Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 02:19 PM JST

PDB ID	:	5B48
Title	:	2-Oxoacid:Ferredoxin Oxidoreductase 1 from Sulfolobus tokodai
Authors	:	Yan, Z.; Maruyama, A.; Arakawa, T.; Fushinobu, S.; Wakagi, T.
Deposited on	:	2016-04-01
Resolution	:	2.50 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:

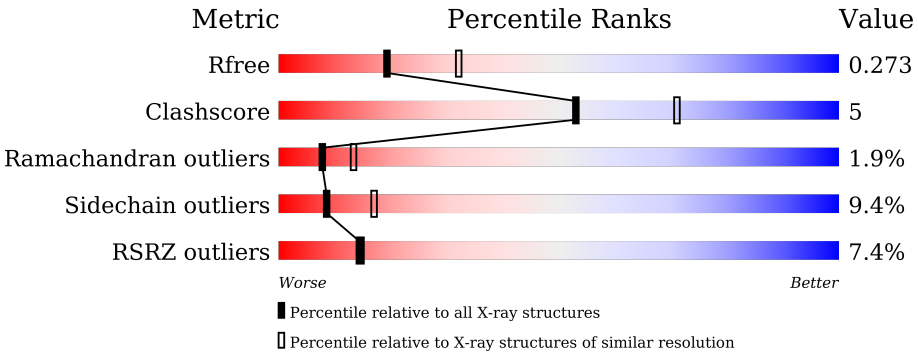
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	627	5% 76% 13% • 8%
1	C	627	7% 72% 15% • 11%
2	B	305	10% 75% 15% • 6%
2	D	305	5% 63% 11% •• 24%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13072 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 2-oxoacid--ferredoxin oxidoreductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4546	2913	756	864	13			
1	C	560	Total	C	N	O	S	0	0	0
			4421	2832	737	841	11			

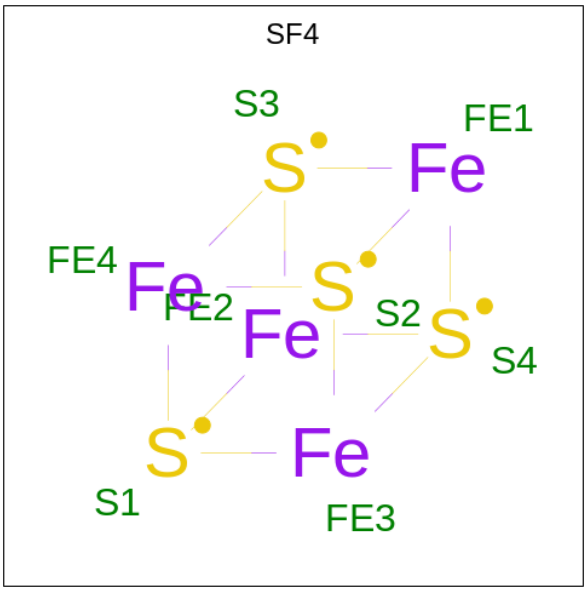
- Molecule 2 is a protein called 2-oxoacid--ferredoxin oxidoreductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2209	1415	377	412	5			
2	D	231	Total	C	N	O	S	0	0	0
			1796	1155	309	331	1			

There are 2 discrepancies between the modelled and reference sequences:

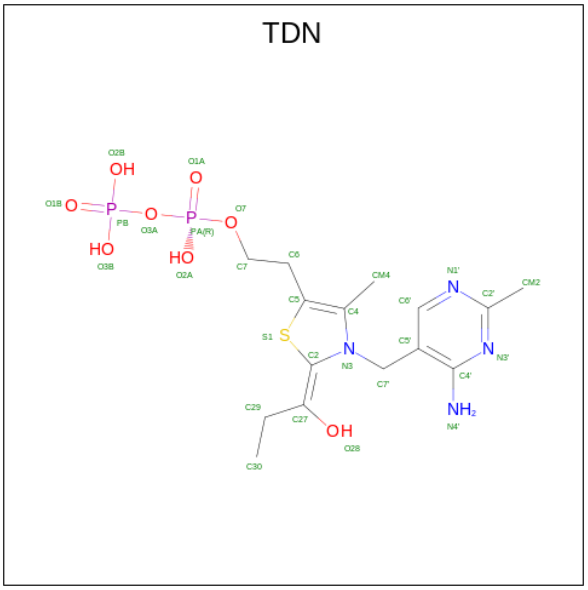
Chain	Residue	Modelled	Actual	Comment	Reference
B	5	THR	LYS	engineered mutation	UNP Q96Y68
D	5	THR	LYS	engineered mutation	UNP Q96Y68

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe S 8 4 4	0	0

- Molecule 4 is 2-[(2E)-3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-2-(1-oxidanylpropylidene)-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: TDN) (formula: $C_{15}H_{24}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P S 30 15 4 8 2 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is water.

