



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:13 AM GMT

PDB ID : 2F2C
Title : X-ray structure of human CDK6-Vcyclinwith the inhibitor aminopurvalanol
Authors : Schulze-Gahmen, U; Lu, H.
Deposited on : 2005-11-16
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

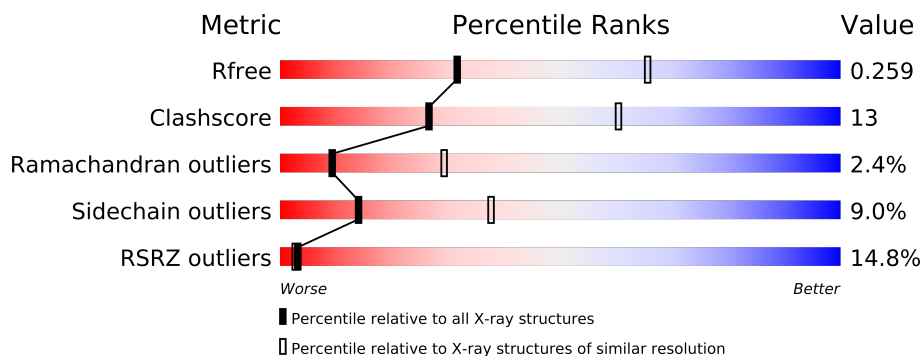
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 ≥ 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	254	
2	B	308	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4059 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 Cyclin homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1903	1228	306	358	11			

- Molecule 2 is a protein called Cell division protein kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	280	Total	C	N	O	S	0	0	0
			2119	1370	351	391	7			

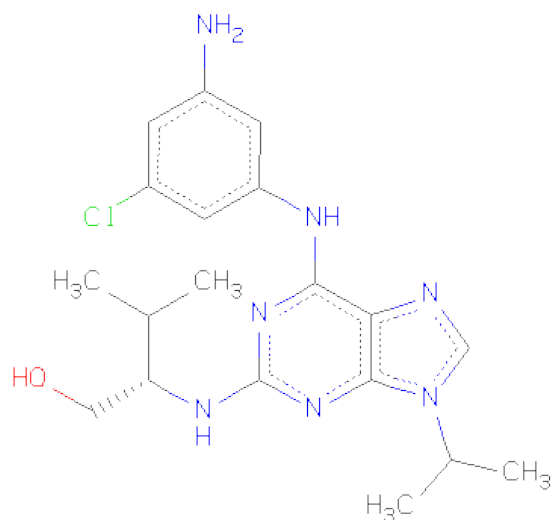
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

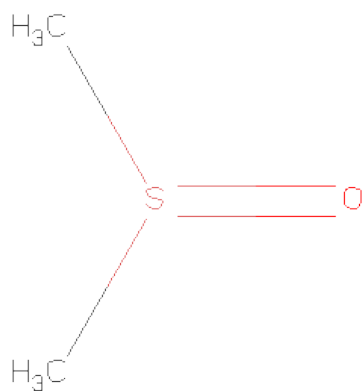
- Molecule 4 is (2S)-2-({6-[(3-AMINO-5-CHLOROPHENYL)AMINO]-9-ISOPROPYL-9 H-PURIN-2-YL}AMINO)-3-METHYLBUTAN-1-OL (three-letter code: AP9) (formula:

C₁₉H₂₆ClN₇O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	B	1	28	19	1	7	1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



