



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 08:44 AM EST

PDB ID : 2O8Y  
Title : Apo IRAK4 Kinase Domain  
Authors : Boriack-Sjodin, P.A.; Mol, C.  
Deposited on : 2006-12-12  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

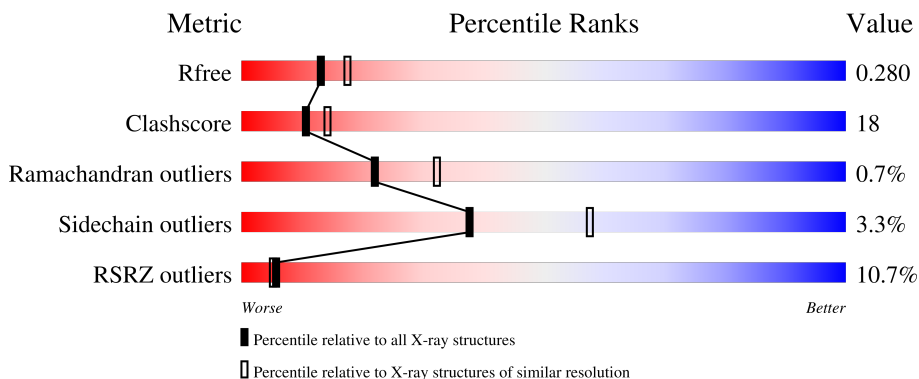
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	298	
1	B	298	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4457 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
			Total	C	N	O	P	S	Se			
1	A	280	2207	1387	371	433	2	5	9	0	0	0
1	B	277	2191	1376	369	430	2	5	9	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	MSE	MET	modified residue	UNP Q9NWZ3
A	237	MSE	MET	modified residue	UNP Q9NWZ3
A	265	MSE	MET	modified residue	UNP Q9NWZ3
A	287	MSE	MET	modified residue	UNP Q9NWZ3
A	342	TPO	THR	modified residue	UNP Q9NWZ3
A	344	MSE	MET	modified residue	UNP Q9NWZ3
A	345	TPO	THR	modified residue	UNP Q9NWZ3
A	355	MSE	MET	modified residue	UNP Q9NWZ3
A	418	MSE	MET	modified residue	UNP Q9NWZ3
A	429	MSE	MET	modified residue	UNP Q9NWZ3
A	457	MSE	MET	modified residue	UNP Q9NWZ3
B	192	MSE	MET	modified residue	UNP Q9NWZ3
B	237	MSE	MET	modified residue	UNP Q9NWZ3
B	265	MSE	MET	modified residue	UNP Q9NWZ3
B	287	MSE	MET	modified residue	UNP Q9NWZ3
B	342	TPO	THR	modified residue	UNP Q9NWZ3
B	344	MSE	MET	modified residue	UNP Q9NWZ3
B	345	TPO	THR	modified residue	UNP Q9NWZ3
B	355	MSE	MET	modified residue	UNP Q9NWZ3
B	418	MSE	MET	modified residue	UNP Q9NWZ3
B	429	MSE	MET	modified residue	UNP Q9NWZ3
B	457	MSE	MET	modified residue	UNP Q9NWZ3

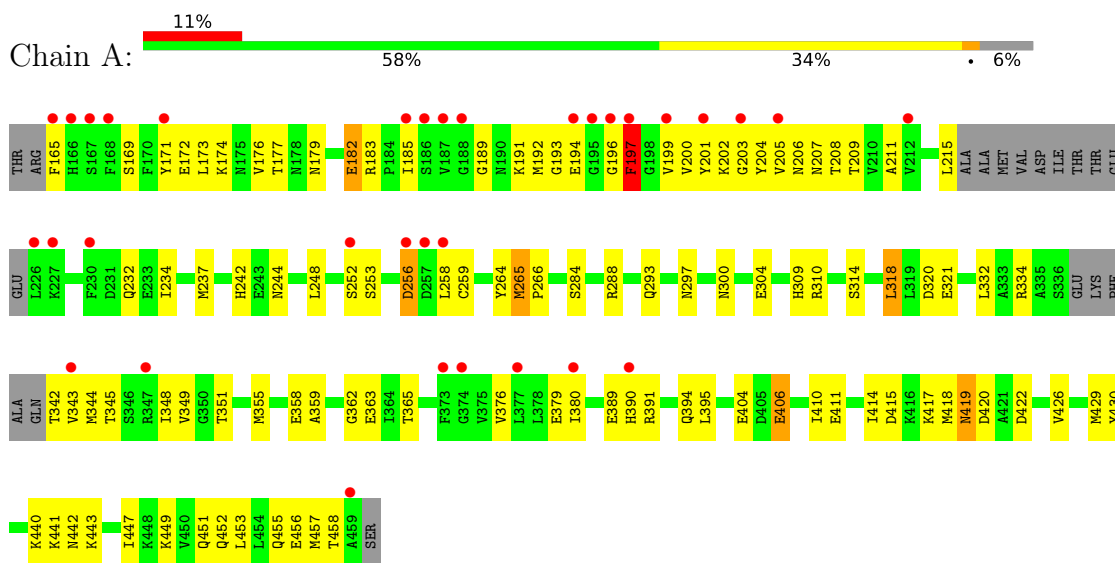
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total 32	O 32	0	0
2	B	27	Total 27	O 27	0	0

