



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2016 – 09:22 PM EST

PDB ID : 5GQR  
Title : Crystal structure of PXY-CLE41-SERK2  
Authors : Chai, J.J.; Zhang, H.Q.  
Deposited on : 2016-08-08  
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (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

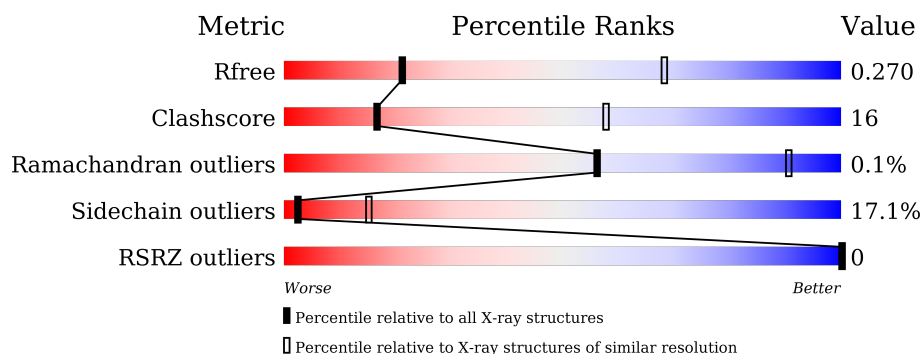
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 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	B	598	<div> <div>54%</div> <div>37%</div> <div>8%</div> <div>.</div> </div>
2	C	12	<div> <div>50%</div> <div>42%</div> <div>8%</div> </div>
3	K	185	<div> <div>65%</div> <div>29%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6160 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 Leucine-rich repeat receptor-like protein kinase TDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	593	Total	C	N	O	S	0	0	0
			4613	2963	765	872	13			

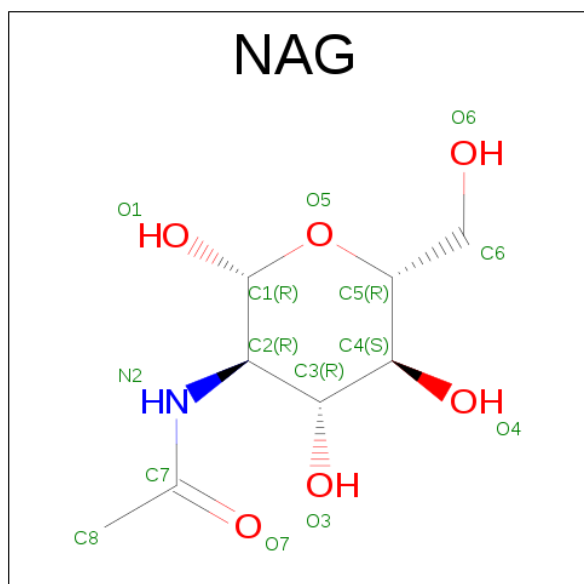
- Molecule 2 is a protein called TDIF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			89	53	16	20			

- Molecule 3 is a protein called Somatic embryogenesis receptor kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	185	Total	C	N	O	S	0	0	0
			1402	883	240	272	7			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

