



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:28 pm GMT

PDB ID : 4AZE  
Title : Human DYRK1A in complex with Leucettine L41  
Authors : Elkins, J.M.; Soundararajan, M.; Muniz, J.R.C.; Tahtouh, T.; Burgy, G.; Durieu, E.; Lozach, O.; Cochet, C.; Schmid, R.S.; Lo, D.C.; Delhommel, F.; Carreaux, F.; Bazureau, J.P.; Meijer, L.; Edwards, A.; Bountra, C.; Knapp, S.  
Deposited on : 2012-06-25  
Resolution : 3.15 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.

---

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 : trunk28620  
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) : recalc28949

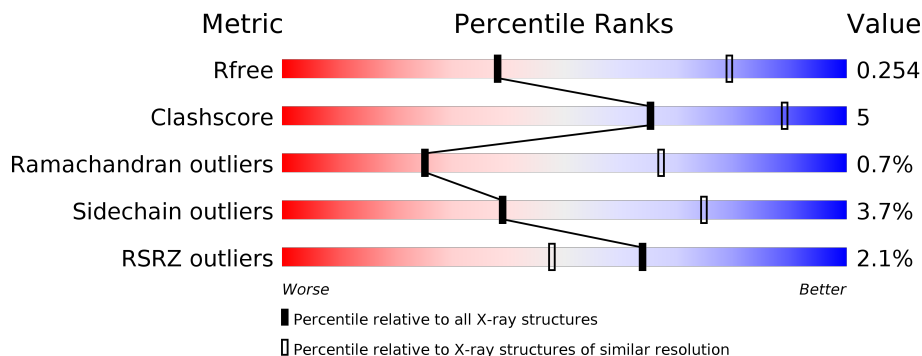
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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	382	<div> <div>80%</div> <div>12% • 8%</div> </div>
1	B	382	<div> <div>%</div> <div>78%</div> <div>12% 9%</div> </div>
1	C	382	<div> <div>4%</div> <div>79%</div> <div>12% • 8%</div> </div>
2	E	4	<div> <div>50%</div> <div>50%</div> </div>
2	F	4	<div> <div>50%</div> <div>50%</div> </div>
2	G	4	<div> <div>25%</div> <div>75%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8613 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	350	Total	C	N	O	P	S	0	0	0
			2844	1826	485	514	2	17			
1	B	347	Total	C	N	O	P	S	0	0	0
			2813	1810	477	508	1	17			
1	C	350	Total	C	N	O	P	S	0	0	0
			2812	1804	478	511	2	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	EXPRESSION TAG	UNP Q13627
A	105	HIS	-	EXPRESSION TAG	UNP Q13627
A	106	HIS	-	EXPRESSION TAG	UNP Q13627
A	107	HIS	-	EXPRESSION TAG	UNP Q13627
A	108	HIS	-	EXPRESSION TAG	UNP Q13627
A	109	HIS	-	EXPRESSION TAG	UNP Q13627
A	110	HIS	-	EXPRESSION TAG	UNP Q13627
A	111	SER	-	EXPRESSION TAG	UNP Q13627
A	112	SER	-	EXPRESSION TAG	UNP Q13627
A	113	GLY	-	EXPRESSION TAG	UNP Q13627
A	114	VAL	-	EXPRESSION TAG	UNP Q13627
A	115	ASP	-	EXPRESSION TAG	UNP Q13627
A	116	LEU	-	EXPRESSION TAG	UNP Q13627
A	117	GLY	-	EXPRESSION TAG	UNP Q13627
A	118	THR	-	EXPRESSION TAG	UNP Q13627
A	119	GLU	-	EXPRESSION TAG	UNP Q13627
A	120	ASN	-	EXPRESSION TAG	UNP Q13627
A	121	LEU	-	EXPRESSION TAG	UNP Q13627
A	122	TYR	-	EXPRESSION TAG	UNP Q13627
A	123	PHE	-	EXPRESSION TAG	UNP Q13627
A	124	GLN	-	EXPRESSION TAG	UNP Q13627
A	125	SER	-	EXPRESSION TAG	UNP Q13627

