



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 04:45 pm GMT

PDB ID : 5UIQ  
Title : Crystal structure of IRAK4 in complex with compound 9  
Authors : Han, S.; Chang, J.S.  
Deposited on : 2017-01-14  
Resolution : 2.64 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](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

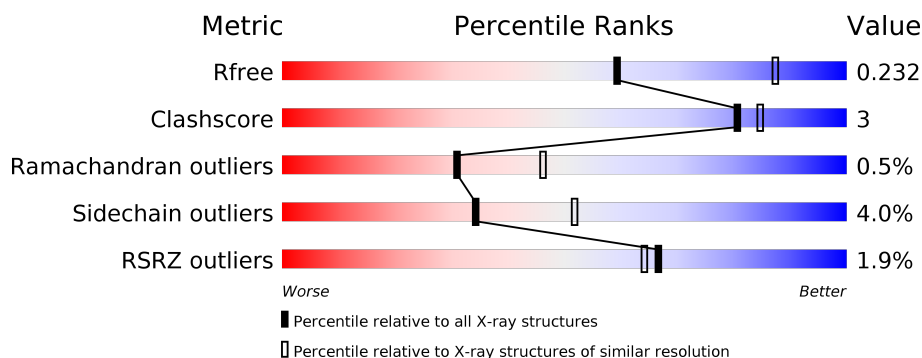
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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))
$R_{free}$	111664	1191 (2.66-2.62)
Clashscore	122126	1233 (2.66-2.62)
Ramachandran outliers	120053	1216 (2.66-2.62)
Sidechain outliers	120020	1216 (2.66-2.62)
RSRZ outliers	108989	1175 (2.66-2.62)

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	323	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>16%</div> </div> </div>
1	B	323	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
1	C	323	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>12%</div> </div> </div>
1	D	323	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8759 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	P	S	0	0	0
			2108	1322	351	418	3	14			
1	B	275	Total	C	N	O	P	S	0	1	0
			2155	1352	366	419	3	15			
1	C	283	Total	C	N	O	P	S	0	0	0
			2214	1387	374	436	3	14			
1	D	274	Total	C	N	O	P	S	0	0	0
			2167	1361	368	421	3	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	GLY	-	expression tag	UNP Q9NWZ3
A	146	GLY	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	138	MET	-	initiating methionine	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3

