



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:56 pm GMT

PDB ID : 3F5X
Title : CDK-2-Cyclin complex with indazole inhibitor 9 bound at its active site
Authors : Kiefer, J.R.; Day, J.E.; Caspers, N.L.; Mathis, K.J.; Kretzmer, K.K.; Weinberg, R.A.; Reitz, B.A.; Stegeman, R.A.; Trujillo, J.I.; Huang, W.; Thorarensen, A.; Xing, L.; Wrightstone, A.; Christine, L.; Compton, R.; Li, X.
Deposited on : 2008-11-04
Resolution : 2.40 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

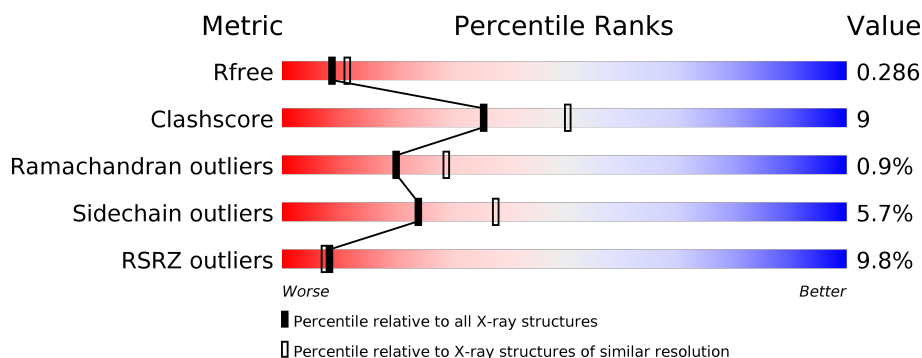
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	298	<div> <div>10%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
1	C	298	<div> <div>12%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	256	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
2	D	256	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9069 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.

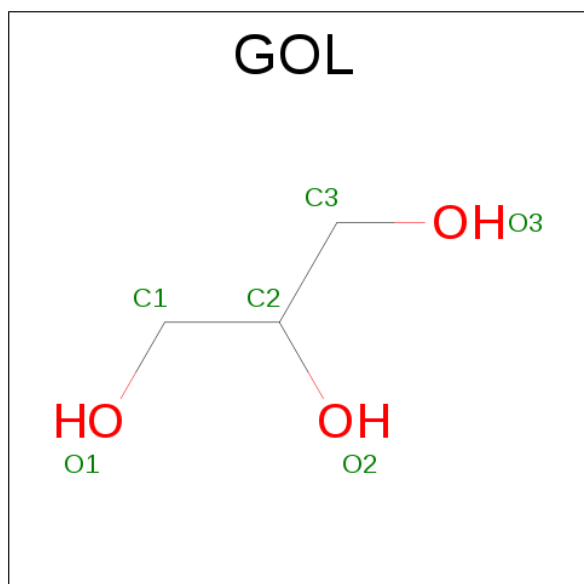
- Molecule 1 is a protein called Cell division protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2390	1555	406	421	8			
1	C	298	Total	C	N	O	S	0	0	0
			2398	1559	408	423	8			

- Molecule 2 is a protein called Cyclin-A2.

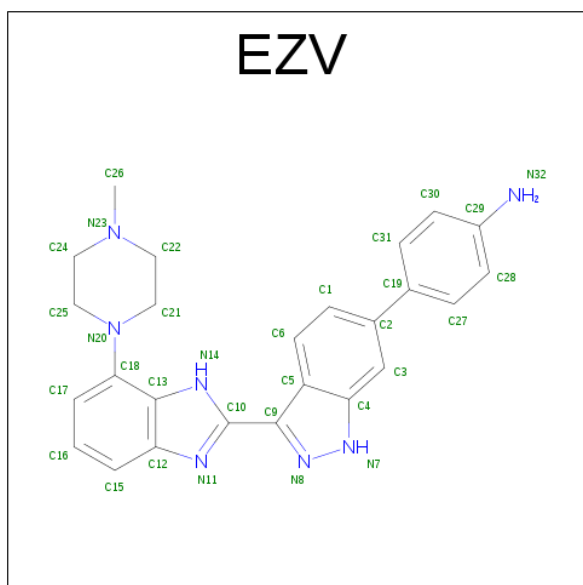
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			2070	1340	337	382	11			
2	D	255	Total	C	N	O	S	0	0	0
			2062	1336	336	379	11			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 4-{3-[7-(4-METHYLPIPERAZIN-1-YL)-1H-BENZIMIDAZOL-2-YL]-1H-INDAZOL-6-YL}ANILINE (three-letter code: EZV) (formula: C₂₅H₂₅N₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			32	25	7		
4	C	1	Total	C	N	0	0
			32	25	7		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

