



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:07 AM GMT

PDB ID : 3W3D  
Title : Crystal structure of smooth muscle G actin DNase I complex  
Authors : Sakabe, N.; Sakabe, K.; Sasaki, K.; Kondo, H.; Shimomur, M.  
Deposited on : 2012-12-20  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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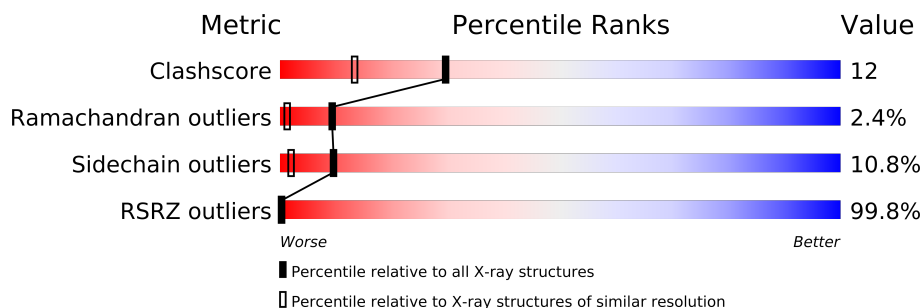
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	374	
2	B	260	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ATP	A	401	-	X
4	CA	B	308	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5472 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Actin, gamma-enteric smooth muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2924	1849	492	562	21	0	0	0

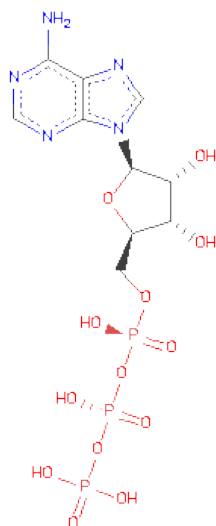
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	GLN	PRO	CONFLICT	UNP P63270

- Molecule 2 is a protein called Deoxyribonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	2049	1298	341	402	8	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 is water.

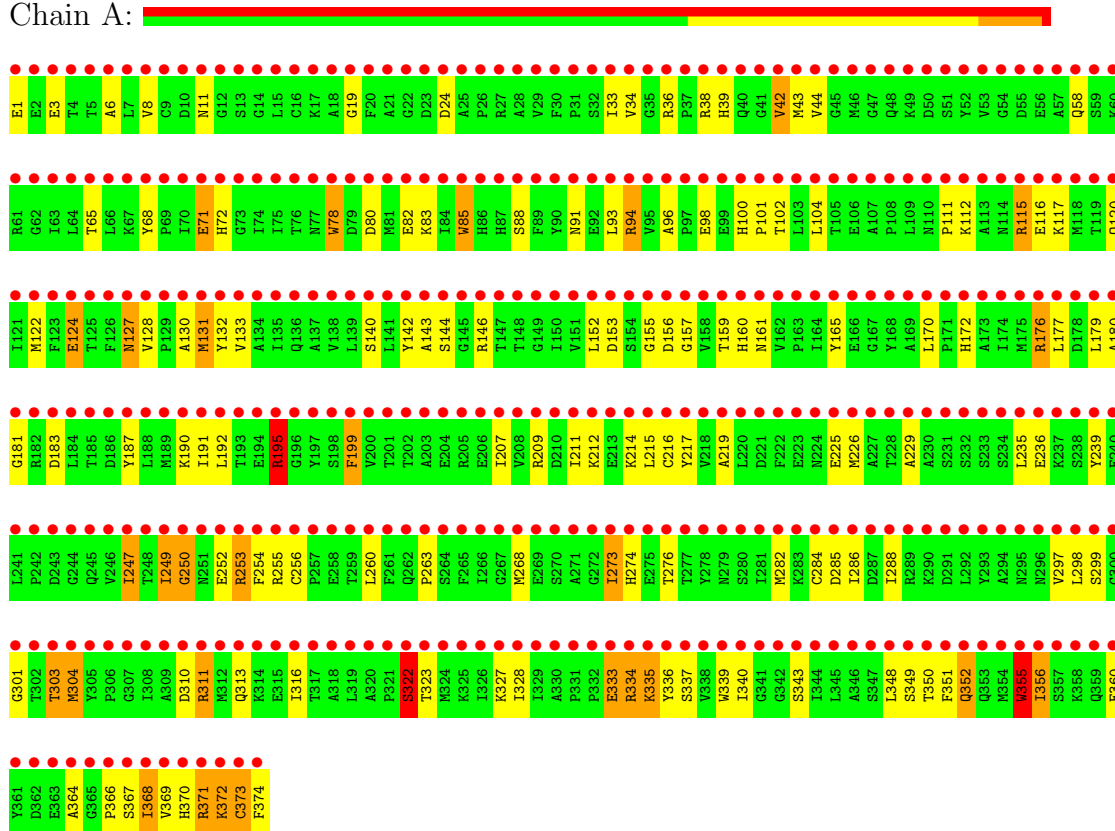
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	188	Total	O	0	0
			188	188		

### 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.

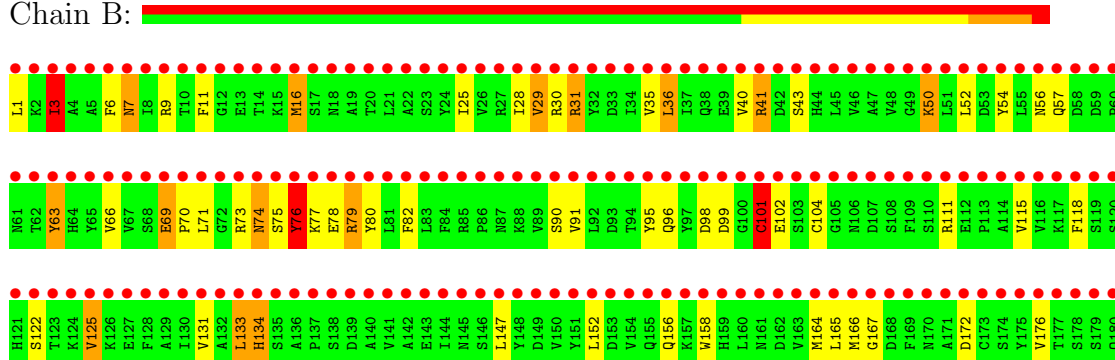
- Molecule 1: Actin, gamma-enteric smooth muscle

Chain A:



- Molecule 2: Deoxyribonuclease-1

Chain B:



W181	●
S182	●
S183	●
I184	●
R185	●
L186	●
R187	●
T188	●
S189	●
S190	●
T191	●
F192	●
Q193	●
W194	●
L195	●
I196	●
P197	●
D198	●
S199	●
A200	●
D201	●
T202	●
T203	●
A204	●
T205	●
S206	●
T207	●
N208	●
C209	●
A210	●
Y211	●
D212	●
R213	●
I214	●
V215	●
V216	●
A217	●
G218	●
S219	●
L220	●
L221	●
Q222	●
S223	●
S224	●
V225	●
V226	●
P227	●
G228	●
S229	●
A230	●
A231	●
F232	●
F233	●
D234	●
F235	●
Q236	●
A237	●
A238	●
Y239	●
G240	●

L241	●
S242	●
N243	●
E244	●
N245	●
A246	●
L247	●
A248	●
I249	●
S250	●
D251	●
H252	●
Y253	●
P254	●
V255	●
E256	●
V257	●
T258	●
I259	●
T260	●

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.00Å 225.30Å 77.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 77.6 (10.00-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.60 (at 1.80Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.196 , (Not available) 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.07 , 18.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 53428 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: BMA, NAG, CA, HIC, ATP, MAN

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	0.85	0/2974	1.57	42/4025 (1.0%)
2	B	0.95	1/2095 (0.0%)	1.79	42/2853 (1.5%)
All	All	0.89	1/5069 (0.0%)	1.67	84/6878 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	158	TRP	CG-CD2	-5.25	1.34	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	ARG	NE-CZ-NH2	12.75	126.68	120.30
2	B	79	ARG	NE-CZ-NH2	11.57	126.08	120.30
2	B	95	TYR	CB-CG-CD1	-11.03	114.38	121.00
2	B	9	ARG	NE-CZ-NH1	-10.31	115.14	120.30
1	A	311	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	A	38	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	A	253	ARG	NE-CZ-NH2	9.44	125.02	120.30
2	B	213	ARG	NE-CZ-NH1	-9.24	115.68	120.30
1	A	78	TRP	CD1-CG-CD2	8.95	113.46	106.30
2	B	31	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	A	371	ARG	NE-CZ-NH2	8.70	124.65	120.30
2	B	194	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	339	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	311	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	A	364	ALA	N-CA-C	8.16	133.04	111.00
2	B	73	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	78	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	A	339	TRP	CE2-CD2-CG	-7.75	101.10	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	A	311	ARG	CA-CB-CG	-7.60	96.68	113.40
2	B	181	TRP	CD1-CG-CD2	7.32	112.16	106.30
2	B	181	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	B	76	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	85	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	355	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	44	VAL	CA-C-N	6.96	130.12	116.20
1	A	78	TRP	CG-CD2-CE3	6.85	140.07	133.90
1	A	334	ARG	NE-CZ-NH1	-6.77	116.91	120.30
2	B	79	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	372	LYS	N-CA-C	6.67	129.02	111.00
1	A	226	MET	CA-CB-CG	6.62	124.56	113.30
2	B	194	TRP	CE2-CD2-CG	-6.59	102.03	107.30
2	B	255	VAL	N-CA-CB	-6.52	97.16	111.50
2	B	255	VAL	CB-CA-C	6.43	123.62	111.40
1	A	78	TRP	CG-CD1-NE1	-6.43	103.67	110.10
2	B	30	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	B	91	VAL	CG1-CB-CG2	-6.38	100.69	110.90
1	A	371	ARG	N-CA-C	6.25	127.88	111.00
2	B	3	ILE	CG1-CB-CG2	-6.22	97.72	111.40
1	A	355	TRP	CD1-CG-CD2	6.20	111.26	106.30
2	B	82	PHE	CB-CG-CD1	-6.19	116.47	120.80
2	B	36	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	216	CYS	CA-CB-SG	-6.16	102.92	114.00
1	A	85	TRP	CE2-CD2-CG	-6.15	102.38	107.30
1	A	65	THR	N-CA-C	-6.12	94.47	111.00
1	A	43	MET	CG-SD-CE	-6.09	90.46	100.20
1	A	322	SER	N-CA-C	6.08	127.40	111.00
2	B	158	TRP	CE2-CD2-CG	-5.98	102.52	107.30
1	A	199	PHE	N-CA-C	-5.97	94.87	111.00
1	A	115	ARG	NE-CZ-NH2	5.94	123.27	120.30
2	B	9	ARG	NE-CZ-NH2	5.88	123.24	120.30
2	B	63	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	B	54	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	68	TYR	CA-CB-CG	5.84	124.50	113.40
1	A	78	TRP	CB-CG-CD1	-5.82	119.43	127.00
2	B	194	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	179	LEU	CA-CB-CG	5.74	128.51	115.30
2	B	6	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	B	181	TRP	CG-CD2-CE3	5.53	138.88	133.90
2	B	188	THR	N-CA-CB	-5.45	99.95	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	MET	CA-CB-CG	5.41	122.50	113.30
2	B	16	MET	CG-SD-CE	-5.41	91.55	100.20
1	A	339	TRP	CG-CD1-NE1	-5.38	104.72	110.10
2	B	80	TYR	CB-CG-CD2	-5.36	117.78	121.00
2	B	213	ARG	NE-CZ-NH2	5.35	122.98	120.30
2	B	185	ARG	NE-CZ-NH2	5.33	122.97	120.30
2	B	189	SER	N-CA-CB	-5.23	102.65	110.50
1	A	322	SER	N-CA-CB	-5.19	102.71	110.50
2	B	176	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	176	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	371	ARG	N-CA-CB	-5.18	101.28	110.60
2	B	41	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	333	GLU	CA-CB-CG	5.16	124.76	113.40
2	B	133	LEU	CA-C-N	-5.15	105.87	117.20
1	A	368	ILE	N-CA-C	5.14	124.88	111.00
2	B	255	VAL	N-CA-C	-5.14	97.13	111.00
2	B	73	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	94	ARG	NE-CZ-NH1	-5.08	117.76	120.30
2	B	176	VAL	CA-CB-CG1	-5.07	103.29	110.90
2	B	29	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	A	255	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	B	172	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	226	MET	N-CA-CB	-5.02	101.57	110.60
1	A	44	VAL	CG1-CB-CG2	-5.02	102.87	110.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2924	0	2887	84	0
2	B	2049	0	1981	38	0
3	A	31	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	83	0	70	0	0
6	A	195	0	0	14	0
6	B	188	0	0	3	0
