	G	13	DA	P-O3'-C3'	6.43	129.85	120.20
3	E	6	DT	P-O3'-C3'	6.41	129.81	120.20
3	E	4	DC	P-O3'-C3'	6.29	129.63	120.20
1	C	223	THR	CA-C-N	6.29	129.40	120.53
1	C	223	THR	C-N-CA	6.29	129.40	120.53
4	F	1	DT	N1-C1'-C2'	6.09	122.64	113.50
4	F	8	DG	P-O5'-C5'	6.06	129.09	120.00
4	F	2	DT	P-O3'-C3'	5.86	128.99	120.20
1	C	332	ILE	CA-C-N	5.86	130.80	122.72
1	C	332	ILE	C-N-CA	5.86	130.80	122.72
1	A	223	THR	CA-C-N	5.81	128.67	120.42
1	A	223	THR	C-N-CA	5.81	128.67	120.42
1	A	252	ASP	CA-CB-CG	5.80	118.40	112.60
4	F	10	DG	P-O3'-C3'	5.80	128.90	120.20
1	A	255	GLU	N-CA-C	5.80	118.60	109.96
1	A	457	ASN	CA-CB-CG	5.79	118.39	112.60
4	F	13	DA	P-O3'-C3'	5.78	128.88	120.20
4	H	13	DA	P-O5'-C5'	5.68	128.53	120.00
1	A	258	GLY	CA-C-N	5.68	128.45	120.28
1	A	258	GLY	C-N-CA	5.68	128.45	120.28
1	C	191	SER	N-CA-C	-5.62	102.45	110.59
1	A	255	GLU	CA-C-N	5.49	130.96	120.97
1	A	255	GLU	C-N-CA	5.49	130.96	120.97
1	C	245	ALA	N-CA-C	-5.48	100.24	109.07
3	E	5	DT	P-O3'-C3'	5.37	128.26	120.20
1	C	66	LEU	CA-C-N	5.37	128.25	120.79
1	C	66	LEU	C-N-CA	5.37	128.25	120.79
3	E	3	DT	P-O5'-C5'	5.36	128.04	120.00
3	E	4	DC	O3'-P-O5'	-5.36	95.96	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	12	DC	N1-C1'-C2'	5.36	121.54	113.50
1	A	54	PRO	N-CA-C	5.33	119.59	111.11
1	C	456	ARG	CA-C-N	5.31	127.65	120.38
1	C	456	ARG	C-N-CA	5.31	127.65	120.38
3	E	15	DT	P-O5'-C5'	5.26	127.89	120.00
1	C	368	GLU	CA-C-N	5.24	126.69	120.14
1	C	368	GLU	C-N-CA	5.24	126.69	120.14
3	E	1	DA	O4'-C1'-N9	5.15	116.12	108.40
1	C	342	GLU	CA-C-N	5.07	131.23	121.54
1	C	342	GLU	C-N-CA	5.07	131.23	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	259	GLU	Peptide
3	E	1	DA	Sidechain

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	A	3339	0	3317	39	0
1	C	3349	0	3322	37	0
2	B	121	0	120	0	0
2	D	121	0	120	2	0
3	E	298	0	172	1	0
3	G	298	0	172	5	0
4	F	311	0	171	1	0
4	H	311	0	171	6	0
5	A	4	0	6	0	0
6	A	3	0	0	0	0
6	C	5	0	0	0	0
All	All	8160	0	7571	85	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 5.

