



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:40 PM UTC

PDB ID : 1VYW / pdb_00001vyw
Title : Structure of CDK2/Cyclin A with PNU-292137
Authors : Pevarello, P.; Brasca, M.G.; Amici, R.; Orsini, P.; Traquandi, G.; Corti, L.; Piutti, C.; Sansonna, P.; Villa, M.; Pierce, B.S.; Pulici, M.; Giordano, P.; Martina, K.; Fritzen, E.L.; Nugent, R.A.; Casale, E.; Cameron, A.; Ciomei, M.; Roletto, F.; Isacchi, A.; Fogliatto, G.; Pesenti, E.; Pastori, W.; Marsiglio, A.; Leach, K.L.; Clare, P.M.; Fiorentini, F.; Varasi, M.; Vulpetti, A.; Warpehoski, M.A.
Deposited on : 2004-05-07
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

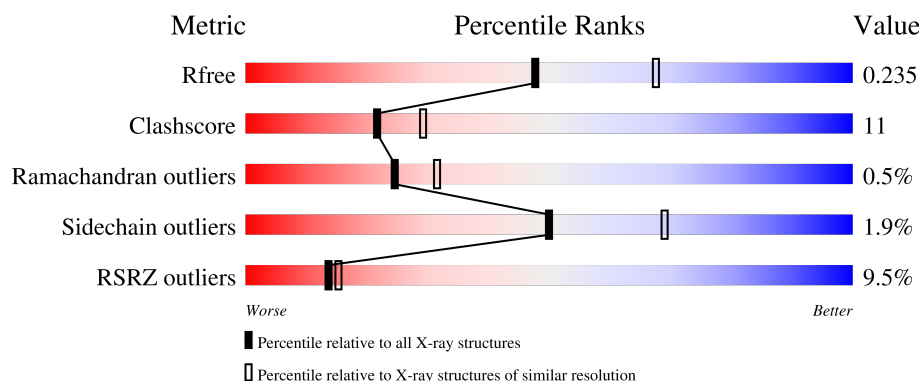
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	309	9% 75% 20% ..
1	C	309	10% 67% 28% ..
2	B	265	11% 72% 23% ..

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	265	7% 77% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9442 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.

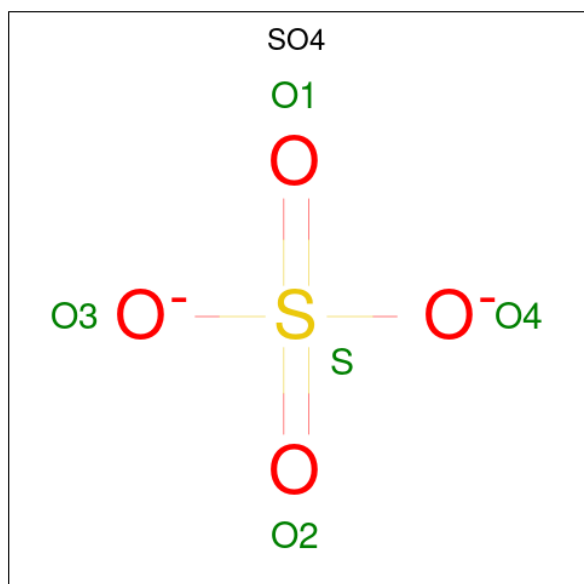
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2427	1579	412	428	8			
1	C	299	Total	C	N	O	S	0	0	0
			2405	1563	409	425	8			

- Molecule 2 is a protein called CYCLIN A2.

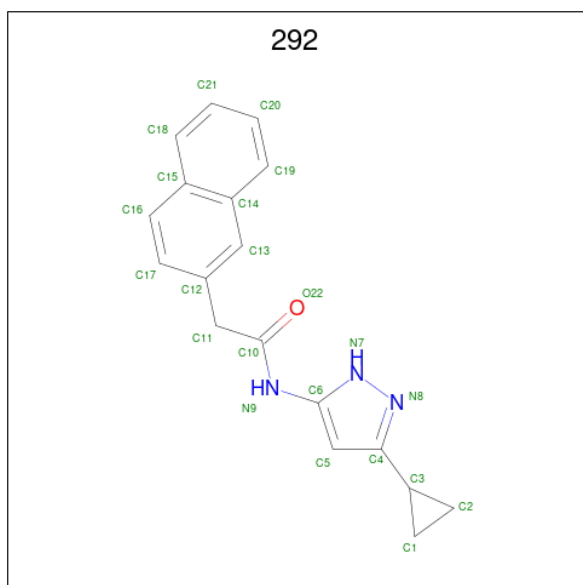
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			
2	D	255	Total	C	N	O	S	0	0	0
			2062	1336	336	379	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is N-(3-CYCLOPROPYL-1H-PYRAZOL-5-YL)-2-(2-NAPHTHYL)ACETAMIDE (CCD ID: 292) (formula: C₁₈H₁₇N₃O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 18 3 1	0	0
4	C	1	Total C N O 22 18 3 1	0	0

