



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:24 PM GMT

PDB ID : 4EOK  
Title : Thr 160 phosphorylated CDK2 H84S, Q85M, K89D - human cyclin A3 complex with the inhibitor NU6102  
Authors : Echalier, A.; Cot, E.; Camasses, A.; Hodimont, E.; Hoh, F.; Sheinerman, F.; Krasinska, L.; Fisher, D.  
Deposited on : 2012-04-14  
Resolution : 2.57 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 (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

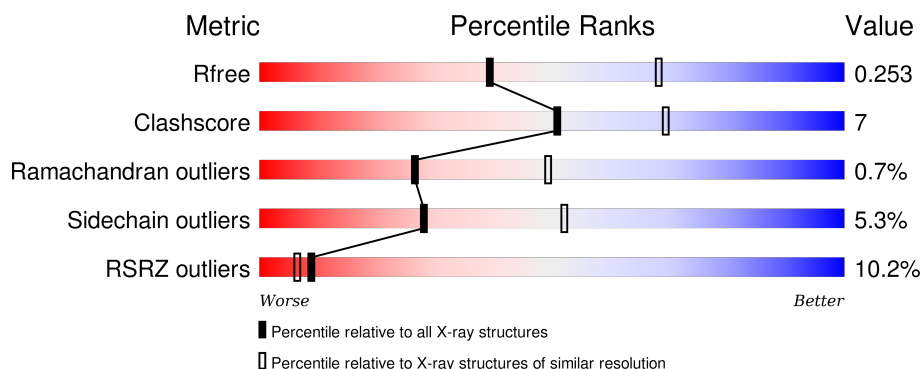
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	300	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	C	300	<div> <div>15%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	B	258	<div> <div>6%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	D	258	<div> <div>16%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8994 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	P	S	0	0	0
			2362	1534	400	418	1	9			
1	C	300	Total	C	N	O	P	S	0	0	0
			2405	1559	406	430	1	9			

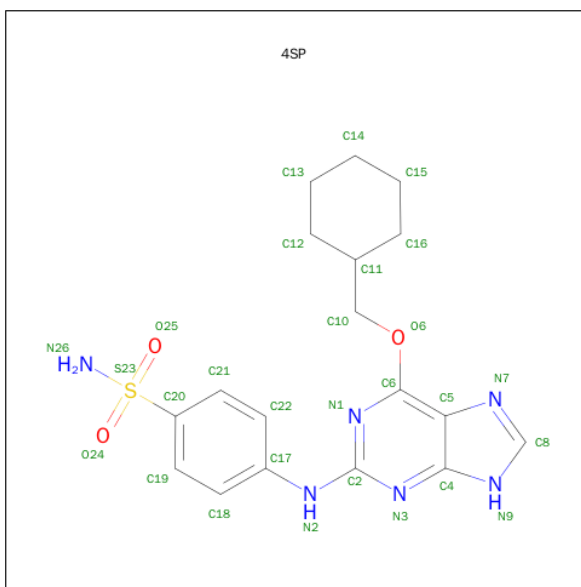
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	EXPRESSION TAG	UNP P24941
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
A	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
A	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
A	89	ASP	LYS	ENGINEERED MUTATION	UNP P24941
C	-2	LEU	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941
C	84	SER	HIS	ENGINEERED MUTATION	UNP P24941
C	85	MET	GLN	ENGINEERED MUTATION	UNP P24941
C	89	ASP	LYS	ENGINEERED MUTATION	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

