



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 05:00 pm BST

PDB ID : 4KDP
Title : TcaR-ssDNA complex crystal structure reveals the novel ssDNA binding mechanism of the MarR family proteins
Authors : Chang, Y.M.; Chen, C.K.-M.; Wang, A.H.-J.
Deposited on : 2013-04-25
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

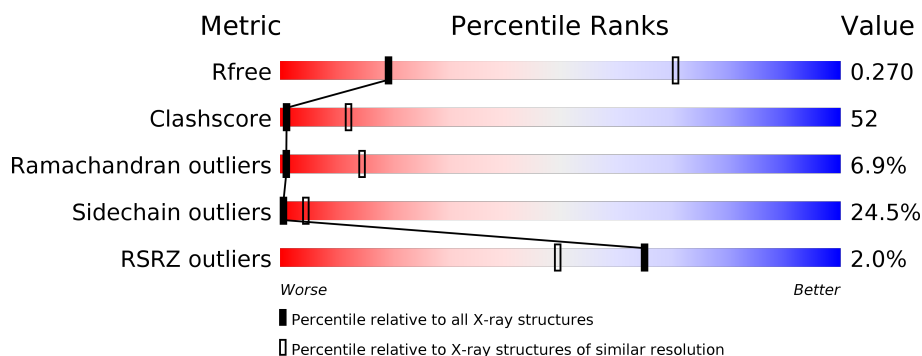
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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	151	<div> <div>3%</div> <div>23% 58% 16%</div> <div>•</div> </div>
1	B	151	<div> <div>3%</div> <div>30% 56% 11%</div> <div>•</div> </div>
1	C	151	<div> <div>4%</div> <div>28% 48% 21%</div> <div>•</div> </div>
1	D	151	<div> <div>3%</div> <div>29% 46% 23%</div> <div>•</div> </div>
1	E	151	<div> <div>%</div> <div>24% 53% 20%</div> <div>••</div> </div>
1	F	151	<div> <div>%</div> <div>30% 51% 17%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	151	
2	H	17	
2	J	17	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	2002	-	-	-	X
4	TRS	F	202	-	-	-	X
4	TRS	J	102	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9084 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 TcaR transcription regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1216	766	214	232	4			
1	B	151	Total	C	N	O	S	0	0	0
			1217	766	214	233	4			
1	C	151	Total	C	N	O	S	0	0	0
			1217	766	214	233	4			
1	D	151	Total	C	N	O	S	0	0	0
			1217	766	214	233	4			
1	E	150	Total	C	N	O	S	0	0	0
			1208	760	213	231	4			
1	F	151	Total	C	N	O	S	0	0	0
			1217	766	214	233	4			
1	G	151	Total	C	N	O	S	0	0	0
			1217	766	214	233	4			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*CP*AP*GP*CP*GP*CP*GP*CP*AP*GP*CP*CP*CP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			
2	J	10	Total	C	N	O	P	0	0	0
			198	94	38	57	9			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	F	1	Total	C	N	O	0	0
			8	4	1	3		
4	H	1	Total	C	N	O	0	0
			8	4	1	3		
4	J	1	Total	C	N	O	0	0
			8	4	1	3		
4	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	8	Total	O	0	0
			8	8		
5	C	16	Total	O	0	0
			16	16		
5	D	16	Total	O	0	0
			16	16		
5	E	7	Total	O	0	0
			7	7		
5	F	7	Total	O	0	0
			7	7		
5	G	10	Total	O	0	0
			10	10		

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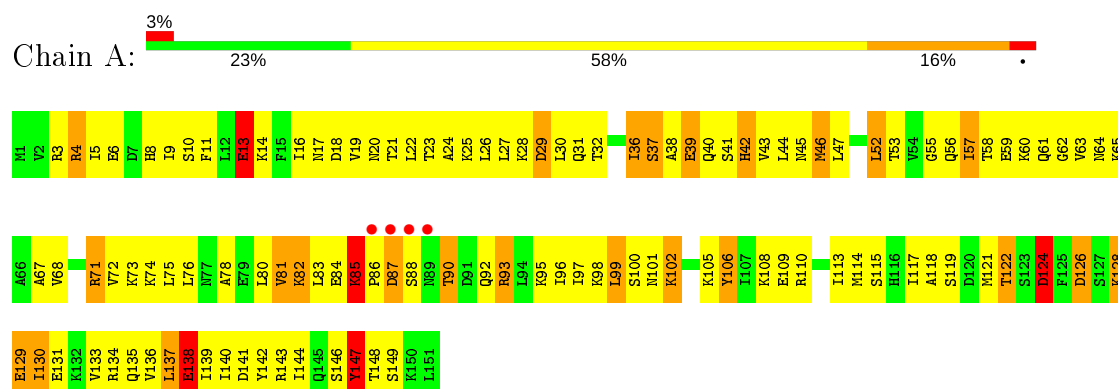
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	8	Total	O	0	0
			8	8		
5	J	10	Total	O	0	0
			10	10		

