



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:05 AM GMT

PDB ID : 3O0G
Title : Crystal Structure of Cdk5:p25 in complex with an ATP analogue
Authors : Mapelli, M.
Deposited on : 2010-07-19
Resolution : 1.95 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

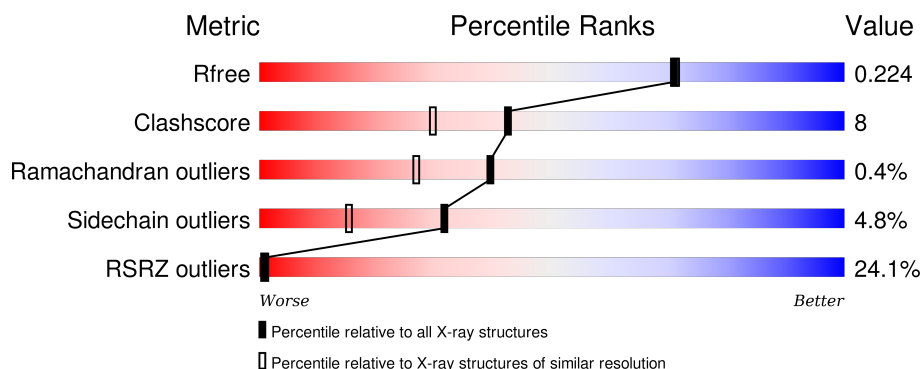
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 $\leq 5\%$. 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	292	<div> <div>16%</div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
1	B	292	<div> <div>16%</div> <div>70%</div> <div>18%</div> <div>• 10%</div> </div>
2	D	149	<div> <div>8%</div> <div>83%</div> <div>17%</div> </div>
2	E	149	<div> <div>66%</div> <div>89%</div> <div>10%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7105 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2325	1492	400	422	11			
1	B	264	Total	C	N	O	S	0	0	0
			2117	1366	366	375	10			

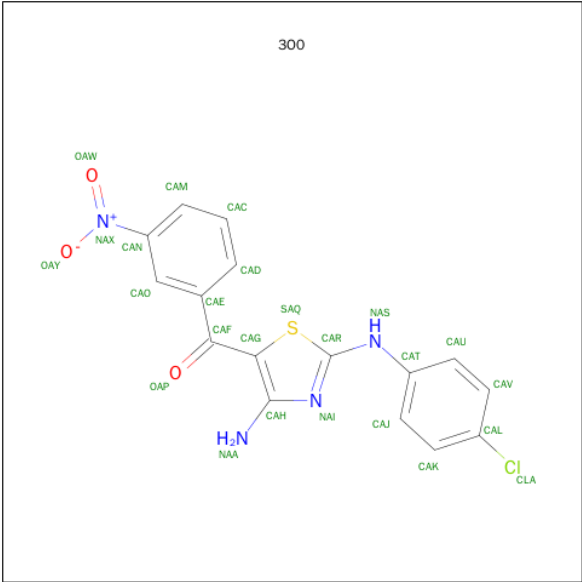
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	ASN	ASP	ENGINEERED MUTATION	UNP Q00535
B	144	ASN	ASP	ENGINEERED MUTATION	UNP Q00535

- Molecule 2 is a protein called Cyclin-dependent kinase 5 activator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	149	Total	C	N	O	S	0	0	0
			1202	771	198	222	11			
2	E	149	Total	C	N	O	S	0	0	0
			1202	771	198	222	11			

- Molecule 3 is {4-AMINO-2-[(4-CHLOROPHENYL)AMINO]-1,3-THIAZOL-5-YL}(3-NITROPHENYL)METHANONE (three-letter code: 3O0) (formula: C₁₆H₁₁ClN₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	B	1	Total	C	Cl	N	O	S	0	0
			25	16	1	4	3	1		