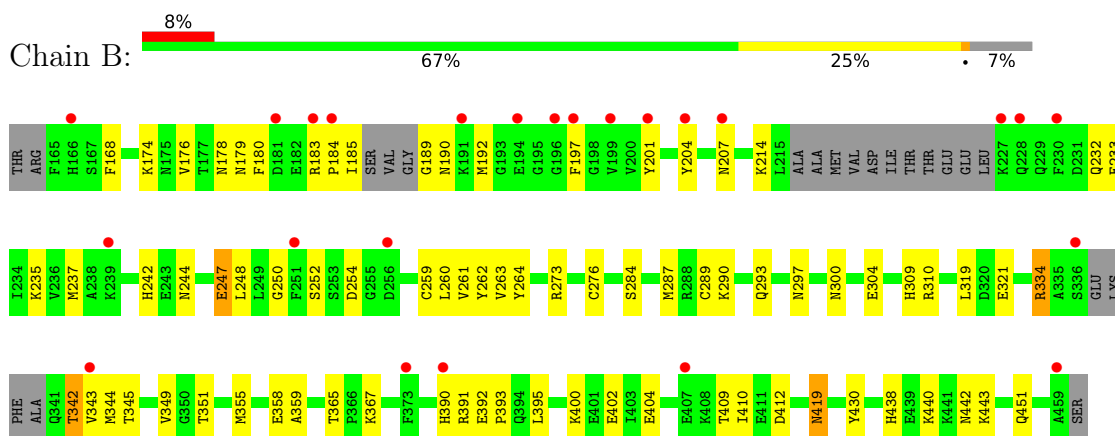
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.15Å 118.64Å 140.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.40 26.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (35.00-2.40) 98.8 (26.91-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.39Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.289 0.237 , 0.280	Depositor DCC
$R_{free}$ test set	1448 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	0.36	0/2212	0.58	0/2964
1	B	0.33	0/2194	0.55	0/2936
All	All	0.35	0/4406	0.56	0/5900

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

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	2207	0	2178	105	0
1	B	2191	0	2155	60	0
2	A	32	0	0	1	0
2	B	27	0	0	0	0
All	All	4457	0	4333	161	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 18.