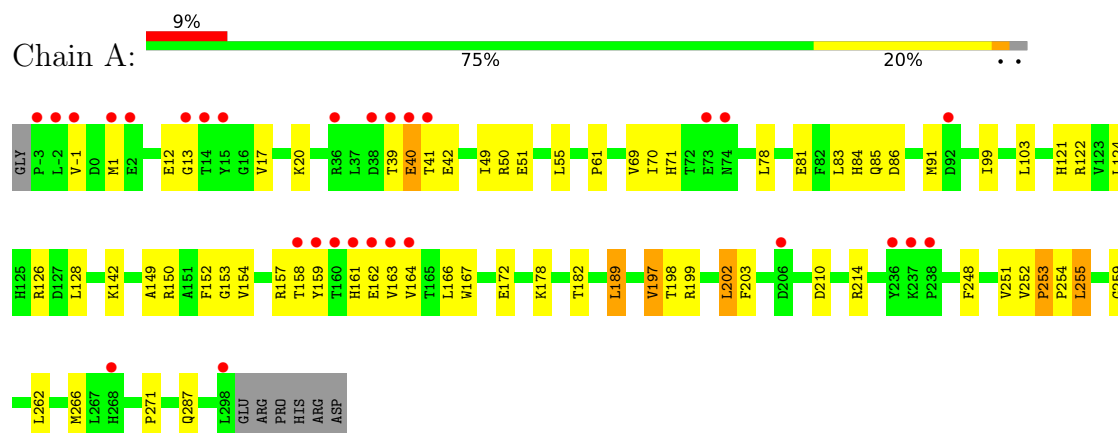
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	153	Total O 153 153	0	0
5	B	66	Total O 66 66	0	0
5	C	55	Total O 55 55	0	0
5	D	136	Total O 136 136	0	0

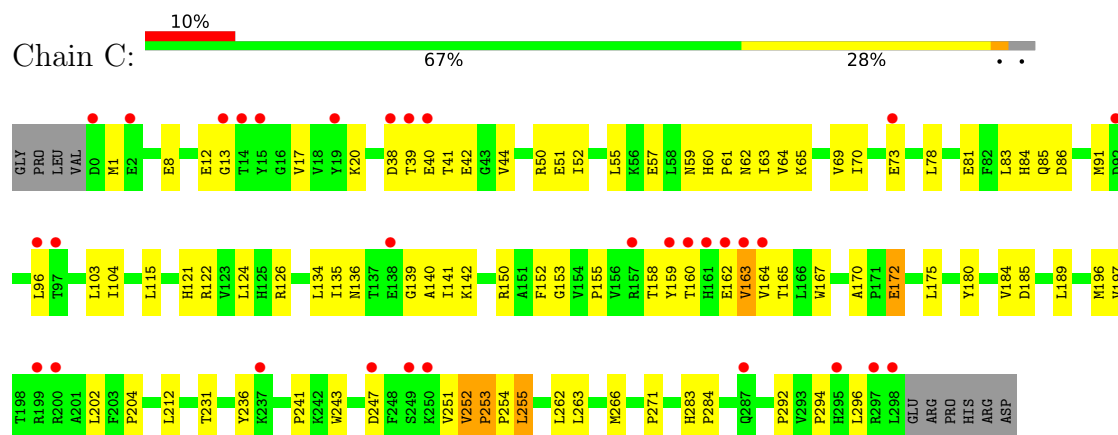
3 Residue-property plots

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

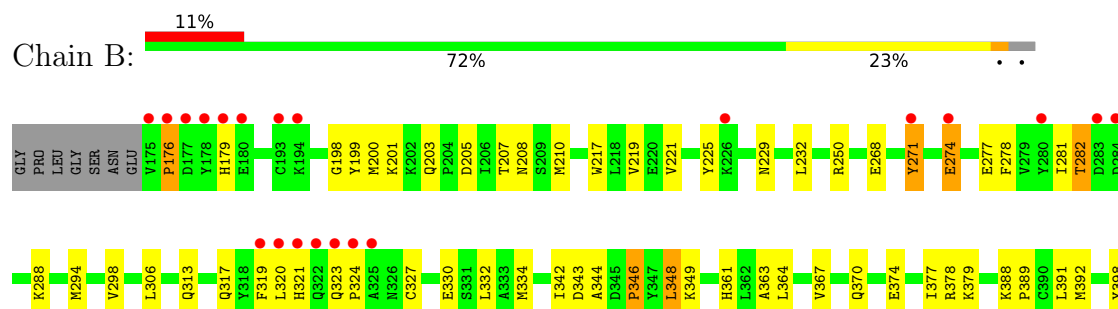
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

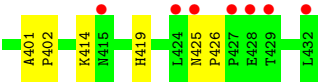


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

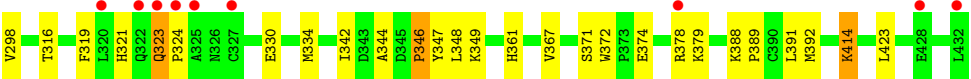
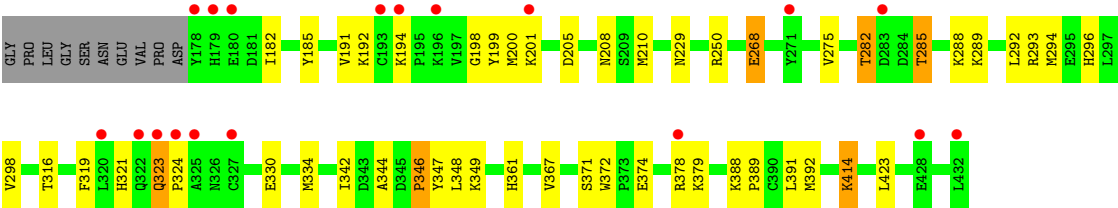
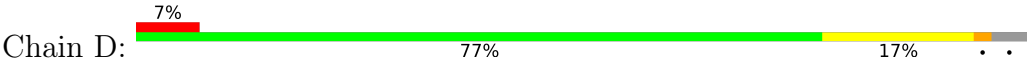


