Full wwPDB X-ray Structure Validation Report (i)

Dec 21, 2016 – 12:11 PM EST

PDB ID	:	5A4Q
Title	:	DYRK1A IN COMPLEX WITH CHLORO BENZOTHIAZOLE FRAGMENT
Authors	:	Rothweiler, U.
Deposited on	:	2015-06-11
Resolution	:	2.37 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:

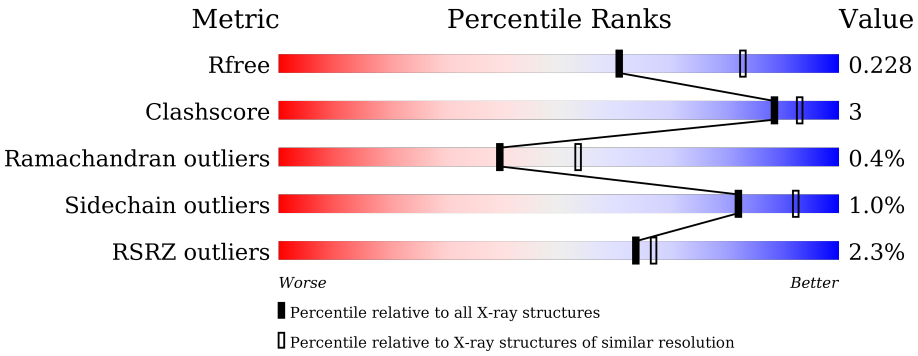
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	368	89% · 7%
1	B	368	84% 7% 9%
1	C	368	5% 79% 11% 10%
1	D	368	2% 85% 6% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11318 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.

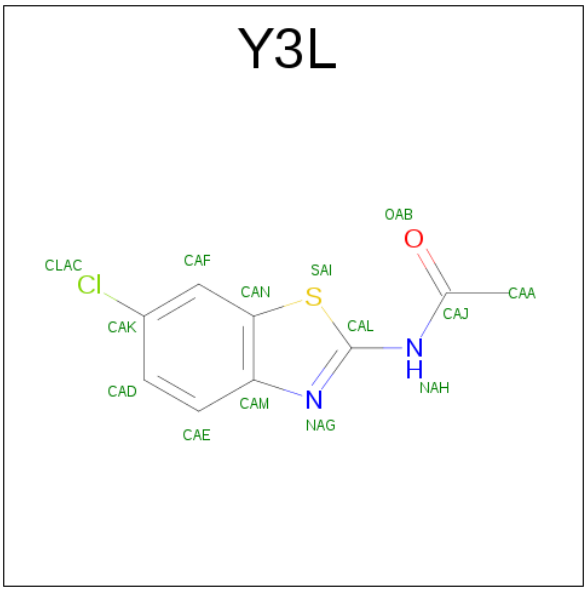
- Molecule 1 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	P	S	0	0	0
			2790	1795	476	501	1	17			
1	B	336	Total	C	N	O	P	S	0	0	0
			2727	1756	467	487	1	16			
1	C	333	Total	C	N	O	P	S	0	0	0
			2668	1718	448	484	1	17			
1	D	335	Total	C	N	O	P	S	0	0	0
			2732	1763	460	491	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	EXPRESSION TAG	UNP Q13627
A	124	ALA	-	EXPRESSION TAG	UNP Q13627
A	125	SER	-	EXPRESSION TAG	UNP Q13627
B	123	GLY	-	EXPRESSION TAG	UNP Q13627
B	124	ALA	-	EXPRESSION TAG	UNP Q13627
B	125	SER	-	EXPRESSION TAG	UNP Q13627
C	123	GLY	-	EXPRESSION TAG	UNP Q13627
C	124	ALA	-	EXPRESSION TAG	UNP Q13627
C	125	SER	-	EXPRESSION TAG	UNP Q13627
D	123	GLY	-	EXPRESSION TAG	UNP Q13627
D	124	ALA	-	EXPRESSION TAG	UNP Q13627
D	125	SER	-	EXPRESSION TAG	UNP Q13627

- Molecule 2 is N-(5-CHLORANYL-1,3-BENZOTHIAZOL-2-YL)ETHANAMIDE (three-letter code: Y3L) (formula: $C_9H_7ClN_2OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			14	9	1	2	1	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			14	9	1	2	1	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			14	9	1	2	1	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			14	9	1	2	1	1		

- Molecule 3 is water.

