



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:34 PM UTC

PDB ID : 1Z69 / pdb_00001z69
Title : Crystal structure of methylenetetrahydromethanopterin reductase (Mer) in complex with coenzyme F420
Authors : Aufhammer, S.W.; Warkentin, E.; Ermler, U.; Hagemeier, C.H.; Thauer, R.K.; Shima, S.
Deposited on : 2005-03-22
Resolution : 2.61 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

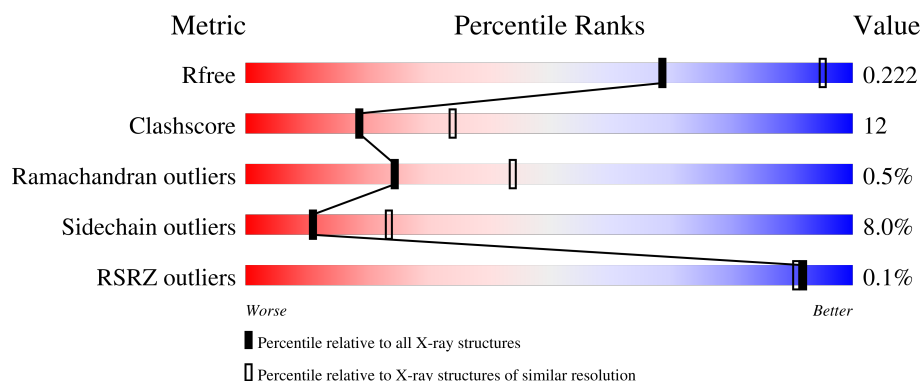
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

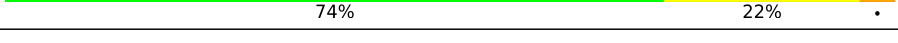
The reported resolution of this entry is 2.61 Å.

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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	327	 74% 21% . .
1	B	327	 72% 25% .
1	C	327	 75% 21% .
1	D	327	 74% 22% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	4001	-	-	X	-
3	CL	D	4002	-	-	X	-

2 Entry composition [i](#)

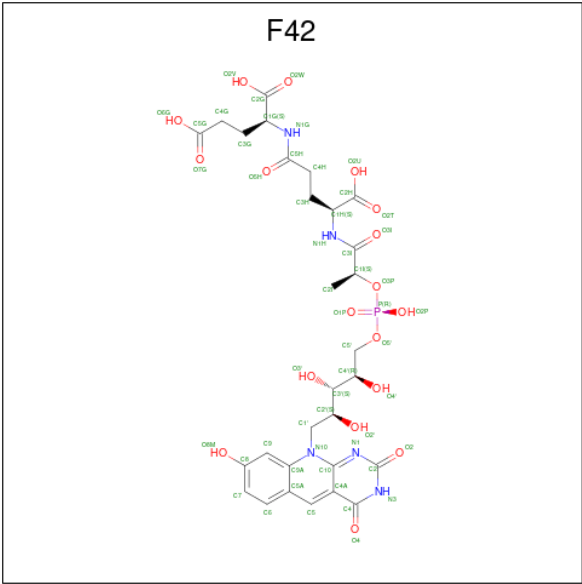
There are 5 unique types of molecules in this entry. The entry contains 10154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coenzyme F420-dependent N(5),N(10)-methylenetetrahydro methanopterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2421	1548	405	456	12			
1	B	327	Total	C	N	O	S	0	0	0
			2421	1548	405	456	12			
1	C	327	Total	C	N	O	S	0	0	0
			2421	1548	405	456	12			
1	D	327	Total	C	N	O	S	0	0	0
			2421	1548	405	456	12			

- Molecule 2 is COENZYME F420 (CCD ID: F42) (formula: C₂₉H₃₆N₅O₁₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	29	5	18	1		
2	B	1	Total	C	N	O	P	0	0
			53	29	5	18	1		

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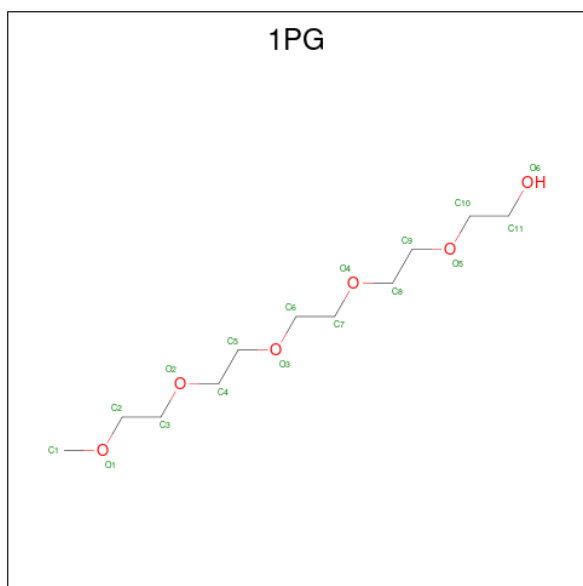
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	29	5	18	1		
2	D	1	Total	C	N	O	P	0	0
			53	29	5	18	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (CCD ID: 1PG) (formula: C₁₁H₂₄O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 17 11 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	42	Total O 42 42	0	0

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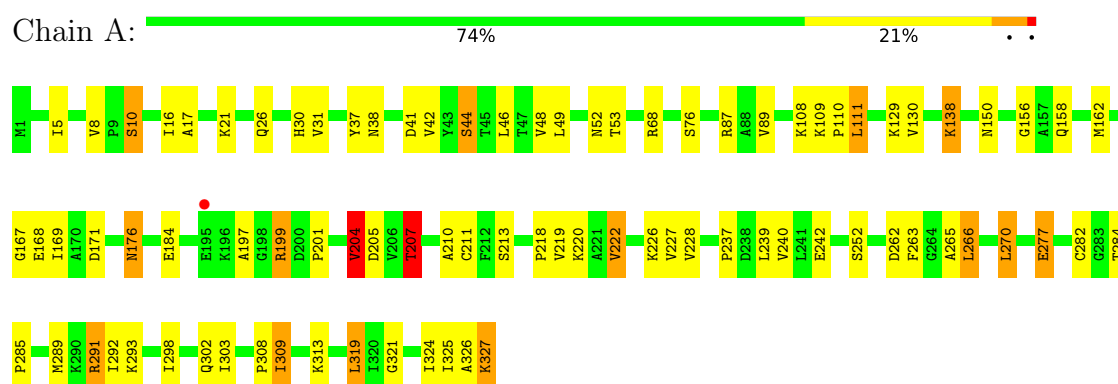
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	62	Total 62	O 62	0	0
5	C	64	Total 64	O 64	0	0
5	D	71	Total 71	O 71	0	0

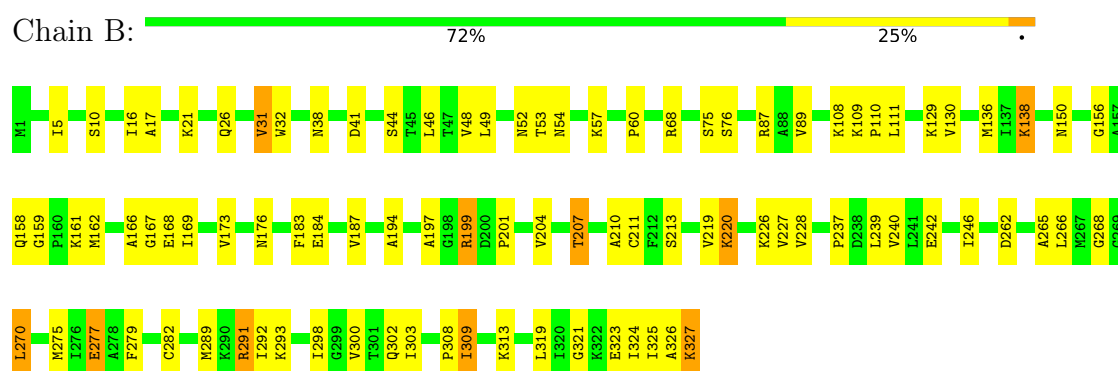
3 Residue-property plots

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.