All (161) 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:192:MSE:HE3	1:A:200:VAL:HG12	1.28	1.11
1:B:284:SER:H	1:B:287:MSE:HE3	1.03	1.06
1:B:284:SER:N	1:B:287:MSE:HE3	1.88	0.88
1:A:194:GLU:HG3	1:A:199:VAL:HG22	1.57	0.85
1:A:215:LEU:HD12	1:A:258:LEU:HB2	1.60	0.83
1:A:265:MSE:HE2	1:A:320:ASP:HB3	1.62	0.81
1:A:265:MSE:HE2	1:A:320:ASP:CB	2.12	0.79
1:B:440:LYS:HB2	1:B:443:LYS:HB2	1.64	0.78
1:B:176:VAL:HG22	1:B:204:TYR:H	1.50	0.75
1:A:265:MSE:HG2	1:A:318:LEU:HB3	1.67	0.75
1:A:266:PRO:HG2	1:A:321:GLU:HG3	1.69	0.75
1:B:232:GLN:NE2	1:B:235:LYS:HZ1	1.86	0.74
1:A:176:VAL:HG22	1:A:204:TYR:H	1.51	0.74
1:A:176:VAL:HG21	1:A:205:VAL:HG23	1.69	0.74
1:A:169:SER:HB3	1:A:172:GLU:HB2	1.71	0.73
1:A:390:HIS:HB3	1:B:391:ARG:HA	1.71	0.73
1:A:237:MSE:HA	1:A:237:MSE:HE2	1.71	0.72
1:A:419:ASN:HD22	1:A:419:ASN:C	1.94	0.71
1:B:310:ARG:HH11	1:B:334:ARG:HG2	1.53	0.70
1:B:232:GLN:HE22	1:B:235:LYS:HZ1	1.40	0.69
1:A:321:GLU:H	1:A:321:GLU:CD	1.98	0.67
1:B:180:PHE:CE1	1:B:214:LYS:HD3	2.30	0.66
1:A:192:MSE:HE2	1:A:201:TYR:C	2.17	0.65
1:A:242:HIS:HE1	1:A:244:ASN:HD22	1.45	0.65
1:B:400:LYS:O	1:B:404:GLU:HG3	1.96	0.65
1:A:192:MSE:HE3	1:A:200:VAL:CG1	2.17	0.65
1:A:215:LEU:HG	1:A:258:LEU:O	1.96	0.65
1:A:391:ARG:HA	1:B:390:HIS:HB3	1.79	0.65
1:B:237:MSE:HA	1:B:237:MSE:HE2	1.79	0.65
1:A:449:LYS:HE2	1:A:453:LEU:HD21	1.79	0.64
1:A:215:LEU:CD1	1:A:258:LEU:HB2	2.27	0.63
1:B:297:ASN:ND2	1:B:451:GLN:HE21	1.96	0.63
1:A:176:VAL:CG2	1:A:204:TYR:H	2.11	0.62
1:B:297:ASN:HD22	1:B:451:GLN:HE21	1.47	0.62
1:A:343:VAL:HG12	1:A:344:MSE:H	1.66	0.61
1:A:191:LYS:NZ	1:A:194:GLU:HB2	2.16	0.61
1:A:192:MSE:HE1	1:A:211:ALA:HA	1.83	0.60
1:A:232:GLN:HE21	1:A:232:GLN:HA	1.67	0.60
1:A:165:PHE:CE1	1:A:248:LEU:HD23	2.37	0.59
1:A:314:SER:HB2	1:A:379:GLU:OE2	2.02	0.59
1:A:415:ASP:HB3	1:A:418:MSE:HE2	1.84	0.59
1:B:367:LYS:HE2	1:B:442:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HG22	1:A:204:TYR:N	2.17	0.58
1:A:351:THR:O	1:A:355:MSE:HG3	2.02	0.58
1:B:409:THR:HG22	1:B:412:ASP:OD2	2.03	0.58
1:A:343:VAL:HG12	1:A:344:MSE:N	2.19	0.58
1:A:440:LYS:HB2	1:A:443:LYS:HB2	1.84	0.58
1:A:173:LEU:HA	1:A:176:VAL:HG12	1.86	0.58
1:B:289:CYS:O	1:B:293:GLN:HG3	2.03	0.58
1:B:204:TYR:CE1	1:B:207:ASN:HA	2.38	0.57
1:A:185:ILE:HD13	1:A:189:GLY:O	2.04	0.57
1:A:173:LEU:C	1:A:176:VAL:HG12	2.25	0.57
1:A:363:GLU:OE2	1:A:441:LYS:HE3	2.05	0.57
1:B:183:ARG:HB3	1:B:184:PRO:HD2	1.85	0.56
1:B:321:GLU:H	1:B:321:GLU:CD	2.08	0.56
