



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:34 PM UTC

PDB ID : 2FM5 / pdb_00002fm5
Title : Crystal structure of PDE4D2 in complex with inhibitor L-869299
Authors : Huai, Q.; Sun, Y.; Wang, H.; Macdonald, D.; Aspiotis, R.; Robinson, H.;
Huang, Z.; Ke, H.
Deposited on : 2006-01-07
Resolution : 2.03 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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

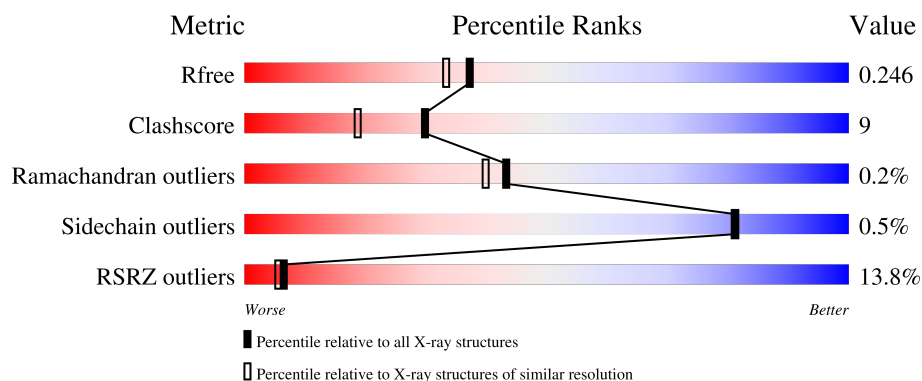
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	361	9% 74% 19% 7%
1	B	361	22% 69% 20% • 9%
1	C	361	13% 72% 18% • 9%
1	D	361	7% 76% 16% • 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11207 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			

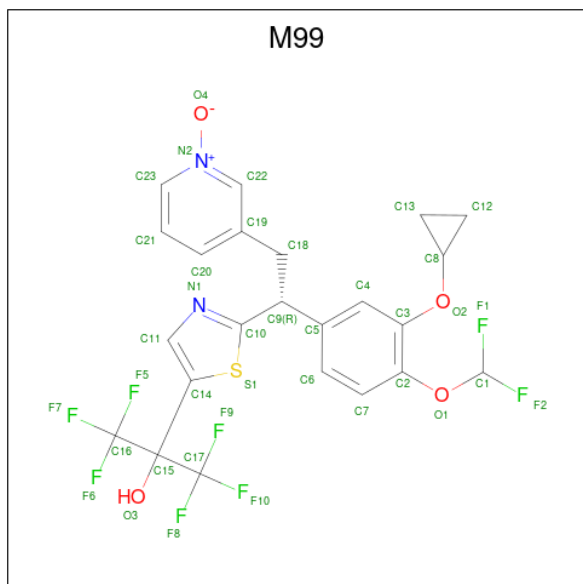
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (R)-3-(2-(3-CYCLOPROPOXY-4-(DIFLUOROMETHOXY)PHENYL)-2-(5-(1,1,1,3,3,3-HEXAFLUORO-2-HYDROXYPROPAN-2-YL)THIAZOL-2-YL)ETHYL)PYRIDINE 1-OXIDE (CCD ID: M99) (formula: $C_{23}H_{18}F_8N_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		
4	B	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		
4	C	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		
4	D	1	Total	C	F	N	O	S	0	0
			38	23	8	2	4	1		

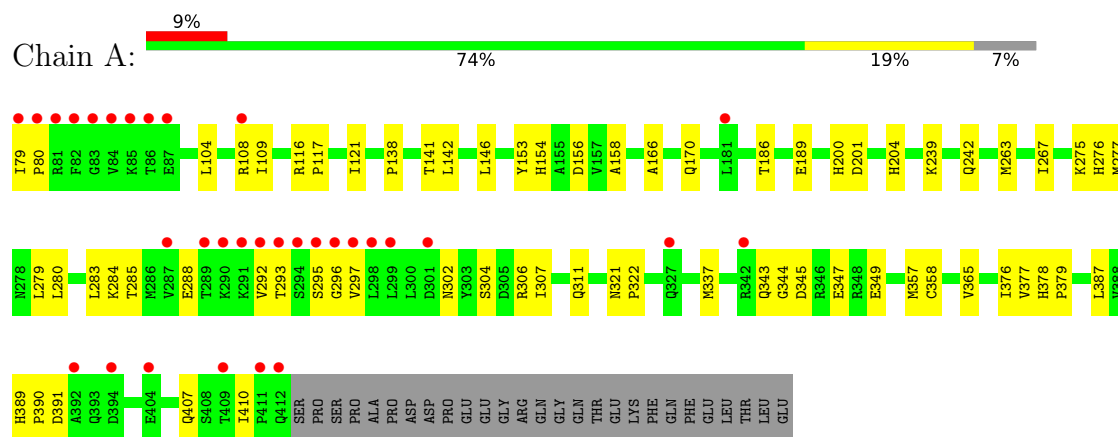
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	74	Total	O	0	0
			74	74		
5	C	76	Total	O	0	0
			76	76		
5	D	104	Total	O	0	0
			104	104		

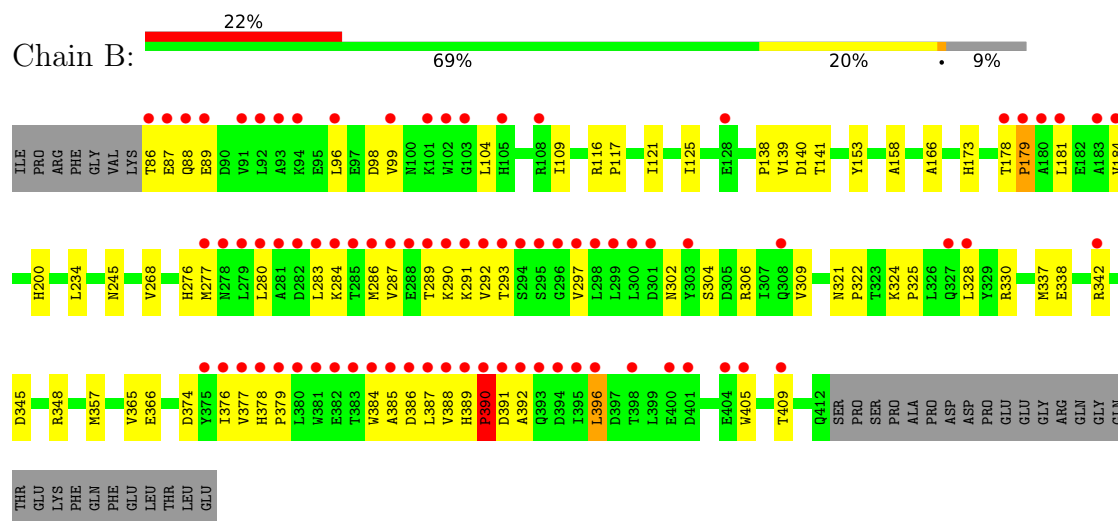
3 Residue-property plots

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.