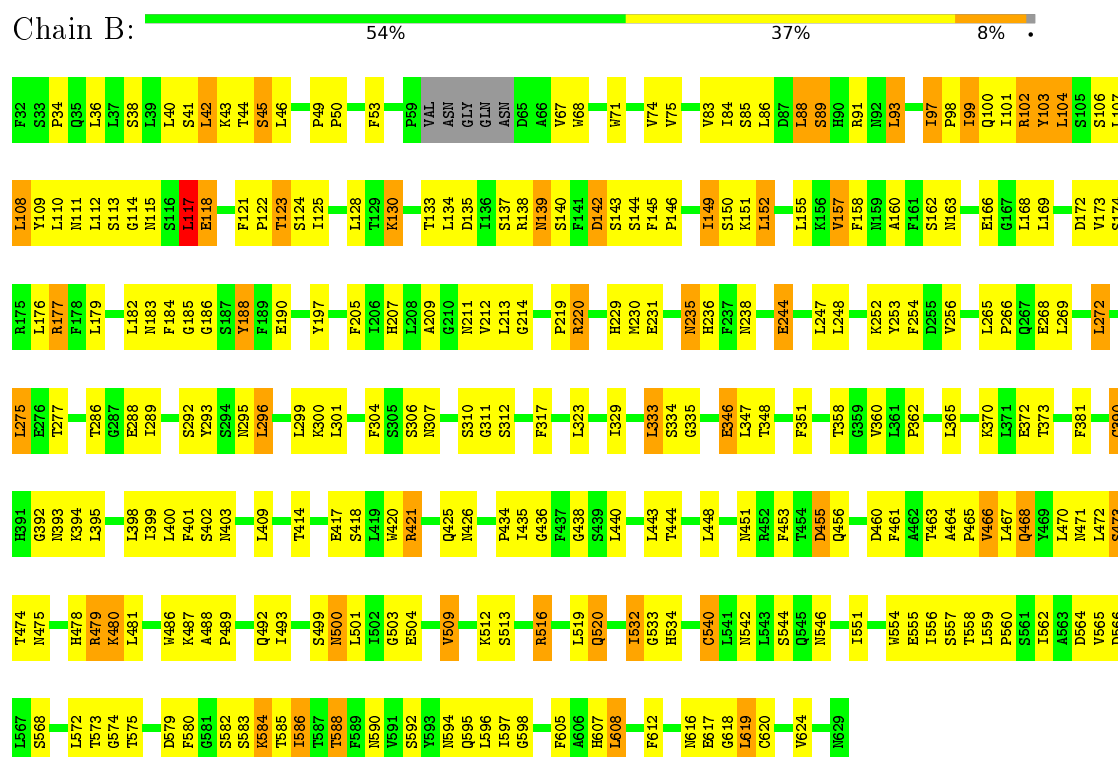


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	K	1	Total 14	C 8	N 1	O 5	0	0
4	K	1	Total 14	C 8	N 1	O 5	0	0

### 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 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.

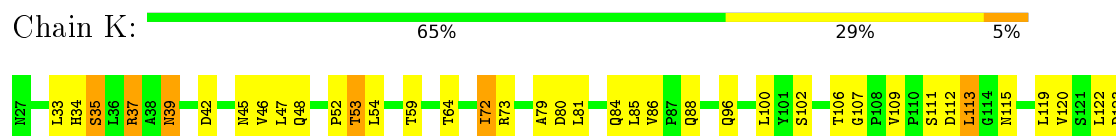
- Molecule 1: Leucine-rich repeat receptor-like protein kinase TDR



- Molecule 2: TDIF



- Molecule 3: Somatic embryogenesis receptor kinase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 <sub>2</sub> 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.42Å 162.42Å 187.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.47 – 3.50 40.47 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.47-3.50) 94.4 (40.47-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.219 , 0.276 0.218 , 0.270	Depositor DCC
$R_{free}$ test set	920 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	91.3	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 27.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	B	0.47	0/4729	0.75	1/6428 (0.0%)
2	C	0.65	0/82	0.95	0/109
3	K	0.48	0/1432	0.72	0/1963
All	All	0.48	0/6243	0.75	1/8500 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	117	LEU	CA-CB-CG	5.68	128.37	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4613	0	4546	167	0
2	C	89	0	78	4	0
3	K	1402	0	1366	35	0
4	B	28	0	26	0	0
4	K	28	0	26	0	0
All	All	6160	0	6042	201	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 16.