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MET	-	EXPRESSION TAG	UNP Q13627
A	127	SER	-	EXPRESSION TAG	UNP Q13627
B	104	MET	-	EXPRESSION TAG	UNP Q13627
B	105	HIS	-	EXPRESSION TAG	UNP Q13627
B	106	HIS	-	EXPRESSION TAG	UNP Q13627
B	107	HIS	-	EXPRESSION TAG	UNP Q13627
B	108	HIS	-	EXPRESSION TAG	UNP Q13627
B	109	HIS	-	EXPRESSION TAG	UNP Q13627
B	110	HIS	-	EXPRESSION TAG	UNP Q13627
B	111	SER	-	EXPRESSION TAG	UNP Q13627
B	112	SER	-	EXPRESSION TAG	UNP Q13627
B	113	GLY	-	EXPRESSION TAG	UNP Q13627
B	114	VAL	-	EXPRESSION TAG	UNP Q13627
B	115	ASP	-	EXPRESSION TAG	UNP Q13627
B	116	LEU	-	EXPRESSION TAG	UNP Q13627
B	117	GLY	-	EXPRESSION TAG	UNP Q13627
B	118	THR	-	EXPRESSION TAG	UNP Q13627
B	119	GLU	-	EXPRESSION TAG	UNP Q13627
B	120	ASN	-	EXPRESSION TAG	UNP Q13627
B	121	LEU	-	EXPRESSION TAG	UNP Q13627
B	122	TYR	-	EXPRESSION TAG	UNP Q13627
B	123	PHE	-	EXPRESSION TAG	UNP Q13627
B	124	GLN	-	EXPRESSION TAG	UNP Q13627
B	125	SER	-	EXPRESSION TAG	UNP Q13627
B	126	MET	-	EXPRESSION TAG	UNP Q13627
B	127	SER	-	EXPRESSION TAG	UNP Q13627
C	104	MET	-	EXPRESSION TAG	UNP Q13627
C	105	HIS	-	EXPRESSION TAG	UNP Q13627
C	106	HIS	-	EXPRESSION TAG	UNP Q13627
C	107	HIS	-	EXPRESSION TAG	UNP Q13627
C	108	HIS	-	EXPRESSION TAG	UNP Q13627
C	109	HIS	-	EXPRESSION TAG	UNP Q13627
C	110	HIS	-	EXPRESSION TAG	UNP Q13627
C	111	SER	-	EXPRESSION TAG	UNP Q13627
C	112	SER	-	EXPRESSION TAG	UNP Q13627
C	113	GLY	-	EXPRESSION TAG	UNP Q13627
C	114	VAL	-	EXPRESSION TAG	UNP Q13627
C	115	ASP	-	EXPRESSION TAG	UNP Q13627
C	116	LEU	-	EXPRESSION TAG	UNP Q13627
C	117	GLY	-	EXPRESSION TAG	UNP Q13627
C	118	THR	-	EXPRESSION TAG	UNP Q13627
C	119	GLU	-	EXPRESSION TAG	UNP Q13627

*Continued on next page...*

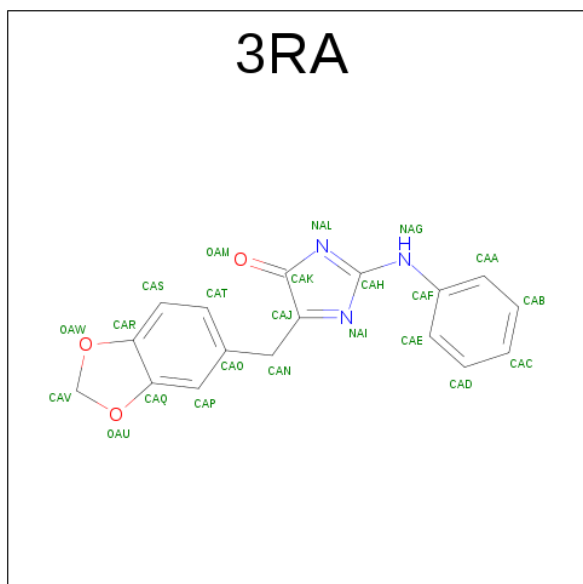
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	120	ASN	-	EXPRESSION TAG	UNP Q13627
C	121	LEU	-	EXPRESSION TAG	UNP Q13627
C	122	TYR	-	EXPRESSION TAG	UNP Q13627
C	123	PHE	-	EXPRESSION TAG	UNP Q13627
C	124	GLN	-	EXPRESSION TAG	UNP Q13627
C	125	SER	-	EXPRESSION TAG	UNP Q13627
C	126	MET	-	EXPRESSION TAG	UNP Q13627
C	127	SER	-	EXPRESSION TAG	UNP Q13627

