Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:38 AM GMT

PDB ID	:	3BHV
Title	:	Structure of phosphorylated Thr160 CDK2/cyclin A in complex with the inhibitor variolin B
Authors	:	Echalier, A.; Bettayeb, K.; Ferandin, Y.; Lozach, O.; Clement, M.; Valette, A.; Liger, F.; Marquet, B.; Morris, J.C.; Endicott, J.A.; Joseph, B.; Meijer, L.
Deposited on	:	2007-11-29
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

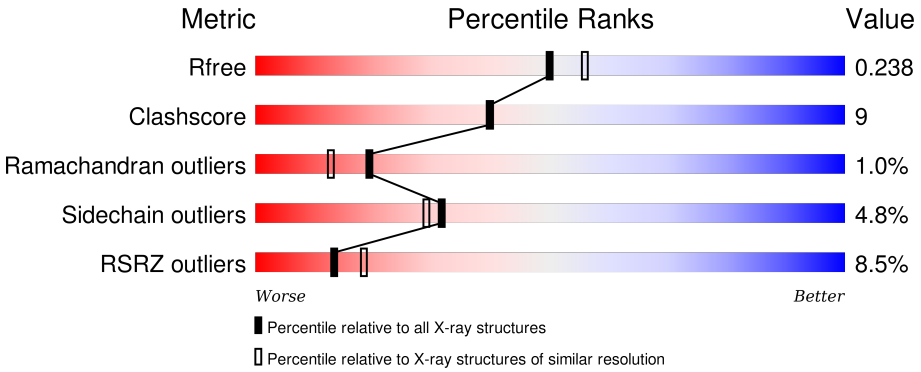
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	300	6% 80% 17%
1	C	300	10% 71% 18% 9%
2	B	262	5% 87% 12%
2	D	262	12% 88% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	2	-	-	-	X
4	VAR	C	299	-	-	-	X
5	SGM	B	2	-	X	X	X
5	SGM	B	3	-	X	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9822 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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	0	7	0
			2435	1580	413	432	1	9			
1	C	272	Total	C	N	O	P	S	0	1	0
			2186	1417	374	387	1	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941

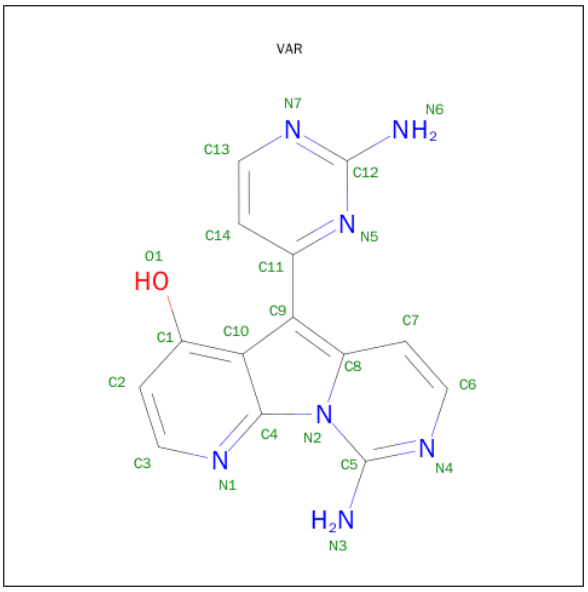
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	3	0
			2130	1379	346	395	10			
2	D	262	Total	C	N	O	S	0	1	0
			2118	1371	344	393	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

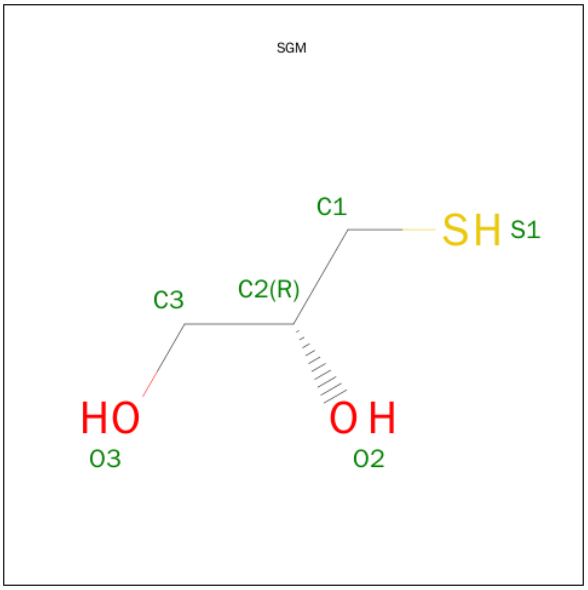
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 9-AMINO-5-(2-AMINOPYRIMIDIN-4-YL)PYRIDO[3',2':4,5]PYRROLO[1,2-C]PYRIMIDIN-4-OL (three-letter code: VAR) (formula: $C_{14}H_{11}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	14	7	1		
4	C	1	Total	C	N	O	0	0
			22	14	7	1		

- Molecule 5 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



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

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

- Molecule 6 is water.