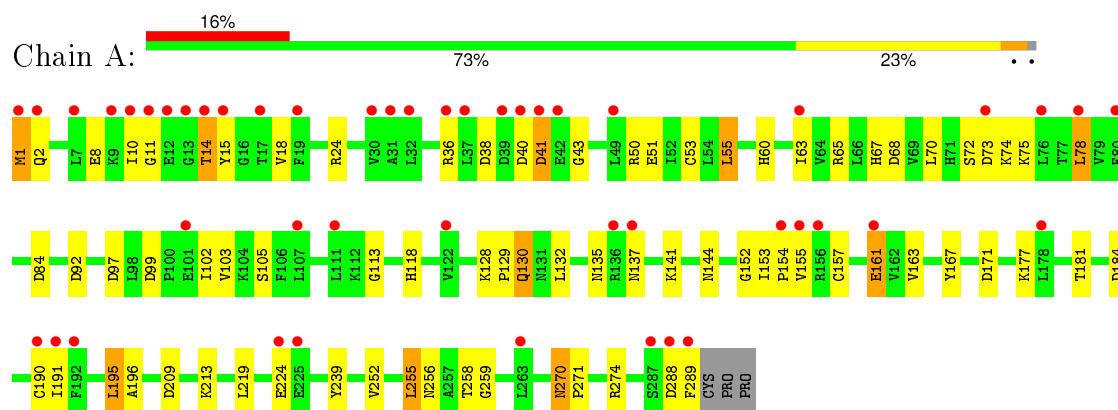
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	D	37	Total	O	0	0
			37	37		
4	B	63	Total	O	0	0
			63	63		
4	E	10	Total	O	0	0
			10	10		

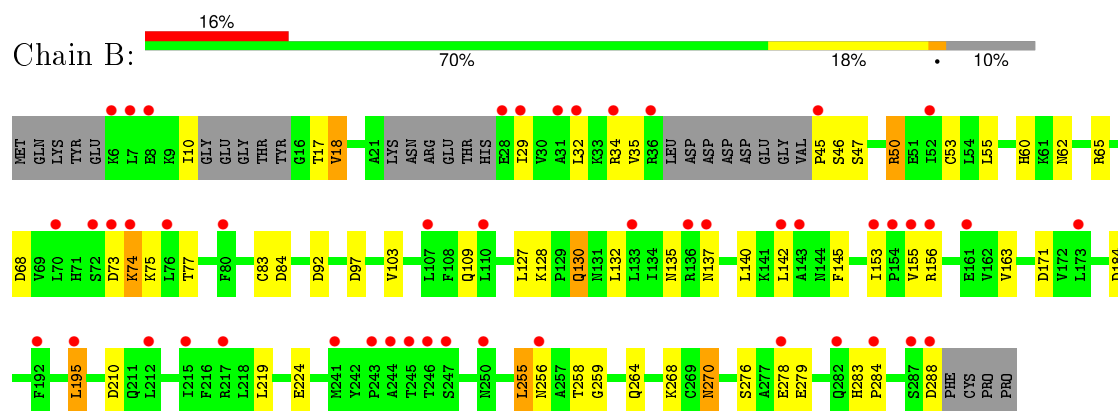
3 Residue-property plots [i](#)

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.

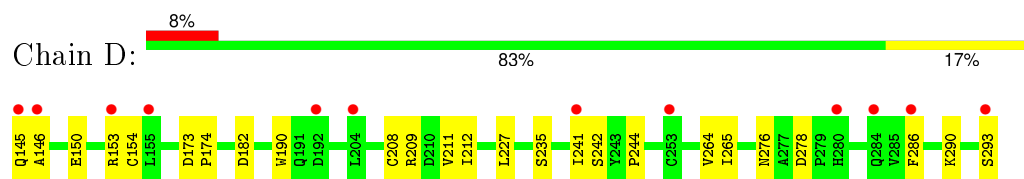
- Molecule 1: Cell division protein kinase 5



