



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:51 PM UTC

PDB ID : 6OD3 / pdb_00006od3
Title : Human TCF4 C-terminal bHLH domain in Complex with 13-bp Oligonucleotide Containing E-box Sequence
Authors : Horton, J.R.; Cheng, X.; Yang, J.
Deposited on : 2019-03-25
Resolution : 1.49 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:

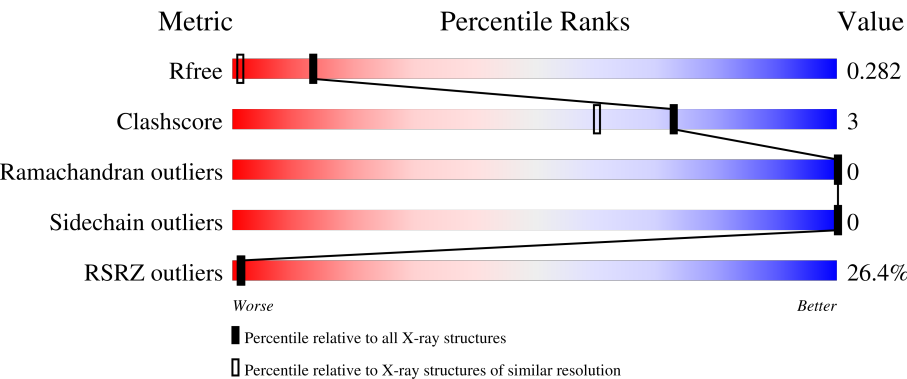
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	62	19% 94% 6%
1	B	62	15% 95% ..
1	E	62	8% 89% 11%
1	F	62	19% 89% 8% .
1	G	62	27% 84% 5% 11%

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Mol	Chain	Length	Quality of chain
1	H	62	44% 90% 8%
1	I	62	58% 90% 5% 5%
1	J	62	27% 76% 8% 16%
2	W	13	62% 31% 8%
2	X	13	8% 62% 38%
2	Y	13	8% 69% 31%
2	Z	13	8% 62% 38%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5160 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 Transcription factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	0	0
			499	309	102	85	3			
1	B	61	Total	C	N	O	S	0	2	0
			518	322	106	86	4			
1	E	62	Total	C	N	O	S	0	1	0
			514	318	106	87	3			
1	F	60	Total	C	N	O	S	0	0	0
			480	298	98	82	2			
1	G	55	Total	C	N	O	S	0	0	0
			409	260	77	71	1			
1	H	61	Total	C	N	O	S	0	0	0
			475	295	96	82	2			
1	I	59	Total	C	N	O	S	0	0	0
			421	268	79	73	1			
1	J	52	Total	C	N	O	S	0	0	0
			402	256	79	66	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	HIS	-	expression tag	UNP P15884
A	568	MET	-	expression tag	UNP P15884
B	567	HIS	-	expression tag	UNP P15884
B	568	MET	-	expression tag	UNP P15884
E	567	HIS	-	expression tag	UNP P15884
E	568	MET	-	expression tag	UNP P15884
F	567	HIS	-	expression tag	UNP P15884
F	568	MET	-	expression tag	UNP P15884
G	567	HIS	-	expression tag	UNP P15884
G	568	MET	-	expression tag	UNP P15884
H	567	HIS	-	expression tag	UNP P15884
H	568	MET	-	expression tag	UNP P15884
I	567	HIS	-	expression tag	UNP P15884

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Chain	Residue	Modelled	Actual	Comment	Reference
I	568	MET	-	expression tag	UNP P15884
J	567	HIS	-	expression tag	UNP P15884
J	568	MET	-	expression tag	UNP P15884