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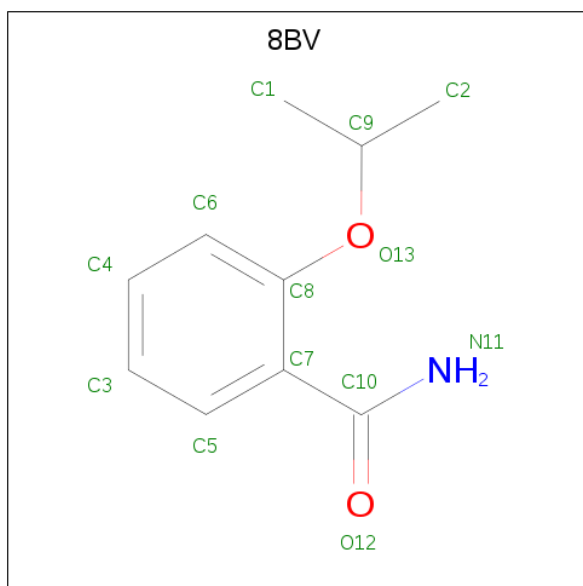
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	138	MET	-	initiating methionine	UNP Q9NWZ3
C	139	HIS	-	expression tag	UNP Q9NWZ3
C	140	HIS	-	expression tag	UNP Q9NWZ3
C	141	HIS	-	expression tag	UNP Q9NWZ3
C	142	HIS	-	expression tag	UNP Q9NWZ3
C	143	HIS	-	expression tag	UNP Q9NWZ3
C	144	HIS	-	expression tag	UNP Q9NWZ3
C	145	GLY	-	expression tag	UNP Q9NWZ3
C	146	GLY	-	expression tag	UNP Q9NWZ3
C	147	GLU	-	expression tag	UNP Q9NWZ3
C	148	ASN	-	expression tag	UNP Q9NWZ3
C	149	LEU	-	expression tag	UNP Q9NWZ3
C	150	TYR	-	expression tag	UNP Q9NWZ3
C	151	PHE	-	expression tag	UNP Q9NWZ3
C	152	GLN	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	138	MET	-	initiating methionine	UNP Q9NWZ3
D	139	HIS	-	expression tag	UNP Q9NWZ3
D	140	HIS	-	expression tag	UNP Q9NWZ3
D	141	HIS	-	expression tag	UNP Q9NWZ3
D	142	HIS	-	expression tag	UNP Q9NWZ3
D	143	HIS	-	expression tag	UNP Q9NWZ3
D	144	HIS	-	expression tag	UNP Q9NWZ3
D	145	GLY	-	expression tag	UNP Q9NWZ3
D	146	GLY	-	expression tag	UNP Q9NWZ3
D	147	GLU	-	expression tag	UNP Q9NWZ3
D	148	ASN	-	expression tag	UNP Q9NWZ3
D	149	LEU	-	expression tag	UNP Q9NWZ3
D	150	TYR	-	expression tag	UNP Q9NWZ3
D	151	PHE	-	expression tag	UNP Q9NWZ3
D	152	GLN	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 2-[(propan-2-yl)oxy]benzamide (three-letter code: 8BV) (formula: C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	10	1	2		
2	B	1	Total	C	N	O	0	0
			13	10	1	2		
2	C	1	Total	C	N	O	0	0
			13	10	1	2		
2	D	1	Total	C	N	O	0	0
			13	10	1	2		

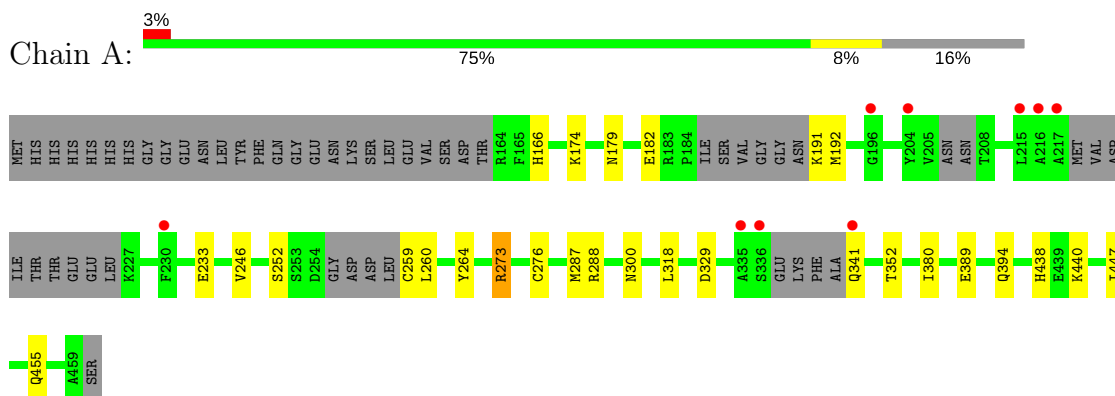
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	13	Total	O	0	0
			13	13		
3	C	11	Total	O	0	0
			11	11		
3	D	16	Total	O	0	0
			16	16		