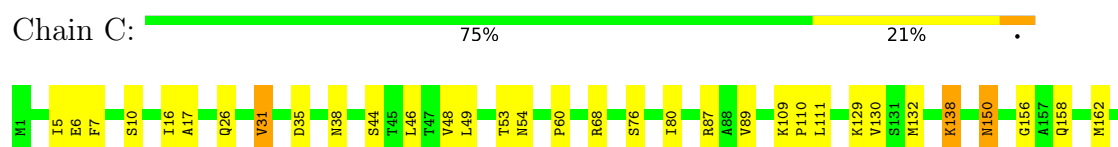
- Molecule 1: Coenzyme F420-dependent N(5),N(10)-methylenetetrahydromethanopterin reductase

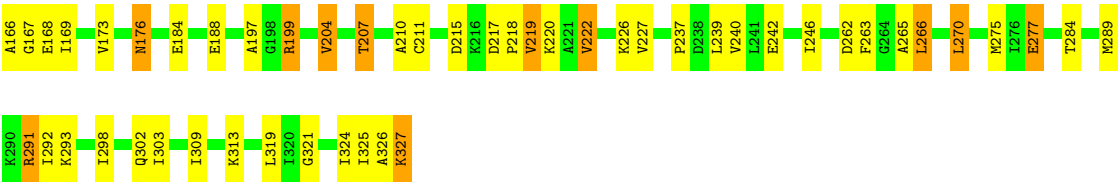


- Molecule 1: Coenzyme F420-dependent N(5),N(10)-methylenetetrahydromethanopterin reductase

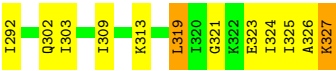


- Molecule 1: Coenzyme F420-dependent N(5),N(10)-methylenetetrahydromethanopterin reductase





• Molecule 1: Coenzyme F420-dependent N(5),N(10)-methylenetetrahydromethanopterin reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.81Å 83.41Å 99.17Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	19.95 – 2.61 19.95 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.95-2.61) 98.6 (19.95-2.61)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.222 0.184 , 0.222	Depositor DCC
R_{free} test set	2016 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l 0.016 for k,h,-l 0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10154	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: 1PG, F42, CL

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	0.66	0/2464	1.04	16/3329 (0.5%)
1	B	0.67	0/2464	1.04	14/3329 (0.4%)
1	C	0.67	0/2464	1.03	15/3329 (0.5%)
1	D	0.68	0/2464	1.07	14/3329 (0.4%)
All	All	0.67	0/9856	1.05	59/13316 (0.4%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	CYS	N-CA-C	-7.43	97.89	109.25
1	B	211	CYS	N-CA-C	-7.30	98.08	109.25
1	B	169	ILE	N-CA-C	7.30	120.64	113.71
1	D	211	CYS	N-CA-C	-7.13	98.34	109.25
1	A	44	SER	N-CA-C	-6.95	103.79	111.36
1	C	44	SER	N-CA-C	-6.89	103.85	111.36
1	D	279	PHE	N-CA-C	6.85	121.30	112.26
1	C	169	ILE	N-CA-C	6.79	120.16	113.71
1	B	313	LYS	N-CA-C	6.71	119.16	111.11
1	C	211	CYS	N-CA-C	-6.67	99.05	109.25
1	A	169	ILE	N-CA-C	6.57	119.95	113.71
1	D	44	SER	N-CA-C	-6.55	104.22	111.36
1	D	313	LYS	N-CA-C	6.46	118.86	111.11
1	D	130	VAL	N-CA-C	6.43	117.55	108.36
1	A	313	LYS	N-CA-C	6.38	118.80	111.02
1	B	44	SER	N-CA-C	-6.36	104.42	111.36
1	C	210	ALA	N-CA-C	6.35	119.91	110.52
1	D	264	GLY	N-CA-C	-6.22	104.80	112.77
1	C	313	LYS	N-CA-C	6.13	118.50	111.02
1	A	129	LYS	N-CA-C	-5.92	99.63	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	VAL	N-CA-C	5.90	116.79	108.36
1	B	184	GLU	N-CA-C	-5.78	105.06	111.36
1	C	129	LYS	N-CA-C	-5.78	99.77	108.96
1	A	184	GLU	N-CA-C	-5.76	105.09	111.36
1	C	10	SER	N-CA-C	-5.75	106.03	113.16
1	A	10	SER	N-CA-C	-5.70	106.09	113.16
1	A	130	VAL	N-CA-C	5.70	116.51	108.36
1	C	130	VAL	N-CA-C	5.67	116.75	108.58
1	C	184	GLU	N-CA-C	-5.61	105.08	111.14
1	B	129	LYS	N-CA-C	-5.58	100.08	108.96
1	C	204	VAL	N-CA-C	5.57	116.25	108.89
1	D	239	LEU	N-CA-C	-5.56	105.12	111.07
1	C	169	ILE	CB-CA-C	-5.56	105.41	110.63
1	C	31	VAL	N-CA-C	-5.53	100.51	108.48
1	A	207	THR	N-CA-C	5.50	118.37	109.40
1	A	204	VAL	N-CA-C	5.48	116.13	108.89
1	A	171	ASP	N-CA-C	-5.45	106.80	113.50
1	A	210	ALA	N-CA-C	5.43	118.84	110.42
1	A	156	GLY	N-CA-C	-5.41	101.53	110.95
1	D	10	SER	N-CA-C	-5.41	106.45	113.16
1	D	169	ILE	N-CA-C	5.38	120.53	109.34
1	D	129	LYS	N-CA-C	-5.38	100.41	108.96
1	D	282	CYS	N-CA-C	5.37	117.42	108.99
1	B	31	VAL	N-CA-C	-5.34	100.80	108.48
1	B	268	GLY	N-CA-C	5.29	120.49	114.67
1	B	210	ALA	N-CA-C	5.27	118.58	110.42
1	C	156	GLY	N-CA-C	-5.26	101.05	111.31
1	C	226	LYS	N-CA-C	5.24	116.67	111.07
1	A	226	LYS	N-CA-C	5.20	117.35	111.11
1	D	274	GLN	N-CA-C	-5.18	105.71	111.36
1	A	30	HIS	CA-C-N	-5.17	115.93	123.06
1	A	30	HIS	C-N-CA	-5.17	115.93	123.06
1	B	156	GLY	N-CA-C	-5.15	101.26	111.31
1	D	210	ALA	N-CA-C	5.15	118.41	110.42
1	D	252	SER	N-CA-C	-5.11	105.41	111.69
1	B	10	SER	N-CA-C	-5.10	106.84	113.16
1	B	226	LYS	N-CA-C	5.06	116.48	111.07
1	B	220	LYS	N-CA-C	-5.05	105.86	111.36
1	C	150	ASN	N-CA-C	5.04	117.46	109.24

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	2421	0	2496	59	0
1	B	2421	0	2496	64	0
1	C	2421	0	2496	55	0
1	D	2421	0	2496	66	0
2	A	53	0	32	5	0
2	B	53	0	32	8	0
2	C	53	0	32	4	0
2	D	53	0	32	9	0
3	B	1	0	0	2	0
3	D	1	0	0	2	0
4	D	17	0	23	4	0
5	A	42	0	0	4	0
5	B	62	0	0	5	0
5	C	64	0	0	4	0
5	D	71	0	0	5	0
All	All	10154	0	10135	239	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 12.