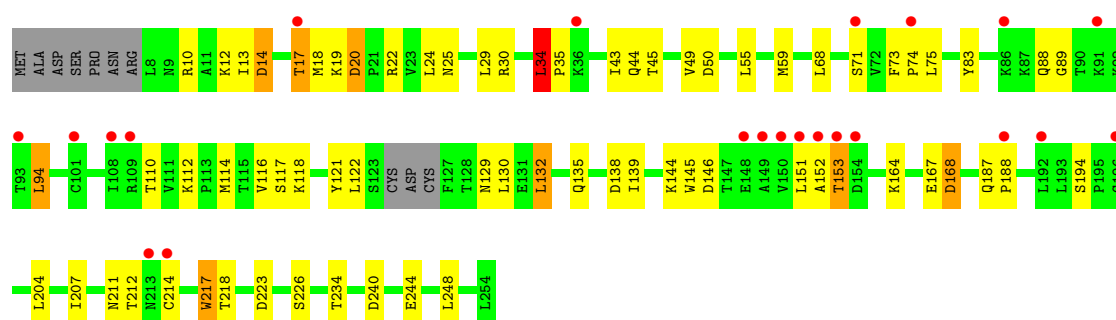
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	B	1	4	2	1	1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

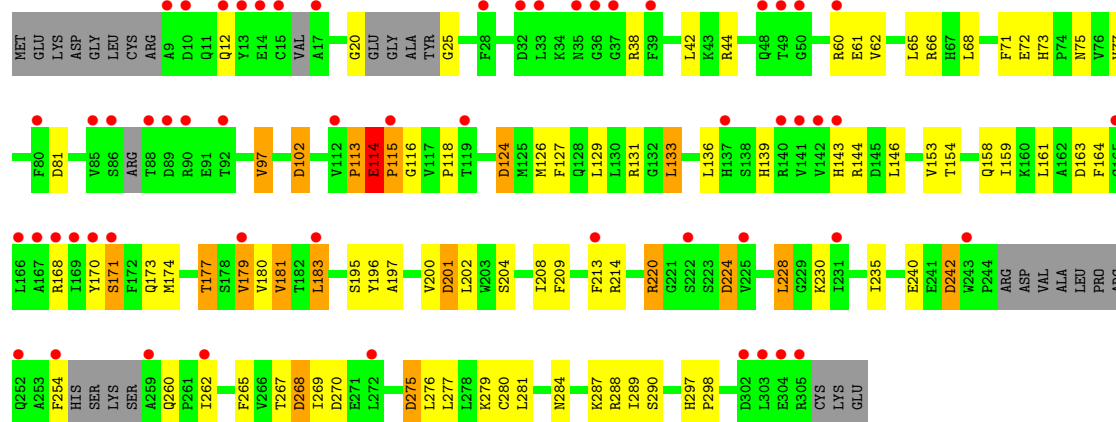
• Molecule 1: Cyclin homolog

Chain A: 



• Molecule 2: Cell division protein kinase 6

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	71.52Å 71.52Å 449.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 36.37 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.80) 96.8 (36.37-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.238 , 0.301 0.253 , 0.259	Depositor DCC
R_{free} test set	903 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 17699 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4059	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AP9, DMS, SO4

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	0.54	0/1934	0.83	8/2632 (0.3%)
2	B	0.69	2/2162 (0.1%)	0.80	8/2943 (0.3%)
All	All	0.62	2/4096 (0.0%)	0.81	16/5575 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	114	GLU	CD-OE2	17.08	1.44	1.25
2	B	114	GLU	CD-OE1	13.31	1.40	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	ASP	CB-CG-OD2	8.08	125.57	118.30
1	A	34	LEU	CA-CB-CG	6.50	130.26	115.30
2	B	124	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	223	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	20	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	50	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	138	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	146	ASP	CB-CG-OD1	5.76	123.49	118.30
2	B	102	ASP	CB-CG-OD2	5.76	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	268	ASP	CB-CG-OD2	5.65	123.38	118.30
2	B	275	ASP	CB-CG-OD2	5.32	123.09	118.30
2	B	115	PRO	N-CD-CG	-5.25	95.32	103.20
1	A	168	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	14	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	242	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	224	ASP	CB-CG-OD2	5.15	122.93	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	114	GLU	Peptide