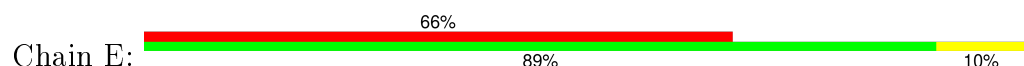
- Molecule 1: Cell division protein kinase 5

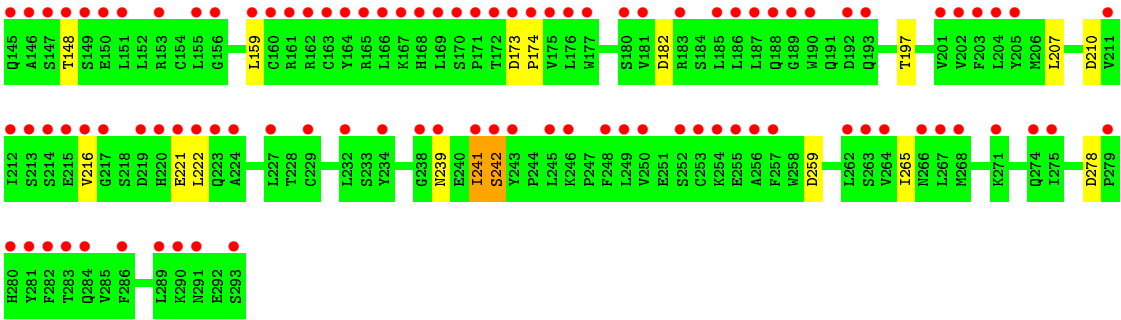


- Molecule 2: Cyclin-dependent kinase 5 activator 1



- Molecule 2: Cyclin-dependent kinase 5 activator 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.12Å 117.12Å 155.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 1.95 19.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.95) 98.0 (19.97-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.256 0.232 , 0.224	Depositor DCC
R_{free} test set	4427 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 62.6	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88261 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7105	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3O0

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	0.58	0/2379	0.82	10/3219 (0.3%)
1	B	0.47	0/2164	0.74	8/2925 (0.3%)
2	D	0.49	0/1230	0.69	2/1667 (0.1%)
2	E	0.35	0/1230	0.62	4/1667 (0.2%)
All	All	0.50	0/7003	0.74	24/9478 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASP	CB-CG-OD2	7.68	125.22	118.30
1	A	68	ASP	CB-CG-OD2	6.58	124.23	118.30
2	D	182	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	84	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	210	ASP	CB-CG-OD2	6.22	123.90	118.30
2	E	278	ASP	CB-CG-OD2	6.06	123.75	118.30
2	D	278	ASP	CB-CG-OD2	5.92	123.63	118.30
2	E	210	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	97	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	78	LEU	CA-CB-CG	5.64	128.26	115.30
1	A	92	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	288	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	40	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	84	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	171	ASP	CB-CG-OD2	5.32	123.08	118.30
2	E	259	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	97	ASP	CB-CG-OD2	5.21	122.98	118.30
1	B	92	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	184	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	209	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	274	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	171	ASP	CB-CG-OD2	5.08	122.87	118.30
2	E	182	ASP	CB-CG-OD2	5.05	122.85	118.30

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	2325	0	2346	60	0
1	B	2117	0	2162	31	0
2	D	1202	0	1187	17	0
2	E	1202	0	1187	11	0
3	B	25	0	11	3	0
4	A	124	0	0	12	0
4	B	63	0	0	4	0
4	D	37	0	0	1	0
4	E	10	0	0	3	0
All	All	7105	0	6893	114	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 8.