- Molecule 2 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			25	12	4	8	1			
2	F	4	Total	C	N	O	P	0	0	0
			25	12	4	8	1			
2	G	4	Total	C	N	O	P	0	0	0
			25	12	4	8	1			

- Molecule 3 is 5-(1,3-BENZODIOXOL-5-YLMETHYL)-2-(PHENYLAMINO)-4H-IMIDAZO L-4-ONE (three-letter code: 3RA) (formula: C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	17	3	3		

Continued on next page...

*Continued from previous page...*

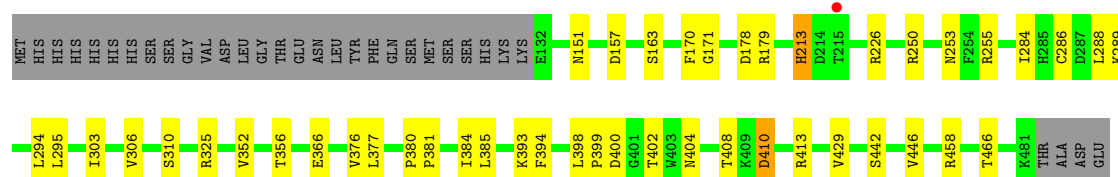
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			23	17	3	3		
3	C	1	Total	C	N	O	0	0
			23	17	3	3		

### 3 Residue-property plots


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.

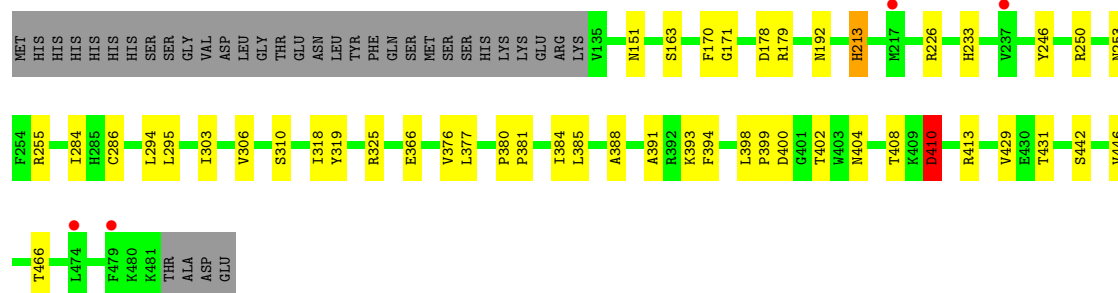
#### • Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain A: 




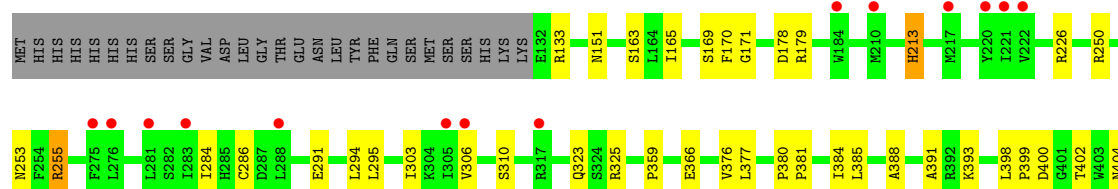
#### • Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain B: 



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

Chain C: 





- Molecule 2: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain E: 50% 50%



- Molecule 2: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain F: 50% 50%



- Molecule 2: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

Chain G: 25% 75%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.65Å 111.65Å 301.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.57 – 3.15 69.70 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (100.57-3.15) 99.7 (69.70-3.15)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.218 , 0.248 0.221 , 0.254	Depositor DCC
$R_{free}$ test set	1883 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: 3RA, PTR, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/2882	0.67	1/3888 (0.0%)
1	B	0.49	0/2855	0.61	0/3854
1	C	0.47	0/2850	0.60	0/3853
All	All	0.50	0/8587	0.62	1/11595 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	CG-CD-NE	6.12	124.65	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	HIS	Peptide
1	B	213	HIS	Peptide
1	C	213	HIS	Peptide