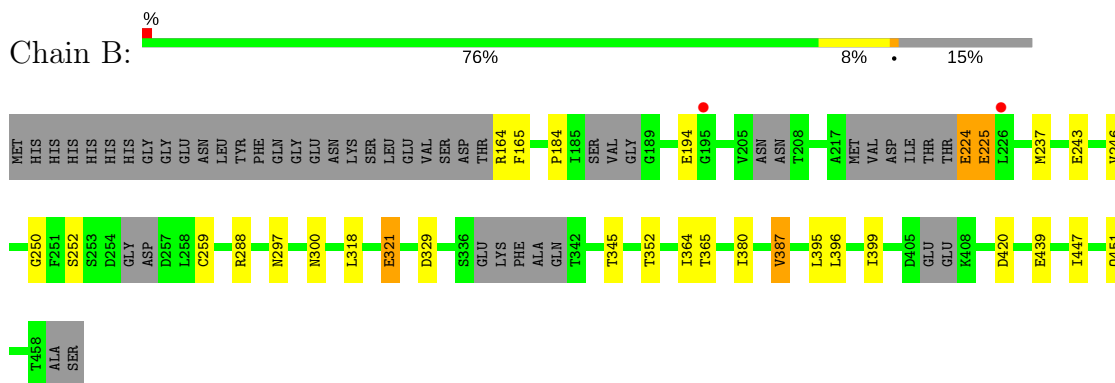
### 3 Residue-property plots [i](#)

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.

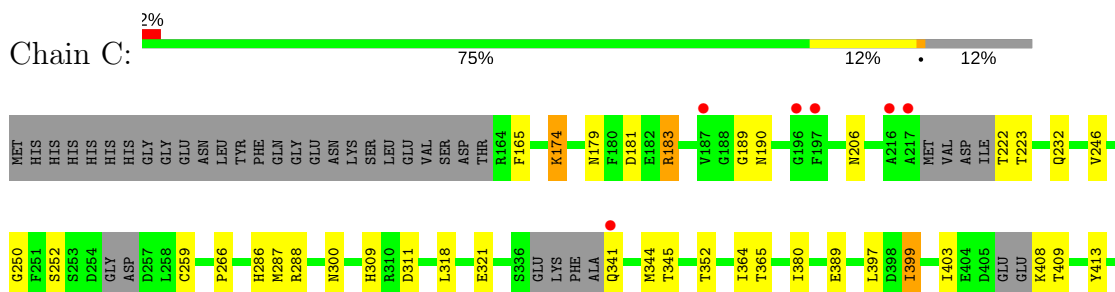
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4

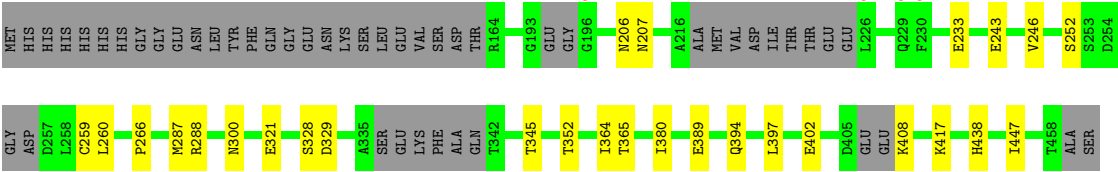


- Molecule 1: Interleukin-1 receptor-associated kinase 4





● Molecule 1: Interleukin-1 receptor-associated kinase 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.06Å 140.80Å 87.99Å 90.00° 124.90° 90.00°	Depositor
Resolution (Å)	19.86 – 2.64 19.86 – 2.64	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.86-2.64) 94.9 (19.86-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.63Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.198 , 0.226 0.202 , 0.232	Depositor DCC
$R_{free}$ test set	1946 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.160 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: TPO, 8BV, SEP

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	0.46	0/2107	0.65	0/2839
1	B	0.48	0/2158	0.65	0/2900
1	C	0.48	0/2215	0.66	0/2985
1	D	0.49	0/2167	0.66	0/2914
All	All	0.48	0/8647	0.66	0/11638