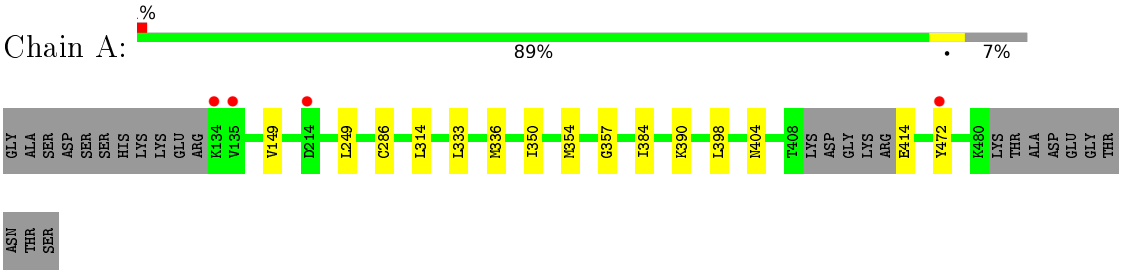
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	71	Total	O	0	0
			71	71		
3	C	60	Total	O	0	0
			60	60		
3	D	87	Total	O	0	0
			87	87		

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.

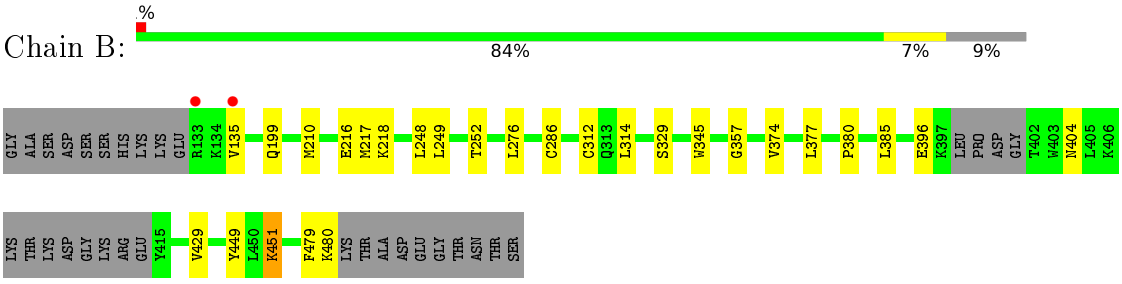
• Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain A:



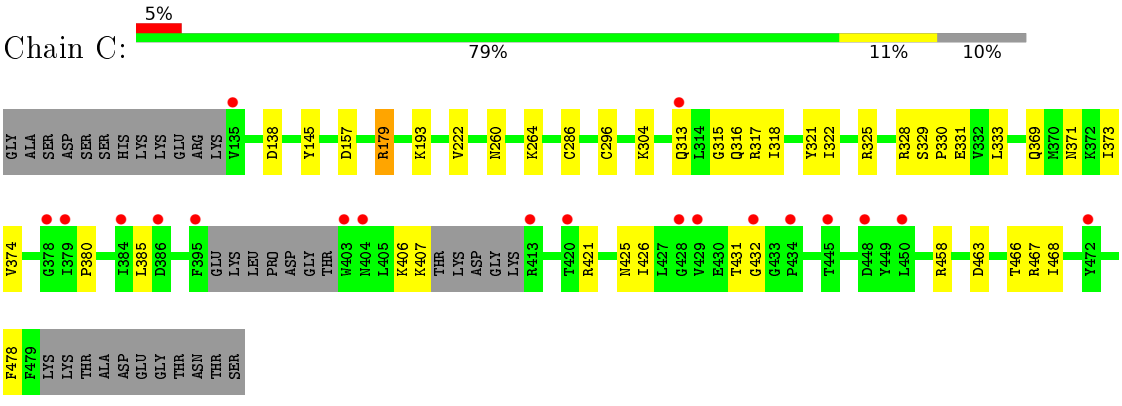
• Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain B:



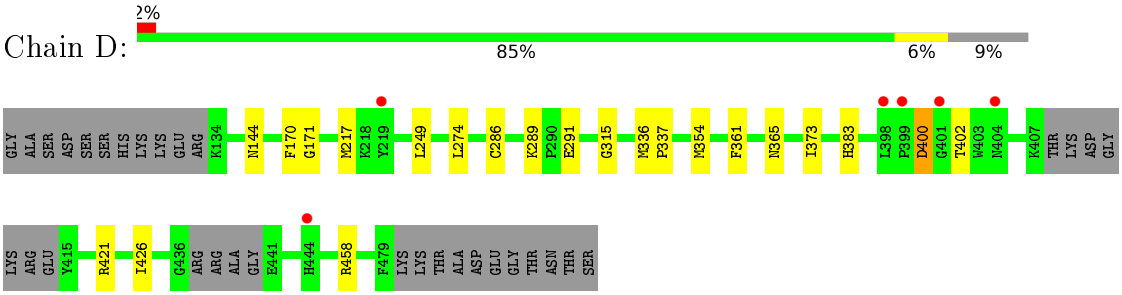
• Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain C:



• Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain D:


2%
85%
6%
9%
GLY ALA SER ASP SER SER HIS LYS LYS GLU ARG K134 N144 F170 G171 M217 K218 Y219 L249 L274 C286 K289 P290 E291 G315 M336 P337 M354 F361 N365 I373 H383 L398 P399 D400 G401 T402 W403 N404 K407 THR LYS ASP GLY
LYS ARG GLU Y415 R421 I426 G436 ARG ARG ALA GLY E441 H444 R458 F479 LYS LYS THR ALA ASP GLU GLY THR ASN THR SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.04Å 88.94Å 229.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 2.37 48.45 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.45-2.37) 99.3 (48.45-2.37)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.207 , 0.243 0.198 , 0.228	Depositor DCC
R_{free} test set	2101 reflections (2.94%)	DCC
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11318	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 3.40% 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, 0.333 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: PTR, Y3L

