



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2017 – 10:25 PM EDT

PDB ID : 5UIS  
Title : Crystal structure of IRAK4 in complex with compound 12  
Authors : Han, S.; Chang, J.S.  
Deposited on : unknown  
Resolution : 2.50 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

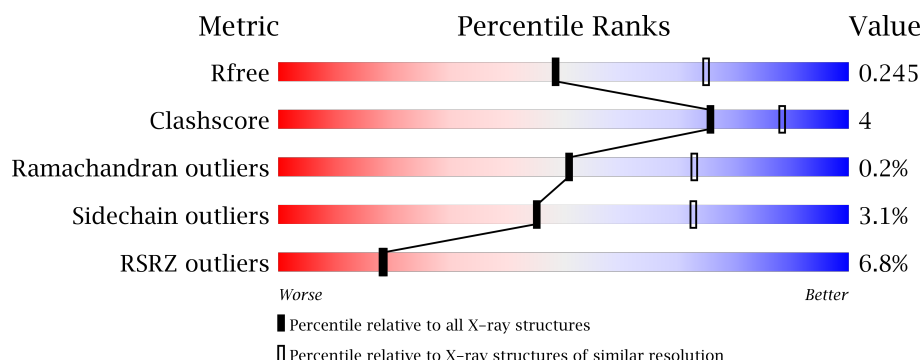
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	323	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>10%</div> <div>16%</div> </div> </div>
1	B	323	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>15%</div> </div> </div>
1	C	323	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>16%</div> </div> </div>
1	D	323	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>9%</div> <div>22%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8743 atoms, of which 92 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	270	Total	C	N	O	P	S	0	0	0
			2124	1337	359	413	1	14			
1	B	275	Total	C	N	O	P	S	0	0	0
			2159	1360	365	419	1	14			
1	C	271	Total	C	N	O	P	S	0	1	0
			2146	1353	364	413	1	15			
1	D	251	Total	C	N	O	P	S	0	0	0
			1989	1259	335	380	1	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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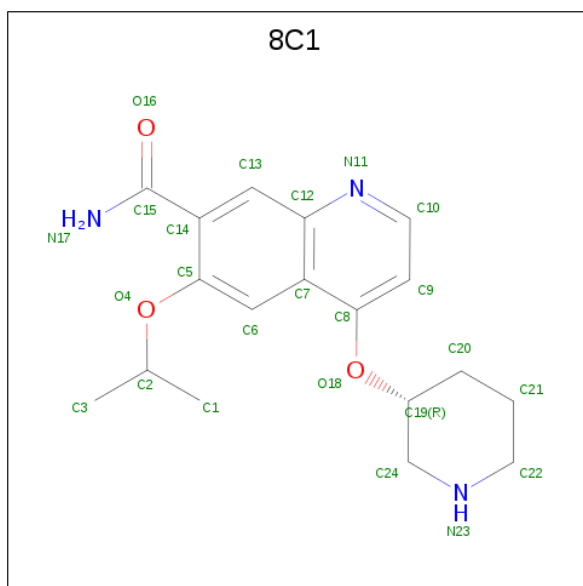
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	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 4-[[[(3R)-piperidin-3-yl]oxy}-6-[(propan-2-yl)oxy]quinoline-7-carboxamide (three-letter code: 8C1) (formula: C<sub>18</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			47	18	23	3	3		
2	B	1	Total	C	H	N	O	0	0
			47	18	23	3	3		
2	C	1	Total	C	H	N	O	0	0
			47	18	23	3	3		
2	D	1	Total	C	H	N	O	0	0
			47	18	23	3	3		

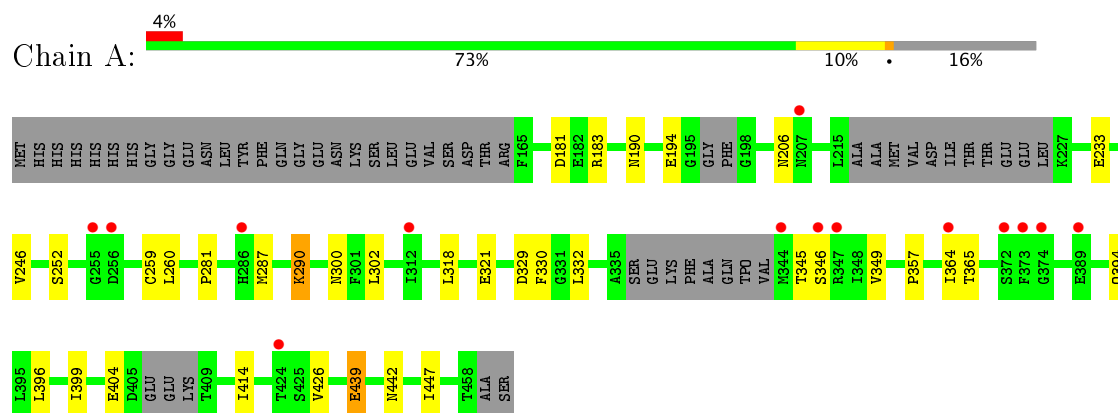
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	36	Total	O	0	0
			36	36		
3	C	38	Total	O	0	0
			38	38		
3	D	29	Total	O	0	0
			29	29		