All (114) 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:A:256:ASN:HD21	1:A:258:THR:HB	1.11	1.09
1:A:135:ASN:HB2	4:A:384:HOH:O	1.52	1.09
1:A:196:ALA:HB1	4:A:411:HOH:O	1.58	1.03
1:A:256:ASN:ND2	1:A:258:THR:HB	1.72	1.02
1:A:135:ASN:CB	4:A:384:HOH:O	2.06	0.99
1:A:60:HIS:HB3	1:A:63:ILE:HD13	1.47	0.94
1:A:1:MET:HG3	1:A:70:LEU:HD13	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:CYS:HA	2:D:212:ILE:HD13	1.54	0.89
1:A:190:CYS:SG	4:A:297:HOH:O	2.29	0.89
2:D:145:GLN:HA	2:D:150:GLU:HG2	1.56	0.88
1:A:11:GLY:HA3	1:A:18:VAL:HB	1.59	0.85
1:A:167:TYR:CD1	1:A:190:CYS:SG	2.71	0.82
1:B:50:ARG:HD2	4:B:346:HOH:O	1.86	0.74
2:E:239:ASN:HA	4:E:294:HOH:O	1.88	0.72
1:A:167:TYR:CE1	1:A:190:CYS:SG	2.83	0.71
1:A:99:ASP:HB3	1:A:102:ILE:HD13	1.72	0.70
1:B:10:ILE:HG13	1:B:18:VAL:HG23	1.74	0.69
1:A:1:MET:HB2	4:A:375:HOH:O	1.90	0.69
1:B:156:ARG:HD2	2:E:197:THR:HG21	1.76	0.67
1:B:34:ARG:HG3	1:B:75:LYS:HE3	1.78	0.65
1:A:73:ASP:CG	1:A:74:LYS:H	1.97	0.65
3:B:293:3O0:SAQ	3:B:293:3O0:HAU	2.38	0.63
1:A:135:ASN:HB3	4:A:384:HOH:O	1.83	0.61
1:A:129:PRO:HD3	1:A:191:ILE:HD11	1.84	0.60
2:D:153:ARG:HH12	2:D:293:SER:HB2	1.67	0.59
1:A:137:ASN:HB2	4:A:384:HOH:O	2.03	0.59
1:A:118:HIS:HD2	4:A:304:HOH:O	1.88	0.56
1:A:51:GLU:CG	1:A:55:LEU:HD22	2.36	0.56
1:B:83:CYS:HA	1:B:135:ASN:HD21	1.70	0.56
1:A:14:THR:HG21	1:A:144:ASN:HB3	1.88	0.55
1:A:256:ASN:ND2	1:A:258:THR:CB	2.60	0.55
2:E:239:ASN:HB2	4:E:297:HOH:O	2.07	0.53
2:E:159:LEU:HD12	2:E:174:PRO:HB3	1.89	0.53
1:A:43:GLY:O	2:D:242:SER:HB2	2.08	0.53
1:B:10:ILE:CG1	1:B:18:VAL:HG23	2.39	0.53
1:B:35:VAL:HG11	1:B:45:PRO:HB3	1.90	0.53
1:A:99:ASP:HB3	1:A:102:ILE:CD1	2.39	0.53
1:B:128:LYS:HG3	1:B:130:GLN:HG2	1.91	0.52
2:E:207:LEU:HD13	4:E:296:HOH:O	2.09	0.52
1:A:129:PRO:HD3	1:A:191:ILE:CD1	2.40	0.52
1:A:2:GLN:O	1:A:24:ARG:NH1	2.43	0.52
1:B:140:LEU:HB2	4:B:339:HOH:O	2.10	0.52
1:A:103:VAL:HG13	1:A:195:LEU:HB3	1.92	0.51
1:A:270:ASN:HD22	1:A:270:ASN:C	2.14	0.51
1:A:15:TYR:O	4:A:379:HOH:O	2.18	0.51
1:B:46:SER:HB3	2:E:242:SER:HA	1.93	0.51
1:A:161:GLU:HA	1:A:161:GLU:OE1	2.11	0.50
2:D:212:ILE:N	2:D:212:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:HIS:HE1	1:B:62:ASN:HD22	1.60	0.49
3:B:293:3O0:HAD	3:B:293:3O0:SAQ	2.52	0.49
1:B:35:VAL:CG1	1:B:45:PRO:HB3	2.42	0.49
1:B:278:GLU:HG3	4:B:336:HOH:O	2.12	0.49
1:A:118:HIS:HE1	1:A:184:ASP:OD1	1.96	0.49
2:D:173:ASP:HB2	2:D:174:PRO:HD3	1.95	0.49
1:A:73:ASP:CG	1:A:74:LYS:N	2.66	0.48
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.94	0.48
1:A:50:ARG:HD3	2:D:235:SER:O	2.13	0.48
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.94	0.47
1:B:153:ILE:O	1:B:155:VAL:HG23	2.15	0.47
1:A:67:HIS:HE1	4:A:325:HOH:O	1.97	0.47
1:B:55:LEU:HD11	1:B:145:PHE:HB2	1.96	0.47