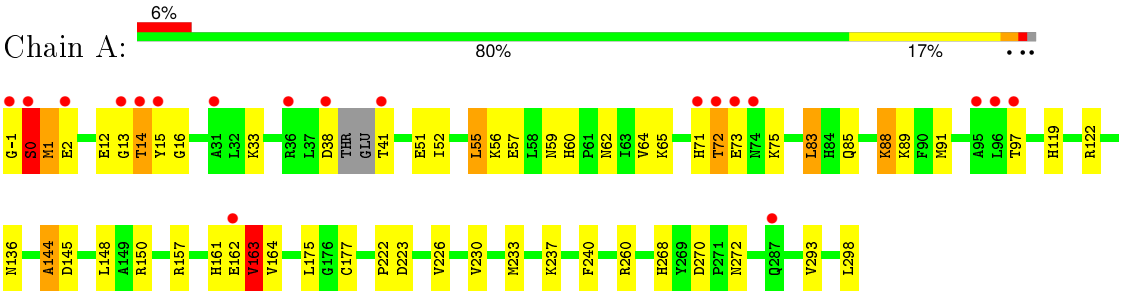
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	296	Total	O	0	0
			296	296		
6	B	244	Total	O	0	0
			244	244		
6	C	175	Total	O	0	0
			175	175		
6	D	174	Total	O	0	0
			174	174		

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.

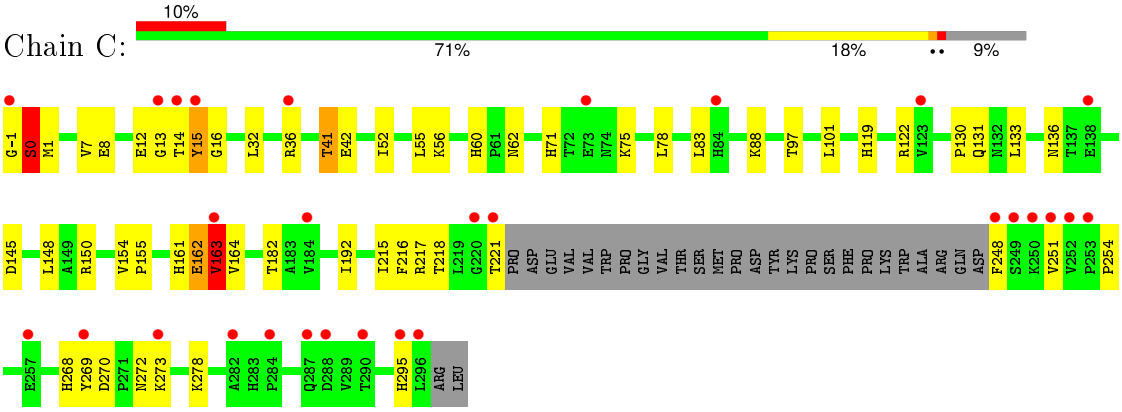
- Molecule 1: Cell division protein kinase 2

Chain A:



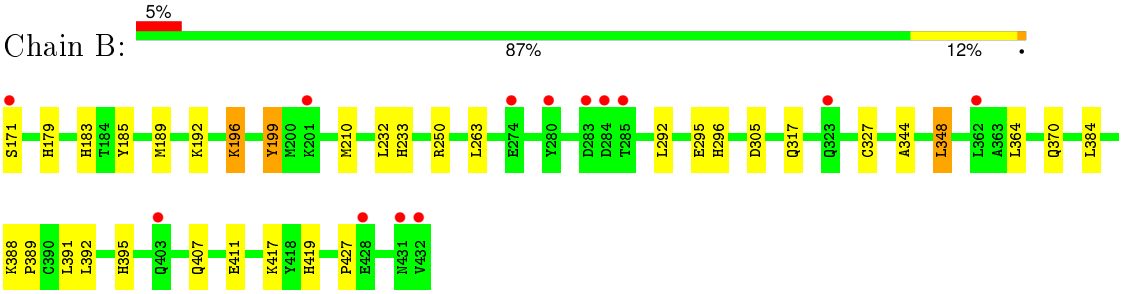
- Molecule 1: Cell division protein kinase 2

Chain C:



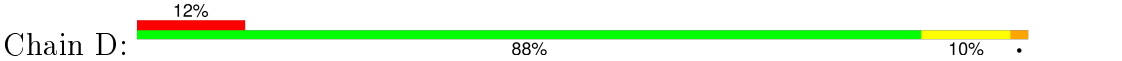
- Molecule 2: Cyclin-A2

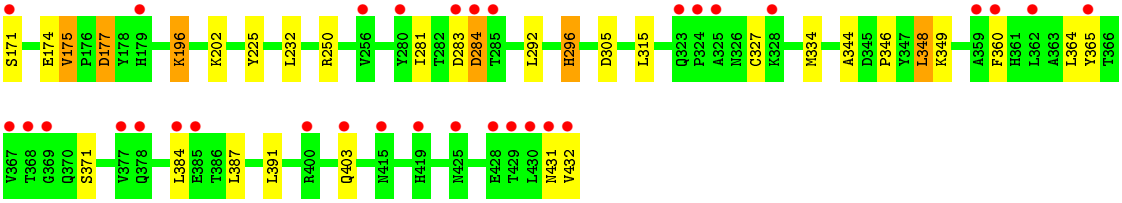
Chain B:



- Molecule 2: Cyclin-A2

Chain D:




S171
E174
V175
P176
D177
Y178
H179
K196
K202
Y225
L232
R250
V256
Y280
I281
T282
D283
D284
T285
L292
H296
D305
L315
Q323
P324
A325
N326
C327
K328
M334
A344
D345
P346
Y347
L348
K349
A359
F360
H361
L362
A363
L364
Y365
T366
V367
T368
G369
Q370
S371
V377
Q378
L384
E385
T386
L387
L391
R400
Q403
N415
H419
N425
E428
T429
L430
N431
V432

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.16Å 133.97Å 147.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.10) 99.7 (19.18-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.229 0.202 , 0.238	Depositor DCC
R_{free} test set	4327 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 86294 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, VAR, MG, SGM

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	0.67	1/2494 (0.0%)	0.70	1/3381 (0.0%)
1	C	0.56	0/2227	0.65	1/3013 (0.0%)
2	B	0.57	0/2190	0.62	0/2978
2	D	0.49	0/2171	0.65	3/2952 (0.1%)
All	All	0.58	1/9082 (0.0%)	0.66	5/12324 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ALA	CA-CB	-5.03	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	VAL	N-CA-C	8.22	133.20	111.00
2	D	174	GLU	N-CA-C	6.47	128.46	111.00
2	D	175	VAL	N-CA-C	-6.43	93.64	111.00
2	D	250	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	C	163	VAL	N-CA-C	5.57	126.04	111.00

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	2435	0	2479	61	0
1	C	2186	0	2246	44	0
2	B	2130	0	2146	26	0
2	D	2118	0	2135	20	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	22	0	11	5	0
4	C	22	0	11	2	0
5	B	12	0	16	16	0
5	D	6	0	7	1	0
6	A	296	0	0	13	0
6	B	244	0	0	5	0
6	C	175	0	0	10	0
6	D	174	0	0	2	0
All	All	9822	0	9051	158	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 9.