All (239) 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:110:PRO:HD2	2:A:328:F42:H1G1	1.34	1.07
1:A:68:ARG:HG2	1:B:68:ARG:HG2	1.44	0.98
1:C:68:ARG:HG2	1:D:68:ARG:HG2	1.50	0.94
1:C:158:GLN:HE22	1:C:176:ASN:H	1.00	0.93
1:B:325:ILE:C	1:B:327:LYS:H	1.78	0.90
1:A:207:THR:HB	1:A:302:GLN:HB3	1.53	0.89
1:C:207:THR:HB	1:C:302:GLN:HB3	1.52	0.89
1:D:207:THR:HB	1:D:302:GLN:HB3	1.54	0.89
1:D:325:ILE:C	1:D:327:LYS:H	1.80	0.89
1:C:158:GLN:NE2	1:C:176:ASN:H	1.71	0.89
1:A:325:ILE:C	1:A:327:LYS:H	1.81	0.88
1:D:109:LYS:HA	2:D:3328:F42:H4G2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LYS:HD2	1:B:136:MET:HE1	1.54	0.87
1:D:217:ASP:OD1	1:D:219:VAL:HG12	1.75	0.87
1:B:207:THR:HB	1:B:302:GLN:HB3	1.56	0.87
1:C:158:GLN:HE22	1:C:176:ASN:N	1.72	0.86
1:A:111:LEU:HB2	2:A:328:F42:H3G2	1.58	0.85
1:A:292:ILE:HG23	1:A:303:ILE:HD12	1.59	0.85
1:C:325:ILE:C	1:C:327:LYS:H	1.84	0.85
1:D:292:ILE:HG23	1:D:303:ILE:HD12	1.58	0.83
1:B:292:ILE:HG23	1:B:303:ILE:HD12	1.59	0.83
1:C:227:VAL:HG22	5:C:4006:HOH:O	1.80	0.81
1:D:111:LEU:H	2:D:3328:F42:H4G1	1.46	0.81
1:A:158:GLN:NE2	1:A:176:ASN:H	1.79	0.81
1:A:158:GLN:HE22	1:A:176:ASN:H	1.30	0.80
1:A:227:VAL:HG22	5:A:4100:HOH:O	1.82	0.79
1:A:292:ILE:HG23	1:A:303:ILE:CD1	2.15	0.77
1:C:158:GLN:NE2	1:C:176:ASN:HB2	2.01	0.75
1:B:108:LYS:CD	1:B:136:MET:HE1	2.19	0.73
1:A:109:LYS:HA	2:A:328:F42:H4G1	1.71	0.70
1:C:111:LEU:H	2:C:2328:F42:H4G1	1.56	0.70
1:C:292:ILE:HG12	1:C:303:ILE:HD13	1.74	0.70
1:A:277:GLU:O	1:A:291:ARG:NH2	2.25	0.70
1:C:277:GLU:O	1:C:291:ARG:NH2	2.26	0.69
1:D:111:LEU:N	2:D:3328:F42:H4G1	2.08	0.69
1:C:292:ILE:HG23	1:C:303:ILE:CD1	2.24	0.68
1:A:158:GLN:HE22	1:A:176:ASN:N	1.90	0.68
1:D:16:ILE:HG22	1:D:49:LEU:HD21	1.75	0.68
1:C:237:PRO:HG2	1:C:240:VAL:HG23	1.76	0.68
1:D:227:VAL:HG22	5:D:4128:HOH:O	1.92	0.68
1:A:237:PRO:HG2	1:A:240:VAL:HG23	1.75	0.68
1:A:16:ILE:HG22	1:A:49:LEU:HD21	1.76	0.67
1:A:5:ILE:HD11	1:A:309:ILE:HD13	1.77	0.67
1:C:16:ILE:HG22	1:C:49:LEU:HD21	1.77	0.66
1:A:325:ILE:C	1:A:327:LYS:N	2.53	0.66
1:D:325:ILE:C	1:D:327:LYS:N	2.54	0.66
1:D:218:PRO:O	1:D:222:VAL:HG13	1.94	0.66
1:D:292:ILE:HG23	1:D:303:ILE:CD1	2.25	0.65
1:C:292:ILE:HG23	1:C:303:ILE:HD12	1.78	0.65
1:D:39:ASN:HD21	4:D:4003:1PG:H22	1.60	0.65
1:B:292:ILE:HG12	1:B:303:ILE:HD13	1.78	0.65
1:B:292:ILE:HG23	1:B:303:ILE:CD1	2.26	0.64
1:C:138:LYS:NZ	5:C:4041:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:PRO:HG2	1:D:240:VAL:HG23	1.79	0.63
1:D:238:ASP:OD2	1:D:248:VAL:HB	1.98	0.63
1:B:5:ILE:HD11	1:B:309:ILE:HD13	1.82	0.62
1:C:5:ILE:HD11	1:C:309:ILE:HD13	1.80	0.62
1:D:138:LYS:NZ	5:D:4050:HOH:O	2.31	0.62
1:C:109:LYS:HA	2:C:2328:F42:H4G2	1.83	0.61
1:B:26:GLN:HE21	1:B:321:GLY:HA3	1.65	0.61
1:D:292:ILE:HG12	1:D:303:ILE:HD13	1.83	0.61
1:B:46:LEU:HD11	1:B:60:PRO:HD3	1.81	0.61
1:C:138:LYS:NZ	1:C:138:LYS:HB3	2.17	0.60
1:B:194:ALA:HB3	5:B:4189:HOH:O	2.01	0.59
1:B:325:ILE:O	1:B:327:LYS:N	2.35	0.59
1:D:138:LYS:NZ	1:D:138:LYS:HB3	2.18	0.59
5:C:4165:HOH:O	1:D:69:ASN:HB2	2.03	0.59
1:B:277:GLU:O	1:B:291:ARG:NH2	2.35	0.58
1:B:237:PRO:HG2	1:B:240:VAL:HG23	1.86	0.58
1:D:159:GLY:HA3	2:D:3328:F42:O2T	2.04	0.58
1:C:217:ASP:OD1	1:C:219:VAL:HG13	2.04	0.57
1:D:324:ILE:O	1:D:327:LYS:HA	2.04	0.57
2:A:328:F42:O2V	2:A:328:F42:H4G2	2.03	0.57
1:B:325:ILE:C	1:B:327:LYS:N	2.50	0.57
1:A:324:ILE:O	1:A:327:LYS:HA	2.04	0.57
1:C:46:LEU:HD11	1:C:60:PRO:HD3	1.87	0.56
1:A:138:LYS:NZ	1:A:138:LYS:HB3	2.21	0.56
1:B:324:ILE:O	1:B:327:LYS:HA	2.05	0.56
1:A:298:ILE:HG22	1:A:298:ILE:O	2.04	0.56
1:A:292:ILE:HG12	1:A:303:ILE:HD13	1.87	0.56
1:A:325:ILE:O	1:A:327:LYS:N	2.37	0.55
1:D:5:ILE:HD11	1:D:309:ILE:HD13	1.88	0.55
1:A:68:ARG:CG	1:B:68:ARG:HG2	2.30	0.55
2:B:1328:F42:H2'	2:B:1328:F42:H9	1.88	0.55
1:A:41:ASP:OD1	5:A:4173:HOH:O	2.18	0.55
1:B:109:LYS:HA	2:B:1328:F42:H4G2	1.89	0.55
1:D:38:ASN:HD22	1:D:38:ASN:H	1.53	0.55
1:D:53:THR:O	3:D:4002:CL:CL	2.61	0.55
1:D:254:ILE:HD11	1:D:275:MET:HE1	1.89	0.55
1:B:16:ILE:HG22	1:B:49:LEU:HD21	1.89	0.54
1:D:109:LYS:CA	2:D:3328:F42:H4G2	2.32	0.54
1:B:38:ASN:HD22	1:B:38:ASN:H	1.55	0.54
1:B:161:LYS:HB2	2:B:1328:F42:O2U	2.08	0.54
1:C:324:ILE:O	1:C:327:LYS:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ALA:HB1	1:C:270:LEU:HD22	1.91	0.53
1:D:26:GLN:HE21	1:D:321:GLY:HA3	1.72	0.53
1:A:265:ALA:HB1	1:A:270:LEU:HD22	1.89	0.53
1:B:289:MET:HE1	1:B:293:LYS:HD2	1.91	0.53
1:D:325:ILE:O	1:D:327:LYS:N	2.39	0.53
1:C:262:ASP:OD2	1:C:265:ALA:HB2	2.09	0.53
1:D:247:PRO:C	1:D:249:GLU:H	2.15	0.53
1:B:53:THR:O	3:B:4001:CL:CL	2.63	0.53
1:C:325:ILE:C	1:C:327:LYS:N	2.56	0.53
1:A:26:GLN:HE21	1:A:321:GLY:HA3	1.73	0.52
1:A:158:GLN:NE2	1:A:176:ASN:HB2	2.25	0.52
1:B:110:PRO:HD2	2:B:1328:F42:H1G1	1.92	0.52
1:D:35:ASP:OD2	1:D:68:ARG:NH2	2.43	0.52
1:D:68:ARG:HB2	5:D:4007:HOH:O	2.10	0.52
1:A:263:PHE:HA	1:A:266:LEU:HD22	1.92	0.51
1:B:246:ILE:HD13	1:B:275:MET:HG2	1.92	0.51
1:B:32:TRP:HE1	1:B:302:GLN:HE22	1.59	0.51
1:B:300:VAL:O	5:B:4199:HOH:O	2.19	0.51
1:D:168:GLU:HG3	1:D:197:ALA:HB2	1.93	0.51
1:B:262:ASP:OD2	1:B:265:ALA:HB2	2.11	0.50
1:C:110:PRO:HD2	2:C:2328:F42:H4G2	1.92	0.50
1:D:159:GLY:HA3	2:D:3328:F42:C2H	2.42	0.50
1:A:227:VAL:HG23	1:A:228:VAL:N	2.24	0.50
3:B:4001:CL:CL	1:C:53:THR:O	2.66	0.50
2:B:1328:F42:C5H	2:B:1328:F42:O2V	2.59	0.50
1:B:68:ARG:HB2	5:B:4045:HOH:O	2.12	0.50
1:C:325:ILE:O	1:C:327:LYS:N	2.44	0.50
1:B:108:LYS:O	1:B:108:LYS:HG2	2.12	0.49
1:B:54:ASN:ND2	1:C:87:ARG:HH21	2.10	0.49
1:D:138:LYS:HB3	1:D:138:LYS:HZ3	1.78	0.49
1:D:167:GLY:O	1:D:199:ARG:HD2	2.12	0.49
1:A:68:ARG:HB2	5:A:4042:HOH:O	2.13	0.49
1:B:159:GLY:HA3	2:B:1328:F42:O2T	2.11	0.49
1:C:26:GLN:HE21	1:C:321:GLY:HA3	1.78	0.49