All (201) 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)
3:K:64:THR:HB	3:K:73:ARG:HB2	1.60	0.81
1:B:438:GLY:HA2	1:B:464:ALA:HB2	1.63	0.81
1:B:219:PRO:HB3	1:B:244:GLU:HG3	1.62	0.80
1:B:213:LEU:HB2	1:B:235:ASN:HD22	1.46	0.78
1:B:421:ARG:HH12	3:K:54:LEU:HD11	1.47	0.78
1:B:565:VAL:H	1:B:588:THR:HG22	1.48	0.77
1:B:448:LEU:O	1:B:451:ASN:ND2	2.21	0.72
1:B:409:LEU:HD23	1:B:434:PRO:HD2	1.72	0.72
1:B:455:ASP:OD1	1:B:479:ARG:NH2	2.24	0.71
1:B:420:TRP:HA	1:B:443:LEU:HA	1.73	0.71
1:B:573:THR:HB	1:B:595:GLN:HB2	1.73	0.70
1:B:292:SER:O	1:B:295:ASN:ND2	2.25	0.69
3:K:183:ASP:OD1	3:K:183:ASP:N	2.25	0.68
1:B:583:SER:HB3	1:B:586:ILE:HD11	1.75	0.68
1:B:346:GLU:OE2	1:B:370:LYS:NZ	2.26	0.67
1:B:444:THR:HG22	1:B:466:VAL:HB	1.76	0.66
1:B:89:SER:HB3	1:B:113:SER:H	1.61	0.65
1:B:555:GLU:O	1:B:558:THR:OG1	2.14	0.65
1:B:390:CYS:O	1:B:393:ASN:N	2.27	0.65
1:B:40:LEU:O	1:B:44:THR:HG23	1.96	0.65
1:B:139:ASN:N	1:B:139:ASN:HD22	1.95	0.64
3:K:39:ASN:O	3:K:39:ASN:ND2	2.28	0.64
1:B:75:VAL:HB	1:B:85:SER:HB3	1.79	0.64
3:K:72:ILE:HG12	3:K:73:ARG:HG3	1.80	0.64
1:B:150:SER:N	1:B:172:ASP:OD2	2.31	0.64
1:B:185:GLY:HA2	1:B:211:ASN:HD21	1.62	0.64
1:B:493:ILE:HG23	1:B:516:ARG:HB3	1.80	0.63
1:B:166:GLU:HA	1:B:188:TYR:O	2.00	0.62
1:B:334:SER:OG	1:B:335:GLY:N	2.30	0.62
1:B:289:ILE:HD11	1:B:333:LEU:HD11	1.80	0.62
1:B:584:LYS:HD2	1:B:585:THR:HG23	1.80	0.62
1:B:137:SER:O	1:B:139:ASN:ND2	2.33	0.62
1:B:214:GLY:HA2	1:B:236:HIS:O	2.00	0.61
3:K:210:CYS:HB2	3:K:211:PRO:HD2	1.83	0.60
1:B:597:ILE:HG22	1:B:618:GLY:HA3	1.85	0.59
3:K:42:ASP:HB2	3:K:47:LEU:HD12	1.83	0.59
1:B:42:LEU:HA	1:B:98:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HB3	1:B:134:LEU:HD12	1.84	0.58
1:B:107:LEU:HD21	1:B:110:LEU:HD13	1.85	0.58
1:B:185:GLY:HA2	1:B:211:ASN:ND2	2.18	0.58
1:B:584:LYS:HE3	1:B:584:LYS:H	1.67	0.58
1:B:499:SER:O	1:B:501:LEU:N	2.36	0.58
1:B:533:GLY:HA2	1:B:559:LEU:HD21	1.86	0.58
1:B:551:ILE:HG22	1:B:574:GLY:HA3	1.86	0.57
3:K:34:HIS:ND1	3:K:52:PRO:HG3	2.19	0.57
1:B:596:LEU:HB2	1:B:616:ASN:ND2	2.19	0.57
1:B:296:LEU:HD13	1:B:299:LEU:HD22	1.87	0.56
1:B:162:SER:HA	1:B:186:GLY:O	2.06	0.56
1:B:456:GLN:HG3	1:B:479:ARG:HG2	1.87	0.56
1:B:138:ARG:C	1:B:139:ASN:HD22	2.08	0.56
1:B:97:ILE:HD12	1:B:122:PRO:HG3	1.87	0.56
3:K:119:LEU:HD23	3:K:140:LEU:HD13	1.86	0.56
3:K:176:ARG:NH1	3:K:199:LEU:HD13	2.21	0.56
1:B:121:PHE:CD1	1:B:122:PRO:HD2	2.40	0.55
1:B:123:THR:HG23	1:B:146:PRO:HB2	1.88	0.55
3:K:79:ALA:HB3	3:K:81:LEU:HG	1.88	0.55
1:B:230:MET:HE1	1:B:254:PHE:HE1	1.72	0.55
3:K:37:ARG:HG2	3:K:47:LEU:HB3	1.88	0.55
1:B:544:SER:O	1:B:546:ASN:ND2	2.39	0.55
1:B:540:CYS:HB2	1:B:564:ASP:HB2	1.88	0.55
1:B:401:PHE:HB2	1:B:425:GLN:HG2	1.89	0.55
1:B:133:THR:HG23	1:B:157:VAL:HB	1.89	0.55
3:K:144:ARG:NH1	3:K:168:GLN:OE1	2.21	0.54
1:B:101:ILE:C	1:B:103:TYR:H	2.10	0.54
1:B:414:THR:HG21	1:B:436:GLY:H	1.73	0.54
1:B:516:ARG:CZ	1:B:540:CYS:HB3	2.37	0.54
3:K:119:LEU:HD21	3:K:122:LEU:HB2	1.89	0.54
1:B:84:ILE:HA	1:B:107:LEU:HA	1.90	0.54
