Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 02:16 pm BST

PDB ID	:	5N28 / pdb_00005n28
Title	:	METHYL-COENZYME M REDUCTASE III FROM METHANOTORRIS FORMICICUS MONOCLINIC FORM
Authors	:	Wagner, T.; Wegner, C.E.; Ermler, U.; Shima, S.
Deposited on	:	2017-02-07
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

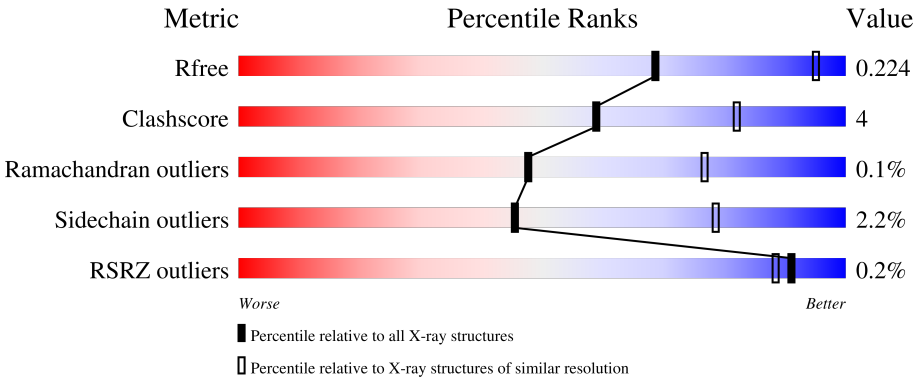
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	552	85% 14%
1	D	552	% 86% 13%
2	B	444	91% 8%
2	E	444	90% 9%
3	C	260	87% 12%

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Mol	Chain	Length	Quality of chain
3	F	260	

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
4	COM	A	601	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19579 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 Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4277	2721	718	816	22			
1	D	547	Total	C	N	O	S	0	0	0
			4268	2716	717	813	22			

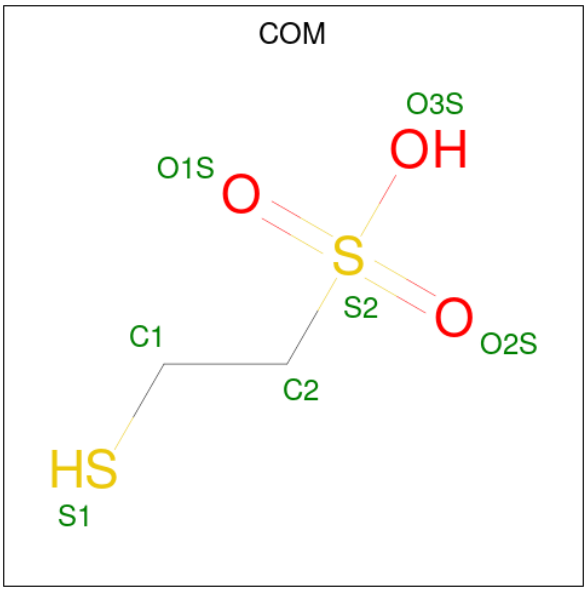
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	443	Total	C	N	O	S	0	0	0
			3324	2123	551	630	20			
2	E	443	Total	C	N	O	S	0	0	0
			3324	2123	551	630	20			

- Molecule 3 is a protein called Methyl-coenzyme M reductase, gamma subunit.

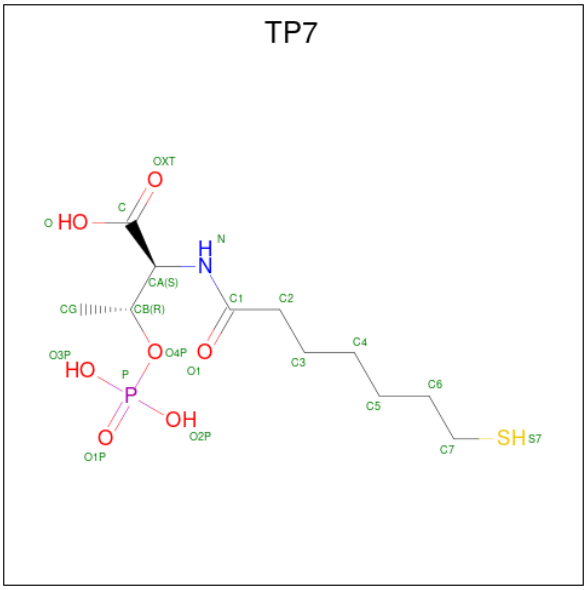
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	0	0
			2113	1331	376	396	10			
3	F	252	Total	C	N	O	S	0	0	0
			2064	1301	369	384	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



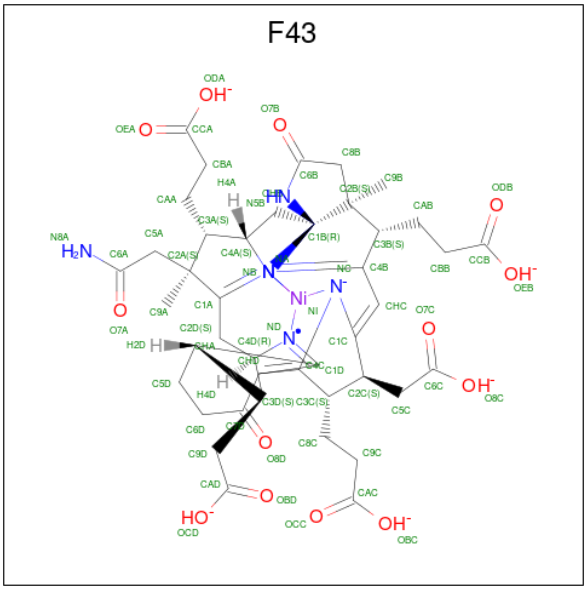
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 7 2 3 2	0	0
4	D	1	Total C O S 7 2 3 2	0	0

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 21 11 1 7 1 1	0	0
5	A	1	Total C N O P S 21 11 1 7 1 1	0	0

- Molecule 6 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N Ni O 62 42 6 1 13	0	0
6	D	1	Total C N Ni O 62 42 6 1 13	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is water.

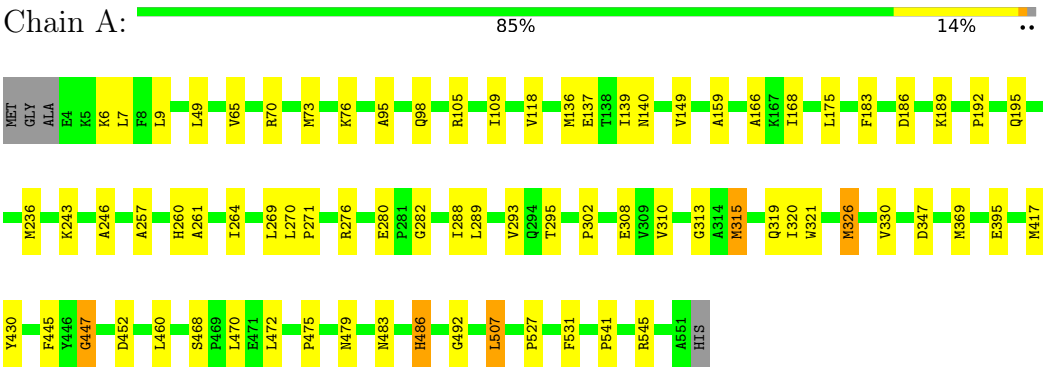
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	9	Total O 9 9	0	0
8	B	9	Total O 9 9	0	0
8	C	3	Total O 3 3	0	0
8	D	5	Total O 5 5	0	0
8	E	2	Total O 2 2	0	0

3 Residue-property plots (i)

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.