1:A:41:ASP:N	1:A:41:ASP:OD1	2.48	0.47
1:B:53:CYS:SG	2:E:265:ILE:HG12	2.55	0.47
1:A:36:ARG:NH2	1:A:38:ASP:OD2	2.48	0.46
1:B:264:GLN:O	1:B:268:LYS:HD3	2.15	0.46
2:D:208:CYS:CA	2:D:212:ILE:HD13	2.37	0.46
1:A:129:PRO:HG3	1:A:191:ILE:HD12	1.97	0.46
1:B:103:VAL:HG13	1:B:195:LEU:HB3	1.97	0.46
1:B:283:HIS:CG	1:B:284:PRO:HD2	2.51	0.46
1:A:128:LYS:HA	1:A:191:ILE:HD11	1.96	0.46
1:A:270:ASN:HD22	1:A:271:PRO:N	2.13	0.46
1:A:72:SER:O	1:A:73:ASP:HB3	2.17	0.45
1:A:105:SER:HA	1:A:289:PHE:CZ	2.52	0.45
2:E:216:VAL:HG11	2:E:222:LEU:HB2	1.99	0.45
1:B:47:SER:OG	2:E:241:ILE:O	2.33	0.45
1:A:51:GLU:HG2	1:A:55:LEU:HD22	1.98	0.44
1:A:153:ILE:O	1:A:155:VAL:HG23	2.17	0.44
1:A:60:HIS:HB3	1:A:63:ILE:CD1	2.32	0.44
2:D:146:ALA:HB1	4:D:296:HOH:O	2.18	0.44
1:B:73:ASP:CG	1:B:74:LYS:H	2.22	0.44
1:A:152:GLY:HA3	2:D:276:ASN:O	2.16	0.44
1:B:270:ASN:HD22	1:B:270:ASN:C	2.22	0.43
1:A:105:SER:HA	1:A:289:PHE:HZ	1.83	0.43
1:A:128:LYS:HG3	1:A:130:GLN:HG2	2.00	0.43
1:B:109:GLN:NE2	4:B:339:HOH:O	2.50	0.43
1:A:270:ASN:HD22	1:A:271:PRO:CD	2.31	0.43
2:D:208:CYS:HA	2:D:212:ILE:CD1	2.38	0.43
1:B:127:LEU:CD2	1:B:142:LEU:HD11	2.49	0.43
2:D:286:PHE:CZ	2:D:290:LYS:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:ILE:N	2:D:212:ILE:CD1	2.82	0.42
1:B:10:ILE:HG13	1:B:18:VAL:CG2	2.45	0.42
2:E:216:VAL:HG13	2:E:221:GLU:HB3	2.02	0.42
1:A:270:ASN:HD22	1:A:271:PRO:HD2	1.84	0.42
1:A:63:ILE:HD11	1:A:113:GLY:HA2	2.01	0.42
1:B:256:ASN:ND2	1:B:258:THR:HB	2.35	0.42
2:E:173:ASP:HB2	2:E:174:PRO:HD3	2.00	0.42
1:A:53:CYS:SG	2:D:265:ILE:HG12	2.60	0.42
1:B:75:LYS:HE2	1:B:77:THR:OG1	2.20	0.42
3:B:293:3O0:SAQ	3:B:293:3O0:CAU	3.07	0.42
2:D:211:VAL:HG21	2:D:264:VAL:HG13	2.01	0.42
1:A:153:ILE:HG23	1:A:154:PRO:HD2	2.02	0.42
1:B:255:LEU:HG	1:B:259:GLY:HA3	2.02	0.42
1:A:252:VAL:HB	4:A:411:HOH:O	2.18	0.41
1:A:155:VAL:HG12	1:A:157:CYS:H	1.85	0.41
1:B:34:ARG:CG	1:B:75:LYS:HE3	2.50	0.41
2:D:190:TRP:CE3	2:D:244:PRO:HD3	2.56	0.40
1:B:276:SER:OG	1:B:279:GLU:HG3	2.22	0.40
2:D:154:CYS:SG	2:D:293:SER:HB3	2.62	0.40
1:A:118:HIS:CD2	1:A:181:THR:HB	2.56	0.40
1:A:36:ARG:HH11	1:A:75:LYS:CG	2.33	0.40
1:A:255:LEU:N	4:A:411:HOH:O	2.54	0.40
1:A:63:ILE:HD12	1:A:63:ILE:N	2.37	0.40
1:B:18:VAL:HA	1:B:32:LEU:O	2.21	0.40
1:A:213:LYS:HG3	1:A:239:TYR:HE2	1.86	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	287/292 (98%)	274 (96%)	12 (4%)	1 (0%)	46	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	256/292 (88%)	243 (95%)	11 (4%)	2 (1%)	24	11
2	D	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
2	E	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
All	All	837/882 (95%)	807 (96%)	27 (3%)	3 (0%)	39	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	VAL
1	B	163	VAL
1	B	29	ILE