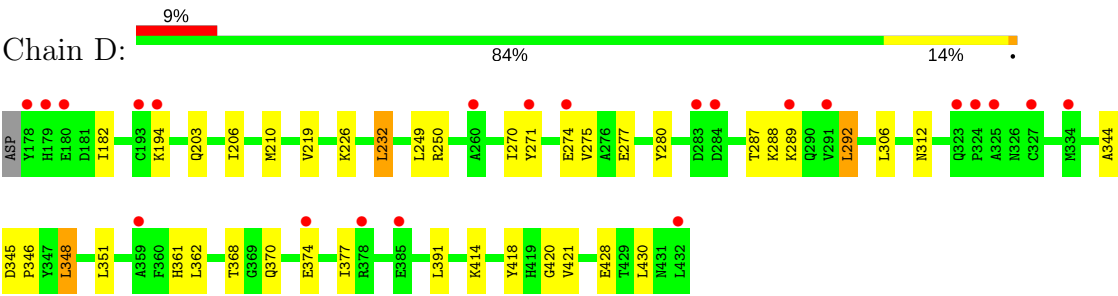


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	10	Total	O	0	0
			10	10		
6	C	3	Total	O	0	0
			3	3		
6	D	14	Total	O	0	0
			14	14		

● Molecule 2: Cyclin-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.05Å 184.05Å 214.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.40) 99.4 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.283 0.268 , 0.286	Depositor DCC
R_{free} test set	4169 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9069	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, EZV, 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	0.42	0/2451	0.60	0/3324
1	C	0.43	0/2460	0.62	3/3338 (0.1%)
2	B	0.40	0/2119	0.53	0/2875
2	D	0.39	0/2111	0.56	0/2864
All	All	0.41	0/9141	0.58	3/12401 (0.0%)

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
1	A	0	1
1	C	2	1
2	D	1	0
All	All	3	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	VAL	N-CA-C	5.70	126.38	111.00
1	C	97	THR	N-CA-CB	5.37	120.50	110.30
1	C	159	TYR	CB-CA-C	5.25	120.90	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	97	THR	CA
1	C	163	VAL	CA

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Mol	Chain	Res	Type	Atom
2	D	280	TYR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	HIS	Peptide
1	C	161	HIS	Peptide