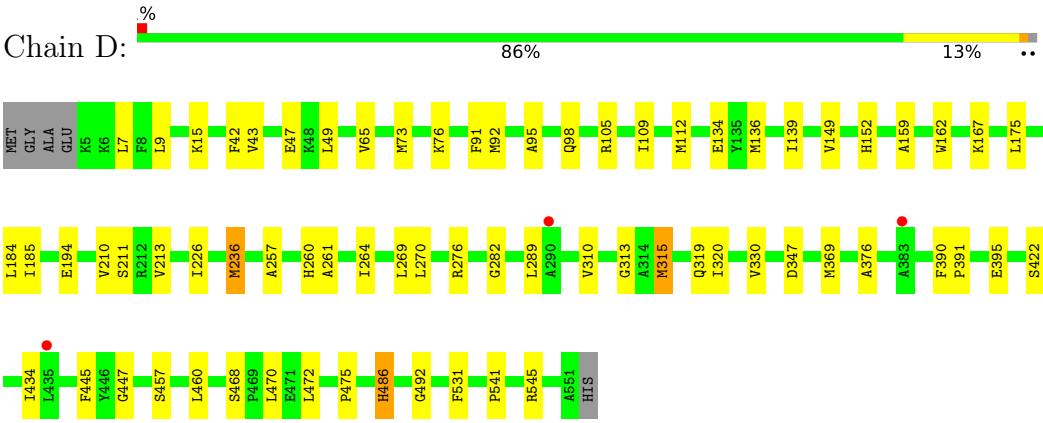
• Molecule 1: Methyl-coenzyme M reductase subunit alpha

Chain A:



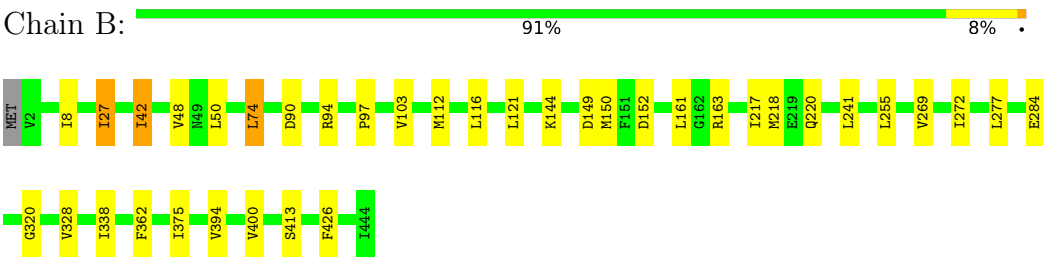
• Molecule 1: Methyl-coenzyme M reductase subunit alpha

Chain D:



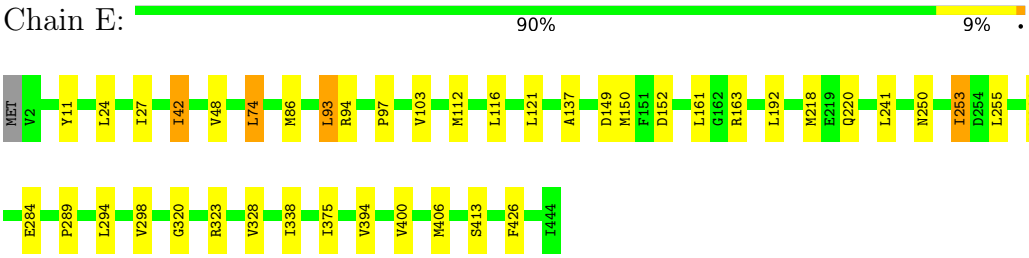
• Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain B:



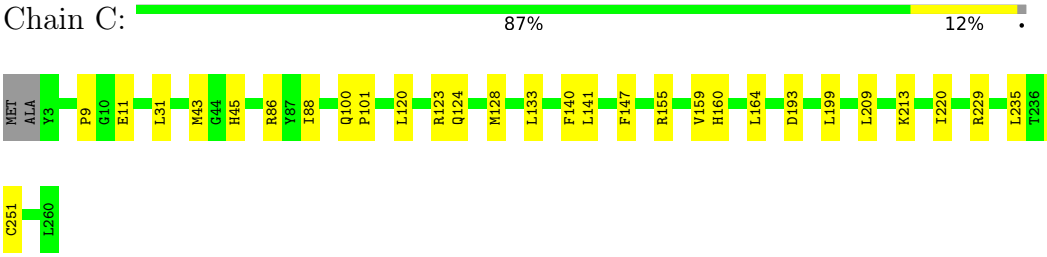
• Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain E:



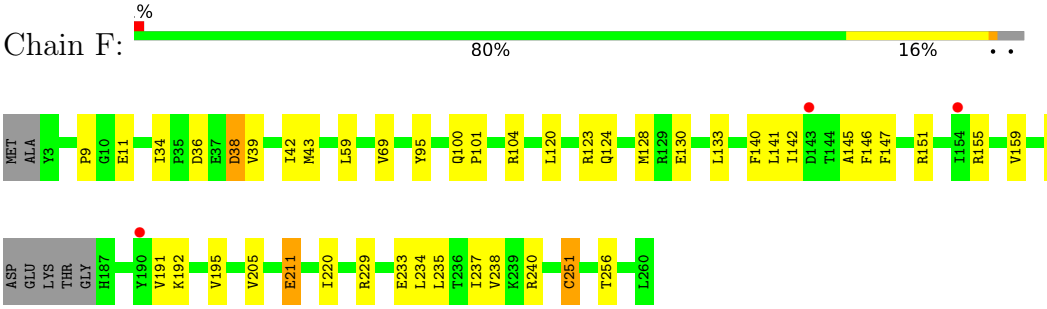
• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain C:



• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.68Å 81.16Å 154.95Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	48.43 – 2.80 48.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.43-2.80) 99.9 (48.43-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.193 , 0.204 0.209 , 0.224	Depositor DCC
R_{free} test set	3016 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19579	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COM, TRX, MHS, GL3, AGM, MGN, F43, K, TP7

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	0.73	1/4319 (0.0%)	1.32	5/5844 (0.1%)
1	D	0.73	1/4310 (0.0%)	1.33	5/5832 (0.1%)
2	B	0.76	0/3382	1.38	5/4590 (0.1%)
2	E	0.76	1/3382 (0.0%)	1.37	5/4590 (0.1%)
3	C	0.73	0/2161	1.31	0/2919
3	F	0.78	1/2110 (0.0%)	1.35	7/2849 (0.2%)
All	All	0.75	4/19664 (0.0%)	1.34	27/26624 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	43	MET	SD-CE	-8.96	1.57	1.79
1	A	326	MET	SD-CE	-7.86	1.59	1.79
1	D	236	MET	SD-CE	-5.42	1.66	1.79
2	E	253	ILE	CG1-CD1	-5.41	1.30	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	298	VAL	N-CA-C	-6.46	105.44	111.45
2	E	298	VAL	N-CA-C	-6.44	105.46	111.45
2	E	149	ASP	CA-C-N	6.02	128.66	120.54
2	E	149	ASP	C-N-CA	6.02	128.66	120.54
3	F	130	GLU	CA-C-N	5.84	128.03	120.44
3	F	130	GLU	C-N-CA	5.84	128.03	120.44
2	B	149	ASP	CA-C-N	5.62	128.13	120.54
2	B	149	ASP	C-N-CA	5.62	128.13	120.54
3	F	38	ASP	CA-C-N	5.58	127.59	120.56
3	F	38	ASP	C-N-CA	5.58	127.59	120.56
1	A	271	PRO	CA-C-N	5.48	127.88	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	PRO	C-N-CA	5.48	127.88	120.38
3	F	145	ALA	CA-C-N	5.42	127.54	120.28
3	F	145	ALA	C-N-CA	5.42	127.54	120.28
1	D	486	HIS	CA-C-N	5.31	127.70	120.54
1	D	486	HIS	C-N-CA	5.31	127.70	120.54
1	A	486	HIS	CA-C-N	5.28	127.66	120.54
1	A	486	HIS	C-N-CA	5.28	127.66	120.54
1	D	65	VAL	N-CA-C	5.25	113.14	108.63
2	B	277	LEU	CA-C-N	5.20	127.25	120.28
2	B	277	LEU	C-N-CA	5.20	127.25	120.28
2	E	277	LEU	CA-C-N	5.20	127.24	120.28
2	E	277	LEU	C-N-CA	5.20	127.24	120.28
1	A	479	ASN	CA-CB-CG	5.14	117.74	112.60
3	F	147	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	194	GLU	CB-CG-CD	5.11	121.28	112.60
1	D	42	PHE	CA-CB-CG	5.09	118.89	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4277	0	4141	61	0
1	D	4268	0	4135	45	0
2	B	3324	0	3372	19	0
2	E	3324	0	3372	24	0
3	C	2113	0	2073	18	0
3	F	2064	0	2030	30	0
4	A	7	0	6	1	0
4	D	7	0	6	1	0
5	A	42	0	38	1	0
6	A	62	0	43	3	0
6	D	62	0	43	2	0
7	A	1	0	0	0	0
8	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	9	0	0	0	0
8	C	3	0	0	0	0
8	D	5	0	0	0	0
8	E	2	0	0	0	0
All	All	19579	0	19259	171	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 4.

