



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:45 PM GMT

PDB ID : 4J9U  
Title : Crystal Structure of the TrkH/TrkA potassium transport complex  
Authors : Cao, Y.; Jin, X.; Huang, H.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)  
Deposited on : 2013-02-17  
Resolution : 3.80 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](mailto: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.

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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

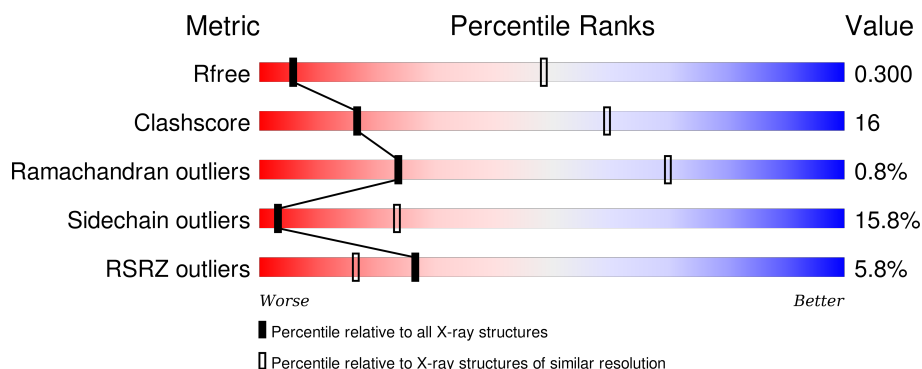
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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  $\geq 3$ , 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	A	485	<div> <div>5%</div> <div>52% 38% 6% 5%</div> </div>
1	B	485	<div> <div>4%</div> <div>53% 36% 6% 5%</div> </div>
1	C	485	<div> <div>8%</div> <div>53% 36% 6% 5%</div> </div>
1	D	485	<div> <div>5%</div> <div>53% 37% 5% 5%</div> </div>
2	E	458	<div> <div>6%</div> <div>58% 34% 6% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	458	
2	G	458	
2	H	458	

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	TBR	A	501	-	-	-	X
3	TBR	B	501	-	-	-	X
3	TBR	C	501	-	-	-	X
3	TBR	D	501	-	-	-	X
3	TBR	D	502	-	-	-	X
3	TBR	D	503	-	-	-	X
3	TBR	E	503	-	-	-	X
3	TBR	F	503	-	-	-	X
3	TBR	G	503	-	-	-	X
3	TBR	H	503	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28567 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.

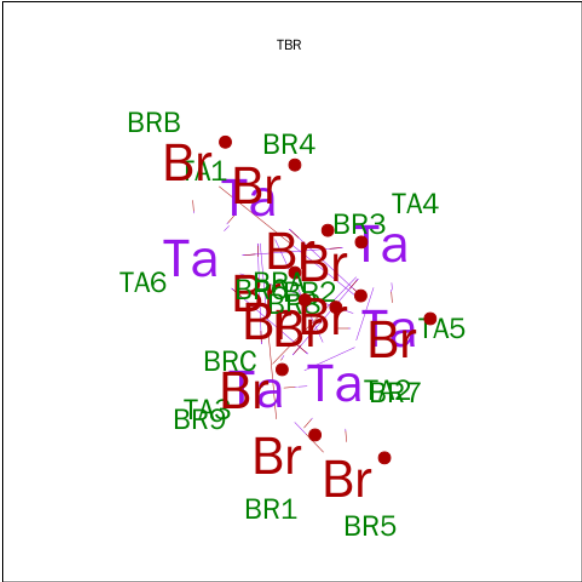
- Molecule 1 is a protein called Trk system potassium uptake protein TrkH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	B	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	C	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			
1	D	462	Total	C	N	O	S	0	0	0
			3569	2389	564	598	18			

- Molecule 2 is a protein called Potassium uptake protein TrkA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	451	Total	C	N	O	S	0	0	0
			3454	2162	611	669	12			
2	F	444	Total	C	N	O	S	0	0	0
			3410	2138	600	660	12			
2	G	452	Total	C	N	O	S	0	0	0
			3468	2174	612	670	12			
2	H	450	Total	C	N	O	S	0	0	0
			3455	2165	610	668	12			