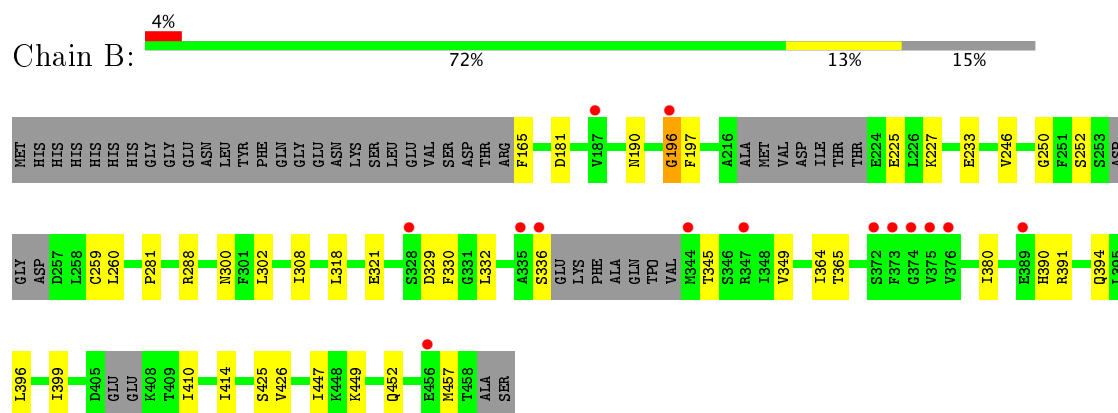
### 3 Residue-property plots [i](#)

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.

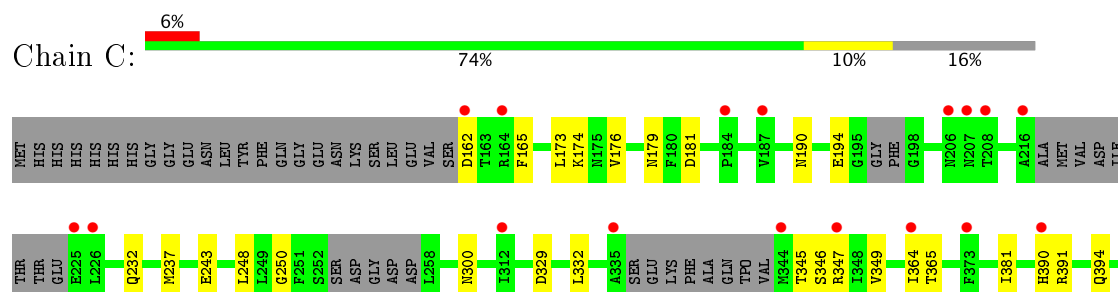
- Molecule 1: Interleukin-1 receptor-associated kinase 4