All (171) 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:395:GLU:HG3	3:F:164:LEU:HD22	1.49	0.92
1:A:70:ARG:HH21	1:A:395:GLU:HG2	1.40	0.87
1:A:276:ARG:NH1	1:A:326:MET:CE	2.46	0.79
3:F:151:ARG:NH1	3:F:211:GLU:HG3	1.98	0.78
1:A:6:LYS:HB2	1:A:9:LEU:HD13	1.67	0.75
1:D:213:VAL:HG21	1:D:226:ILE:HD12	1.71	0.73
2:E:86:MET:HG3	2:E:103:VAL:HG12	1.70	0.72
3:F:104:ARG:HG2	3:F:146:PHE:HE1	1.54	0.72
3:F:104:ARG:HG2	3:F:146:PHE:CE1	2.28	0.69
1:A:70:ARG:HH11	1:D:152:HIS:HD2	1.40	0.68
1:A:276:ARG:NH1	1:A:326:MET:HE1	2.09	0.68
2:B:217:ILE:HG22	2:B:218:MET:HE2	1.76	0.67
1:A:70:ARG:NH1	1:D:152:HIS:CD2	2.64	0.66
1:A:70:ARG:NH2	1:A:395:GLU:HG2	2.09	0.65
1:A:70:ARG:HD2	3:C:160:HIS:NE2	2.13	0.64
1:A:295:THR:HG21	1:A:308:GLU:HB2	1.79	0.63
1:D:213:VAL:CG2	1:D:226:ILE:HD12	2.28	0.63
3:F:151:ARG:HH11	3:F:211:GLU:HG3	1.63	0.63
2:B:90:ASP:HB2	2:B:103:VAL:HG21	1.81	0.63
1:A:276:ARG:NH1	1:A:326:MET:HE2	2.15	0.61
2:E:328:VAL:HG21	2:E:394:VAL:HA	1.83	0.60
2:B:328:VAL:HG21	2:B:394:VAL:HA	1.84	0.60
3:F:251:CYS:HB3	3:F:256:THR:HG21	1.82	0.60
6:A:604:F43:H9A1	1:D:330:VAL:HB	1.84	0.60
3:F:34:ILE:CD1	3:F:205:VAL:HA	2.31	0.60
3:F:34:ILE:HD11	3:F:205:VAL:HA	1.84	0.60
2:E:323:ARG:HG3	3:F:59:LEU:HD11	1.84	0.60
3:F:140:PHE:HD1	3:F:141:LEU:HD23	1.66	0.59
1:A:330:VAL:HB	6:D:601:F43:H9A1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:LEU:HD21	2:E:152:ASP:HB3	1.83	0.59
1:A:70:ARG:HH11	1:D:152:HIS:CD2	2.19	0.59
2:B:74:LEU:HD21	2:B:152:ASP:HB3	1.84	0.59
3:C:31:LEU:HD13	3:C:209:LEU:HD11	1.84	0.59
2:E:253:ILE:HD12	3:F:69:VAL:HG22	1.84	0.58
2:E:255:LEU:HD11	2:E:272:ILE:HD13	1.86	0.58
1:D:167:LYS:HE2	1:D:182:LYS:O	2.03	0.57
1:A:70:ARG:HH12	1:A:73:MET:HG3	1.70	0.56
2:B:255:LEU:HD11	2:B:272:ILE:HD13	1.88	0.56
1:A:257:ALA:HA	1:A:261:ALA:HB3	1.86	0.55
1:A:288:ILE:HG13	1:A:507:LEU:HD12	1.87	0.55
3:C:141:LEU:O	3:C:147:PHE:HB2	2.07	0.55
1:A:276:ARG:HH12	1:A:326:MET:HE2	1.72	0.54
3:F:9:PRO:HG3	3:F:237:ILE:HG21	1.89	0.54
2:E:24:LEU:O	2:E:27:ILE:HG13	2.07	0.54
1:A:472:LEU:HD22	2:E:163:ARG:HG3	1.90	0.54
1:A:49:LEU:HD11	1:D:159:ALA:HA	1.89	0.54
3:C:120:LEU:HD22	3:C:123:ARG:HE	1.73	0.53
1:A:321:TRP:CH2	1:A:326:MET:HE3	2.43	0.53
1:D:9:LEU:HD21	1:D:390:PHE:HE1	1.72	0.53
1:D:109:ILE:HG12	1:D:210:VAL:HG22	1.90	0.53
3:F:191:VAL:HG23	3:F:192:LYS:HG3	1.90	0.53
1:A:276:ARG:HH12	1:A:326:MET:CE	2.19	0.53
1:A:109:ILE:HG12	1:A:210:VAL:HG22	1.89	0.53
3:F:120:LEU:HD22	3:F:123:ARG:HE	1.74	0.52
1:D:91:PHE:CE1	1:D:92:MET:HE3	2.44	0.52
2:B:163:ARG:HG3	1:D:472:LEU:HD22	1.91	0.52
1:A:308:GLU:OE2	1:A:527:PRO:HD2	2.10	0.52
1:D:429:TRX:HD1	1:D:430:TYR:CD1	2.44	0.52
2:E:269:VAL:HG11	2:E:338:ILE:HG22	1.91	0.52
2:B:294:LEU:HD11	3:C:240:ARG:HG2	1.91	0.52
2:B:269:VAL:HG11	2:B:338:ILE:HG22	1.91	0.52
1:D:315:MET:HG2	1:D:531:PHE:CZ	2.45	0.51
1:A:445:PHE:HB2	4:A:601:COM:O3S	2.10	0.51
1:A:246:ALA:HB1	6:A:604:F43:H9B1	1.92	0.51
1:A:429:TRX:HD1	1:A:430:TYR:CD1	2.45	0.50
3:C:9:PRO:HG3	3:C:237:ILE:HG21	1.93	0.50
3:C:101:PRO:HA	3:C:124:GLN:HG3	1.93	0.50
3:F:101:PRO:HA	3:F:124:GLN:HG3	1.94	0.50
1:D:95:ALA:HB1	1:D:541:PRO:HG3	1.95	0.49
1:D:429:TRX:HZ2	1:D:486:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:ASP:HB2	2:B:103:VAL:CG2	2.42	0.49
1:A:118:VAL:HG22	2:E:406:MET:HG3	1.94	0.49
2:B:42:ILE:HG13	2:B:426:PHE:HE1	1.78	0.49
1:A:95:ALA:HB1	1:A:541:PRO:HG3	1.94	0.48
2:E:192:LEU:HD22	2:E:218:MET:HE1	1.94	0.48
3:C:43:MET:HB3	3:C:45:HIS:CD2	2.48	0.48
1:D:136:MET:HA	1:D:139:ILE:HG22	1.95	0.48
1:A:136:MET:HA	1:A:139:ILE:HG22	1.96	0.48
2:E:93:LEU:HD11	2:E:137:ALA:HB2	1.96	0.48
2:E:42:ILE:HG13	2:E:426:PHE:HE1	1.78	0.48
1:A:137:GLU:HG3	1:A:183:PHE:CZ	2.48	0.48
1:A:429:TRX:HZ2	1:A:486:HIS:CD2	2.48	0.48
1:A:483:ASN:HA	5:A:603:TP7:S7	2.54	0.48
1:D:391:PRO:HB3	3:F:95:TYR:OH	2.14	0.48
1:A:6:LYS:HB2	1:A:9:LEU:CD1	2.41	0.48
3:C:140:PHE:HD1	3:C:141:LEU:HD23	1.79	0.48
1:D:236:MET:HE2	6:D:601:F43:HBA1	1.95	0.48
2:E:253:ILE:HD12	3:F:69:VAL:CG2	2.44	0.48
1:D:7:LEU:HB2	1:D:347:ASP:HB2	1.96	0.47
1:A:276:ARG:HH11	1:A:326:MET:HE1	1.78	0.47
3:C:100:GLN:HE21	3:C:220:ILE:HB	1.80	0.47
1:A:243:LYS:HB3	3:F:195:VAL:HG11	1.97	0.47
1:A:7:LEU:HB2	1:A:347:ASP:HB2	1.97	0.47
1:A:49:LEU:HD13	1:D:162:TRP:HB3	1.97	0.47