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*TP*AP*CP*AP*CP*GP*TP*GP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	13	Total	C	N	O	P	0	0	0
			262	127	47	76	12			
2	W	12	Total	C	N	O	P	0	0	0
			246	118	44	72	12			
2	Y	13	Total	C	N	O	P	0	0	0
			262	127	47	76	12			
2	Z	13	Total	C	N	O	P	0	0	0
			262	127	47	76	12			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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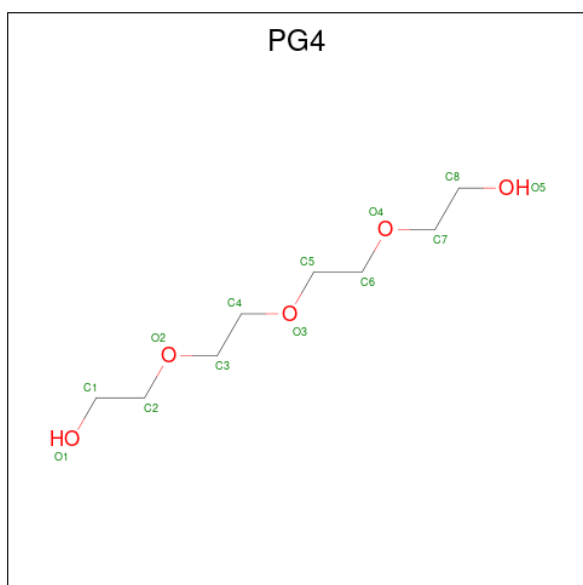
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Z	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			13	8	5		

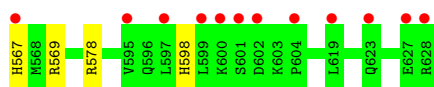
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	32	Total	O	0	0
			32	32		
6	X	34	Total	O	0	0
			34	34		
6	W	28	Total	O	0	0
			28	28		
6	E	46	Total	O	0	0
			46	46		
6	F	38	Total	O	0	0
			38	38		
6	Y	32	Total	O	0	0
			32	32		
6	Z	21	Total	O	0	0
			21	21		
6	G	22	Total	O	0	0
			22	22		
6	H	32	Total	O	0	0
			32	32		
6	I	13	Total	O	0	0
			13	13		
6	J	17	Total	O	0	0
			17	17		

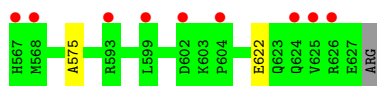
3 Residue-property plots [i](#)

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.

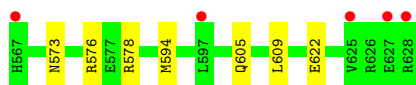
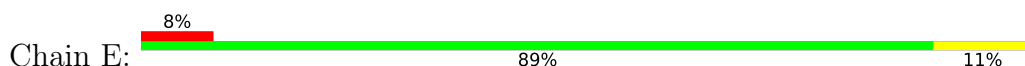
- Molecule 1: Transcription factor 4



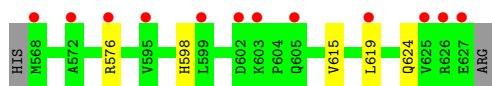
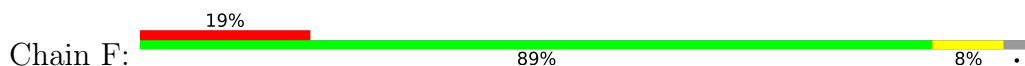
- Molecule 1: Transcription factor 4



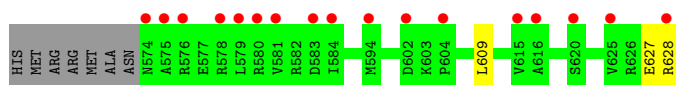
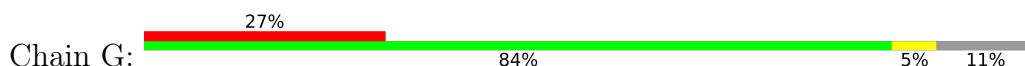
- Molecule 1: Transcription factor 4