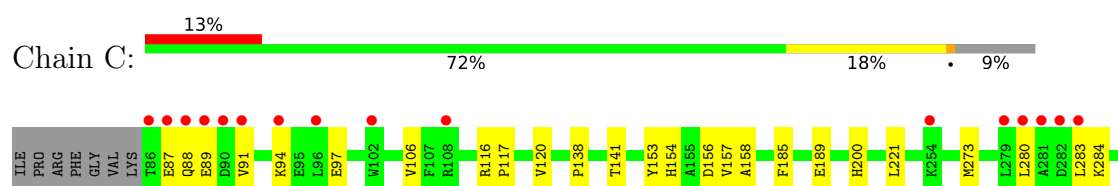
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

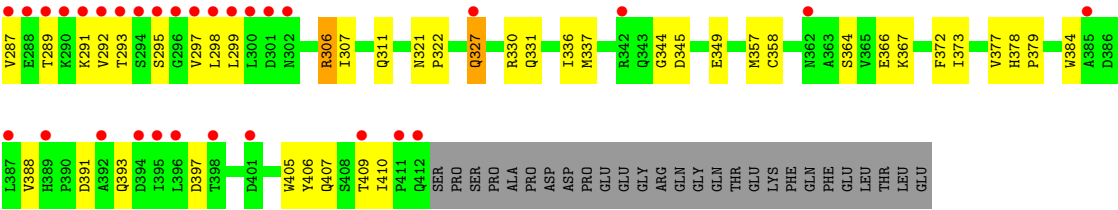


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

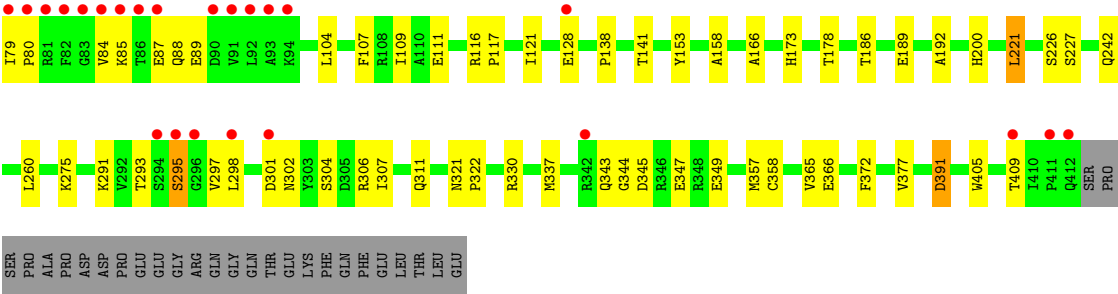
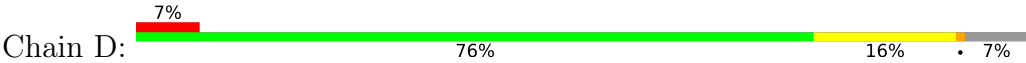


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.36Å 112.81Å 161.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.03 30.00 – 2.03	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.03) 91.4 (30.00-2.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.260 0.219 , 0.246	Depositor DCC
R_{free} test set	11254 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	1.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11207	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: M99, MG, ZN

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	0/2760	0.85	5/3749 (0.1%)
1	B	0.37	0/2701	0.83	5/3670 (0.1%)
1	C	0.38	0/2701	0.85	5/3670 (0.1%)
1	D	0.42	0/2760	0.87	9/3749 (0.2%)
All	All	0.40	0/10922	0.85	24/14838 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	HIS	N-CA-C	7.48	122.06	112.34
1	A	158	ALA	N-CA-C	7.39	118.98	111.07
1	D	295	SER	N-CA-C	-7.37	100.18	110.35
1	D	200	HIS	N-CA-C	7.21	120.98	111.75
1	A	153	TYR	N-CA-C	-7.21	97.94	109.76
1	D	153	TYR	N-CA-C	-7.20	98.88	110.32
1	A	200	HIS	N-CA-C	7.18	120.94	111.75
1	D	301	ASP	N-CA-C	6.91	120.18	111.69
1	D	158	ALA	N-CA-C	6.72	118.61	111.28
1	B	200	HIS	N-CA-C	6.60	120.92	112.34
1	A	377	VAL	N-CA-C	6.29	116.40	110.30
1	C	391	ASP	N-CA-C	6.25	118.89	111.33
1	B	377	VAL	N-CA-C	6.16	116.27	110.30
1	B	158	ALA	N-CA-C	5.79	117.27	111.07
1	C	106	VAL	N-CA-C	5.66	116.39	110.62
1	C	153	TYR	N-CA-C	-5.61	100.56	109.76
1	C	158	ALA	N-CA-C	5.60	117.06	111.07
1	D	88	GLN	N-CA-C	-5.58	106.51	113.15
1	B	153	TYR	N-CA-C	-5.43	100.86	109.76
1	D	297	VAL	N-CA-C	5.29	116.94	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	391	ASP	N-CA-C	5.21	117.36	111.11
1	B	374	ASP	N-CA-C	5.20	116.76	111.14
1	A	391	ASP	N-CA-C	5.16	117.30	111.11
1	D	377	VAL	N-CA-C	5.13	115.34	110.42