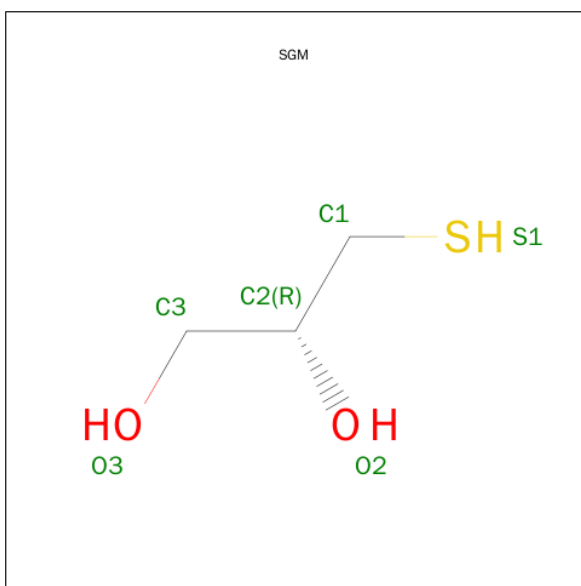
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2083	1350	339	383	11				
2	D	256	Total	C	N	O	S		0	0	0
			2068	1339	337	381	11				

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (three-letter code: 4SP) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	18	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			28	18	6	3	1		

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula:  $C_3H_8O_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		
4	D	1	Total	C	O	S	0	0
			6	3	2	1		

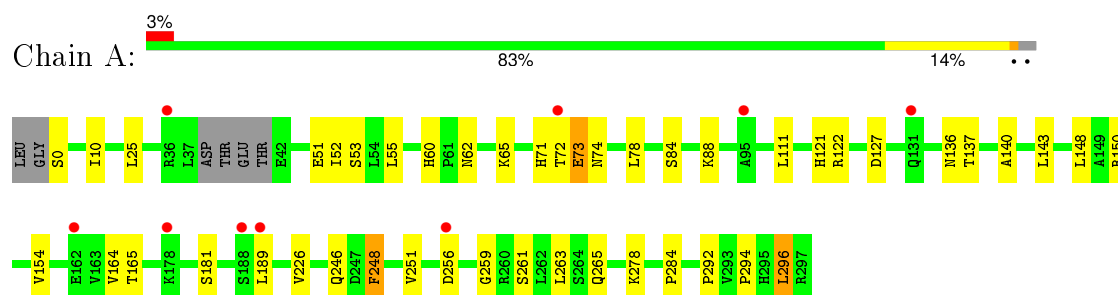
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	1	Total 1	O 1	0	0

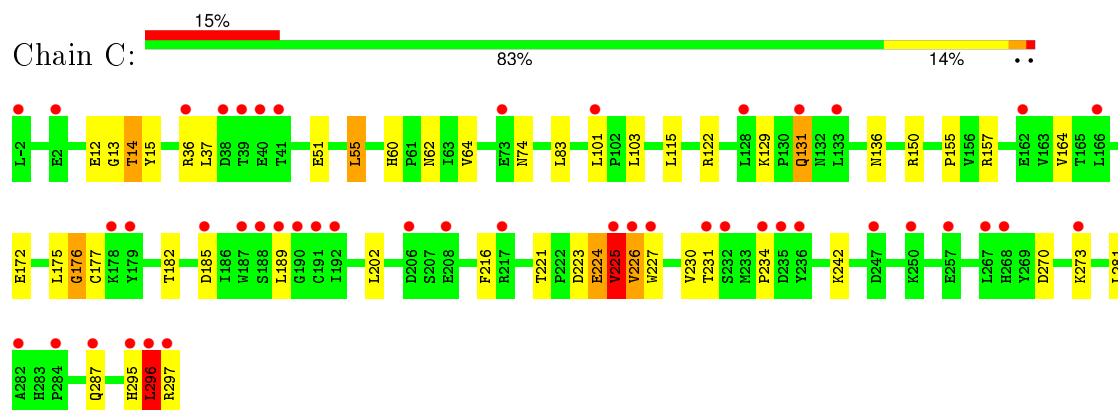
### 3 Residue-property plots [i](#)

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.