All (158) 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:15:TYR:HB2	1:C:16:GLY:CA	1.78	1.10
1:C:15:TYR:HB2	1:C:16:GLY:HA3	1.31	1.09
1:A:13[B]:GLY:O	1:A:14[B]:THR:OG1	1.74	1.05
5:B:2:SGM:C2	5:B:2:SGM:C1	2.35	1.04
5:B:2:SGM:S1	5:B:2:SGM:C1	2.49	1.00
5:B:2:SGM:C2	5:B:2:SGM:C3	2.42	0.96
5:B:3:SGM:C1	5:B:3:SGM:S1	2.53	0.96
4:A:299:VAR:H7	6:A:531:HOH:O	1.67	0.95
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.02	0.94
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.88	0.92
1:A:175:LEU:HD13	1:A:233:MET:CE	2.02	0.89
5:B:3:SGM:C1	5:B:3:SGM:C2	2.52	0.87
1:A:161:HIS:HD2	6:A:355:HOH:O	1.60	0.84
2:D:305:ASP:HB3	5:D:1:SGM:H12	1.59	0.84
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.93	0.83
4:A:299:VAR:O1	4:A:299:VAR:H14	1.79	0.82
1:A:272:ASN:OD1	2:B:171:SER:HB3	1.80	0.82
2:B:327:CYS:SG	5:B:3:SGM:S1	2.64	0.80
1:C:15:TYR:CB	1:C:16:GLY:HA3	1.99	0.79
5:B:3:SGM:C2	5:B:3:SGM:C3	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG23	1:A:233:MET:CE	2.12	0.79
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.65	0.78
6:A:530:HOH:O	2:B:171:SER:HB2	1.85	0.77
1:C:41:THR:HG23	6:C:433:HOH:O	1.84	0.76
1:A:60:HIS:HD2	1:A:62:ASN:H	1.34	0.74
1:C:15:TYR:HB2	1:C:16:GLY:HA2	1.69	0.73
1:A:12:GLU:HG2	1:A:13[B]:GLY:HA3	1.70	0.73
1:A:15[B]:TYR:CD1	1:A:16[B]:GLY:N	2.57	0.72
1:C:60:HIS:HD2	1:C:62:ASN:H	1.33	0.72
1:C:60:HIS:CD2	1:C:62:ASN:H	2.08	0.71
2:B:192:LYS:O	5:B:2:SGM:H31	1.91	0.70
1:A:13[A]:GLY:HA3	1:A:16[A]:GLY:O	1.92	0.69
4:A:299:VAR:N5	6:A:531:HOH:O	2.26	0.69
1:A:13[B]:GLY:C	1:A:14[B]:THR:OG1	2.31	0.69
5:B:2:SGM:C1	5:B:2:SGM:C3	2.71	0.68
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.58	0.67
1:A:230:VAL:HG23	1:A:233:MET:HE1	1.76	0.67
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.77	0.67
1:A:230:VAL:HG23	1:A:233:MET:HE2	1.76	0.66
1:A:60:HIS:CD2	1:A:62:ASN:H	2.14	0.66
2:B:305:ASP:OD2	5:B:2:SGM:H2	1.96	0.66
1:A:-1:GLY:CA	1:A:0:SER:CB	2.74	0.65
2:B:210:MET:HE1	2:B:250:ARG:CB	2.27	0.64
1:C:15:TYR:CB	1:C:16:GLY:CA	2.59	0.64
1:A:230:VAL:CG2	1:A:233:MET:HE2	2.28	0.62
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.68	0.62
1:A:-1:GLY:HA3	1:A:0:SER:CB	2.30	0.61
1:C:268:HIS:HD2	1:C:270:ASP:H	1.47	0.61
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.78	0.61
2:B:233:HIS:HD2	6:B:443:HOH:O	1.84	0.61
1:C:278:LYS:HE3	2:D:177:ASP:O	2.00	0.61
1:A:72:THR:HG22	1:A:73:GLU:H	1.66	0.61
1:A:72:THR:HB	6:A:467:HOH:O	2.01	0.60
1:A:260:ARG:HD3	6:A:336:HOH:O	2.00	0.60
1:A:175:LEU:HD13	1:A:233:MET:HE1	1.83	0.60
1:C:218:THR:HG23	1:C:251:VAL:HG21	1.85	0.59
1:A:-1:GLY:HA3	1:A:0:SER:HB2	1.84	0.58
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.85	0.58
1:C:161:HIS:O	1:C:162:GLU:C	2.38	0.58
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.85	0.57
5:B:2:SGM:C3	5:B:2:SGM:H12	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.85	0.57
2:B:189:MET:CE	5:B:2:SGM:O2	2.52	0.56
1:A:64:VAL:HB	6:A:311:HOH:O	2.06	0.56
2:D:315:LEU:HD13	2:D:334:MET:HE3	1.88	0.56
1:A:12:GLU:CG	1:A:13[B]:GLY:HA3	2.36	0.56
2:B:395:HIS:HE1	2:B:427:PRO:O	1.89	0.56
2:B:183:HIS:HD2	6:B:554:HOH:O	1.87	0.56
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.88	0.55
1:C:272:ASN:OD1	2:D:171:SER:N	2.40	0.55
1:C:119:HIS:HD2	6:C:563:HOH:O	1.89	0.54
2:D:346:PRO:O	2:D:349:LYS:HG2	2.08	0.54
1:A:272:ASN:CG	2:B:171:SER:HB3	2.28	0.54
1:C:295:HIS:CD2	1:C:295:HIS:H	2.24	0.54
5:B:2:SGM:H31	5:B:2:SGM:H12	1.90	0.53
1:A:15[B]:TYR:OH	4:A:299:VAR:H13	2.07	0.53
2:B:196:LYS:HG3	2:B:199:TYR:HB3	1.91	0.52
1:A:38:ASP:O	1:A:41:THR:N	2.42	0.52
1:A:119:HIS:HD2	6:B:543:HOH:O	1.93	0.52
1:A:-1:GLY:HA2	1:A:0:SER:OG	2.10	0.51
1:A:268:HIS:HD2	1:A:270:ASP:H	1.58	0.51
1:C:52:ILE:O	1:C:56:LYS:HG2	2.11	0.51
1:A:175:LEU:CD1	1:A:233:MET:HE3	2.39	0.51