- Molecule 3 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: Br<sub>12</sub>Ta<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	C	1	Total	Br	Ta	0	0
			18	12	6		
3	C	1	Total	Br	Ta	0	0
			18	12	6		
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	D	1	Total	Br	Ta	0	0
			18	12	6		
3	E	1	Total	Br	Ta	0	0
			18	12	6		
3	E	1	Total	Br	Ta	0	0
			18	12	6		
3	F	1	Total	Br	Ta	0	0
			18	12	6		
3	F	1	Total	Br	Ta	0	0
			18	12	6		

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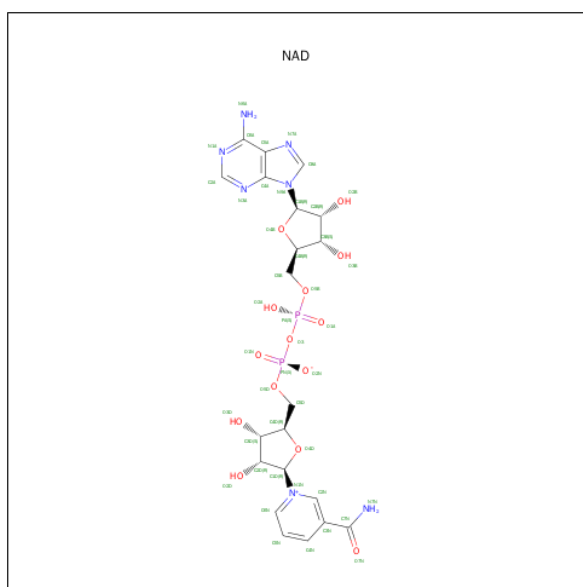
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	Br	Ta	0	0
			18	12	6		
3	G	1	Total	Br	Ta	0	0
			18	12	6		
3	H	1	Total	Br	Ta	0	0
			18	12	6		
3	H	1	Total	Br	Ta	0	0
			18	12	6		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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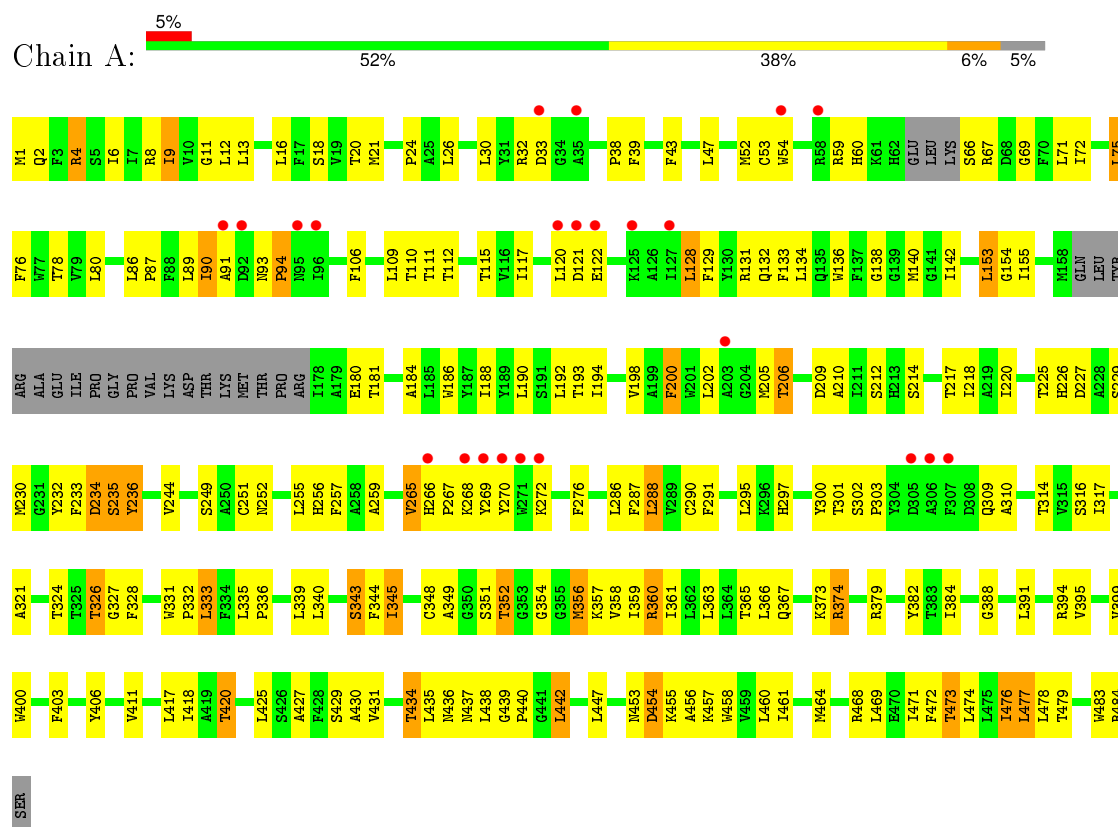
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

