Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:47 AM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

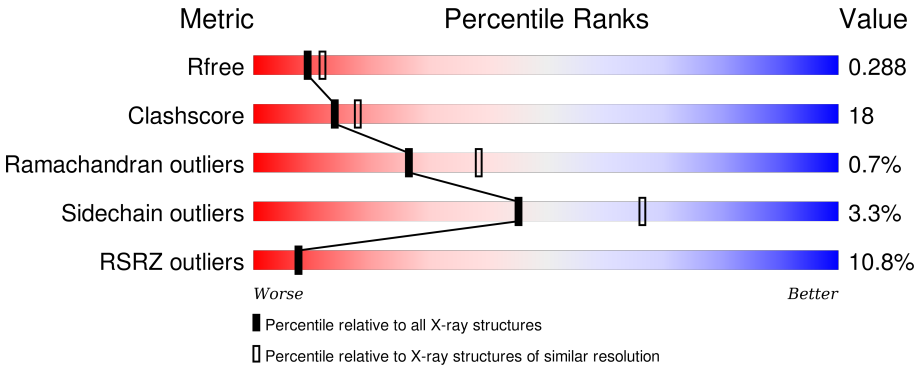
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	11% 58% 33% • 6%
1	B	298	8% 67% 25% • 7%

2 Entry composition

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
1	A	280	Total	C	N	O	P	S	Se	0	0	0
			2207	1387	371	433	2	5	9			
1	B	277	Total	C	N	O	P	S	Se	0	0	0
			2191	1376	369	430	2	5	9			

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.

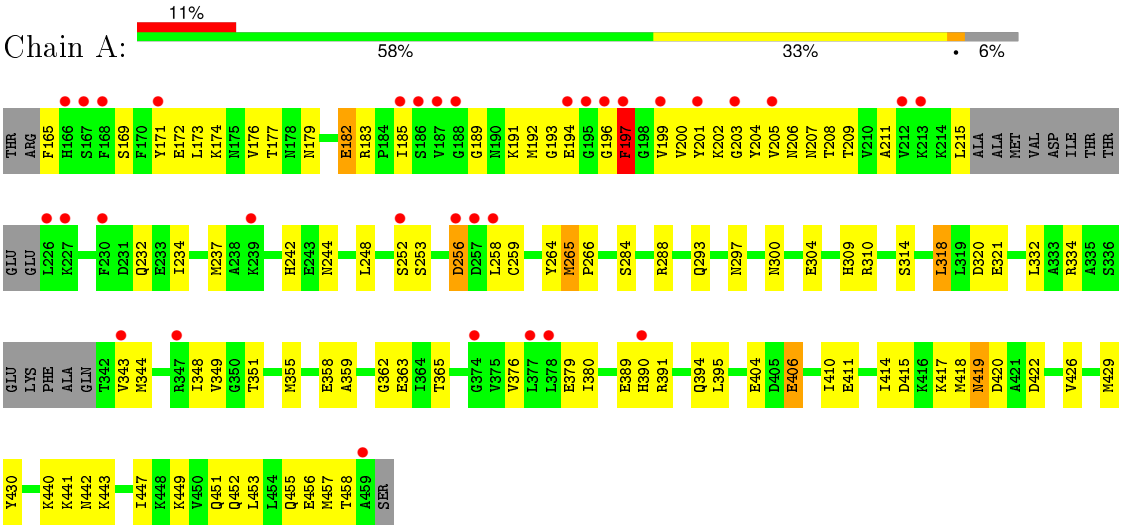
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	27	Total O 27 27	0	0

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.