1:B:176:VAL:CG2	1:B:204:TYR:H	2.18	0.56
1:A:192:MSE:HE2	1:A:202:LYS:N	2.21	0.56
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.86	0.56
1:B:176:VAL:HG21	1:B:204:TYR:C	2.26	0.55
1:A:300:ASN:O	1:A:304:GLU:HG3	2.06	0.55
1:A:173:LEU:O	1:A:176:VAL:HG12	2.06	0.55
1:A:265:MSE:HA	1:A:265:MSE:HE3	1.89	0.55
1:B:185:ILE:HD13	1:B:189:GLY:O	2.06	0.55
1:B:176:VAL:HG21	1:B:204:TYR:O	2.07	0.55
1:A:297:ASN:HD22	1:A:451:GLN:HE21	1.55	0.55
1:A:192:MSE:SE	1:A:264:TYR:HE2	2.40	0.54
1:A:173:LEU:HA	1:A:176:VAL:CG1	2.37	0.54
1:B:310:ARG:NH1	1:B:334:ARG:HG2	2.23	0.54
1:A:419:ASN:C	1:A:419:ASN:ND2	2.60	0.54
1:A:234:ILE:HG12	1:A:248:LEU:HD21	1.91	0.53
1:B:300:ASN:O	1:B:304:GLU:HG3	2.08	0.53
1:A:203:GLY:O	1:A:209:THR:HA	2.09	0.53
1:A:390:HIS:O	1:B:390:HIS:O	2.27	0.53
1:B:342:TPO:HG23	1:B:343:VAL:N	2.24	0.53
1:B:235:LYS:HB3	1:B:235:LYS:NZ	2.23	0.53
1:A:419:ASN:HD22	1:A:420:ASP:N	2.07	0.52
1:B:343:VAL:HG22	1:B:344:MSE:N	2.24	0.52
1:B:232:GLN:NE2	1:B:235:LYS:NZ	2.56	0.52
1:A:422:ASP:O	1:A:426:VAL:HG23	2.10	0.51
1:B:410:ILE:HD13	1:B:430:TYR:CD2	2.45	0.51
1:A:176:VAL:HG23	1:A:204:TYR:O	2.10	0.51
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.91	0.51
1:A:176:VAL:HG21	1:A:205:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD13	1:A:430:TYR:CD2	2.44	0.51
1:A:300:ASN:HD22	1:A:447:ILE:HG23	1.75	0.51
1:B:179:ASN:O	1:B:180:PHE:HB2	2.11	0.51
1:B:351:THR:O	1:B:355:MSE:HG3	2.11	0.51
1:B:176:VAL:HG22	1:B:176:VAL:O	2.11	0.50
1:A:264:TYR:O	1:A:266:PRO:HD3	2.11	0.50
1:B:180:PHE:CD1	1:B:214:LYS:HD3	2.47	0.50
1:A:232:GLN:HA	1:A:232:GLN:NE2	2.26	0.50
1:A:264:TYR:O	1:A:265:MSE:HE3	2.12	0.50
1:A:297:ASN:ND2	1:A:451:GLN:HE21	2.10	0.49
1:B:391:ARG:HG2	1:B:392:GLU:N	2.28	0.49
1:A:176:VAL:CG2	1:A:204:TYR:N	2.74	0.49
1:A:389:GLU:HA	1:A:394:GLN:OE1	2.13	0.48
1:A:183:ARG:CB	1:A:183:ARG:HH11	2.27	0.48
1:A:191:LYS:HE3	1:A:193:GLY:C	2.33	0.48
1:B:438:HIS:CG	1:B:443:LYS:HB3	2.49	0.48
1:B:192:MSE:SE	1:B:264:TYR:HE2	2.47	0.48
1:B:235:LYS:HB3	1:B:235:LYS:HZ3	1.77	0.48
1:B:242:HIS:HE1	1:B:244:ASN:HD22	1.62	0.48
1:B:358:GLU:HG2	1:B:359:ALA:N	2.28	0.48
1:A:358:GLU:HG2	1:A:359:ALA:N	2.28	0.47
1:B:310:ARG:NH2	1:B:349:VAL:HG22	2.30	0.47
1:A:173:LEU:CA	1:A:176:VAL:HG12	2.44	0.47
1:A:411:GLU:HA	1:A:414:ILE:HD12	1.95	0.47
1:A:171:TYR:O	1:A:174:LYS:N	2.47	0.47
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.79	0.47
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.97	0.47
1:A:191:LYS:HZ1	1:A:194:GLU:HB2	1.80	0.46