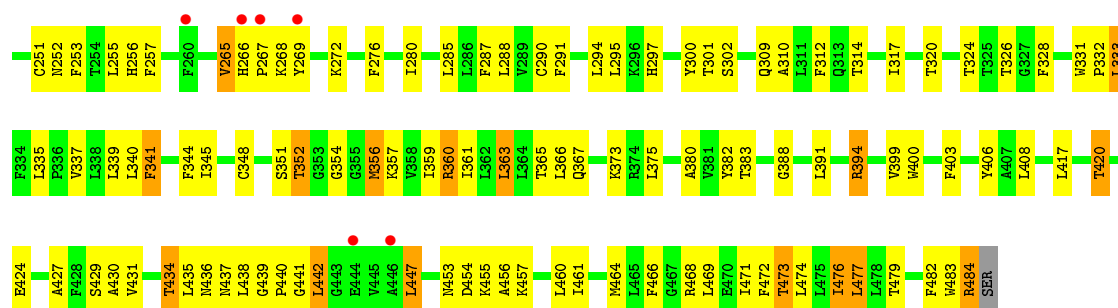
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

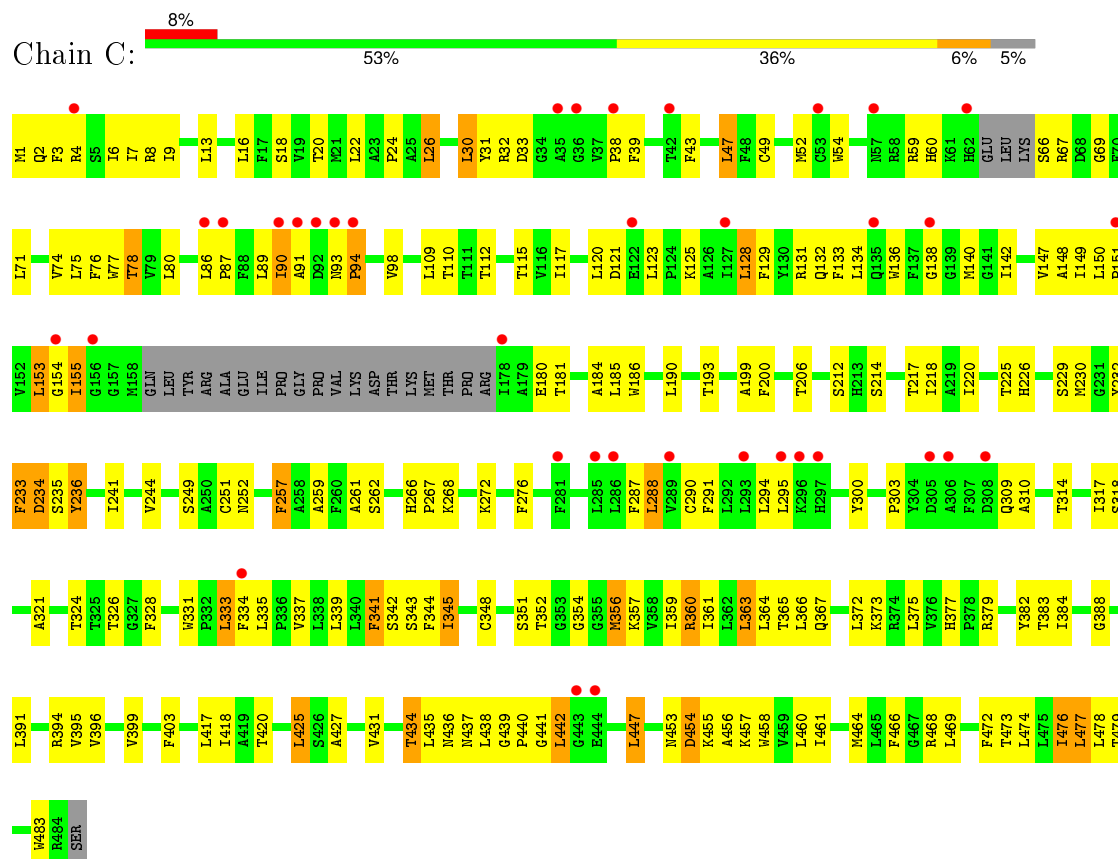
- Molecule 1: Trk system potassium uptake protein TrkH