3:C:128:MET:HG2	3:C:133:LEU:HD13	1.97	0.46
3:F:38:ASP:O	3:F:42:ILE:HG12	2.15	0.46
1:D:9:LEU:HD21	1:D:390:PHE:CE1	2.50	0.46
1:D:109:ILE:HB	1:D:264:ILE:HB	1.97	0.46
2:E:289:PRO:HB2	3:F:11:GLU:HG2	1.98	0.46
1:A:136:MET:HE3	1:A:168:ILE:HB	1.98	0.46
1:A:186:ASP:HB3	1:A:189:LYS:HB2	1.98	0.46
1:A:315:MET:HG2	1:A:531:PHE:CZ	2.51	0.46
3:C:88:ILE:HG22	3:C:133:LEU:HD11	1.98	0.45
3:F:100:GLN:HE21	3:F:220:ILE:HB	1.81	0.45
1:A:49:LEU:CD1	1:D:159:ALA:HA	2.45	0.45
2:E:294:LEU:HD11	3:F:240:ARG:HG2	1.97	0.45
3:C:160:HIS:CE1	3:C:164:LEU:HD11	2.51	0.45
1:A:236:MET:HE2	6:A:604:F43:HBA1	1.99	0.45
2:B:94:ARG:HD3	2:B:97:PRO:HA	1.98	0.45
2:B:48:VAL:HG12	2:B:50:LEU:HD12	1.99	0.45
2:B:220:GLN:HG3	2:B:241:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:229:ARG:HA	3:F:235:LEU:HD11	1.99	0.45
1:A:109:ILE:HB	1:A:264:ILE:HB	1.98	0.45
1:D:105:ARG:O	1:D:226:ILE:HG13	2.17	0.45
1:A:289:LEU:HD21	1:A:313:GLY:HA2	1.99	0.44
1:D:7:LEU:HD13	1:D:347:ASP:HA	1.99	0.44
2:B:150:MET:HG2	1:D:460:LEU:HD13	2.00	0.44
3:F:11:GLU:HG3	3:F:233:GLU:HB2	1.98	0.44
1:A:105:ARG:O	1:A:226:ILE:HG13	2.17	0.44
1:D:257:ALA:HA	1:D:261:ALA:HB3	1.98	0.44
2:E:220:GLN:HG3	2:E:241:LEU:HB2	1.98	0.44
1:A:545:ARG:HD3	1:D:98:GLN:OE1	2.18	0.44
2:E:42:ILE:HG13	2:E:426:PHE:CE1	2.53	0.44
1:D:289:LEU:HD21	1:D:313:GLY:HA2	1.99	0.44
2:E:93:LEU:CD1	2:E:137:ALA:HB2	2.48	0.44
1:A:430:TYR:CD1	1:A:452:ASP:HA	2.53	0.43
1:D:315:MET:O	1:D:319:GLN:HB2	2.17	0.43
2:B:42:ILE:HG13	2:B:426:PHE:CE1	2.53	0.43
3:C:229:ARG:HA	3:C:235:LEU:HD11	2.00	0.43
1:A:7:LEU:HD12	1:A:347:ASP:HA	2.01	0.43
1:A:422:SER:HB2	1:A:470:LEU:HB3	2.00	0.43
1:A:447:GL3:HA1	2:B:362:PHE:HB2	2.01	0.43
3:C:86:ARG:HD3	3:C:86:ARG:HA	1.87	0.43
1:D:310:VAL:HG22	1:D:492:GLY:HA3	2.01	0.43
1:A:460:LEU:HD13	2:E:150:MET:HG2	2.00	0.43
2:B:48:VAL:HB	2:B:112:MET:HB3	2.01	0.43
3:F:34:ILE:HD12	3:F:205:VAL:HA	2.01	0.42
1:A:315:MET:O	1:A:319:GLN:HB2	2.19	0.42
1:A:159:ALA:HA	1:D:49:LEU:HD11	2.01	0.42
2:E:94:ARG:HD3	2:E:97:PRO:HA	2.01	0.42
3:F:128:MET:HB3	3:F:133:LEU:HB2	2.01	0.42
1:A:310:VAL:HG22	1:A:492:GLY:HA3	2.01	0.42
1:D:180:ASP:HB3	1:D:182:LYS:HG2	2.01	0.42
1:D:422:SER:HB2	1:D:470:LEU:HB3	2.01	0.42
3:F:36:ASP:O	3:F:39:VAL:HB	2.18	0.42
3:F:155:ARG:HG3	3:F:159:VAL:HG12	2.01	0.42
1:D:43:VAL:O	1:D:47:GLU:HG2	2.20	0.41
1:D:445:PHE:HB2	4:D:602:COM:O2S	2.20	0.41
3:F:39:VAL:HG22	3:F:142:ILE:HD13	2.01	0.41
1:A:293:VAL:HG12	1:A:295:THR:HG22	2.02	0.41
1:D:15:LYS:NZ	1:D:73:MET:HB3	2.35	0.41
1:A:282:GLY:HA2	1:A:475:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PRO:HB2	1:A:417:MET:HE1	2.03	0.41
2:B:320:GLY:HA2	2:B:400:VAL:HG11	2.02	0.41
3:C:155:ARG:HG3	3:C:159:VAL:HG12	2.01	0.41
1:A:98:GLN:OE1	1:D:545:ARG:HD3	2.21	0.41
1:A:270:LEU:HD12	1:A:276:ARG:HB2	2.02	0.41
1:A:140:ASN:HD21	1:A:166:ALA:H	1.69	0.41
2:B:8:ILE:HD11	2:B:27:ILE:HD13	2.03	0.41
1:D:376:ALA:HB3	1:D:431:LEU:HD23	2.02	0.41
1:D:434:ILE:HG22	3:F:238:VAL:HG13	2.02	0.41
1:A:192:PRO:HD2	1:A:195:GLN:OE1	2.20	0.41
1:A:276:ARG:HG2	1:A:280:GLU:HG3	2.03	0.41
3:C:209:LEU:HD22	3:C:213:LYS:HG2	2.03	0.41
1:D:282:GLY:HA2	1:D:475:PRO:HB2	2.03	0.40
1:D:184:LEU:HD12	1:D:185:ILE:N	2.37	0.40
2:E:11:TYR:CG	2:E:250:ASN:HB2	2.55	0.40
2:E:48:VAL:HB	2:E:112:MET:HB3	2.02	0.40
1:D:270:LEU:HD12	1:D:276:ARG:HB2	2.03	0.40
3:C:193:ASP:HB3	3:C:199:LEU:HD21	2.04	0.40
2:E:320:GLY:HA2	2:E:400:VAL:HG11	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	541/552 (98%)	513 (95%)	27 (5%)	1 (0%)	43	72
1	D	540/552 (98%)	515 (95%)	24 (4%)	1 (0%)	43	72
2	B	441/444 (99%)	428 (97%)	13 (3%)	0	100	100
2	E	441/444 (99%)	429 (97%)	12 (3%)	0	100	100
3	C	256/260 (98%)	247 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	248/260 (95%)	240 (97%)	8 (3%)	0	100 100
All	All	2467/2512 (98%)	2372 (96%)	93 (4%)	2 (0%)	48 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER
1	D	468	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	436/438 (100%)	426 (98%)	10 (2%)	44 78
1	D	435/438 (99%)	424 (98%)	11 (2%)	42 76
2	B	350/351 (100%)	340 (97%)	10 (3%)	37 73
2	E	350/351 (100%)	341 (97%)	9 (3%)	40 75
3	C	228/229 (100%)	226 (99%)	2 (1%)	70 89
3	F	223/229 (97%)	220 (99%)	3 (1%)	61 86
All	All	2022/2036 (99%)	1977 (98%)	45 (2%)	45 78