1:B:178:ASN:HB2	1:B:190:ASN:ND2	2.30	0.46
1:A:192:MSE:SE	1:A:264:TYR:CE2	3.19	0.46
1:A:449:LYS:HE2	1:A:453:LEU:CD2	2.45	0.46
1:B:247:GLU:OE2	1:B:263:VAL:HG21	2.16	0.46
1:B:419:ASN:HD22	1:B:419:ASN:N	2.13	0.45
1:A:429:MSE:HB2	1:A:457:MSE:SE	2.67	0.45
1:A:440:LYS:HA	1:A:440:LYS:HE3	1.99	0.45
1:B:393:PRO:HD3	1:B:402:GLU:OE1	2.16	0.45
1:A:452:GLN:O	1:A:456:GLU:HG3	2.17	0.45
1:B:273:ARG:HG3	1:B:319:LEU:HD12	1.97	0.45
1:A:253:SER:HA	1:A:258:LEU:CD2	2.47	0.45
1:A:310:ARG:HH11	1:A:334:ARG:HG2	1.81	0.45
1:A:391:ARG:HD3	2:A:482:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:HA	1:A:174:LYS:HE2	1.98	0.45
1:B:310:ARG:NH1	1:B:334:ARG:CG	2.80	0.45
1:A:293:GLN:HE22	1:A:458:THR:HG21	1.82	0.45
1:B:342:TPO:CG2	1:B:343:VAL:N	2.79	0.45
1:A:206:ASN:O	1:A:207:ASN:HB2	2.17	0.44
1:A:310:ARG:HD3	1:A:332:LEU:O	2.17	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	2.00	0.44
1:A:176:VAL:HG13	1:A:177:THR:HG23	1.99	0.44
1:A:404:GLU:C	1:A:406:GLU:H	2.19	0.44
1:A:182:GLU:H	1:A:182:GLU:HG2	1.57	0.43
1:A:171:TYR:CD1	1:A:172:GLU:N	2.86	0.43
1:B:290:LYS:HD3	1:B:290:LYS:HA	1.65	0.43
1:A:310:ARG:NH2	1:A:349:VAL:HG22	2.33	0.43
1:A:242:HIS:CE1	1:A:244:ASN:HD22	2.29	0.43
1:A:417:LYS:HD2	1:B:276:CYS:HB2	2.01	0.43
1:B:201:TYR:CE1	1:B:214:LYS:HE3	2.54	0.43
1:B:409:THR:HG23	1:B:412:ASP:H	1.83	0.43
1:A:165:PHE:CZ	1:A:248:LEU:HD23	2.54	0.43
1:A:348:ILE:HG12	1:A:362:GLY:HA2	2.00	0.42
1:A:174:LYS:O	1:A:179:ASN:HA	2.19	0.42
1:A:192:MSE:HE2	1:A:202:LYS:CA	2.49	0.42
1:A:376:VAL:O	1:A:380:ILE:HG13	2.20	0.42
1:A:442:ASN:HD22	1:A:442:ASN:HA	1.69	0.42
1:B:168:PHE:HE1	1:B:250:GLY:HA3	1.85	0.42
1:A:183:ARG:CB	1:A:183:ARG:NH1	2.83	0.41
1:B:248:LEU:HD12	1:B:261:VAL:O	2.20	0.41
1:A:171:TYR:HA	1:A:174:LYS:HB3	2.03	0.41
1:A:196:GLY:O	1:A:197:PHE:C	2.59	0.41
1:A:266:PRO:HD2	1:A:320:ASP:HA	2.02	0.41
1:B:248:LEU:HD13	1:B:262:TYR:CE1	2.56	0.41
1:A:191:LYS:C	1:A:191:LYS:HD3	2.41	0.40
1:A:284:SER:O	1:A:288:ARG:HG3	2.21	0.40
1:A:309:HIS:O	1:A:310:ARG:HB2	2.21	0.40
1:A:206:ASN:C	1:A:208:THR:H	2.24	0.40
1:B:309:HIS:O	1:B:310:ARG:HB2	2.21	0.40
1:A:293:GLN:HE22	1:A:458:THR:CG2	2.35	0.40
1:A:174:LYS:O	1:A:179:ASN:N	2.52	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	273/298 (92%)	256 (94%)	14 (5%)	3 (1%)	14	20
1	B	267/298 (90%)	250 (94%)	16 (6%)	1 (0%)	34	48
All	All	540/596 (91%)	506 (94%)	30 (6%)	4 (1%)	22	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	256	ASP
1	B	254	ASP
1	A	406	GLU