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	2390	0	2443	50	0
1	C	2398	0	2450	69	0
2	B	2070	0	2091	32	0
2	D	2062	0	2087	33	0
3	A	6	0	8	2	0
3	C	6	0	8	0	0
4	A	32	0	25	5	0
4	C	32	0	25	3	0
5	D	5	0	0	0	0
6	A	41	0	0	0	0
6	B	10	0	0	0	0
6	C	3	0	0	0	0
6	D	14	0	0	0	0
All	All	9069	0	9137	166	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 (166) 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:163:VAL:HG23	1:A:164:VAL:HG23	1.46	0.96
1:C:1:MET:HE2	1:C:70:ILE:HD13	1.54	0.89
1:A:126:ARG:O	1:A:164:VAL:HG22	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LYS:NZ	4:C:300:EZV:H28	1.94	0.83
1:A:33:LYS:NZ	4:A:300:EZV:H28	1.96	0.80
1:C:148:LEU:HD11	1:C:163:VAL:CG2	2.13	0.79
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.64	0.78
1:C:152:PHE:CE2	2:D:182:ILE:CD1	2.67	0.77
1:A:227:TRP:O	1:A:230:VAL:HG22	1.85	0.76
1:C:148:LEU:CD1	1:C:163:VAL:HB	2.15	0.76
1:A:163:VAL:CG2	1:A:164:VAL:HG23	2.18	0.74
2:D:210:MET:HE1	2:D:250:ARG:CB	2.18	0.73
1:C:152:PHE:CE2	2:D:182:ILE:HD11	2.23	0.73
1:A:197:VAL:HG11	1:A:255:LEU:HD13	1.72	0.72
1:C:1:MET:CE	1:C:70:ILE:HD13	2.19	0.72
1:C:33:LYS:HZ1	4:C:300:EZV:H28	1.55	0.71
1:A:128:LEU:HD13	1:A:189:LEU:HD13	1.73	0.70
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.27	0.70
1:C:227:TRP:O	1:C:230:VAL:HG22	1.92	0.69
1:C:148:LEU:HD11	1:C:163:VAL:HG21	1.73	0.69
2:B:194:LYS:HE3	2:B:351:LEU:HD21	1.74	0.68
1:A:33:LYS:HZ1	4:A:300:EZV:H28	1.58	0.68
1:C:197:VAL:HG11	1:C:255:LEU:HD13	1.76	0.68
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.76	0.67
1:C:158:THR:HG22	1:C:180:TYR:CD1	2.31	0.65
1:C:158:THR:HA	1:C:180:TYR:CE1	2.31	0.65
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.80	0.64
1:A:1:MET:CE	1:A:70:ILE:HD13	2.29	0.63
1:C:163:VAL:O	1:C:164:VAL:C	2.36	0.62
1:C:227:TRP:CD2	1:C:230:VAL:HG13	2.34	0.62
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.35	0.61
1:A:96:LEU:O	1:A:97:THR:HG23	1.99	0.61
1:C:152:PHE:CZ	2:D:182:ILE:HD11	2.35	0.61
2:B:221:VAL:HG11	2:B:281:ILE:HD13	1.83	0.60
1:C:51:GLU:O	1:C:55:LEU:HB2	2.02	0.60
2:B:210:MET:CE	2:B:250:ARG:HB2	2.31	0.60
1:A:1:MET:HE2	1:A:70:ILE:HD13	1.83	0.60
1:A:51:GLU:OE2	4:A:300:EZV:N32	2.34	0.59
1:A:163:VAL:CG2	1:A:164:VAL:N	2.65	0.59
1:C:227:TRP:CG	1:C:230:VAL:HG13	2.39	0.58
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.86	0.57
1:A:152:PHE:CE2	2:B:182:ILE:CD1	2.87	0.57
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.87	0.57
1:A:73:GLU:CG	1:A:74:ASN:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.86	0.56
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.86	0.56
1:A:122:ARG:HB3	2:B:182:ILE:HD13	1.88	0.56
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.88	0.55
1:C:30:VAL:HG21	1:C:79:VAL:CG1	2.36	0.55
1:C:73:GLU:CG	1:C:74:ASN:H	2.20	0.55
1:C:148:LEU:HD11	1:C:163:VAL:CB	2.37	0.55
1:A:163:VAL:O	1:A:164:VAL:C	2.44	0.55