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.92	0.51
2:B:388:LYS:HE2	2:B:392:LEU:HD11	1.92	0.51
2:D:387:LEU:O	2:D:391:LEU:HB2	2.11	0.51
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.93	0.50
1:A:-1:GLY:CA	1:A:0:SER:OG	2.59	0.50
1:C:7:VAL:HG12	1:C:8:GLU:HG2	1.92	0.50
1:C:0:SER:HA	6:C:420:HOH:O	2.11	0.50
1:A:59[A]:ASN:HD21	1:A:65:LYS:HE3	1.76	0.50
1:C:161:HIS:O	1:C:162:GLU:O	2.29	0.50
2:D:283:ASP:O	2:D:284:ASP:CB	2.59	0.50
1:A:52:ILE:O	1:A:56:LYS:HG2	2.12	0.50
1:A:13[B]:GLY:HA2	1:A:16[B]:GLY:O	2.12	0.49
1:A:161:HIS:O	1:A:161:HIS:CG	2.64	0.49
1:A:223:ASP:H	1:A:226:VAL:HG12	1.76	0.49
5:B:2:SGM:C2	5:B:2:SGM:O2	2.61	0.49
2:B:179[A]:HIS:CE1	6:B:490:HOH:O	2.66	0.49
1:A:60:HIS:HE1	6:A:443:HOH:O	1.96	0.49
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.96	0.47
5:B:3:SGM:C2	5:B:3:SGM:S1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ARG:HH11	1:C:75:LYS:HE3	1.80	0.47
1:C:216:PHE:HB3	1:C:221:THR:HG23	1.97	0.47
1:C:1:MET:HE1	1:C:32:LEU:HD13	1.97	0.46
5:B:3:SGM:C2	5:B:3:SGM:O2	2.63	0.46
1:C:-1:GLY:O	1:C:0:SER:O	2.32	0.46
2:D:283:ASP:O	2:D:284:ASP:HB3	2.15	0.46
1:A:175:LEU:CD1	1:A:233:MET:CE	2.84	0.46
4:C:299:VAR:O1	4:C:299:VAR:H14	2.16	0.46
2:D:365:TYR:OH	2:D:431:ASN:OD1	2.34	0.46
1:C:161:HIS:HD2	6:C:374:HOH:O	1.98	0.45
1:C:36:ARG:NH1	1:C:75:LYS:HE3	2.31	0.45
1:C:248:PHE:N	6:C:348:HOH:O	2.50	0.45
1:A:85:GLN:HG2	1:A:298:LEU:HG	1.97	0.45
1:A:237:LYS:HD3	1:A:240:PHE:CE1	2.51	0.45
2:B:407:GLN:O	2:B:411:GLU:HG2	2.16	0.45
1:A:13[A]:GLY:CA	1:A:16[A]:GLY:O	2.64	0.45
2:D:360:PHE:O	2:D:364:LEU:HB2	2.17	0.45
1:A:88:LYS:HE3	6:A:378:HOH:O	2.17	0.44
1:C:13:GLY:C	1:C:15:TYR:H	2.21	0.44
1:C:270:ASP:HB3	1:C:273:LYS:HB2	2.00	0.44
4:C:299:VAR:H7	4:C:299:VAR:N5	2.32	0.44
1:C:254:PRO:HA	6:C:459:HOH:O	2.16	0.44
6:C:434:HOH:O	2:D:296:HIS:HD2	2.00	0.44
1:A:162:GLU:HG2	1:A:163:VAL:H	1.82	0.44
1:A:15[B]:TYR:CD1	1:A:33:LYS:HE3	2.53	0.44
1:A:57:GLU:HB3	2:B:185:TYR:OH	2.18	0.44
2:D:196:LYS:HE3	6:D:688:HOH:O	2.17	0.43
2:B:196:LYS:CG	2:B:199:TYR:HB3	2.48	0.43
1:A:51:GLU:O	1:A:55:LEU:HB2	2.19	0.43
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.54	0.43
6:C:434:HOH:O	2:D:296:HIS:CD2	2.72	0.43
1:C:119:HIS:CD2	1:C:182:THR:HB	2.54	0.43
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.00	0.43
2:D:225:TYR:HE2	2:D:281:ILE:HG21	1.83	0.43
2:B:364:LEU:HG	2:B:370:GLN:HB2	2.01	0.43
1:C:41:THR:HB	1:C:42:GLU:H	1.38	0.42
2:D:327:CYS:HB2	6:D:683:HOH:O	2.18	0.42
1:A:12:GLU:HA	1:A:13[A]:GLY:HA3	1.85	0.42
1:A:177[B]:CYS:SG	1:A:233:MET:SD	3.18	0.42
1:A:0:SER:HB3	1:A:1:MET:H	1.45	0.42
1:C:12:GLU:HG2	1:C:16:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HA	1:A:91:MET:CE	2.51	0.41
1:A:157:ARG:HD3	6:A:483:HOH:O	2.19	0.41
2:B:263:LEU:HD21	2:B:295:GLU:HG3	2.02	0.41
1:C:161:HIS:CE1	6:C:360:HOH:O	2.72	0.41
1:A:222:PRO:HA	1:A:226:VAL:HG11	2.03	0.41
2:B:171:SER:HB2	6:B:592:HOH:O	2.20	0.41
1:C:215:ILE:HG22	1:C:269:TYR:HE1	1.85	0.41
1:A:162:GLU:HA	6:A:525:HOH:O	2.19	0.41
1:A:161:HIS:CD2	6:A:355:HOH:O	2.49	0.41
1:C:41:THR:HG21	6:C:407:HOH:O	2.19	0.41
1:A:162:GLU:HG2	1:A:163:VAL:N	2.36	0.41
1:C:154:VAL:HA	1:C:155:PRO:HA	1.97	0.41
1:C:52:ILE:HD11	1:C:78:LEU:HD21	2.03	0.40
1:A:89:LYS:HE2	6:A:534:HOH:O	2.20	0.40
1:A:64:VAL:HG11	4:A:299:VAR:HN3	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	A	300/300 (100%)	289 (96%)	5 (2%)	6 (2%)	9 4
1	C	268/300 (89%)	255 (95%)	8 (3%)	5 (2%)	10 4
2	B	263/262 (100%)	261 (99%)	2 (1%)	0	100 100
2	D	261/262 (100%)	256 (98%)	4 (2%)	1 (0%)	39 37
All	All	1092/1124 (97%)	1061 (97%)	19 (2%)	12 (1%)	19 11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	163	VAL
1	C	0	SER
1	C	162	GLU
1	C	163	VAL
1	A	14[A]	THR
1	A	14[B]	THR
1	A	164	VAL
2	D	284	ASP
1	C	164	VAL
1	C	145	ASP
1	A	145	ASP