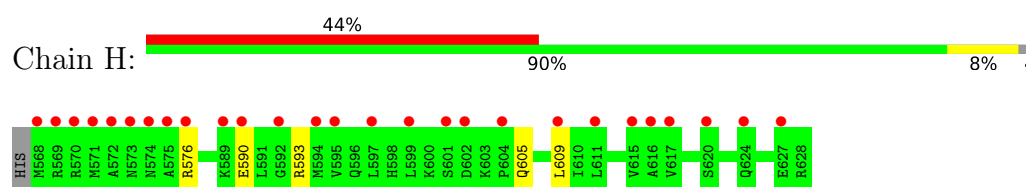
- Molecule 1: Transcription factor 4



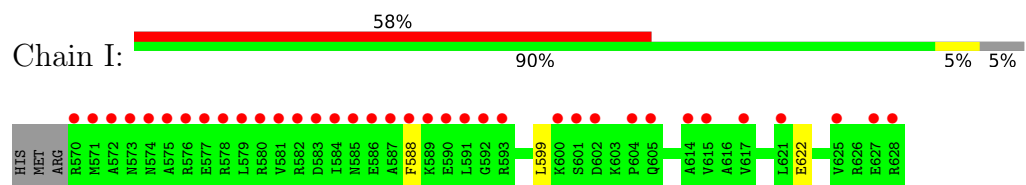
- Molecule 1: Transcription factor 4



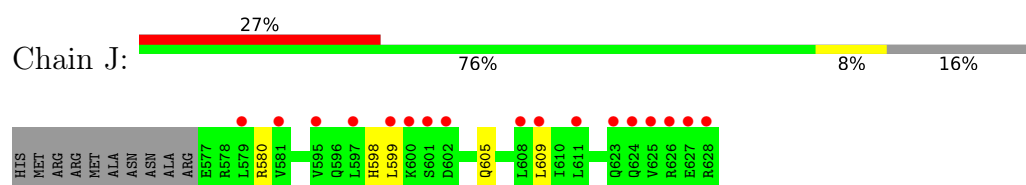
- Molecule 1: Transcription factor 4



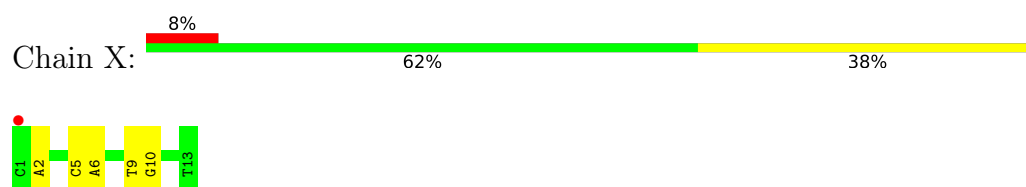
- Molecule 1: Transcription factor 4



- Molecule 1: Transcription factor 4



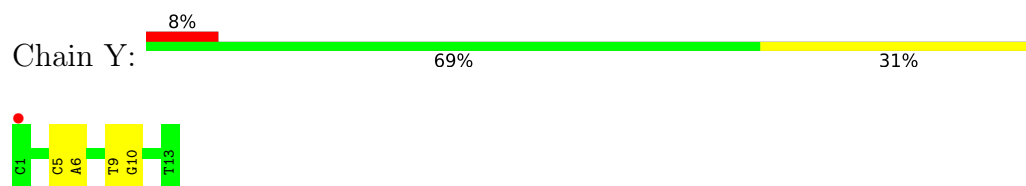
- Molecule 2: DNA (5'-D(*CP*AP*TP*AP*CP*AP*CP*GP*TP*GP*TP*AP*T)-3')