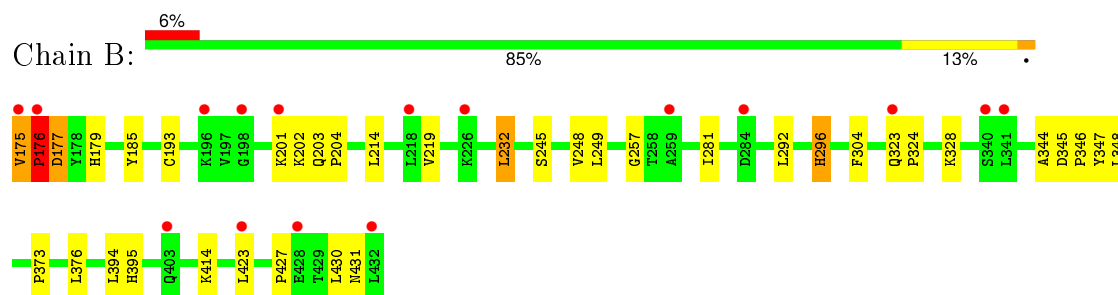
- Molecule 1: Cyclin-dependent kinase 2



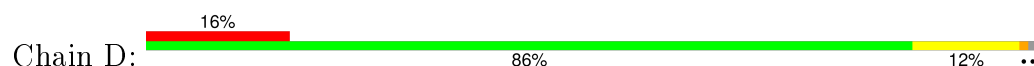
- Molecule 1: Cyclin-dependent kinase 2

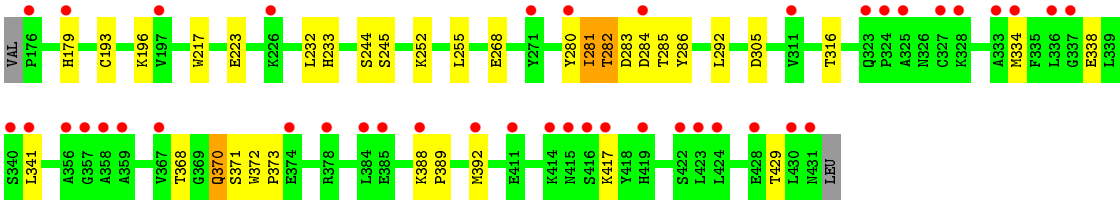


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.23Å 136.01Å 171.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.57 29.23 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.57) 99.2 (29.23-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.259 0.220 , 0.253	Depositor DCC
$R_{free}$ test set	2845 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55634 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, SGM, 4SP

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	0.43	0/2410	0.58	0/3267
1	C	0.47	0/2454	0.60	3/3329 (0.1%)
2	B	0.48	0/2133	0.56	0/2897
2	D	0.38	0/2118	0.52	0/2875
All	All	0.44	0/9115	0.56	3/12368 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	LEU	CB-CA-C	-9.99	91.22	110.20
1	C	297	ARG	N-CA-CB	8.68	126.23	110.60
1	C	224	GLU	N-CA-C	-5.17	97.05	111.00

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	A	2362	0	2408	27	0
1	C	2405	0	2447	59	0
2	B	2083	0	2106	26	0
2	D	2068	0	2088	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	22	0	0
3	C	28	0	22	2	0
4	B	6	0	7	1	0
4	D	6	0	8	2	0
5	A	7	0	0	0	0
5	B	1	0	0	0	0
All	All	8994	0	9108	125	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 7.