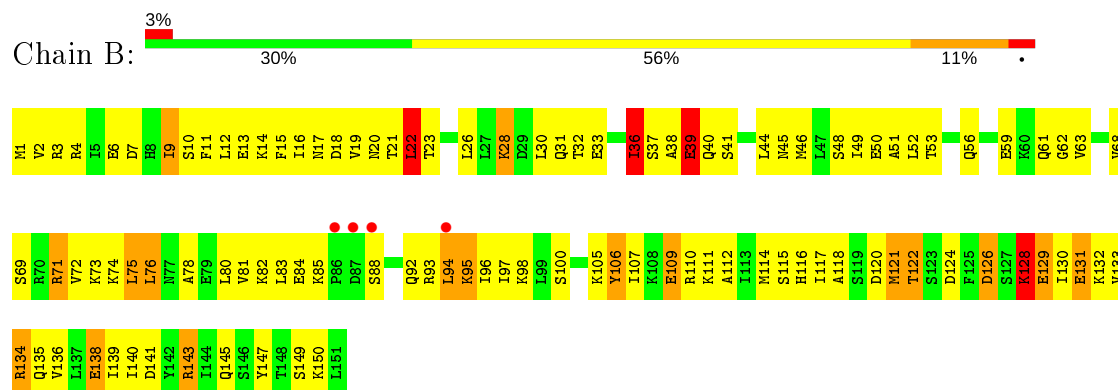
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

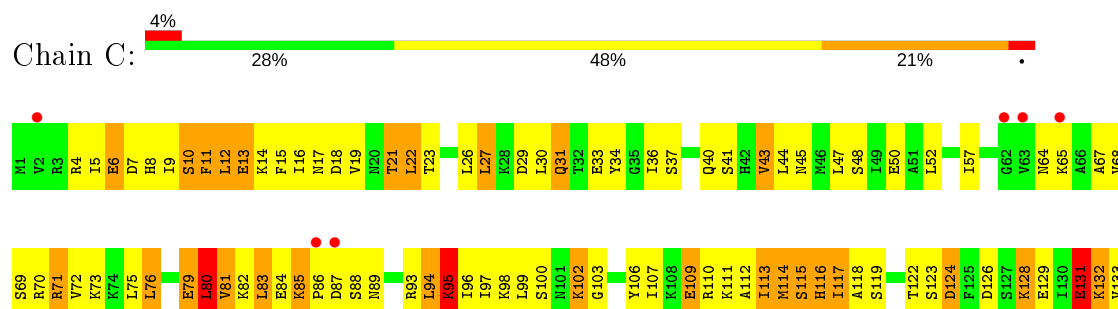
- Molecule 1: TcaR transcription regulator



- Molecule 1: TcaR transcription regulator



- Molecule 1: TcaR transcription regulator



R134
Q135
V136
L137
E138
I139
I140
D141
Y142
R143
I144
Q145
S146
Y147
S149
K150
L151

- Molecule 1: TcaR transcription regulator

Chain D: 

R1 V2 R3 R4 I5 E6 E7 H8 I9 S10 F11 L12 E13 I16 I17 D18 V19 N20 T21 T22 T23 L26 L27 K28 D29 L30 Q31 Y34 G35 I36 S37 A38 E39 Q40 S41 S42 V43 L44 M46 L47 S48 I49 E50 A51 L52 T53 V54 I57 T58 E59 K60 K61 G62 V63 I64

K65 A66 A67 V68 S69 R70 R71 R72 L75 L76 N77 A78 E79 L80 I81 K82 L83 E84 K85 P86 D87 S88 N89 T90 D91 K95 I96 I97 K98 L99 S100 N101 K102 G103 K104 K105 Y106 E109 R110 N111 A112 I113 M114 S115 R116 I117 T118 S119 D120 M121 T122 S123 D124 F125 K128 E129