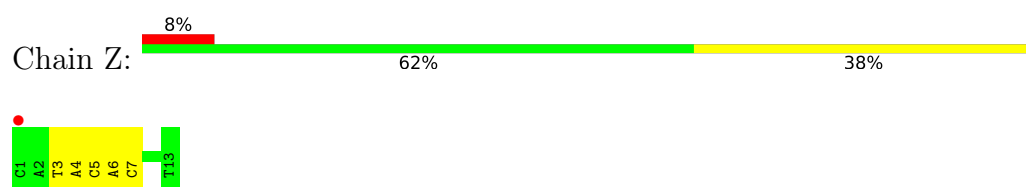
- Molecule 2: DNA (5'-D(*CP*AP*TP*AP*CP*AP*CP*GP*TP*GP*TP*AP*T)-3')



- Molecule 2: DNA (5'-D(*CP*AP*TP*AP*CP*AP*CP*GP*TP*GP*TP*AP*T)-3')



- Molecule 2: DNA (5'-D(*CP*AP*TP*AP*CP*AP*CP*GP*TP*GP*TP*AP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.18Å 58.95Å 62.72Å 104.63° 90.34° 94.86°	Depositor
Resolution (Å)	37.90 – 1.49 37.90 – 1.49	Depositor EDS
% Data completeness (in resolution range)	79.8 (37.90-1.49) 73.9 (37.90-1.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.50Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.221 , 0.237 (Not available) , 0.282	Depositor DCC
R_{free} test set	1901 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.1	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	0.95	EDS
Total number of atoms	5160	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.83% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PG4, 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	0.09	0/503	0.24	0/674
1	B	0.08	0/528	0.25	0/703
1	E	0.09	0/521	0.25	0/696
1	F	0.08	0/483	0.23	0/647
1	G	0.07	0/412	0.21	0/556
1	H	0.09	0/478	0.25	0/643
1	I	0.07	0/424	0.22	0/576
1	J	0.08	0/405	0.26	0/546
2	W	0.19	0/275	0.39	0/422
2	X	0.20	0/293	0.39	0/450
2	Y	0.19	0/293	0.39	0/450
2	Z	0.18	0/293	0.37	0/450
All	All	0.12	0/4908	0.28	0/6813

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	499	0	515	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	518	0	559	2	0
1	E	514	0	541	6	0
1	F	480	0	502	5	0
1	G	409	0	413	2	0
1	H	475	0	484	3	0
1	I	421	0	409	2	0
1	J	402	0	416	4	0
2	W	246	0	137	3	0
2	X	262	0	149	3	0
2	Y	262	0	149	2	0
2	Z	262	0	149	3	0
3	A	16	0	24	1	0
3	B	8	0	12	0	0
3	H	4	0	6	0	0
3	J	4	0	6	0	0
3	W	4	0	6	0	0
3	Y	4	0	6	0	0
3	Z	4	0	6	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	J	13	0	18	1	0
6	A	36	0	0	0	0
6	B	32	0	0	0	0
6	E	46	0	0	0	0
6	F	38	0	0	2	0
6	G	22	0	0	0	0
6	H	32	0	0	0	0
6	I	13	0	0	0	0
6	J	17	0	0	1	0
6	W	28	0	0	0	0
6	X	34	0	0	0	0
6	Y	32	0	0	0	0
6	Z	21	0	0	0	0
All	All	5160	0	4507	30	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 3.