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	1903	0	1961	44	0
2	B	2119	0	2028	67	0
3	B	5	0	0	2	0
4	B	28	0	26	3	0
5	B	4	0	6	3	0
All	All	4059	0	4021	107	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 13.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:202:LEU:HD13	2:B:289:ILE:O	1.71	0.88
1:A:55:LEU:HD22	1:A:94:LEU:HD22	1.57	0.85
2:B:60:ARG:NH1	2:B:168:ARG:HD2	1.97	0.80
1:A:68:LEU:HD11	1:A:114:MET:HE2	1.63	0.79
1:A:68:LEU:HD11	1:A:114:MET:CE	2.17	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:ASP:O	1:A:244:GLU:HG2	1.87	0.74
2:B:114:GLU:O	2:B:116:GLY:N	2.22	0.73
1:A:116:VAL:HG23	1:A:132:LEU:HD12	1.68	0.73
2:B:60:ARG:HH12	2:B:168:ARG:HD2	1.55	0.72
2:B:168:ARG:HE	2:B:174:MET:HE1	1.59	0.68
1:A:12:LYS:HD2	1:A:13:ILE:H	1.58	0.67
2:B:267:THR:O	2:B:268:ASP:HB2	1.94	0.67
2:B:235:ILE:HD13	2:B:281:LEU:O	1.96	0.66
1:A:30:ARG:HD3	2:B:139:HIS:ND1	2.13	0.64
1:A:44:GLN:HE22	1:A:89:GLY:H	1.46	0.64
1:A:34:LEU:HB2	1:A:35:PRO:CD	2.28	0.63
2:B:20:GLY:HA3	4:B:401:AP9:H141	1.81	0.62
1:A:12:LYS:CD	1:A:13:ILE:H	2.11	0.62
2:B:114:GLU:C	2:B:116:GLY:H	2.04	0.61
1:A:207:ILE:O	1:A:211:ASN:HA	2.01	0.60
2:B:144:ARG:NH1	3:B:402:SO4:O3	2.36	0.59
2:B:129:LEU:HD12	2:B:161:LEU:HD21	1.86	0.58
1:A:34:LEU:HB2	1:A:35:PRO:HD2	1.86	0.58
1:A:116:VAL:HG23	1:A:132:LEU:CD1	2.32	0.58
2:B:68:LEU:HB2	5:B:403:DMS:H12	1.86	0.58
2:B:214:ARG:HD2	2:B:265:PHE:O	2.03	0.57
1:A:17:THR:HG22	1:A:18:MET:HG3	1.87	0.57
1:A:19:LYS:HE2	1:A:167:GLU:OE2	2.05	0.56
2:B:242:ASP:HB3	2:B:284:ASN:HB2	1.88	0.56
1:A:12:LYS:HD2	1:A:13:ILE:N	2.21	0.55
2:B:65:LEU:HA	5:B:403:DMS:H13	1.89	0.55
2:B:127:PHE:CE2	2:B:131:ARG:HD3	2.42	0.54
2:B:114:GLU:C	2:B:116:GLY:N	2.60	0.54
1:A:49:VAL:CG1	1:A:188:PRO:HB3	2.38	0.54
1:A:45:THR:H	1:A:88:GLN:NE2	2.07	0.53
2:B:143:HIS:O	2:B:201:ASP:OD1	2.25	0.53
2:B:171:SER:O	2:B:174:MET:HG2	2.09	0.53
2:B:228:LEU:HD12	2:B:254:PHE:CE2	2.43	0.53
1:A:217:TRP:C	1:A:217:TRP:CD1	2.82	0.53
2:B:168:ARG:HE	2:B:174:MET:CE	2.22	0.52
1:A:211:ASN:O	1:A:214:CYS:HB3	2.10	0.52
1:A:43:ILE:HG22	1:A:43:ILE:O	2.10	0.52
2:B:275:ASP:HB3	2:B:297:HIS:HE2	1.73	0.52
2:B:235:ILE:CD1	2:B:281:LEU:O	2.57	0.52
2:B:262:ILE:HG12	2:B:277:LEU:HD23	1.91	0.52
1:A:43:ILE:O	1:A:43:ILE:CG2	2.59	0.51
2:B:183:LEU:HD23	2:B:183:LEU:H	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:65:LEU:O	5:B:403:DMS:H11	2.12	0.50
2:B:177:THR:N	3:B:402:SO4:O2	2.38	0.49
2:B:153:VAL:HA	2:B:158:GLN:O	2.12	0.49
1:A:121:TYR:HD2	1:A:122:LEU:HD12	1.77	0.49
2:B:126:MET:HG3	2:B:209:PHE:CD1	2.48	0.49
2:B:279:LYS:HG2	2:B:289:ILE:HD13	1.95	0.48