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	2108	0	2025	12	0
1	B	2155	0	2118	15	0
1	C	2214	0	2153	14	0
1	D	2167	0	2147	12	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
2	C	13	0	0	0	0
2	D	13	0	0	0	0
3	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	0	0
3	C	11	0	0	0	0
3	D	16	0	0	0	0
All	All	8759	0	8443	50	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 (50) 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:297:ASN:ND2	1:B:451:GLN:HE21	1.91	0.68
1:A:438:HIS:HD2	1:A:440:LYS:H	1.48	0.62
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.82	0.61
1:B:321:GLU:O	1:D:243:GLU:HB2	2.01	0.61
1:B:387:VAL:HG13	1:B:395:LEU:HD23	1.85	0.59
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.86	0.57
1:C:286:HIS:HD2	1:C:420:ASP:OD2	1.90	0.54
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.89	0.54
1:C:399:ILE:HG12	1:C:413:TYR:CE1	2.44	0.53
1:B:396:LEU:O	1:B:399:ILE:HG12	2.07	0.53
1:B:297:ASN:HD22	1:B:451:GLN:HE21	1.57	0.53
1:A:182:GLU:HA	1:A:191:LYS:HB2	1.91	0.52
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.91	0.51
1:B:387:VAL:CG1	1:B:395:LEU:HD23	2.42	0.50
1:C:246:VAL:HG11	1:C:318:LEU:HD12	1.94	0.50
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.94	0.49
1:A:192:MET:CE	1:A:264:TYR:HE1	2.26	0.49
1:D:345:TPO:HB	1:D:364:ILE:HD11	1.94	0.49
1:D:266:PRO:HG3	1:D:321:GLU:HG3	1.94	0.49
1:C:181:ASP:HB3	1:C:190:ASN:HB2	1.95	0.49
1:C:309:HIS:HD2	1:C:311:ASP:H	1.61	0.48
1:C:266:PRO:HG3	1:C:321:GLU:HG3	1.94	0.48
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.95	0.48
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.96	0.48
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.94	0.48
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.95	0.47
1:B:345:TPO:HB	1:B:364:ILE:HD11	1.96	0.47
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.97	0.47
1:A:276:CYS:HB2	1:D:417:LYS:HD3	1.96	0.47
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:TPO:HB	1:C:364:ILE:HD11	1.97	0.46
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.97	0.46
1:D:288:ARG:HB3	1:D:380:ILE:HG23	1.98	0.46
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.98	0.46
1:D:402:GLU:HB3	1:D:408:LYS:HD2	1.98	0.46
1:B:420:ASP:HA	1:D:207:ASN:O	2.16	0.45
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.97	0.45
1:D:389:GLU:HA	1:D:394:GLN:HE21	1.82	0.44
1:D:246:VAL:HG21	1:D:328:SER:HB3	2.00	0.44
1:B:252:SER:HB3	1:B:259:CYS:HB2	2.00	0.44
1:C:403:ILE:HG23	1:C:409:THR:HA	2.02	0.42
1:A:389:GLU:HA	1:A:394:GLN:HE21	1.85	0.42
1:B:237:MET:HE3	1:B:237:MET:HA	2.02	0.42
1:D:233:GLU:HG2	1:D:260:LEU:HD13	2.02	0.41
1:C:174:LYS:HG3	1:C:179:ASN:HA	2.02	0.41
1:C:183:ARG:HB3	1:C:189:GLY:HA3	2.02	0.41
1:A:233:GLU:HG2	1:A:260:LEU:HD13	2.03	0.41
1:A:174:LYS:HG2	1:A:179:ASN:HA	2.02	0.40
1:A:273:ARG:HD3	1:A:273:ARG:HA	1.67	0.40
1:B:224:GLU:CD	1:B:225:GLU:H	2.25	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	256/323 (79%)	245 (96%)	10 (4%)	1 (0%)	36	52
1	B	260/323 (80%)	253 (97%)	5 (2%)	2 (1%)	21	31
1	C	270/323 (84%)	260 (96%)	9 (3%)	1 (0%)	36	52
1	D	260/323 (80%)	251 (96%)	8 (3%)	1 (0%)	36	52
All	All	1046/1292 (81%)	1009 (96%)	32 (3%)	5 (0%)	31	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	PRO
1	B	329	ASP
1	A	329	ASP
1	C	206	ASN
1	D	329	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	223/278 (80%)	217 (97%)	6 (3%)	48	67
1	B	231/278 (83%)	221 (96%)	10 (4%)	32	49
1	C	238/278 (86%)	223 (94%)	15 (6%)	20	30
1	D	236/278 (85%)	230 (98%)	6 (2%)	50	70
All	All	928/1112 (84%)	891 (96%)	37 (4%)	34	52