All (30) 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:I:588:PHE:HB3	1:I:599:LEU:HD22	1.77	0.66
1:E:594:MET:HE1	1:F:615:VAL:HG13	1.83	0.59
3:A:704:EDO:H22	2:X:2:DA:C8	2.41	0.56
2:X:5:DC:H2''	2:X:6:DA:C8	2.43	0.54
1:G:627:GLU:O	1:G:628:ARG:NE	2.40	0.54
1:H:590:GLU:OE2	1:H:593:ARG:NH2	2.41	0.54
1:H:605:GLN:HA	1:H:609:LEU:HD23	1.91	0.52
1:B:575:ALA:HB3	1:F:619:LEU:HD12	1.93	0.51
1:F:576:ARG:NH2	6:F:702:HOH:O	2.44	0.50
2:W:9:DT:H1'	1:H:576:ARG:HH22	1.79	0.48
1:F:624:GLN:NE2	6:F:703:HOH:O	2.47	0.48
1:I:622:GLU:OE1	1:J:598:HIS:NE2	2.40	0.48
2:W:5:DC:H2''	2:W:6:DA:C8	2.50	0.46
2:Z:5:DC:H2''	2:Z:6:DA:C8	2.51	0.46
1:A:578:ARG:NE	2:W:7:DC:OP2	2.45	0.46
1:E:578:ARG:NE	2:Z:7:DC:OP2	2.46	0.46
2:X:9:DT:H2''	2:X:10:DG:C8	2.51	0.46
1:J:605:GLN:HA	1:J:609:LEU:HD23	1.99	0.45
1:J:599:LEU:HD23	1:J:599:LEU:HA	1.76	0.45
2:Y:5:DC:H2''	2:Y:6:DA:C8	2.53	0.44
1:A:598:HIS:NE2	1:B:622:GLU:OE2	2.35	0.43
1:A:567:HIS:CE1	1:A:569:ARG:HB3	2.53	0.43
1:E:573:ASN:OD1	1:E:576[B]:ARG:NH2	2.46	0.43
1:J:580:ARG:NH1	6:J:801:HOH:O	2.38	0.43
1:E:605:GLN:HA	1:E:609:LEU:HD23	2.00	0.43
2:Y:9:DT:H2''	2:Y:10:DG:C8	2.54	0.42
1:E:576[B]:ARG:HG2	1:G:609:LEU:HD13	2.01	0.42
1:E:622:GLU:OE2	1:F:598:HIS:NE2	2.36	0.41
2:Z:3:DT:H2''	2:Z:4:DA:C8	2.57	0.41
5:J:702:PG4:H41	5:J:702:PG4:H21	1.91	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	
1	A	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
1	B	61/62 (98%)	61 (100%)	0	0	100	100
1	E	61/62 (98%)	61 (100%)	0	0	100	100
1	F	58/62 (94%)	58 (100%)	0	0	100	100
1	G	53/62 (86%)	52 (98%)	1 (2%)	0	100	100
1	H	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
1	I	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	J	50/62 (81%)	50 (100%)	0	0	100	100
All	All	459/496 (92%)	455 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	52/56 (93%)	52 (100%)	0	100	100
1	B	57/56 (102%)	57 (100%)	0	100	100
1	E	55/56 (98%)	55 (100%)	0	100	100
1	F	50/56 (89%)	50 (100%)	0	100	100
1	G	40/56 (71%)	40 (100%)	0	100	100
1	H	48/56 (86%)	48 (100%)	0	100	100
1	I	38/56 (68%)	38 (100%)	0	100	100
1	J	40/56 (71%)	40 (100%)	0	100	100
All	All	380/448 (85%)	380 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	605	GLN
1	A	613	GLN
1	B	585	ASN
1	E	605	GLN
1	E	613	GLN
1	I	624	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](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	EDO	Y	101	-	3,3,3	0.42	0	2,2,2	0.38	0