1:B:101:ILE:HG22	1:B:102:ARG:H	1.72	0.54
1:B:460:ASP:O	1:B:463:THR:OG1	2.17	0.54
3:K:34:HIS:CG	3:K:52:PRO:HG3	2.44	0.53
1:B:594:ASN:N	1:B:616:ASN:OD1	2.38	0.52
1:B:370:LYS:HA	1:B:394:LYS:HE2	1.90	0.52
1:B:312:SER:HA	1:B:334:SER:O	2.10	0.52
1:B:186:GLY:O	2:C:93:HIS:HB3	2.09	0.52
1:B:43:LYS:HA	1:B:53:PHE:CE2	2.45	0.52
1:B:598:GLY:O	1:B:619:LEU:HD12	2.10	0.52
3:K:182:PRO:HG2	3:K:187:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:HD12	1:B:443:LEU:HD22	1.92	0.51
1:B:329:ILE:HD11	1:B:351:PHE:HD2	1.76	0.51
1:B:362:PRO:O	1:B:365:LEU:HB2	2.11	0.51
1:B:475:ASN:H	1:B:499:SER:HB3	1.75	0.51
1:B:329:ILE:HD11	1:B:351:PHE:CD2	2.46	0.50
1:B:420:TRP:CE3	1:B:421:ARG:HB2	2.46	0.50
1:B:605:PHE:HA	1:B:608:LEU:HG	1.94	0.50
1:B:68:TRP:HA	1:B:71:TRP:CE2	2.47	0.50
1:B:100:GLN:O	1:B:103:TYR:HB2	2.11	0.50
3:K:106:THR:OG1	3:K:107:GLY:N	2.45	0.50
1:B:421:ARG:NH1	2:C:104:ASN:O	2.45	0.50
1:B:487:LYS:HG2	1:B:509:VAL:HG13	1.93	0.50
1:B:566:ASP:OD1	1:B:590:ASN:HB3	2.12	0.49
1:B:135:ASP:OD1	1:B:137:SER:OG	2.27	0.49
1:B:465:PRO:HA	1:B:489:PRO:HG2	1.93	0.49
2:C:100:ASN:OD1	2:C:102:ILE:HG23	2.13	0.49
1:B:253:TYR:CE2	1:B:277:THR:HG21	2.46	0.49
3:K:178:SER:HA	3:K:200:ASP:O	2.11	0.49
1:B:177:ARG:HG2	1:B:177:ARG:H	1.48	0.49
1:B:46:LEU:HD13	1:B:93:LEU:HD11	1.95	0.49
1:B:34:PRO:O	1:B:38:SER:HB2	2.13	0.48
1:B:304:PHE:O	1:B:307:ASN:ND2	2.37	0.48
1:B:470:LEU:HD11	1:B:472:LEU:HD21	1.94	0.48
1:B:168:LEU:HA	1:B:190:GLU:O	2.14	0.48
1:B:293:TYR:C	1:B:295:ASN:H	2.16	0.48
1:B:41:SER:O	1:B:45:SER:HB3	2.13	0.48
1:B:480:LYS:HD3	1:B:503:GLY:HA3	1.95	0.48
1:B:486:TRP:HH2	1:B:519:LEU:HD11	1.79	0.48
1:B:266:PRO:HD2	1:B:269:LEU:HD12	1.96	0.48
1:B:86:LEU:HG	1:B:88:LEU:HD21	1.96	0.48
3:K:45:ASN:HB3	3:K:48:GLN:HB2	1.96	0.48
1:B:142:ASP:CG	1:B:143:SER:N	2.66	0.47
1:B:390:CYS:O	1:B:392:GLY:N	2.47	0.47
1:B:499:SER:O	1:B:499:SER:OG	2.25	0.47
3:K:176:ARG:HH11	3:K:199:LEU:HD13	1.80	0.47
1:B:468:GLN:HG2	1:B:492:GLN:HE21	1.79	0.47
1:B:109:TYR:CE1	1:B:111:ASN:HB2	2.49	0.47
1:B:398:LEU:HD11	1:B:400:LEU:HG	1.96	0.47
1:B:572:LEU:HB2	1:B:594:ASN:OD1	2.14	0.46
1:B:99:ILE:HD12	1:B:99:ILE:H	1.80	0.46
1:B:471:ASN:OD1	1:B:473:SER:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:84:GLN:HG2	3:K:107:GLY:HA3	1.97	0.46
1:B:235:ASN:OD1	1:B:235:ASN:N	2.47	0.46
1:B:596:LEU:HB2	1:B:616:ASN:HD22	1.79	0.46
1:B:179:LEU:HD21	1:B:182:LEU:HB2	1.98	0.46
1:B:138:ARG:HA	1:B:162:SER:HB3	1.96	0.46
1:B:149:ILE:HD12	1:B:152:LEU:HD23	1.98	0.45
3:K:53:THR:OG1	3:K:53:THR:O	2.34	0.45
1:B:118:GLU:HB2	1:B:140:SER:HB3	1.99	0.45
1:B:448:LEU:HD22	1:B:453:PHE:CE2	2.51	0.45
1:B:158:PHE:CZ	1:B:160:ALA:HB2	2.52	0.45
1:B:288:GLU:HG2	1:B:311:GLY:HA3	1.98	0.45
1:B:213:LEU:HD12	1:B:235:ASN:ND2	2.32	0.45
1:B:300:LYS:O	1:B:323:LEU:HD12	2.16	0.45
3:K:135:ASP:OD1	3:K:158:PRO:HB3	2.16	0.45
1:B:520:GLN:H	1:B:520:GLN:HG3	1.10	0.44
3:K:147:ARG:HG2	3:K:171:ASP:HB3	1.99	0.44
1:B:532:ILE:HG21	1:B:556:ILE:HG12	2.00	0.44
1:B:289:ILE:H	1:B:289:ILE:HD12	1.81	0.44