## 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	2844	0	2803	22	0
1	B	2813	0	2768	29	0
1	C	2812	0	2731	25	0
2	E	25	0	9	1	0
2	F	25	0	9	1	0
2	G	25	0	9	3	0
3	A	23	0	13	2	0
3	B	23	0	13	2	0
3	C	23	0	13	4	0
All	All	8613	0	8368	80	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 5.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LYS:NZ	2:G:900:SEP:O1P	2.11	0.80
1:B:431:THR:HG21	1:C:437:ARG:HG2	1.69	0.75
3:C:700:3RA:HAA	3:C:700:3RA:NAI	2.04	0.72
1:B:376:VAL:HG12	1:B:377:LEU:HD23	1.73	0.69
1:A:398:LEU:HD11	1:A:404:ASN:ND2	2.10	0.66
1:B:376:VAL:HG12	1:B:377:LEU:CD2	2.27	0.65
1:B:246:TYR:CE1	1:C:413:ARG:HD2	2.32	0.64
1:A:376:VAL:HG12	1:A:377:LEU:HD23	1.80	0.64
1:B:151:ASN:ND2	1:B:163:SER:HA	2.13	0.63
1:A:295:LEU:HD23	1:A:303:ILE:HG22	1.81	0.62
1:B:295:LEU:HD23	1:B:303:ILE:HG22	1.83	0.60
1:C:295:LEU:HD23	1:C:303:ILE:HG22	1.82	0.60
1:C:376:VAL:HG12	1:C:377:LEU:HD23	1.83	0.60
3:B:700:3RA:NAI	3:B:700:3RA:HAP	2.16	0.60
1:C:381:PRO:HD2	1:C:384:ILE:HD12	1.84	0.59
1:A:376:VAL:HG12	1:A:377:LEU:CD2	2.33	0.59
1:B:151:ASN:HD22	1:B:163:SER:HA	1.67	0.58
1:A:366:GLU:OE1	1:A:393:LYS:NZ	2.38	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:LEU:HD11	1:B:404:ASN:ND2	2.20	0.57
1:C:376:VAL:HG12	1:C:377:LEU:CD2	2.34	0.57
3:C:700:3RA:HAP	3:C:700:3RA:NAI	2.20	0.57
1:B:381:PRO:HD2	1:B:384:ILE:HD12	1.86	0.56
1:A:151:ASN:ND2	1:A:163:SER:HA	2.20	0.55
1:C:151:ASN:ND2	1:C:163:SER:HA	2.21	0.55
1:A:151:ASN:HD22	1:A:163:SER:HA	1.73	0.54
1:B:366:GLU:OE1	1:B:393:LYS:NZ	2.40	0.54
1:C:398:LEU:HD11	1:C:404:ASN:ND2	2.24	0.54
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.90	0.52
1:A:284:ILE:HG22	1:A:286:CYS:SG	2.49	0.52
1:A:381:PRO:HD2	1:A:384:ILE:HD12	1.92	0.51
1:B:429:VAL:O	1:B:446:VAL:HG22	2.10	0.51
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.91	0.51
3:C:700:3RA:CAA	3:C:700:3RA:NAI	2.70	0.50
1:B:400:ASP:OD1	1:B:402:THR:HG23	2.12	0.50
1:C:151:ASN:HD22	1:C:163:SER:HA	1.77	0.49
1:A:170:PHE:CD1	1:A:171:GLY:N	2.82	0.48
1:B:284:ILE:HG22	1:B:286:CYS:SG	2.53	0.48
1:C:366:GLU:OE1	1:C:393:LYS:NZ	2.45	0.48
2:E:901:UNK:O	2:E:902:UNK:CB	2.62	0.48
2:F:901:UNK:O	2:F:902:UNK:CB	2.62	0.48