I130 E131 K132 V133 R134 Q135 V136 L137 E138 I139 I140 D141 Y142 R143 I144 Q145 S146 Y147 T148 L151

- Molecule 1: TcaR transcription regulator

Chain E: 

R1 V2 R3 I5 E6 D7 H8 I9 S10 F11 L12 E13 K14 F15 I16 N17 D18 V19 K20 T21 T22 T23 L26 L27 K28 D29 L30 Q31 Y34 S37 A38 E39 Q40 S41 S42 V43 L44 M46 L47 S48 I49 L52 T53 V54 G55 Q56 I57 T58 E59 K60 K61 G62 V63 I64 A66

A67 V68 S69 R70 R71 R72 K73 R74 L75 L76 E79 E80 R81 K82 L83 E84 K85 P86 D87 S88 N89 T90 D91 K95 I96 I97 K98 L99 S100 N101 K102 G103 K104 K105 Y106 I107 I108 E109 E110 A111 A112 I113 M114 I117 A118 S119 D120 M121 T122 S123 D124 F125 D126 K128 A66

E129 I130 E131 K132 V133 R134 Q135 V136 L137 E138 I139 I140 D141 Y142 R143 I144 Q145 S146 Y147 T148 S149 K150 LEU

- Molecule 1: TcaR transcription regulator

Chain F: 

M1 V2 R3 R4 I5 E6 D7 H8 I9 S10 F11 L12 E13 K14 F15 I16 N17 D18 V19 N20 T21 T22 T23 L26 L27 K28 D29 L30 Q31 I36 S37 Q40 V43 L44 M45 M46 L47 S48 I49 E50 A51 L52 T53 V54 G55 Q56 I57 T58 E59 K60 Q61 K62 V63 M64 K65 V68

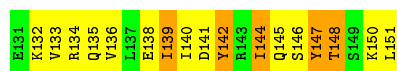
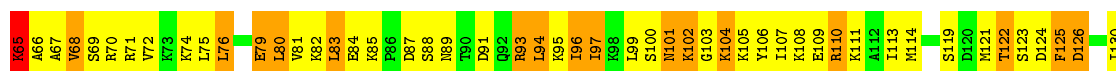
S69 R70 R71 V72 K73 R74 L75 L76 M77 L80 V81 K82 L83 E84 K85 S88 D91 Q92 R93 L94 K95 I96 I97 K98 R99 S100 N101 K105 Y106 I107 K108 E109 R110 I113 M114 S115 I116 I117 A118 M121 T122 F125 D126 S127 K128 E129 I130 Q131 E132 V133 R134 V136

L137 E138 I139 I140 D141 Y142 R143 I144 Q145 T148 S149 K150 L151

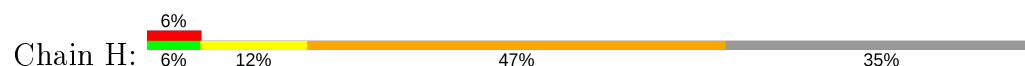
- Molecule 1: TcaR transcription regulator

Chain G: 

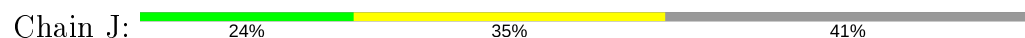
R1 R4 I5 E6 D7 H8 I9 S10 E13 K14 F15 I16 M17 D18 V19 L22 T23 A24 K25 L26 L27 K28 D29 L30 Q31 T32 E33 Y34 G35 I36 S37 A38 E39 Q40 S41 S42 V43 L44 M46 L47 S48 I49 E50 A51 L52 T53 Q56 I57 T58 E59 K60 K61 G62 V63 I64



- Molecule 2: DNA (5'-D(*CP*GP*CP*AP*GP*CP*GP*CP*GP*CP*AP*GP*CP*CP*CP*TP
*A)-3')