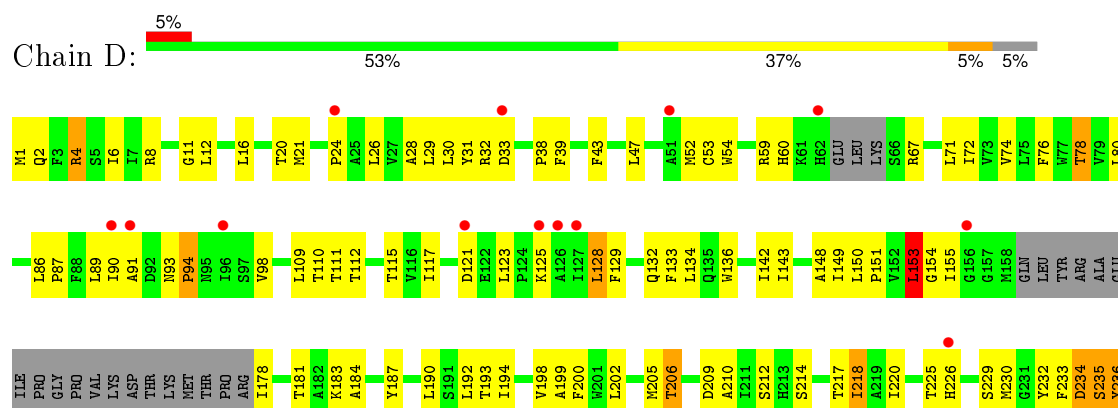




• Molecule 1: Trk system potassium uptake protein TrkH



• Molecule 1: Trk system potassium uptake protein TrkH







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.72Å 146.63Å 163.67Å 90.00° 99.32° 90.00°	Depositor
Resolution (Å)	49.79 – 3.80 49.79 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.79-3.80) 99.6 (49.79-3.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.232 , 0.280 0.258 , 0.300	Depositor DCC
$R_{free}$ test set	3130 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	118.3	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 61321 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	28567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.8858e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: K, TBR, NAD

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	0.30	0/3670	0.55	0/5000
1	B	0.30	0/3670	0.56	0/5000
1	C	0.30	0/3670	0.54	0/5000
1	D	0.28	0/3670	0.54	1/5000 (0.0%)
2	E	0.27	0/3498	0.54	0/4743
2	F	0.27	0/3451	0.54	0/4676
2	G	0.28	0/3513	0.54	0/4763
2	H	0.28	0/3500	0.56	0/4746
All	All	0.29	0/28642	0.55	1/38928 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	LEU	CA-CB-CG	5.31	127.52	115.30

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	3569	0	3638	144	0
1	B	3569	0	3638	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3569	0	3638	132	0
1	D	3569	0	3638	129	0
2	E	3454	0	3489	105	0
2	F	3410	0	3458	110	0
2	G	3468	0	3507	113	0
2	H	3455	0	3497	108	0
3	A	54	0	0	0	0
3	B	36	0	0	0	0
3	C	36	0	0	1	0
3	D	54	0	0	2	0
3	E	36	0	0	3	0
3	F	36	0	0	2	0
3	G	36	0	0	3	0
3	H	36	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	E	44	0	26	5	0
5	F	44	0	26	3	0
5	G	44	0	26	5	0
5	H	44	0	26	5	0
All	All	28567	0	28607	941	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 16.

The worst 5 of 941 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:B:420:THR:HG21	1:B:456:ALA:HB2	1.50	0.94
2:F:3:ILE:HG22	2:F:68:MET:HB3	1.59	0.85
1:A:420:THR:HG21	1:A:456:ALA:HB2	1.58	0.85
1:B:132:GLN:HG3	1:B:212:SER:HB2	1.57	0.84
1:D:420:THR:HG21	1:D:456:ALA:HB2	1.60	0.83