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	273	ARG
1	A	287	MET
1	A	341	GLN
1	A	352	THR
1	A	455	GLN
1	B	164	ARG
1	B	194	GLU
1	B	224	GLU
1	B	225	GLU
1	B	243	GLU
1	B	321	GLU
1	B	352	THR
1	B	365	THR
1	B	387	VAL

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Mol	Chain	Res	Type
1	B	439	GLU
1	C	174	LYS
1	C	183	ARG
1	C	222	THR
1	C	223	THR
1	C	232	GLN
1	C	287	MET
1	C	341	GLN
1	C	344	MET
1	C	352	THR
1	C	365	THR
1	C	389	GLU
1	C	397	LEU
1	C	399	ILE
1	C	408	LYS
1	C	458	THR
1	D	206	ASN
1	D	287	MET
1	D	352	THR
1	D	365	THR
1	D	397	LEU
1	D	438	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	438	HIS
1	A	455	GLN
1	B	190	ASN
1	B	229	GLN
1	B	297	ASN
1	B	305	ASN
1	B	394	GLN
1	C	175	ASN
1	C	190	ASN
1	C	232	GLN
1	C	286	HIS
1	C	305	ASN
1	C	309	HIS
1	D	190	ASN
1	D	206	ASN

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Mol	Chain	Res	Type
1	D	207	ASN
1	D	232	GLN
1	D	305	ASN
1	D	394	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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$
1	TPO	A	342	1	9,10,11	1.60	2 (22%)	11,14,16	2.39	3 (27%)
1	TPO	A	345	1	9,10,11	1.58	2 (22%)	11,14,16	1.19	1 (9%)
1	SEP	A	346	1	9,9,10	1.14	1 (11%)	9,12,14	2.13	2 (22%)
1	TPO	B	342	1	9,10,11	1.44	1 (11%)	11,14,16	1.22	1 (9%)
1	TPO	B	345	1	9,10,11	1.30	1 (11%)	11,14,16	1.47	2 (18%)
1	SEP	B	346	1	9,9,10	0.95	0	9,12,14	1.52	3 (33%)
1	TPO	C	342	1	9,10,11	1.64	2 (22%)	11,14,16	2.13	3 (27%)
1	TPO	C	345	1	9,10,11	1.52	3 (33%)	11,14,16	1.08	0
1	SEP	C	346	1	9,9,10	0.90	0	9,12,14	2.17	2 (22%)
1	TPO	D	342	1	9,10,11	1.18	1 (11%)	11,14,16	1.44	2 (18%)
1	TPO	D	345	1	9,10,11	1.35	1 (11%)	11,14,16	1.44	1 (9%)
1	SEP	D	346	1	9,9,10	1.21	1 (11%)	9,12,14	2.23	1 (11%)