• Molecule 2: CYCLIN A2





● 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	184.22Å 184.22Å 214.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.86-2.30) 99.0 (29.86-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.31Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.229 , 0.258 (Not available) , 0.235	Depositor DCC
R_{free} test set	3556 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	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	0.94	EDS
Total number of atoms	9442	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: SO4, 292

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	0.44	0/2490	0.94	8/3381 (0.2%)
1	C	0.39	0/2467	0.91	8/3349 (0.2%)
2	B	0.39	0/2134	0.89	8/2897 (0.3%)
2	D	0.44	0/2111	0.90	7/2864 (0.2%)
All	All	0.42	0/9202	0.91	31/12491 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	HIS	N-CA-C	8.02	120.93	111.71
1	C	153	GLY	N-CA-C	-7.11	104.89	113.99
1	A	253	PRO	N-CA-C	6.99	119.23	110.70
1	A	20	LYS	N-CA-C	-6.99	99.16	110.20
1	A	153	GLY	N-CA-C	-6.92	105.13	113.99
1	A	81	GLU	N-CA-C	-6.87	101.46	110.53
2	B	342	ILE	N-CA-C	6.79	117.58	110.72
1	C	84	HIS	N-CA-C	6.78	118.67	111.28
2	D	268	GLU	N-CA-C	6.78	121.68	113.41
2	B	414	LYS	N-CA-C	-6.58	104.28	112.90
1	C	20	LYS	N-CA-C	-6.24	99.11	109.46
2	D	285	THR	N-CA-C	-6.06	104.59	112.23
2	D	367	VAL	N-CA-C	6.05	116.69	110.82
2	D	342	ILE	N-CA-C	6.04	116.83	110.72
2	D	414	LYS	N-CA-C	-5.87	105.95	113.23
2	D	347	TYR	N-CA-C	5.83	119.92	112.34
2	B	377	ILE	N-CA-C	-5.58	105.09	110.72
1	A	167	TRP	N-CA-C	5.55	118.86	111.75
2	B	367	VAL	N-CA-C	5.52	117.02	111.00
2	D	282	THR	N-CA-C	-5.52	106.22	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	VAL	CA-C-N	5.34	125.27	119.76
1	C	44	VAL	C-N-CA	5.34	125.27	119.76
2	B	268	GLU	N-CA-C	5.30	119.75	113.12
1	A	166	LEU	N-CA-C	5.24	120.02	111.37
1	A	197	VAL	N-CA-C	5.22	115.44	110.53
1	C	253	PRO	N-CA-C	5.20	117.05	110.70
1	C	252	VAL	CA-C-N	5.15	125.69	120.38
1	C	252	VAL	C-N-CA	5.15	125.69	120.38
2	B	203	GLN	N-CA-C	-5.11	103.33	109.72
2	B	282	THR	N-CA-C	-5.07	106.68	112.92
2	B	343	ASP	N-CA-C	5.01	116.86	107.99