All	All	5472	0	4950	122	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:99:ASP:HB3	2:B:104:CYS:HB3	1.59	0.83
2:B:207:THR:HG23	2:B:209:CYS:SG	2.19	0.82
2:B:56:ASN:HD21	2:B:63:TYR:H	1.34	0.74
1:A:219:ALA:HB1	1:A:225:GLU:HG3	1.73	0.70
1:A:239:TYR:HB3	1:A:247:ILE:HG22	1.75	0.69
1:A:191:ILE:HG21	1:A:252:GLU:HG3	1.75	0.67
2:B:74:ASN:HA	2:B:77:LYS:NZ	2.12	0.65
1:A:144:SER:HB2	1:A:146:ARG:HG2	1.78	0.64
1:A:152:LEU:HD11	1:A:273:ILE:HD12	1.79	0.64
2:B:11:PHE:HD2	2:B:40:VAL:HG13	1.64	0.63
2:B:239:TYR:HB2	2:B:241:LEU:HD13	1.82	0.61
1:A:122:MET:HB3	1:A:128:VAL:HG21	1.83	0.60
1:A:34:VAL:HG21	1:A:80:ASP:HB3	1.82	0.60
1:A:187:TYR:O	1:A:190:LYS:HB3	2.03	0.59
1:A:334:ARG:HA	1:A:337:SER:OG	2.02	0.59
2:B:3:ILE:HD11	2:B:164:MET:SD	2.44	0.58
1:A:219:ALA:CB	1:A:225:GLU:HG3	2.34	0.57
1:A:298:LEU:HB3	1:A:303:THR:HG23	1.85	0.57
1:A:195:ARG:NH1	1:A:249:ILE:HA	2.21	0.56
1:A:282:MET:SD	6:A:531:HOH:O	2.58	0.56
1:A:301:GLY:HA3	3:A:401:ATP:O4'	2.06	0.56
1:A:8:VAL:HG21	1:A:343:SER:HA	1.88	0.56
1:A:352:GLN:HA	1:A:355:TRP:HE3	1.71	0.55
1:A:153:ASP:HA	1:A:299:SER:O	2.06	0.55
1:A:161:ASN:HD22	1:A:276:THR:HG22	1.70	0.55
2:B:41:ARG:NE	2:B:76:TYR:HE1	2.05	0.55
2:B:70:PRO:HD3	2:B:79:ARG:NH2	2.22	0.55
1:A:301:GLY:O	1:A:304:MET:HB2	2.07	0.55
1:A:72:HIC:HD2	1:A:157:GLY:O	2.07	0.54
2:B:131:VAL:HG13	2:B:165:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:ARG:O	1:A:212:LYS:HB3	2.07	0.54
2:B:101:CYS:O	2:B:104:CYS:HB2	2.08	0.53
1:A:316:ILE:HD12	1:A:328:ILE:HD11	1.90	0.53
1:A:217:TYR:O	1:A:254:PHE:HA	2.09	0.53
1:A:98:GLU:HA	1:A:127:ASN:O	2.09	0.52
2:B:56:ASN:ND2	2:B:63:TYR:H	2.04	0.52
1:A:88:SER:O	1:A:93:LEU:HB2	2.10	0.52
1:A:229:ALA:HB2	1:A:235:LEU:HD12	1.91	0.52
2:B:224:SER:O	2:B:260:THR:HG22	2.10	0.52
1:A:192:LEU:HD21	1:A:211:ILE:HD11	1.92	0.52
1:A:249:ILE:HB	1:A:252:GLU:HB2	1.92	0.51
1:A:152:LEU:HD21	1:A:273:ILE:HG23	1.92	0.51
1:A:42:VAL:HG12	2:B:66:VAL:HG13	1.92	0.51
2:B:133:LEU:O	2:B:167:GLY:HA3	2.11	0.51
1:A:122:MET:HB3	1:A:128:VAL:CG2	2.41	0.51
1:A:102:THR:O	1:A:131:MET:HA	2.11	0.50
1:A:24:ASP:HB2	6:A:516:HOH:O	2.11	0.50
1:A:33:ILE:HD11	1:A:58:GLN:HB2	1.94	0.49
1:A:160:HIS:CE1	1:A:176:ARG:HG3	2.47	0.49
2:B:28:ILE:O	2:B:31:ARG:HG3	2.12	0.49
1:A:142:TYR:HA	1:A:146:ARG:O	2.12	0.49
2:B:210:ALA:O	2:B:213:ARG:HD3	2.13	0.49
1:A:112:LYS:HB3	6:A:659:HOH:O	2.13	0.49
1:A:159:THR:HG21	1:A:273:ILE:HD11	1.93	0.49
1:A:170:LEU:HD12	1:A:284:CYS:SG	2.53	0.48
1:A:71:GLU:HB3	6:A:576:HOH:O	2.13	0.48
1:A:112:LYS:HZ3	1:A:369:VAL:H	1.61	0.48
2:B:11:PHE:HB3	2:B:40:VAL:HA	1.96	0.48
2:B:78:GLU:OE2	2:B:134:HIS:HD2	1.96	0.47
2:B:236:GLN:NE2	2:B:243:ASN:HA	2.29	0.47
1:A:120:GLN:O	1:A:124:GLU:HB2	2.14	0.47
2:B:50:LYS:HE3	2:B:50:LYS:HA	1.96	0.47
1:A:239:TYR:HB3	1:A:247:ILE:CG2	2.44	0.47
1:A:249:ILE:H	1:A:249:ILE:HD13	1.78	0.47
2:B:96:GLN:HG2	6:B:532:HOH:O	2.15	0.47
1:A:263:PRO:HB3	1:A:268:MET:HB3	1.97	0.47
2:B:90:SER:O	2:B:118:PHE:HA	2.15	0.47
2:B:1:LEU:N	6:B:568:HOH:O	2.48	0.46
1:A:39:HIS:HA	6:A:672:HOH:O	2.16	0.46
2:B:74:ASN:HA	2:B:77:LYS:HZ1	1.81	0.46
1:A:19:GLY:HA3	6:A:626:HOH:O	2.16	0.46
2:B:197:PRO:HA	6:B:513:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:LEU:HB3	1:A:199:PHE:HE1	1.81	0.46
1:A:215:LEU:O	1:A:253:ARG:HD2	2.14	0.46
1:A:336:TYR:O	1:A:340:ILE:HG13	2.16	0.45
1:A:183:ASP:HB3	6:A:588:HOH:O	2.16	0.45
1:A:170:LEU:HB3	1:A:373:CYS:HB3	1.97	0.45
1:A:11:ASN:ND2	1:A:85:TRP:HE1	2.14	0.45
1:A:239:TYR:HA	6:A:618:HOH:O	2.16	0.45
1:A:152:LEU:CD2	1:A:273:ILE:HG23	2.47	0.45
1:A:115:ARG:HD3	1:A:368:ILE:HG12	1.99	0.45
2:B:70:PRO:HB3	2:B:77:LYS:HB3	2.00	0.44
2:B:11:PHE:CD2	2:B:40:VAL:HG13	2.50	0.44
1:A:304:MET:HB3	3:A:401:ATP:C6	2.53	0.44
1:A:101:PRO:HA	1:A:130:ALA:O	2.18	0.44
2:B:7:ASN:C	2:B:7:ASN:HD22	2.21	0.44
2:B:125:VAL:HG13	2:B:220:LEU:HB3	2.00	0.44
2:B:29:VAL:HG13	2:B:35:VAL:HG11	1.99	0.44
1:A:3:GLU:HB3	6:A:597:HOH:O	2.17	0.44
1:A:165:TYR:HB3	1:A:170:LEU:HD21	2.00	0.44
1:A:369:VAL:HG23	1:A:371:ARG:NH1	2.33	0.44
2:B:214:ILE:HG13	2:B:255:VAL:HG13	1.98	0.44
1:A:239:TYR:HE2	6:A:633:HOH:O	2.00	0.43
1:A:349:SER:HA	1:A:352:GLN:OE1	2.19	0.43
1:A:297:VAL:HG23	6:A:584:HOH:O	2.17	0.43
1:A:348:LEU:HB3	1:A:350:THR:OG1	2.19	0.43
1:A:368:ILE:HG21	6:A:646:HOH:O	2.17	0.43
1:A:236:GLU:HA	1:A:250:GLY:HA2	2.00	0.43
2:B:69:GLU:O	2:B:71:LEU:HG	2.19	0.42
1:A:78:TRP:CD2	1:A:117:LYS:HG2	2.55	0.42
1:A:91:ASN:O	1:A:94:ARG:HD3	2.19	0.42
2:B:16:MET:CE	2:B:25:ILE:HD12	2.49	0.42
1:A:132:TYR:CG	1:A:351:PHE:HZ	2.38	0.42
1:A:335:LYS:HE3	1:A:335:LYS:HB2	1.86	0.42
2:B:147:LEU:HA	2:B:147:LEU:HD12	1.89	0.42
1:A:303:THR:HG22	1:A:334:ARG:HE	1.85	0.42
2:B:230:ALA:HA	2:B:256:GLU:O	2.20	0.41
2:B:3:ILE:HD11	2:B:166:MET:SD	2.60	0.41
1:A:131:MET:O	1:A:356:ILE:HG23	2.20	0.41
1:A:155:GLY:O	1:A:180:ALA:HB1	2.21	0.41
1:A:153:ASP:O	1:A:159:THR:HA	2.20	0.41
1:A:115:ARG:HD2	1:A:368:ILE:HD11	2.02	0.41
1:A:6:ALA:HA	1:A:101:PRO:HD2	2.02	0.41
1:A:96:ALA:O	1:A:100:HIS:HD2	2.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:156:ASP:HB2	3:A:401:ATP:H5'1	2.03	0.41
1:A:172:HIS:HB2	1:A:373:CYS:O	2.21	0.41
1:A:104:LEU:O	1:A:133:VAL:HA	2.20	0.41
1:A:214:LYS:HE2	6:A:633:HOH:O	2.21	0.40
3:A:401:ATP:H1'	6:A:506:HOH:O	2.21	0.40
1:A:140:SER:O	1:A:143:ALA:HB3	2.20	0.40
1:A:285:ASP:O	1:A:288:ILE:HG12	2.21	0.40
2:B:187:ARG:HD3	2:B:194:TRP:CE2	2.56	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	371/374 (99%)	339 (91%)	22 (6%)	10 (3%)	8	1
2	B	258/260 (99%)	244 (95%)	9 (4%)	5 (2%)	12	2
All	All	629/634 (99%)	583 (93%)	31 (5%)	15 (2%)	9	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	SER
1	A	367	SER
1	A	373	CYS
1	A	286	ILE
1	A	372	LYS
2	B	57	GLN
1	A	195	ARG
2	B	43	SER
1	A	273	ILE
2	B	75	SER
2	B	74	ASN
2	B	101	CYS