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	266/263 (101%)	253 (95%)	13 (5%)	31	28
1	C	238/263 (90%)	225 (94%)	13 (6%)	27	23
2	B	238/235 (101%)	230 (97%)	8 (3%)	44	45
2	D	236/235 (100%)	224 (95%)	12 (5%)	29	26
All	All	978/996 (98%)	932 (95%)	46 (5%)	31	30

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	1	MET
1	A	2	GLU
1	A	55	LEU
1	A	72	THR
1	A	75	LYS
1	A	83	LEU
1	A	88	LYS
1	A	97	THR
1	A	122	ARG

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Mol	Chain	Res	Type
1	A	148	LEU
1	A	150	ARG
1	A	293	VAL
2	B	196	LYS
2	B	199	TYR
2	B	232	LEU
2	B	292	LEU
2	B	348	LEU
2	B	384	LEU
2	B	391	LEU
2	B	417	LYS
1	C	0	SER
1	C	14	THR
1	C	15	TYR
1	C	41	THR
1	C	55	LEU
1	C	97	THR
1	C	101	LEU
1	C	122	ARG
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	217	ARG
2	D	175	VAL
2	D	177	ASP
2	D	196	LYS
2	D	202	LYS
2	D	232	LEU
2	D	292	LEU
2	D	296	HIS
2	D	348	LEU
2	D	371	SER
2	D	384	LEU
2	D	403	GLN
2	D	432	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	119	HIS
1	A	161	HIS
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS
1	C	119	HIS
1	C	265	GLN
1	C	268	HIS
1	C	295	HIS
2	D	173	ASN
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	396	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	2.45	3 (37%)	7,14,16	1.40	2 (28%)
1	TPO	C	160	1	8,10,11	2.12	3 (37%)	7,14,16	1.25	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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	-4.27	1.37	1.51
1	A	160	TPO	P-O2P	-4.04	1.40	1.54
1	C	160	TPO	P-O2P	-3.38	1.42	1.54
1	C	160	TPO	P-O3P	-3.21	1.43	1.54
1	C	160	TPO	P-O1P	-3.07	1.41	1.51
1	A	160	TPO	P-O3P	-3.01	1.43	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	O-C-CA	-2.36	119.21	125.44
1	A	160	TPO	O-C-CA	-2.09	119.91	125.44
1	A	160	TPO	C-CA-N	2.24	114.50	109.83