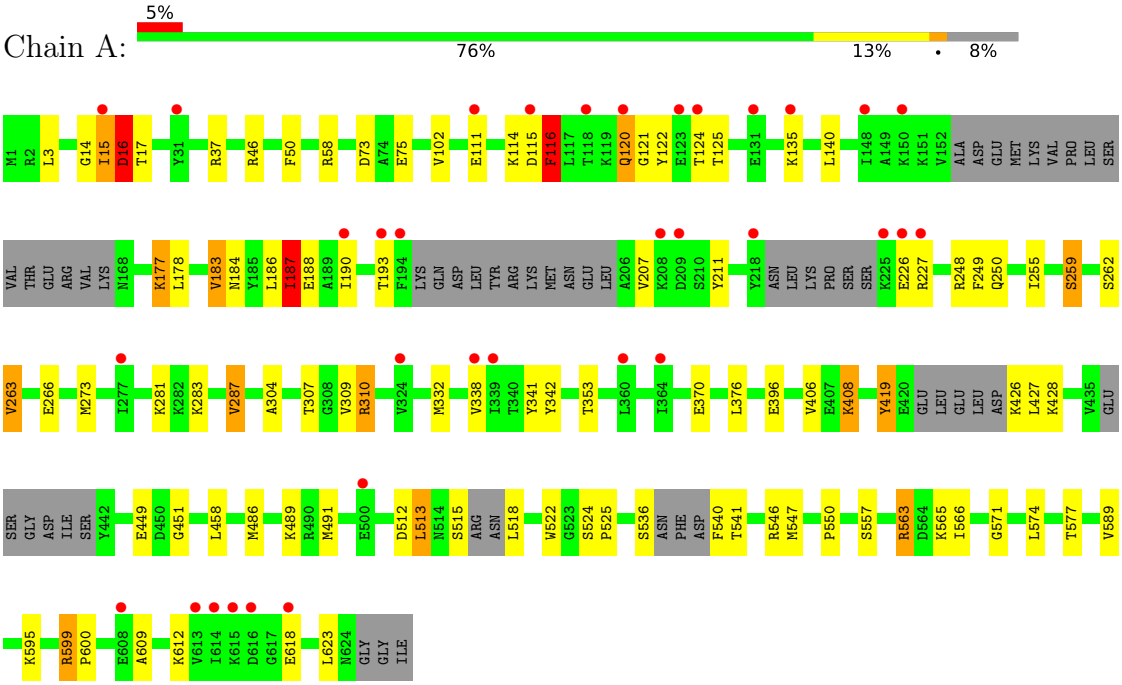
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	5	Total O 5 5	0	0
6	C	23	Total O 23 23	0	0
6	D	8	Total O 8 8	0	0

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.

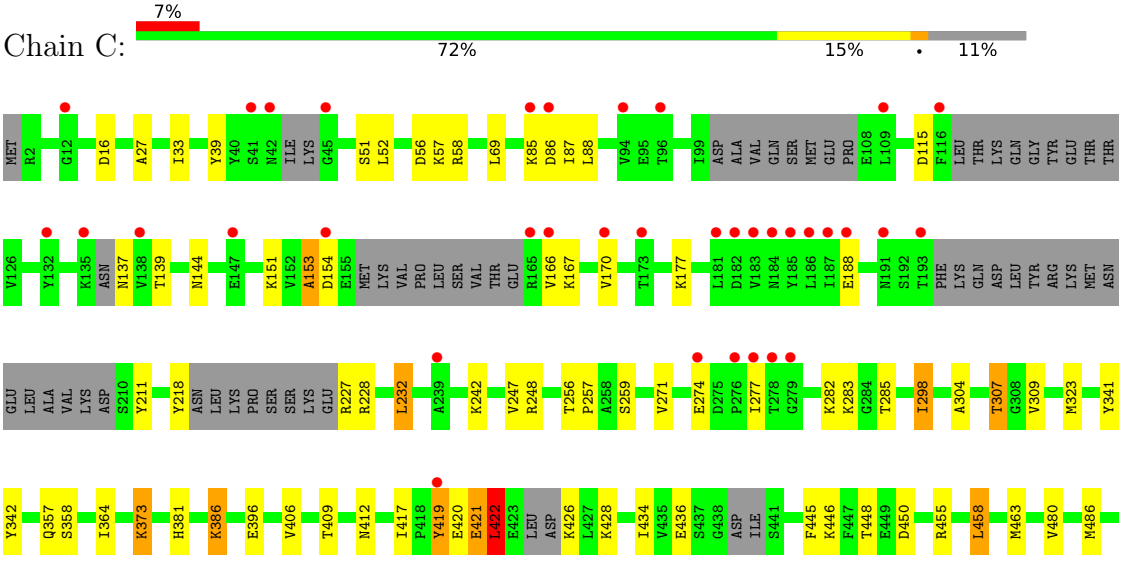
• Molecule 1: 2-oxoacid--ferredoxin oxidoreductase alpha subunit

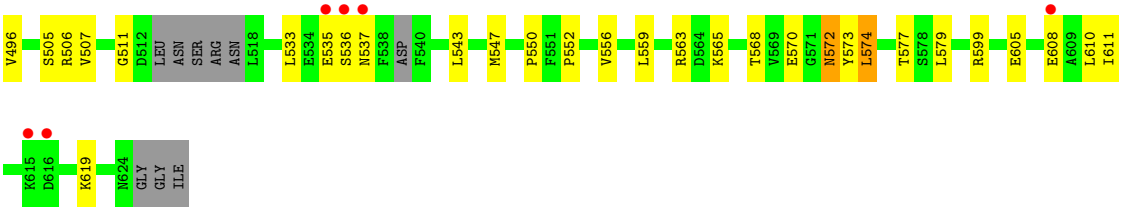
Chain A:



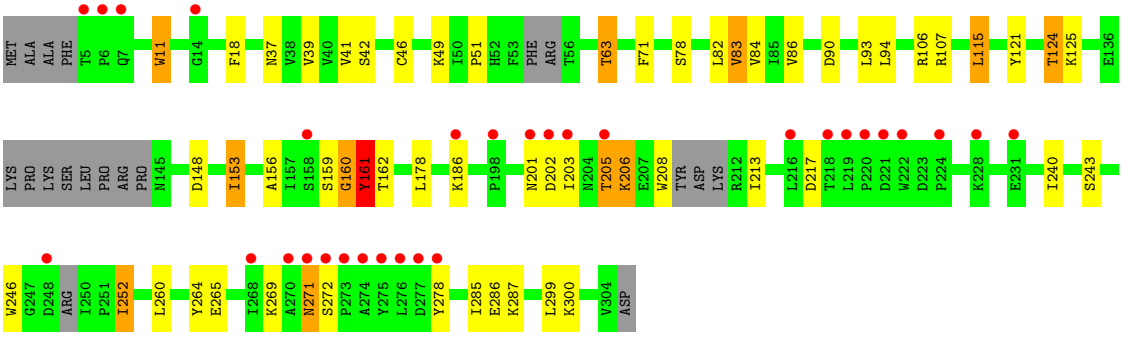
• Molecule 1: 2-oxoacid--ferredoxin oxidoreductase alpha subunit