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Mol	Chain	Res	Type
1	A	250	GLY
1	A	366	PRO
1	A	181	GLY

### 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	316/316 (100%)	282 (89%)	34 (11%)	9	2
2	B	229/229 (100%)	204 (89%)	25 (11%)	9	2
All	All	545/545 (100%)	486 (89%)	59 (11%)	9	2

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	36	ARG
1	A	42	VAL
1	A	71	GLU
1	A	82	GLU
1	A	83	LYS
1	A	111	PRO
1	A	116	GLU
1	A	124	GLU
1	A	127	ASN
1	A	177	LEU
1	A	195	ARG
1	A	207	ILE
1	A	247	ILE
1	A	249	ILE
1	A	256	CYS
1	A	260	LEU
1	A	274	HIS
1	A	303	THR
1	A	304	MET
1	A	310	ASP
1	A	311	ARG

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	322	SER
1	A	323	THR
1	A	327	LYS
1	A	333	GLU
1	A	335	LYS
1	A	352	GLN
1	A	355	TRP
1	A	356	ILE
1	A	360	GLU
1	A	370	HIS
1	A	374	PHE
2	B	3	ILE
2	B	7	ASN
2	B	36	LEU
2	B	50	LYS
2	B	52	LEU
2	B	69	GLU
2	B	76	TYR
2	B	98	ASP
2	B	101	CYS
2	B	102	GLU
2	B	111	ARG
2	B	115	VAL
2	B	122	SER
2	B	125	VAL
2	B	134	HIS
2	B	152	LEU
2	B	156	GLN
2	B	183	SER
2	B	188	THR
2	B	199	SER
2	B	206	SER
2	B	207	THR
2	B	225	VAL
2	B	243	ASN
2	B	255	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN

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Mol	Chain	Res	Type
1	A	110	ASN
1	A	160	HIS
1	A	161	ASN
2	B	7	ASN
2	B	44	HIS
2	B	56	ASN
2	B	134	HIS
2	B	161	ASN
2	B	193	GLN
2	B	222	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
1	HIC	A	72	1	11,11,12	5.94	6 (54%)	12,14,16	3.42	5 (41%)

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	HIC	A	72	1	-	0/4/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	HIC	O-C	18.32	1.24	1.11
1	A	72	HIC	CD2-NE2	-4.17	1.31	1.37
1	A	72	HIC	CE1-NE2	-3.60	1.31	1.36
1	A	72	HIC	CD2-CG	2.78	1.39	1.36
1	A	72	HIC	CA-C	2.73	1.53	1.48
1	A	72	HIC	CE1-ND1	-2.20	1.30	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIC	CG-CD2-NE2	-6.86	99.38	107.19
1	A	72	HIC	CD2-NE2-CE1	6.42	118.31	107.95
1	A	72	HIC	CG-CB-CA	4.61	120.15	113.85
1	A	72	HIC	ND1-CE1-NE2	-4.23	102.60	112.55
1	A	72	HIC	CE1-ND1-CG	2.96	110.52	104.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