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	0.56	0/2838	0.69	0/3829
1	B	0.49	0/2772	0.65	0/3739
1	C	0.49	0/2714	0.68	1/3675 (0.0%)
1	D	0.52	0/2779	0.66	1/3750 (0.0%)
All	All	0.51	0/11103	0.67	2/14993 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	179	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	458	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	2790	0	2776	7	0
1	B	2727	0	2708	13	0
1	C	2668	0	2577	21	0
1	D	2732	0	2715	14	0
2	A	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	0	1	0
2	C	14	0	0	1	0
2	D	14	0	0	1	0
3	A	127	0	0	1	0
3	B	71	0	0	0	0
3	C	60	0	0	1	0
3	D	87	0	0	1	0
All	All	11318	0	10776	55	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 (55) 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:C:296:CYS:SG	3:C:2028:HOH:O	2.47	0.73
2:A:1482:Y3L:CAA	2:A:1482:Y3L:SAI	2.81	0.68
1:A:314:LEU:O	1:D:315:GLY:HA2	1.96	0.64
2:C:1481:Y3L:CAA	2:C:1481:Y3L:SAI	2.88	0.62
2:B:1482:Y3L:CAA	2:B:1482:Y3L:SAI	2.91	0.59
3:A:2022:HOH:O	1:B:199:GLN:NE2	2.35	0.58
1:B:216:GLU:O	1:B:218:LYS:N	2.37	0.58
1:D:400:ASP:N	1:D:400:ASP:OD1	2.37	0.58
1:C:321:PTR:O2P	1:C:325:ARG:NH1	2.38	0.56
1:C:431:THR:HG22	1:C:432:GLY:H	1.71	0.56
1:C:331:GLU:OE2	1:C:467:ARG:NH1	2.40	0.55
1:C:425:ASN:O	1:C:426:ILE:HB	2.08	0.54
1:C:380:PRO:HB2	1:C:385:LEU:HD11	1.92	0.51
1:B:248:LEU:O	1:B:252:THR:HG23	2.12	0.50
1:C:316:GLN:O	1:C:318:ILE:N	2.46	0.49
1:B:479:PHE:O	1:B:480:LYS:HB2	2.13	0.49
1:C:145:TYR:CZ	1:C:193:LYS:HE3	2.47	0.49
2:D:1481:Y3L:SAI	2:D:1481:Y3L:CAA	3.02	0.48
1:C:458:ARG:HG3	1:C:468:ILE:HB	1.95	0.48
1:C:371:ASN:HA	1:C:374:VAL:HG22	1.95	0.48
1:D:421:ARG:HG2	1:D:426:ILE:HD11	1.96	0.48
1:C:260:ASN:O	1:C:264:LYS:HG3	2.14	0.47
1:C:369:GLN:O	1:C:373:ILE:HD12	2.15	0.47
1:D:289:LYS:HE3	1:D:291:GLU:HG2	1.98	0.46
1:C:431:THR:HG22	1:C:432:GLY:N	2.31	0.46
1:C:330:PRO:HA	1:C:333:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PRO:HB2	1:B:385:LEU:HD13	1.99	0.44
1:A:333:LEU:O	1:A:390:LYS:HE3	2.18	0.44
1:B:314:LEU:O	1:C:315:GLY:HA2	2.17	0.43
1:C:138:ASP:OD1	1:D:365:ASN:HB2	2.17	0.43
1:A:350:ILE:O	1:A:354:MET:HG2	2.17	0.43
1:D:336:MET:HB3	1:D:337:PRO:HD2	2.00	0.43
1:B:329:SER:HA	1:B:345:TRP:CD1	2.54	0.43
1:B:210:MET:CE	1:B:276:LEU:HD22	2.49	0.43
1:D:217:MET:SD	1:D:274:LEU:HD23	2.59	0.43
1:D:144:ASN:ND2	3:D:2002:HOH:O	2.51	0.42
1:C:222:VAL:HA	1:C:304:LYS:HD3	2.01	0.42
1:C:322:ILE:O	1:C:328:ARG:NH1	2.51	0.42
1:D:249:LEU:HD11	1:D:354:MET:HE2	2.00	0.42
1:A:472:TYR:OH	1:D:383:HIS:HB2	2.18	0.42
1:D:289:LYS:HG3	1:D:291:GLU:HG2	2.02	0.42
1:D:289:LYS:HE3	1:D:291:GLU:CG	2.49	0.42
1:B:249:LEU:HD22	1:B:357:GLY:HA2	2.00	0.42
1:C:406:LYS:O	1:C:407:LYS:C	2.59	0.41
1:C:157:ASP:O	1:C:179:ARG:NH2	2.53	0.41
1:B:429:VAL:HG22	1:B:449:TYR:HB3	2.03	0.41
1:C:463:ASP:HB3	1:C:466:THR:OG1	2.21	0.41
1:B:396:GLU:N	1:B:404:ASN:O	2.48	0.41
1:D:361:PHE:CE1	1:D:373:ILE:HA	2.56	0.41
1:B:451:LYS:N	1:B:451:LYS:HD3	2.35	0.41
1:D:170:PHE:CD1	1:D:171:GLY:N	2.89	0.41
1:A:336:MET:HE1	1:A:384:ILE:HG23	2.04	0.40
1:A:398:LEU:HD11	1:A:404:ASN:OD1	2.22	0.40
1:A:249:LEU:HD22	1:A:357:GLY:HA2	2.02	0.40
1:B:374:VAL:O	1:B:377:LEU:O	2.40	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	337/368 (92%)	323 (96%)	14 (4%)	0	100 100
1	B	329/368 (89%)	317 (96%)	11 (3%)	1 (0%)	46 61
1	C	326/368 (89%)	302 (93%)	20 (6%)	4 (1%)	16 21
1	D	328/368 (89%)	312 (95%)	16 (5%)	0	100 100
All	All	1320/1472 (90%)	1254 (95%)	61 (5%)	5 (0%)	39 53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	MET
1	C	478	PHE
1	C	421	ARG
1	C	313	GLN
1	C	317	ARG