2:B:168:ARG:NE	2:B:174:MET:HE1	2.28	0.48
2:B:204:SER:O	2:B:208:ILE:HD12	2.14	0.48
1:A:20:ASP:OD1	1:A:22:ARG:HG2	2.13	0.48
2:B:209:PHE:CE2	2:B:276:LEU:HD23	2.49	0.48
2:B:25:GLY:HA3	2:B:44:ARG:O	2.13	0.48
2:B:77:VAL:HG21	4:B:401:AP9:H102	1.96	0.48
2:B:133:LEU:HD11	2:B:146:LEU:HD11	1.94	0.47
2:B:280:CYS:O	2:B:288:ARG:HD3	2.13	0.47
1:A:151:LEU:O	1:A:152:ALA:C	2.53	0.47
2:B:220:ARG:O	2:B:230:LYS:NZ	2.48	0.47
2:B:213:PHE:CE1	2:B:269:ILE:HA	2.50	0.47
1:A:240:ASP:O	1:A:244:GLU:CG	2.61	0.46
2:B:154:THR:OG1	2:B:158:GLN:HB3	2.15	0.46
1:A:145:TRP:HB3	2:B:62:VAL:HG11	1.98	0.46
2:B:202:LEU:CD1	2:B:290:SER:HA	2.46	0.45
1:A:19:LYS:CE	1:A:167:GLU:OE2	2.64	0.45
2:B:42:LEU:CD2	2:B:97:VAL:HG13	2.46	0.45
1:A:10:ARG:HD3	2:B:173:GLN:O	2.16	0.45
1:A:121:TYR:CD2	1:A:122:LEU:HD12	2.52	0.45
1:A:116:VAL:C	1:A:118:LYS:H	2.21	0.44
2:B:196:TYR:HB2	2:B:200:VAL:HG21	2.00	0.44
2:B:61:GLU:HG3	2:B:164:PHE:HB2	1.99	0.44
2:B:113:PRO:O	2:B:114:GLU:O	2.35	0.44
2:B:71:PHE:CZ	2:B:139:HIS:HE1	2.36	0.44
2:B:177:THR:HB	2:B:179:VAL:HG23	1.99	0.43
2:B:153:VAL:HG12	2:B:159:ILE:HD13	2.00	0.43
2:B:180:VAL:HG13	2:B:181:VAL:HG23	1.99	0.43
1:A:55:LEU:O	1:A:59:MET:HG3	2.18	0.42
1:A:121:TYR:HD2	1:A:122:LEU:CD1	2.32	0.42
2:B:196:TYR:HB2	2:B:200:VAL:CG2	2.49	0.42
1:A:12:LYS:CG	1:A:13:ILE:H	2.32	0.42
1:A:151:LEU:C	1:A:153:THR:N	2.69	0.42
2:B:73:HIS:HE1	2:B:75:ASN:HB2	1.84	0.42
1:A:73:PHE:HB3	1:A:74:PRO:HD3	2.02	0.42
2:B:42:LEU:HD21	2:B:97:VAL:HG13	2.00	0.42
2:B:77:VAL:HG21	4:B:401:AP9:C10	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:202:LEU:HD11	2:B:290:SER:HA	2.02	0.42
2:B:81:ASP:HB2	2:B:97:VAL:CG2	2.50	0.41
1:A:45:THR:H	1:A:88:GLN:HE21	1.66	0.41
1:A:83:TYR:CE1	1:A:139:ILE:HA	2.55	0.41
2:B:81:ASP:HB2	2:B:97:VAL:HG23	2.02	0.41
1:A:204:LEU:HD22	1:A:217:TRP:CD1	2.55	0.41
1:A:135:GLN:HE21	1:A:139:ILE:HG13	1.85	0.41
2:B:73:HIS:CE1	2:B:75:ASN:HB2	2.56	0.41
2:B:170:TYR:CE2	2:B:197:ALA:HA	2.56	0.41
1:A:14:ASP:OD2	2:B:197:ALA:HB1	2.21	0.41
2:B:275:ASP:O	2:B:279:LYS:HB2	2.21	0.41
1:A:217:TRP:O	1:A:218:THR:C	2.60	0.41
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.91	0.41
2:B:114:GLU:HA	2:B:114:GLU:OE2	2.21	0.40
2:B:168:ARG:NE	2:B:174:MET:CE	2.83	0.40
1:A:22:ARG:HA	1:A:25:ASN:HB2	2.02	0.40
1:A:187:GLN:NE2	1:A:187:GLN:HA	2.36	0.40
2:B:262:ILE:HG12	2:B:277:LEU:CD2	2.51	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	240/254 (94%)	210 (88%)	28 (12%)	2 (1%)	27	65
2	B	268/308 (87%)	229 (85%)	29 (11%)	10 (4%)	5	16
All	All	508/562 (90%)	439 (86%)	57 (11%)	12 (2%)	9	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	72	GLU
2	B	114	GLU