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	2427	0	2481	55	0
1	C	2405	0	2454	66	0
2	B	2084	0	2107	43	0
2	D	2062	0	2087	43	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	22	0	17	1	0
4	C	22	0	17	2	0
5	A	153	0	0	3	0
5	B	66	0	0	2	0
5	C	55	0	0	1	0
5	D	136	0	0	3	0
All	All	9442	0	9163	196	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 11.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LEU:HG	1:C:266:MET:HE2	1.35	1.07
1:A:262:LEU:HG	1:A:266:MET:HE2	1.36	1.04
1:C:163:VAL:HG23	1:C:164:VAL:H	1.33	0.92
2:D:323:GLN:HB2	2:D:324:PRO:HD3	1.54	0.86
1:C:1:MET:HE3	1:C:70:ILE:HG12	1.58	0.85
1:C:83:LEU:H	4:C:2300:292:H7	1.23	0.84
1:C:91:MET:HE3	1:C:196:MET:HG2	1.60	0.80
1:C:163:VAL:HG21	1:C:180:TYR:OH	1.82	0.80
2:B:210:MET:HE1	2:B:250:ARG:HG2	1.62	0.80
2:D:323:GLN:HE21	2:D:324:PRO:HD3	1.47	0.79
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.64	0.78
2:D:323:GLN:NE2	2:D:323:GLN:H	1.82	0.77
1:A:83:LEU:H	4:A:2300:292:H7	1.31	0.77
1:A:126:ARG:O	1:A:164:VAL:HG22	1.85	0.77
2:D:229:ASN:HD22	2:D:334:MET:HE3	1.54	0.72
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.70	0.72
1:A:262:LEU:HG	1:A:266:MET:CE	2.17	0.72
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.53	0.72
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.75	0.68
1:A:158:THR:HG21	5:A:2092:HOH:O	1.91	0.68
1:C:51:GLU:O	1:C:55:LEU:HB2	1.94	0.68
1:C:61:PRO:O	1:C:142:LYS:HE2	1.96	0.66
2:D:275:VAL:HG21	2:D:292:LEU:HD21	1.77	0.66
2:B:321:HIS:NE2	2:B:379:LYS:HD2	2.10	0.66
2:D:321:HIS:NE2	2:D:379:LYS:HD2	2.12	0.65
2:B:205:ASP:OD2	2:B:250:ARG:HG3	1.97	0.65
2:D:346:PRO:O	2:D:349:LYS:HG2	1.97	0.65
2:D:374:GLU:HG3	2:D:378:ARG:NH1	2.11	0.65
2:B:229:ASN:HD22	2:B:334:MET:HE3	1.64	0.63
1:A:-1:VAL:HG11	2:D:296:HIS:CE1	2.34	0.63
2:D:344:ALA:O	2:D:348:LEU:HB2	1.99	0.62
2:D:198:GLY:O	2:D:201:LYS:HG2	1.99	0.62
1:C:126:ARG:O	1:C:164:VAL:HG22	2.00	0.62
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.36	0.61
1:A:262:LEU:CG	1:A:266:MET:HE2	2.22	0.61
2:D:289:LYS:O	2:D:293:ARG:HG3	2.01	0.60
2:B:278:PHE:O	2:B:282:THR:HG23	2.01	0.60
1:C:12:GLU:HG2	1:C:17:VAL:HG13	1.82	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.01	0.60
1:A:121:HIS:O	1:A:122:ARG:HG3	2.01	0.60
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.36	0.60
1:A:210:ASP:O	1:A:214:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:C:70:ILE:CG1	2.32	0.60
1:C:163:VAL:HG23	1:C:164:VAL:N	2.12	0.60
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.18	0.58
2:B:346:PRO:O	2:B:349:LYS:HG2	2.04	0.58
1:C:158:THR:HA	1:C:180:TYR:CE2	2.38	0.58
1:A:41:THR:HB	2:B:288:LYS:HZ1	1.69	0.58
1:C:91:MET:HE3	1:C:196:MET:CG	2.33	0.58
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.86	0.57
1:A:41:THR:HB	2:B:288:LYS:NZ	2.19	0.57
1:A:126:ARG:NH2	1:A:150:ARG:HD2	2.20	0.57
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.05	0.56
2:D:210:MET:HE1	2:D:250:ARG:HG2	1.87	0.56
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.40	0.56
1:C:155:PRO:HD3	2:D:316:THR:HG21	1.86	0.56
2:B:176:PRO:HD2	2:B:179:HIS:HD2	1.70	0.56
2:D:194:LYS:HE2	5:D:2093:HOH:O	2.06	0.56
2:B:198:GLY:O	2:B:201:LYS:HG2	2.06	0.55
1:A:1:MET:HE3	1:A:70:ILE:HG12	1.89	0.55
1:A:50:ARG:NH1	1:A:150:ARG:NH2	2.54	0.55
1:A:197:VAL:CG1	1:A:254:PRO:HG2	2.37	0.55
1:C:263:LEU:HA	1:C:266:MET:HE3	1.89	0.55
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.21	0.55
1:C:163:VAL:CG2	1:C:164:VAL:H	2.09	0.54
2:B:294:MET:O	2:B:298:VAL:HG23	2.07	0.54
1:C:70:ILE:HD12	1:C:70:ILE:N	2.22	0.54
1:C:69:VAL:C	1:C:70:ILE:HD12	2.33	0.54
2:B:179:HIS:NE2	2:B:320:LEU:HD12	2.22	0.54
1:A:126:ARG:CZ	1:A:150:ARG:HD2	2.37	0.54
2:B:207:THR:OG1	2:B:210:MET:HG3	2.08	0.53
1:A:149:ALA:O	1:A:150:ARG:HG3	2.08	0.53
2:D:414:LYS:HE2	2:D:423:LEU:HD21	1.90	0.53
2:D:388:LYS:O	2:D:392:MET:HG2	2.08	0.53
1:C:165:THR:HG22	5:C:2037:HOH:O	2.09	0.53
2:D:289:LYS:HD3	5:D:2073:HOH:O	2.08	0.52
1:C:62:ASN:HA	1:C:142:LYS:HG2	1.92	0.52
1:C:134:LEU:O	1:C:141:ILE:HA	2.10	0.52
2:D:205:ASP:OD1	2:D:250:ARG:NH1	2.43	0.52
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.92	0.52
2:B:374:GLU:HG3	2:B:378:ARG:NH1	2.25	0.52
2:D:323:GLN:HB2	2:D:324:PRO:CD	2.35	0.52
2:B:205:ASP:OD1	2:B:250:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.92	0.51
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.91	0.51
1:A:159:TYR:CE2	1:A:162:GLU:HG3	2.45	0.51
2:D:205:ASP:OD2	2:D:250:ARG:HG3	2.10	0.51
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.93	0.51
1:C:39:THR:HG22	1:C:39:THR:O	2.12	0.50
1:A:121:HIS:C	1:A:122:ARG:HG3	2.37	0.50
1:C:38:ASP:HB3	1:C:42:GLU:HB3	1.94	0.50
2:D:371:SER:O	2:D:372:TRP:C	2.54	0.50
1:A:12:GLU:OE2	1:A:17:VAL:HG22	2.12	0.49
1:A:157:ARG:HH12	1:A:178:LYS:HE2	1.78	0.49
1:A:159:TYR:CD2	1:A:162:GLU:HG3	2.47	0.49
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.94	0.49
1:A:1:MET:HE3	1:A:70:ILE:CG1	2.43	0.49
1:A:91:MET:HE2	5:A:2098:HOH:O	2.13	0.49