7 carbohydrates 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
5	NAG	B	301	2,5	12,14,15	1.11	1 (8%)	15,19,21	0.89	1 (6%)
5	NAG	B	302	5	12,14,15	1.18	0	15,19,21	1.55	3 (20%)
5	BMA	B	303	5	10,11,12	1.60	3 (30%)	11,15,17	1.45	2 (18%)
5	MAN	B	304	5	10,11,12	1.61	3 (30%)	11,15,17	1.03	1 (9%)
5	BMA	B	305	5	10,11,12	0.87	0	11,15,17	1.10	1 (9%)
5	BMA	B	306	5	10,11,12	1.13	1 (10%)	11,15,17	1.30	1 (9%)
5	MAN	B	307	5	10,11,12	1.08	1 (10%)	11,15,17	1.76	3 (27%)

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
5	NAG	B	301	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	302	5	-	0/6/23/26	0/1/1/1
5	BMA	B	303	5	-	0/2/19/22	0/1/1/1
5	MAN	B	304	5	-	0/2/19/22	0/1/1/1
5	BMA	B	305	5	-	0/2/19/22	0/1/1/1
5	BMA	B	306	5	-	0/2/19/22	0/1/1/1
5	MAN	B	307	5	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	304	MAN	C4-C5	3.32	1.60	1.53
5	B	303	BMA	O3-C3	2.96	1.50	1.43
5	B	303	BMA	C3-C2	2.78	1.59	1.52
5	B	301	NAG	C4-C5	2.71	1.59	1.53
5	B	306	BMA	C3-C2	2.69	1.58	1.52
5	B	307	MAN	C4-C5	2.35	1.58	1.53
5	B	304	MAN	C4-C3	2.25	1.58	1.52
5	B	303	BMA	C4-C3	2.13	1.58	1.52
5	B	304	MAN	O3-C3	2.08	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	307	MAN	C3-C4-C5	3.57	116.58	110.20
5	B	302	NAG	C3-C4-C5	-3.53	103.89	110.20
5	B	303	BMA	C3-C4-C5	2.90	115.39	110.20
5	B	306	BMA	O3-C3-C2	2.68	114.84	109.94
5	B	305	BMA	O5-C5-C4	-2.37	107.65	110.65
5	B	307	MAN	O5-C5-C6	2.35	109.44	106.98
5	B	301	NAG	C2-N2-C7	2.32	126.98	123.09
5	B	303	BMA	O5-C5-C6	2.27	109.36	106.98
5	B	302	NAG	C3-C2-N2	-2.21	108.39	111.76
5	B	302	NAG	C4-C3-C2	-2.10	106.19	111.32
5	B	307	MAN	O5-C5-C4	-2.05	108.05	110.65
5	B	304	MAN	C3-C4-C5	2.03	113.83	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
3	ATP	A	401	4	33,33,33	1.40	6 (18%)	52,52,52	1.46	4 (7%)

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	ATP	A	401	4	-	0/22/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ATP	C2'-C1'	-4.14	1.47	1.53
3	A	401	ATP	PB-O3B	2.62	1.64	1.59
3	A	401	ATP	PG-O3B	2.44	1.64	1.60
3	A	401	ATP	PG-O3G	-2.39	1.46	1.54
3	A	401	ATP	C8-N7	-2.36	1.30	1.34
3	A	401	ATP	C5-C4	-2.02	1.35	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ATP	O4'-C1'-N9	5.43	113.49	108.44
3	A	401	ATP	C4'-O4'-C1'	-4.79	104.55	109.75
3	A	401	ATP	C1'-N9-C4	-2.31	122.64	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	401	ATP	O4'-C4'-C3'	2.10	109.43	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	374/374 (100%)	10.58	374 (100%) 0 0	10, 34, 64, 72	0
2	B	260/260 (100%)	9.62	260 (100%) 0 0	4, 16, 42, 57	0
All	All	634/634 (100%)	10.19	634 (100%) 0 0	4, 26, 61, 72	0

All (634) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ALA	41.8
2	B	228	GLY	30.8
1	A	155	GLY	30.3
1	A	368	ILE	29.0
1	A	143	ALA	24.8
1	A	102	THR	23.6
2	B	209	CYS	23.5
1	A	246	VAL	23.0
2	B	8	ILE	22.7
1	A	139	LEU	21.6
1	A	2	GLU	20.9
2	B	241	LEU	20.8
1	A	168	TYR	20.6
1	A	93	LEU	20.4
2	B	200	ALA	20.3
1	A	217	TYR	20.1
1	A	242	PRO	20.0
2	B	21	LEU	19.8
1	A	348	LEU	19.7
1	A	172	HIS	19.7
1	A	150	ILE	19.4
1	A	173	ALA	19.3
1	A	218	VAL	19.1
1	A	288	ILE	18.9

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Mol	Chain	Res	Type	RSRZ
1	A	371	ARG	18.8
1	A	15	LEU	18.8
2	B	152	LEU	18.7
1	A	369	VAL	18.4
1	A	300	GLY	18.3
1	A	324	MET	18.3
2	B	97	TYR	18.1
1	A	59	SER	17.8
1	A	34	VAL	17.7
1	A	25	ALA	17.7
2	B	227	PRO	17.6
1	A	241	LEU	17.5
2	B	55	LEU	17.5
1	A	374	PHE	17.4
1	A	355	TRP	17.3
2	B	159	HIS	17.3
1	A	364	ALA	17.2
1	A	167	GLY	17.1
1	A	211	ILE	17.1
1	A	203	ALA	17.0
1	A	365	GLY	17.0
1	A	344	ILE	16.9
1	A	165	TYR	16.9
1	A	326	ILE	16.9
1	A	86	HIS	16.7
1	A	32	SER	16.7
1	A	24	ASP	16.5
1	A	18	ALA	16.5
1	A	68	TYR	16.5
1	A	349	SER	16.5
1	A	276	THR	16.5
1	A	356	ILE	16.4
1	A	275	GLU	16.3
1	A	363	GLU	16.3
1	A	85	TRP	16.2
1	A	100	HIS	15.9
1	A	319	LEU	15.9
1	A	50	ASP	15.8
1	A	373	CYS	15.7
2	B	5	ALA	15.7
1	A	3	GLU	15.6
1	A	282	MET	15.5

