Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 08:35 AM EST

PDB ID	:	6CUZ
Title	:	Engineered TrpB from Pyrococcus furiosus, PfTrpB7E6 with (2S,3R)-ethylserine bound as the amino-acrylate
Authors	:	Scheele, R.A.; Buller, A.R.; Boville, C.E.; Arnold, F.H.
Deposited on	:	2018-03-27
Resolution	:	1.75 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:

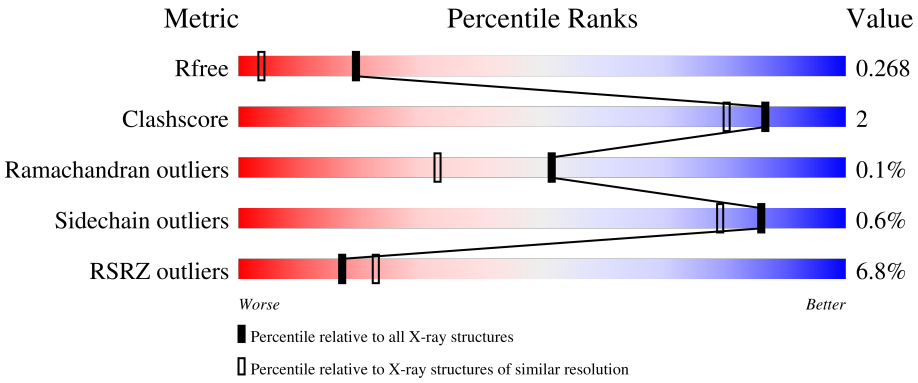
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	388	4% 92% 6% ·
1	D	388	8% 94% 5% ·
2	B	388	9% 91% 6% ·
2	C	388	5% 93% · · ·

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11996 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 Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	1	0
			2878	1834	498	534	12			
1	D	385	Total	C	N	O	S	0	0	0
			2860	1820	492	536	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	engineered mutation	UNP Q8U093
A	17	GLY	GLU	engineered mutation	UNP Q8U093
A	91	PRO	LEU	engineered mutation	UNP Q8U093
A	95	LEU	PHE	engineered mutation	UNP Q8U093
A	161	ALA	LEU	engineered mutation	UNP Q8U093
A	173	GLU	VAL	engineered mutation	UNP Q8U093
A	274	LEU	PHE	engineered mutation	UNP Q8U093
A	292	SER	THR	engineered mutation	UNP Q8U093
A	384	ALA	VAL	engineered mutation	UNP Q8U093
D	16	VAL	ILE	engineered mutation	UNP Q8U093
D	17	GLY	GLU	engineered mutation	UNP Q8U093
D	91	PRO	LEU	engineered mutation	UNP Q8U093
D	95	LEU	PHE	engineered mutation	UNP Q8U093
D	161	ALA	LEU	engineered mutation	UNP Q8U093
D	173	GLU	VAL	engineered mutation	UNP Q8U093
D	274	LEU	PHE	engineered mutation	UNP Q8U093
D	292	SER	THR	engineered mutation	UNP Q8U093
D	384	ALA	VAL	engineered mutation	UNP Q8U093

- Molecule 2 is a protein called Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	376	Total	C	N	O	P	S	0	1	0
			2818	1799	483	524	1	11			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	377	Total	C	N	O	P	S	0	0	0
			2833	1811	480	529	1	12			

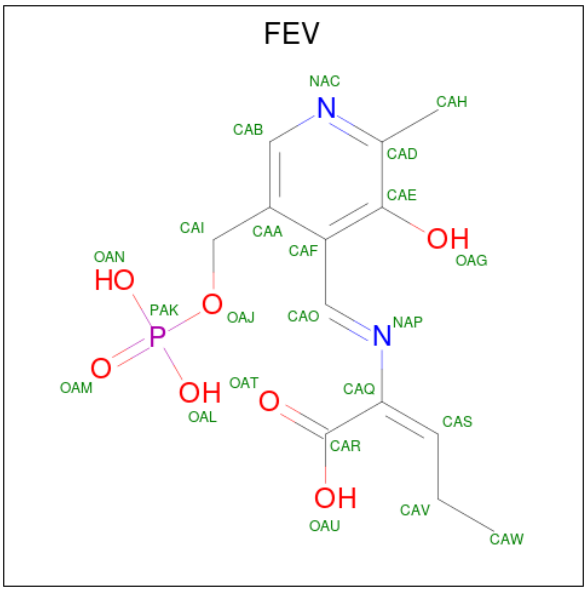
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	VAL	ILE	engineered mutation	UNP Q8U093
B	17	GLY	GLU	engineered mutation	UNP Q8U093
B	91	PRO	LEU	engineered mutation	UNP Q8U093
B	95	LEU	PHE	engineered mutation	UNP Q8U093
B	161	ALA	LEU	engineered mutation	UNP Q8U093
B	173	GLU	VAL	engineered mutation	UNP Q8U093
B	274	LEU	PHE	engineered mutation	UNP Q8U093
B	292	SER	THR	engineered mutation	UNP Q8U093
B	384	ALA	VAL	engineered mutation	UNP Q8U093
C	16	VAL	ILE	engineered mutation	UNP Q8U093
C	17	GLY	GLU	engineered mutation	UNP Q8U093
C	91	PRO	LEU	engineered mutation	UNP Q8U093
C	95	LEU	PHE	engineered mutation	UNP Q8U093
C	161	ALA	LEU	engineered mutation	UNP Q8U093
C	173	GLU	VAL	engineered mutation	UNP Q8U093
C	274	LEU	PHE	engineered mutation	UNP Q8U093
C	292	SER	THR	engineered mutation	UNP Q8U093
C	384	ALA	VAL	engineered mutation	UNP Q8U093