- Molecule 2: DNA (5'-D(*CP*GP*CP*AP*GP*CP*GP*CP*GP*CP*AP*GP*CP*CP*CP*TP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.90Å 91.90Å 261.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.00 – 3.60 29.88 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (16.00-3.60) 98.5 (29.88-3.61)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.285 0.242 , 0.270	Depositor DCC
R_{free} test set	756 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	138.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 112.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9084	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: TRS, 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	0.98	4/1226 (0.3%)	0.90	2/1640 (0.1%)
1	B	0.94	1/1227 (0.1%)	0.88	2/1640 (0.1%)
1	C	1.02	3/1227 (0.2%)	0.94	4/1640 (0.2%)
1	D	0.90	1/1227 (0.1%)	0.92	0/1640
1	E	1.00	3/1218 (0.2%)	0.87	1/1629 (0.1%)
1	F	0.91	2/1227 (0.2%)	0.88	0/1640
1	G	0.90	1/1227 (0.1%)	0.90	0/1640
2	H	2.90	15/249 (6.0%)	1.72	6/382 (1.6%)
2	J	2.17	1/221 (0.5%)	1.40	1/338 (0.3%)
All	All	1.10	31/9049 (0.3%)	0.95	16/12189 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
2	H	0	2
2	J	0	1
All	All	0	5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	DC	N1-C2	12.64	1.52	1.40
2	H	8	DC	N1-C2	9.04	1.49	1.40
1	E	138	GLU	CG-CD	8.71	1.65	1.51
2	H	3	DC	N1-C2	8.62	1.48	1.40
2	H	8	DC	C3'-C2'	8.22	1.62	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	H	7	DG	O4'-C4'-C3'	-6.61	101.86	104.50
1	B	143	ARG	NE-CZ-NH1	-6.13	117.24	120.30
2	H	8	DC	O4'-C1'-N1	6.07	112.25	108.00
1	A	124	ASP	CB-CG-OD2	-6.03	112.87	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	70	ARG	Sidechain
1	G	147	TYR	Sidechain
2	H	1	DC	Sidechain
2	H	2	DG	Sidechain
2	J	2	DG	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	1216	0	1290	156	0
1	B	1217	0	1290	160	0
1	C	1217	0	1290	146	0
1	D	1217	0	1290	146	0
1	E	1208	0	1279	163	0
1	F	1217	0	1290	145	0
1	G	1217	0	1290	142	0
2	H	222	0	123	19	0
2	J	198	0	112	4	0
3	B	8	0	12	0	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
3	H	8	0	12	0	0
4	B	8	0	12	0	0
4	F	8	0	12	0	0
4	H	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	16	0	24	0	0
5	A	9	0	0	0	0
5	B	8	0	0	0	0
5	C	16	0	0	0	0
5	D	16	0	0	0	0
5	E	7	0	0	1	0
5	F	7	0	0	1	0
5	G	10	0	0	1	0
5	H	8	0	0	0	0
5	J	10	0	0	0	0
All	All	9084	0	9350	955	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 52.

The worst 5 of 955 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:79:GLU:HB3	1:C:102:LYS:HD3	1.30	1.14
1:D:72:VAL:HA	1:D:75:LEU:HD12	1.14	1.14
1:F:118:ALA:O	1:F:122:THR:HG22	1.52	1.10
1:B:14:LYS:HE3	1:D:142:TYR:OH	1.52	1.10
1:A:16:ILE:HG12	1:B:16:ILE:HD11	1.34	1.08

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	149/151 (99%)	103 (69%)	38 (26%)	8 (5%)	2	19
1	B	149/151 (99%)	108 (72%)	32 (22%)	9 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	149/151 (99%)	105 (70%)	32 (22%)	12 (8%)	1	11
1	D	149/151 (99%)	110 (74%)	24 (16%)	15 (10%)	0	7
1	E	148/151 (98%)	102 (69%)	32 (22%)	14 (10%)	0	8
1	F	149/151 (99%)	109 (73%)	33 (22%)	7 (5%)	2	22
1	G	149/151 (99%)	113 (76%)	29 (20%)	7 (5%)	2	22
All	All	1042/1057 (99%)	750 (72%)	220 (21%)	72 (7%)	1	14

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	63	VAL
1	B	121	MET
1	B	150	LYS
1	C	29	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/139 (100%)	108 (78%)	31 (22%)	1	6
1	B	139/139 (100%)	114 (82%)	25 (18%)	1	11
1	C	139/139 (100%)	104 (75%)	35 (25%)	0	4
1	D	139/139 (100%)	98 (70%)	41 (30%)	0	2
1	E	138/139 (99%)	105 (76%)	33 (24%)	0	4
1	F	139/139 (100%)	107 (77%)	32 (23%)	1	5
1	G	139/139 (100%)	98 (70%)	41 (30%)	0	2
All	All	972/973 (100%)	734 (76%)	238 (24%)	0	4