2:B:200:MET:SD	2:B:206:ILE:HD12	2.46	0.55
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.43	0.54
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.88	0.54
2:D:275:VAL:HG11	2:D:292:LEU:HD13	1.89	0.54
1:C:223:ASP:H	1:C:226:VAL:HG12	1.73	0.54
1:A:47:THR:HG23	1:A:147:GLY:CA	2.37	0.54
1:C:159:TYR:CE1	1:C:162:GLU:HG3	2.42	0.54
1:C:159:TYR:HB3	2:D:270:ILE:HD13	1.90	0.54
2:D:194:LYS:HE3	2:D:351:LEU:HD21	1.90	0.54
1:A:152:PHE:CZ	2:B:182:ILE:HD11	2.43	0.53
1:A:73:GLU:HG2	1:A:74:ASN:H	1.73	0.53
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.91	0.53
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.91	0.52
1:A:51:GLU:OE2	4:A:300:EZV:H28	2.10	0.52
1:C:162:GLU:OE1	1:C:163:VAL:HG23	2.10	0.52
1:A:51:GLU:O	1:A:55:LEU:HB2	2.09	0.51
1:C:148:LEU:HD11	1:C:163:VAL:HB	1.89	0.51
1:A:115:LEU:HD22	1:A:119:HIS:CE1	2.46	0.51
1:A:33:LYS:HZ3	4:A:300:EZV:H28	1.73	0.51
1:C:69:VAL:HG13	1:C:76:LEU:HD21	1.92	0.51
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.93	0.51
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.22	0.51
2:D:287:THR:HG22	2:D:289:LYS:H	1.76	0.50
1:A:115:LEU:HD12	1:A:189:LEU:HD22	1.94	0.50
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.94	0.50
2:B:203:GLN:HG2	2:B:206:ILE:HG13	1.94	0.50
2:B:221:VAL:CG1	2:B:281:ILE:HD13	2.42	0.49
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.95	0.49
1:C:158:THR:HG22	1:C:180:TYR:CE1	2.46	0.49
2:B:418:TYR:O	2:B:421:VAL:HG13	2.12	0.49
1:C:159:TYR:CZ	1:C:162:GLU:HG3	2.47	0.49
1:A:163:VAL:HG22	1:A:164:VAL:N	2.28	0.48
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:HD21	1:C:207:SER:C	2.33	0.48
2:B:399:LEU:HD23	2:B:426:PRO:HG2	1.95	0.48
2:D:210:MET:CE	2:D:250:ARG:HB2	2.43	0.48
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.95	0.48
2:B:287:THR:HG22	2:B:289:LYS:H	1.79	0.48
1:C:161:HIS:HB2	2:D:271:TYR:OH	2.14	0.48
1:A:111:LEU:CD2	1:A:133:LEU:HD22	2.44	0.48
1:A:96:LEU:HG	1:A:96:LEU:O	2.14	0.48
1:C:197:VAL:CG1	1:C:255:LEU:HD13	2.42	0.48
1:A:73:GLU:CG	1:A:74:ASN:N	2.78	0.47
1:C:73:GLU:HG2	1:C:74:ASN:H	1.79	0.47
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.49	0.47
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.97	0.47
2:D:287:THR:HG22	2:D:288:LYS:N	2.30	0.47
1:C:148:LEU:CD1	1:C:163:VAL:CG2	2.91	0.46
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.50	0.46
1:C:33:LYS:HZ3	4:C:300:EZV:H28	1.78	0.46
1:C:135:ILE:HD12	1:C:296:LEU:HD21	1.97	0.46
1:A:152:PHE:CE2	2:B:182:ILE:HD11	2.50	0.46
1:A:227:TRP:CE3	1:A:230:VAL:CG1	2.99	0.46
1:C:162:GLU:CD	1:C:163:VAL:HG23	2.37	0.46
1:A:40:GLU:O	2:B:288:LYS:HD3	2.16	0.45
1:C:158:THR:HG22	1:C:180:TYR:CG	2.51	0.45
1:C:181:SER:O	1:C:184:VAL:HG22	2.16	0.45
2:B:230:GLU:OE2	2:B:313:GLN:NE2	2.47	0.45
1:C:119:HIS:CE1	1:C:182:THR:HB	2.51	0.45
2:B:222:GLY:HA2	2:B:227:LEU:HD12	1.99	0.45
1:C:159:TYR:CG	2:D:270:ILE:CG2	3.00	0.45