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	76	LYS
1	A	149	VAL
1	A	175	LEU
1	A	211	SER
1	A	269	LEU
1	A	315	MET
1	A	320	ILE
1	A	369	MET

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Mol	Chain	Res	Type
1	A	507	LEU
2	B	27	ILE
2	B	42	ILE
2	B	74	LEU
2	B	116	LEU
2	B	121	LEU
2	B	144	LYS
2	B	161	LEU
2	B	284	GLU
2	B	375	ILE
2	B	413	SER
3	C	11	GLU
3	C	251	CYS
1	D	76	LYS
1	D	112	MET
1	D	134	GLU
1	D	149	VAL
1	D	175	LEU
1	D	211	SER
1	D	269	LEU
1	D	315	MET
1	D	320	ILE
1	D	369	MET
1	D	457	SER
2	E	42	ILE
2	E	74	LEU
2	E	93	LEU
2	E	116	LEU
2	E	121	LEU
2	E	161	LEU
2	E	284	GLU
2	E	375	ILE
2	E	413	SER
3	F	211	GLU
3	F	234	LEU
3	F	251	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	140	ASN

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	319	GLN
1	A	334	GLN
1	A	487	GLN
1	A	495	GLN
1	A	508	ASN
2	B	133	ASN
3	C	124	GLN
1	D	319	GLN
1	D	487	GLN
1	D	495	GLN
1	D	508	ASN
2	E	133	ASN
2	E	262	ASN
3	F	45	HIS
3	F	77	ASN
3	F	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TRX	A	429	1	15,16,17	1.77	2 (13%)	19,22,24	1.70	3 (15%)
1	GL3	D	447	1	2,3,4	2.54	1 (50%)	1,2,4	0.07	0
1	AGM	D	274	1	10,11,12	0.47	0	6,13,15	0.85	0
1	MHS	D	260	1	10,11,12	1.27	1 (10%)	6,14,16	2.89	3 (50%)
1	MGN	A	402	1	6,9,10	0.57	0	5,12,14	0.39	0
1	AGM	A	274	1	10,11,12	0.46	0	6,13,15	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MHS	A	260	1	10,11,12	1.20	0	6,14,16	2.96	2 (33%)
1	MGN	D	402	1	6,9,10	0.60	0	5,12,14	0.31	0
1	TRX	D	429	1	15,16,17	1.74	2 (13%)	19,22,24	1.80	4 (21%)
1	GL3	A	447	1	2,3,4	2.67	1 (50%)	1,2,4	0.04	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
1	TRX	A	429	1	-	0/5/6/8	0/2/2/2
1	GL3	D	447	1	-	1/1/1/2	-
1	AGM	D	274	1	-	2/10/11/13	-
1	MHS	D	260	1	-	0/5/6/8	0/1/1/1
1	MGN	A	402	1	-	0/7/9/12	-
1	AGM	A	274	1	-	2/10/11/13	-
1	MHS	A	260	1	-	0/5/6/8	0/1/1/1
1	MGN	D	402	1	-	0/7/9/12	-
1	TRX	D	429	1	-	0/5/6/8	0/2/2/2
1	GL3	A	447	1	-	1/1/1/2	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	429	TRX	CD2-CE2	5.50	1.48	1.41
1	D	429	TRX	CD2-CE2	5.47	1.48	1.41
1	A	447	GL3	C-S	-3.78	1.67	1.80
1	D	447	GL3	C-S	-3.60	1.68	1.80
1	D	429	TRX	CD2-CG	2.30	1.47	1.44
1	A	429	TRX	CD2-CG	2.23	1.47	1.44
1	D	260	MHS	CD2-NE2	-2.01	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	MHS	ND1-CE1-NE2	-6.32	109.23	112.93
1	D	260	MHS	ND1-CE1-NE2	-5.89	109.49	112.93
1	D	429	TRX	CZ2-CE2-CD2	-5.32	118.08	122.45
1	A	429	TRX	CZ2-CE2-CD2	-4.86	118.46	122.45
1	D	429	TRX	CE3-CD2-CE2	2.82	121.86	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	429	TRX	CE3-CD2-CE2	2.54	121.56	118.83
1	A	260	MHS	CD2-NE2-CE1	2.35	108.08	105.22
1	D	260	MHS	CD2-NE2-CE1	2.20	107.90	105.22
1	D	260	MHS	CM-ND1-CG	2.14	129.01	126.70
1	D	429	TRX	CZ3-CE3-CD2	-2.13	117.48	120.94
1	A	429	TRX	CZ3-CE3-CD2	-2.05	117.61	120.94
1	D	429	TRX	CZ2-CE2-NE1	2.02	134.73	131.69

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	447	GL3	S-C-CA-N
1	A	447	GL3	S-C-CA-N
1	A	274	AGM	CE2-CD-CG-CB
1	A	274	AGM	NE1-CD-CG-CB
1	D	274	AGM	CE2-CD-CG-CB
1	D	274	AGM	NE1-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	429	TRX	2	0
1	D	429	TRX	2	0
1	A	447	GL3	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	COM	A	601	-	6,6,6	1.40	2 (33%)	7,8,8	3.19	4 (57%)
5	TP7	A	603	-	19,20,20	0.63	0	24,26,26	0.99	1 (4%)
6	F43	D	601	1	61,71,71	2.03	6 (9%)	64,118,118	1.37	11 (17%)
4	COM	D	602	-	6,6,6	1.30	1 (16%)	7,8,8	2.94	4 (57%)
5	TP7	A	602	-	19,20,20	0.62	0	24,26,26	0.97	0
6	F43	A	604	1	61,71,71	2.04	6 (9%)	64,118,118	1.38	10 (15%)

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	COM	A	601	-	-	2/4/4/4	-
5	TP7	A	603	-	-	3/24/24/24	-
6	F43	D	601	1	-	10/28/185/185	-
4	COM	D	602	-	-	0/4/4/4	-
5	TP7	A	602	-	-	4/24/24/24	-
6	F43	A	604	1	-	9/28/185/185	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	604	F43	NI-NA	7.81	2.06	1.89
6	D	601	F43	NI-NA	7.63	2.06	1.89
6	A	604	F43	NI-NB	7.50	2.05	1.89
6	D	601	F43	NI-NB	7.45	2.05	1.89
6	D	601	F43	NI-ND	6.95	2.04	1.89
6	A	604	F43	NI-ND	6.82	2.04	1.89
6	D	601	F43	CHD-C1D	-6.14	1.35	1.43
6	A	604	F43	CHD-C1D	-6.10	1.35	1.43
6	D	601	F43	CHC-C4B	2.74	1.47	1.39
6	A	604	F43	CHC-C4B	2.65	1.46	1.39
4	A	601	COM	O1S-S2	2.34	1.51	1.45
6	D	601	F43	C4D-ND	-2.34	1.45	1.49
6	A	604	F43	C4D-ND	-2.27	1.45	1.49
4	A	601	COM	O2S-S2	2.15	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	COM	O1S-S2	2.10	1.51	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	602	COM	O1S-S2-C2	5.18	113.16	106.92
4	A	601	COM	O1S-S2-C2	5.07	113.02	106.92
4	A	601	COM	O2S-S2-C2	4.48	112.31	106.92
4	A	601	COM	O2S-S2-O1S	-4.32	98.99	113.95
4	D	602	COM	O2S-S2-O1S	-3.55	101.68	113.95
6	A	604	F43	O7B-C6B-C8B	-3.39	122.46	126.59
4	D	602	COM	O2S-S2-C2	3.04	110.58	106.92
6	D	601	F43	CAB-C3B-C2B	-2.91	112.92	119.09
6	A	604	F43	CAB-C3B-C2B	-2.83	113.11	119.09
6	D	601	F43	O7B-C6B-C8B	-2.79	123.18	126.59
4	D	602	COM	O3S-S2-C2	2.73	110.19	105.77
6	A	604	F43	C4D-ND-C1D	2.64	111.99	108.51
6	A	604	F43	CBA-CAA-C3A	-2.62	107.99	114.43
6	D	601	F43	CBA-CAA-C3A	-2.60	108.03	114.43
6	D	601	F43	OEA-CCA-CBA	-2.58	114.79	123.08
6	D	601	F43	C4D-ND-C1D	2.58	111.90	108.51
6	A	604	F43	OEA-CCA-CBA	-2.50	115.06	123.08
6	A	604	F43	ODA-CCA-CBA	2.47	121.98	114.03
6	D	601	F43	ODA-CCA-CBA	2.44	121.86	114.03
6	A	604	F43	C9A-C2A-C3A	2.32	116.40	112.98
4	A	601	COM	O3S-S2-C2	2.24	109.39	105.77
6	A	604	F43	C2B-C1B-NB	2.23	105.17	101.84
6	D	601	F43	C2B-C1B-NB	2.20	105.13	101.84
5	A	603	TP7	C2-C1-N	-2.09	112.21	115.83
6	D	601	F43	O8D-C7D-C6D	-2.09	117.44	120.86
6	D	601	F43	ODB-CCB-CBB	-2.05	116.48	123.08
6	D	601	F43	C9A-C2A-C3A	2.04	115.99	112.98
6	A	604	F43	O8D-C7D-C6D	-2.04	117.53	120.86
6	A	604	F43	C9D-C3D-C4D	-2.01	109.36	114.67
6	D	601	F43	OCD-CAD-C9D	2.00	120.49	114.07

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	COM	C1-C2-S2-O2S
5	A	602	TP7	CB-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
5	A	603	TP7	CB-O4P-P-O2P
6	A	604	F43	C4A-C3A-CAA-CBA
6	D	601	F43	C4A-C3A-CAA-CBA
5	A	603	TP7	O1-C1-N-CA
5	A	602	TP7	O1-C1-N-CA
5	A	603	TP7	C2-C1-N-CA
5	A	602	TP7	C2-C1-N-CA
6	A	604	F43	C2A-C3A-CAA-CBA
6	D	601	F43	C2A-C3A-CAA-CBA
6	A	604	F43	C4B-C3B-CAB-CBB
6	D	601	F43	C4B-C3B-CAB-CBB
6	A	604	F43	C3D-C9D-CAD-OCD
6	D	601	F43	C3D-C9D-CAD-OCD
6	A	604	F43	C3D-C9D-CAD-OBD
6	D	601	F43	C3D-C9D-CAD-OBD
6	D	601	F43	CAB-CBB-CCB-OEB
6	A	604	F43	CAB-CBB-CCB-OEB
6	A	604	F43	CAB-CBB-CCB-ODB
5	A	602	TP7	CB-O4P-P-O1P
6	D	601	F43	CAB-CBB-CCB-ODB
4	A	601	COM	C1-C2-S2-O3S
6	A	604	F43	C2D-C3D-C9D-CAD
6	A	604	F43	C4D-C3D-C9D-CAD
6	D	601	F43	C2D-C3D-C9D-CAD
6	D	601	F43	C4D-C3D-C9D-CAD
6	D	601	F43	CAA-CBA-CCA-ODA

There are no ring outliers.