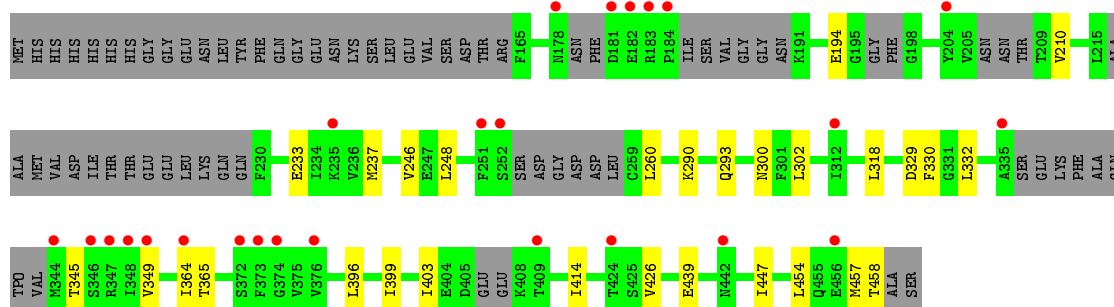


- Molecule 1: Interleukin-1 receptor-associated kinase 4



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.14Å 141.13Å 87.44Å 90.00° 124.72° 90.00°	Depositor
Resolution (Å)	25.36 – 2.50 25.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (25.36-2.50) 99.5 (25.36-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.234 , 0.250 0.227 , 0.245	Depositor DCC
$R_{free}$ test set	2517 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.098 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.36% 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, 8C1

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	0.45	0/2146	0.65	0/2888
1	B	0.45	0/2181	0.64	0/2934
1	C	0.46	0/2167	0.65	0/2914
1	D	0.45	0/2006	0.65	0/2691
All	All	0.45	0/8500	0.65	0/11427

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	2124	0	2095	15	0
1	B	2159	0	2135	22	0
1	C	2146	0	2128	14	0
1	D	1989	0	1979	13	0
2	A	24	23	0	0	0
2	B	24	23	0	0	0
2	C	24	23	0	0	0
2	D	24	23	0	0	0
3	A	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	0	0	0	0
3	C	38	0	0	0	0
3	D	29	0	0	0	0
All	All	8651	92	8337	60	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 4.

All (60) 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:A:321:GLU:HG3	1:B:281:PRO:HD3	1.64	0.79
1:B:196:GLY:H	1:B:197:PHE:HA	1.55	0.70
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.78	0.65
1:B:196:GLY:N	1:B:197:PHE:HA	2.13	0.64
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.80	0.64
1:C:237:MET:HG2	1:C:248:LEU:HB2	1.81	0.62
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.84	0.60
1:D:399:ILE:O	1:D:403:ILE:HG12	2.01	0.60
1:B:390:HIS:O	1:C:391:ARG:HA	2.02	0.59
1:B:391:ARG:HA	1:C:390:HIS:O	2.03	0.59
1:C:237:MET:HG2	1:C:248:LEU:CB	2.35	0.56
1:D:293:GLN:HE22	1:D:458:THR:HB	1.71	0.56
1:A:357:PRO:HG3	1:A:439:GLU:HG3	1.90	0.53
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.90	0.53
1:D:237:MET:HG2	1:D:248:LEU:HB2	1.92	0.52
1:C:381:ILE:HG21	1:C:410:ILE:HD11	1.92	0.51
1:C:181:ASP:HB3	1:C:190:ASN:HD22	1.75	0.51
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.92	0.51
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.93	0.50
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.93	0.49
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.94	0.49
1:A:181:ASP:HB3	1:A:190:ASN:HD22	1.77	0.49
1:B:332:LEU:HD22	1:B:349:VAL:HG21	1.97	0.47
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.96	0.47
1:A:281:PRO:HD3	1:B:321:GLU:HG3	1.97	0.47
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.95	0.47
1:D:237:MET:HG2	1:D:248:LEU:CB	2.45	0.46
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.80	0.46
1:D:332:LEU:HD22	1:D:349:VAL:HG21	1.98	0.46
1:A:332:LEU:HD22	1:A:349:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.81	0.45
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.98	0.45
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.99	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.44
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.99	0.44
1:C:174:LYS:HG2	1:C:179:ASN:HA	2.00	0.44
1:B:396:LEU:O	1:B:399:ILE:HG12	2.18	0.44
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.00	0.44
1:B:181:ASP:HB3	1:B:190:ASN:HD22	1.82	0.43
1:C:414:ILE:HG12	1:C:426:VAL:HG11	1.99	0.43
1:C:300:ASN:HA	1:C:447:ILE:HG21	2.01	0.43
1:D:233:GLU:HG2	1:D:260:LEU:HD13	2.01	0.43
1:C:425:SER:O	1:C:457:MET:HE3	2.18	0.43
1:D:396:LEU:O	1:D:399:ILE:HG12	2.19	0.43
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.00	0.43
1:A:396:LEU:O	1:A:399:ILE:HG12	2.19	0.43
1:A:287:MET:CE	1:A:290:LYS:HD2	2.48	0.43
1:B:345:TPO:HB	1:B:364:ILE:HD11	2.01	0.42
1:B:410:ILE:O	1:B:414:ILE:HG13	2.20	0.42
1:C:345:TPO:HB	1:C:364:ILE:HD11	2.02	0.42
1:D:345:TPO:HB	1:D:364:ILE:HD11	2.02	0.42
1:A:181:ASP:OD1	1:A:183:ARG:HD3	2.19	0.42
1:D:454:LEU:O	1:D:457:MET:HG2	2.20	0.42
1:B:288:ARG:HB3	1:B:380:ILE:HG23	2.01	0.42
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.85	0.41
1:C:332:LEU:HD22	1:C:349:VAL:HG21	2.02	0.41
1:B:425:SER:O	1:B:457:MET:HE3	2.20	0.41
1:B:449:LYS:HA	1:B:452:GLN:HG2	2.03	0.41
1:A:345:TPO:HB	1:A:364:ILE:HD11	2.02	0.41
1:B:308:ILE:HD11	1:B:336:SER:HB3	2.02	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	259/323 (80%)	249 (96%)	9 (4%)	1 (0%)	38	59
1	B	264/323 (82%)	256 (97%)	7 (3%)	1 (0%)	38	59
1	C	259/323 (80%)	252 (97%)	7 (3%)	0	100	100
1	D	232/323 (72%)	227 (98%)	5 (2%)	0	100	100
All	All	1014/1292 (78%)	984 (97%)	28 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	GLU
1	B	196	GLY