3	EDO	A	704	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	B	701	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	A	701	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	H	701	-	3,3,3	0.43	0	2,2,2	0.40	0
5	PG4	J	702	-	12,12,12	0.54	0	11,11,11	0.23	0
3	EDO	A	703	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	W	101	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	Z	101	-	3,3,3	0.43	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	J	701	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	A	702	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	B	702	-	3,3,3	0.42	0	2,2,2	0.38	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
3	EDO	Y	101	-	-	0/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	B	701	-	-	0/1/1/1	-
3	EDO	A	701	-	-	0/1/1/1	-
3	EDO	H	701	-	-	0/1/1/1	-
5	PG4	J	702	-	-	4/10/10/10	-
3	EDO	A	703	-	-	0/1/1/1	-
3	EDO	W	101	-	-	0/1/1/1	-
3	EDO	Z	101	-	-	0/1/1/1	-
3	EDO	J	701	-	-	0/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	702	PG4	C5-C6-O4-C7
5	J	702	PG4	O2-C3-C4-O3
5	J	702	PG4	C3-C4-O3-C5
5	J	702	PG4	C8-C7-O4-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	EDO	1	0
5	J	702	PG4	1	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	A	62/62 (100%)	1.27	12 (19%) 3 2	18, 30, 68, 79	0
1	B	61/62 (98%)	1.03	9 (14%) 5 6	14, 26, 55, 71	2 (3%)
1	E	62/62 (100%)	1.08	5 (8%) 18 20	12, 30, 52, 83	1 (1%)
1	F	60/62 (96%)	1.29	12 (20%) 3 2	19, 32, 66, 74	0
1	G	55/62 (88%)	1.81	17 (30%) 1 1	20, 38, 73, 86	0
1	H	61/62 (98%)	1.91	27 (44%) 0 0	26, 40, 61, 75	0
1	I	59/62 (95%)	2.39	36 (61%) 0 0	25, 45, 110, 131	0
1	J	52/62 (83%)	1.85	17 (32%) 1 1	29, 46, 76, 86	0
2	W	12/13 (92%)	0.56	0 100 100	22, 26, 43, 47	0
2	X	13/13 (100%)	0.66	1 (7%) 19 21	20, 29, 37, 53	0
2	Y	13/13 (100%)	0.77	1 (7%) 19 21	21, 30, 36, 52	0
2	Z	13/13 (100%)	0.77	1 (7%) 19 21	23, 30, 40, 69	0
All	All	523/548 (95%)	1.48	138 (26%) 1 1	12, 36, 74, 131	3 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	581	VAL	6.9
1	I	581	VAL	5.9
1	E	628	ARG	5.8
1	I	575	ALA	5.4
1	A	597	LEU	5.2
1	H	572	ALA	5.1
1	G	574	ASN	5.0
1	I	572	ALA	5.0
1	I	577	GLU	4.8
1	E	597	LEU	4.7
1	I	628	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	599	LEU	4.7
1	J	602	ASP	4.6
1	J	599	LEU	4.6
2	Z	1	DC	4.5
1	F	599	LEU	4.3
1	G	616	ALA	4.3
1	J	581	VAL	4.3
1	I	579	LEU	4.2
1	I	570	ARG	4.2
1	I	574	ASN	4.2
1	J	600	LYS	4.2
1	E	567	HIS	4.1
1	G	579	LEU	4.1
1	I	627	GLU	4.1
1	A	628	ARG	3.9
1	F	625	VAL	3.8
1	H	604	PRO	3.7
1	H	568	MET	3.7
1	I	580	ARG	3.7
1	I	573	ASN	3.6
1	J	609	LEU	3.6
1	E	625	VAL	3.6
1	A	601	SER	3.5
1	A	599	LEU	3.5