Chain C:

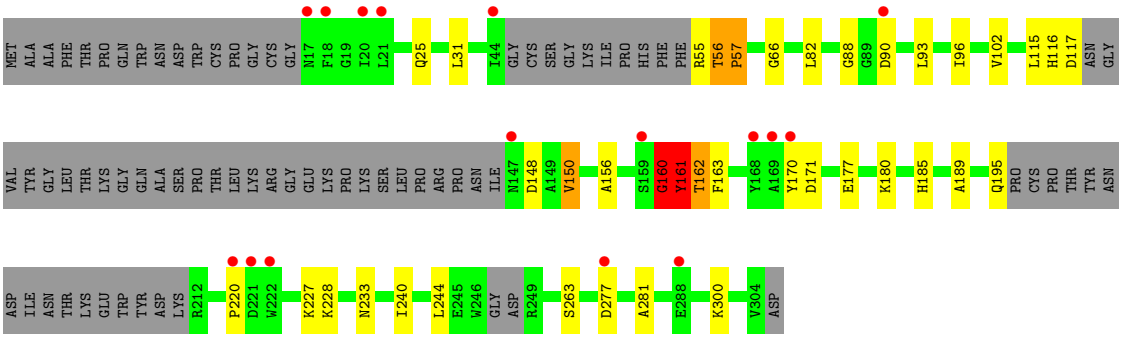




• Molecule 2: 2-oxoacid--ferredoxin oxidoreductase beta subunit



• Molecule 2: 2-oxoacid--ferredoxin oxidoreductase beta subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.15Å 145.88Å 170.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.47 – 2.50 36.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.47-2.50) 99.0 (36.47-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.211 , 0.278 0.212 , 0.273	Depositor DCC
R_{free} test set	3274 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13072	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: MG, TDN, SF4

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	0.68	0/4629	0.86	6/6253 (0.1%)
1	C	0.65	0/4498	0.84	5/6069 (0.1%)
2	B	0.69	2/2254 (0.1%)	0.90	4/3060 (0.1%)
2	D	0.63	0/1825	0.85	1/2471 (0.0%)
All	All	0.67	2/13206 (0.0%)	0.86	16/17853 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	2
2	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	ASP	CB-CG	6.70	1.65	1.51
2	B	265	GLU	CD-OE1	-5.92	1.19	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	455	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	310	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	C	422	LEU	CA-CB-CG	6.73	130.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	11	TRP	CA-CB-CG	5.90	124.92	113.70
1	A	58	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	B	161	TYR	N-CA-CB	5.64	120.76	110.60
1	A	376	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	572	ASN	CB-CA-C	-5.43	99.53	110.40
1	A	115	ASP	C-N-CA	5.23	134.76	121.70
1	C	574	LEU	CA-CB-CG	5.13	127.09	115.30
1	C	458	LEU	CB-CG-CD1	5.09	119.66	111.00
2	D	161	TYR	N-CA-CB	5.09	119.77	110.60
1	A	183	VAL	CB-CA-C	-5.05	101.81	111.40
2	B	217	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	248	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	B	160	GLY	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ILE	Peptide
2	B	159	SER	Peptide
2	B	51	PRO	Peptide
1	C	511	GLY	Peptide
2	D	160	GLY	Peptide

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	4546	0	4572	66	0
1	C	4421	0	4428	39	0
2	B	2209	0	2227	30	0
2	D	1796	0	1855	13	0
3	B	8	0	0	0	0
4	B	30	0	0	0	0
5	B	1	0	0	0	0
6	A	25	0	0	1	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	23	0	0	1	0
6	D	8	0	0	0	0
All	All	13072	0	13082	141	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 5.