1:B:87:ARG:HH21	1:C:54:ASN:ND2	2.10	0.49
1:C:17:ALA:HA	1:C:49:LEU:HD22	1.95	0.48
1:D:205:ASP:O	1:D:207:THR:HG22	2.13	0.48
1:B:17:ALA:HA	1:B:49:LEU:HD22	1.94	0.48
1:C:168:GLU:HG3	1:C:197:ALA:HB2	1.94	0.48
1:B:109:LYS:HG2	2:B:1328:F42:O7G	2.14	0.48
1:B:158:GLN:HB2	2:B:1328:F42:H5'2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLU:HG3	1:B:197:ALA:HB2	1.95	0.48
1:A:41:ASP:OD2	1:A:44:SER:N	2.40	0.48
1:A:168:GLU:HG3	1:A:197:ALA:HB2	1.96	0.47
1:C:111:LEU:CD1	1:C:162:MET:HE2	2.44	0.47
1:B:298:ILE:O	1:B:298:ILE:HG22	2.14	0.47
1:C:166:ALA:HB1	1:C:173:VAL:HG22	1.94	0.47
1:C:218:PRO:HB3	1:C:284:THR:HG23	1.96	0.47
1:C:298:ILE:HG22	1:C:298:ILE:O	2.14	0.47
1:A:21:LYS:HD3	1:A:52:ASN:O	2.14	0.47
1:A:218:PRO:O	1:A:222:VAL:HG13	2.14	0.47
1:B:213:SER:HB3	1:B:282:CYS:HB2	1.97	0.47
1:B:292:ILE:HG12	1:B:303:ILE:CD1	2.44	0.47
1:B:323:GLU:HA	1:B:323:GLU:OE2	2.14	0.47
1:D:217:ASP:OD1	1:D:219:VAL:CG1	2.57	0.47
1:D:227:VAL:HG23	1:D:228:VAL:H	1.79	0.47
1:D:247:PRO:C	1:D:249:GLU:N	2.71	0.47
1:D:38:ASN:H	1:D:38:ASN:ND2	2.12	0.47
1:A:38:ASN:H	1:A:38:ASN:HD22	1.63	0.47
1:C:246:ILE:HD13	1:C:275:MET:HG2	1.97	0.47
1:A:87:ARG:HH21	1:D:54:ASN:ND2	2.12	0.47
1:A:201:PRO:O	1:A:204:VAL:HG13	2.14	0.47
1:D:217:ASP:OD1	1:D:217:ASP:C	2.57	0.46
1:B:57:LYS:NZ	5:B:4216:HOH:O	2.47	0.46
1:C:218:PRO:O	1:C:222:VAL:HG13	2.15	0.46
1:A:111:LEU:HD13	1:A:162:MET:HE2	1.96	0.46
1:A:213:SER:O	1:A:282:CYS:HB2	2.15	0.46
1:B:46:LEU:CD1	1:B:60:PRO:HD3	2.44	0.46
1:C:218:PRO:HD3	1:C:284:THR:HG22	1.98	0.46
1:A:308:PRO:O	1:A:309:ILE:HB	2.16	0.46
1:B:38:ASN:H	1:B:38:ASN:ND2	2.13	0.46
2:C:2328:F42:H2'	2:C:2328:F42:H9	1.97	0.45
1:D:254:ILE:CD1	1:D:275:MET:HE1	2.46	0.45
1:A:298:ILE:O	1:A:298:ILE:CG2	2.64	0.45
1:D:32:TRP:HE1	1:D:302:GLN:HE22	1.65	0.45
1:B:108:LYS:CG	1:B:136:MET:HE1	2.46	0.45
1:C:263:PHE:HA	1:C:266:LEU:HD22	1.98	0.45
1:D:111:LEU:HB2	2:D:3328:F42:C3G	2.47	0.44
1:D:213:SER:HB3	1:D:282:CYS:CB	2.47	0.44
1:A:262:ASP:OD2	1:A:265:ALA:HB2	2.18	0.44
1:D:17:ALA:HA	1:D:49:LEU:HD22	2.00	0.44
1:C:167:GLY:O	1:C:199:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLY:O	1:A:199:ARG:HD2	2.18	0.43
1:D:246:ILE:HA	1:D:247:PRO:HD3	1.89	0.43
1:D:323:GLU:OE2	1:D:323:GLU:HA	2.18	0.43
1:C:289:MET:O	1:C:293:LYS:HG3	2.18	0.43
1:B:167:GLY:O	1:B:199:ARG:HD2	2.18	0.43
1:B:265:ALA:HB1	1:B:270:LEU:HD22	1.98	0.43
1:D:8:VAL:HG21	4:D:4003:1PG:H71	1.99	0.43
1:A:285:PRO:HD2	5:A:4209:HOH:O	2.17	0.43
1:C:46:LEU:CB	1:C:80:ILE:HD13	2.49	0.43
1:C:215:ASP:O	1:C:284:THR:HA	2.18	0.43
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.84	0.43
1:C:237:PRO:HG2	1:C:240:VAL:CG2	2.47	0.43
1:A:41:ASP:HB2	1:B:76:SER:HA	2.00	0.43
1:B:308:PRO:O	1:B:309:ILE:HB	2.19	0.43
1:B:166:ALA:HB1	1:B:173:VAL:HG22	2.00	0.43
1:C:38:ASN:H	1:C:38:ASN:HD22	1.66	0.43
1:A:53:THR:O	3:D:4002:CL:CL	2.74	0.42
1:B:289:MET:CE	1:B:293:LYS:HD2	2.48	0.42
1:A:37:TYR:O	1:B:75:SER:HB2	2.19	0.42
1:A:205:ASP:O	1:A:207:THR:HG22	2.19	0.42
1:D:36:HIS:CE1	4:D:4003:1PG:H51	2.55	0.42
1:D:110:PRO:HD2	2:D:3328:F42:H1G1	2.00	0.42
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.91	0.42
1:D:244:HIS:O	1:D:246:ILE:HG13	2.18	0.42
1:D:148:ALA:HA	5:D:4536:HOH:O	2.19	0.42
1:D:39:ASN:ND2	4:D:4003:1PG:H22	2.31	0.42
1:D:41:ASP:OD2	1:D:44:SER:N	2.47	0.42
1:A:237:PRO:HG2	1:A:240:VAL:CG2	2.47	0.42
1:A:109:LYS:CA	2:A:328:F42:H4G1	2.44	0.42
1:A:218:PRO:HB3	1:A:284:THR:HG23	2.02	0.42
1:D:21:LYS:HD3	1:D:52:ASN:O	2.20	0.42
1:D:291:ARG:NH1	5:D:4510:HOH:O	2.51	0.42
1:B:138:LYS:NZ	1:B:138:LYS:HB3	2.34	0.41
1:C:6:GLU:HG2	1:C:7:PHE:N	2.30	0.41
1:D:33:ILE:HD11	1:D:49:LEU:HD11	2.02	0.41
1:A:17:ALA:HA	1:A:49:LEU:HD22	2.01	0.41
1:A:76:SER:HA	1:B:41:ASP:HB2	2.02	0.41
1:D:122:ARG:HG2	1:D:122:ARG:HH11	1.85	0.41
1:A:42:VAL:O	1:A:46:LEU:HG	2.21	0.41
1:B:246:ILE:HD12	1:B:279:PHE:HE1	1.85	0.41
1:A:8:VAL:C	1:A:10:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LYS:HD3	1:B:52:ASN:O	2.20	0.41
1:B:111:LEU:HD13	1:B:162:MET:HE2	2.03	0.41
1:B:183:PHE:O	1:B:187:VAL:HG23	2.20	0.41
1:C:46:LEU:CD1	1:C:60:PRO:HD3	2.50	0.41
1:C:132:MET:HE2	1:C:132:MET:HB3	1.89	0.41
1:D:227:VAL:HG23	1:D:228:VAL:N	2.35	0.41
1:D:239:LEU:C	1:D:239:LEU:HD23	2.46	0.41
1:B:227:VAL:HG23	1:B:228:VAL:N	2.36	0.41
1:C:138:LYS:HB3	1:C:138:LYS:HZ3	1.85	0.41
1:C:188:GLU:OE1	5:C:4214:HOH:O	2.22	0.41
1:D:111:LEU:CD1	1:D:162:MET:HE2	2.51	0.40
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.82	0.40
1:B:289:MET:O	1:B:293:LYS:HG3	2.21	0.40
1:C:111:LEU:HD13	1:C:162:MET:HE2	2.03	0.40
1:B:201:PRO:HB3	5:B:4189:HOH:O	2.21	0.40
1:C:35:ASP:OD2	1:C:68:ARG:NH2	2.55	0.40
1:C:76:SER:HA	1:D:41:ASP:HB2	2.02	0.40
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.87	0.40
2:D:3328:F42:H2'	2:D:3328:F42:H9	2.03	0.40
1:A:8:VAL:O	1:A:10:SER:N	2.49	0.40
1:A:289:MET:O	1:A:293:LYS:HG3	2.21	0.40
1:D:319:LEU:HD23	1:D:319:LEU:HA	1.95	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	325/327 (99%)	310 (95%)	13 (4%)	2 (1%)	21	39
1	B	325/327 (99%)	308 (95%)	15 (5%)	2 (1%)	21	39
1	C	325/327 (99%)	311 (96%)	13 (4%)	1 (0%)	36	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	325/327 (99%)	307 (94%)	17 (5%)	1 (0%)	36	56
All	All	1300/1308 (99%)	1236 (95%)	58 (4%)	6 (0%)	24	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	326	ALA
1	B	326	ALA
1	C	326	ALA
1	A	326	ALA
1	A	309	ILE
1	B	309	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/251 (100%)	228 (91%)	23 (9%)	8	18
1	B	251/251 (100%)	233 (93%)	18 (7%)	13	28
1	C	251/251 (100%)	231 (92%)	20 (8%)	11	23
1	D	251/251 (100%)	232 (92%)	19 (8%)	12	26
All	All	1004/1004 (100%)	924 (92%)	80 (8%)	11	23