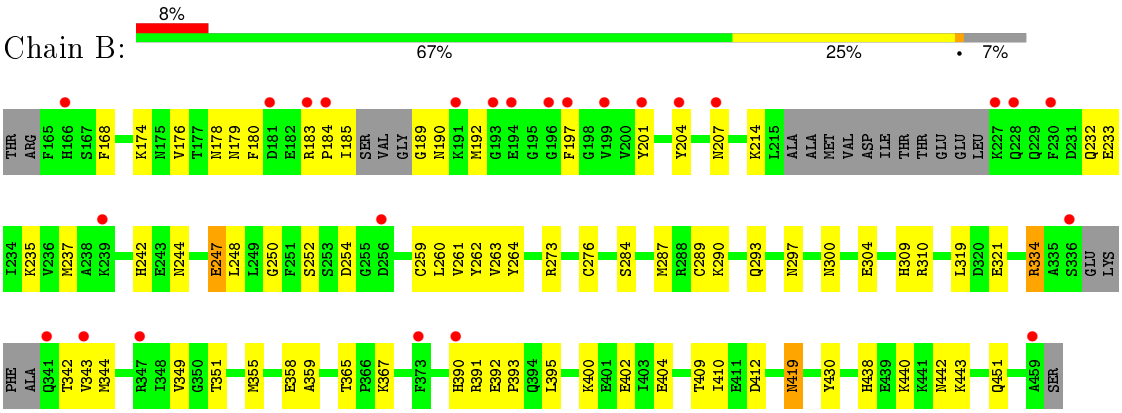
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.47 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.289 0.242 , 0.288	Depositor DCC
R_{free} test set	1448 reflections (4.91%)	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29503 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4457	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:HE2	1:A:237:MSE:HA	1.71	0.72
1:A:419:ASN:C	1:A:419:ASN:HD22	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:CD	1:A:321:GLU:H	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:B:400:LYS:O	1:B:404:GLU:HG3	1.96	0.65
1:A:242:HIS:HE1	1:A:244:ASN:HD22	1.45	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:HE2	1:B:237:MSE:HA	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:HA	1:A:232:GLN:HE21	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:CD	1:B:321:GLU:H	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:NZ	1:B:235:LYS:HB3	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:B:179:ASN:O	1:B:180:PHE:HB2	2.11	0.51
1:A:300:ASN:HD22	1:A:447:ILE:HG23	1.75	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: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:A:183:ARG:CB	1:A:183:ARG:HH11	2.27	0.48
1:B:235:LYS:HZ3	1:B:235:LYS:HB3	1.77	0.48
1:B:192:MSE:SE	1:B:264:TYR:HE2	2.47	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:B:310:ARG:NH2	1:B:349:VAL:HG22	2.30	0.47
1:A:358:GLU:HG2	1:A:359:ALA:N	2.28	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:N	1:B:419:ASN:HD22	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:B:273:ARG:HG3	1:B:319:LEU:HD12	1.97	0.45
1:A:452:GLN:O	1:A:456:GLU:HG3	2.17	0.45
1:A:253:SER:HA	1:A:258:LEU:CD2	2.47	0.45
1:A:391:ARG:HD3	2:A:482:HOH:O	2.17	0.45
1:A:310:ARG:HH11	1:A:334:ARG:HG2	1.81	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:B:342:TPO:CG2	1:B:343:VAL:N	2.79	0.45
1:A:293:GLN:HE22	1:A:458:THR:HG21	1.82	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:HA	1:B:290:LYS:HD3	1.65	0.43
1:A:310:ARG:NH2	1:A:349:VAL:HG22	2.33	0.43
1:B:201:TYR:CE1	1:B:214:LYS:HE3	2.54	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: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:HA	1:A:442:ASN:HD22	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:266:PRO:HD2	1:A:320:ASP:HA	2.02	0.41
1:A:171:TYR:HA	1:A:174:LYS:HB3	2.03	0.41
1:B:248:LEU:HD13	1:B:262:TYR:CE1	2.56	0.41
1:A:196:GLY:O	1:A:197:PHE:C	2.59	0.41
1:A:191:LYS:C	1:A:191:LYS:HD3	2.41	0.40
1:A:309:HIS:O	1:A:310:ARG:HB2	2.21	0.40
1:A:284:SER:O	1:A:288:ARG:HG3	2.21	0.40
1:B:309:HIS:O	1:B:310:ARG:HB2	2.21	0.40
1:A:206:ASN:C	1:A:208:THR:H	2.24	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