All (141) 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:184:ASN:CA	1:A:187:ILE:HD11	1.25	1.55
1:A:184:ASN:HA	1:A:187:ILE:CD1	1.49	1.40
1:A:184:ASN:C	1:A:187:ILE:HD11	1.66	1.16
1:A:183:VAL:O	1:A:187:ILE:CD1	1.93	1.15
1:A:184:ASN:CA	1:A:187:ILE:CD1	2.16	1.14
1:A:183:VAL:O	1:A:187:ILE:HD13	1.52	1.06
1:A:184:ASN:HA	1:A:187:ILE:HD11	0.93	0.90
1:A:515:SER:C	1:A:518:LEU:N	2.29	0.86
1:A:187:ILE:HG12	1:A:188:GLU:H	1.43	0.84
1:A:184:ASN:N	1:A:187:ILE:HD11	1.95	0.81
1:A:187:ILE:HD13	1:A:187:ILE:H	1.43	0.81
1:A:15:ILE:O	1:A:17:THR:N	2.16	0.78
1:A:183:VAL:C	1:A:187:ILE:CD1	2.53	0.78
1:A:184:ASN:C	1:A:187:ILE:CD1	2.47	0.76
2:B:37:ASN:O	2:B:82:LEU:O	2.04	0.74
1:A:184:ASN:HA	1:A:187:ILE:HD12	1.66	0.71
1:C:58:ARG:NH1	1:C:421:GLU:OE2	2.24	0.71
1:A:184:ASN:HA	1:A:187:ILE:CG1	2.22	0.69
1:A:183:VAL:O	1:A:187:ILE:HD12	1.88	0.69
1:A:262:SER:O	1:A:263:VAL:HB	1.93	0.68
1:A:75:GLU:HG3	1:A:102:VAL:HG11	1.75	0.68
1:A:177:LYS:HG2	1:A:211:TYR:CE1	2.31	0.66
1:A:513:LEU:HD23	1:A:540:PHE:N	2.12	0.65
1:C:421:GLU:HA	1:C:422:LEU:HB3	1.79	0.64
1:A:183:VAL:CG1	1:A:211:TYR:CE1	2.82	0.63
1:A:16:ASP:N	1:A:16:ASP:OD1	2.27	0.62
2:D:156:ALA:O	2:D:161:TYR:HB2	2.00	0.60
1:A:491:MET:HG2	1:C:573:TYR:CD1	2.38	0.59
2:B:156:ALA:O	2:B:161:TYR:HB2	2.02	0.59
1:A:187:ILE:HG12	1:A:188:GLU:N	2.16	0.59
1:C:419:TYR:O	1:C:421:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:GLY:HA2	2:B:161:TYR:HB2	1.85	0.58
1:A:184:ASN:N	1:A:187:ILE:CD1	2.61	0.57
1:A:46:ARG:HD3	6:A:724:HOH:O	2.05	0.57
1:A:486:MET:HE1	1:A:489:LYS:CE	2.35	0.57
1:A:515:SER:O	1:A:518:LEU:N	2.38	0.56
1:A:73:ASP:OD1	1:A:75:GLU:N	2.39	0.56
1:C:570:GLU:OE2	1:C:577:THR:HG22	2.04	0.56
1:C:248:ARG:HB2	1:C:309:VAL:CG2	2.37	0.55
1:C:304:ALA:O	1:C:307:THR:HB	2.07	0.54
1:A:15:ILE:HD12	1:A:16:ASP:OD1	2.08	0.54
1:C:232:LEU:HB2	1:C:417:ILE:HD12	1.90	0.53
1:A:599:ARG:HG3	1:A:600:PRO:HD2	1.90	0.53
1:C:69:LEU:HD23	1:C:88:LEU:HD13	1.91	0.53
2:B:78:SER:HB3	1:C:307:THR:HG21	1.90	0.53
1:A:342:TYR:HA	1:A:406:VAL:O	2.10	0.52
2:B:107:ARG:HG2	2:B:264:TYR:CD1	2.45	0.52
1:C:86:ASP:OD2	1:C:218:TYR:OH	2.22	0.52
2:B:121:TYR:HB3	2:B:124:THR:HG22	1.91	0.51
1:A:187:ILE:HD13	1:A:187:ILE:N	2.19	0.51
1:A:522:TRP:CD1	1:A:577:THR:HG21	2.46	0.51
2:B:63:THR:CG2	2:B:71:PHE:CD1	2.94	0.51
1:A:259:SER:O	1:A:262:SER:O	2.28	0.51
1:A:14:GLY:O	1:A:15:ILE:HG13	2.11	0.50
2:D:88:GLY:HA3	2:D:93:LEU:CD1	2.42	0.50
1:C:58:ARG:HD3	6:C:723:HOH:O	2.11	0.50
1:A:566:ILE:HG22	1:A:589:VAL:HG23	1.94	0.49
1:A:120:GLN:HB2	1:A:121:GLY:HA2	1.95	0.49
1:A:307:THR:CG2	2:D:281:ALA:HB2	2.42	0.49
1:C:608:GLU:HA	1:C:611:ILE:HD12	1.95	0.49
1:A:183:VAL:HG13	1:A:211:TYR:CE1	2.48	0.49
1:A:566:ILE:O	1:A:589:VAL:HG22	2.13	0.48
2:B:11:TRP:CH2	2:B:46:CYS:O	2.67	0.48
2:B:90:ASP:HA	2:B:115:LEU:HD21	1.95	0.48
1:C:357:GLN:O	1:C:572:ASN:OD1	2.31	0.48
1:C:421:GLU:CA	1:C:422:LEU:HB3	2.43	0.48
2:B:272:SER:HB3	1:C:285:THR:HG21	1.96	0.48
1:A:451:GLY:HA2	1:A:489:LYS:HG3	1.97	0.47
1:C:381:HIS:HB2	1:C:417:ILE:HD11	1.96	0.47
1:C:543:LEU:HD22	1:C:559:LEU:HD23	1.95	0.47
1:C:177:LYS:HD3	1:C:211:TYR:O	2.15	0.47
1:C:386:LYS:HE3	1:C:422:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HG12	2:B:84:VAL:HG22	1.97	0.47
2:B:153:ILE:HG13	2:B:243:SER:HB2	1.97	0.47
1:A:541:THR:OG1	1:A:563:ARG:NH2	2.48	0.46
2:B:42:SER:O	2:B:63:THR:OG1	2.21	0.46
2:B:206:LYS:N	2:B:206:LYS:HD3	2.30	0.46
1:C:342:TYR:HA	1:C:406:VAL:O	2.15	0.46
1:C:256:THR:HB	1:C:257:PRO:HD3	1.98	0.46
1:C:115:ASP:OD1	1:C:115:ASP:N	2.49	0.46
1:C:364:ILE:O	1:C:373:LYS:HE2	2.15	0.46
1:A:304:ALA:O	1:A:307:THR:HB	2.16	0.45
1:C:27:ALA:HB2	1:C:33:ILE:CD1	2.46	0.45
1:C:450:ASP:HB2	1:C:496:VAL:HG21	1.98	0.45
2:B:160:GLY:CA	2:B:161:TYR:HB2	2.45	0.45
1:C:298:ILE:HG12	1:C:323:MET:HB3	1.98	0.45
2:B:63:THR:HG22	2:B:71:PHE:CE1	2.52	0.45
2:B:269:LYS:O	2:B:271:ASN:N	2.49	0.45
1:A:207:VAL:O	1:A:211:TYR:HB2	2.17	0.45
2:B:78:SER:CB	1:C:307:THR:HG21	2.47	0.44
1:C:242:LYS:HB3	1:C:247:VAL:HG11	1.98	0.44
2:D:90:ASP:O	2:D:93:LEU:O	2.34	0.44
2:D:56:THR:HB	2:D:57:PRO:CD	2.47	0.44
1:C:506:ARG:HB3	1:C:547:MET:HB3	1.99	0.44
1:A:37:ARG:HG2	1:A:50:PHE:CE2	2.53	0.44
1:A:486:MET:HE1	1:A:489:LYS:HE2	1.99	0.44
2:B:213:ILE:HD12	2:B:252:ILE:HD12	1.98	0.44
1:A:547:MET:SD	1:A:550:PRO:HD2	2.57	0.44
1:C:445:PHE:HB3	1:C:486:MET:HE1	2.00	0.44
2:B:11:TRP:HB2	2:B:18:PHE:CE2	2.54	0.43
1:C:547:MET:SD	1:C:550:PRO:HD2	2.58	0.43
2:D:31:LEU:HD11	2:D:180:LYS:HA	1.99	0.43
2:D:162:THR:HG23	2:D:185:HIS:CE1	2.53	0.43
1:A:14:GLY:C	1:A:15:ILE:HG13	2.38	0.43
1:A:183:VAL:C	1:A:187:ILE:HD11	2.30	0.43
1:C:27:ALA:HB2	1:C:33:ILE:HD12	1.99	0.43
2:D:156:ALA:O	2:D:160:GLY:N	2.48	0.43
2:B:240:ILE:HG13	2:D:240:ILE:HG21	2.00	0.43
2:B:206:LYS:N	2:B:206:LYS:CD	2.82	0.42
1:A:426:LYS:C	1:A:427:LEU:HD12	2.40	0.42
1:A:524:SER:N	1:A:525:PRO:CD	2.83	0.42
1:C:570:GLU:CD	1:C:577:THR:HG22	2.40	0.42
1:A:353:THR:O	1:A:408:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:GLY:HA2	1:A:595:LYS:O	2.19	0.42
2:D:163:PHE:CD1	2:D:189:ALA:HB1	2.55	0.42
1:A:609:ALA:HB2	1:A:623:LEU:HD21	2.01	0.42
2:B:94:LEU:HD11	2:B:115:LEU:HD11	2.01	0.42
2:D:66:GLY:HA3	2:D:96:ILE:HG23	2.02	0.42
1:A:186:LEU:O	1:A:190:ILE:N	2.52	0.42
1:A:249:PHE:CD2	1:A:287:VAL:CG2	3.03	0.42
2:B:11:TRP:CH2	2:B:49:LYS:HB2	2.55	0.42
2:B:11:TRP:HB2	2:B:18:PHE:CZ	2.55	0.42
2:D:170:TYR:O	2:D:170:TYR:CD1	2.73	0.42
1:A:262:SER:O	1:A:263:VAL:CB	2.67	0.41
2:B:106:ARG:HD2	2:D:150:VAL:HG13	2.01	0.41
1:A:114:LYS:C	1:A:116:PHE:O	2.59	0.41
2:B:82:LEU:O	2:B:83:VAL:CB	2.68	0.41
1:A:522:TRP:HD1	1:A:577:THR:HG21	1.85	0.41
1:C:153:ALA:HA	1:C:154:ASP:C	2.41	0.41
1:C:552:PRO:O	1:C:556:VAL:HG23	2.20	0.41
1:A:122:TYR:N	1:A:122:TYR:CD1	2.89	0.41
1:A:183:VAL:HG13	1:A:211:TYR:CZ	2.56	0.41
1:A:249:PHE:CD2	1:A:287:VAL:HG22	2.56	0.41
2:B:41:VAL:O	2:B:86:VAL:HA	2.21	0.41
1:C:87:ILE:HD13	1:C:139:THR:HB	2.03	0.41
1:C:421:GLU:HA	1:C:422:LEU:CB	2.48	0.40
2:B:213:ILE:HG23	2:B:252:ILE:HD12	2.03	0.40
1:C:247:VAL:O	1:C:247:VAL:HG13	2.22	0.40
1:A:309:VAL:HG12	1:A:310:ARG:O	2.22	0.40
1:A:486:MET:HE1	1:A:489:LYS:HE3	2.03	0.40
2:B:201:ASN:OD1	2:B:203:ILE:O	2.40	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	560/627 (89%)	522 (93%)	26 (5%)	12 (2%)	7 11
1	C	536/627 (86%)	506 (94%)	22 (4%)	8 (2%)	10 18
2	B	276/305 (90%)	248 (90%)	23 (8%)	5 (2%)	8 14
2	D	221/305 (72%)	201 (91%)	14 (6%)	6 (3%)	5 7
All	All	1593/1864 (86%)	1477 (93%)	85 (5%)	31 (2%)	8 13