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
1	TPO	A	342	1	-	0/8/11/13	0/0/0/0
1	TPO	A	345	1	-	1/8/11/13	0/0/0/0
1	SEP	A	346	1	-	0/5/8/10	0/0/0/0
1	TPO	B	342	1	-	0/8/11/13	0/0/0/0
1	TPO	B	345	1	-	1/8/11/13	0/0/0/0
1	SEP	B	346	1	-	0/5/8/10	0/0/0/0
1	TPO	C	342	1	-	1/8/11/13	0/0/0/0
1	TPO	C	345	1	-	1/8/11/13	0/0/0/0
1	SEP	C	346	1	-	0/5/8/10	0/0/0/0
1	TPO	D	342	1	-	0/8/11/13	0/0/0/0
1	TPO	D	345	1	-	1/8/11/13	0/0/0/0
1	SEP	D	346	1	-	0/5/8/10	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	TPO	P-OG1	-2.05	1.55	1.59
1	D	342	TPO	CA-C	2.06	1.53	1.50
1	A	345	TPO	CB-CA	2.08	1.57	1.53
1	A	342	TPO	CG2-CB	2.14	1.56	1.51
1	C	345	TPO	CA-C	2.23	1.53	1.50
1	C	345	TPO	CB-CA	2.34	1.58	1.53
1	C	342	TPO	CG2-CB	2.35	1.57	1.51
1	B	342	TPO	CA-C	2.39	1.53	1.50
1	A	346	SEP	CA-C	2.60	1.53	1.50
1	D	346	SEP	CA-C	2.63	1.53	1.50
1	D	345	TPO	CA-C	2.76	1.53	1.50
1	B	345	TPO	CA-C	2.90	1.54	1.50
1	C	342	TPO	CA-C	3.12	1.54	1.50
1	A	345	TPO	CA-C	3.28	1.54	1.50
1	A	342	TPO	CA-C	3.28	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	P-OG1-CB	-4.27	110.30	123.21
1	C	342	TPO	P-OG1-CB	-3.82	111.66	123.21
1	C	342	TPO	O-C-CA	-2.38	119.54	125.09
1	B	345	TPO	O-C-CA	-2.33	119.66	125.09
1	D	342	TPO	P-OG1-CB	-2.29	116.29	123.21
1	B	342	TPO	OG1-P-O1P	-2.22	100.83	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	P-OG-CB	-2.18	112.30	118.30
1	A	345	TPO	O-C-CA	-2.05	120.31	125.09
1	B	346	SEP	P-OG-CB	-2.02	112.72	118.30
1	B	346	SEP	O3P-P-OG	2.03	112.12	106.73
1	B	345	TPO	O3P-P-OG1	2.34	116.49	105.99
1	A	342	TPO	O2P-P-OG1	2.35	116.53	105.99
1	A	346	SEP	O3P-P-OG	2.37	113.04	106.73
1	D	345	TPO	O3P-P-OG1	2.47	117.06	105.99
1	D	342	TPO	O3P-P-OG1	2.80	118.55	105.99
1	B	346	SEP	OG-CB-CA	2.91	111.04	108.17
1	C	342	TPO	CG2-CB-CA	4.25	121.77	113.07
1	A	346	SEP	OG-CB-CA	4.92	113.02	108.17
1	C	346	SEP	OG-CB-CA	5.16	113.26	108.17
1	A	342	TPO	CG2-CB-CA	5.41	124.13	113.07
1	D	346	SEP	OG-CB-CA	5.71	113.80	108.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	342	TPO	OG1-CB-CA-N
1	D	345	TPO	OG1-CB-CA-N
1	B	345	TPO	OG1-CB-CA-N
1	C	345	TPO	OG1-CB-CA-N
1	A	345	TPO	OG1-CB-CA-N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0
1	C	345	TPO	1	0
1	D	345	TPO	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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
2	8BV	A	501	-	13,13,13	0.92	1 (7%)	17,17,17	1.18	1 (5%)
2	8BV	B	501	-	13,13,13	1.11	1 (7%)	17,17,17	1.40	3 (17%)
2	8BV	C	501	-	13,13,13	1.02	1 (7%)	17,17,17	1.29	3 (17%)
2	8BV	D	501	-	13,13,13	1.02	1 (7%)	17,17,17	1.45	3 (17%)