All (125) 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)
2:B:193:CYS:SG	4:B:501:SGM:S1	2.32	1.27
1:C:224:GLU:OE2	1:C:231:THR:OG1	1.64	1.14
1:C:225:VAL:O	1:C:226:VAL:HG12	1.47	1.12
1:C:224:GLU:O	1:C:225:VAL:HG12	1.56	1.05
1:C:227:TRP:O	1:C:230:VAL:HG23	1.57	1.04
2:D:368:THR:OG1	2:D:370:GLN:HG3	1.66	0.95
1:A:73:GLU:HG3	1:A:74:ASN:HA	1.46	0.93
1:C:14:THR:HG22	1:C:15:TYR:H	1.36	0.90
1:C:14:THR:CG2	1:C:15:TYR:N	2.35	0.90
1:C:14:THR:HG23	1:C:15:TYR:HD2	1.38	0.89
1:C:14:THR:HG22	1:C:15:TYR:N	1.88	0.87
1:A:60:HIS:HD2	1:A:62:ASN:H	1.17	0.87
1:C:226:VAL:CG1	1:C:227:TRP:N	2.39	0.85
2:D:371:SER:O	2:D:373:PRO:HD3	1.75	0.85
1:C:295:HIS:O	1:C:296:LEU:HD12	1.76	0.84
1:C:295:HIS:C	1:C:296:LEU:HG	1.96	0.84
1:C:223:ASP:O	1:C:225:VAL:O	1.97	0.82
2:D:282:THR:HG23	2:D:285:THR:OG1	1.79	0.82
1:A:136:ASN:HD21	1:A:140:ALA:HB3	1.46	0.81
1:C:295:HIS:O	1:C:296:LEU:CG	2.30	0.79
1:A:278:LYS:NZ	2:B:177:ASP:O	2.13	0.79
1:C:295:HIS:O	1:C:296:LEU:CD1	2.30	0.79
1:C:295:HIS:O	1:C:296:LEU:HG	1.82	0.79
1:C:225:VAL:O	1:C:226:VAL:CG1	2.29	0.78
1:C:224:GLU:O	1:C:225:VAL:CG1	2.30	0.78
1:C:227:TRP:O	1:C:230:VAL:CG2	2.32	0.77
1:C:14:THR:HG23	1:C:15:TYR:CD2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:O	1:C:226:VAL:HG12	1.86	0.75
1:C:226:VAL:HG12	1:C:227:TRP:H	1.53	0.73
1:C:226:VAL:HG13	1:C:227:TRP:N	2.04	0.72
1:C:225:VAL:HG12	1:C:225:VAL:O	1.88	0.71
1:C:225:VAL:CG1	1:C:225:VAL:O	2.35	0.71
2:D:371:SER:O	2:D:372:TRP:C	2.30	0.70
2:D:282:THR:HG23	2:D:282:THR:O	1.92	0.68
2:D:193:CYS:SG	4:D:501:SGM:S1	2.71	0.68
1:C:157:ARG:HH22	2:D:268:GLU:HG3	1.61	0.65
1:C:14:THR:CG2	1:C:15:TYR:CD2	2.79	0.65
1:C:175:LEU:O	1:C:177:CYS:N	2.30	0.65
2:D:371:SER:O	2:D:373:PRO:CD	2.46	0.63
1:A:256:ASP:HB3	1:A:259:GLY:H	1.62	0.63
2:D:282:THR:CG2	2:D:282:THR:O	2.42	0.62
1:C:224:GLU:O	1:C:225:VAL:CB	2.49	0.60
1:C:223:ASP:C	1:C:224:GLU:O	2.32	0.60
1:C:176:GLY:O	1:C:234:PRO:HG2	2.02	0.59
1:C:14:THR:CG2	1:C:15:TYR:HD2	2.12	0.57
1:A:73:GLU:CG	1:A:74:ASN:HA	2.27	0.57
1:A:60:HIS:CD2	1:A:62:ASN:H	2.10	0.56
1:C:175:LEU:O	1:C:176:GLY:C	2.42	0.56
1:A:294:PRO:HG2	1:A:296:LEU:HD22	1.86	0.56
1:C:13:GLY:O	1:C:14:THR:HG22	2.07	0.55
2:B:347:TYR:OH	2:B:394:LEU:HA	2.06	0.55
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.90	0.54
2:D:305:ASP:HB3	4:D:501:SGM:H12	1.90	0.54
1:C:224:GLU:C	1:C:225:VAL:O	2.46	0.53
1:A:71:HIS:HE2	2:B:296:HIS:CE1	2.26	0.53
1:A:71:HIS:HE2	2:B:296:HIS:CD2	2.27	0.53
2:B:175:VAL:O	2:B:176:PRO:O	2.28	0.52
1:C:14:THR:HG23	1:C:15:TYR:N	2.20	0.52
1:C:224:GLU:OE2	1:C:231:THR:CB	2.57	0.51
2:D:388:LYS:O	2:D:392:MET:HG2	2.10	0.51
1:C:227:TRP:HB3	1:C:230:VAL:HG21	1.92	0.51
1:C:51:GLU:O	1:C:55:LEU:HB2	2.10	0.51
1:A:51:GLU:O	1:A:55:LEU:HB2	2.10	0.51
2:D:233:HIS:CD2	2:D:341:LEU:HD11	2.46	0.51
2:D:282:THR:O	2:D:283:ASP:HB2	2.11	0.51
1:C:270:ASP:HB3	1:C:273:LYS:HB2	1.91	0.50
2:B:175:VAL:C	2:B:176:PRO:O	2.50	0.50
1:C:224:GLU:O	1:C:225:VAL:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:368:THR:CB	2:D:370:GLN:HG3	2.41	0.49