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	48	VAL
1	A	89	VAL
1	A	108	LYS
1	A	111	LEU
1	A	138	LYS
1	A	150	ASN
1	A	176	ASN

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Mol	Chain	Res	Type
1	A	199	ARG
1	A	204	VAL
1	A	207	THR
1	A	219	VAL
1	A	220	LYS
1	A	222	VAL
1	A	239	LEU
1	A	242	GLU
1	A	252	SER
1	A	266	LEU
1	A	270	LEU
1	A	277	GLU
1	A	291	ARG
1	A	319	LEU
1	A	327	LYS
1	B	31	VAL
1	B	48	VAL
1	B	89	VAL
1	B	138	LYS
1	B	150	ASN
1	B	176	ASN
1	B	199	ARG
1	B	204	VAL
1	B	207	THR
1	B	219	VAL
1	B	220	LYS
1	B	239	LEU
1	B	242	GLU
1	B	266	LEU
1	B	270	LEU
1	B	277	GLU
1	B	291	ARG
1	B	327	LYS
1	C	31	VAL
1	C	48	VAL
1	C	89	VAL
1	C	138	LYS
1	C	150	ASN
1	C	176	ASN
1	C	199	ARG
1	C	204	VAL
1	C	207	THR

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Mol	Chain	Res	Type
1	C	219	VAL
1	C	220	LYS
1	C	222	VAL
1	C	239	LEU
1	C	242	GLU
1	C	266	LEU
1	C	270	LEU
1	C	277	GLU
1	C	291	ARG
1	C	319	LEU
1	C	327	LYS
1	D	31	VAL
1	D	38	ASN
1	D	48	VAL
1	D	89	VAL
1	D	138	LYS
1	D	150	ASN
1	D	158	GLN
1	D	176	ASN
1	D	199	ARG
1	D	204	VAL
1	D	207	THR
1	D	222	VAL
1	D	248	VAL
1	D	252	SER
1	D	266	LEU
1	D	270	LEU
1	D	291	ARG
1	D	319	LEU
1	D	327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	GLN
1	A	38	ASN
1	A	54	ASN
1	A	158	GLN
1	B	25	GLN
1	B	26	GLN
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	54	ASN
1	B	158	GLN
1	B	302	GLN
1	C	25	GLN
1	C	26	GLN
1	C	38	ASN
1	C	54	ASN
1	C	158	GLN
1	C	302	GLN
1	D	25	GLN
1	D	26	GLN
1	D	38	ASN
1	D	39	ASN
1	D	54	ASN
1	D	253	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
2	F42	C	2328	-	54,55,55	1.77	14 (25%)	73,79,79	2.05	12 (16%)
4	1PG	D	4003	-	16,16,16	1.61	3 (18%)	15,15,15	0.58	0
2	F42	B	1328	-	54,55,55	1.96	16 (29%)	73,79,79	1.81	13 (17%)
2	F42	D	3328	-	54,55,55	1.85	8 (14%)	73,79,79	2.53	15 (20%)
2	F42	A	328	-	54,55,55	1.56	9 (16%)	73,79,79	1.57	13 (17%)

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
2	F42	C	2328	-	-	14/53/53/53	0/3/3/3
4	1PG	D	4003	-	-	6/14/14/14	-
2	F42	B	1328	-	-	14/53/53/53	0/3/3/3
2	F42	D	3328	-	-	9/53/53/53	0/3/3/3
2	F42	A	328	-	-	13/53/53/53	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3328	F42	C5A-C9A	5.98	1.51	1.41
2	D	3328	F42	C5-C4A	5.60	1.47	1.35
2	B	1328	F42	C1'-C2'	5.56	1.60	1.52
2	D	3328	F42	C7-C6	4.81	1.46	1.38
2	B	1328	F42	C5A-C9A	4.75	1.49	1.41
2	D	3328	F42	C7-C8	4.41	1.47	1.39
2	B	1328	F42	C5-C4A	4.40	1.44	1.35
2	C	2328	F42	C5-C4A	4.39	1.44	1.35
2	C	2328	F42	C5A-C9A	4.33	1.48	1.41
2	B	1328	F42	C7-C6	4.05	1.45	1.38
2	A	328	F42	C5-C4A	3.95	1.43	1.35
2	A	328	F42	C7-C6	3.87	1.45	1.38
2	D	3328	F42	C2-N1	-3.76	1.28	1.36
2	C	2328	F42	C1'-C2'	3.72	1.57	1.52
2	A	328	F42	C7-C8	3.67	1.45	1.39
2	C	2328	F42	C7-C6	3.67	1.44	1.38
2	B	1328	F42	C9-C9A	3.64	1.45	1.39
2	D	3328	F42	C6-C5A	3.64	1.47	1.41
2	A	328	F42	C5A-C9A	3.60	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1328	F42	C7-C8	3.41	1.45	1.39
2	A	328	F42	C4'-C3'	3.22	1.59	1.53
2	B	1328	F42	C9-C8	3.16	1.43	1.39
2	C	2328	F42	P-O3P	-3.08	1.49	1.59
2	C	2328	F42	P-O5'	-3.08	1.47	1.59
2	B	1328	F42	C5'-C4'	2.97	1.55	1.51
2	C	2328	F42	C9-C9A	2.85	1.44	1.39
2	C	2328	F42	C7-C8	2.84	1.44	1.39
2	B	1328	F42	C6-C5A	2.81	1.45	1.41
2	C	2328	F42	C9-C8	2.74	1.43	1.39
2	D	3328	F42	C9-C9A	2.71	1.44	1.39
2	A	328	F42	P-O3P	-2.70	1.51	1.59
2	A	328	F42	C1'-C2'	2.61	1.56	1.52
2	B	1328	F42	C2'-C3'	-2.60	1.48	1.53
2	B	1328	F42	C10-N10	2.53	1.42	1.37
2	C	2328	F42	P-O1P	-2.50	1.42	1.50
2	B	1328	F42	C1'-N10	2.43	1.53	1.47
2	C	2328	F42	C10-N1	2.42	1.38	1.33
2	B	1328	F42	C4A-C4	2.42	1.49	1.45
4	D	4003	1PG	C3-C2	2.35	1.60	1.49
2	C	2328	F42	C2-N1	-2.33	1.31	1.36
2	A	328	F42	C2-N1	-2.27	1.31	1.36
2	B	1328	F42	P-O2P	-2.27	1.44	1.55
2	A	328	F42	C9-C9A	2.23	1.43	1.39
2	B	1328	F42	C2-N1	-2.22	1.31	1.36
2	B	1328	F42	C10-N1	2.20	1.37	1.33
2	C	2328	F42	C4-N3	2.15	1.42	1.38
4	D	4003	1PG	C7-C6	2.15	1.59	1.49
2	D	3328	F42	P-O2P	-2.09	1.45	1.55
2	C	2328	F42	P-O2P	-2.06	1.45	1.55
4	D	4003	1PG	C5-C4	2.01	1.59	1.49

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3328	F42	C4-C4A-C10	-12.57	110.89	117.48
2	D	3328	F42	C5A-C5-C4A	-10.86	111.44	122.06
2	C	2328	F42	C4-C4A-C10	-8.54	113.00	117.48
2	B	1328	F42	C4-C4A-C10	-7.47	113.57	117.48
2	C	2328	F42	C5A-C5-C4A	-6.63	115.58	122.06
2	C	2328	F42	C4'-C3'-C2'	-5.87	103.79	113.57
2	B	1328	F42	C9A-C9-C8	5.44	126.01	117.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3328	F42	C9A-C9-C8	5.30	125.81	117.95
2	A	328	F42	C7-C8-C9	-5.04	114.66	120.19
2	A	328	F42	C9A-C9-C8	4.99	125.35	117.95
2	D	3328	F42	O8M-C8-C7	4.28	131.91	120.00
2	B	1328	F42	C10-N1-C2	4.19	125.92	116.85
2	C	2328	F42	C1'-C2'-C3'	4.16	120.94	109.66
2	C	2328	F42	C10-N1-C2	4.11	125.75	116.85
2	C	2328	F42	C7-C8-C9	-4.11	115.68	120.19
2	D	3328	F42	C7-C8-C9	-3.98	115.83	120.19
2	B	1328	F42	C5A-C5-C4A	-3.84	118.31	122.06
2	B	1328	F42	C7-C8-C9	-3.80	116.02	120.19
2	A	328	F42	C4-C4A-C10	-3.77	115.50	117.48
2	C	2328	F42	O2-C2-N3	3.68	125.63	118.58
2	D	3328	F42	C4-N3-C2	-3.50	119.43	125.64
2	B	1328	F42	C1'-C2'-C3'	3.46	119.03	109.66
2	D	3328	F42	C6-C5A-C9A	-3.44	114.02	118.63
2	A	328	F42	C10-N1-C2	3.21	123.79	116.85
2	D	3328	F42	C4A-C4-N3	3.11	119.89	114.45
2	B	1328	F42	O4-C4-N3	-3.07	114.34	120.11
2	D	3328	F42	C10-N1-C2	3.05	123.45	116.85
2	D	3328	F42	C1'-C2'-C3'	3.01	117.82	109.66
2	B	1328	F42	C9-C9A-C5A	-3.01	116.52	119.81
2	A	328	F42	O8M-C8-C7	2.96	128.26	120.00
2	D	3328	F42	O8M-C8-C9	-2.92	112.22	119.85
2	D	3328	F42	O2'-C2'-C3'	2.82	115.86	109.25
2	C	2328	F42	C9A-C5A-C5	2.77	121.59	119.18
2	A	328	F42	C5A-C5-C4A	-2.73	119.40	122.06
2	D	3328	F42	C5-C4A-C4	2.63	124.99	119.30
2	A	328	F42	C4A-C4-N3	2.59	118.98	114.45
2	A	328	F42	C6-C7-C8	2.58	122.61	119.88
2	B	1328	F42	C4A-C4-N3	2.57	118.95	114.45
2	A	328	F42	O2'-C2'-C3'	2.48	115.04	109.25
2	D	3328	F42	O2-C2-N1	-2.45	117.73	121.80
2	A	328	F42	O3'-C3'-C4'	2.35	114.28	108.93
2	C	2328	F42	C9A-C9-C8	2.34	121.43	117.95
2	A	328	F42	O4-C4-C4A	-2.27	120.97	125.98
2	C	2328	F42	C6-C5A-C9A	-2.25	115.61	118.63
2	B	1328	F42	C9-C9A-N10	2.24	124.87	121.85
2	D	3328	F42	O4-C4-N3	-2.19	115.99	120.11
2	B	1328	F42	C4'-C3'-C2'	-2.17	109.97	113.57
2	B	1328	F42	O2-C2-N3	2.07	122.55	118.58
2	C	2328	F42	O2'-C2'-C1'	2.06	118.67	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1328	F42	O2'-C2'-C1'	2.06	118.66	110.20
2	C	2328	F42	O3'-C3'-C2'	2.03	113.53	108.93
2	A	328	F42	O2P-P-O1P	2.02	121.85	112.44
2	A	328	F42	O2-C2-N3	2.01	122.45	118.58