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	2704	0	2664	46	0
1	B	2647	0	2599	54	0
1	C	2647	0	2599	45	0
1	D	2704	0	2664	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	38	0	17	2	0
4	B	38	0	17	1	0
4	C	38	0	17	3	0
4	D	38	0	17	2	0
5	A	91	0	0	1	0
5	B	74	0	0	2	0
5	C	76	0	0	0	0
5	D	104	0	0	2	0
All	All	11207	0	10594	183	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 (183) 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:D:337:MET:HE2	1:D:365:VAL:HG22	1.42	1.00
1:A:292:VAL:HG12	1:A:293:THR:H	1.31	0.94
1:B:337:MET:HE2	1:B:365:VAL:HG22	1.49	0.92
1:C:292:VAL:HG22	1:C:293:THR:H	1.43	0.83
1:B:276:HIS:HD2	1:B:277:MET:HE2	1.47	0.78
1:D:337:MET:CE	1:D:365:VAL:HG22	2.15	0.74
1:C:273:MET:HE2	4:C:603:M99:H111	1.69	0.73
1:B:287:VAL:HG22	1:B:387:LEU:HD13	1.71	0.72
1:B:286:MET:HE1	1:B:309:VAL:HG22	1.71	0.72
1:B:96:LEU:O	1:B:99:VAL:HG23	1.90	0.70
1:D:221:LEU:C	1:D:221:LEU:HD23	2.17	0.70
1:D:79:ILE:N	1:D:80:PRO:HD2	2.07	0.69
1:B:276:HIS:CD2	1:B:277:MET:HE2	2.28	0.69
1:B:386:ASP:O	1:B:389:HIS:HB2	1.94	0.67
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.77	0.67
1:B:325:PRO:HG2	1:B:328:LEU:HD12	1.76	0.66
1:A:295:SER:C	1:A:297:VAL:H	2.04	0.65
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.31	0.65
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.32	0.65
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.79	0.64
1:A:357:MET:SD	4:A:601:M99:H122	2.39	0.63
1:C:366:GLU:HG2	1:C:409:THR:HG22	1.80	0.63
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.82	0.62
1:B:104:LEU:HD11	1:B:109:ILE:HD11	1.81	0.62
1:A:337:MET:HE3	1:A:365:VAL:HG13	1.81	0.62
1:B:283:LEU:O	1:B:287:VAL:HG23	2.00	0.62
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.81	0.61
1:C:292:VAL:HG22	1:C:293:THR:N	2.14	0.61
1:A:79:ILE:N	1:A:80:PRO:HD2	2.15	0.61
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.33	0.61
1:C:293:THR:HG22	1:C:297:VAL:O	2.00	0.61
1:D:79:ILE:N	1:D:79:ILE:HD12	2.17	0.60
1:B:330:ARG:HD3	1:B:405:TRP:CH2	2.37	0.59
1:A:292:VAL:HG12	1:A:293:THR:N	2.07	0.59
1:A:345:ASP:O	1:A:349:GLU:HG3	2.02	0.59
1:D:138:PRO:HG2	1:D:141:THR:OG1	2.04	0.57
1:A:307:ILE:O	1:A:311:GLN:HG3	2.04	0.57
1:C:291:LYS:O	1:C:299:LEU:HB3	2.05	0.56
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.87	0.56
1:B:286:MET:HE1	1:B:309:VAL:CG2	2.36	0.56
5:B:641:HOH:O	1:D:84:VAL:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:THR:HG23	1:C:295:SER:H	1.70	0.56
1:A:280:LEU:HG	1:A:284:LYS:HE3	1.89	0.55
1:D:85:LYS:HD2	5:D:663:HOH:O	2.05	0.55
1:A:283:LEU:HD11	1:A:387:LEU:HD22	1.89	0.54
1:D:275:LYS:HE2	5:D:636:HOH:O	2.08	0.54
1:B:378:HIS:HB3	1:B:379:PRO:HD3	1.88	0.54
1:C:138:PRO:HG2	1:C:141:THR:OG1	2.08	0.54
1:B:357:MET:SD	4:B:602:M99:H122	2.47	0.54
1:D:221:LEU:HD23	1:D:221:LEU:O	2.08	0.54
1:C:221:LEU:HD23	1:C:221:LEU:O	2.09	0.53
1:C:407:GLN:NE2	1:C:410:ILE:HD12	2.24	0.53
1:A:302:ASN:OD1	1:A:304:SER:HB3	2.08	0.53
1:A:79:ILE:N	1:A:80:PRO:CD	2.71	0.53
1:A:275:LYS:O	1:A:279:LEU:HB2	2.08	0.53
1:D:107:PHE:O	1:D:111:GLU:HG3	2.09	0.53
1:D:366:GLU:HG2	1:D:409:THR:HG22	1.90	0.53
1:C:393:GLN:HE21	1:C:397:ASP:CG	2.17	0.52
1:C:357:MET:SD	4:C:603:M99:H122	2.48	0.52
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.91	0.52
1:C:384:TRP:O	1:C:388:VAL:HG22	2.09	0.52
1:B:385:ALA:HA	1:B:392:ALA:HB3	1.91	0.52
1:A:292:VAL:CG1	1:A:293:THR:H	2.14	0.52
1:B:178:THR:O	1:B:178:THR:HG23	2.11	0.51
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.92	0.51
1:D:343:GLN:O	1:D:347:GLU:HG3	2.10	0.51
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.76	0.50
1:C:378:HIS:HB3	1:C:379:PRO:HD3	1.93	0.50
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.46	0.50
1:B:280:LEU:HG	1:B:284:LYS:HE3	1.94	0.50
1:D:121:ILE:HD12	1:D:166:ALA:HB1	1.94	0.50
1:C:366:GLU:H	1:C:366:GLU:CD	2.20	0.50
1:D:357:MET:SD	4:D:604:M99:H122	2.51	0.50
1:D:307:ILE:O	1:D:311:GLN:HG3	2.12	0.50
1:D:79:ILE:N	1:D:80:PRO:CD	2.76	0.49
1:C:221:LEU:HD23	1:C:221:LEU:C	2.37	0.49
1:C:372:PHE:CG	4:C:603:M99:H132	2.48	0.49
1:A:239:LYS:HE3	5:A:627:HOH:O	2.11	0.49
1:A:295:SER:C	1:A:297:VAL:N	2.70	0.49
1:C:87:GLU:O	1:C:91:VAL:HG23	2.13	0.49
1:D:116:ARG:N	1:D:117:PRO:CD	2.76	0.49
1:B:116:ARG:N	1:B:117:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:GLY:HA3	1:C:358:CYS:O	2.13	0.48
1:B:286:MET:HE2	1:B:387:LEU:HD11	1.94	0.48
1:B:289:THR:O	1:B:291:LYS:HG3	2.14	0.48
1:B:302:ASN:O	1:B:306:ARG:HG3	2.13	0.48
1:C:116:ARG:N	1:C:117:PRO:CD	2.77	0.48
1:D:87:GLU:C	1:D:89:GLU:H	2.20	0.48
1:B:389:HIS:ND1	1:B:390:PRO:HB3	2.28	0.47
1:D:344:GLY:HA3	1:D:358:CYS:O	2.13	0.47
1:A:344:GLY:HA3	1:A:358:CYS:O	2.14	0.47
1:A:201:ASP:O	1:A:204:HIS:HB2	2.13	0.47
1:B:86:THR:O	1:B:89:GLU:HB3	2.15	0.47
1:B:324:LYS:HB3	1:B:325:PRO:HD2	1.96	0.47
1:B:384:TRP:O	1:B:388:VAL:HG22	2.15	0.47
1:C:345:ASP:O	1:C:349:GLU:HG3	2.14	0.47
1:A:337:MET:HE3	1:A:365:VAL:HA	1.97	0.47
1:C:94:LYS:O	1:C:97:GLU:HB2	2.15	0.47
1:B:178:THR:HG22	1:B:181:LEU:HD12	1.96	0.47
1:D:366:GLU:HG2	1:D:409:THR:CG2	2.44	0.47
1:B:389:HIS:CE1	1:B:390:PRO:HB3	2.51	0.47
1:D:372:PHE:CD1	4:D:604:M99:H132	2.51	0.46
1:A:138:PRO:HG2	1:A:141:THR:OG1	2.15	0.46
1:B:389:HIS:HA	1:B:390:PRO:HA	1.66	0.46
1:D:345:ASP:O	1:D:349:GLU:HG3	2.15	0.46
1:C:116:ARG:O	1:C:120:VAL:HG22	2.15	0.46
1:C:407:GLN:CD	1:C:410:ILE:HD12	2.40	0.46
1:A:116:ARG:N	1:A:117:PRO:CD	2.78	0.46
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.45	0.46
1:C:289:THR:O	1:C:289:THR:HG22	2.16	0.46
1:A:295:SER:O	1:A:297:VAL:N	2.47	0.46
1:B:138:PRO:HG2	1:B:141:THR:OG1	2.15	0.46
1:B:292:VAL:HG12	1:B:293:THR:N	2.29	0.46
1:D:186:THR:OG1	1:D:189:GLU:HG3	2.15	0.46
1:A:276:HIS:HD2	1:A:277:MET:HE2	1.81	0.45
1:C:293:THR:HG22	1:C:297:VAL:N	2.31	0.45
1:B:287:VAL:HG22	1:B:387:LEU:CD1	2.45	0.45
1:C:88:GLN:HE22	1:C:89:GLU:HB2	1.82	0.45
1:C:406:TYR:O	1:C:409:THR:HB	2.17	0.45
1:C:185:PHE:HD1	1:C:306:ARG:HH12	1.64	0.44
1:C:289:THR:O	1:C:291:LYS:HG2	2.16	0.44
1:A:239:LYS:HD2	1:A:242:GLN:OE1	2.17	0.44
1:B:302:ASN:OD1	1:B:304:SER:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:VAL:HG13	1:B:140:ASP:N	2.33	0.44
1:D:291:LYS:O	1:D:298:LEU:HD12	2.16	0.44
1:B:87:GLU:HG3	1:B:88:GLN:HG3	1.99	0.44
1:B:138:PRO:HG2	1:B:141:THR:CB	2.48	0.44
1:B:345:ASP:HA	1:B:348:ARG:NH1	2.32	0.44
1:A:242:GLN:NE2	1:D:242:GLN:OE1	2.50	0.44
1:B:87:GLU:HG3	1:B:88:GLN:N	2.33	0.44
1:D:293:THR:O	1:D:295:SER:O	2.36	0.44
1:C:373:ILE:HA	1:C:377:VAL:HB	2.00	0.44
1:A:285:THR:O	1:A:288:GLU:HB2	2.18	0.43
1:A:142:LEU:O	1:A:146:LEU:HG	2.18	0.43
1:D:192:ALA:HB2	1:D:260:LEU:HD12	2.00	0.43
1:D:226:SER:O	1:D:227:SER:C	2.62	0.43
1:B:289:THR:O	1:B:290:LYS:C	2.62	0.43
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.34	0.43
1:D:104:LEU:HD11	1:D:109:ILE:HD11	2.00	0.43
1:B:179:PRO:HD2	1:B:391:ASP:CG	2.44	0.43
1:B:386:ASP:O	1:B:389:HIS:N	2.45	0.43
1:D:178:THR:OG1	1:D:391:ASP:HB3	2.19	0.42
1:D:302:ASN:OD1	1:D:304:SER:HB3	2.19	0.42
1:A:343:GLN:O	1:A:347:GLU:HG3	2.20	0.42
1:B:184:VAL:HG23	1:B:297:VAL:HG11	2.00	0.42
1:C:280:LEU:HG	1:C:284:LYS:HE3	2.01	0.42
1:A:154:HIS:CD2	1:A:154:HIS:N	2.87	0.42
1:D:221:LEU:C	1:D:221:LEU:CD2	2.86	0.42
1:A:357:MET:HE1	4:A:601:M99:F6	2.10	0.42
1:A:121:ILE:HD12	1:A:166:ALA:HB1	2.01	0.42
1:C:297:VAL:HG12	1:C:298:LEU:N	2.34	0.42
1:C:307:ILE:O	1:C:311:GLN:HG3	2.19	0.42
1:C:336:ILE:HG23	1:C:337:MET:HE2	2.01	0.42
1:A:154:HIS:HB3	1:A:156:ASP:OD1	2.20	0.42
1:C:327:GLN:O	1:C:331:GLN:HG3	2.19	0.42
1:A:302:ASN:O	1:A:306:ARG:HG3	2.19	0.42
1:A:376:ILE:C	1:A:379:PRO:HD2	2.45	0.42
1:B:121:ILE:HD12	1:B:166:ALA:HB1	2.02	0.42
1:D:302:ASN:O	1:D:306:ARG:HG3	2.20	0.42
1:A:186:THR:OG1	1:A:189:GLU:HG3	2.20	0.41
1:A:407:GLN:OE1	1:A:410:ILE:HD12	2.20	0.41
1:B:396:LEU:O	1:B:396:LEU:HD23	2.20	0.41
1:D:128:GLU:OE1	1:D:173:HIS:NE2	2.53	0.41
1:B:96:LEU:C	1:B:98:ASP:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.48	0.41
1:B:376:ILE:C	1:B:379:PRO:HD2	2.45	0.41
1:C:293:THR:HG23	1:C:295:SER:N	2.34	0.41
1:A:292:VAL:HG12	1:A:295:SER:O	2.21	0.41
1:C:94:LYS:HD2	1:C:97:GLU:CD	2.46	0.41
1:C:154:HIS:HB3	1:C:156:ASP:OD1	2.21	0.41
1:D:87:GLU:H	1:D:87:GLU:HG2	1.68	0.41
1:B:283:LEU:HD11	1:B:387:LEU:HD22	2.03	0.41
1:C:154:HIS:HB2	1:C:157:VAL:HG23	2.03	0.41
1:B:125:ILE:HD13	1:B:173:HIS:HB2	2.03	0.41
1:C:283:LEU:O	1:C:287:VAL:HG23	2.21	0.41
1:A:263:MET:O	1:A:267:ILE:HG13	2.21	0.41
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.51	0.41
1:B:245:ASN:ND2	5:B:665:HOH:O	2.50	0.41
1:A:378:HIS:HB3	1:A:379:PRO:HD3	2.03	0.40
1:C:364:SER:HB3	1:C:367:LYS:HB3	2.03	0.40
1:C:189:GLU:OE2	1:C:306:ARG:NH1	2.54	0.40
1:B:234:LEU:HG	1:B:268:VAL:HG11	2.03	0.40
1:D:138:PRO:HG2	1:D:141:THR:CB	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	332/361 (92%)	318 (96%)	13 (4%)	1 (0%)	36	31
1	B	325/361 (90%)	295 (91%)	29 (9%)	1 (0%)	36	31
1	C	325/361 (90%)	310 (95%)	15 (5%)	0	100	100
1	D	332/361 (92%)	317 (96%)	15 (4%)	0	100	100
All	All	1314/1444 (91%)	1240 (94%)	72 (6%)	2 (0%)	43	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	PRO
1	A	296	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/329 (93%)	305 (100%)	0	100	100
1	B	299/329 (91%)	296 (99%)	3 (1%)	68	71
1	C	299/329 (91%)	297 (99%)	2 (1%)	76	77
1	D	305/329 (93%)	304 (100%)	1 (0%)	86	86
All	All	1208/1316 (92%)	1202 (100%)	6 (0%)	81	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	PRO
1	B	390	PRO
1	B	396	LEU
1	C	306	ARG
1	C	327	GLN
1	D	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	210	GLN
1	A	245	ASN
1	A	250	GLN
1	A	258	GLN
1	A	308	GLN
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	369	GLN
1	A	389	HIS
1	B	123	HIS
1	B	210	GLN
1	B	245	ASN
1	B	308	GLN
1	B	369	GLN
1	B	407	GLN
1	C	88	GLN
1	C	210	GLN
1	C	214	ASN
1	C	242	GLN
1	C	245	ASN
1	C	250	GLN
1	C	308	GLN
1	C	327	GLN
1	C	331	GLN
1	C	393	GLN
1	C	407	GLN
1	D	123	HIS
1	D	127	GLN
1	D	210	GLN
1	D	245	ASN
1	D	321	ASN
1	D	369	GLN
1	D	378	HIS
1	D	407	GLN