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	273/298 (92%)	256 (94%)	14 (5%)	3 (1%)	17 25
1	B	267/298 (90%)	250 (94%)	16 (6%)	1 (0%)	39 56
All	All	540/596 (91%)	506 (94%)	30 (6%)	4 (1%)	26 38

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

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%)	41 62
1	B	240/248 (97%)	233 (97%)	7 (3%)	50 71
All	All	482/496 (97%)	466 (97%)	16 (3%)	45 66

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

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	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

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	342	1	8,10,11	1.72	1 (12%)	7,14,16	1.49	1 (14%)
1	TPO	A	345	1	8,10,11	1.73	1 (12%)	7,14,16	1.55	1 (14%)
1	TPO	B	342	1	8,10,11	1.66	1 (12%)	7,14,16	1.54	1 (14%)
1	TPO	B	345	1	8,10,11	1.64	1 (12%)	7,14,16	1.53	1 (14%)

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	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-O2P	-4.06	1.40	1.54
1	A	342	TPO	P-O2P	-3.93	1.40	1.54
1	B	342	TPO	P-O2P	-3.89	1.40	1.54
1	B	345	TPO	P-O2P	-3.83	1.40	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	TPO	O2P-P-O1P	2.70	119.26	110.58
1	B	342	TPO	O2P-P-O1P	2.70	119.28	110.58
1	B	345	TPO	O2P-P-O1P	2.71	119.29	110.58
1	A	345	TPO	O2P-P-O1P	2.72	119.33	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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 carbohydrates 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 (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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	269/298 (90%)	0.57	33 (12%) 5 5	22, 46, 76, 89	0
1	B	266/298 (89%)	0.37	25 (9%) 11 10	23, 44, 93, 103	0
All	All	535/596 (89%)	0.47	58 (10%) 8 8	22, 45, 87, 103	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PHE	6.7
1	A	194	GLU	5.4
1	A	196	GLY	4.8
1	A	195	GLY	4.5
1	A	256	ASP	4.5
1	A	197	PHE	4.5
1	A	186	SER	4.4
1	A	185	ILE	4.0
1	A	347	ARG	3.9
1	B	207	ASN	3.8
1	B	194	GLU	3.8
1	A	201	TYR	3.8
1	B	230	PHE	3.8
1	A	258	LEU	3.6
1	B	197	PHE	3.6
1	A	168	PHE	3.5
1	A	226	LEU	3.5
1	A	203	GLY	3.5
1	B	256	ASP	3.4
1	B	181	ASP	3.2
1	B	204	TYR	3.2
1	B	459	ALA	3.1
1	A	188	GLY	3.0
1	A	167	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	239	LYS	2.9
1	B	183	ARG	2.9
1	B	336	SER	2.8
1	B	166	HIS	2.8
1	B	196	GLY	2.7
1	A	227	LYS	2.7
1	B	199	VAL	2.7
1	B	227	LYS	2.7
1	A	257	ASP	2.6
1	A	459	ALA	2.6
1	A	171	TYR	2.6
1	B	191	LYS	2.6
1	A	187	VAL	2.6
1	B	343	VAL	2.6
1	B	201	TYR	2.4
1	A	205	VAL	2.4
1	B	228	GLN	2.4
1	B	390	HIS	2.4
1	A	343	VAL	2.4
1	A	239	LYS	2.3
1	A	213	LYS	2.3
1	A	252	SER	2.3
1	A	374	GLY	2.3
1	A	166	HIS	2.2
1	A	378	LEU	2.2
1	A	212	VAL	2.1
1	A	390	HIS	2.1
1	B	341	GLN	2.1
1	B	373	PHE	2.1
1	B	347	ARG	2.1
1	A	377	LEU	2.1
1	B	184	PRO	2.0
1	A	199	VAL	2.0
1	B	193	GLY	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^{th} 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^2)	Q<0.9
1	TPO	A	342	11/12	0.92	0.11	-	68,69,75,75	0
1	TPO	A	345	11/12	0.96	0.12	-	61,62,64,64	0
1	TPO	B	345	11/12	0.94	0.15	-	60,63,66,66	0
1	TPO	B	342	11/12	0.93	0.15	-	71,73,75,75	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.