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	328	F42	C5'-O5'-P-O3P
2	B	1328	F42	C4H-C5H-N1G-C1G
2	B	1328	F42	O5H-C5H-N1G-C1G
2	C	2328	F42	O2'-C2'-C3'-O3'
2	C	2328	F42	C5'-O5'-P-O1P
2	C	2328	F42	C4H-C5H-N1G-C1G
2	C	2328	F42	O5H-C5H-N1G-C1G
2	C	2328	F42	C3G-C1G-N1G-C5H
2	D	3328	F42	C5'-O5'-P-O1P
2	D	3328	F42	C5'-O5'-P-O3P
2	D	3328	F42	C4H-C5H-N1G-C1G
2	D	3328	F42	O5H-C5H-N1G-C1G
2	D	3328	F42	C3G-C1G-N1G-C5H
2	B	1328	F42	C2G-C1G-N1G-C5H
2	B	1328	F42	N1H-C1H-C3H-C4H
4	D	4003	1PG	C3-C2-O1-C1
2	A	328	F42	C4H-C5H-N1G-C1G
2	C	2328	F42	O2'-C2'-C3'-C4'
2	A	328	F42	C1H-C3H-C4H-C5H
2	B	1328	F42	C2H-C1H-C3H-C4H
2	B	1328	F42	C2G-C1G-C3G-C4G
4	D	4003	1PG	O5-C10-C11-O6
2	B	1328	F42	O2'-C2'-C3'-C4'
2	C	2328	F42	N1G-C1G-C2G-O2W
4	D	4003	1PG	O1-C2-C3-O2
4	D	4003	1PG	O2-C4-C5-O3
2	A	328	F42	O3P-C1I-C3I-O3I
2	C	2328	F42	O3P-C1I-C3I-O3I
2	A	328	F42	C3G-C1G-C2G-O2W
2	B	1328	F42	O2'-C2'-C3'-O3'
2	C	2328	F42	C1G-C3G-C4G-C5G
2	C	2328	F42	C2I-C1I-C3I-O3I
2	D	3328	F42	N1G-C1G-C2G-O2V

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Mol	Chain	Res	Type	Atoms
4	D	4003	1PG	C11-C10-O5-C9
2	A	328	F42	C3G-C1G-C2G-O2V
2	C	2328	F42	C3H-C4H-C5H-O5H
2	A	328	F42	C5'-O5'-P-O1P
2	B	1328	F42	C5'-O5'-P-O1P
2	B	1328	F42	C3G-C1G-C2G-O2W
2	B	1328	F42	C3G-C1G-C2G-O2V
2	D	3328	F42	C3G-C4G-C5G-O7G
2	B	1328	F42	C3G-C4G-C5G-O6G
4	D	4003	1PG	C9-C8-O4-C7
2	B	1328	F42	C4'-C5'-O5'-P
2	B	1328	F42	C3G-C4G-C5G-O7G
2	C	2328	F42	C3G-C4G-C5G-O7G
2	A	328	F42	O2'-C2'-C3'-C4'
2	C	2328	F42	C3G-C4G-C5G-O6G
2	D	3328	F42	C3G-C4G-C5G-O6G
2	D	3328	F42	N1G-C1G-C2G-O2W
2	C	2328	F42	C3H-C4H-C5H-N1G
2	A	328	F42	C2I-C1I-C3I-O3I
2	A	328	F42	N1G-C1G-C2G-O2W
2	A	328	F42	C3G-C4G-C5G-O7G
2	A	328	F42	C3G-C4G-C5G-O6G
2	A	328	F42	C3G-C1G-N1G-C5H

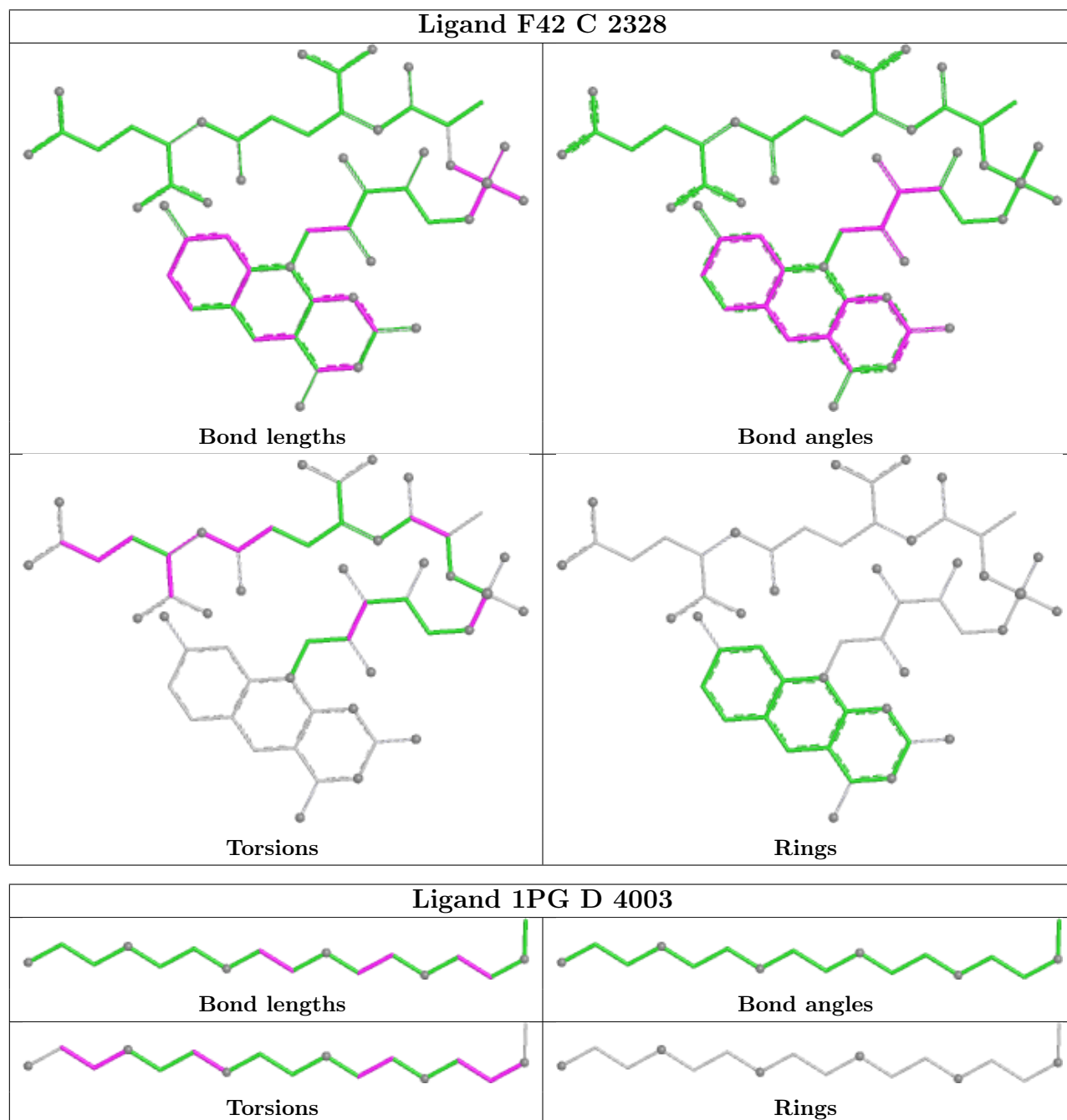
There are no ring outliers.