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

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	M99	D	604	-	39,41,41	1.67	9 (23%)	51,63,63	1.79	3 (5%)
4	M99	A	601	-	39,41,41	1.66	9 (23%)	51,63,63	1.79	3 (5%)
4	M99	B	602	-	39,41,41	1.71	9 (23%)	51,63,63	1.79	3 (5%)
4	M99	C	603	-	39,41,41	1.66	9 (23%)	51,63,63	1.76	3 (5%)

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	M99	D	604	-	-	3/42/46/46	0/4/4/4
4	M99	A	601	-	-	3/42/46/46	0/4/4/4
4	M99	B	602	-	-	3/42/46/46	0/4/4/4
4	M99	C	603	-	-	3/42/46/46	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	M99	C11-N1	4.25	1.45	1.37
4	D	604	M99	C11-C14	4.07	1.41	1.34
4	C	603	M99	C11-C14	3.96	1.41	1.34
4	B	602	M99	C11-N1	3.94	1.45	1.37
4	A	601	M99	C11-C14	3.91	1.41	1.34
4	B	602	M99	C11-C14	3.89	1.41	1.34
4	A	601	M99	C10-S1	-3.81	1.66	1.75
4	C	603	M99	C10-S1	-3.81	1.66	1.75
4	D	604	M99	C11-N1	3.78	1.44	1.37
4	D	604	M99	C10-S1	-3.76	1.66	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	M99	C10-S1	-3.68	1.67	1.75
4	A	601	M99	C11-N1	3.41	1.44	1.37
4	D	604	M99	C13-C8	3.29	1.54	1.48
4	C	603	M99	C13-C8	3.22	1.54	1.48
4	B	602	M99	C12-C8	3.20	1.53	1.48
4	D	604	M99	C12-C8	3.19	1.53	1.48
4	C	603	M99	C12-C8	3.15	1.53	1.48
4	B	602	M99	C13-C8	3.14	1.53	1.48
4	B	602	M99	C17-C15	3.07	1.57	1.53
4	A	601	M99	C13-C8	2.97	1.53	1.48
4	A	601	M99	C12-C8	2.97	1.53	1.48
4	A	601	M99	C14-S1	-2.93	1.67	1.73
4	B	602	M99	C22-N2	2.73	1.40	1.35
4	D	604	M99	C22-N2	2.73	1.40	1.35
4	A	601	M99	C17-C15	2.62	1.56	1.53
4	D	604	M99	C14-S1	-2.59	1.67	1.73
4	C	603	M99	C22-N2	2.59	1.40	1.35
4	B	602	M99	C14-S1	-2.59	1.67	1.73
4	A	601	M99	C22-N2	2.46	1.40	1.35
4	B	602	M99	C16-C15	2.39	1.56	1.53
4	C	603	M99	C17-C15	2.35	1.56	1.53
4	C	603	M99	C14-S1	-2.30	1.68	1.73
4	D	604	M99	C17-C15	2.25	1.56	1.53
4	D	604	M99	C16-C15	2.25	1.56	1.53
4	C	603	M99	C16-C15	2.22	1.56	1.53
4	A	601	M99	C16-C15	2.05	1.56	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	M99	C14-C11-N1	-9.88	107.01	117.10
4	D	604	M99	C14-C11-N1	-9.86	107.03	117.10
4	A	601	M99	C14-C11-N1	-9.77	107.12	117.10
4	C	603	M99	C14-C11-N1	-9.77	107.13	117.10
4	A	601	M99	C11-C14-S1	5.16	113.63	108.93
4	B	602	M99	C11-C14-S1	5.15	113.63	108.93
4	D	604	M99	C11-C14-S1	5.02	113.51	108.93
4	C	603	M99	C11-C14-S1	4.68	113.20	108.93
4	C	603	M99	S1-C10-N1	-3.53	111.16	115.98
4	B	602	M99	S1-C10-N1	-3.51	111.18	115.98
4	A	601	M99	S1-C10-N1	-3.44	111.28	115.98
4	D	604	M99	S1-C10-N1	-3.38	111.37	115.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