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.99	0.45
1:A:47:THR:HG23	1:A:147:GLY:HA3	1.99	0.45
2:B:194:LYS:CE	2:B:351:LEU:HD21	2.45	0.45
2:B:319:PHE:HE2	2:B:334:MET:CE	2.30	0.44
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.47	0.44
2:B:287:THR:HG22	2:B:288:LYS:N	2.31	0.44
2:D:418:TYR:O	2:D:421:VAL:HG13	2.16	0.44
2:B:404:HIS:O	2:B:407:GLN:NE2	2.45	0.44
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.48	0.44
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.47	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
2:B:210:MET:HE1	2:B:250:ARG:CB	2.48	0.44
1:C:101:LEU:N	1:C:102:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:HG23	1:C:103:LEU:HD23	1.99	0.44
2:D:203:GLN:HG2	2:D:206:ILE:CG1	2.48	0.44
2:B:210:MET:CE	2:B:250:ARG:CB	2.96	0.43
1:A:122:ARG:HB3	2:B:182:ILE:CD1	2.49	0.43
1:C:172:GLU:HG2	1:C:271:PRO:HG3	2.00	0.43
2:D:275:VAL:HG11	2:D:292:LEU:CD1	2.47	0.43
1:C:30:VAL:HG22	1:C:80:PHE:O	2.19	0.43
1:C:1:MET:CE	1:C:70:ILE:CD1	2.95	0.43
1:A:197:VAL:CG1	1:A:255:LEU:HD13	2.46	0.43
1:C:122:ARG:HD2	1:C:122:ARG:O	2.19	0.43
1:C:159:TYR:CG	2:D:270:ILE:HG21	2.53	0.43
2:D:362:LEU:HD13	2:D:430:LEU:HD21	2.01	0.43
1:C:202:LEU:HD13	1:C:203:PHE:CZ	2.54	0.42
1:C:231:THR:HA	1:C:236:TYR:CD1	2.53	0.42
1:C:122:ARG:HB3	2:D:182:ILE:HD13	2.01	0.42
1:C:159:TYR:CD1	2:D:270:ILE:CG2	3.02	0.42
1:A:166:LEU:HD21	1:A:207:SER:C	2.40	0.42
1:C:164:VAL:O	1:C:165:THR:C	2.55	0.42
1:A:67:LEU:HB3	3:A:299:GOL:C1	2.50	0.42
1:C:38:ASP:OD2	1:C:41:THR:OG1	2.32	0.42
2:B:414:LYS:HA	2:B:420:GLY:HA2	2.02	0.42
2:D:368:THR:HB	2:D:370:GLN:HE21	1.85	0.42
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.35	0.42
1:C:163:VAL:O	1:C:164:VAL:O	2.38	0.42
1:C:148:LEU:CD1	1:C:163:VAL:CB	2.89	0.41
1:C:39:THR:O	1:C:39:THR:HG22	2.20	0.41
2:B:347:TYR:OH	2:B:394:LEU:HA	2.20	0.41
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.19	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.55	0.41
1:C:96:LEU:HG	1:C:96:LEU:O	2.19	0.41
1:A:124:LEU:HD21	1:A:182:THR:HA	2.03	0.41
1:A:67:LEU:HB3	3:A:299:GOL:H12	2.03	0.41
1:A:1:MET:HE1	1:A:70:ILE:HD13	2.02	0.41
1:A:164:VAL:O	1:A:165:THR:C	2.59	0.41
1:C:154:VAL:HG21	2:D:312:ASN:ND2	2.36	0.41
2:D:194:LYS:CE	2:D:351:LEU:HD21	2.50	0.41
1:C:97:THR:HG23	1:C:199:ARG:NH1	2.36	0.40
2:D:274:GLU:HG3	2:D:277:GLU:HG2	2.03	0.40
2:D:345:ASP:HA	2:D:346:PRO:HA	1.93	0.40
2:D:362:LEU:CD1	2:D:430:LEU:HD21	2.51	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	293/298 (98%)	279 (95%)	10 (3%)	4 (1%)	13	18
1	C	296/298 (99%)	282 (95%)	8 (3%)	6 (2%)	9	10
2	B	254/256 (99%)	251 (99%)	3 (1%)	0	100	100
2	D	253/256 (99%)	251 (99%)	2 (1%)	0	100	100
All	All	1096/1108 (99%)	1063 (97%)	23 (2%)	10 (1%)	20	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	97	THR
1	C	163	VAL
1	C	164	VAL
1	A	97	THR
1	C	73	GLU
1	A	73	GLU
1	A	161	HIS
1	C	161	HIS
1	C	165	THR