5 monomers are involved in 30 short contacts:

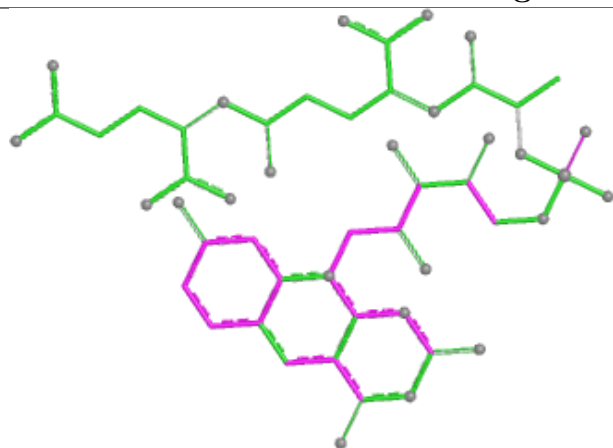
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2328	F42	4	0
4	D	4003	1PG	4	0
2	B	1328	F42	8	0
2	D	3328	F42	9	0
2	A	328	F42	5	0

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

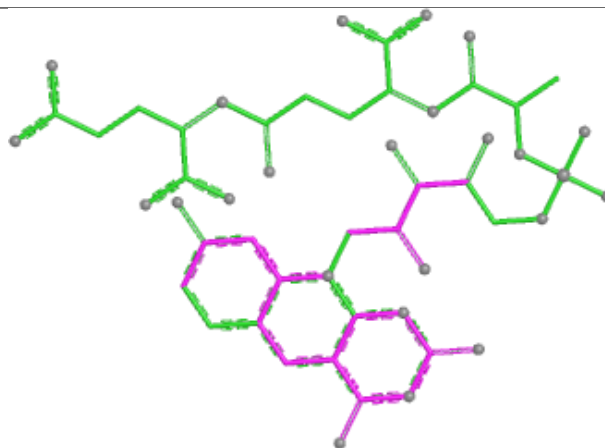
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



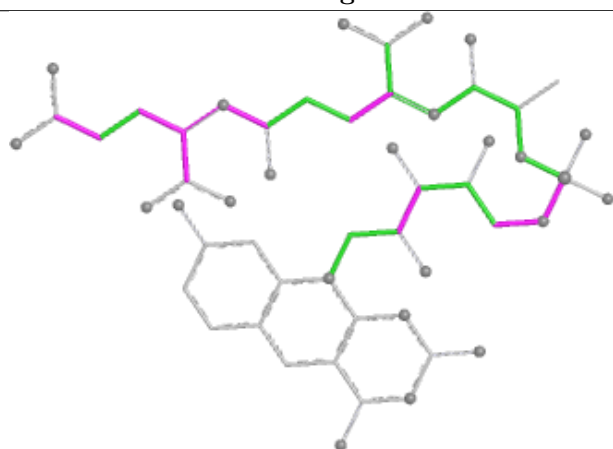
Ligand F42 B 1328



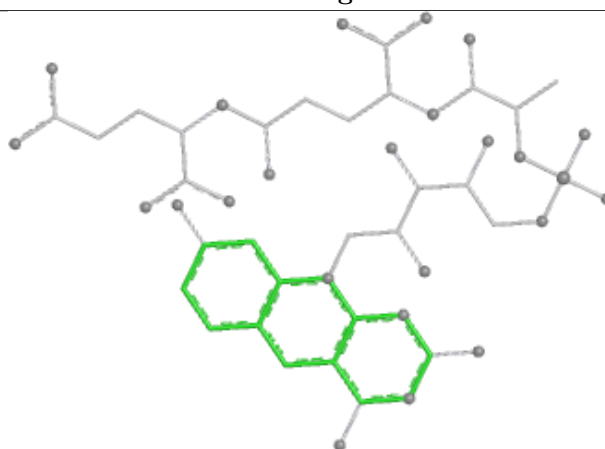
Bond lengths



Bond angles

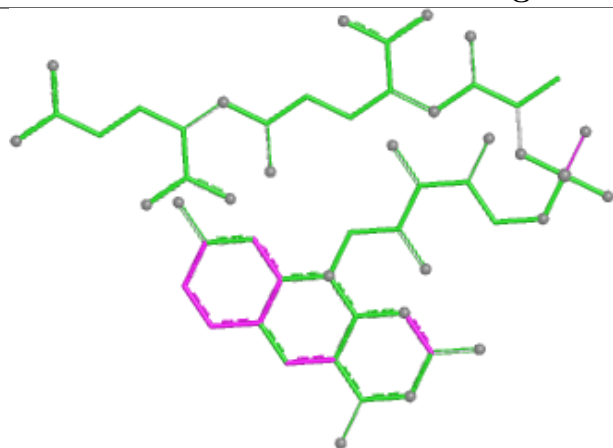


Torsions

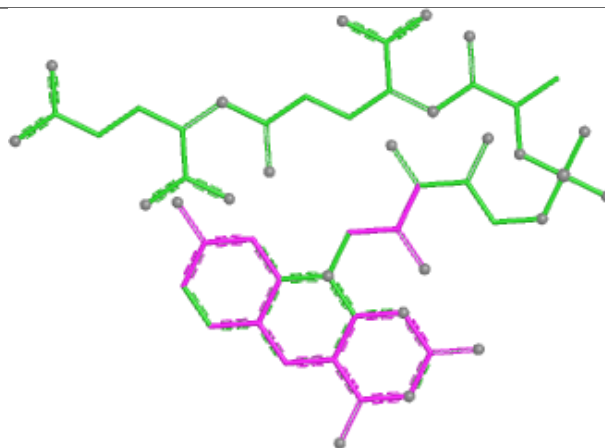


Rings

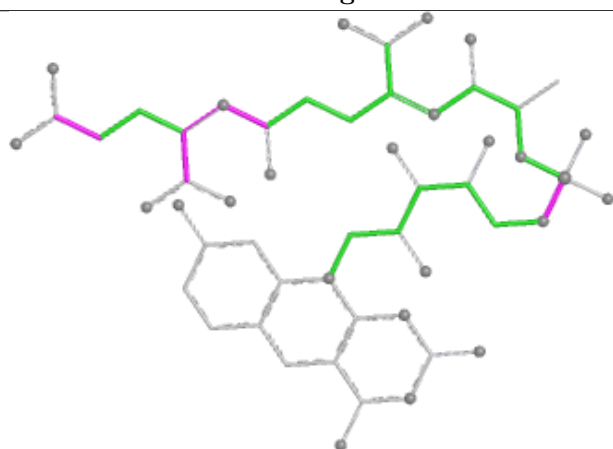
Ligand F42 D 3328



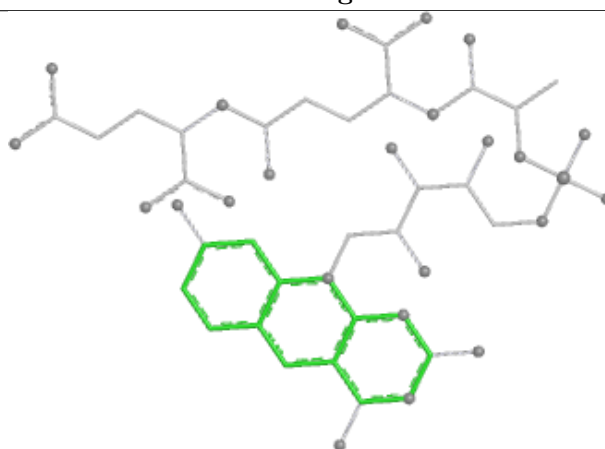
Bond lengths



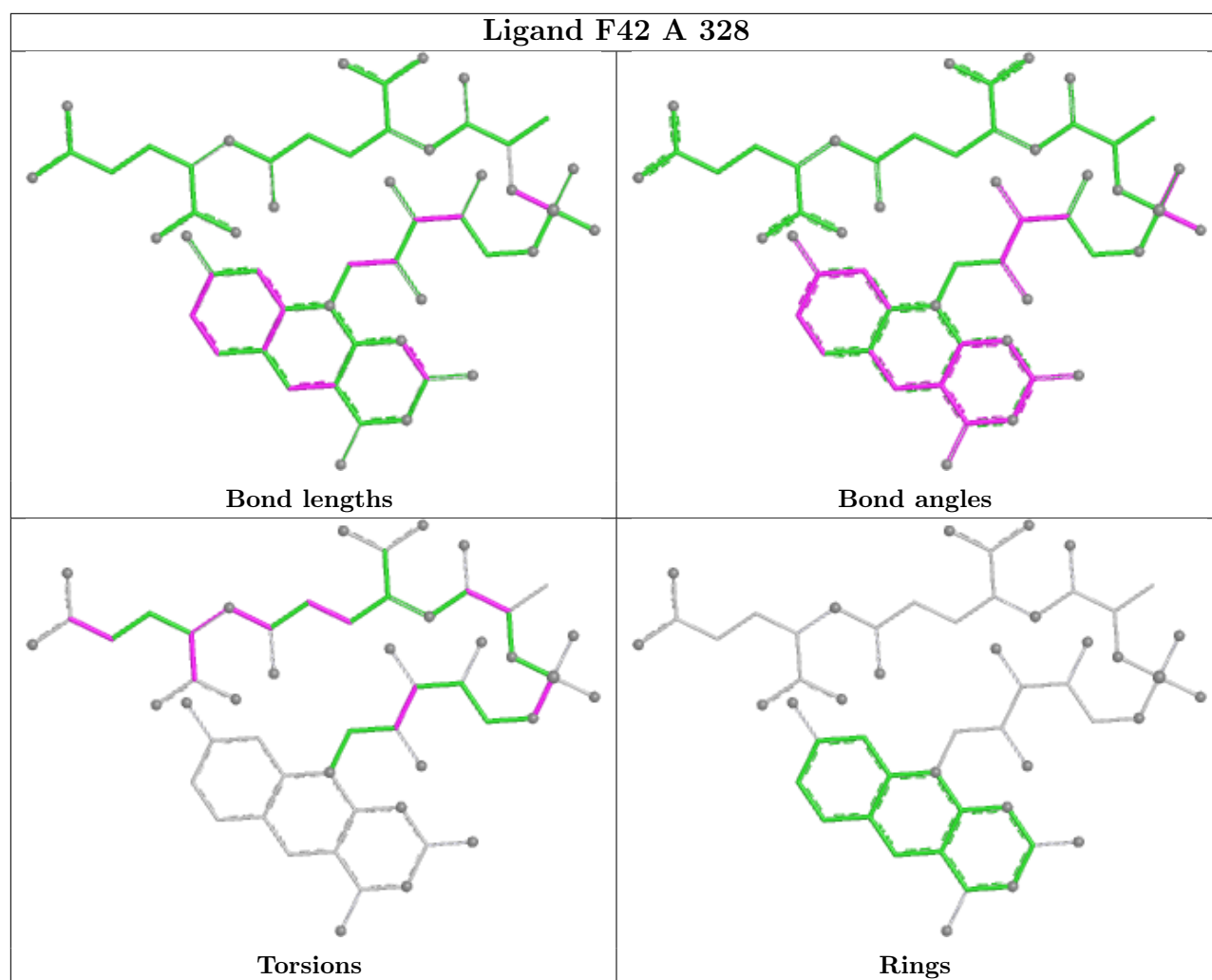
Bond angles



Torsions



Rings



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	327/327 (100%)	-0.36	1 (0%) 90 88	10, 27, 56, 72	0
1	B	327/327 (100%)	-0.51	0 100 100	10, 24, 54, 69	0
1	C	327/327 (100%)	-0.51	0 100 100	9, 25, 54, 69	0
1	D	327/327 (100%)	-0.44	0 100 100	8, 26, 53, 74	0
All	All	1308/1308 (100%)	-0.45	1 (0%) 92 91	8, 26, 55, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLU	2.1