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	456/485 (94%)	386 (85%)	66 (14%)	4 (1%)	21	68
1	B	456/485 (94%)	385 (84%)	68 (15%)	3 (1%)	26	72
1	C	456/485 (94%)	385 (84%)	66 (14%)	5 (1%)	17	65
1	D	456/485 (94%)	387 (85%)	66 (14%)	3 (1%)	26	72
2	E	445/458 (97%)	395 (89%)	45 (10%)	5 (1%)	17	65
2	F	436/458 (95%)	393 (90%)	41 (9%)	2 (0%)	34	77
2	G	446/458 (97%)	391 (88%)	50 (11%)	5 (1%)	17	65
2	H	446/458 (97%)	401 (90%)	42 (9%)	3 (1%)	26	72
All	All	3597/3772 (95%)	3123 (87%)	444 (12%)	30 (1%)	24	70

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	456	PHE
2	F	165	PRO
1	C	262	SER
2	E	93	PRO
2	E	165	PRO

### 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	374/395 (95%)	310 (83%)	64 (17%)	2	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	374/395 (95%)	311 (83%)	63 (17%)	2	19
1	C	374/395 (95%)	318 (85%)	56 (15%)	3	26
1	D	374/395 (95%)	315 (84%)	59 (16%)	3	23
2	E	370/378 (98%)	312 (84%)	58 (16%)	3	24
2	F	366/378 (97%)	309 (84%)	57 (16%)	3	24
2	G	372/378 (98%)	320 (86%)	52 (14%)	4	29
2	H	370/378 (98%)	309 (84%)	61 (16%)	3	20
All	All	2974/3092 (96%)	2504 (84%)	470 (16%)	3	23

5 of 470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	234	ASP
2	E	198	GLN
2	H	254	THR
1	D	324	THR
1	D	476	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	367	GLN
1	D	239	ASN
2	G	297	GLN
1	C	239	ASN
2	G	265	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	TBR	A	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	A	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	A	503	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	C	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	C	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	D	501	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	D	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	D	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	E	501	-	38,48,48	0.92	2 (5%)	47,73,73	1.76	7 (14%)
3	TBR	E	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	E	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	F	501	-	38,48,48	0.93	2 (5%)	47,73,73	1.56	7 (14%)
3	TBR	F	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	F	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	G	501	-	38,48,48	0.89	1 (2%)	47,73,73	1.59	7 (14%)
3	TBR	G	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	G	503	-	0,36,36	0.00	-	0,180,180	0.00	-
5	NAD	H	501	-	38,48,48	0.89	1 (2%)	47,73,73	1.66	7 (14%)
3	TBR	H	502	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	H	503	-	0,36,36	0.00	-	0,180,180	0.00	-

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	TBR	A	501	-	-	0/0/696/696	0/0/19/19
3	TBR	A	502	-	-	0/0/696/696	0/0/19/19
3	TBR	A	503	-	-	0/0/696/696	0/0/19/19
3	TBR	B	501	-	-	0/0/696/696	0/0/19/19
3	TBR	B	502	-	-	0/0/696/696	0/0/19/19
3	TBR	C	501	-	-	0/0/696/696	0/0/19/19
3	TBR	C	502	-	-	0/0/696/696	0/0/19/19
3	TBR	D	501	-	-	0/0/696/696	0/0/19/19
3	TBR	D	502	-	-	0/0/696/696	0/0/19/19
3	TBR	D	503	-	-	0/0/696/696	0/0/19/19
5	NAD	E	501	-	-	0/22/62/62	0/5/5/5
3	TBR	E	502	-	-	0/0/696/696	0/0/19/19
3	TBR	E	503	-	-	0/0/696/696	0/0/19/19
5	NAD	F	501	-	-	0/22/62/62	0/5/5/5
3	TBR	F	502	-	-	0/0/696/696	0/0/19/19
3	TBR	F	503	-	-	0/0/696/696	0/0/19/19
5	NAD	G	501	-	-	0/22/62/62	0/5/5/5
3	TBR	G	502	-	-	0/0/696/696	0/0/19/19
3	TBR	G	503	-	-	0/0/696/696	0/0/19/19
5	NAD	H	501	-	-	0/22/62/62	0/5/5/5
3	TBR	H	502	-	-	0/0/696/696	0/0/19/19
3	TBR	H	503	-	-	0/0/696/696	0/0/19/19