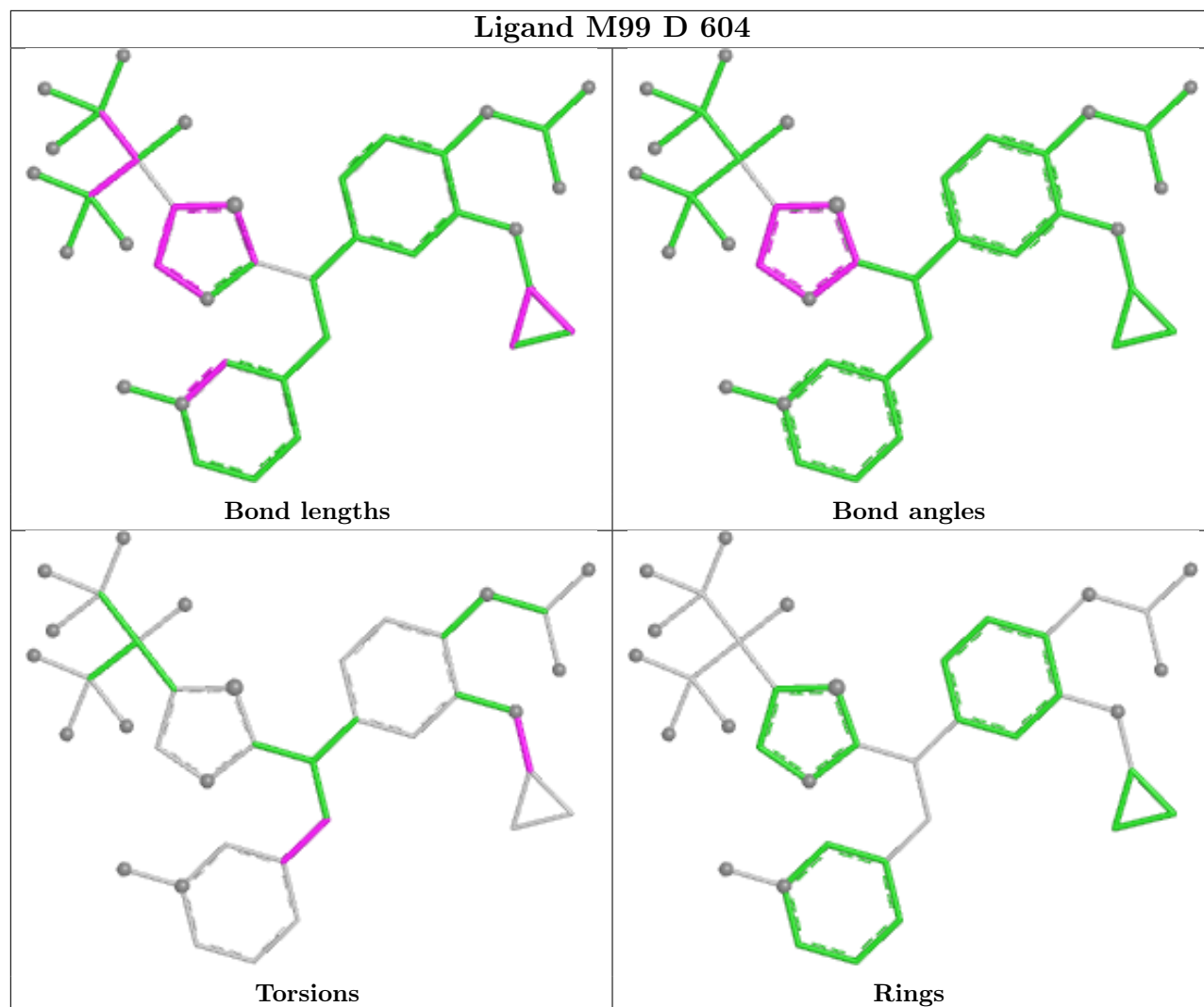
Mol	Chain	Res	Type	Atoms
4	A	601	M99	C13-C8-O2-C3
4	B	602	M99	C13-C8-O2-C3
4	C	603	M99	C13-C8-O2-C3
4	D	604	M99	C13-C8-O2-C3
4	D	604	M99	C9-C18-C19-C20
4	A	601	M99	C9-C18-C19-C20
4	B	602	M99	C9-C18-C19-C20
4	C	603	M99	C9-C18-C19-C20
4	A	601	M99	C9-C18-C19-C22
4	B	602	M99	C9-C18-C19-C22
4	C	603	M99	C9-C18-C19-C22
4	D	604	M99	C9-C18-C19-C22

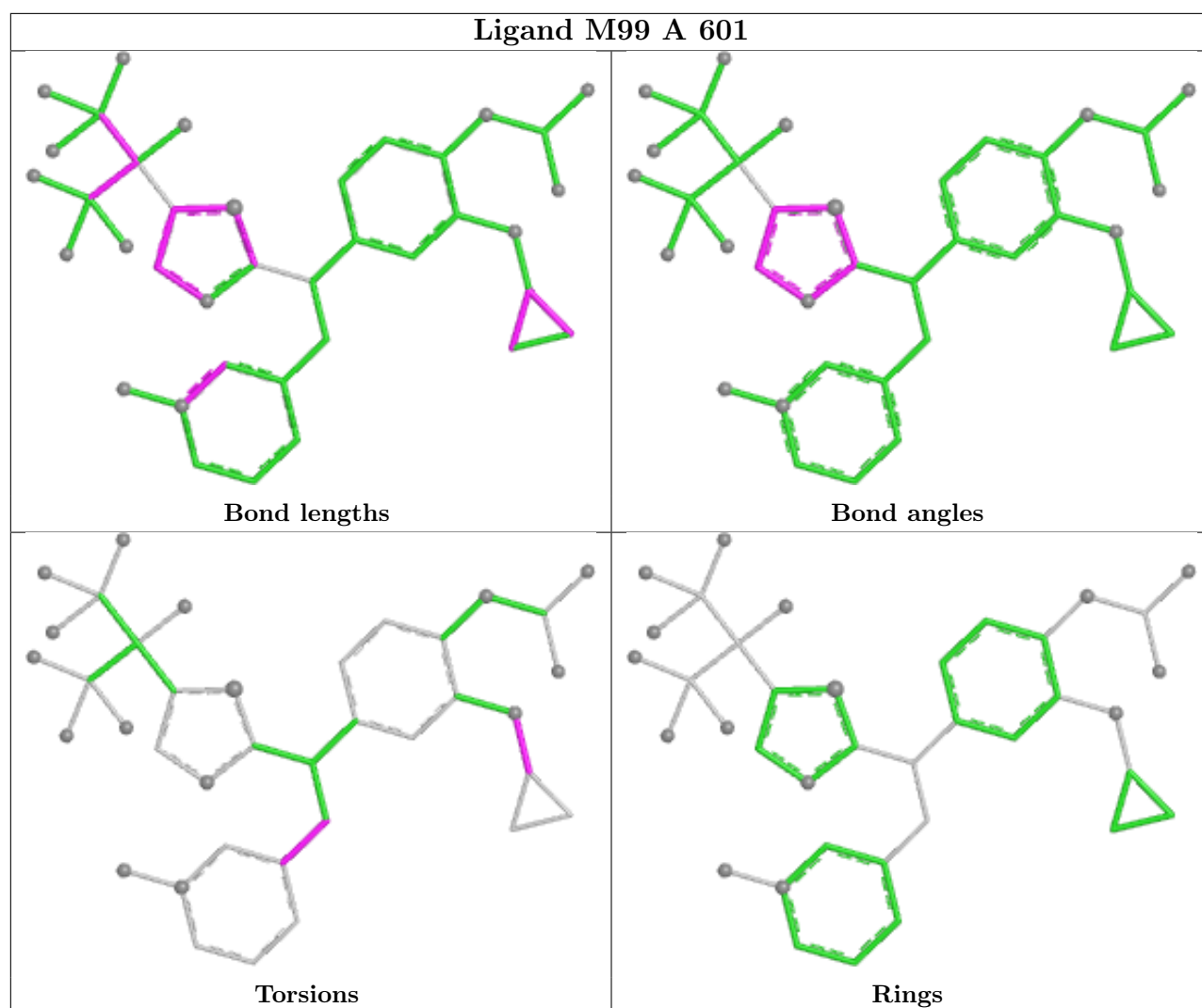
There are no ring outliers.