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Mol	Chain	Res	Type	RSRZ
1	A	372	LYS	15.4
2	B	204	ALA	15.3
1	A	178	ASP	15.3
2	B	106	ASN	15.1
1	A	79	ASP	15.0
2	B	165	LEU	14.9
2	B	43	SER	14.9
2	B	188	THR	14.9
1	A	329	ILE	14.8
1	A	133	VAL	14.8
2	B	41	ARG	14.7
2	B	254	PRO	14.6
1	A	269	GLU	14.6
2	B	146	SER	14.6
2	B	192	PHE	14.5
1	A	350	THR	14.5
1	A	191	ILE	14.5
2	B	154	VAL	14.5
1	A	229	ALA	14.4
2	B	253	TYR	14.4
1	A	224	ASN	14.4
1	A	74	ILE	14.4
2	B	142	ALA	14.3
1	A	142	TYR	14.3
1	A	147	THR	14.3
1	A	339	TRP	14.2
1	A	256	CYS	14.2
1	A	200	VAL	14.2
1	A	110	ASN	14.1
2	B	35	VAL	14.1
2	B	84	PHE	14.0
1	A	119	THR	13.9
2	B	17	SER	13.8
1	A	199	PHE	13.7
2	B	257	VAL	13.7
2	B	28	ILE	13.7
2	B	248	ALA	13.7
2	B	121	HIS	13.7
1	A	254	PHE	13.7
1	A	360	GLU	13.7
1	A	265	PHE	13.6
2	B	110	SER	13.6

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Mol	Chain	Res	Type	RSRZ
1	A	94	ARG	13.6
1	A	207	ILE	13.6
2	B	145	ASN	13.5
1	A	310	ASP	13.4
1	A	362	ASP	13.4
2	B	218	GLY	13.4
1	A	126	PHE	13.4
1	A	120	GLN	13.3
1	A	116	GLU	13.3
1	A	353	GLN	13.3
2	B	101	CYS	13.2
2	B	245	MET	13.2
1	A	215	LEU	13.2
1	A	80	ASP	13.1
1	A	286	ILE	13.1
1	A	347	SER	13.0
1	A	98	GLU	13.0
2	B	113	PRO	12.9
1	A	233	SER	12.9
1	A	358	LYS	12.8
2	B	260	THR	12.8
1	A	292	LEU	12.8
1	A	361	TYR	12.8
1	A	222	PHE	12.7
1	A	278	TYR	12.7
2	B	175	TYR	12.7
2	B	32	TYR	12.7
2	B	52	LEU	12.7
1	A	132	TYR	12.7
1	A	359	GLN	12.6
1	A	1	GLU	12.5
1	A	354	MET	12.5
1	A	370	HIS	12.5
2	B	83	LEU	12.5
2	B	239	TYR	12.5
2	B	29	VAL	12.5
2	B	61	ASN	12.4
1	A	306	PRO	12.4
1	A	249	ILE	12.4
2	B	195	LEU	12.4
1	A	296	ASN	12.3
2	B	74	ASN	12.3

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Mol	Chain	Res	Type	RSRZ
2	B	76	TYR	12.2
1	A	260	LEU	12.2
1	A	232	SER	12.1
2	B	235	PHE	12.1
2	B	176	VAL	12.1
1	A	129	PRO	12.0
2	B	94	THR	12.0
2	B	11	PHE	12.0
1	A	186	ASP	12.0
2	B	20	THR	12.0
1	A	134	ALA	12.0
1	A	36	ARG	11.9
1	A	20	PHE	11.9
1	A	320	ALA	11.9
1	A	128	VAL	11.9
2	B	22	ALA	11.9
1	A	312	MET	11.9
1	A	112	LYS	11.8
2	B	16	MET	11.8
1	A	248	THR	11.8
2	B	86	PRO	11.8
2	B	147	LEU	11.8
1	A	287	ASP	11.8
2	B	99	ASP	11.8
2	B	128	PHE	11.7
2	B	126	LYS	11.7
1	A	289	ARG	11.7
1	A	144	SER	11.7
1	A	12	GLY	11.7
1	A	338	VAL	11.6
1	A	152	LEU	11.6
2	B	75	SER	11.6
2	B	224	SER	11.6
2	B	158	TRP	11.5
1	A	46	MET	11.5
2	B	155	GLN	11.5
1	A	87	HIS	11.5
1	A	316	ILE	11.4
1	A	201	THR	11.4
2	B	36	LEU	11.3
1	A	5	THR	11.3
2	B	229	SER	11.3

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Mol	Chain	Res	Type	RSRZ
1	A	162	VAL	11.3
2	B	71	LEU	11.3
2	B	95	TYR	11.3
1	A	366	PRO	11.2
1	A	65	THR	11.2
2	B	96	GLN	11.2
1	A	182	ARG	11.2
1	A	197	TYR	11.2
1	A	334	ARG	11.2
1	A	40	GLN	11.1
2	B	34	ILE	11.1
2	B	194	TRP	11.1
2	B	240	GLY	11.1
1	A	323	THR	11.0
1	A	337	SER	11.0
1	A	301	GLY	11.0
1	A	351	PHE	11.0
2	B	231	ALA	10.9
1	A	22	GLY	10.9
2	B	103	SER	10.9
2	B	26	VAL	10.8
2	B	104	CYS	10.8
1	A	14	GLY	10.8
2	B	172	ASP	10.8
2	B	184	ILE	10.7
1	A	77	ASN	10.7
1	A	251	ASN	10.7
1	A	223	GLU	10.7
1	A	63	ILE	10.7
1	A	210	ASP	10.7
2	B	136	ALA	10.6
1	A	61	ARG	10.6
2	B	170	ASN	10.6
1	A	121	ILE	10.6
2	B	250	SER	10.6
2	B	23	SER	10.6
2	B	221	LEU	10.6
1	A	298	LEU	10.6
1	A	268	MET	10.6
1	A	64	LEU	10.6
1	A	7	LEU	10.5
2	B	199	SER	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	193	THR	10.5
2	B	6	PHE	10.5
2	B	220	LEU	10.5
2	B	207	THR	10.4
1	A	161	ASN	10.4
1	A	235	LEU	10.4
1	A	205	ARG	10.4
1	A	124	GLU	10.4
2	B	161	ASN	10.4
1	A	45	GLY	10.4
1	A	196	GLY	10.4
1	A	240	GLU	10.4
1	A	158	VAL	10.4
1	A	104	LEU	10.3
2	B	212	ASP	10.3
1	A	314	LYS	10.3
1	A	184	LEU	10.3
2	B	1	LEU	10.3
1	A	156	ASP	10.3
2	B	64	HIS	10.3
1	A	83	LYS	10.3
1	A	29	VAL	10.2
2	B	181	TRP	10.2
2	B	135	SER	10.2
2	B	89	VAL	10.2
1	A	239	TYR	10.1
1	A	113	ALA	10.1
2	B	160	LEU	10.1
2	B	211	TYR	10.1
2	B	49	GLY	10.1
2	B	233	PHE	10.1
1	A	226	MET	10.0
1	A	8	VAL	10.0
1	A	151	VAL	10.0
1	A	131	MET	10.0
1	A	245	GLN	10.0
1	A	103	LEU	10.0
2	B	137	PRO	10.0
2	B	169	PHE	10.0
1	A	299	SER	10.0
1	A	91	ASN	9.9
1	A	44	VAL	9.9