1:B:444:THR:HA	1:B:467:LEU:HA	2.00	0.44
1:B:145:PHE:HA	1:B:146:PRO:HD2	1.72	0.44
3:K:112:ASP:O	3:K:115:ASN:HB2	2.18	0.44
1:B:151:LYS:HB2	1:B:151:LYS:HE2	1.78	0.44
1:B:174:SER:HB2	1:B:197:TYR:HD1	1.83	0.44
1:B:93:LEU:O	1:B:115:ASN:HB3	2.18	0.44
1:B:565:VAL:N	1:B:588:THR:HG22	2.24	0.43
1:B:130:LYS:HA	1:B:130:LYS:HD2	1.65	0.43
1:B:532:ILE:C	1:B:534:HIS:H	2.21	0.43
1:B:584:LYS:CE	1:B:584:LYS:H	2.31	0.43
1:B:139:ASN:N	1:B:139:ASN:ND2	2.65	0.43
1:B:138:ARG:HH12	2:C:94:GLU:CD	2.21	0.43
1:B:478:HIS:CD2	1:B:500:ASN:HB3	2.53	0.43
1:B:46:LEU:HD22	1:B:93:LEU:HG	1.98	0.43
1:B:488:ALA:HA	1:B:489:PRO:HD3	1.80	0.43
1:B:512:LYS:HG2	1:B:513:SER:OG	2.18	0.43
1:B:272:LEU:HD13	1:B:275:LEU:HD13	1.99	0.43
1:B:347:LEU:HD12	1:B:348:THR:H	1.83	0.43
1:B:74:VAL:HG13	1:B:83:VAL:HG13	2.01	0.43
1:B:152:LEU:HB3	1:B:155:LEU:HB2	2.00	0.42
1:B:381:PHE:HB2	1:B:403:ASN:OD1	2.19	0.42
1:B:252:LYS:HA	1:B:275:LEU:HA	2.01	0.42
1:B:608:LEU:HD13	1:B:612:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:H	1:B:139:ASN:HD21	1.67	0.42
1:B:481:LEU:H	1:B:481:LEU:HD12	1.85	0.42
1:B:616:ASN:HB3	1:B:619:LEU:HD22	2.01	0.42
1:B:117:LEU:O	1:B:117:LEU:HD23	2.20	0.42
1:B:139:ASN:O	1:B:163:ASN:HA	2.19	0.42
1:B:205:PHE:CE2	1:B:229:HIS:CD2	3.08	0.42
1:B:220:ARG:O	1:B:220:ARG:HG3	2.19	0.42
1:B:293:TYR:C	1:B:295:ASN:N	2.72	0.42
1:B:89:SER:HA	1:B:115:ASN:HD21	1.84	0.42
3:K:113:LEU:HA	3:K:113:LEU:HD12	1.86	0.42
3:K:35:SER:HB2	3:K:86:VAL:HG21	2.01	0.42
1:B:207:HIS:CE1	1:B:209:ALA:HB3	2.54	0.42
1:B:207:HIS:HA	1:B:231:GLU:O	2.20	0.41
1:B:149:ILE:HG23	1:B:172:ASP:OD2	2.20	0.41
1:B:562:ILE:O	1:B:562:ILE:HG23	2.20	0.41
1:B:114:GLY:H	1:B:139:ASN:ND2	2.19	0.41
1:B:481:LEU:HD11	1:B:501:LEU:HD13	2.02	0.41
1:B:88:LEU:HB2	1:B:91:ARG:HD2	2.02	0.41
1:B:607:HIS:ND1	3:K:168:GLN:HG2	2.35	0.41
1:B:104:LEU:HD12	1:B:104:LEU:H	1.86	0.41
1:B:253:TYR:HA	1:B:277:THR:HB	2.01	0.41
1:B:448:LEU:HD23	1:B:448:LEU:HA	1.91	0.41
1:B:520:GLN:HG2	1:B:542:ASN:CG	2.40	0.41
3:K:33:LEU:HD23	3:K:33:LEU:HA	1.94	0.41
3:K:96:GLN:O	3:K:119:LEU:HD12	2.20	0.41
1:B:40:LEU:O	1:B:43:LYS:HB3	2.20	0.41
1:B:584:LYS:CD	1:B:585:THR:HG23	2.50	0.41
1:B:453:PHE:HB2	1:B:475:ASN:OD1	2.21	0.41
3:K:180:SER:HA	3:K:202:CYS:O	2.21	0.41
3:K:156:PRO:HA	3:K:178:SER:O	2.21	0.40
1:B:108:LEU:H	1:B:108:LEU:HG	1.66	0.40
1:B:93:LEU:HD23	1:B:115:ASN:HB3	2.03	0.40
1:B:372:GLU:O	1:B:395:LEU:HA	2.20	0.40
3:K:123:ASP:HB3	3:K:125:TYR:CE1	2.57	0.40
3:K:39:ASN:HD22	3:K:39:ASN:C	2.19	0.40
3:K:85:LEU:HD21	3:K:100:LEU:CD1	2.51	0.40
1:B:253:TYR:CD2	1:B:277:THR:HG21	2.56	0.40
1:B:520:GLN:HE21	1:B:542:ASN:HB3	1.86	0.40
1:B:559:LEU:HA	1:B:560:PRO:HD3	1.69	0.40
1:B:402:SER:HA	1:B:426:ASN:HB2	2.03	0.40
1:B:49:PRO:HA	1:B:50:PRO:HD3	1.87	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	B	589/598 (98%)	555 (94%)	33 (6%)	1 (0%)	52	88
2	C	9/12 (75%)	9 (100%)	0	0	100	100
3	K	183/185 (99%)	170 (93%)	13 (7%)	0	100	100
All	All	781/795 (98%)	734 (94%)	46 (6%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	500	ASN