All (85) 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)
1:C:230:HIS:CD2	1:C:237:HIS:HE1	1.84	0.96
1:C:230:HIS:HD2	1:C:237:HIS:CE1	1.87	0.91
1:C:230:HIS:HD2	1:C:237:HIS:HE1	0.96	0.91
1:A:230:HIS:HD2	1:A:237:HIS:HE1	1.16	0.87
1:A:230:HIS:HD2	1:A:237:HIS:CE1	1.93	0.86
1:A:230:HIS:CD2	1:A:237:HIS:HE1	2.02	0.74
1:A:162:ARG:NH1	1:A:165:PHE:HB2	2.06	0.71
1:C:389:ASN:HB3	1:C:390:GLY:HA3	1.75	0.69
1:A:131:ILE:O	1:A:133:ASN:HA	1.96	0.65
1:C:307:SER:HB3	1:C:310:HIS:CE1	2.33	0.63
1:C:75:LEU:HB2	1:C:100:TYR:HB2	1.81	0.62
3:G:10:DC:H42	4:H:8:DG:H1	1.46	0.62
1:A:136:GLN:HE22	1:A:138:MET:HE3	1.68	0.58
1:C:86:TYR:O	1:C:89:GLU:HG2	2.01	0.58
1:A:70:GLY:HA2	1:A:104:SER:OG	2.03	0.57
1:A:251:LEU:HD21	1:A:275:LYS:HB2	1.85	0.57
1:A:129:ILE:HD12	1:A:169:VAL:HG22	1.87	0.56
1:A:230:HIS:CD2	1:A:237:HIS:CE1	2.83	0.56
1:A:389:ASN:N	1:A:390:GLY:HA2	2.20	0.56
1:A:294:ASP:HB2	1:A:299:LEU:HD11	1.87	0.55
3:G:12:DC:H42	4:H:6:DG:H1	1.55	0.55
1:C:73:THR:HB	1:C:102:MET:HB2	1.89	0.55
1:A:129:ILE:HG12	1:A:154:LEU:HD11	1.89	0.55
1:A:86:TYR:H	1:A:89:GLU:HG3	1.71	0.55
1:C:217:ASN:HB3	1:C:326:LEU:HD21	1.89	0.55
1:C:230:HIS:CD2	1:C:237:HIS:CE1	2.75	0.54
3:G:3:DT:H2'	3:G:4:DC:C6	2.43	0.54
1:A:58:THR:HG22	1:A:370:MET:HE1	1.89	0.53
1:A:308:GLN:NE2	1:A:358:SER:HB2	2.24	0.53
1:C:190:ILE:HD11	1:C:309:LEU:HD12	1.90	0.53
1:A:309:LEU:HD21	1:A:357:ILE:HD12	1.91	0.52
1:A:388:LEU:HB3	1:A:390:GLY:HA2	1.91	0.52
4:H:2:DT:H2'	4:H:3:DA:C8	2.45	0.52
1:A:62:MET:HG2	1:A:414:ASP:HA	1.92	0.52
1:C:389:ASN:CB	1:C:390:GLY:HA3	2.40	0.52
1:C:70:GLY:HA2	1:C:104:SER:OG	2.11	0.51
1:C:171:MET:HB3	1:C:179:ILE:HD12	1.93	0.51
1:C:261:PHE:CZ	1:C:275:LYS:HG2	2.47	0.50
2:D:196:ASP:HA	2:D:197:ASN:HB2	1.94	0.50
1:C:78:HIS:HD2	1:C:79:ALA:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HG22	1:C:134:SER:HB3	1.94	0.49
3:E:14:DG:H2'	3:E:15:DT:C6	2.48	0.49
1:A:58:THR:HG23	1:A:61:ALA:H	1.78	0.48
1:A:322:MET:HB3	1:A:333:GLN:HG2	1.94	0.48
1:C:234:GLY:HA2	1:C:283:MET:HE1	1.94	0.48
1:A:75:LEU:HB2	1:A:100:TYR:HB2	1.96	0.48
1:A:308:GLN:HE22	1:A:358:SER:HB2	1.78	0.47
1:A:257:GLU:HG2	1:A:287:ARG:NE	2.30	0.47
1:C:216:PHE:HB3	1:C:228:TYR:CD1	2.50	0.47
1:C:199:SER:OG	1:C:201:LYS:HG2	2.15	0.47
1:C:134:SER:C	1:C:136:GLN:H	2.23	0.46
1:C:84:LYS:HA	1:C:156:ILE:HD12	1.98	0.46
1:C:405:THR:H	1:C:408:LEU:HD12	1.81	0.46
1:C:321:ARG:HB3	1:C:336:ALA:HB3	1.98	0.46
1:A:389:ASN:HB2	1:A:396:MET:HB2	1.99	0.45
1:A:222:GLN:HG3	3:G:13:DA:H5'	1.98	0.45
1:A:322:MET:HG3	1:A:333:GLN:HE21	1.81	0.45
1:C:131:ILE:O	1:C:133:ASN:N	2.50	0.45
1:C:218:ARG:HD3	1:C:226:THR:OG1	2.17	0.45
1:A:81:VAL:HB	1:A:190:ILE:HD12	1.98	0.44
1:C:124:GLN:NE2	1:C:125:PRO:HD2	2.32	0.44
1:C:126:CYS:O	1:C:171:MET:HG2	2.18	0.44
1:C:109:LYS:HG3	1:C:113:MET:HE2	2.00	0.44
1:C:382:VAL:O	1:C:401:GLY:HA3	2.18	0.44
3:G:10:DC:N4	4:H:8:DG:H1	2.14	0.43
1:A:232:GLU:HG2	1:A:237:HIS:CE1	2.54	0.43
1:A:261:PHE:CZ	1:A:275:LYS:HG2	2.53	0.43
4:F:5:DT:H2''	4:F:6:DG:C8	2.54	0.43
1:A:237:HIS:HD2	1:A:329:GLU:OE1	2.01	0.43
1:A:295:LYS:HE3	4:H:10:DG:H5''	2.01	0.42
1:A:64:ASN:HA	1:A:67:LYS:HD2	2.00	0.42
1:C:322:MET:HB3	1:C:333:GLN:HG2	2.00	0.42
4:H:6:DG:H2''	4:H:7:DT:H71	2.00	0.42
1:C:227:ARG:HB3	1:C:238:ALA:HB1	2.02	0.42
1:C:422:ARG:HD2	1:C:428:LEU:HD12	2.02	0.42
1:A:288:LEU:HD13	1:A:314:PHE:HB3	2.00	0.42
1:A:81:VAL:HG12	1:A:188:LYS:HB3	2.02	0.42
1:C:132:GLY:HA3	1:C:162:ARG:HH12	1.85	0.41
1:A:179:ILE:O	1:A:377:VAL:HG22	2.20	0.41
1:C:284:ALA:O	2:D:190:VAL:HA	2.20	0.41
1:A:111:GLU:O	1:A:115:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ARG:HD2	1:C:414:ASP:O	2.20	0.40
1:C:379:PRO:HB2	1:C:403:ASN:HB3	2.02	0.40
1:A:186:ARG:HH11	1:A:186:ARG:HB2	1.86	0.40
1:A:275:LYS:NZ	1:A:285:LEU:O	2.54	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	
1	A	420/427 (98%)	397 (94%)	23 (6%)	0	100	100
1	C	420/427 (98%)	391 (93%)	26 (6%)	3 (1%)	18	35
2	B	13/28 (46%)	12 (92%)	1 (8%)	0	100	100
2	D	13/28 (46%)	13 (100%)	0	0	100	100
All	All	866/910 (95%)	813 (94%)	50 (6%)	3 (0%)	36	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	GLY
1	C	134	SER
1	C	389	ASN