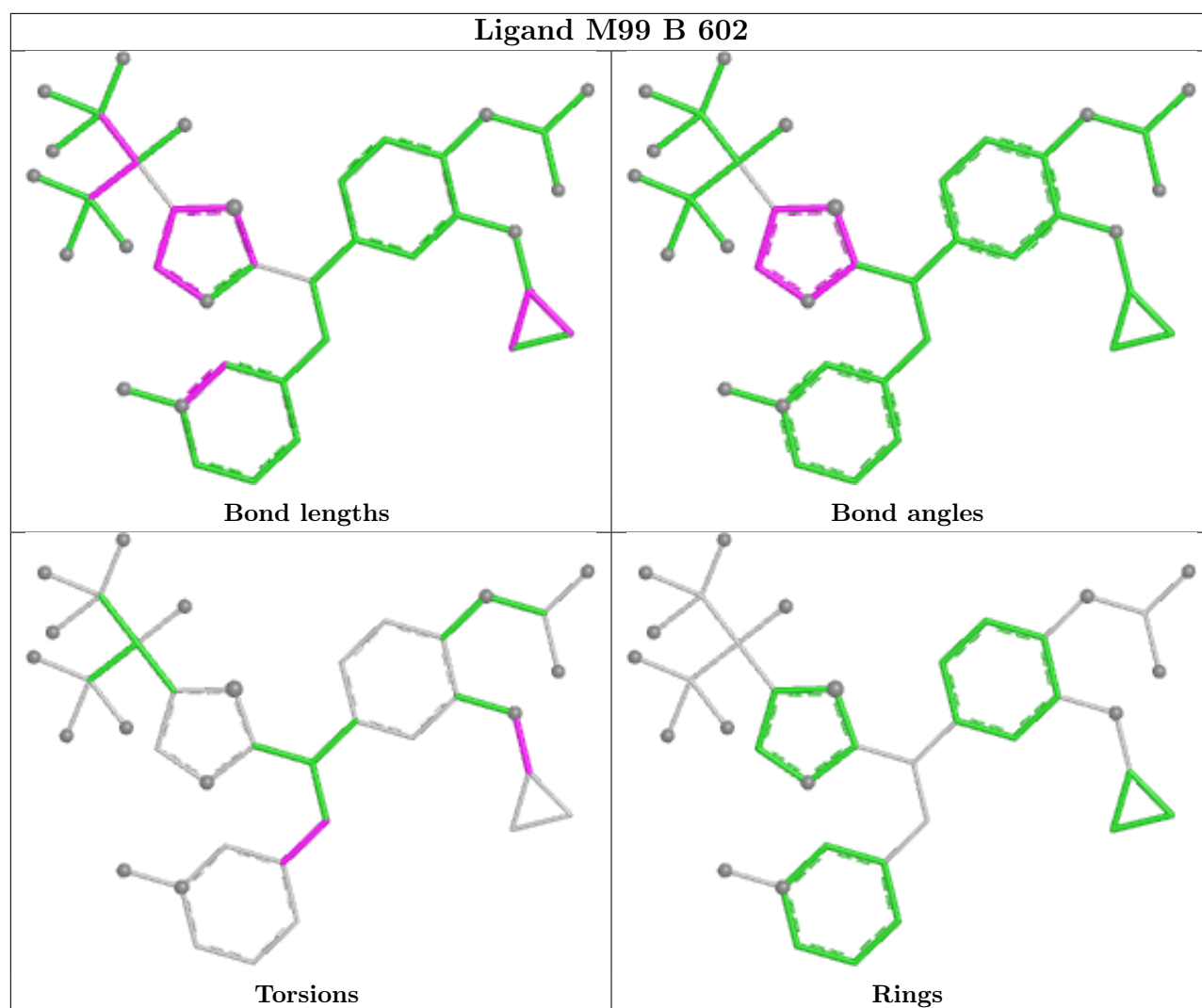
4 monomers are involved in 8 short contacts:

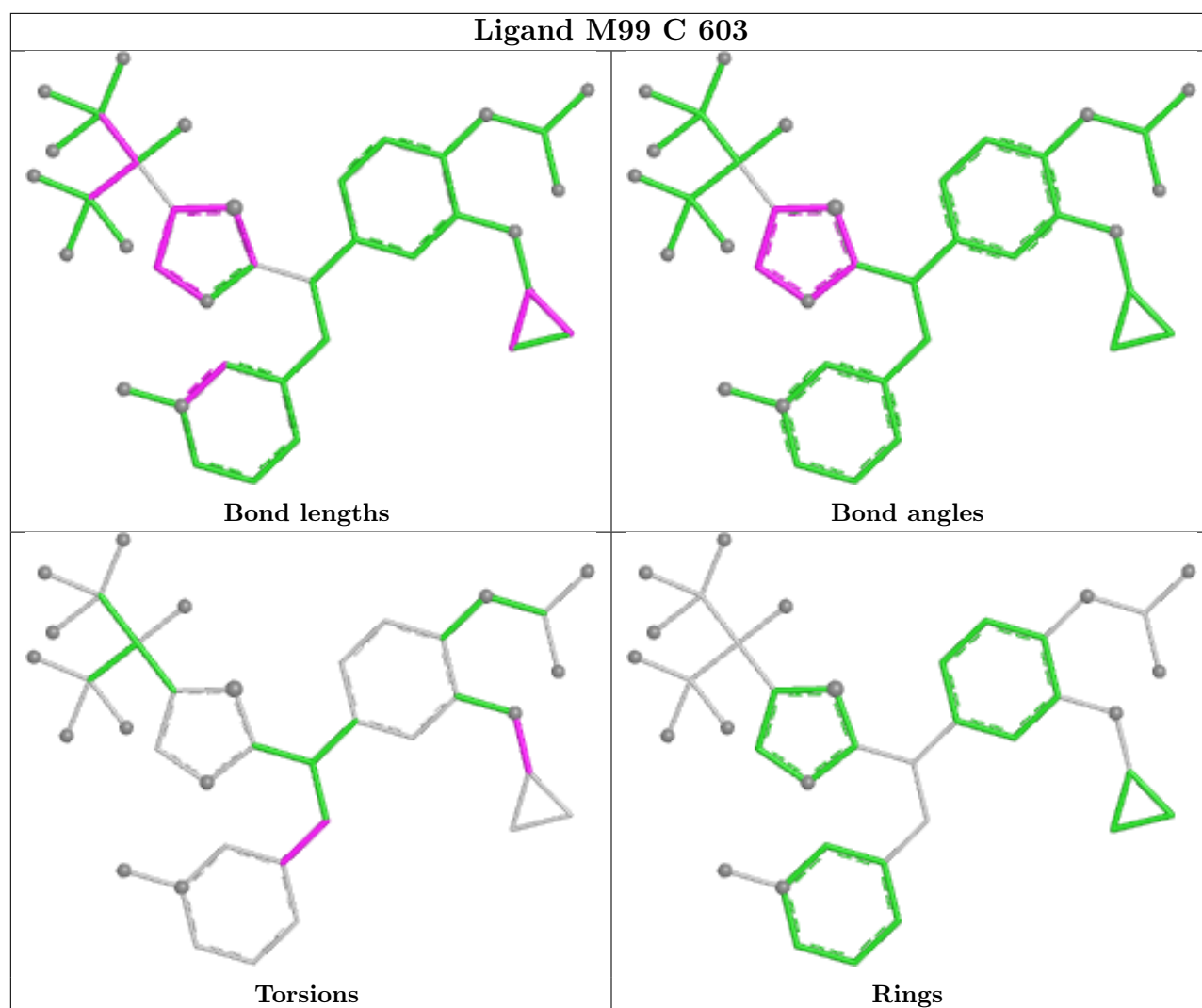
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	604	M99	2	0
4	A	601	M99	2	0
4	B	602	M99	1	0
4	C	603	M99	3	0