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	16	ASP
1	A	116	PHE
1	A	120	GLN
1	A	419	TYR
2	B	125	LYS
1	C	16	ASP
2	D	57	PRO
1	A	193	THR
2	B	161	TYR
2	B	271	ASN
1	C	153	ALA
1	C	277	ILE
1	C	419	TYR
1	C	536	SER
2	D	160	GLY
1	A	512	ASP
1	C	422	LEU
2	D	56	THR
1	A	370	GLU
2	D	161	TYR
2	D	171	ASP
2	B	205	THR
1	C	170	VAL
1	A	187	ILE
1	A	226	GLU
1	A	618	GLU
2	B	83	VAL
1	C	420	GLU
2	D	220	PRO
1	A	263	VAL

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	488/535 (91%)	451 (92%)	37 (8%)	13 25
1	C	473/535 (88%)	420 (89%)	53 (11%)	6 11
2	B	239/256 (93%)	217 (91%)	22 (9%)	9 18
2	D	194/256 (76%)	175 (90%)	19 (10%)	8 15
All	All	1394/1582 (88%)	1263 (91%)	131 (9%)	8 17

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	16	ASP
1	A	111	GLU
1	A	116	PHE
1	A	124	THR
1	A	125	THR
1	A	135	LYS
1	A	140	LEU
1	A	177	LYS
1	A	178	LEU
1	A	187	ILE
1	A	227	ARG
1	A	250	GLN
1	A	259	SER
1	A	266	GLU
1	A	273	MET
1	A	281	LYS
1	A	283	LYS
1	A	287	VAL
1	A	332	MET
1	A	338	VAL
1	A	341	TYR
1	A	396	GLU
1	A	408	LYS