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.95	0.49
2:B:214:LEU:HD11	2:B:257:GLY:HA3	1.93	0.49
1:C:216:PHE:HB3	1:C:221:THR:HG22	1.95	0.49
1:A:0:SER:HA	1:A:72:THR:HG22	1.95	0.48
2:B:430:LEU:O	2:B:431:ASN:HB2	2.13	0.48
1:A:111:LEU:HD13	1:A:189:LEU:HD21	1.95	0.48
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.96	0.48
1:A:127:ASP:OD1	1:A:165:THR:HG23	2.14	0.48
2:B:395:HIS:HE1	2:B:427:PRO:O	1.97	0.47
1:C:172:GLU:O	1:C:177:CYS:HB2	2.14	0.47
2:B:176:PRO:HG2	2:B:179:HIS:CE1	2.50	0.47
1:A:25:LEU:O	2:D:252:LYS:HG3	2.15	0.47
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.21	0.46
1:C:227:TRP:NE1	1:C:270:ASP:HA	2.30	0.46
1:C:223:ASP:O	1:C:224:GLU:C	2.54	0.46
2:B:176:PRO:C	2:B:177:ASP:OD2	2.54	0.46
1:C:224:GLU:HG2	1:C:224:GLU:H	1.45	0.45
2:D:196:LYS:HB2	2:D:244:SER:HB3	1.99	0.45
2:B:177:ASP:OD2	2:B:177:ASP:N	2.48	0.44
1:C:155:PRO:HD2	2:D:316:THR:HB	1.98	0.44
1:C:129:LYS:HG3	1:C:131:GLN:HG2	2.00	0.44
1:C:225:VAL:O	1:C:226:VAL:CB	2.64	0.44
1:A:0:SER:HA	1:A:72:THR:CG2	2.47	0.44
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.99	0.44
1:A:71:HIS:NE2	2:B:296:HIS:NE2	2.59	0.44
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.88	0.44
2:B:203:GLN:HA	2:B:204:PRO:HD3	1.87	0.44
2:D:334:MET:O	2:D:338:GLU:HB2	2.18	0.43
2:D:280:TYR:C	2:D:282:THR:H	2.22	0.43
1:A:53:SER:HB3	2:B:304:PHE:O	2.18	0.43
1:A:71:HIS:CE1	1:A:73:GLU:HB2	2.53	0.43
2:D:284:ASP:O	2:D:285:THR:C	2.57	0.43
1:A:121:HIS:HD2	2:B:185:TYR:CE1	2.36	0.43
2:B:376:LEU:HA	2:B:376:LEU:HD23	1.75	0.43
1:A:246:GLN:HE21	1:A:251:VAL:HG22	1.83	0.43
1:C:227:TRP:CD2	1:C:230:VAL:HG22	2.54	0.42
1:A:248:PHE:HE2	1:A:263:LEU:HG	1.84	0.42
1:A:137:THR:HG22	1:A:296:LEU:HD21	2.02	0.42
1:C:13:GLY:O	1:C:14:THR:CB	2.68	0.42
2:B:373:PRO:HD2	2:B:376:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CD2	1:C:62:ASN:H	2.38	0.42
1:A:261:SER:O	1:A:265:GLN:HG3	2.20	0.42
1:A:52:ILE:HD11	1:A:78:LEU:HD21	2.00	0.42
2:D:217:TRP:CZ2	2:D:281:ILE:HD12	2.55	0.42
2:D:255:LEU:HB2	2:D:286:TYR:CE1	2.55	0.41
1:C:227:TRP:CZ3	1:C:230:VAL:HG13	2.54	0.41
1:C:64:VAL:HG21	3:C:301:ASP:C8	2.50	0.41
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.56	0.41
2:B:345:ASP:HA	2:B:346:PRO:HA	1.82	0.41
1:C:83:LEU:HD12	1:C:136:ASN:HB3	2.01	0.41
2:B:414:LYS:HE3	2:B:423:LEU:HD21	2.03	0.40
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.97	0.40
1:C:227:TRP:CD1	1:C:270:ASP:HA	2.56	0.40
2:B:323:GLN:HA	2:B:324:PRO:HA	1.81	0.40
1:C:64:VAL:HG21	3:C:301:ASP:H8	2.03	0.40
2:B:248:VAL:HG12	2:B:249:LEU:O	2.21	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	289/300 (96%)	272 (94%)	15 (5%)	2 (1%)	26	49
1	C	297/300 (99%)	280 (94%)	13 (4%)	4 (1%)	15	29
2	B	256/258 (99%)	250 (98%)	5 (2%)	1 (0%)	39	63
2	D	254/258 (98%)	240 (94%)	13 (5%)	1 (0%)	39	63
All	All	1096/1116 (98%)	1042 (95%)	46 (4%)	8 (1%)	26	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	PRO
1	C	176	GLY
1	C	164	VAL
1	C	225	VAL
1	A	164	VAL
2	D	281	ILE
1	A	73	GLU
1	C	182	THR