1:B:246:TYR:CE1	1:C:413:ARG:CD	2.97	0.47
1:A:429:VAL:O	1:A:446:VAL:HG22	2.13	0.47
1:B:380:PRO:HD2	1:B:385:LEU:HD11	1.96	0.47
1:A:400:ASP:OD1	1:A:402:THR:HG23	2.14	0.46
1:C:294:LEU:HD13	1:C:306:VAL:CG2	2.45	0.46
1:A:178:ASP:OD2	1:A:226:ARG:NH2	2.48	0.46
1:B:294:LEU:HD13	1:B:306:VAL:HG21	1.97	0.46
1:C:170:PHE:CD1	1:C:171:GLY:N	2.85	0.46
1:C:255:ARG:NH2	1:C:437:ARG:O	2.50	0.45
1:B:170:PHE:CD1	1:B:171:GLY:N	2.84	0.45
1:B:294:LEU:HD13	1:B:306:VAL:CG2	2.47	0.45
1:C:284:ILE:HG22	1:C:286:CYS:SG	2.57	0.45
1:A:398:LEU:HB3	1:A:399:PRO:HD2	2.00	0.44
1:A:380:PRO:HD2	1:A:385:LEU:HD11	1.99	0.44
2:G:901:UNK:O	2:G:902:UNK:CB	2.65	0.44
1:A:398:LEU:HD11	1:A:404:ASN:HD21	1.80	0.44
1:B:318:ILE:O	1:B:319:TYR:CD1	2.71	0.44
1:C:165:ILE:HD12	3:C:700:3RA:HAV	2.00	0.44
1:C:294:LEU:HD13	1:C:306:VAL:HG21	1.99	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LYS:HD3	1:A:394:PHE:CZ	2.53	0.43
1:A:413:ARG:O	1:A:413:ARG:HG2	2.17	0.43
1:B:398:LEU:HB3	1:B:399:PRO:HD2	2.00	0.43
1:B:393:LYS:HD3	1:B:394:PHE:CZ	2.54	0.42
1:C:429:VAL:O	1:C:446:VAL:HG22	2.18	0.42
1:C:380:PRO:HD2	1:C:385:LEU:HD11	2.01	0.42
1:C:398:LEU:HB3	1:C:399:PRO:HD2	2.00	0.42
3:A:700:3RA:NAI	3:A:700:3RA:CAA	2.82	0.42
1:B:413:ARG:NE	1:C:291:GLU:OE2	2.51	0.42
1:B:410:ASP:HB3	1:C:169:SER:HA	2.01	0.42
1:A:288:LEU:O	1:A:289:LYS:HB3	2.20	0.42
1:A:294:LEU:HD13	1:A:306:VAL:CG2	2.49	0.42
1:A:294:LEU:N	1:A:294:LEU:HD12	2.35	0.42
1:C:178:ASP:OD2	1:C:226:ARG:NH2	2.53	0.41
1:C:400:ASP:OD1	1:C:402:THR:HG23	2.20	0.41
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.54	0.41
1:B:178:ASP:OD2	1:B:226:ARG:NH2	2.54	0.41
1:B:393:LYS:CE	2:G:900:SEP:O1P	2.68	0.41
1:A:352:VAL:O	1:A:356:THR:HG23	2.21	0.40
3:A:700:3RA:HAP	3:A:700:3RA:NAI	2.37	0.40
1:B:294:LEU:HD23	3:B:700:3RA:HAVA	2.03	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	346/382 (91%)	314 (91%)	30 (9%)	2 (1%)	28	70
1	B	343/382 (90%)	315 (92%)	26 (8%)	2 (1%)	28	70
1	C	346/382 (91%)	316 (91%)	27 (8%)	3 (1%)	20	62
All	All	1035/1146 (90%)	945 (91%)	83 (8%)	7 (1%)	25	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	410	ASP
1	B	410	ASP
1	C	410	ASP
1	B	253	ASN
1	C	253	ASN
1	C	323	GLN