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	257/260 (99%)	239 (93%)	18 (7%)	19	6
1	B	235/260 (90%)	222 (94%)	13 (6%)	27	12
2	D	138/139 (99%)	135 (98%)	3 (2%)	60	51
2	E	138/139 (99%)	135 (98%)	3 (2%)	60	51
All	All	768/798 (96%)	731 (95%)	37 (5%)	31	15

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	GLU
1	A	10	ILE
1	A	14	THR
1	A	41	ASP
1	A	55	LEU
1	A	65	ARG
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	130	GLN
1	A	132	LEU
1	A	141	LYS
1	A	161	GLU
1	A	177	LYS
1	A	195	LEU
1	A	219	LEU
1	A	224	GLU
1	A	255	LEU
1	A	270	ASN
2	D	209	ARG
2	D	227	LEU
2	D	241	ILE
1	B	17	THR
1	B	18	VAL
1	B	50	ARG
1	B	65	ARG
1	B	74	LYS
1	B	130	GLN
1	B	132	LEU
1	B	137	ASN
1	B	195	LEU
1	B	219	LEU
1	B	224	GLU
1	B	255	LEU
1	B	270	ASN
2	E	148	THR
2	E	241	ILE
2	E	242	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	67	HIS
1	A	118	HIS
1	A	135	ASN
1	A	206	ASN
1	A	226	GLN
1	A	256	ASN
1	A	270	ASN
1	B	62	ASN

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Mol	Chain	Res	Type
1	B	135	ASN
1	B	226	GLN
1	B	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
3	3O0	B	293	-	21,27,27	2.57	4 (19%)	25,38,38	0.89	1 (4%)