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(Å ²)	Q<0.9
4	1PG	D	4003	17/17	0.84	0.15	47,53,58,59	0

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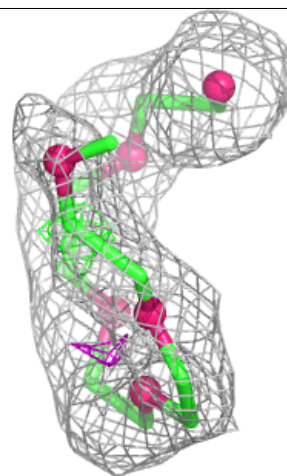
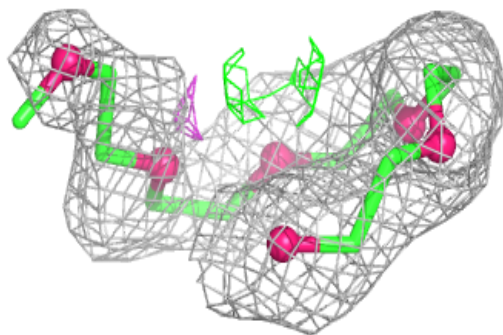
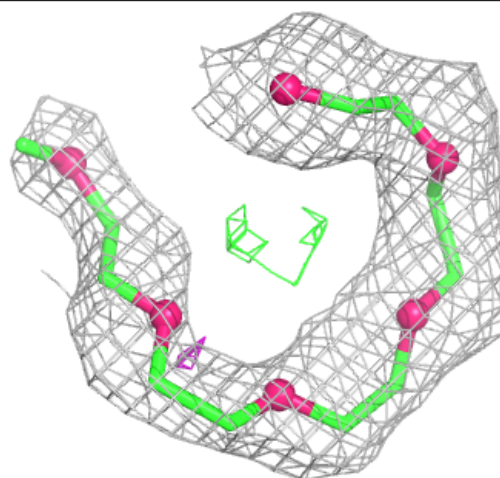
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	F42	B	1328	53/53	0.89	0.11	37,50,84,90	0
3	CL	B	4001	1/1	0.92	0.06	30,30,30,30	0
2	F42	C	2328	53/53	0.92	0.10	29,47,72,74	0
2	F42	A	328	53/53	0.93	0.09	21,38,63,69	0
3	CL	D	4002	1/1	0.93	0.05	25,25,25,25	0
2	F42	D	3328	53/53	0.93	0.09	16,34,75,79	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.

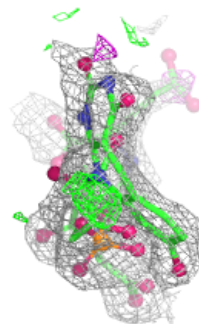
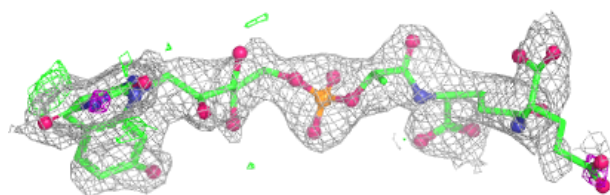
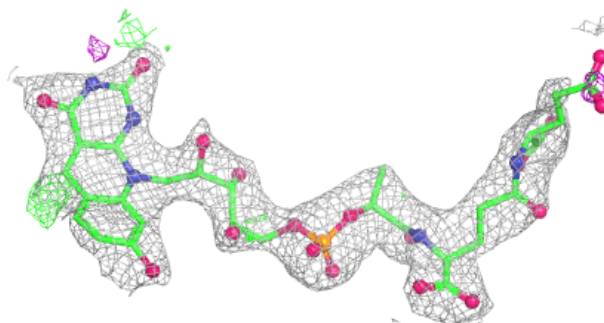
Electron density around 1PG D 4003:

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

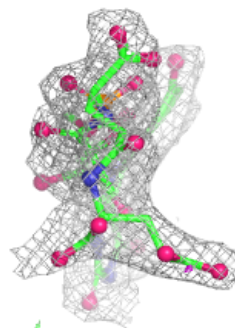
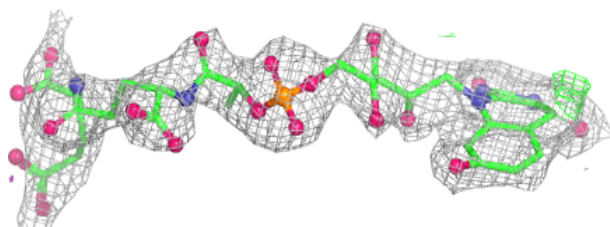
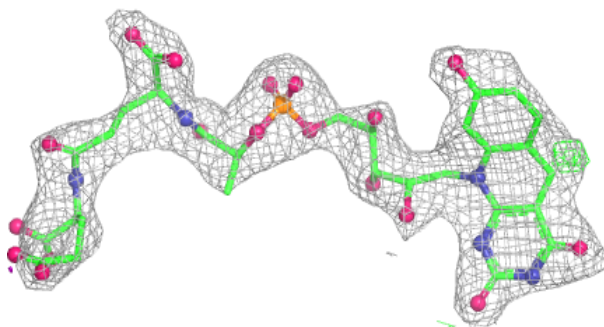


Electron density around F42 B 1328:

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

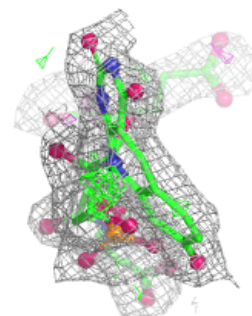
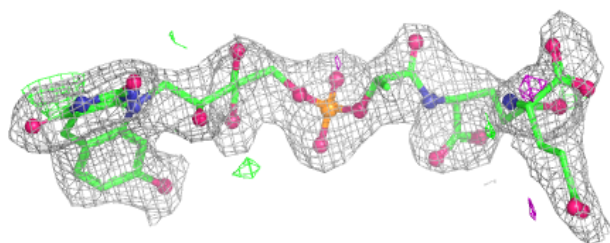
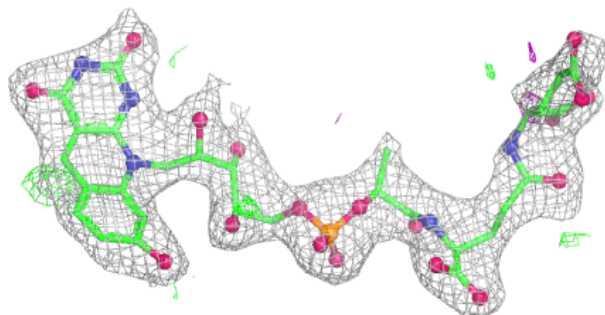
**Electron density around F42 C 2328:**

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

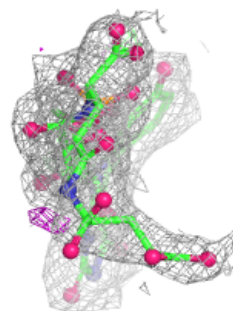
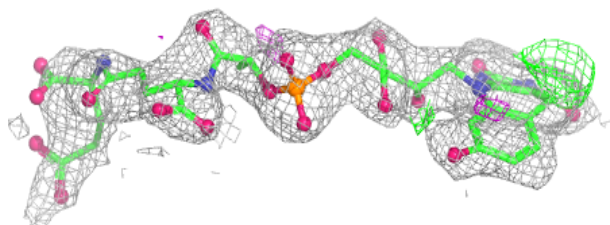
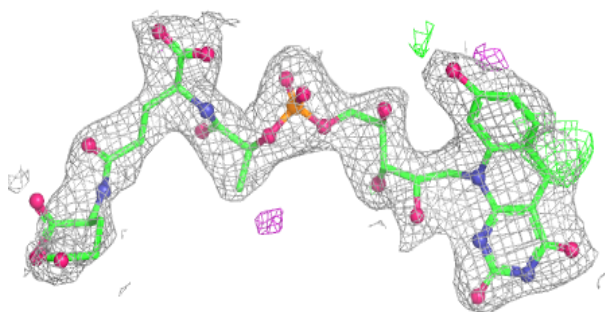


Electron density around F42 A 328:

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

**Electron density around F42 D 3328:**

$2mF_o-DF_c$ (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.