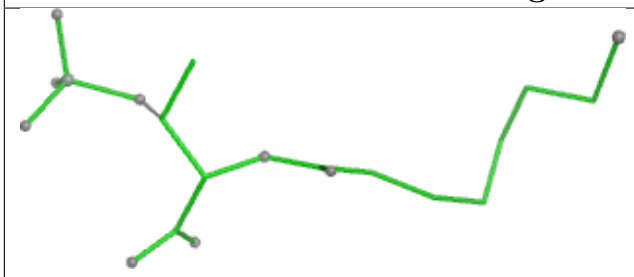
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	COM	1	0
5	A	603	TP7	1	0
6	D	601	F43	2	0
4	D	602	COM	1	0
6	A	604	F43	3	0

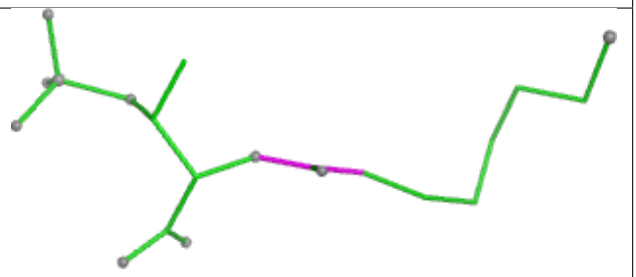
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