### 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	B	529/533 (99%)	435 (82%)	94 (18%)	2	13
2	C	10/10 (100%)	8 (80%)	2 (20%)	1	9
3	K	164/169 (97%)	140 (85%)	24 (15%)	4	22
All	All	703/712 (99%)	583 (83%)	120 (17%)	2	15

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	LEU
1	B	42	LEU
1	B	45	SER
1	B	67	VAL
1	B	88	LEU
1	B	89	SER
1	B	93	LEU
1	B	97	ILE
1	B	99	ILE
1	B	102	ARG
1	B	103	TYR
1	B	104	LEU
1	B	106	SER
1	B	108	LEU
1	B	112	LEU
1	B	117	LEU
1	B	118	GLU
1	B	123	THR
1	B	124	SER
1	B	125	ILE
1	B	128	LEU
1	B	130	LYS
1	B	139	ASN
1	B	142	ASP
1	B	144	SER
1	B	149	ILE
1	B	152	LEU
1	B	157	VAL
1	B	169	LEU
1	B	173	VAL
1	B	176	LEU
1	B	177	ARG
1	B	183	ASN
1	B	184	PHE
1	B	188	TYR
1	B	212	VAL
1	B	220	ARG
1	B	235	ASN
1	B	238	ASN
1	B	244	GLU
1	B	247	LEU
1	B	248	LEU
1	B	256	VAL