### 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	234/279 (84%)	225 (96%)	9 (4%)	38	64
1	B	237/279 (85%)	232 (98%)	5 (2%)	59	83
1	C	236/279 (85%)	227 (96%)	9 (4%)	38	64
1	D	219/279 (78%)	213 (97%)	6 (3%)	50	77
All	All	926/1116 (83%)	897 (97%)	29 (3%)	45	73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	206	ASN
1	A	290	LYS
1	A	329	ASP
1	A	346	SER
1	A	365	THR

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Mol	Chain	Res	Type
1	A	394	GLN
1	A	439	GLU
1	A	442	ASN
1	B	225	GLU
1	B	227	LYS
1	B	329	ASP
1	B	365	THR
1	B	394	GLN
1	C	162	ASP
1	C	194	GLU
1	C	232	GLN
1	C	243	GLU
1	C	329	ASP
1	C	346	SER
1	C	347	ARG
1	C	365	THR
1	C	394	GLN
1	D	194	GLU
1	D	210	VAL
1	D	290	LYS
1	D	329	ASP
1	D	365	THR
1	D	439	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	206	ASN
1	A	207	ASN
1	B	179	ASN
1	B	190	ASN
1	B	394	GLN
1	C	190	ASN
1	D	293	GLN
1	D	451	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	345	1	9,10,11	1.68	2 (22%)	10,14,16	1.47	3 (30%)
1	TPO	B	345	1	9,10,11	1.70	2 (22%)	10,14,16	1.62	3 (30%)
1	TPO	C	345	1	9,10,11	1.65	2 (22%)	10,14,16	1.44	3 (30%)
1	TPO	D	345	1	9,10,11	1.58	2 (22%)	10,14,16	1.53	3 (30%)