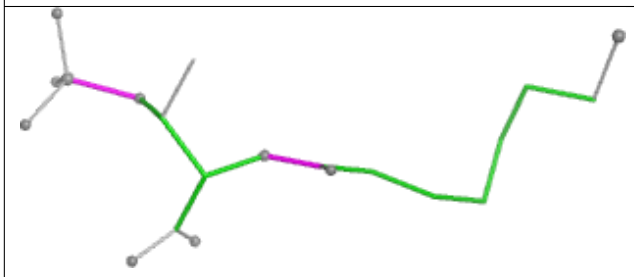
Ligand TP7 A 603



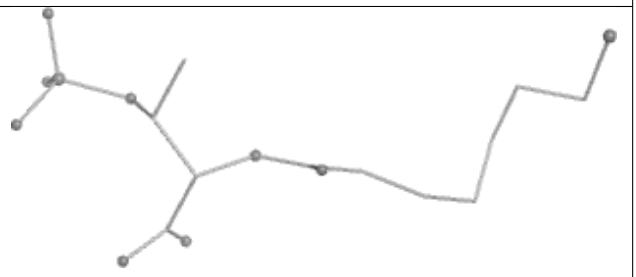
Bond lengths



Bond angles

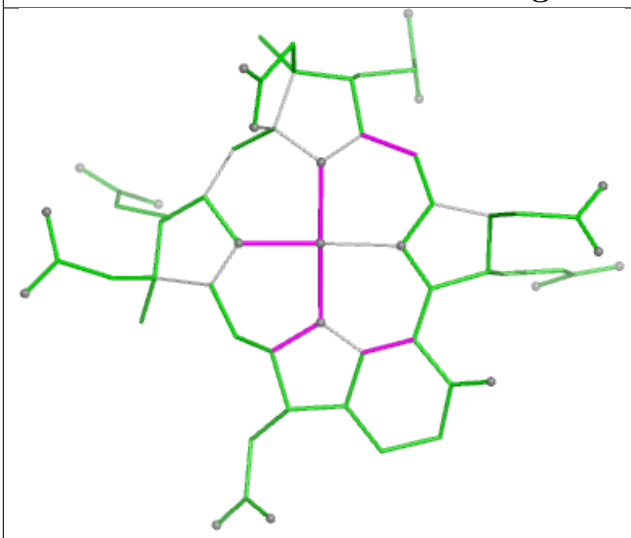


Torsions

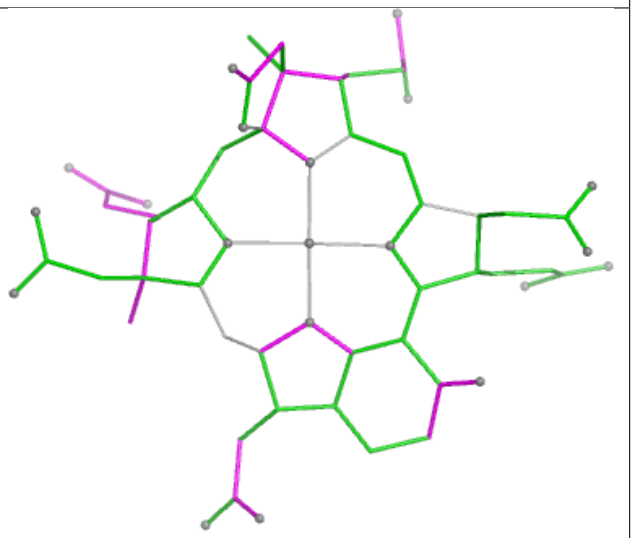


Rings

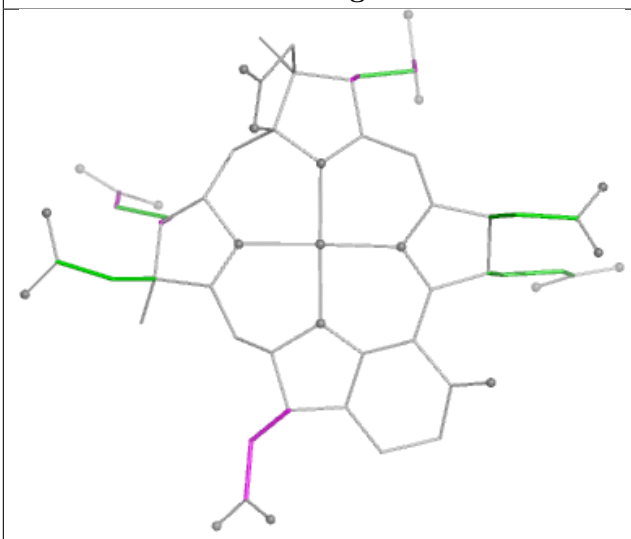
Ligand F43 D 601



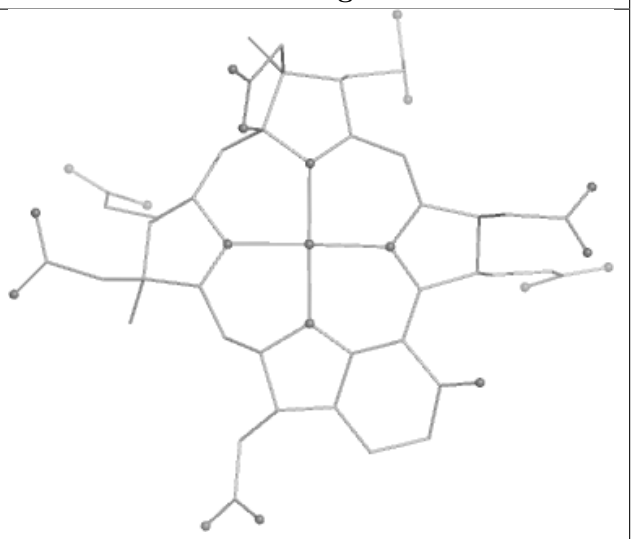
Bond lengths



Bond angles

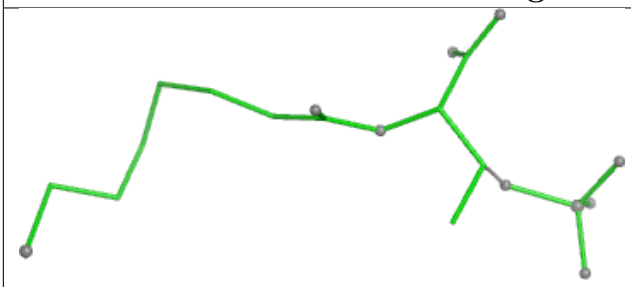


Torsions

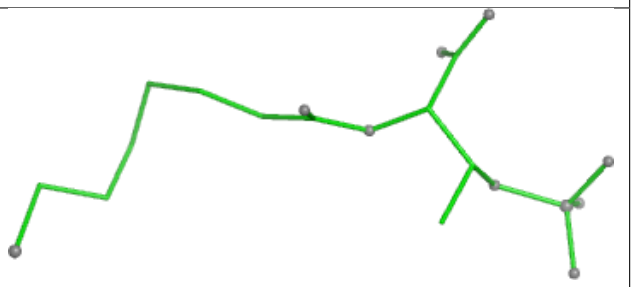


Rings

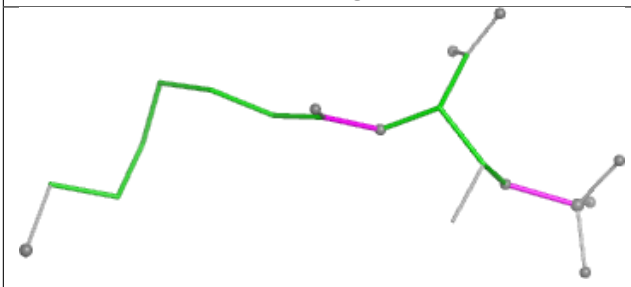
Ligand TP7 A 602



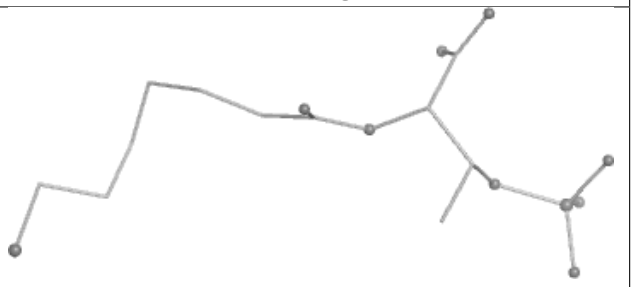
Bond lengths



Bond angles

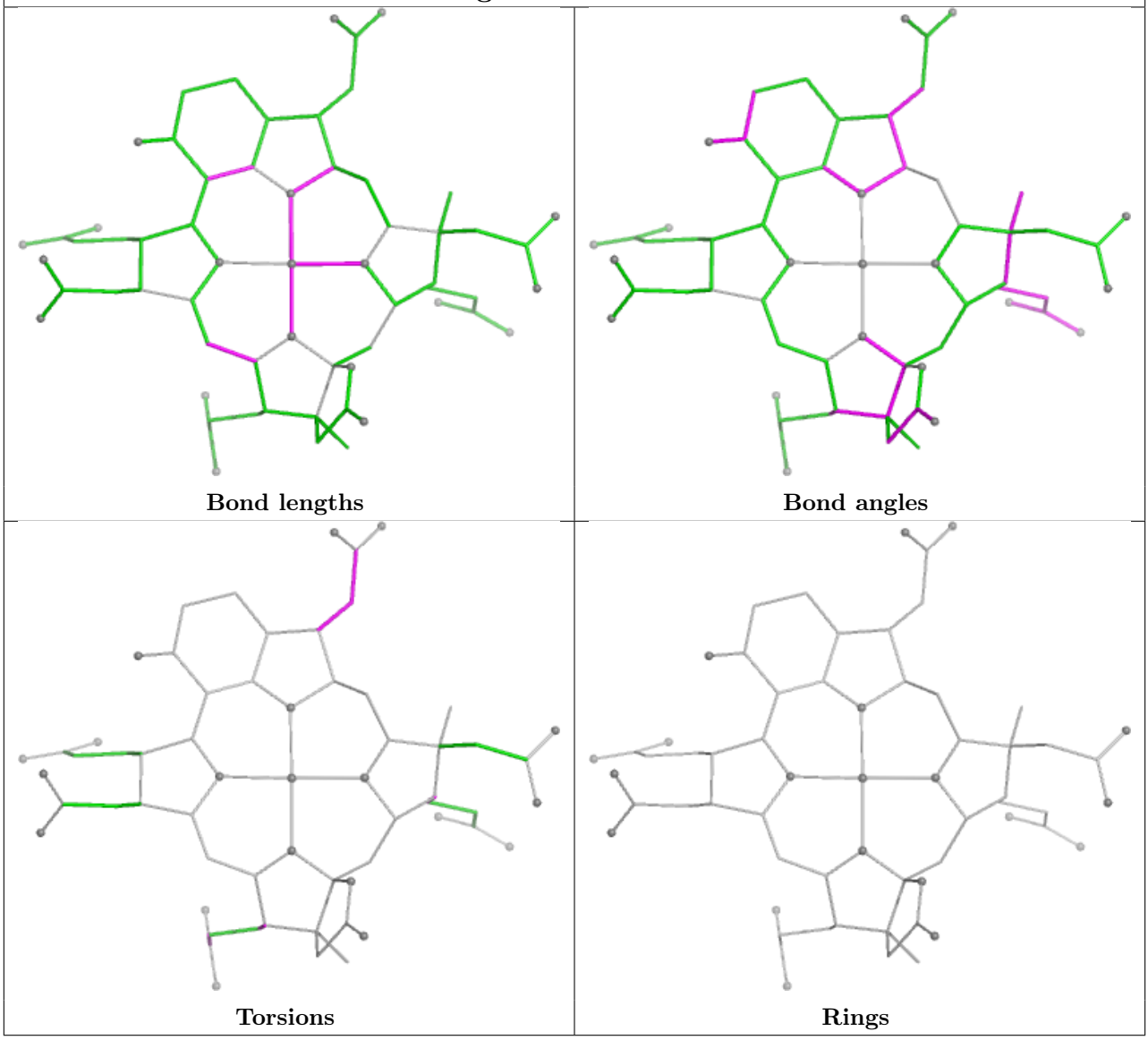


Torsions



Rings

Ligand F43 A 604



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	543/552 (98%)	-0.21	0 100 100	49, 86, 132, 150	0
1	D	542/552 (98%)	-0.10	3 (0%) 85 80	52, 91, 141, 176	0
2	B	443/444 (99%)	-0.47	0 100 100	44, 68, 102, 118	0
2	E	443/444 (99%)	-0.27	0 100 100	55, 85, 122, 155	0
3	C	258/260 (99%)	-0.35	0 100 100	58, 94, 127, 153	0
3	F	252/260 (96%)	0.18	3 (1%) 76 68	91, 142, 185, 208	0
All	All	2481/2512 (98%)	-0.22	6 (0%) 91 88	44, 88, 150, 208	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	154	ILE	3.2
1	D	290	ALA	2.8
3	F	143	ASP	2.4
3	F	190	TYR	2.4
1	D	383	ALA	2.4
1	D	435	LEU	2.2

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

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
1	MHS	D	260	11/12	0.92	0.08	62,66,67,67	0
1	TRX	D	429	15/16	0.92	0.09	75,76,84,84	0
1	GL3	A	447	4/5	0.93	0.09	59,60,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MHS	A	260	11/12	0.94	0.11	65,65,71,71	0
1	AGM	D	274	12/13	0.95	0.08	52,53,56,57	0
1	MGN	D	402	10/11	0.95	0.11	92,93,96,97	0
1	AGM	A	274	12/13	0.95	0.08	47,48,51,51	0
1	TRX	A	429	15/16	0.96	0.07	55,56,63,63	0
1	MGN	A	402	10/11	0.96	0.09	68,69,72,72	0
1	GL3	D	447	4/5	0.96	0.05	82,83,84,85	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

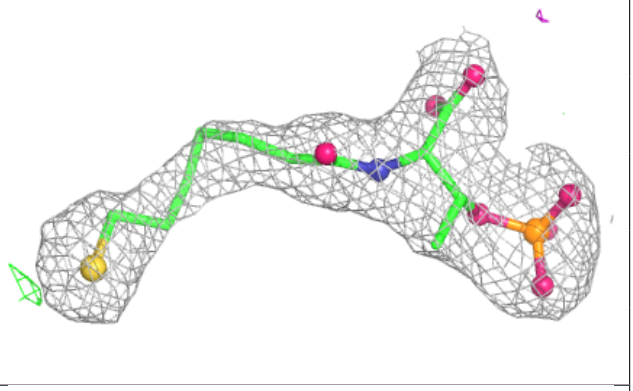
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

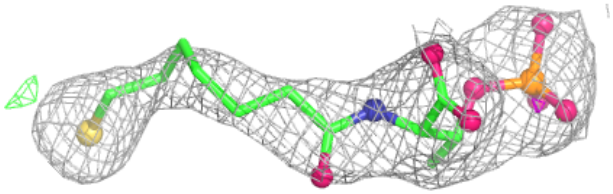
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COM	D	602	7/7	0.93	0.08	98,100,101,102	0
5	TP7	A	602	21/21	0.94	0.09	77,80,83,84	0
6	F43	A	604	62/62	0.94	0.09	83,86,95,102	0
5	TP7	A	603	21/21	0.95	0.09	64,71,76,77	0
4	COM	A	601	7/7	0.96	0.09	66,68,71,73	0
6	F43	D	601	62/62	0.96	0.07	60,66,74,76	0
7	K	A	605	1/1	0.96	0.05	72,72,72,72	0