### 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	299/338 (88%)	288 (96%)	11 (4%)	39	75
1	B	296/338 (88%)	286 (97%)	10 (3%)	42	76
1	C	291/338 (86%)	279 (96%)	12 (4%)	35	71
All	All	886/1014 (87%)	853 (96%)	33 (4%)	39	75

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ASP
1	A	179	ARG
1	A	213	HIS
1	A	250	ARG
1	A	255	ARG
1	A	310	SER
1	A	325	ARG
1	A	408	THR
1	A	410	ASP
1	A	442	SER
1	A	466	THR
1	B	179	ARG
1	B	213	HIS
1	B	250	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	255	ARG
1	B	310	SER
1	B	325	ARG
1	B	408	THR
1	B	410	ASP
1	B	442	SER
1	B	466	THR
1	C	133	ARG
1	C	179	ARG
1	C	213	HIS
1	C	250	ARG
1	C	255	ARG
1	C	310	SER
1	C	325	ARG
1	C	359	PRO
1	C	408	THR
1	C	410	ASP
1	C	442	SER
1	C	466	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	198	ASN
1	A	251	ASN
1	A	404	ASN
1	B	151	ASN
1	B	251	ASN
1	B	404	ASN
1	C	151	ASN
1	C	198	ASN
1	C	251	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	SEP	A	301	1	9,9,10	0.75	0	9,12,14	1.83	2 (22%)
1	PTR	A	321	1	15,16,17	0.84	0	19,22,24	1.11	1 (5%)
1	SEP	B	301	1	5,5,10	1.39	1 (20%)	1,5,14	1.71	0
1	PTR	B	321	1	15,16,17	0.70	0	19,22,24	1.09	2 (10%)
1	SEP	C	301	1	9,9,10	0.83	0	9,12,14	1.80	2 (22%)
1	PTR	C	321	1	15,16,17	0.74	0	19,22,24	0.93	0
2	SEP	E	900	2	9,9,10	0.89	1 (11%)	9,12,14	1.57	2 (22%)
2	SEP	F	900	2	9,9,10	0.91	1 (11%)	9,12,14	1.61	2 (22%)
2	SEP	G	900	2	9,9,10	0.91	0	9,12,14	1.66	2 (22%)

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	SEP	A	301	1	-	0/5/8/10	0/0/0/0
1	PTR	A	321	1	-	0/9/11/13	0/1/1/1
1	SEP	B	301	1	-	0/2/4/10	0/0/0/0
1	PTR	B	321	1	-	0/9/11/13	0/1/1/1
1	SEP	C	301	1	-	0/5/8/10	0/0/0/0
1	PTR	C	321	1	-	0/9/11/13	0/1/1/1
2	SEP	E	900	2	-	0/5/8/10	0/0/0/0
2	SEP	F	900	2	-	0/5/8/10	0/0/0/0
2	SEP	G	900	2	-	0/5/8/10	0/0/0/0

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	SEP	CA-C	2.03	1.52	1.50
2	F	900	SEP	CA-C	2.18	1.53	1.50
1	B	301	SEP	CA-C	2.95	1.54	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	900	SEP	OG-P-O1P	-2.39	99.78	106.47
2	F	900	SEP	O2P-P-OG	-2.26	100.73	106.73
2	E	900	SEP	O2P-P-OG	-2.25	100.76	106.73
1	B	321	PTR	CB-CA-C	-2.17	107.23	111.41
2	F	900	SEP	OG-P-O1P	-2.13	100.50	106.47
2	G	900	SEP	O2P-P-OG	-2.03	101.34	106.73
1	B	321	PTR	O3P-P-O2P	2.11	116.14	107.61
2	E	900	SEP	O3P-P-O2P	2.17	116.39	107.61
1	A	321	PTR	O3P-P-O2P	2.45	117.51	107.61
1	C	301	SEP	OG-CB-CA	2.53	110.66	108.17
1	A	301	SEP	OG-CB-CA	3.10	111.22	108.17
1	A	301	SEP	P-OG-CB	3.59	128.20	118.30
1	C	301	SEP	P-OG-CB	3.66	128.37	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	900	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
3	3RA	A	700	-	25,26,26	2.82	5 (20%)	27,36,36	1.86	5 (18%)
3	3RA	B	700	-	25,26,26	2.69	5 (20%)	27,36,36	1.68	6 (22%)
3	3RA	C	700	-	25,26,26	2.47	4 (16%)	27,36,36	1.75	6 (22%)