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	334/361 (92%)	0.44	32 (9%) 13 12	13, 23, 59, 81	0
1	B	327/361 (90%)	1.19	80 (24%) 2 1	14, 31, 64, 87	0
1	C	327/361 (90%)	0.71	47 (14%) 6 5	13, 29, 63, 77	0
1	D	334/361 (92%)	0.30	24 (7%) 21 20	12, 23, 44, 80	0
All	All	1322/1444 (91%)	0.66	183 (13%) 6 5	12, 26, 62, 87	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	VAL	9.4
1	B	287	VAL	8.9
1	A	79	ILE	8.7
1	B	387	LEU	8.0
1	D	79	ILE	7.8
1	B	385	ALA	6.6
1	A	80	PRO	6.6
1	B	390	PRO	6.5
1	B	392	ALA	6.4
1	B	296	GLY	6.4
1	B	292	VAL	5.8
1	D	296	GLY	5.8
1	A	81	ARG	5.6
1	B	388	VAL	5.6
1	D	82	PHE	5.5
1	B	299	LEU	5.2
1	B	281	ALA	5.2
1	A	82	PHE	5.1
1	B	295	SER	5.1
1	B	389	HIS	5.1
1	B	283	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	5.1
1	D	85	LYS	5.0
1	A	298	LEU	5.0
1	B	391	ASP	4.9
1	D	80	PRO	4.9
1	C	298	LEU	4.8
1	D	86	THR	4.8
1	B	289	THR	4.8
1	D	83	GLY	4.7
1	A	411	PRO	4.6
1	B	383	THR	4.6
1	B	88	GLN	4.6
1	D	412	GLN	4.5
1	B	179	PRO	4.5
1	C	287	VAL	4.5
1	B	293	THR	4.4
1	C	297	VAL	4.4
1	B	301	ASP	4.3
1	B	180	ALA	4.3
1	C	293	THR	4.3
1	B	384	TRP	4.2
1	C	86	THR	4.1
1	B	290	LYS	4.0
1	B	294	SER	4.0
1	C	88	GLN	4.0
1	A	293	THR	4.0
1	A	412	GLN	4.0
1	B	291	LYS	4.0
1	B	297	VAL	3.9
1	B	396	LEU	3.8
1	B	183	ALA	3.8
1	C	300	LEU	3.8
1	C	392	ALA	3.7
1	C	294	SER	3.7
1	B	285	THR	3.7
1	B	181	LEU	3.6
1	B	298	LEU	3.6
1	B	395	ILE	3.6
1	A	83	GLY	3.5
1	C	411	PRO	3.5
1	A	291	LYS	3.5
1	A	301	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	294	SER	3.4
1	B	300	LEU	3.4
1	C	301	ASP	3.3
1	C	295	SER	3.3
1	B	394	ASP	3.3
1	C	90	ASP	3.3
1	B	386	ASP	3.3
1	A	289	THR	3.2
1	B	284	LYS	3.2
1	D	295	SER	3.2
1	A	297	VAL	3.2
1	A	290	LYS	3.2
1	B	86	THR	3.2
1	B	278	ASN	3.2
1	B	91	VAL	3.2
1	B	280	LEU	3.2
1	A	299	LEU	3.1
1	C	279	LEU	3.1
1	A	295	SER	3.1
1	B	99	VAL	3.1
1	B	405	TRP	3.1
1	C	282	ASP	3.1
1	C	91	VAL	3.0
1	B	282	ASP	3.0
1	C	296	GLY	3.0
1	B	286	MET	3.0
1	D	81	ARG	3.0
1	A	84	VAL	3.0
1	C	292	VAL	3.0
1	D	294	SER	2.9
1	B	184	VAL	2.9
1	B	288	GLU	2.9
1	B	178	THR	2.9
1	D	93	ALA	2.9
1	B	92	LEU	2.8
1	B	308	GLN	2.8
1	B	404	GLU	2.8
1	D	91	VAL	2.8
1	B	93	ALA	2.8
1	C	387	LEU	2.8
1	C	289	THR	2.8
1	B	102	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	395	ILE	2.7
1	B	103	GLY	2.7
1	B	393	GLN	2.7
1	C	409	THR	2.7
1	A	342	ARG	2.7
1	A	87	GLU	2.6
1	A	409	THR	2.6
1	C	401	ASP	2.6
1	B	377	VAL	2.6
1	C	385	ALA	2.6
1	C	108	ARG	2.6
1	C	299	LEU	2.6
1	D	94	LYS	2.6
1	A	394	ASP	2.6
1	A	108	ARG	2.6
1	D	87	GLU	2.6
1	C	394	ASP	2.6
1	A	392	ALA	2.5
1	C	94	LYS	2.5
1	B	96	LEU	2.5
1	B	381	TRP	2.5
1	D	301	ASP	2.5
1	C	412	GLN	2.5
1	D	409	THR	2.5
1	C	281	ALA	2.5
1	B	279	LEU	2.5
1	B	342	ARG	2.5
1	B	379	PRO	2.4
1	C	283	LEU	2.4
1	C	302	ASN	2.4
1	A	292	VAL	2.4
1	D	90	ASP	2.4
1	B	376	ILE	2.4
1	B	380	LEU	2.4
1	B	89	GLU	2.4
1	C	254	LYS	2.4
1	B	398	THR	2.4
1	B	375	TYR	2.3
1	B	94	LYS	2.3
1	C	396	LEU	2.3
1	D	298	LEU	2.3
1	C	290	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	378	HIS	2.3
1	B	401	ASP	2.3
1	C	280	LEU	2.3
1	B	277	MET	2.3
1	D	128	GLU	2.3
1	A	287	VAL	2.3
1	C	362	ASN	2.3
1	B	101	LYS	2.3
1	C	288	GLU	2.2
1	C	327	GLN	2.2
1	B	108	ARG	2.2
1	B	128	GLU	2.2
1	A	85	LYS	2.2
1	A	404	GLU	2.2
1	B	382	GLU	2.2
1	C	87	GLU	2.2
1	D	92	LEU	2.2
1	B	105	HIS	2.2
1	B	409	THR	2.2
1	C	89	GLU	2.2
1	B	327	GLN	2.2
1	C	398	THR	2.1
1	C	102	TRP	2.1
1	A	181	LEU	2.1
1	A	86	THR	2.1
1	D	411	PRO	2.1
1	C	389	HIS	2.1
1	B	87	GLU	2.1
1	B	400	GLU	2.1
1	A	327	GLN	2.1
1	B	303	TYR	2.1
1	C	342	ARG	2.1
1	B	328	LEU	2.0
1	C	96	LEU	2.0
1	C	291	LYS	2.0
1	D	342	ARG	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 oligosaccharides in this entry.