### 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	258/263 (98%)	244 (95%)	14 (5%)	27	51
1	C	263/263 (100%)	245 (93%)	18 (7%)	20	38
2	B	232/232 (100%)	221 (95%)	11 (5%)	32	58
2	D	230/232 (99%)	221 (96%)	9 (4%)	39	66
All	All	983/990 (99%)	931 (95%)	52 (5%)	28	52

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	65	LYS
1	A	84	SER
1	A	88	LYS
1	A	122	ARG
1	A	143	LEU
1	A	148	LEU
1	A	150	ARG
1	A	181	SER
1	A	226	VAL
1	A	248	PHE
1	A	284	PRO
1	A	292	PRO
1	A	296	LEU

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Mol	Chain	Res	Type
2	B	175	VAL
2	B	176	PRO
2	B	177	ASP
2	B	201	LYS
2	B	202	LYS
2	B	232	LEU
2	B	245	SER
2	B	281	ILE
2	B	292	LEU
2	B	296	HIS
2	B	328	LYS
1	C	12	GLU
1	C	14	THR
1	C	36	ARG
1	C	37	LEU
1	C	55	LEU
1	C	74	ASN
1	C	101	LEU
1	C	103	LEU
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	202	LEU
1	C	225	VAL
1	C	226	VAL
1	C	242	LYS
1	C	281	LEU
1	C	287	GLN
1	C	296	LEU
2	D	179	HIS
2	D	223	GLU
2	D	232	LEU
2	D	245	SER
2	D	282	THR
2	D	292	LEU
2	D	370	GLN
2	D	417	LYS
2	D	429	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	246	GLN
1	A	265	GLN
2	B	179	HIS
2	B	183	HIS
2	B	233	HIS
2	B	317	GLN
2	B	395	HIS
1	C	60	HIS
1	C	119	HIS
1	C	131	GLN
2	D	233	HIS
2	D	254	GLN
2	D	323	GLN
2	D	370	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	160	1	8,10,11	0.64	0	7,14,16	1.46	0
1	TPO	C	160	1	8,10,11	0.65	0	7,14,16	1.42	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	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

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	C	160	TPO	O-C-CA	-2.02	120.11	125.44