1:C:104:ILE:HG23	1:C:196:MET:HE3	1.95	0.48
1:C:57:GLU:HG2	2:D:185:TYR:OH	2.13	0.48
1:A:40:GLU:N	1:A:40:GLU:OE1	2.46	0.48
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.48	0.48
1:A:39:THR:HG22	1:A:39:THR:O	2.13	0.48
2:B:199:TYR:C	2:B:199:TYR:CD1	2.91	0.47
1:C:121:HIS:C	1:C:122:ARG:HG3	2.39	0.47
1:C:197:VAL:CG1	1:C:254:PRO:HG2	2.44	0.47
1:C:241:PRO:HB2	1:C:243:TRP:CZ3	2.49	0.47
1:A:-1:VAL:HG13	1:C:73:GLU:OE2	2.15	0.47
2:D:199:TYR:C	2:D:199:TYR:CD1	2.93	0.47
1:A:85:GLN:HG3	1:A:86:ASP:N	2.29	0.47
1:C:8:GLU:OE2	4:C:2300:292:H2O	2.15	0.47
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.50	0.47
2:D:323:GLN:H	2:D:323:GLN:CD	2.23	0.47
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.50	0.47
1:A:12:GLU:HG3	1:A:13:GLY:H	1.79	0.46
2:D:200:MET:HG2	2:D:208:ASN:ND2	2.30	0.46
1:C:63:ILE:O	1:C:64:VAL:C	2.59	0.46
2:B:210:MET:HE1	2:B:250:ARG:CG	2.39	0.46
1:C:150:ARG:HH22	2:D:268:GLU:C	2.24	0.46
1:A:287:GLN:HB3	5:A:2142:HOH:O	2.15	0.46
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.50	0.46
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.97	0.46
1:C:197:VAL:HG11	1:C:255:LEU:HD13	1.98	0.46
2:B:313:GLN:O	2:B:317:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.97	0.46
2:D:191:VAL:O	2:D:191:VAL:HG12	2.16	0.46
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.98	0.45
1:A:50:ARG:HH12	1:A:150:ARG:NH2	2.14	0.45
2:B:281:ILE:C	2:B:281:ILE:HD12	2.41	0.45
2:B:319:PHE:CE2	2:B:330:GLU:HG2	2.51	0.45
1:C:40:GLU:HG3	1:C:41:THR:HG23	1.96	0.45
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.52	0.45
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.98	0.45
2:B:217:TRP:O	2:B:221:VAL:HG23	2.16	0.45
1:C:164:VAL:O	1:C:165:THR:C	2.59	0.45
1:C:1:MET:HA	1:C:1:MET:HE2	1.99	0.45
2:B:274:GLU:HG2	2:B:277:GLU:HG2	1.99	0.44
2:B:327:CYS:HB3	2:B:419:HIS:NE2	2.32	0.44
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.82	0.44
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.53	0.44
1:C:121:HIS:O	1:C:122:ARG:HG3	2.18	0.44
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.53	0.44
1:C:175:LEU:HD21	1:C:212:LEU:HD21	2.00	0.44
1:A:71:HIS:CD2	5:B:2038:HOH:O	2.69	0.44
1:A:124:LEU:HD21	1:A:182:THR:HA	2.00	0.43
1:C:12:GLU:HB3	1:C:13:GLY:H	1.64	0.43
1:A:40:GLU:HG2	1:A:42:GLU:H	1.83	0.43
2:B:219:VAL:HG22	2:B:232:LEU:HD21	2.00	0.43
1:A:128:LEU:HD13	1:A:189:LEU:HD13	2.00	0.43
2:B:398:TYR:CE1	2:B:426:PRO:HG3	2.54	0.43
2:D:191:VAL:O	2:D:191:VAL:CG1	2.65	0.43
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.53	0.43
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.81	0.43
1:C:40:GLU:O	2:D:288:LYS:HD2	2.19	0.43
1:C:159:TYR:O	1:C:160:THR:C	2.61	0.43
1:A:159:TYR:CE2	1:A:161:HIS:HB2	2.54	0.43
2:D:323:GLN:HE21	2:D:324:PRO:CD	2.25	0.43
1:A:159:TYR:CZ	1:A:161:HIS:HB2	2.54	0.42
2:D:192:LYS:C	2:D:194:LYS:H	2.26	0.42
1:A:252:VAL:N	1:A:253:PRO:HD3	2.35	0.42
1:A:124:LEU:CD2	1:A:182:THR:HA	2.49	0.42
2:B:425:ASN:HA	2:B:426:PRO:HD3	1.89	0.42
1:C:60:HIS:ND1	1:C:61:PRO:HD2	2.35	0.42
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.49	0.42
1:A:198:THR:O	1:A:199:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:LEU:HG	2:B:370:GLN:HB2	2.02	0.42
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.01	0.42
1:A:71:HIS:HD2	5:B:2038:HOH:O	2.01	0.42
1:A:159:TYR:HD2	1:A:162:GLU:HB2	1.85	0.42
1:C:65:LYS:H	1:C:81:GLU:HG2	1.84	0.42
1:C:85:GLN:HG3	1:C:86:ASP:N	2.35	0.42
2:D:334:MET:HE1	5:D:2082:HOH:O	2.18	0.42
1:C:50:ARG:NH1	1:C:150:ARG:NH2	2.68	0.42
1:A:61:PRO:O	1:A:142:LYS:HE2	2.19	0.41
2:B:323:GLN:HB2	2:B:324:PRO:HD3	2.01	0.41
2:B:323:GLN:N	2:B:324:PRO:HD2	2.35	0.41
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.55	0.41
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.82	0.41
1:C:135:ILE:HD12	1:C:296:LEU:HD21	2.01	0.41
1:C:159:TYR:HB2	1:C:163:VAL:HG13	2.03	0.41
2:D:330:GLU:O	2:D:334:MET:HG2	2.21	0.41
1:A:69:VAL:C	1:A:70:ILE:HD12	2.46	0.41
1:C:247:ASP:O	1:C:251:VAL:HG23	2.21	0.41
1:A:40:GLU:O	1:A:41:THR:C	2.64	0.41
2:D:294:MET:O	2:D:298:VAL:HG23	2.21	0.41
1:C:103:LEU:HD13	1:C:292:PRO:HB2	2.03	0.41
1:C:172:GLU:HG2	1:C:271:PRO:HG3	2.02	0.40
2:B:374:GLU:HG3	2:B:378:ARG:HH11	1.85	0.40
2:D:282:THR:O	2:D:285:THR:OG1	2.35	0.40
1:A:159:TYR:CE1	2:B:271:TYR:CE2	3.09	0.40
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.92	0.40
1:C:152:PHE:CE2	2:D:182:ILE:HD11	2.55	0.40
1:A:99:ILE:HG23	1:A:103:LEU:HD23	2.04	0.40
1:A:251:VAL:C	1:A:253:PRO:HD3	2.46	0.40
2:B:388:LYS:O	2:B:392:MET:HG2	2.22	0.40
1:C:115:LEU:HD21	1:C:185:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/309 (97%)	292 (97%)	7 (2%)	1 (0%)	36	46
1	C	297/309 (96%)	283 (95%)	11 (4%)	3 (1%)	12	15
2	B	256/265 (97%)	247 (96%)	8 (3%)	1 (0%)	30	38
2	D	253/265 (96%)	247 (98%)	6 (2%)	0	100	100
All	All	1106/1148 (96%)	1069 (97%)	32 (3%)	5 (0%)	24	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLU
1	A	40	GLU
1	C	96	LEU
1	C	163	VAL
2	B	176	PRO