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Mol	Chain	Res	Type
1	A	419	TYR
1	A	428	LYS
1	A	449	GLU
1	A	458	LEU
1	A	513	LEU
1	A	536	SER
1	A	546	ARG
1	A	557	SER
1	A	563	ARG
1	A	565	LYS
1	A	574	LEU
1	A	599	ARG
1	A	612	LYS
2	B	63	THR
2	B	93	LEU
2	B	115	LEU
2	B	124	THR
2	B	148	ASP
2	B	153	ILE
2	B	162	THR
2	B	178	LEU
2	B	186	LYS
2	B	202	ASP
2	B	205	THR
2	B	206	LYS
2	B	208	TRP
2	B	246	TRP
2	B	252	ILE
2	B	260	LEU
2	B	278	TYR
2	B	285	ILE
2	B	286	GLU
2	B	287	LYS
2	B	299	LEU
2	B	300	LYS
1	C	39	TYR
1	C	51	SER
1	C	52	LEU
1	C	56	ASP
1	C	57	LYS
1	C	85	LYS
1	C	137	ASN

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Mol	Chain	Res	Type
1	C	144	ASN
1	C	151	LYS
1	C	166	VAL
1	C	167	LYS
1	C	188	GLU
1	C	227	ARG
1	C	228	ARG
1	C	232	LEU
1	C	259	SER
1	C	271	VAL
1	C	274	GLU
1	C	282	LYS
1	C	283	LYS
1	C	298	ILE
1	C	307	THR
1	C	341	TYR
1	C	358	SER
1	C	373	LYS
1	C	386	LYS
1	C	396	GLU
1	C	409	THR
1	C	412	ASN
1	C	421	GLU
1	C	426	LYS
1	C	428	LYS
1	C	434	ILE
1	C	436	GLU
1	C	446	LYS
1	C	448	THR
1	C	458	LEU
1	C	463	MET
1	C	480	VAL
1	C	505	SER
1	C	507	VAL
1	C	533	LEU
1	C	535	GLU
1	C	537	ASN
1	C	563	ARG
1	C	565	LYS
1	C	568	THR
1	C	574	LEU
1	C	579	LEU

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Mol	Chain	Res	Type
1	C	599	ARG
1	C	605	GLU
1	C	610	LEU
1	C	619	LYS
2	D	25	GLN
2	D	55	ARG
2	D	82	LEU
2	D	102	VAL
2	D	115	LEU
2	D	116	HIS
2	D	117	ASP
2	D	148	ASP
2	D	150	VAL
2	D	162	THR
2	D	177	GLU
2	D	195	GLN
2	D	227	LYS
2	D	228	LYS
2	D	233	ASN
2	D	244	LEU
2	D	263	SER
2	D	277	ASP
2	D	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	591	ASN
1	C	11	GLN
1	C	144	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	TDN	B	402	5	28,31,31	2.75	9 (32%)	33,46,46	2.09	14 (42%)
3	SF4	B	401	2	0,12,12	-	-	-		

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	TDN	B	402	5	-	8/19/23/23	0/2/2/2
3	SF4	B	401	2	-	-	0/6/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	TDN	C6-C5	-7.59	1.36	1.50
4	B	402	TDN	C5-S1	-7.51	1.58	1.74
4	B	402	TDN	C7'-C5'	-4.65	1.43	1.51
4	B	402	TDN	C7'-N3	3.57	1.52	1.47
4	B	402	TDN	CM2-C2'	-3.43	1.39	1.49
4	B	402	TDN	CM4-C4	3.15	1.54	1.49
4	B	402	TDN	C6'-N1'	2.76	1.40	1.34
4	B	402	TDN	PA-O7	2.43	1.69	1.59
4	B	402	TDN	PB-O3B	-2.23	1.46	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	402	TDN	C5'-C7'-N3	4.81	119.23	113.13
4	B	402	TDN	C7-C6-C5	4.01	125.46	112.73
4	B	402	TDN	C6-C5-C4	3.49	137.08	128.20
4	B	402	TDN	O3B-PB-O2B	2.97	118.97	107.64
4	B	402	TDN	CM2-C2'-N3'	2.86	121.62	117.15
4	B	402	TDN	C4-C5-S1	-2.74	108.14	110.59
4	B	402	TDN	O3A-PB-O1B	-2.64	96.55	111.19
4	B	402	TDN	O2B-PB-O3A	-2.56	96.05	104.64
4	B	402	TDN	N1'-C2'-N3'	-2.55	121.14	125.54
4	B	402	TDN	C7'-C5'-C4'	2.35	124.94	122.56
4	B	402	TDN	O2B-PB-O1B	2.10	118.91	110.68
4	B	402	TDN	C6-C5-S1	-2.07	114.74	119.20
4	B	402	TDN	C2'-N3'-C4'	2.05	121.28	118.08
4	B	402	TDN	C7'-C5'-C6'	-2.01	118.42	121.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