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Mol	Chain	Res	Type
2	B	115	PRO
1	A	117	SER
1	A	212	THR
2	B	113	PRO
2	B	181	VAL
2	B	12	GLN
2	B	38	ARG
2	B	163	ASP
2	B	298	PRO
2	B	260	GLN

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	216/234 (92%)	195 (90%)	21 (10%)	12	32
2	B	217/272 (80%)	199 (92%)	18 (8%)	16	42
All	All	433/506 (86%)	394 (91%)	39 (9%)	14	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	24	LEU
1	A	29	LEU
1	A	34	LEU
1	A	71	SER
1	A	75	LEU
1	A	94	LEU
1	A	110	THR
1	A	112	LYS
1	A	129	ASN
1	A	130	LEU
1	A	132	LEU
1	A	144	LYS
1	A	153	THR
1	A	164	LYS

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Mol	Chain	Res	Type
1	A	168	ASP
1	A	194	SER
1	A	217	TRP
1	A	226	SER
1	A	234	THR
1	A	248	LEU
2	B	66	ARG
2	B	97	VAL
2	B	102	ASP
2	B	118	PRO
2	B	124	ASP
2	B	133	LEU
2	B	136	LEU
2	B	171	SER
2	B	177	THR
2	B	179	VAL
2	B	183	LEU
2	B	195	SER
2	B	220	ARG
2	B	224	ASP
2	B	228	LEU
2	B	240	GLU
2	B	270	ASP
2	B	287	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	44	GLN
1	A	88	GLN
1	A	95	GLN
1	A	129	ASN
1	A	135	GLN
1	A	187	GLN
2	B	67	HIS
2	B	158	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	AP9	B	401	-	30,30,30	2.24	5 (16%)	43,43,43	2.24	11 (25%)
3	SO4	B	402	-	4,4,4	0.37	0	6,6,6	0.43	0
5	DMS	B	403	-	3,3,3	2.86	1 (33%)	3,3,3	1.02	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	AP9	B	401	-	-	2/18/18/18	0/1/3/3
3	SO4	B	402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	403	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	AP9	C5A-CL1	-10.21	1.50	1.74
5	B	403	DMS	O-S	4.81	1.82	1.50
4	B	401	AP9	C5-C4	3.09	1.47	1.40
4	B	401	AP9	C6-N1	2.66	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	AP9	C6-C5	2.56	1.49	1.44
4	B	401	AP9	C1A-N6	-2.47	1.35	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	AP9	C2-N3-C4	6.06	122.75	115.15
4	B	401	AP9	C5-C4-N3	-5.64	117.77	125.94
4	B	401	AP9	N3-C4-N9	5.57	135.08	126.91
4	B	401	AP9	N2-C2-N1	4.52	123.24	116.94
4	B	401	AP9	C2-N2-C12	4.47	128.18	123.42
4	B	401	AP9	C4-C5-N7	-4.28	105.85	109.52
4	B	401	AP9	C5-C6-N1	-2.86	117.32	120.45
4	B	401	AP9	N3-C2-N1	-2.69	122.04	126.19
4	B	401	AP9	N6-C6-N1	2.63	123.69	119.09
4	B	401	AP9	C2-N1-C6	2.33	121.82	116.97
4	B	401	AP9	C11-C9-C10	-2.12	106.45	113.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	AP9	C11-C9-N9-C8
4	B	401	AP9	C11-C9-N9-C4