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Mol	Chain	Res	Type
1	B	265	LEU
1	B	268	GLU
1	B	272	LEU
1	B	275	LEU
1	B	286	THR
1	B	296	LEU
1	B	301	LEU
1	B	306	SER
1	B	310	SER
1	B	317	PHE
1	B	333	LEU
1	B	346	GLU
1	B	358	THR
1	B	360	VAL
1	B	373	THR
1	B	390	CYS
1	B	399	ILE
1	B	417	GLU
1	B	418	SER
1	B	421	ARG
1	B	435	ILE
1	B	455	ASP
1	B	461	PHE
1	B	466	VAL
1	B	468	GLN
1	B	473	SER
1	B	474	THR
1	B	479	ARG
1	B	480	LYS
1	B	504	GLU
1	B	509	VAL
1	B	516	ARG
1	B	520	GLN
1	B	532	ILE
1	B	540	CYS
1	B	554	TRP
1	B	557	SER
1	B	568	SER
1	B	575	THR
1	B	579	ASP
1	B	580	PHE
1	B	582	SER

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Mol	Chain	Res	Type
1	B	584	LYS
1	B	586	ILE
1	B	588	THR
1	B	592	SER
1	B	608	LEU
1	B	617	GLU
1	B	619	LEU
1	B	620	CYS
1	B	624	VAL
2	C	102	ILE
2	C	103	SER
3	K	35	SER
3	K	37	ARG
3	K	39	ASN
3	K	46	VAL
3	K	53	THR
3	K	59	THR
3	K	72	ILE
3	K	80	ASP
3	K	88	GLN
3	K	102	SER
3	K	109	VAL
3	K	111	SER
3	K	113	LEU
3	K	120	VAL
3	K	130	THR
3	K	140	LEU
3	K	142	LYS
3	K	165	MET
3	K	168	GLN
3	K	176	ARG
3	K	183	ASP
3	K	189	LEU
3	K	206	THR
3	K	208	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	139	ASN
1	B	229	HIS
1	B	378	ASN