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	345	1	-	1/8/11/13	0/0/0/0
1	TPO	B	345	1	-	1/8/11/13	0/0/0/0
1	TPO	C	345	1	-	1/8/11/13	0/0/0/0
1	TPO	D	345	1	-	1/8/11/13	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	P-OG1	-2.94	1.54	1.59
1	A	345	TPO	CG2-CB	2.00	1.56	1.51
1	D	345	TPO	CB-CA	2.12	1.57	1.53
1	C	345	TPO	CB-CA	2.33	1.58	1.53
1	B	345	TPO	CA-C	3.18	1.54	1.50
1	D	345	TPO	CA-C	3.21	1.54	1.50
1	C	345	TPO	CA-C	3.39	1.54	1.50
1	A	345	TPO	CA-C	3.92	1.55	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	TPO	O-C-CA	-2.04	120.38	125.15
1	B	345	TPO	O-C-CA	-2.04	120.39	125.15
1	D	345	TPO	O-C-CA	-2.03	120.41	125.15
1	A	345	TPO	O-C-CA	-2.01	120.47	125.15
1	C	345	TPO	OG1-P-O1P	2.07	117.38	109.26
1	B	345	TPO	CG2-CB-CA	2.16	117.22	113.22
1	A	345	TPO	O2P-P-OG1	2.41	116.94	106.00
1	D	345	TPO	O2P-P-OG1	2.48	117.26	106.00
1	C	345	TPO	C-CA-N	2.97	115.86	109.86
1	D	345	TPO	C-CA-N	3.00	115.92	109.86
1	A	345	TPO	C-CA-N	3.05	116.01	109.86
1	B	345	TPO	C-CA-N	3.47	116.85	109.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	8C1	A	800	-	25,26,26	3.57	7 (28%)	29,36,36	1.82	5 (17%)
2	8C1	B	801	-	25,26,26	3.50	7 (28%)	29,36,36	1.84	6 (20%)
2	8C1	C	501	-	25,26,26	3.52	8 (32%)	29,36,36	1.87	6 (20%)
2	8C1	D	501	-	25,26,26	3.53	8 (32%)	29,36,36	1.83	5 (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	8C1	A	800	-	-	1/12/32/32	0/3/3/3
2	8C1	B	801	-	-	1/12/32/32	0/3/3/3
2	8C1	C	501	-	-	1/12/32/32	0/3/3/3
2	8C1	D	501	-	-	1/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	8C1	C13-C14	-8.30	1.38	1.53
2	A	800	8C1	C13-C14	-8.29	1.38	1.53
2	D	501	8C1	C13-C14	-8.29	1.38	1.53
2	C	501	8C1	C13-C14	-8.22	1.38	1.53
2	A	800	8C1	C14-C5	-8.18	1.41	1.53
2	C	501	8C1	C13-C12	-8.12	1.41	1.51
2	D	501	8C1	C13-C12	-8.12	1.41	1.51
2	B	801	8C1	C13-C12	-8.08	1.41	1.51
2	C	501	8C1	C14-C5	-8.04	1.41	1.53
2	B	801	8C1	C14-C5	-8.02	1.41	1.53
2	A	800	8C1	C13-C12	-8.00	1.41	1.51
2	D	501	8C1	C14-C5	-7.97	1.41	1.53
2	A	800	8C1	C6-C5	-7.66	1.37	1.51
2	C	501	8C1	C6-C5	-7.54	1.37	1.51
2	D	501	8C1	C6-C5	-7.53	1.37	1.51
2	B	801	8C1	C6-C5	-7.45	1.37	1.51
2	A	800	8C1	C6-C7	-5.22	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	8C1	C6-C7	-4.91	1.43	1.51
2	C	501	8C1	C6-C7	-4.89	1.43	1.51
2	B	801	8C1	C6-C7	-4.80	1.43	1.51
2	A	800	8C1	O4-C5	-4.08	1.38	1.44
2	D	501	8C1	O4-C5	-3.95	1.38	1.44
2	C	501	8C1	O4-C5	-3.83	1.38	1.44
2	B	801	8C1	O4-C5	-3.64	1.38	1.44
2	C	501	8C1	C8-C7	2.00	1.42	1.40
2	D	501	8C1	C8-C7	2.01	1.42	1.40
2	B	801	8C1	C12-N11	2.93	1.37	1.34
2	C	501	8C1	C12-N11	2.97	1.37	1.34
2	A	800	8C1	C12-N11	2.98	1.37	1.34
2	D	501	8C1	C12-N11	2.99	1.37	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	8C1	C6-C7-C12	-2.77	118.91	121.14
2	C	501	8C1	C6-C7-C12	-2.74	118.94	121.14
2	D	501	8C1	C6-C7-C12	-2.71	118.96	121.14
2	A	800	8C1	C6-C7-C12	-2.61	119.04	121.14
2	C	501	8C1	O18-C8-C7	-2.14	113.01	114.07
2	B	801	8C1	C6-C7-C8	2.03	124.23	120.13
2	A	800	8C1	C7-C6-C5	3.31	120.01	111.50
2	C	501	8C1	C7-C6-C5	3.36	120.12	111.50
2	D	501	8C1	C7-C6-C5	3.36	120.13	111.50
2	B	801	8C1	C7-C6-C5	3.39	120.21	111.50
2	D	501	8C1	O4-C5-C6	3.72	123.26	109.15
2	C	501	8C1	O4-C5-C6	3.74	123.32	109.15
2	A	800	8C1	O4-C5-C6	3.75	123.35	109.15
2	B	801	8C1	O4-C5-C6	3.84	123.69	109.15
2	A	800	8C1	C5-C14-C15	4.42	125.49	112.59
2	C	501	8C1	C5-C14-C15	4.49	125.69	112.59
2	B	801	8C1	C5-C14-C15	4.53	125.80	112.59
2	D	501	8C1	C5-C14-C15	4.60	126.02	112.59
2	A	800	8C1	C12-C13-C14	5.18	120.98	113.97
2	C	501	8C1	C12-C13-C14	5.27	121.11	113.97
2	D	501	8C1	C12-C13-C14	5.34	121.19	113.97
2	B	801	8C1	C12-C13-C14	5.38	121.25	113.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	8C1	C2-O4-C5-C6
2	C	501	8C1	C2-O4-C5-C6
2	D	501	8C1	C2-O4-C5-C6
2	A	800	8C1	C2-O4-C5-C6