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)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	VAR	A	299	-	20,25,25	1.50	4 (20%)	20,37,37	3.70	13 (65%)
5	SGM	B	2	-	5,5,5	31.87	5 (100%)	5,5,5	9.72	4 (80%)
5	SGM	B	3	-	5,5,5	34.57	5 (100%)	5,5,5	14.43	5 (100%)
4	VAR	C	299	-	20,25,25	1.56	3 (15%)	20,37,37	4.17	11 (55%)
5	SGM	D	1	-	5,5,5	0.51	0	5,5,5	0.61	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
4	VAR	A	299	-	-	0/1/4/4	0/4/4/4
5	SGM	B	2	-	-	0/4/4/4	0/0/0/0
5	SGM	B	3	-	-	0/4/4/4	0/0/0/0
4	VAR	C	299	-	-	0/1/4/4	0/4/4/4
5	SGM	D	1	-	-	0/4/4/4	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	299	VAR	C10-C4	2.08	1.48	1.43
4	A	299	VAR	C7-C6	2.65	1.39	1.36
4	C	299	VAR	C7-C6	2.84	1.40	1.36
4	A	299	VAR	C1-C10	3.04	1.49	1.43
4	C	299	VAR	C1-C10	3.36	1.49	1.43
4	C	299	VAR	C9-C8	3.89	1.50	1.41
4	A	299	VAR	C9-C8	3.91	1.50	1.41
5	B	2	SGM	C3-C2	23.58	2.42	1.52
5	B	3	SGM	C3-C2	28.60	2.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	SGM	C1-C2	30.34	2.35	1.50
5	B	2	SGM	C1-S1	30.36	2.49	1.81
5	B	3	SGM	C1-S1	32.46	2.53	1.81
5	B	2	SGM	O3-C3	33.73	2.87	1.42
5	B	3	SGM	O3-C3	33.91	2.88	1.42
5	B	3	SGM	C1-C2	36.68	2.52	1.50
5	B	2	SGM	O2-C2	39.26	2.61	1.43
5	B	3	SGM	O2-C2	40.10	2.63	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	3	SGM	C2-C1-S1	-24.44	73.39	113.91
5	B	2	SGM	C1-C2-C3	-17.10	69.14	112.29
5	B	3	SGM	C1-C2-C3	-15.62	72.89	112.29
5	B	2	SGM	C2-C1-S1	-11.07	95.56	113.91
5	B	3	SGM	O3-C3-C2	-9.71	63.11	110.18
5	B	3	SGM	O2-C2-C1	-8.58	79.76	108.99
4	C	299	VAR	C9-C10-C4	-8.29	100.92	107.54
4	A	299	VAR	C9-C10-C4	-7.19	101.80	107.54
5	B	2	SGM	O3-C3-C2	-6.84	77.02	110.18
4	C	299	VAR	N7-C12-N5	-5.83	119.69	125.78
5	B	3	SGM	O2-C2-C3	-5.70	82.51	108.65
4	A	299	VAR	C2-C1-C10	-4.99	116.73	120.58
4	C	299	VAR	C2-C1-C10	-4.98	116.74	120.58
4	A	299	VAR	N7-C12-N5	-4.74	120.83	125.78
4	C	299	VAR	C7-C6-N4	-4.68	119.77	123.91
4	A	299	VAR	C7-C6-N4	-4.45	119.98	123.91
4	A	299	VAR	C14-C13-N7	-4.00	119.34	123.90
4	C	299	VAR	C14-C13-N7	-3.59	119.80	123.90
5	B	2	SGM	O2-C2-C1	-2.83	99.35	108.99
4	A	299	VAR	N3-C5-N4	2.19	119.13	117.07
4	A	299	VAR	C3-N1-C4	2.22	119.79	116.86
4	A	299	VAR	N3-C5-N2	2.29	121.55	118.42
4	A	299	VAR	C13-C14-C11	2.34	119.50	117.26
4	C	299	VAR	N3-C5-N4	2.40	119.33	117.07
4	A	299	VAR	N6-C12-N7	2.67	119.80	117.39
4	C	299	VAR	C3-N1-C4	3.01	120.84	116.86
4	A	299	VAR	C13-N7-C12	4.78	120.62	116.32
4	C	299	VAR	C6-N4-C5	5.06	120.74	116.92
4	A	299	VAR	C6-N4-C5	5.26	120.90	116.92
4	C	299	VAR	C13-N7-C12	5.44	121.21	116.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	299	VAR	N6-C12-N7	5.95	122.75	117.39
4	A	299	VAR	C11-N5-C12	7.23	120.26	116.34