6.4 Ligands

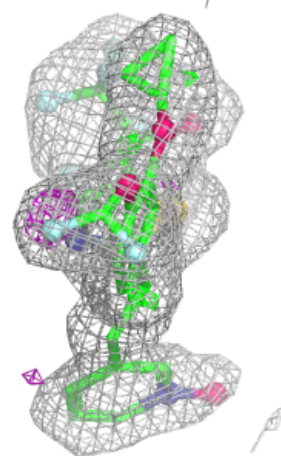
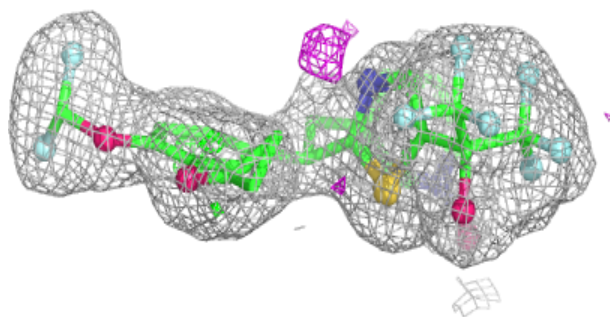
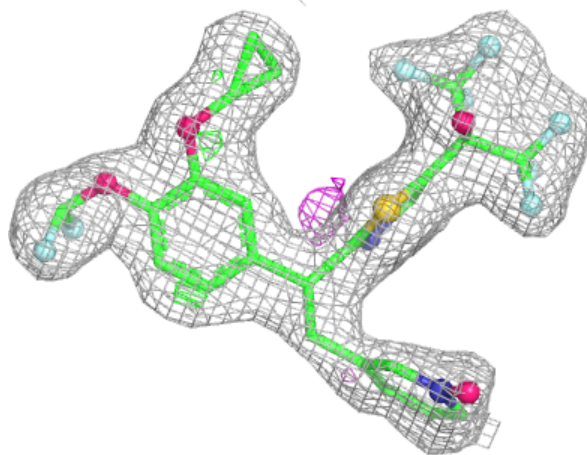
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	M99	C	603	38/38	0.89	0.13	36,45,54,55	0
4	M99	B	602	38/38	0.90	0.12	32,42,49,51	0
4	M99	A	601	38/38	0.91	0.10	28,34,43,44	0
3	MG	B	504	1/1	0.92	0.06	20,20,20,20	0
4	M99	D	604	38/38	0.92	0.10	29,35,47,48	0
3	MG	C	506	1/1	0.95	0.08	22,22,22,22	0
3	MG	D	508	1/1	0.95	0.07	19,19,19,19	0
2	ZN	B	503	1/1	0.97	0.09	26,26,26,26	0
3	MG	A	502	1/1	0.98	0.11	20,20,20,20	0
2	ZN	C	505	1/1	0.98	0.07	25,25,25,25	0
2	ZN	A	501	1/1	0.99	0.06	23,23,23,23	0
2	ZN	D	507	1/1	0.99	0.05	21,21,21,21	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.

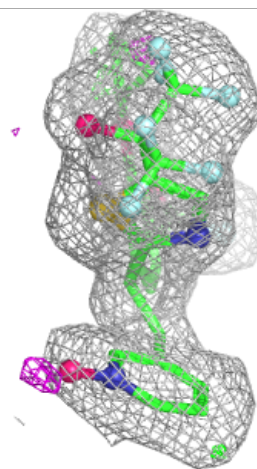
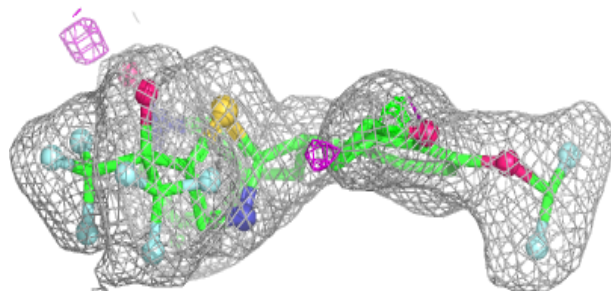
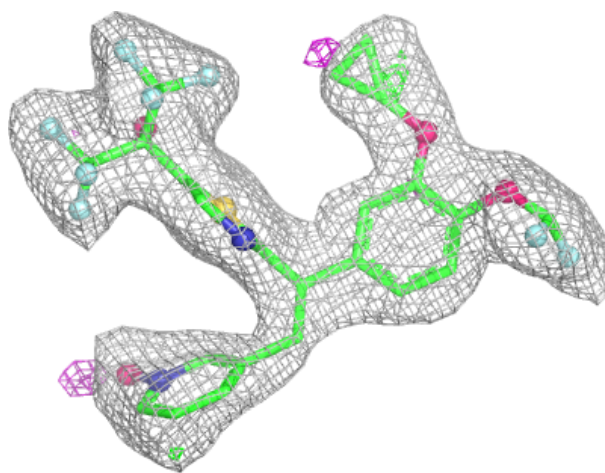
Electron density around M99 C 603:

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



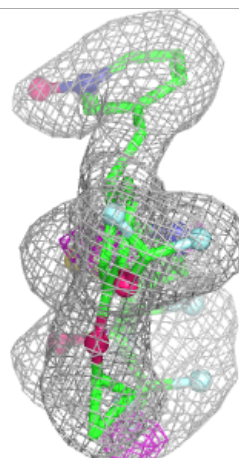
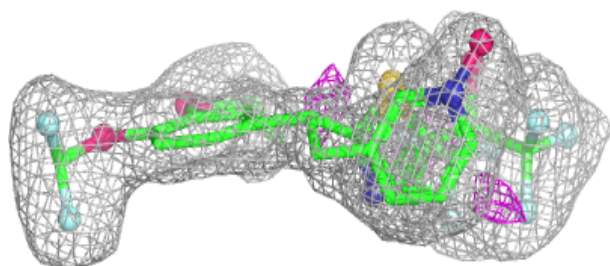
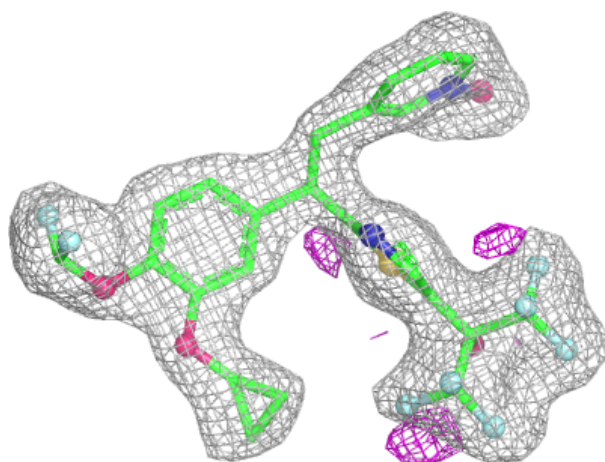
Electron density around M99 B 602:

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



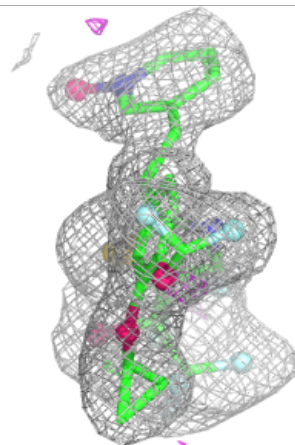
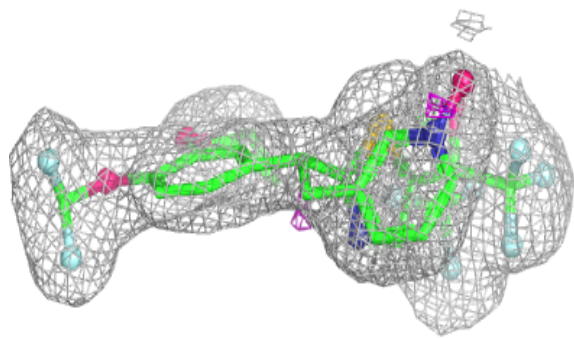
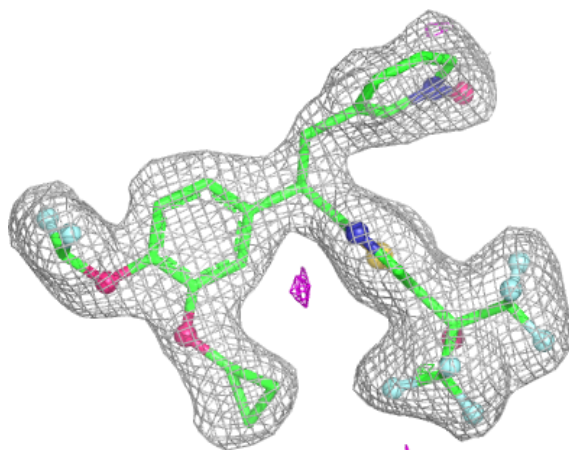
Electron density around M99 A 601:

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



Electron density around M99 D 604:

$2mF_o-DF_c$ (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.