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	65	LYS
1	E	5	ILE
1	G	89	ASN
1	D	89	ASN
1	D	121	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	42	HIS
1	E	40	GLN
1	G	101	ASN
1	E	17	ASN
1	B	40	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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
3	EDO	H	102	-	3,3,3	0.51	0	2,2,2	0.16	0
3	EDO	E	201	-	3,3,3	0.47	0	2,2,2	0.12	0
4	TRS	B	2003	-	7,7,7	0.38	0	9,9,9	0.65	0
4	TRS	F	202	-	7,7,7	0.39	0	9,9,9	0.52	0
3	EDO	B	2002	-	3,3,3	0.49	0	2,2,2	0.16	0
3	EDO	H	101	-	3,3,3	0.50	0	2,2,2	0.06	0
3	EDO	B	2001	-	3,3,3	0.46	0	2,2,2	0.38	0
4	TRS	J	101	-	7,7,7	0.46	0	9,9,9	0.74	0
3	EDO	F	201	-	3,3,3	0.48	0	2,2,2	0.08	0
4	TRS	J	102	-	7,7,7	0.70	0	9,9,9	0.50	0
4	TRS	H	103	-	7,7,7	0.50	0	9,9,9	0.70	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	H	102	-	-	0/1/1/1	-
3	EDO	E	201	-	-	0/1/1/1	-
4	TRS	B	2003	-	-	0/9/9/9	-
4	TRS	F	202	-	-	0/9/9/9	-
3	EDO	B	2002	-	-	0/1/1/1	-
3	EDO	H	101	-	-	0/1/1/1	-
3	EDO	B	2001	-	-	0/1/1/1	-
4	TRS	J	101	-	-	0/9/9/9	-
3	EDO	F	201	-	-	0/1/1/1	-
4	TRS	J	102	-	-	0/9/9/9	-
4	TRS	H	103	-	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	103	TRS	N-C-C1-O1
4	H	103	TRS	C2-C-C1-O1
4	H	103	TRS	C3-C-C1-O1

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	151/151 (100%)	-0.49	4 (2%) 56 40	45, 112, 157, 165	0
1	B	151/151 (100%)	-0.47	4 (2%) 56 40	61, 107, 160, 166	0
1	C	151/151 (100%)	-0.40	6 (3%) 38 25	56, 109, 157, 171	0
1	D	151/151 (100%)	-0.48	4 (2%) 56 40	51, 106, 157, 166	0
1	E	150/151 (99%)	-0.58	1 (0%) 87 78	57, 109, 157, 166	0
1	F	151/151 (100%)	-0.41	2 (1%) 77 63	57, 113, 157, 163	0
1	G	151/151 (100%)	-0.72	0 100 100	58, 109, 153, 166	0
2	H	11/17 (64%)	0.95	1 (9%) 9 5	130, 137, 143, 145	0
2	J	10/17 (58%)	0.66	0 100 100	129, 138, 141, 142	0
All	All	1077/1091 (98%)	-0.48	22 (2%) 65 49	45, 110, 158, 171	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	ASP	3.8
2	H	11	DA	3.7
1	A	88	SER	3.7
1	A	87	ASP	3.5
1	A	86	PRO	3.4

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. 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(\AA^2)	Q<0.9
3	EDO	H	101	4/4	0.53	0.38	103,107,108,109	0
3	EDO	B	2002	4/4	0.58	0.53	102,105,105,106	0
3	EDO	F	201	4/4	0.61	0.29	109,110,111,112	0
4	TRS	F	202	8/8	0.62	0.87	145,146,147,148	0
4	TRS	J	102	8/8	0.65	0.64	142,144,145,146	0
3	EDO	E	201	4/4	0.72	0.39	106,110,111,113	0
3	EDO	B	2001	4/4	0.79	0.22	116,118,119,120	0
3	EDO	H	102	4/4	0.81	0.56	121,123,124,124	0
4	TRS	H	103	8/8	0.83	0.23	126,128,129,131	0
4	TRS	J	101	8/8	0.85	0.25	136,137,138,138	0
4	TRS	B	2003	8/8	0.92	0.17	142,144,145,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.