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Mol	Chain	Res	Type	RSRZ
2	B	91	VAL	9.9
1	A	137	ALA	9.8
2	B	109	PHE	9.8
2	B	81	LEU	9.8
1	A	130	ALA	9.8
2	B	73	ARG	9.8
1	A	114	ASN	9.8
2	B	134	HIS	9.7
2	B	201	ASP	9.7
2	B	173	CYS	9.7
2	B	196	ILE	9.7
1	A	179	LEU	9.7
1	A	255	ARG	9.7
1	A	322	SER	9.7
1	A	228	THR	9.7
2	B	255	VAL	9.7
2	B	214	ILE	9.7
2	B	62	THR	9.7
2	B	249	ILE	9.7
1	A	135	ILE	9.6
1	A	313	GLN	9.6
1	A	352	GLN	9.6
1	A	51	SER	9.6
2	B	217	ALA	9.6
2	B	50	LYS	9.6
2	B	162	ASP	9.6
1	A	164	ILE	9.6
2	B	82	PHE	9.5
1	A	75	ILE	9.5
2	B	167	GLY	9.5
2	B	92	LEU	9.5
1	A	219	ALA	9.5
1	A	76	THR	9.5
2	B	216	VAL	9.5
1	A	293	TYR	9.5
1	A	141	LEU	9.5
2	B	244	GLU	9.5
1	A	204	GLU	9.5
1	A	73	GLY	9.5
1	A	176	ARG	9.5
2	B	57	GLN	9.5
1	A	216	CYS	9.4

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Mol	Chain	Res	Type	RSRZ
2	B	60	PRO	9.4
1	A	123	PHE	9.4
1	A	271	ALA	9.4
1	A	27	ARG	9.4
1	A	10	ASP	9.3
2	B	19	ALA	9.3
1	A	78	TRP	9.3
1	A	42	VAL	9.3
1	A	244	GLY	9.3
1	A	41	GLY	9.3
1	A	325	LYS	9.3
2	B	115	VAL	9.3
1	A	17	LYS	9.3
1	A	345	LEU	9.3
2	B	67	VAL	9.2
1	A	127	ASN	9.2
1	A	247	ILE	9.2
1	A	259	THR	9.2
1	A	261	PHE	9.2
2	B	58	ASP	9.1
1	A	47	GLY	9.1
2	B	123	THR	9.1
1	A	227	ALA	9.1
1	A	294	ALA	9.1
1	A	194	GLU	9.1
1	A	4	THR	9.1
2	B	45	LEU	9.1
2	B	131	VAL	9.1
2	B	102	GLU	9.1
1	A	236	GLU	9.0
1	A	214	LYS	9.0
1	A	148	THR	9.0
1	A	39	HIS	9.0
1	A	321	PRO	9.0
1	A	195	ARG	8.9
1	A	274	HIS	8.9
2	B	40	VAL	8.9
1	A	221	ASP	8.9
1	A	317	THR	8.9
2	B	153	ASP	8.9
1	A	69	PRO	8.9
1	A	225	GLU	8.8

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Mol	Chain	Res	Type	RSRZ
2	B	107	ASP	8.8
1	A	31	PRO	8.8
1	A	52	TYR	8.8
2	B	24	TYR	8.8
1	A	9	CYS	8.8
1	A	252	GLU	8.8
2	B	190	SER	8.8
2	B	208	ASN	8.8
2	B	47	ALA	8.8
2	B	256	GLU	8.8
1	A	96	ALA	8.7
1	A	343	SER	8.7
2	B	54	TYR	8.7
2	B	148	TYR	8.7
1	A	146	ARG	8.7
1	A	346	ALA	8.6
2	B	129	ALA	8.6
2	B	132	ALA	8.6
1	A	67	LYS	8.6
2	B	232	PRO	8.6
1	A	125	THR	8.5
2	B	122	SER	8.5
2	B	37	ILE	8.5
1	A	92	GLU	8.5
1	A	89	PHE	8.5
1	A	206	GLU	8.5
1	A	101	PRO	8.5
2	B	120	SER	8.5
2	B	252	HIS	8.5
1	A	198	SER	8.5
1	A	108	PRO	8.5
1	A	202	THR	8.5
1	A	262	GLN	8.5
1	A	54	GLY	8.4
1	A	170	LEU	8.4
1	A	220	LEU	8.4
1	A	16	CYS	8.4
2	B	10	THR	8.4
2	B	230	ALA	8.4
1	A	281	ILE	8.4
2	B	205	THR	8.4
1	A	230	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
2	B	69	GLU	8.3
2	B	151	TYR	8.3
2	B	171	ALA	8.3
1	A	48	GLN	8.3
2	B	127	GLU	8.3
1	A	291	ASP	8.3
2	B	124	LYS	8.3
1	A	335	LYS	8.2
1	A	311	ARG	8.2
2	B	65	TYR	8.2
1	A	283	LYS	8.2
2	B	215	VAL	8.2
2	B	27	ARG	8.2
1	A	264	SER	8.2
1	A	190	LYS	8.2
1	A	267	GLY	8.2
2	B	189	SER	8.2
1	A	84	ILE	8.2
2	B	118	PHE	8.2
1	A	66	LEU	8.1
1	A	189	MET	8.1
1	A	280	SER	8.1
2	B	149	ASP	8.1
1	A	118	MET	8.1
1	A	159	THR	8.1
2	B	51	LEU	8.1
2	B	210	ALA	8.1
1	A	183	ASP	8.0
1	A	37	PRO	8.0
1	A	305	TYR	8.0
1	A	157	GLY	8.0
2	B	44	HIS	8.0
1	A	53	VAL	8.0
2	B	125	VAL	8.0
2	B	259	LEU	8.0
2	B	7	ASN	7.9
2	B	53	ASP	7.9
1	A	95	VAL	7.9
1	A	115	ARG	7.9
1	A	70	ILE	7.9
1	A	327	LYS	7.9
1	A	187	TYR	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	7.9
2	B	12	GLY	7.9
1	A	23	ASP	7.9
1	A	174	ILE	7.8
2	B	9	ARG	7.8
1	A	175	MET	7.8
1	A	11	ASN	7.8
2	B	141	VAL	7.8
1	A	290	LYS	7.8
2	B	138	SER	7.8
1	A	357	SER	7.7
1	A	330	ALA	7.7
1	A	13	SER	7.7
2	B	203	THR	7.6
1	A	243	ASP	7.6
1	A	295	ASN	7.6
2	B	198	ASP	7.6
2	B	108	SER	7.6
1	A	49	LYS	7.5
1	A	231	SER	7.5
2	B	119	SER	7.5
2	B	98	ASP	7.5
2	B	191	THR	7.5
1	A	208	VAL	7.5
2	B	177	THR	7.5
2	B	3	ILE	7.4
1	A	213	GLU	7.4
2	B	222	GLN	7.4
1	A	90	TYR	7.4
1	A	258	GLU	7.4
2	B	93	ASP	7.4
2	B	133	LEU	7.4
1	A	238	SER	7.3
2	B	174	SER	7.3
1	A	284	CYS	7.3
1	A	307	GLY	7.3
1	A	122	MET	7.3
2	B	88	LYS	7.3
2	B	251	ASP	7.3
2	B	164	MET	7.3
2	B	258	THR	7.3
2	B	183	SER	7.3