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	262/263 (100%)	246 (94%)	16 (6%)	22	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	263/263 (100%)	238 (90%)	25 (10%)	10	14
2	B	230/230 (100%)	222 (96%)	8 (4%)	41	61
2	D	229/230 (100%)	222 (97%)	7 (3%)	45	66
All	All	984/986 (100%)	928 (94%)	56 (6%)	24	38

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	87	LEU
1	A	97	THR
1	A	115	LEU
1	A	122	ARG
1	A	154	VAL
1	A	157	ARG
1	A	159	TYR
1	A	162	GLU
1	A	200	ARG
1	A	202	LEU
1	A	230	VAL
1	A	246	GLN
1	A	255	LEU
1	A	257	GLU
1	A	297	ARG
2	B	196	LYS
2	B	232	LEU
2	B	292	LEU
2	B	323	GLN
2	B	348	LEU
2	B	391	LEU
2	B	392	MET
2	B	407	GLN
1	C	2	GLU
1	C	14	THR
1	C	30	VAL
1	C	41	THR
1	C	74	ASN
1	C	75	LYS
1	C	76	LEU
1	C	87	LEU
1	C	97	THR

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Mol	Chain	Res	Type
1	C	122	ARG
1	C	159	TYR
1	C	160	THR
1	C	161	HIS
1	C	162	GLU
1	C	163	VAL
1	C	172	GLU
1	C	202	LEU
1	C	212	LEU
1	C	230	VAL
1	C	232	SER
1	C	239	SER
1	C	252	VAL
1	C	255	LEU
1	C	257	GLU
1	C	297	ARG
2	D	226	LYS
2	D	232	LEU
2	D	249	LEU
2	D	280	TYR
2	D	292	LEU
2	D	348	LEU
2	D	428	GLU