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	300/324 (93%)	297 (99%)	3 (1%)	82 92
1	B	291/324 (90%)	287 (99%)	4 (1%)	74 88
1	C	280/324 (86%)	278 (99%)	2 (1%)	88 95
1	D	295/324 (91%)	292 (99%)	3 (1%)	82 92
All	All	1166/1296 (90%)	1154 (99%)	12 (1%)	82 92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	VAL
1	A	286	CYS
1	A	414	GLU
1	B	135	VAL
1	B	286	CYS
1	B	312	CYS

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Mol	Chain	Res	Type
1	B	451	LYS
1	C	286	CYS
1	C	329	SER
1	D	286	CYS
1	D	400	ASP
1	D	402	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	404	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	PTR	A	321	1	13,16,17	0.92	0	19,22,24	0.94	0
1	PTR	B	321	1	13,16,17	0.80	0	19,22,24	1.20	2 (10%)
1	PTR	C	321	1	13,16,17	0.80	0	19,22,24	0.99	1 (5%)
1	PTR	D	321	1	13,16,17	0.75	0	19,22,24	1.13	2 (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	PTR	A	321	1	-	0/9/11/13	0/1/1/1
1	PTR	B	321	1	-	0/9/11/13	0/1/1/1
1	PTR	C	321	1	-	0/9/11/13	0/1/1/1
1	PTR	D	321	1	-	0/9/11/13	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	PTR	O2P-P-OH	-2.52	97.45	105.47
1	D	321	PTR	O3P-P-OH	-2.01	99.08	105.47
1	D	321	PTR	O2P-P-O1P	2.37	118.37	110.63
1	C	321	PTR	O3P-P-O2P	2.69	117.32	107.44
1	B	321	PTR	O3P-P-O2P	3.22	119.28	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	321	PTR	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	Y3L	A	1482	-	12,15,15	1.83	4 (33%)	11,21,21	2.38	5 (45%)
2	Y3L	B	1482	-	12,15,15	1.90	3 (25%)	11,21,21	2.24	4 (36%)
2	Y3L	C	1481	-	12,15,15	1.91	2 (16%)	11,21,21	1.87	4 (36%)
2	Y3L	D	1481	-	12,15,15	2.04	3 (25%)	11,21,21	2.11	4 (36%)

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	Y3L	A	1482	-	-	0/2/4/4	0/2/2/2
2	Y3L	B	1482	-	-	0/2/4/4	0/2/2/2
2	Y3L	C	1481	-	-	0/2/4/4	0/2/2/2
2	Y3L	D	1481	-	-	0/2/4/4	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1481	Y3L	CAE-CAM	-4.78	1.33	1.41
2	D	1481	Y3L	CAE-CAM	-4.26	1.34	1.41
2	A	1482	Y3L	CAE-CAM	-3.97	1.34	1.41
2	B	1482	Y3L	CAE-CAM	-3.73	1.35	1.41
2	A	1482	Y3L	CAL-NAH	-2.50	1.32	1.36
2	A	1482	Y3L	CAF-CAN	-2.40	1.33	1.37
2	C	1481	Y3L	CAF-CAN	-2.36	1.33	1.37
2	B	1482	Y3L	CAF-CAN	-2.33	1.33	1.37
2	A	1482	Y3L	CAM-CAN	-2.14	1.35	1.42
2	D	1481	Y3L	CAF-CAN	-2.09	1.34	1.37
2	B	1482	Y3L	CAK-CLAC	2.94	1.81	1.74
2	D	1481	Y3L	CAK-CLAC	3.40	1.82	1.74