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	267/273 (98%)	260 (97%)	7 (3%)	40	59
1	C	264/273 (97%)	258 (98%)	6 (2%)	44	63
2	B	232/237 (98%)	228 (98%)	4 (2%)	53	72
2	D	229/237 (97%)	227 (99%)	2 (1%)	70	84
All	All	992/1020 (97%)	973 (98%)	19 (2%)	50	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	154	VAL
1	A	163	VAL

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	202	LEU
1	A	248	PHE
1	A	255	LEU
2	B	271	TYR
2	B	274	GLU
2	B	346	PRO
2	B	348	LEU
1	C	59	ASN
1	C	172	GLU
1	C	184	VAL
1	C	202	LEU
1	C	252	VAL
1	C	255	LEU
2	D	323	GLN
2	D	346	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	113	GLN
1	A	161	HIS
1	A	268	HIS
1	A	295	HIS
2	B	208	ASN
2	B	296	HIS
2	B	322	GLN
2	B	425	ASN
1	C	59	ASN
1	C	62	ASN
1	C	131	GLN
2	D	208	ASN
2	D	229	ASN
2	D	296	HIS
2	D	313	GLN
2	D	322	GLN
2	D	323	GLN
2	D	396	GLN
2	D	425	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	292	A	2300	-	25,25,25	2.71	9 (36%)	30,35,35	0.91	2 (6%)
3	SO4	D	1433	-	4,4,4	0.80	0	6,6,6	0.33	0
4	292	C	2300	-	25,25,25	2.67	10 (40%)	30,35,35	0.91	2 (6%)
3	SO4	A	1300	-	4,4,4	0.95	0	6,6,6	0.26	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	292	A	2300	-	-	0/10/14/14	0/4/4/4
4	292	C	2300	-	-	0/10/14/14	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2300	292	C6-N9	9.36	1.46	1.39
4	C	2300	292	C6-N9	9.11	1.46	1.39
4	A	2300	292	C3-C4	5.70	1.55	1.49
4	C	2300	292	C3-C4	5.63	1.55	1.49
4	A	2300	292	C15-C14	3.41	1.50	1.42
4	C	2300	292	C15-C14	3.06	1.49	1.42
4	A	2300	292	C20-C19	2.87	1.42	1.36
4	A	2300	292	C21-C18	2.78	1.42	1.36
4	C	2300	292	C6-N7	2.62	1.39	1.34
4	C	2300	292	C20-C19	2.58	1.42	1.36
4	C	2300	292	C21-C18	2.51	1.42	1.36
4	A	2300	292	C13-C12	2.34	1.42	1.37
4	A	2300	292	C16-C17	2.33	1.41	1.36
4	C	2300	292	C16-C17	2.31	1.41	1.36
4	C	2300	292	C17-C12	2.29	1.43	1.38
4	A	2300	292	C17-C12	2.24	1.43	1.38
4	C	2300	292	C13-C12	2.13	1.42	1.37
4	C	2300	292	C21-C20	2.10	1.42	1.38
4	A	2300	292	C21-C20	2.06	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2300	292	C2-C3-C4	-2.21	116.79	119.63
4	A	2300	292	C5-C4-N8	-2.13	107.42	111.39
4	C	2300	292	C2-C3-C4	-2.11	116.91	119.63
4	C	2300	292	C5-C4-N8	-2.04	107.59	111.39

There are no chirality outliers.

There are no torsion outliers.