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	59	ASN
1	A	74	ASN
2	B	208	ASN
2	B	312	ASN
2	B	317	GLN
2	B	323	GLN
2	B	404	HIS
1	C	287	GLN
2	D	208	ASN
2	D	296	HIS
2	D	370	GLN
2	D	415	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GOL	A	299	-	5,5,5	0.34	0	5,5,5	0.37	0
4	EZV	A	300	-	35,37,37	1.15	3 (8%)	34,54,54	1.79	7 (20%)
3	GOL	C	299	-	5,5,5	0.31	0	5,5,5	0.16	0
4	EZV	C	300	-	35,37,37	1.14	3 (8%)	34,54,54	1.80	8 (23%)
5	SO4	D	1	-	4,4,4	0.16	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	299	-	-	0/4/4/4	0/0/0/0
4	EZV	A	300	-	-	0/8/22/22	0/6/6/6
3	GOL	C	299	-	-	0/4/4/4	0/0/0/0
4	EZV	C	300	-	-	0/8/22/22	0/6/6/6
5	SO4	D	1	-	-	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	C	300	EZV	C10-N14	-3.24	1.31	1.35
4	A	300	EZV	C10-N14	-3.24	1.31	1.35
4	A	300	EZV	C3-C4	-2.62	1.37	1.41
4	C	300	EZV	C3-C4	-2.40	1.38	1.41
4	C	300	EZV	C15-C12	-2.12	1.38	1.41
4	A	300	EZV	C15-C12	-2.12	1.38	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	300	EZV	C16-C15-C12	-3.90	114.19	120.07
4	C	300	EZV	C21-C22-N23	-3.89	106.33	110.79
4	C	300	EZV	C1-C6-C5	-3.86	115.87	121.14
4	A	300	EZV	C1-C6-C5	-3.83	115.90	121.14
4	C	300	EZV	C16-C15-C12	-3.77	114.39	120.07
4	C	300	EZV	C25-C24-N23	-3.14	107.19	110.79
4	A	300	EZV	C21-C22-N23	-3.11	107.23	110.79
4	A	300	EZV	C17-C18-C13	-2.66	114.84	119.89
4	C	300	EZV	C17-C18-C13	-2.63	114.89	119.89
4	C	300	EZV	C21-N20-C18	-2.22	109.95	116.33
4	A	300	EZV	C21-N20-C18	-2.17	110.11	116.33
4	A	300	EZV	C3-C4-C5	2.48	124.31	121.14
4	C	300	EZV	C3-C4-C5	2.67	124.55	121.14
4	C	300	EZV	C24-N23-C22	3.26	113.82	109.47
4	A	300	EZV	C24-N23-C22	4.60	115.61	109.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	299	GOL	2	0
4	A	300	EZV	5	0
4	C	300	EZV	3	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, 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	297/298 (99%)	0.62	31 (10%) 7 6	42, 52, 71, 77	0
1	C	298/298 (100%)	0.64	35 (11%) 5 5	42, 53, 74, 92	0
2	B	256/256 (100%)	0.26	20 (7%) 14 12	41, 51, 68, 78	0
2	D	255/256 (99%)	0.44	22 (8%) 11 10	40, 50, 66, 75	0
All	All	1106/1108 (99%)	0.50	108 (9%) 8 7	40, 52, 70, 92	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	LEU	10.6
1	A	39	THR	9.7
2	B	323	GLN	8.6
2	D	323	GLN	8.0
1	C	161	HIS	7.7
1	A	161	HIS	7.3
1	C	162	GLU	7.2
1	A	15	TYR	7.0
1	C	163	VAL	6.8
1	C	298	LEU	6.8
1	A	40	GLU	6.6
1	C	15	TYR	6.5
1	C	14	THR	6.5
2	D	324	PRO	6.4
1	C	41	THR	6.2
1	C	40	GLU	6.2
1	C	13	GLY	5.5
1	C	12	GLU	5.3
1	C	97	THR	5.2
2	D	193	CYS	5.1
1	C	71	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	178	TYR	4.6
2	B	324	PRO	4.5
2	D	283	ASP	4.5
2	D	178	TYR	4.2
2	B	284	ASP	4.2
1	A	13	GLY	4.2
1	C	159	TYR	4.1
1	A	160	THR	4.0
1	C	164	VAL	4.0
2	B	432	LEU	3.9
1	A	41	THR	3.9
2	D	378	ARG	3.9
1	A	162	GLU	3.9
1	A	38	ASP	3.7
1	C	36	ARG	3.7
1	A	159	TYR	3.7
1	C	39	THR	3.7
1	C	38	ASP	3.6
1	C	74	ASN	3.6
1	A	12	GLU	3.5
2	B	271	TYR	3.5
1	A	36	ARG	3.5
1	A	14	THR	3.5
2	B	177	ASP	3.5
2	B	283	ASP	3.4
1	C	160	THR	3.4
2	B	378	ARG	3.2
2	D	325	ALA	3.2
1	C	206	ASP	3.2
1	A	287	GLN	3.2
2	D	284	ASP	3.1
2	D	327	CYS	3.0
1	C	287	GLN	3.0
2	D	359	ALA	3.0
1	C	297	ARG	3.0
1	C	250	LYS	3.0
1	C	257	GLU	2.9
1	C	247	ASP	2.8
1	C	295	HIS	2.8
2	D	432	LEU	2.8
1	A	71	HIS	2.8
1	C	288	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	280	TYR	2.7
1	A	92	ASP	2.6
2	B	374	GLU	2.6
2	D	374	GLU	2.6
2	B	193	CYS	2.6
1	A	32	LEU	2.6
2	B	205	ASP	2.6
1	A	31	ALA	2.5
1	C	16	GLY	2.5
1	A	73	GLU	2.5
2	B	179	HIS	2.5
1	C	72	THR	2.5
2	B	226	LYS	2.5
1	A	298	LEU	2.4
1	A	87	LEU	2.4
2	B	403	GLN	2.3
2	D	271	TYR	2.3
2	D	260	ALA	2.3
1	C	165	THR	2.3
1	A	164	VAL	2.3
1	C	73	GLU	2.3
1	C	200	ARG	2.2
1	A	74	ASN	2.2
2	D	179	HIS	2.2
1	C	59	ASN	2.2
2	D	291	VAL	2.2
1	A	273	LYS	2.2
1	A	107	TYR	2.1
1	A	108	LEU	2.1
1	A	16	GLY	2.1
2	B	293	ARG	2.1
2	B	180	GLU	2.1
2	D	180	GLU	2.1
1	A	96	LEU	2.1
1	A	206	ASP	2.1
2	B	194	LYS	2.1
2	D	334	MET	2.1
2	D	289	LYS	2.1
1	A	178	LYS	2.1
2	D	385	GLU	2.1
2	D	194	LYS	2.0
1	C	22	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.0
2	D	274	GLU	2.0
2	B	416	SER	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(Å ²)	Q<0.9
3	GOL	C	299	6/6	0.87	0.22	1.82	65,66,66,66	0
4	EZV	C	300	32/32	0.82	0.23	1.00	72,73,75,75	0
3	GOL	A	299	6/6	0.88	0.19	0.51	52,53,54,55	0
4	EZV	A	300	32/32	0.92	0.15	-0.72	46,49,50,51	0
5	SO4	D	1	5/5	0.89	0.31	-	106,106,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.