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1481	Y3L	CAD-CAK-CAF	-3.03	117.77	121.87
2	A	1482	Y3L	OAB-CAJ-CAA	-2.96	116.62	122.07
2	B	1482	Y3L	CAD-CAK-CAF	-2.79	118.09	121.87
2	B	1482	Y3L	OAB-CAJ-NAH	-2.75	119.71	123.08
2	C	1481	Y3L	CAD-CAK-CAF	-2.64	118.30	121.87
2	A	1482	Y3L	CAD-CAK-CAF	-2.51	118.48	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1481	Y3L	OAB-CAJ-NAH	-2.32	120.23	123.08
2	C	1481	Y3L	OAB-CAJ-NAH	-2.09	120.51	123.08
2	A	1482	Y3L	OAB-CAJ-NAH	-2.04	120.58	123.08
2	C	1481	Y3L	CAN-CAM-NAG	2.22	113.27	108.12
2	A	1482	Y3L	CAN-CAM-NAG	2.25	113.32	108.12
2	D	1481	Y3L	CAN-CAM-NAG	2.57	114.07	108.12
2	B	1482	Y3L	CAD-CAK-CLAC	2.85	124.16	119.35
2	C	1481	Y3L	CAA-CAJ-NAH	3.85	120.58	115.01
2	D	1481	Y3L	CAA-CAJ-NAH	4.28	121.19	115.01
2	B	1482	Y3L	CAA-CAJ-NAH	4.57	121.62	115.01
2	A	1482	Y3L	CAA-CAJ-NAH	5.38	122.78	115.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1482	Y3L	1	0
2	B	1482	Y3L	1	0
2	C	1481	Y3L	1	0
2	D	1481	Y3L	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	341/368 (92%)	-0.23	4 (1%) 81 83	23, 35, 58, 94	0
1	B	335/368 (91%)	-0.14	2 (0%) 90 91	29, 47, 83, 112	0
1	C	332/368 (90%)	0.17	19 (5%) 27 31	27, 56, 90, 112	0
1	D	334/368 (90%)	0.04	6 (1%) 71 74	27, 47, 79, 105	0
All	All	1342/1472 (91%)	-0.04	31 (2%) 64 67	23, 46, 84, 112	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	6.5
1	B	133	ARG	6.4
1	D	398	LEU	4.4
1	C	472	TYR	3.9
1	C	450	LEU	3.9
1	C	395	PHE	3.7
1	C	403	TRP	3.6
1	C	404	ASN	3.4
1	D	219	TYR	3.4
1	D	399	PRO	3.4
1	A	134	LYS	3.2
1	A	472	TYR	3.1
1	C	428	GLY	3.1
1	B	135	VAL	3.0
1	C	413	ARG	2.9
1	A	214	ASP	2.8
1	C	384	ILE	2.8
1	D	404	ASN	2.7
1	C	378	GLY	2.5
1	C	386	ASP	2.5
1	C	432	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	444	HIS	2.3
1	A	135	VAL	2.3
1	C	434	PRO	2.3
1	D	401	GLY	2.2
1	C	420	THR	2.2
1	C	429	VAL	2.1
1	C	448	ASP	2.1
1	C	445	THR	2.0
1	C	313	GLN	2.0
1	C	379	ILE	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	PTR	B	321	16/17	0.97	0.11	-	45,49,50,52	0
1	PTR	A	321	16/17	0.97	0.13	-	31,32,35,35	0
1	PTR	D	321	16/17	0.96	0.12	-	33,41,46,46	0
1	PTR	C	321	16/17	0.95	0.12	-	48,51,54,56	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^{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
2	Y3L	A	1482	14/14	0.96	0.11	-0.80	31,34,37,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	Y3L	C	1481	14/14	0.96	0.10	-0.84	34,38,41,41	0
2	Y3L	B	1482	14/14	0.97	0.11	-0.86	37,41,50,54	0
2	Y3L	D	1481	14/14	0.97	0.10	-0.86	43,48,65,68	0

6.5 Other polymers (i)

There are no such residues in this entry.