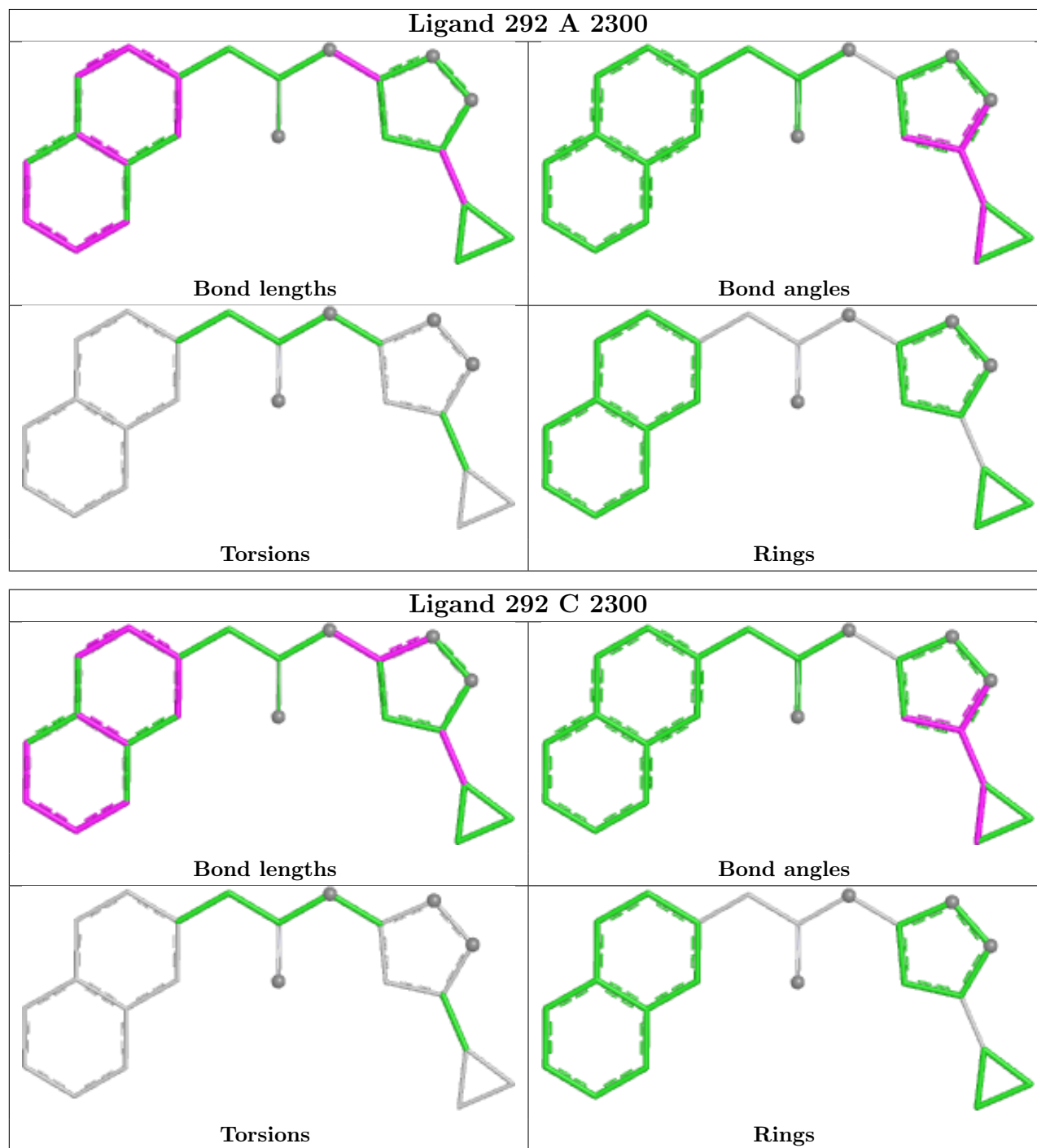
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2300	292	1	0
4	C	2300	292	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	302/309 (97%)	0.36	29 (9%) 13 15	28, 39, 71, 85	0
1	C	299/309 (96%)	0.98	31 (10%) 11 13	34, 54, 74, 86	0
2	B	258/265 (97%)	0.70	28 (10%) 10 12	34, 49, 71, 86	0
2	D	255/265 (96%)	0.20	18 (7%) 22 24	28, 37, 64, 86	0
All	All	1114/1148 (97%)	0.57	106 (9%) 14 15	28, 45, 72, 86	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	323	GLN	8.7
1	C	159	TYR	7.5
1	A	15	TYR	7.2
1	C	15	TYR	6.7
2	D	193	CYS	6.4
2	B	324	PRO	6.4
1	A	159	TYR	6.3
2	B	323	GLN	6.2
2	B	175	VAL	6.0
1	A	-3	PRO	5.9
1	A	162	GLU	5.9
1	C	163	VAL	5.6
1	C	295	HIS	5.1
2	D	324	PRO	5.1
2	B	271	TYR	5.0
1	A	41	THR	4.8
2	B	177	ASP	4.8
2	D	178	TYR	4.7
1	A	164	VAL	4.7
1	A	161	HIS	4.7
1	A	163	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	193	CYS	4.4
1	A	-2	LEU	4.3
1	C	298	LEU	4.3
1	C	96	LEU	4.2
2	B	178	TYR	4.2
1	C	161	HIS	4.0
1	C	200	ARG	4.0
1	C	0	ASP	4.0
1	C	40	GLU	3.9
2	B	283	ASP	3.9
1	A	-1	VAL	3.8
1	C	13	GLY	3.8
1	C	162	GLU	3.8
1	A	40	GLU	3.7
1	A	298	LEU	3.6
2	B	179	HIS	3.6
1	C	160	THR	3.6
2	D	194	LYS	3.5
1	A	13	GLY	3.4
2	D	179	HIS	3.4
1	C	2	GLU	3.3
2	D	180	GLU	3.3
1	A	160	THR	3.2
2	B	432	LEU	3.2
2	D	325	ALA	3.0
1	C	97	THR	3.0
1	C	297	ARG	3.0
1	A	2	GLU	3.0
1	A	14	THR	3.0
2	B	325	ALA	2.9
2	D	320	LEU	2.9
1	C	14	THR	2.9
2	D	201	LYS	2.8
1	C	19	TYR	2.8
2	D	283	ASP	2.8
1	A	36	ARG	2.8
1	C	39	THR	2.7
1	A	38	ASP	2.7
1	A	39	THR	2.7
2	B	194	LYS	2.7
1	A	158	THR	2.7
2	B	284	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	164	VAL	2.7
2	D	271	TYR	2.6
1	C	138	GLU	2.6
2	B	180	GLU	2.6
1	A	206	ASP	2.6
1	C	157	ARG	2.5
2	B	320	LEU	2.5
1	C	237	LYS	2.5
1	A	238	PRO	2.5
2	D	322	GLN	2.5
2	B	280	TYR	2.4
2	B	424	LEU	2.4
1	C	73	GLU	2.4
2	D	428	GLU	2.4
2	D	327	CYS	2.4
2	B	425	ASN	2.4
2	B	176	PRO	2.4
1	C	92	ASP	2.3
1	A	236	TYR	2.3
2	B	226	LYS	2.3
1	A	73	GLU	2.3
2	B	322	GLN	2.3
2	B	427	PRO	2.3
2	B	415	ASN	2.3
2	D	432	LEU	2.2
2	D	378	ARG	2.2
1	A	92	ASP	2.2
1	A	1	MET	2.2
1	A	268	HIS	2.2
2	D	196	LYS	2.2
1	C	38	ASP	2.2
1	C	249	SER	2.2
1	C	199	ARG	2.1
1	A	237	LYS	2.1
2	B	428	GLU	2.1
1	C	250	LYS	2.1
2	B	274	GLU	2.1
1	A	74	ASN	2.1
1	C	247	ASP	2.1
2	B	321	HIS	2.1
2	B	319	PHE	2.1
2	B	429	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	287	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