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
2	8BV	A	501	-	-	0/8/8/8	0/1/1/1
2	8BV	B	501	-	-	0/8/8/8	0/1/1/1
2	8BV	C	501	-	-	0/8/8/8	0/1/1/1
2	8BV	D	501	-	-	0/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	8BV	C10-N11	2.61	1.38	1.33
2	C	501	8BV	C10-N11	2.63	1.38	1.33
2	B	501	8BV	C10-N11	2.65	1.38	1.33
2	D	501	8BV	C10-N11	2.95	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	8BV	C8-O13-C9	-3.09	113.80	119.58
2	B	501	8BV	C8-O13-C9	-3.03	113.93	119.58
2	B	501	8BV	C8-C7-C10	-2.57	123.20	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	8BV	C8-O13-C9	-2.50	114.92	119.58
2	D	501	8BV	O13-C8-C6	-2.43	118.22	123.88
2	C	501	8BV	C5-C7-C8	2.02	120.84	118.21
2	C	501	8BV	O13-C8-C7	2.09	120.20	116.57
2	B	501	8BV	C5-C7-C8	2.42	121.35	118.21
2	D	501	8BV	O13-C9-C1	2.58	117.17	107.92
2	D	501	8BV	O13-C8-C7	3.01	121.81	116.57

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, 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	268/323 (82%)	-0.20	9 (3%)	45 41	31, 56, 116, 151	0
1	B	272/323 (84%)	-0.30	2 (0%)	87 86	30, 53, 97, 134	0
1	C	280/323 (86%)	-0.23	6 (2%)	63 59	28, 54, 105, 141	0
1	D	271/323 (83%)	-0.30	4 (1%)	73 70	30, 52, 94, 131	0
All	All	1091/1292 (84%)	-0.26	21 (1%)	66 64	28, 54, 104, 151	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	LEU	5.6
1	A	216	ALA	4.8
1	B	226	LEU	4.3
1	A	196	GLY	4.1
1	C	187	VAL	4.1
1	A	230	PHE	3.9
1	C	216	ALA	3.5
1	A	336	SER	3.4
1	C	196	GLY	3.3
1	D	230	PHE	2.9
1	A	217	ALA	2.8
1	C	341	GLN	2.8
1	C	217	ALA	2.7
1	D	196	GLY	2.7
1	C	197	PHE	2.6
1	D	229	GLN	2.6
1	A	215	LEU	2.6
1	B	195	GLY	2.2
1	A	341	GLN	2.1
1	A	204	TYR	2.1
1	A	335	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	346	10/11	0.83	0.11	100,108,121,122	0
1	TPO	D	342	11/12	0.85	0.17	92,94,104,104	0
1	SEP	B	346	10/11	0.87	0.12	80,88,98,99	0
1	TPO	C	342	11/12	0.88	0.20	100,100,104,105	0
1	TPO	A	342	11/12	0.88	0.19	99,100,104,106	0
1	SEP	C	346	10/11	0.89	0.12	85,94,104,105	0
1	SEP	D	346	10/11	0.90	0.15	85,93,103,104	0
1	TPO	B	342	11/12	0.93	0.16	87,90,93,94	0
1	TPO	A	345	11/12	0.95	0.09	89,95,99,99	0
1	TPO	B	345	11/12	0.95	0.12	68,74,79,79	0
1	TPO	C	345	11/12	0.97	0.12	72,78,84,85	0
1	TPO	D	345	11/12	0.97	0.11	73,79,83,85	0

## 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	8BV	D	501	13/13	0.94	0.17	46,46,49,50	0
2	8BV	B	501	13/13	0.97	0.14	39,41,44,46	0
2	8BV	C	501	13/13	0.97	0.17	54,56,59,60	0
2	8BV	A	501	13/13	0.97	0.14	47,49,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.