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	269/323 (83%)	0.13	14 (5%)	28 29	29, 47, 75, 90	18 (6%)
1	B	274/323 (84%)	0.18	14 (5%)	29 30	30, 50, 75, 97	18 (6%)
1	C	270/323 (83%)	0.26	19 (7%)	17 17	31, 50, 83, 111	17 (6%)
1	D	250/323 (77%)	0.28	25 (10%)	8 7	30, 52, 84, 98	18 (7%)
All	All	1063/1292 (82%)	0.21	72 (6%)	18 18	29, 49, 80, 111	71 (6%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207	ASN	6.2
1	C	206	ASN	4.6
1	D	409	THR	4.5
1	D	184	PRO	4.3
1	C	226	LEU	4.3
1	D	183	ARG	4.3
1	D	349	VAL	4.0
1	C	162	ASP	3.9
1	D	204	TYR	3.9
1	D	344	MET	3.7
1	D	347	ARG	3.5
1	A	344	MET	3.4
1	A	255	GLY	3.4
1	A	347	ARG	3.4
1	B	389	GLU	3.3
1	B	456	GLU	3.3
1	A	346	SER	3.3
1	C	216	ALA	3.2
1	A	372	SER	3.1
1	D	346	SER	3.1
1	D	182	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	344	MET	3.0
1	A	256	ASP	2.9
1	D	364	ILE	2.9
1	D	376	VAL	2.9
1	D	335	ALA	2.9
1	B	347	ARG	2.9
1	A	389	GLU	2.9
1	D	373	PHE	2.9
1	D	251	PHE	2.8
1	C	390	HIS	2.8
1	B	196	GLY	2.8
1	D	372	SER	2.8
1	A	364	ILE	2.8
1	D	235	LYS	2.7
1	C	409	THR	2.7
1	C	187	VAL	2.7
1	B	374	GLY	2.6
1	D	181	ASP	2.6
1	C	344	MET	2.6
1	A	424	THR	2.5
1	D	456	GLU	2.5
1	A	207	ASN	2.5
1	D	348	ILE	2.5
1	D	178	ASN	2.5
1	B	373	PHE	2.4
1	B	372	SER	2.4
1	D	252	SER	2.4
1	D	312	ILE	2.4
1	C	373	PHE	2.4
1	A	374	GLY	2.3
1	B	375	VAL	2.3
1	B	376	VAL	2.3
1	A	373	PHE	2.3
1	D	424	THR	2.3
1	C	164	ARG	2.3
1	B	335	ALA	2.3
1	C	412	ASP	2.2
1	C	364	ILE	2.2
1	D	442	ASN	2.2
1	C	312	ILE	2.2
1	D	374	GLY	2.2
1	C	184	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	286	HIS	2.2
1	C	208	THR	2.1
1	B	336	SER	2.1
1	B	328	SER	2.1
1	B	187	VAL	2.1
1	C	225	GLU	2.0
1	A	312	ILE	2.0
1	C	347	ARG	2.0
1	C	335	ALA	2.0

## 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. 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
1	TPO	B	345	11/12	0.95	0.31	-	71,75,79,79	0
1	TPO	A	345	11/12	0.92	0.32	-	74,77,80,81	0
1	TPO	D	345	11/12	0.95	0.34	-	82,88,92,94	0
1	TPO	C	345	11/12	0.92	0.20	-	71,76,80,80	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. 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
2	8C1	D	501	24/24	0.94	0.12	-0.66	42,45,52,53	0
2	8C1	B	801	24/24	0.96	0.12	-0.72	39,43,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	8C1	A	800	24/24	0.94	0.12	-0.80	31,36,41,43	0
2	8C1	C	501	24/24	0.93	0.11	-1.05	36,40,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.