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
3	3RA	A	700	-	-	0/8/26/26	0/4/4/4
3	3RA	B	700	-	-	0/8/26/26	0/4/4/4
3	3RA	C	700	-	-	0/8/26/26	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	3RA	CAN-CAJ	-9.14	1.40	1.50
3	B	700	3RA	CAN-CAJ	-9.12	1.40	1.50
3	C	700	3RA	CAN-CAJ	-8.53	1.41	1.50
3	A	700	3RA	CAN-CAO	-6.52	1.40	1.51
3	B	700	3RA	CAN-CAO	-6.41	1.41	1.51
3	C	700	3RA	CAN-CAO	-5.91	1.41	1.51
3	A	700	3RA	CAK-CAJ	-5.59	1.38	1.49
3	B	700	3RA	CAK-CAJ	-5.04	1.39	1.49
3	C	700	3RA	CAK-CAJ	-4.32	1.41	1.49
3	A	700	3RA	CAF-NAG	-4.29	1.33	1.41
3	C	700	3RA	CAF-NAG	-3.33	1.35	1.41
3	B	700	3RA	CAF-NAG	-3.12	1.35	1.41
3	A	700	3RA	CAK-NAL	-3.08	1.32	1.37
3	B	700	3RA	OAW-CAR	-2.46	1.34	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	700	3RA	CAK-CAJ-NAI	-5.18	105.34	111.59
3	A	700	3RA	CAK-CAJ-NAI	-4.64	105.99	111.59
3	B	700	3RA	CAK-CAJ-NAI	-3.87	106.92	111.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	3RA	OAW-CAV-OAU	-3.62	102.44	108.10
3	A	700	3RA	OAW-CAV-OAU	-3.03	103.37	108.10
3	A	700	3RA	CAN-CAO-CAT	-2.54	117.22	120.89
3	B	700	3RA	CAV-OAU-CAQ	-2.35	102.20	105.35
3	C	700	3RA	CAP-CAQ-CAR	-2.12	119.23	122.01
3	C	700	3RA	OAW-CAR-CAS	2.03	131.29	127.86
3	B	700	3RA	OAW-CAR-CAS	2.07	131.36	127.86
3	B	700	3RA	OAU-CAQ-CAP	2.17	130.75	127.86
3	C	700	3RA	CAN-CAO-CAP	2.21	123.85	120.41
3	A	700	3RA	OAU-CAQ-CAP	2.41	131.06	127.86
3	C	700	3RA	OAU-CAQ-CAP	2.67	131.40	127.86
3	B	700	3RA	CAO-CAN-CAJ	3.63	122.57	113.75
3	C	700	3RA	CAO-CAN-CAJ	3.77	122.91	113.75
3	A	700	3RA	CAO-CAN-CAJ	4.93	125.73	113.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	3RA	2	0
3	B	700	3RA	2	0
3	C	700	3RA	4	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<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	348/382 (91%)	-0.21	1 (0%) 93 92	44, 76, 115, 190	0
1	B	345/382 (90%)	-0.05	4 (1%) 79 66	65, 98, 142, 191	0
1	C	348/382 (91%)	0.29	17 (4%) 30 16	77, 146, 205, 234	0
2	E	0/4	-	-	-	-
2	F	0/4	-	-	-	-
2	G	0/4	-	-	-	-
All	All	1041/1158 (89%)	0.01	22 (2%) 64 48	44, 101, 181, 234	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	MET	6.9
1	C	222	VAL	5.3
1	C	305	ILE	5.1
1	C	210	MET	4.3
1	B	217	MET	3.5
1	C	317	ARG	3.0
1	B	474	LEU	3.0
1	C	306	VAL	2.8
1	C	283	ILE	2.7
1	C	220	TYR	2.6
1	C	478	PHE	2.6
1	C	221	ILE	2.6
1	C	410	ASP	2.6
1	B	237	VAL	2.5
1	C	275	PHE	2.5
1	C	276	LEU	2.5
1	B	479	PHE	2.4
1	A	215	THR	2.4
1	C	479	PHE	2.3
1	C	184	TRP	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	281	LEU	2.1
1	C	288	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	PTR	B	321	16/17	0.94	0.22	-	76,79,82,82	0
1	SEP	A	301	10/11	0.86	0.22	-	92,112,151,156	0
1	PTR	A	321	16/17	0.95	0.20	-	61,64,68,71	0
1	SEP	B	301	6/11	0.90	0.19	-	113,120,124,128	0
1	SEP	C	301	10/11	0.83	0.24	-	174,186,218,221	0
1	PTR	C	321	16/17	0.87	0.24	-	120,134,143,152	0
2	SEP	G	900	10/11	0.87	0.18	-	114,138,170,182	0
2	SEP	F	900	10/11	0.78	0.28	-	135,157,179,197	0
2	SEP	E	900	10/11	0.85	0.23	-	97,113,151,160	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
3	3RA	A	700	23/23	0.98	0.26	0.94	49,55,57,63	0
3	3RA	B	700	23/23	0.93	0.30	0.82	61,70,78,80	0
3	3RA	C	700	23/23	0.93	0.33	0.02	74,83,87,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.