### 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	242/248 (98%)	233 (96%)	9 (4%)	34	53
1	B	240/248 (97%)	233 (97%)	7 (3%)	42	62
All	All	482/496 (97%)	466 (97%)	16 (3%)	38	57

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	197	PHE

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	265	MSE
1	A	318	LEU
1	A	365	THR
1	A	395	LEU
1	A	419	ASN
1	A	455	GLN
1	B	174	LYS
1	B	197	PHE
1	B	247	GLU
1	B	334	ARG
1	B	365	THR
1	B	395	LEU
1	B	419	ASN

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

Mol	Chain	Res	Type
1	A	175	ASN
1	A	178	ASN
1	A	190	ASN
1	A	232	GLN
1	A	244	ASN
1	A	293	GLN
1	A	297	ASN
1	A	300	ASN
1	A	419	ASN
1	A	442	ASN
1	A	455	GLN
1	B	179	ASN
1	B	190	ASN
1	B	206	ASN
1	B	232	GLN
1	B	244	ASN
1	B	297	ASN
1	B	300	ASN
1	B	419	ASN
1	B	442	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	8,10,11	1.67	1 (12%)	10,14,16	1.25	1 (10%)
1	TPO	B	345	1	8,10,11	1.60	1 (12%)	10,14,16	1.27	1 (10%)
1	TPO	B	342	1	8,10,11	1.61	1 (12%)	10,14,16	1.23	1 (10%)
1	TPO	A	342	1	8,10,11	1.66	1 (12%)	10,14,16	1.24	1 (10%)

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	-	3/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-O2P	-3.82	1.40	1.54
1	A	342	TPO	P-O2P	-3.70	1.40	1.54
1	B	342	TPO	P-O2P	-3.66	1.40	1.54
1	B	345	TPO	P-O2P	-3.61	1.40	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	345	TPO	O2P-P-O1P	2.21	119.33	110.68
1	B	345	TPO	O2P-P-O1P	2.20	119.29	110.68
1	B	342	TPO	O2P-P-O1P	2.20	119.28	110.68
1	A	342	TPO	O2P-P-O1P	2.19	119.26	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	A	342	TPO	CA-CB-OG1-P
1	A	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CB-OG1-P-O3P
1	B	342	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	342	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	269/298 (90%)	0.50	33 (12%) <b>4</b> <b>3</b>	22, 46, 76, 89	0
1	B	266/298 (89%)	0.31	24 (9%) <b>9</b> <b>8</b>	23, 44, 93, 103	0
All	All	535/596 (89%)	0.40	57 (10%) <b>6</b> <b>5</b>	22, 45, 87, 103	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PHE	6.2
1	A	194	GLU	5.0
1	A	186	SER	4.5
1	A	196	GLY	4.5
1	A	197	PHE	4.3
1	A	256	ASP	4.2
1	A	195	GLY	4.0
1	A	201	TYR	4.0
1	B	197	PHE	3.7
1	A	258	LEU	3.7
1	A	168	PHE	3.7
1	B	194	GLU	3.6
1	A	185	ILE	3.6
1	A	347	ARG	3.5
1	A	203	GLY	3.4
1	A	188	GLY	3.3
1	B	207	ASN	3.3
1	B	336	SER	3.3
1	B	204	TYR	3.1
1	A	167	SER	3.1
1	B	181	ASP	3.0
1	B	196	GLY	3.0
1	A	226	LEU	3.0
1	B	459	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	256	ASP	2.9
1	A	459	ALA	2.8
1	B	228	GLN	2.7
1	B	239	LYS	2.7
1	B	183	ARG	2.6
1	A	187	VAL	2.6
1	B	191	LYS	2.6
1	A	171	TYR	2.6
1	A	252	SER	2.5
1	A	166	HIS	2.5
1	B	199	VAL	2.4
1	B	230	PHE	2.4
1	B	343	VAL	2.4
1	B	390	HIS	2.4
1	A	227	LYS	2.4
1	B	201	TYR	2.4
1	A	205	VAL	2.3
1	B	166	HIS	2.3
1	B	184	PRO	2.3
1	A	377	LEU	2.3
1	A	257	ASP	2.2
1	A	390	HIS	2.1
1	A	374	GLY	2.1
1	A	343	VAL	2.1
1	A	373	PHE	2.1
1	A	199	VAL	2.1
1	B	373	PHE	2.1
1	A	212	VAL	2.1
1	A	380	ILE	2.0
1	A	165	PHE	2.0
1	B	251	PHE	2.0
1	B	407	GLU	2.0
1	B	227	LYS	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. 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( $\text{\AA}^2$ )	Q<0.9
1	TPO	A	342	11/12	0.92	0.11	68,69,75,75	0
1	TPO	B	342	11/12	0.93	0.13	71,73,75,75	0
1	TPO	B	345	11/12	0.94	0.14	60,63,66,66	0
1	TPO	A	345	11/12	0.96	0.11	61,62,64,64	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.