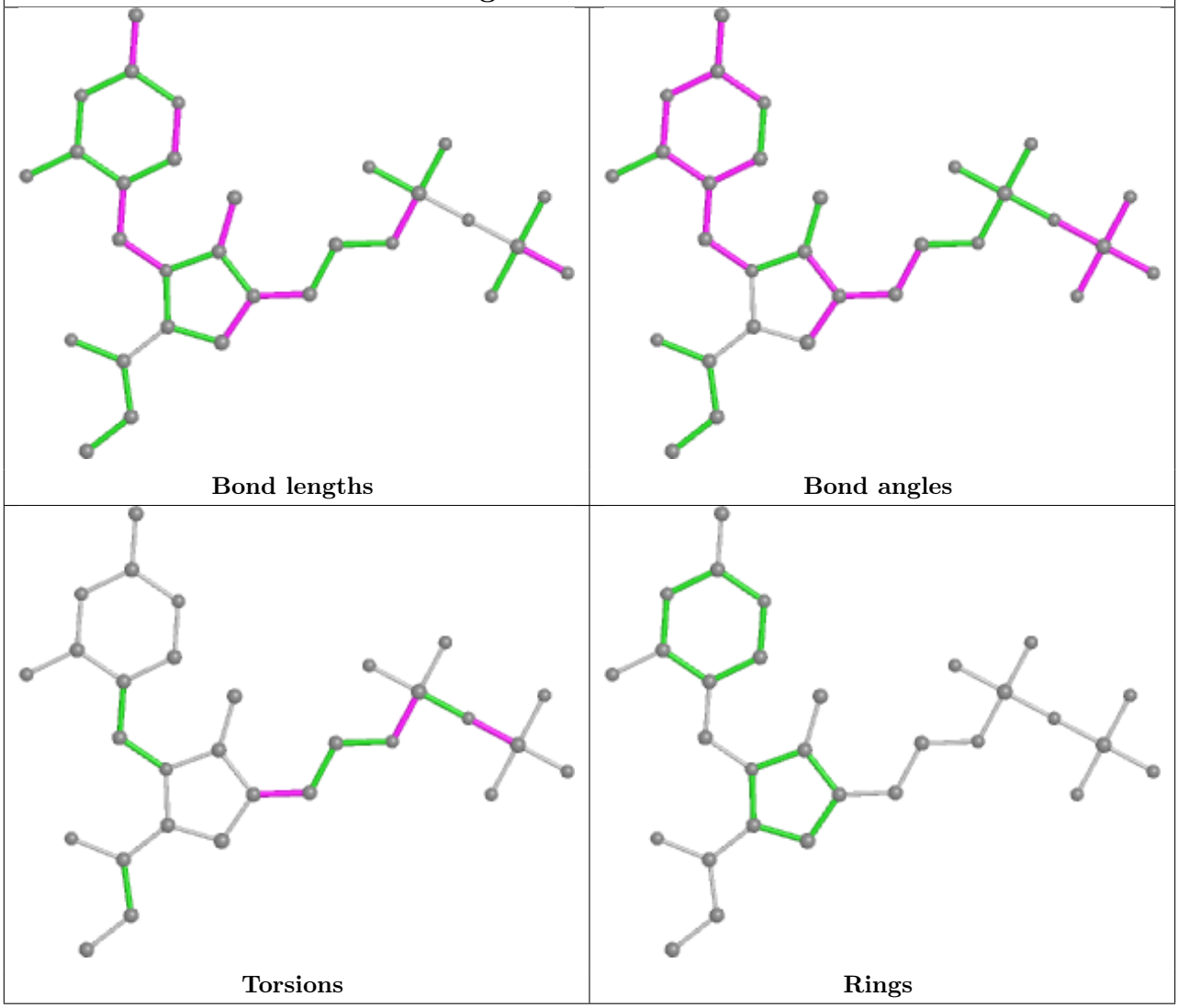
Mol	Chain	Res	Type	Atoms
4	B	402	TDN	PA-O3A-PB-O2B
4	B	402	TDN	PA-O3A-PB-O3B
4	B	402	TDN	C7-O7-PA-O1A
4	B	402	TDN	C7-O7-PA-O2A
4	B	402	TDN	C4-C5-C6-C7
4	B	402	TDN	S1-C5-C6-C7
4	B	402	TDN	C7-O7-PA-O3A
4	B	402	TDN	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 TDN B 402



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	576/627 (91%)	0.31	34 (5%) 22 23	37, 62, 107, 143	0
1	C	560/627 (89%)	0.32	42 (7%) 14 14	34, 62, 106, 131	0
2	B	286/305 (93%)	0.52	31 (10%) 5 5	38, 66, 101, 146	0
2	D	231/305 (75%)	0.39	16 (6%) 16 17	42, 65, 100, 137	0
All	All	1653/1864 (88%)	0.36	123 (7%) 14 15	34, 63, 105, 146	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	220	PRO	7.6
1	A	194	PHE	6.2
2	B	6	PRO	6.2
2	D	170	TYR	5.8
1	C	277	ILE	5.4
1	C	181	LEU	4.9
1	A	225	LYS	4.9
2	B	274	ALA	4.7
1	C	274	GLU	4.7
1	A	111	GLU	4.4
2	D	147	ASN	4.4
2	D	221	ASP	4.4
1	A	209	ASP	4.4
2	B	277	ASP	4.2
2	B	14	GLY	4.1
2	D	288	GLU	4.1
1	C	186	LEU	4.1
1	C	191	ASN	4.1
2	B	219	LEU	4.0
1	C	94	VAL	3.9
1	C	187	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	270	ALA	3.9
1	A	616	ASP	3.9
1	C	86	ASP	3.7
1	A	123	GLU	3.7
2	B	220	PRO	3.7
2	D	21	LEU	3.6
1	C	116	PHE	3.5
2	B	202	ASP	3.5
1	C	183	VAL	3.5
1	A	115	ASP	3.5
1	C	182	ASP	3.4
1	A	277	ILE	3.4
1	A	150	LYS	3.4
1	C	138	VAL	3.4
2	B	273	PRO	3.4
2	D	222	TRP	3.3
1	A	124	THR	3.3
1	A	208	LYS	3.3
1	C	85	LYS	3.3
1	A	31	TYR	3.3
1	C	170	VAL	3.3
2	B	216	LEU	3.2
1	C	419	TYR	3.2
2	B	221	ASP	3.2
1	A	131	GLU	3.2
1	C	135	LYS	3.2
1	C	278	THR	3.2
1	C	165	ARG	3.1
1	C	154	ASP	3.0
2	B	278	TYR	3.0
1	C	535	GLU	3.0
1	A	190	ILE	2.9
1	A	226	GLU	2.9
1	C	276	PRO	2.9
1	A	615	LYS	2.9
2	B	272	SER	2.8
1	C	616	ASP	2.8
1	A	193	THR	2.7
1	A	364	ILE	2.7
1	A	118	THR	2.7
1	C	132	TYR	2.6
1	A	218	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	618	GLU	2.6
1	C	188	GLU	2.6
1	A	120	GLN	2.6
1	A	613	VAL	2.6
2	B	271	ASN	2.6
2	B	5	THR	2.6
1	C	239	ALA	2.5
2	B	224	PRO	2.5
1	C	185	TYR	2.5
2	B	268	ILE	2.5
2	D	168	TYR	2.5
1	C	166	VAL	2.5
1	C	184	ASN	2.5
1	A	15	ILE	2.5
1	A	227	ARG	2.5
1	A	360	LEU	2.5
1	C	279	GLY	2.5
2	B	276	LEU	2.5
2	D	17	ASN	2.4
1	C	608	GLU	2.4
2	D	44	ILE	2.4
1	C	173	THR	2.4
2	B	158	SER	2.4
2	D	18	PHE	2.4
2	B	248	ASP	2.4
1	A	324	VAL	2.4
2	B	198	PRO	2.4
2	B	7	GLN	2.3
2	B	275	TYR	2.3
1	C	537	ASN	2.3
1	C	193	THR	2.3
2	B	186	LYS	2.3
2	B	222	TRP	2.3
2	B	231	GLU	2.3
2	D	90	ASP	2.2
1	C	41	SER	2.2
2	B	205	THR	2.2
1	C	109	LEU	2.2
1	A	614	ILE	2.2
1	A	500	GLU	2.2
2	B	218	THR	2.2
1	C	536	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	228	LYS	2.2
2	D	20	ILE	2.2
2	D	159	SER	2.2
1	A	339	ILE	2.1
2	B	203	ILE	2.1
1	C	147	GLU	2.1
2	B	201	ASN	2.1
1	C	12	GLY	2.1
1	C	45	GLY	2.1
1	C	615	LYS	2.1
1	A	148	ILE	2.0
1	A	135	LYS	2.0
2	D	169	ALA	2.0
1	A	338	VAL	2.0
1	C	42	ASN	2.0
1	A	608	GLU	2.0
1	C	96	THR	2.0
2	D	277	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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.