4	C	299	VAR	C11-N5-C12	8.49	120.94	116.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	299	VAR	5	0
5	B	2	SGM	10	0
5	B	3	SGM	6	0
4	C	299	VAR	2	0
5	D	1	SGM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	297/300 (99%)	0.22	19 (6%) 23 30	15, 28, 51, 62	0
1	C	271/300 (90%)	0.55	29 (10%) 8 11	22, 38, 61, 87	0
2	B	262/262 (100%)	0.17	13 (4%) 32 41	16, 32, 44, 55	0
2	D	262/262 (100%)	0.67	32 (12%) 5 7	20, 39, 58, 75	0
All	All	1092/1124 (97%)	0.40	93 (8%) 13 18	15, 35, 55, 87	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	SER	10.0
2	D	171	SER	8.5
2	D	432	VAL	7.9
1	A	96	LEU	7.6
2	B	171	SER	6.1
1	C	14	THR	6.0
1	C	251	VAL	5.9
2	B	432	VAL	5.8
1	C	221	THR	5.7
2	D	283	ASP	5.7
2	D	284	ASP	5.6
1	C	248	PHE	5.3
1	C	13	GLY	5.2
1	C	250	LYS	5.2
1	A	97	THR	5.0
2	D	323	GLN	4.9
1	C	287	GLN	4.8
2	D	428	GLU	4.6
2	D	365	TYR	4.5
2	D	431	ASN	4.5
1	C	296	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	4.2
1	A	95	ALA	4.2
2	B	323	GLN	4.0
1	A	0	SER	4.0
1	A	73	GLU	4.0
2	D	324	PRO	3.8
1	A	36	ARG	3.8
2	D	400	ARG	3.8
1	A	14[A]	THR	3.7
1	C	15	TYR	3.6
1	A	162	GLU	3.6
1	C	295	HIS	3.5
1	C	269	TYR	3.4
2	B	283[A]	ASP	3.4
1	A	15[A]	TYR	3.3
2	D	429	THR	3.3
2	D	378	GLN	3.2
1	C	-1	GLY	3.2
1	C	220	GLY	3.2
2	D	385	GLU	3.1
2	D	403	GLN	3.1
2	D	285	THR	3.1
1	C	253	PRO	3.1
2	D	328	LYS	3.1
2	D	377	VAL	3.0
1	C	84	HIS	3.0
1	A	38	ASP	3.0
2	D	430	LEU	3.0
1	A	-1	GLY	2.9
2	D	362	LEU	2.9
1	C	282	ALA	2.8
2	D	280	TYR	2.8
1	A	13[A]	GLY	2.8
2	B	284	ASP	2.8
2	D	367	VAL	2.8
2	D	359	ALA	2.7
2	B	201	LYS	2.7
2	B	431	ASN	2.7
2	B	403	GLN	2.7
1	A	71	HIS	2.7
1	A	2	GLU	2.7
1	C	252	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	285	THR	2.6
1	A	74	ASN	2.6
1	C	257	GLU	2.6
2	B	280	TYR	2.6
1	C	36	ARG	2.5
2	D	415	ASN	2.5
2	B	274	GLU	2.5
1	C	73	GLU	2.4
2	B	428	GLU	2.4
2	D	425	ASN	2.4
1	A	72	THR	2.3
2	B	362	LEU	2.3
2	D	384	LEU	2.3
1	A	31	ALA	2.3
2	D	419	HIS	2.3
1	C	184	VAL	2.3
1	C	284	PRO	2.3
1	C	290	THR	2.3
2	D	369	GLY	2.2
2	D	368	THR	2.2
1	C	288	ASP	2.2
1	C	163	VAL	2.2
2	D	179	HIS	2.2
2	D	256	VAL	2.2
1	C	273	LYS	2.1
2	D	325	ALA	2.1
2	D	360	PHE	2.1
1	C	138	GLU	2.0
1	C	123	VAL	2.0
1	A	287	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	C	160	11/12	0.99	0.07	-	35,38,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	A	160	11/12	0.98	0.07	-	24,28,30,31	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
5	SGM	B	3	6/6	0.72	0.35	11.62	78,80,80,80	0
5	SGM	B	2	6/6	0.79	0.36	6.99	44,47,50,55	0
3	MG	D	2	1/1	0.98	0.23	3.62	31,31,31,31	0
4	VAR	C	299	22/22	0.69	0.25	2.07	46,47,50,50	0
5	SGM	D	1	6/6	0.90	0.20	1.39	44,51,52,54	0
4	VAR	A	299	22/22	0.75	0.19	0.64	34,34,40,40	0
3	MG	B	1	1/1	0.98	0.15	0.10	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.