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Mol	Chain	Res	Type
1	B	492	GLN
3	K	62	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	HYP	C	99	2	6,8,9	1.78	2 (33%)	5,10,12	2.25	2 (40%)

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	HYP	C	99	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	99	HYP	CB-CA	-2.80	1.48	1.54
2	C	99	HYP	CB-CG	-2.22	1.47	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	99	HYP	O-C-CA	-2.86	117.89	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	99	HYP	CB-CG-CD	3.68	107.58	103.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	$\# Z  > 2$
4	NAG	B	701	1	14,14,15	0.55	0	15,19,21	1.24	1 (6%)
4	NAG	B	702	1	14,14,15	0.55	0	15,19,21	1.43	2 (13%)
4	NAG	K	301	3	14,14,15	0.45	0	15,19,21	1.20	1 (6%)
4	NAG	K	302	3	14,14,15	1.08	1 (7%)	15,19,21	2.30	3 (20%)

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
4	NAG	B	701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	702	1	-	0/6/23/26	0/1/1/1
4	NAG	K	301	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	302	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	302	NAG	O7-C7	2.24	1.28	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	302	NAG	C3-C4-C5	-3.93	103.22	110.23
4	B	702	NAG	O4-C4-C3	2.19	115.29	110.36
4	K	302	NAG	O4-C4-C3	2.33	115.61	110.36
4	B	701	NAG	C1-O5-C5	2.88	116.38	112.14
4	K	301	NAG	C2-N2-C7	3.31	127.41	123.11
4	B	702	NAG	C1-O5-C5	4.00	118.02	112.14
4	K	302	NAG	C1-O5-C5	6.61	121.86	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	B	593/598 (99%)	-0.45	0 100 100	50, 78, 108, 135	0
2	C	11/12 (91%)	-0.62	0 100 100	55, 67, 75, 78	0
3	K	185/185 (100%)	-0.34	0 100 100	54, 68, 99, 129	0
All	All	789/795 (99%)	-0.43	0 100 100	50, 75, 106, 135	0

There are no RSRZ outliers to report.

### 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
2	HYP	C	99	8/9	0.97	0.16	-	76,78,79,80	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	702	14/15	0.85	0.32	0.70	70,70,71,71	0
4	NAG	B	701	14/15	0.89	0.22	-	96,100,102,103	0
4	NAG	K	302	14/15	0.87	0.22	-	79,81,84,85	0
4	NAG	K	301	14/15	0.70	0.32	-	89,90,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.