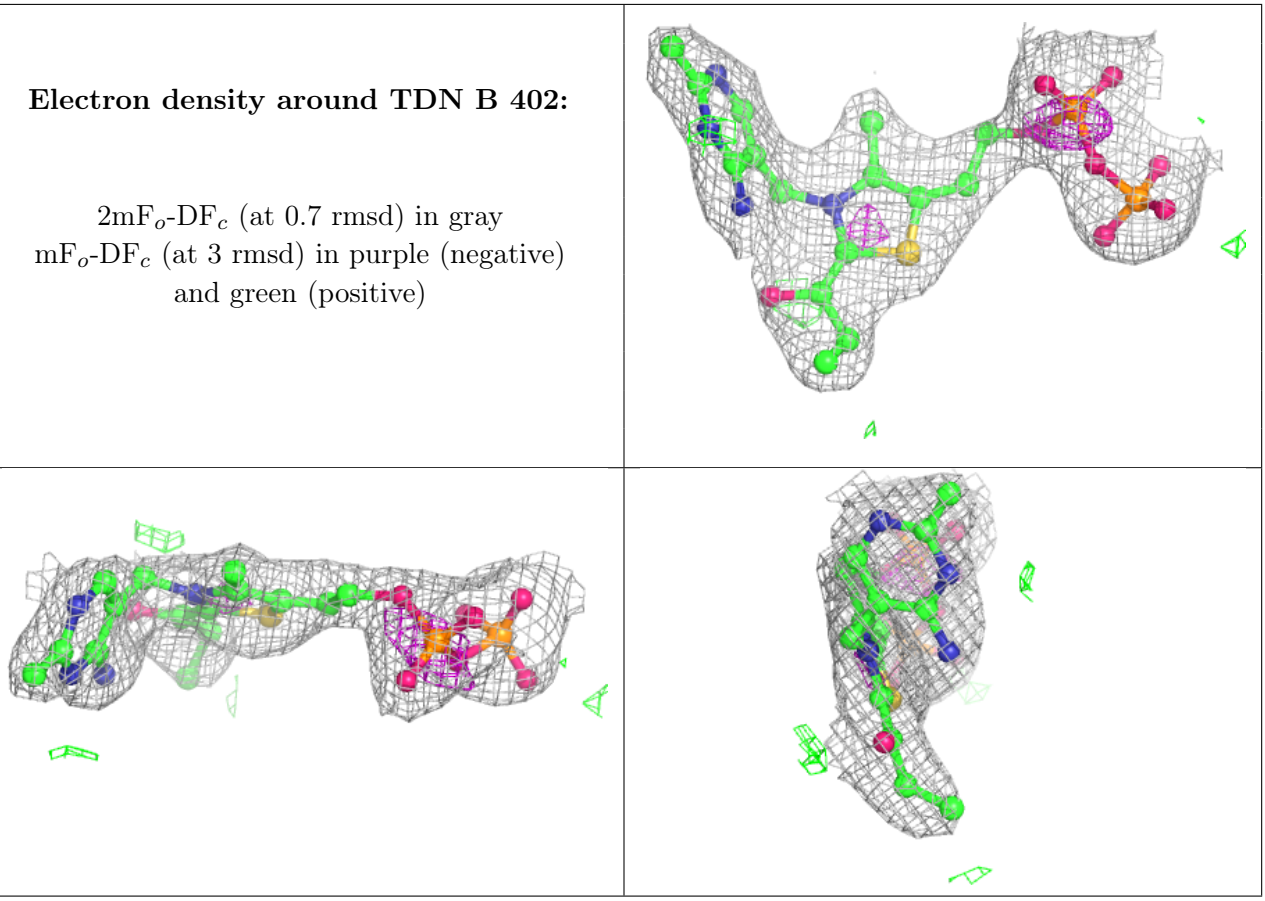
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	403	1/1	0.84	0.08	61,61,61,61	0
4	TDN	B	402	30/30	0.95	0.14	47,58,66,68	0
3	SF4	B	401	8/8	0.99	0.03	55,58,65,66	0

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 TDN B 402:

$2mF_o$-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.