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	$\# Z  > 2$
3	4SP	A	301	-	28,31,31	2.38	7 (25%)	35,44,44	2.27	9 (25%)
4	SGM	B	501	-	5,5,5	0.40	0	5,5,5	0.66	0
3	4SP	C	301	-	28,31,31	2.51	8 (28%)	35,44,44	2.16	8 (22%)
4	SGM	D	501	-	5,5,5	0.42	0	5,5,5	0.62	0

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	4SP	A	301	-	-	0/15/23/23	0/4/4/4
4	SGM	B	501	-	-	0/4/4/4	0/0/0/0
3	4SP	C	301	-	-	0/15/23/23	0/4/4/4
4	SGM	D	501	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	4SP	C20-S23	-10.42	1.61	1.77
3	A	301	4SP	C20-S23	-9.93	1.62	1.77
3	A	301	4SP	S23-N26	-3.75	1.52	1.60
3	C	301	4SP	S23-N26	-3.46	1.52	1.60
3	C	301	4SP	C17-N2	-2.03	1.36	1.40
3	A	301	4SP	O6-C6	2.24	1.36	1.35
3	A	301	4SP	C6-N1	2.51	1.36	1.31
3	C	301	4SP	C6-N1	2.69	1.36	1.31
3	A	301	4SP	C5-C4	2.73	1.46	1.40
3	A	301	4SP	O24-S23	2.79	1.48	1.43
3	C	301	4SP	C5-C4	2.82	1.46	1.40
3	C	301	4SP	O24-S23	2.99	1.48	1.43
3	C	301	4SP	O25-S23	3.09	1.49	1.43
3	A	301	4SP	O25-S23	3.20	1.49	1.43
3	C	301	4SP	O6-C6	3.34	1.37	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	4SP	O25-S23-O24	-7.16	108.74	118.80
3	C	301	4SP	O25-S23-O24	-5.98	110.40	118.80
3	A	301	4SP	N3-C2-N1	-3.89	120.26	126.22
3	A	301	4SP	C4-C5-N7	-3.74	106.04	109.48
3	C	301	4SP	C4-C5-N7	-3.49	106.27	109.48
3	C	301	4SP	N3-C2-N1	-3.23	121.27	126.22
3	C	301	4SP	C5-C6-N1	-3.17	118.21	123.81
3	A	301	4SP	C5-C6-N1	-2.68	119.08	123.81
3	A	301	4SP	C16-C11-C10	-2.12	107.00	111.47
3	C	301	4SP	C2-N3-C4	2.03	117.53	115.09
3	C	301	4SP	O6-C6-C5	2.15	118.44	115.07
3	A	301	4SP	O25-S23-C20	2.67	110.69	107.39
3	A	301	4SP	C2-N3-C4	2.95	118.64	115.09
3	A	301	4SP	O6-C6-C5	3.37	120.33	115.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	4SP	C2-N1-C6	5.60	123.30	115.32
3	A	301	4SP	C2-N1-C6	5.73	123.48	115.32
3	C	301	4SP	C10-O6-C6	5.91	123.41	117.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	SGM	1	0
3	C	301	4SP	2	0
4	D	501	SGM	2	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	293/300 (97%)	0.06	9 (3%) 52 48	29, 43, 71, 84	2 (0%)
1	C	299/300 (99%)	0.71	46 (15%) 3 2	54, 75, 109, 130	1 (0%)
2	B	258/258 (100%)	0.23	16 (6%) 24 20	33, 54, 75, 86	0
2	D	256/258 (99%)	0.82	42 (16%) 2 1	46, 75, 119, 136	0
All	All	1106/1116 (99%)	0.45	113 (10%) 9 6	29, 61, 107, 136	3 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	VAL	9.5
1	C	40	GLU	7.8
2	D	428	GLU	6.9
2	D	423	LEU	5.0
1	C	178	LYS	4.8