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	501	NAD	O4B-C1B	2.07	1.43	1.41
5	F	501	NAD	O4B-C1B	2.21	1.44	1.41
5	H	501	NAD	C5A-C4A	3.28	1.47	1.40
5	G	501	NAD	C5A-C4A	3.30	1.47	1.40
5	E	501	NAD	C5A-C4A	3.39	1.48	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	NAD	N3A-C2A-N1A	-5.90	124.37	128.89
5	F	501	NAD	N3A-C2A-N1A	-5.88	124.39	128.89
5	G	501	NAD	N3A-C2A-N1A	-5.69	124.54	128.89
5	E	501	NAD	N3A-C2A-N1A	-5.59	124.62	128.89
5	E	501	NAD	C4B-O4B-C1B	-5.13	104.09	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	TBR	1	0
3	D	501	TBR	1	0
3	D	502	TBR	1	0
5	E	501	NAD	5	0
3	E	503	TBR	3	0
5	F	501	NAD	3	0
3	F	502	TBR	1	0
3	F	503	TBR	1	0
5	G	501	NAD	5	0
3	G	502	TBR	1	0
3	G	503	TBR	2	0
5	H	501	NAD	5	0
3	H	502	TBR	1	0
3	H	503	TBR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	462/485 (95%)	0.03	23 (4%)	32	21	31, 70, 118, 155	0
1	B	462/485 (95%)	0.08	18 (3%)	43	29	29, 75, 127, 165	0
1	C	462/485 (95%)	0.27	37 (8%)	15	9	39, 94, 142, 173	0
1	D	462/485 (95%)	0.14	23 (4%)	32	21	41, 87, 139, 163	0
2	E	451/458 (98%)	0.21	28 (6%)	24	14	39, 84, 158, 186	0
2	F	444/458 (96%)	0.21	28 (6%)	23	14	43, 80, 132, 161	0
2	G	452/458 (98%)	0.15	20 (4%)	38	25	43, 89, 158, 181	0
2	H	450/458 (98%)	0.30	35 (7%)	16	9	43, 88, 158, 183	0
All	All	3645/3772 (96%)	0.17	212 (5%)	26	16	29, 83, 146, 186	0

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ASP	7.2
2	H	390	THR	5.7
1	C	93	ASN	5.5
1	B	266	HIS	5.1
2	H	171	LEU	5.0

### 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 ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	TBR	G	503	18/18	0.88	0.47	1.64	53,122,192,197	18
3	TBR	B	501	18/18	0.96	0.51	1.62	41,95,161,539	18
3	TBR	D	503	18/18	0.54	0.53	1.48	73,128,323,367	18
3	TBR	D	502	18/18	0.94	0.45	1.25	45,104,211,261	18
3	TBR	A	502	18/18	0.97	0.36	1.12	86,125,275,297	18
3	TBR	H	503	18/18	0.93	0.40	0.99	52,92,184,211	18
3	TBR	A	501	18/18	0.97	0.53	0.91	86,145,324,330	18
3	TBR	C	501	18/18	0.98	0.50	0.87	50,93,125,189	18
3	TBR	G	502	18/18	0.86	0.34	0.57	70,139,259,285	18
3	TBR	D	501	18/18	0.97	0.47	0.56	31,77,99,170	18
4	K	D	504	1/1	0.93	0.22	0.54	119,119,119,119	0
3	TBR	F	503	18/18	0.88	0.46	0.53	49,80,197,198	18
3	TBR	E	503	18/18	0.90	0.43	0.42	48,100,209,232	18
3	TBR	C	502	18/18	0.97	0.37	0.12	81,131,298,309	18
5	NAD	G	501	44/44	0.92	0.21	-0.15	36,58,82,115	0
5	NAD	H	501	44/44	0.93	0.24	-0.18	41,62,102,117	0
5	NAD	E	501	44/44	0.92	0.20	-0.24	33,54,84,122	0
3	TBR	B	502	18/18	0.97	0.33	-0.33	74,116,217,295	18
5	NAD	F	501	44/44	0.95	0.21	-0.39	40,70,92,125	0
3	TBR	A	503	18/18	0.77	0.28	-0.61	99,160,345,346	18
4	K	C	503	1/1	0.76	0.08	-2.05	103,103,103,103	0
3	TBR	F	502	18/18	0.86	0.13	-2.05	81,118,256,309	18
4	K	B	503	1/1	0.92	0.11	-2.22	73,73,73,73	0
4	K	A	504	1/1	0.98	0.12	-2.59	66,66,66,66	0
3	TBR	H	502	18/18	0.90	0.17	-	83,180,334,361	18
3	TBR	E	502	18/18	0.81	0.33	-	59,128,282,314	18

## 6.5 Other polymers [i](#)

There are no such residues in this entry.