5.3.2 Protein sidechains [i](#)

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	
1	A	371/375 (99%)	342 (92%)	29 (8%)	11	25
1	C	372/375 (99%)	355 (95%)	17 (5%)	24	48
2	B	13/22 (59%)	13 (100%)	0	100	100
2	D	13/22 (59%)	13 (100%)	0	100	100
All	All	769/794 (97%)	723 (94%)	46 (6%)	17	36

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

Mol	Chain	Res	Type
1	A	56	ARG
1	A	68	GLU
1	A	77	LEU
1	A	129	ILE
1	A	135	ASP
1	A	139	GLN
1	A	143	LEU
1	A	144	GLU
1	A	147	ASN
1	A	159	SER
1	A	168	SER
1	A	186	ARG
1	A	199	SER
1	A	204	ASP
1	A	219	LEU
1	A	248	ILE
1	A	251	LEU
1	A	257	GLU
1	A	262	THR
1	A	295	LYS
1	A	304	ASP
1	A	307	SER
1	A	337	THR
1	A	348	ILE
1	A	358	SER
1	A	386	LEU
1	A	444	VAL
1	A	445	ARG
1	A	453	THR
1	C	68	GLU
1	C	83	GLN

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Mol	Chain	Res	Type
1	C	120	GLU
1	C	147	ASN
1	C	156	ILE
1	C	192	LYS
1	C	212	LYS
1	C	280	VAL
1	C	283	MET
1	C	296	GLN
1	C	304	ASP
1	C	328	GLN
1	C	333	GLN
1	C	428	LEU
1	C	439	GLU
1	C	453	THR
1	C	464	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	124	GLN
1	A	136	GLN
1	A	202	ASN
1	A	217	ASN
1	A	230	HIS
1	A	237	HIS
1	A	333	GLN
1	A	389	ASN
1	A	407	ASN
1	C	64	ASN
1	C	72	GLN
1	C	78	HIS
1	C	83	GLN
1	C	124	GLN
1	C	142	ASN
1	C	198	GLN
1	C	217	ASN
1	C	230	HIS
1	C	235	ASN
1	C	237	HIS
1	C	328	GLN
1	C	335	GLN

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Mol	Chain	Res	Type
1	C	389	ASN
1	C	446	GLN
1	C	449	GLN
1	C	457	ASN
2	D	197	ASN

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](#)

1 ligand is 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	501	-	3,3,3	0.77	0	2,2,2	0.23	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	501	-	-	0/1/1/1	-

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.

No monomer is involved in short contacts.

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	A	420/427 (98%)	-0.15	5 (1%) 76 71	57, 99, 151, 183	2 (0%)
1	C	421/427 (98%)	-0.18	2 (0%) 87 85	58, 100, 151, 177	1 (0%)
2	B	15/28 (53%)	-0.11	0 100 100	68, 92, 126, 137	0
2	D	15/28 (53%)	-0.06	1 (6%) 24 17	75, 90, 134, 150	0
3	E	15/15 (100%)	0.04	0 100 100	102, 122, 136, 143	0
3	G	15/15 (100%)	0.54	2 (13%) 7 5	138, 145, 179, 192	0
4	F	15/15 (100%)	-0.18	0 100 100	90, 129, 149, 153	0
4	H	15/15 (100%)	0.63	0 100 100	128, 150, 190, 193	0
All	All	931/970 (95%)	-0.13	10 (1%) 78 73	57, 102, 156, 193	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164[A]	HIS	3.6
3	G	15	DT	3.3
1	A	221	SER	3.2
1	A	472	PRO	2.8
1	A	53	PRO	2.8
1	A	377	VAL	2.6
1	C	192	LYS	2.3
1	C	394	VAL	2.1
2	D	197	ASN	2.1
3	G	1	DA	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	501	4/4	0.92	0.13	83,83,85,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.