1	F	568	MET	3.5
1	A	602	ASP	3.4
1	J	579	LEU	3.3
1	I	587	ALA	3.3
1	F	627	GLU	3.3
1	J	627	GLU	3.3
1	G	575	ALA	3.3
1	I	600	LYS	3.2
1	I	592	GLY	3.2
1	H	574	ASN	3.2
1	H	601	SER	3.2
1	G	584	ILE	3.2
1	G	628	ARG	3.2
1	A	600	LYS	3.2
1	G	576	ARG	3.1
1	H	616	ALA	3.1
1	H	570	ARG	3.1
1	H	624	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	584	ILE	3.1
1	B	567	HIS	3.0
1	J	625	VAL	3.0
1	H	571	MET	3.0
1	I	571	MET	3.0
1	J	597	LEU	3.0
1	I	576	ARG	2.9
1	J	611	LEU	2.9
1	J	628	ARG	2.9
1	B	626	ARG	2.9
1	J	624	GLN	2.8
1	F	576	ARG	2.8
1	H	589	LYS	2.8
1	J	601	SER	2.8
1	I	586	GLU	2.8
1	I	614	ALA	2.7
1	G	580	ARG	2.7
1	I	578	ARG	2.7
1	A	567	HIS	2.7
1	B	625	VAL	2.6
1	H	569	ARG	2.6
1	E	627	GLU	2.6
1	H	590	GLU	2.6
1	F	605	GLN	2.6
1	I	583	ASP	2.6
1	H	609	LEU	2.6
1	I	615	VAL	2.6
1	I	621	LEU	2.5
1	H	602	ASP	2.5
1	B	604	PRO	2.5
1	A	619	LEU	2.5
1	H	597	LEU	2.5
1	A	604	PRO	2.5
1	G	625	VAL	2.5
1	I	585	ASN	2.5
1	J	608	LEU	2.5
1	I	604	PRO	2.5
1	H	594	MET	2.5
1	H	595	VAL	2.5
1	F	602	ASP	2.5
1	G	620	SER	2.4
2	Y	1	DC	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	573	ASN	2.4
1	F	595	VAL	2.4
1	H	617	VAL	2.4
1	I	589	LYS	2.4
1	F	619	LEU	2.4
1	A	627	GLU	2.4
1	H	592	GLY	2.4
1	F	572	ALA	2.3
1	G	615	VAL	2.3
1	I	602	ASP	2.3
1	B	593[A]	ARG	2.3
1	J	626	ARG	2.3
1	H	575	ALA	2.3
1	I	588	PHE	2.3
1	G	604	PRO	2.3
1	I	593	ARG	2.3
1	I	590	GLU	2.3
1	B	602	ASP	2.2
1	F	626	ARG	2.2
2	X	1	DC	2.2
1	I	625	VAL	2.2
1	H	611	LEU	2.2
1	G	578	ARG	2.2
1	H	620	SER	2.2
1	J	595	VAL	2.2
1	I	582	ARG	2.2
1	I	601	SER	2.2
1	J	623	GLN	2.2
1	G	602	ASP	2.2
1	A	595	VAL	2.2
1	H	627	GLU	2.2
1	I	617	VAL	2.2
1	A	623	GLN	2.1
1	B	624	GLN	2.1
1	B	568	MET	2.1
1	H	576	ARG	2.1
1	H	615	VAL	2.1
1	G	583	ASP	2.1
1	G	594	MET	2.1
1	I	591	LEU	2.0
1	F	603	LYS	2.0
1	I	605	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	599	LEU	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(Å ²)	Q<0.9
3	EDO	B	701	4/4	0.70	0.15	41,47,49,51	0
3	EDO	Y	101	4/4	0.73	0.20	60,60,61,61	0
3	EDO	J	701	4/4	0.76	0.15	59,61,61,62	0
3	EDO	Z	101	4/4	0.77	0.26	48,51,52,53	0
5	PG4	J	702	13/13	0.77	0.16	54,58,64,64	0
3	EDO	A	703	4/4	0.78	0.15	56,56,56,57	0
3	EDO	A	702	4/4	0.83	0.14	39,44,46,47	0
3	EDO	A	704	4/4	0.84	0.21	46,47,54,55	0
3	EDO	A	701	4/4	0.87	0.14	58,58,59,59	0
3	EDO	W	101	4/4	0.88	0.14	50,54,55,57	0
3	EDO	H	701	4/4	0.89	0.15	63,65,66,66	0
3	EDO	B	702	4/4	0.91	0.13	49,50,51,54	0
4	CL	E	701	1/1	0.98	0.06	22,22,22,22	0
4	CL	B	703	1/1	0.98	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.