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Mol	Chain	Res	Type	RSRZ
2	B	90	SER	7.2
2	B	112	GLU	7.2
2	B	139	ASP	7.2
2	B	163	VAL	7.2
1	A	33	ILE	7.2
1	A	109	LEU	7.2
2	B	178	SER	7.2
2	B	4	ALA	7.2
2	B	180	GLN	7.2
1	A	263	PRO	7.2
2	B	156	GLN	7.2
2	B	13	GLU	7.2
2	B	223	SER	7.2
2	B	140	ALA	7.1
1	A	56	GLU	7.1
2	B	243	ASN	7.1
1	A	341	GLY	7.1
1	A	308	ILE	7.1
2	B	150	VAL	7.1
1	A	107	ALA	7.0
2	B	87	ASN	7.0
1	A	266	ILE	7.0
1	A	332	PRO	7.0
1	A	145	GLY	6.9
2	B	30	ARG	6.9
2	B	85	ARG	6.9
2	B	144	ILE	6.9
2	B	70	PRO	6.9
1	A	185	THR	6.8
2	B	246	ALA	6.8
2	B	116	VAL	6.8
2	B	63	TYR	6.6
1	A	38	ARG	6.6
2	B	179	SER	6.6
1	A	209	ARG	6.6
2	B	238	ALA	6.6
2	B	166	MET	6.6
2	B	100	GLY	6.5
2	B	48	VAL	6.5
2	B	72	GLY	6.5
2	B	66	VAL	6.5
1	A	136	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
2	B	117	LYS	6.5
2	B	225	VAL	6.4
1	A	97	PRO	6.4
1	A	140	SER	6.4
1	A	62	GLY	6.4
2	B	42	ASP	6.3
1	A	285	ASP	6.3
2	B	206	SER	6.3
1	A	71	GLU	6.3
1	A	55	ASP	6.3
1	A	328	ILE	6.2
2	B	111	ARG	6.2
1	A	192	LEU	6.2
1	A	253	ARG	6.2
2	B	247	LEU	6.2
1	A	166	GLU	6.2
1	A	303	THR	6.2
2	B	186	LEU	6.1
2	B	31	ARG	6.1
2	B	157	LYS	6.1
1	A	270	SER	6.1
2	B	182	SER	6.1
1	A	106	GLU	6.1
1	A	315	GLU	6.0
2	B	202	THR	6.0
2	B	185	ARG	6.0
2	B	80	TYR	6.0
2	B	130	ILE	6.0
2	B	39	GLU	6.0
1	A	212	LYS	6.0
2	B	56	ASN	5.9
2	B	68	SER	5.9
1	A	58	GLN	5.9
2	B	33	ASP	5.9
1	A	153	ASP	5.9
1	A	273	ILE	5.9
2	B	193	GLN	5.9
2	B	187	ARG	5.9
2	B	79	ARG	5.9
1	A	43	MET	5.8
1	A	181	GLY	5.8
2	B	213	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	138	VAL	5.8
2	B	105	GLY	5.8
1	A	180	ALA	5.7
1	A	367	SER	5.7
2	B	219	SER	5.7
1	A	272	GLY	5.7
2	B	78	GLU	5.6
2	B	143	GLU	5.6
1	A	160	HIS	5.6
1	A	28	ALA	5.6
2	B	168	ASP	5.6
2	B	46	VAL	5.6
1	A	105	THR	5.6
2	B	242	SER	5.6
1	A	30	PHE	5.5
1	A	336	TYR	5.5
1	A	6	ALA	5.5
2	B	226	VAL	5.5
1	A	35	GLY	5.5
2	B	2	LYS	5.4
1	A	237	LYS	5.4
1	A	149	GLY	5.3
1	A	57	ALA	5.3
1	A	82	GLU	5.3
1	A	333	GLU	5.3
2	B	114	ALA	5.3
1	A	26	PRO	5.3
1	A	154	SER	5.3
2	B	38	GLN	5.2
2	B	236	GLN	5.2
2	B	59	ASP	5.1
1	A	163	PRO	5.1
1	A	88	SER	5.1
1	A	234	SER	5.1
1	A	279	ASN	5.1
1	A	171	PRO	5.0
2	B	77	LYS	5.0
1	A	250	GLY	5.0
1	A	304	MET	5.0
2	B	237	ALA	4.9
2	B	25	ILE	4.8
1	A	188	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	342	GLY	4.7
1	A	302	THR	4.7
1	A	277	THR	4.7
1	A	117	LYS	4.6
2	B	197	PRO	4.6
1	A	297	VAL	4.6
1	A	99	GLU	4.5
1	A	19	GLY	4.4
1	A	257	PRO	4.3
1	A	331	PRO	4.3
1	A	111	PRO	4.3
2	B	18	ASN	4.3
2	B	14	THR	4.3
1	A	309	ALA	4.2
1	A	318	ALA	4.2
2	B	234	ASP	4.1
1	A	340	ILE	4.0
1	A	81	MET	4.0
1	A	60	LYS	3.9
2	B	15	LYS	3.4
1	A	72	HIC	3.0
1	A	169	ALA	3.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	HIC	A	72	11/12	0.61	-0.50	14,18,23,26	0

## 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	302	14/15	0.83	0.48	53,58,60,61	0
5	MAN	B	307	11/12	1.21	0.07	65,70,72,73	0
5	NAG	B	301	14/15	0.52	-1.20	36,40,45,49	0
5	BMA	B	305	11/12	0.99	-	62,64,66,67	0
5	MAN	B	304	11/12	1.45	-	60,62,63,65	0
5	BMA	B	303	11/12	0.72	-	60,63,65,67	0
5	BMA	B	306	11/12	1.21	-	66,68,70,71	0

## 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	B	308	1/1	0.75	0.81	15,15,15,15	0
3	ATP	A	401	31/31	0.50	-0.69	11,19,26,28	0
4	CA	A	402	1/1	0.18	-4.18	29,29,29,29	0

## 6.5 Other polymers

There are no such residues in this entry.