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	3O0	B	293	-	-	0/10/16/16	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	293	3O0	CAT-NAS	-2.79	1.34	1.40
3	B	293	3O0	CAG-CAH	-2.60	1.40	1.44
3	B	293	3O0	CAE-CAF	2.02	1.53	1.49
3	B	293	3O0	OAW-NAX	10.47	1.43	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	293	3O0	CAM-CAN-NAX	2.88	121.81	119.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	293	3O0	3	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, 95th 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	289/292 (98%)	0.95	47 (16%) 2 4	23, 34, 60, 73	0
1	B	264/292 (90%)	1.11	48 (18%) 2 2	27, 45, 79, 116	0
2	D	149/149 (100%)	0.56	12 (8%) 15 23	26, 35, 53, 63	0
2	E	149/149 (100%)	3.45	98 (65%) 0 0	55, 89, 127, 140	0
All	All	851/882 (96%)	1.37	205 (24%) 1 1	23, 41, 102, 140	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	THR	15.8
2	E	187	LEU	15.4
2	E	290	LYS	11.8
2	E	168	HIS	11.6
2	E	241	ILE	11.2
2	E	212	ILE	10.6
1	B	288	ASP	9.5
1	B	73	ASP	8.5
1	B	244	ALA	8.4
2	E	217	GLY	8.4
2	E	146	ALA	8.4
1	A	41	ASP	8.2
2	E	176	LEU	8.0
2	E	166	LEU	7.8
1	A	288	ASP	7.6
2	E	249	LEU	7.4
2	E	215	GLU	7.4
2	E	220	HIS	7.3
2	E	180	SER	7.3
1	B	28	GLU	7.0
1	A	40	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
2	E	189	GLY	6.7
1	A	2	GLN	6.6
1	B	154	PRO	6.5
2	D	146	ALA	6.4
1	A	1	MET	6.4
2	E	186	LEU	6.4
1	A	136	ARG	6.4
2	E	267	LEU	6.3
1	A	12	GLU	6.2
1	A	14	THR	6.1
2	E	156	GLY	6.1
2	E	181	VAL	6.0
2	E	159	LEU	6.0
1	B	287	SER	5.9
2	E	167	LYS	5.8
2	E	262	LEU	5.8
2	E	242	SER	5.6
1	B	72	SER	5.6
2	E	183	ARG	5.5
1	A	156	ARG	5.5
2	E	164	TYR	5.5
1	B	29	ILE	5.3
2	E	161	ARG	5.3
2	E	172	THR	5.3
2	E	291	ASN	5.3
1	A	13	GLY	5.3
2	E	153	ARG	5.3
2	E	246	LYS	5.3
2	E	216	VAL	5.2
1	A	73	ASP	5.2
1	A	39	ASP	5.1
1	B	156	ARG	5.1
2	E	252	SER	5.0
2	E	177	TRP	5.0
1	B	136	ARG	5.0
2	E	190	TRP	5.0
2	E	280	HIS	5.0
2	E	239	ASN	4.9
2	E	245	LEU	4.9
2	E	279	PRO	4.9
2	E	193	GLN	4.8
1	A	11	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	169	LEU	4.7
2	E	211	VAL	4.7
2	E	192	ASP	4.6
2	D	241	ILE	4.6
1	B	247	SER	4.6
1	A	154	PRO	4.6
2	E	253	CYS	4.6
2	E	255	GLU	4.5
1	B	250	ASN	4.5
1	B	246	THR	4.4
1	B	155	VAL	4.4
1	B	36	ARG	4.4
2	E	219	ASP	4.3
1	A	7	LEU	4.3
1	B	107	LEU	4.3
2	E	188	GLN	4.2
2	E	250	VAL	4.1
2	E	171	PRO	4.1
2	D	145	GLN	4.1
2	E	283	THR	4.0