1	C	73	GLU	4.6
2	D	416	SER	4.6
1	C	282	ALA	4.6
1	A	72	THR	4.5
2	D	337	GLY	4.5
2	D	323	GLN	4.5
1	C	284	PRO	4.4
1	C	287	GLN	4.2
1	C	179	TYR	4.2
1	C	297	ARG	4.2
2	D	328	LYS	4.1
2	D	340	SER	4.1
1	C	189	LEU	4.0
1	A	131	GLN	4.0
2	D	280	TYR	4.0
2	D	197	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	324	PRO	3.9
2	D	414	LYS	3.7
2	D	311	VAL	3.7
1	C	232	SER	3.7
1	A	256	ASP	3.7
2	D	431	ASN	3.6
1	A	162	GLU	3.5
1	C	39	THR	3.5
1	C	190	GLY	3.4
1	C	2	GLU	3.4
2	B	176	PRO	3.3
2	D	367	VAL	3.3
1	C	247	ASP	3.3
2	D	359	ALA	3.2
2	D	325	ALA	3.2
1	C	166	LEU	3.2
1	A	36	ARG	3.2
1	C	188	SER	3.1
1	C	-2	LEU	3.1
2	D	333	ALA	3.1
2	D	424	LEU	3.1
2	D	378	ARG	3.1
2	B	428	GLU	3.1
1	C	295	HIS	3.1
2	B	201	LYS	3.1
2	D	358	ALA	3.0
1	C	296	LEU	2.9
1	C	225	VAL	2.9
2	B	323	GLN	2.8
2	B	284	ASP	2.8
1	C	257	GLU	2.8
1	C	234	PRO	2.7
1	C	250	LYS	2.7
1	C	235	ASP	2.7
2	D	356	ALA	2.7
2	D	226	LYS	2.7
2	D	271	TYR	2.7
2	D	415	ASN	2.7
2	D	341	LEU	2.6
1	C	226	VAL	2.6
2	D	417	LYS	2.6
2	B	196	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	226	LYS	2.6
2	D	176	PRO	2.5
2	B	341	LEU	2.5
2	B	198	GLY	2.5
2	B	432	LEU	2.5
1	A	95	ALA	2.5
1	C	187	TRP	2.4
1	C	217	ARG	2.4
1	C	191	CYS	2.4
1	C	128	LEU	2.4
2	D	392	MET	2.4
1	C	133	LEU	2.4
1	C	267	LEU	2.4
1	C	192	ILE	2.4
2	D	179	HIS	2.4
1	C	41	THR	2.3
2	B	340	SER	2.3
2	D	284	ASP	2.3
2	D	384	LEU	2.3
2	D	388	LYS	2.3
1	C	268	HIS	2.3
1	C	162	GLU	2.3
1	C	131	GLN	2.3
1	C	185	ASP	2.3
1	C	36	ARG	2.3
2	D	430	LEU	2.3
2	B	423	LEU	2.2
1	C	208	GLU	2.2
1	C	227	TRP	2.2
1	C	273	LYS	2.2
1	A	188	SER	2.2
2	B	218	LEU	2.2
2	D	357	GLY	2.2
1	C	206	ASP	2.2
2	D	411	GLU	2.2
1	C	231	THR	2.2
1	A	178	LYS	2.2
2	D	419	HIS	2.2
2	B	259	ALA	2.1
2	D	334	MET	2.1
1	C	38	ASP	2.1
1	A	189	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	101	LEU	2.1
2	D	327	CYS	2.1
2	D	385	GLU	2.1
2	D	336	LEU	2.0
2	B	403	GLN	2.0
2	D	374	GLU	2.0
2	D	422	SER	2.0
1	C	236	TYR	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<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	TPO	A	160	11/12	0.97	0.11	-	39,42,43,43	0
1	TPO	C	160	11/12	0.95	0.12	-	65,71,74,75	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
4	SGM	B	501	6/6	0.86	0.27	1.87	68,68,69,70	0
3	4SP	C	301	28/28	0.87	0.19	0.18	68,69,75,75	0
4	SGM	D	501	6/6	0.86	0.18	0.18	79,79,80,81	0
3	4SP	A	301	28/28	0.95	0.13	-0.62	43,47,52,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.