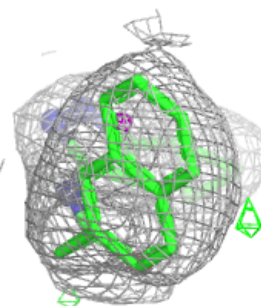
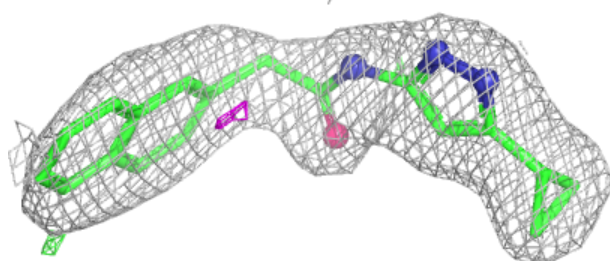
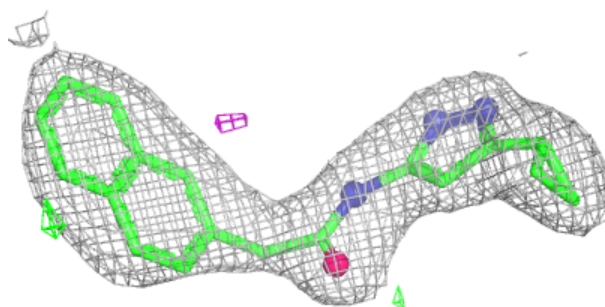
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1300	5/5	0.85	0.11	83,83,84,85	0
4	292	C	2300	22/22	0.90	0.12	43,52,56,57	0
3	SO4	D	1433	5/5	0.92	0.15	82,82,83,83	0
4	292	A	2300	22/22	0.96	0.07	30,35,41,41	0

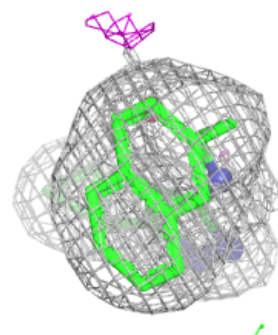
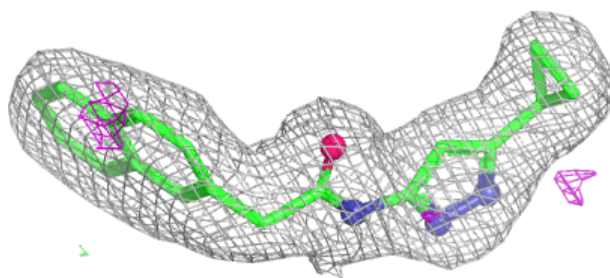
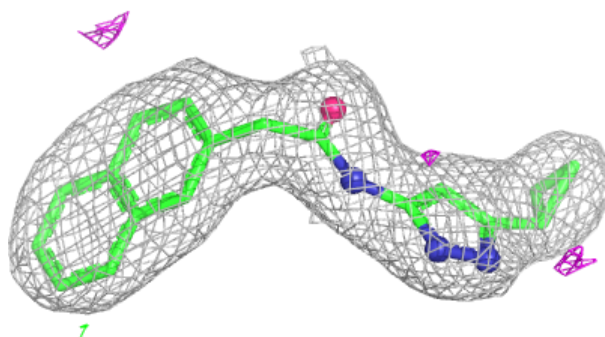
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 292 C 2300:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 292 A 2300:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.