2	E	293	SER	4.0
2	E	170	SER	3.9
2	E	243	TYR	3.8
2	E	256	ALA	3.8
2	E	202	VAL	3.7
1	A	42	GLU	3.7
2	E	213	SER	3.7
2	E	205	TYR	3.7
2	E	286	PHE	3.7
1	A	224	GLU	3.7
2	E	147	SER	3.6
2	E	224	ALA	3.6
2	E	227	LEU	3.6
1	A	190	CYS	3.5
1	B	282	GLN	3.4
2	E	145	GLN	3.4
1	A	36	ARG	3.4
1	B	153	ILE	3.4
1	B	7	LEU	3.3
2	E	163	CYS	3.3
1	B	74	LYS	3.2
1	A	225	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	293	SER	3.2
2	E	160	CYS	3.2
1	A	19	PHE	3.2
1	A	32	LEU	3.2
2	E	148	THR	3.2
2	E	149	SER	3.2
1	B	161	GLU	3.2
2	E	282	PHE	3.2
1	B	137	ASN	3.1
2	E	203	PHE	3.1
1	A	37	LEU	3.1
2	E	248	PHE	3.1
2	E	229	CYS	3.1
2	E	271	LYS	3.1
1	B	212	LEU	3.1
2	D	280	HIS	3.1
1	A	10	ILE	3.1
2	E	150	GLU	3.0
1	B	45	PRO	3.0
2	E	275	ILE	3.0
2	E	263	SER	3.0
1	A	289	PHE	3.0
1	B	8	GLU	3.0
2	E	221	GLU	3.0
1	A	137	ASN	2.9
1	B	173	LEU	2.9
2	E	165	ARG	2.9
2	E	266	ASN	2.8
2	E	204	LEU	2.8
2	E	201	VAL	2.8
1	A	15	TYR	2.8
2	E	234	TYR	2.8
1	B	284	PRO	2.8
1	B	6	LYS	2.8
1	A	17	THR	2.8
2	E	257	PHE	2.7
2	D	155	LEU	2.7
2	D	192	ASP	2.7
2	E	175	VAL	2.7
2	E	254	LYS	2.7
1	A	178	LEU	2.7
1	A	287	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	31	ALA	2.6
1	B	192	PHE	2.6
1	A	9	LYS	2.6
1	A	31	ALA	2.6
1	A	49	LEU	2.6
1	A	76	LEU	2.6
1	B	278	GLU	2.6
2	D	204	LEU	2.5
2	E	281	TYR	2.5
2	E	289	LEU	2.5
1	A	155	VAL	2.5
2	E	173	ASP	2.5
1	B	76	LEU	2.5
2	E	268	MET	2.4
1	B	143	ALA	2.4
1	A	191	ILE	2.4
1	B	243	PRO	2.4
2	E	214	SER	2.4
1	A	78	LEU	2.3
2	E	274	GLN	2.3
1	A	80	PHE	2.3
1	A	161	GLU	2.3
2	E	232	LEU	2.3
2	E	264	VAL	2.3
1	B	142	LEU	2.3
2	E	238	GLY	2.3
1	B	110	LEU	2.3
1	B	215	ILE	2.3
2	D	284	GLN	2.2
2	E	223	GLN	2.2
2	E	284	GLN	2.2
1	B	80	PHE	2.2
2	E	155	LEU	2.2
2	E	185	LEU	2.2
2	D	253	CYS	2.2
1	A	192	PHE	2.2
1	B	52	ILE	2.2
1	A	263	LEU	2.2
1	A	122	VAL	2.2
1	B	217	ARG	2.2
1	B	32	LEU	2.2
2	E	222	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	162	ARG	2.2
2	D	153	ARG	2.2
1	A	30	VAL	2.2
1	A	101	GLU	2.1
1	B	70	LEU	2.1
2	E	174	PRO	2.1
1	B	241	MET	2.1
1	A	107	LEU	2.1
1	B	195	LEU	2.1
1	B	34	ARG	2.1
1	B	133	LEU	2.1
2	E	151	LEU	2.1
1	A	63	ILE	2.0
1	A	111	LEU	2.0
2	D	286	PHE	2.0
1	B	256	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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(\AA^2)	Q<0.9
3	3O0	B	293	25/25	0.86	0.14	-0.05	43,47,62,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.