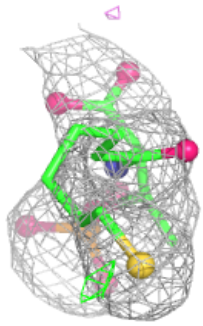
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TP7 A 602:

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

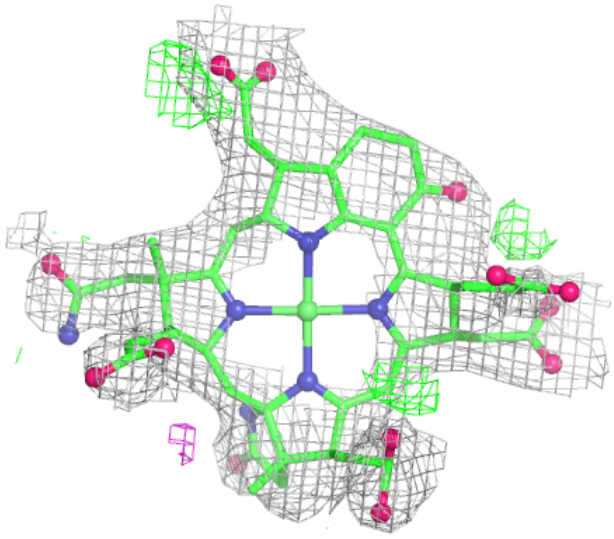


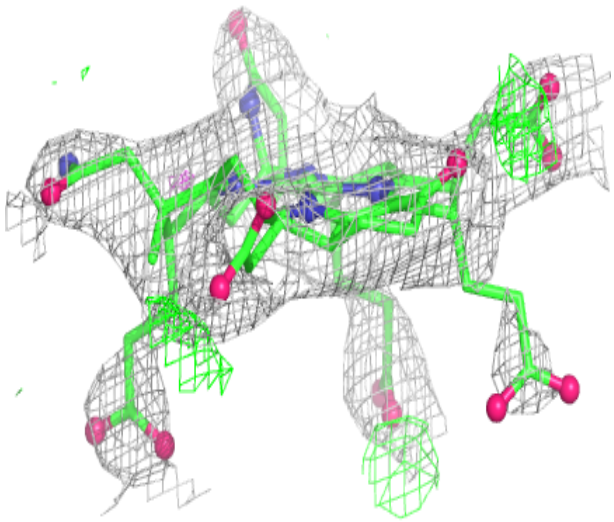


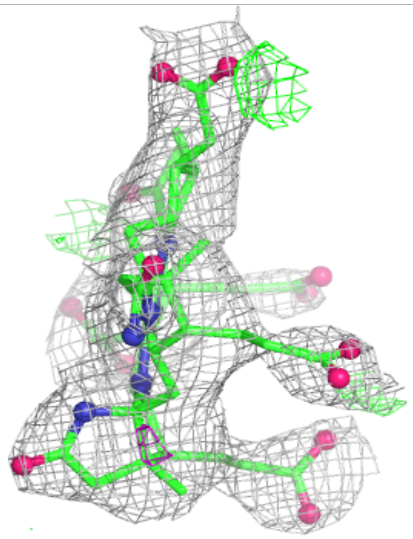


Electron density around F43 A 604:

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

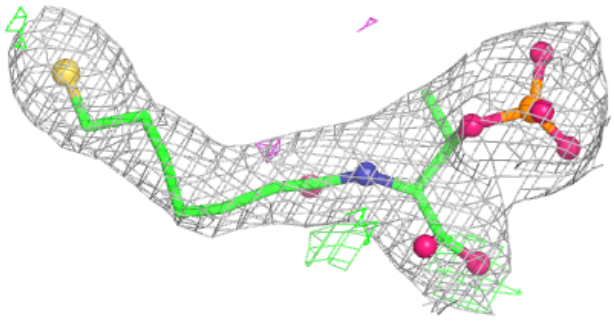


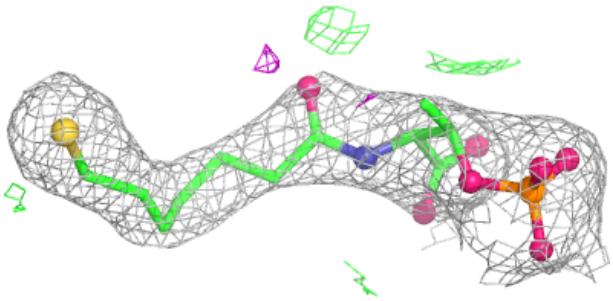


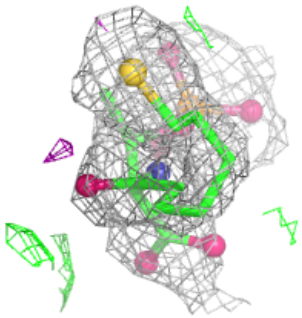


Electron density around TP7 A 603:

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

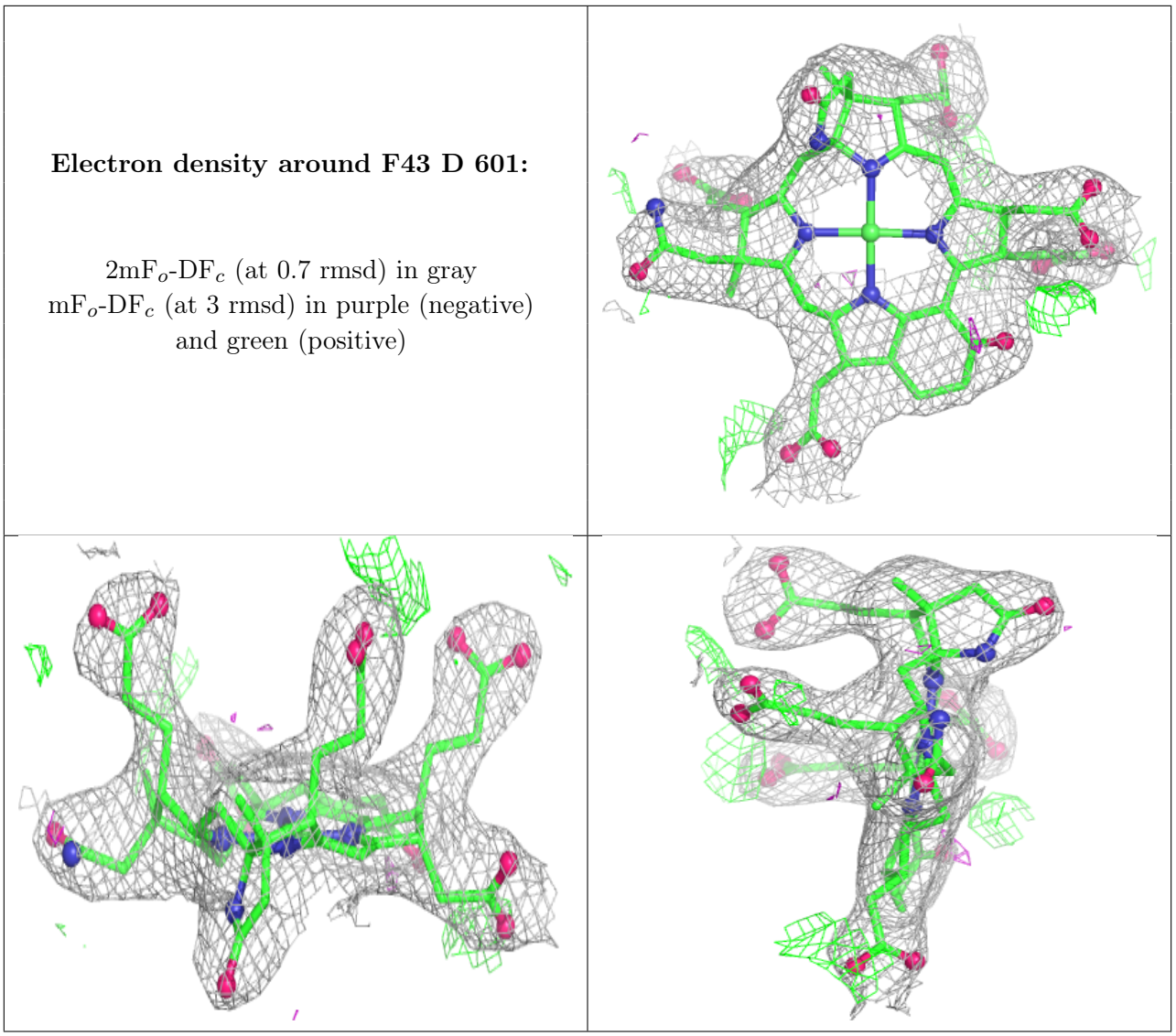






Electron density around F43 D 601:

$2mF_o$-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

There are no such residues in this entry.