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, 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	244/254 (96%)	0.55	22 (9%)	10 8	62, 72, 86, 95	0
2	B	280/308 (90%)	0.98	56 (20%)	2 1	65, 72, 87, 102	0
All	All	524/562 (93%)	0.78	78 (14%)	3 2	62, 72, 87, 102	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	86	SER	6.8
2	B	9	ALA	5.8
2	B	15	CYS	5.6
2	B	169	ILE	5.4
2	B	36	GLY	4.6
2	B	35	ASN	4.5
2	B	32	ASP	4.3
2	B	167	ALA	4.1
2	B	252	GLN	4.1
2	B	33	LEU	4.1
2	B	302	ASP	3.8
1	A	213	ASN	3.7
2	B	183	LEU	3.6
1	A	91	LYS	3.5
2	B	142	VAL	3.5
2	B	304	GLU	3.4
2	B	171	SER	3.4
2	B	17	ALA	3.4
2	B	141	VAL	3.3
2	B	115	PRO	3.3
2	B	243	TRP	3.3
1	A	36	LYS	3.2
2	B	259	ALA	3.2
2	B	262	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	254	PHE	3.0
2	B	89	ASP	3.0
2	B	88	THR	3.0
2	B	39	PHE	2.9
2	B	14	GLU	2.9
1	A	109	ARG	2.8
2	B	49	THR	2.8
2	B	60	ARG	2.8
2	B	12	GLN	2.7
2	B	168	ARG	2.7
1	A	71	SER	2.7
2	B	272	LEU	2.7
2	B	170	TYR	2.6
1	A	192	LEU	2.6
1	A	152	ALA	2.5
2	B	137	HIS	2.5
1	A	93	THR	2.5
2	B	13	TYR	2.5
2	B	80	PHE	2.5
2	B	305	ARG	2.5
1	A	149	ALA	2.5
2	B	179	VAL	2.4
2	B	90	ARG	2.4
2	B	165	GLY	2.4
2	B	222	SER	2.4
1	A	101	CYS	2.4
1	A	154	ASP	2.4
1	A	86	LYS	2.3
2	B	85	VAL	2.3
2	B	28	PHE	2.3
1	A	74	PRO	2.3
1	A	188	PRO	2.3
2	B	166	LEU	2.3
1	A	17	THR	2.3
2	B	50	GLY	2.3
1	A	153	THR	2.3
2	B	112	VAL	2.3
1	A	214	CYS	2.3
2	B	119	THR	2.2
1	A	151	LEU	2.2
2	B	303	LEU	2.2
2	B	10	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	140	ARG	2.1
2	B	143	HIS	2.1
2	B	231	ILE	2.1
2	B	37	GLY	2.1
2	B	92	THR	2.1
2	B	48	GLN	2.0
2	B	213	PHE	2.0
2	B	225	VAL	2.0
1	A	108	ILE	2.0
1	A	150	VAL	2.0
1	A	148	GLU	2.0
1	A	196	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	AP9	B	401	28/28	0.32	1.92	78,80,81,81	0
5	DMS	B	403	4/4	0.25	0.76	87,87,87,88	0
3	SO4	B	402	5/5	0.27	-0.34	94,95,97,97	0

6.5 Other polymers ⓘ

There are no such residues in this entry.