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

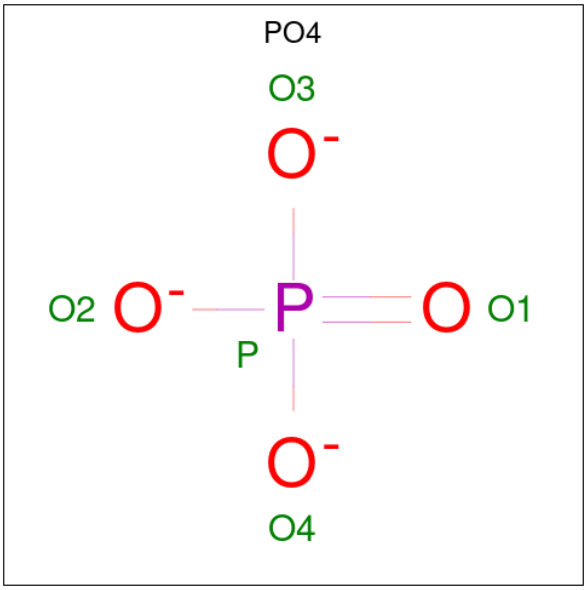
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	2	Total	Na	0	0
			2	2		

- Molecule 4 is (2E)-2-[(E)-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)amino]pent-2-enoic acid (three-letter code: FEV) (formula: $C_{13}H_{17}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	13	2	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	13	2	7	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	O	P		0	0
			5	4	1			

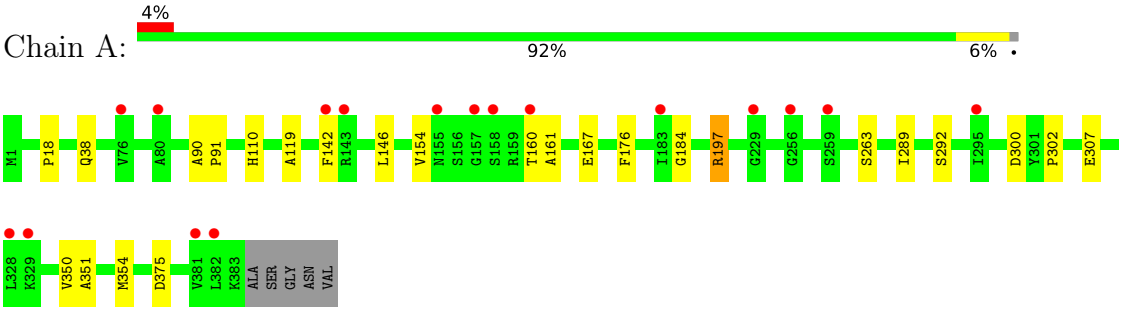
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	145	Total O 145 145	0	0
6	B	117	Total O 117 117	0	0
6	C	145	Total O 145 145	0	0
6	D	143	Total O 143 143	0	0

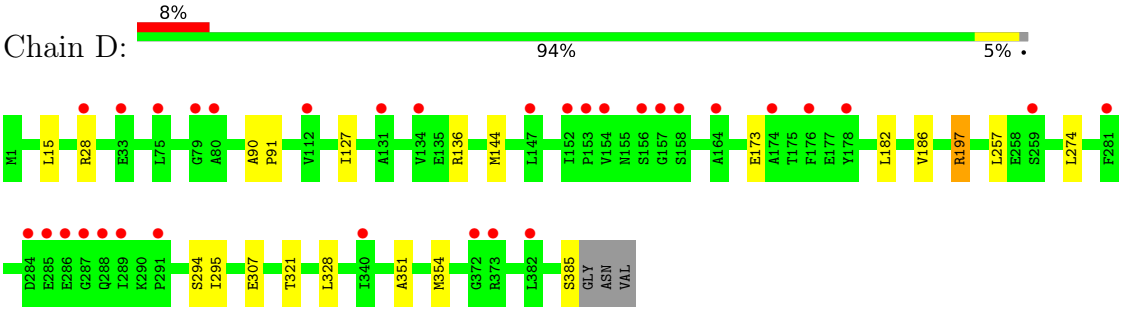
3 Residue-property plots (i)

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.

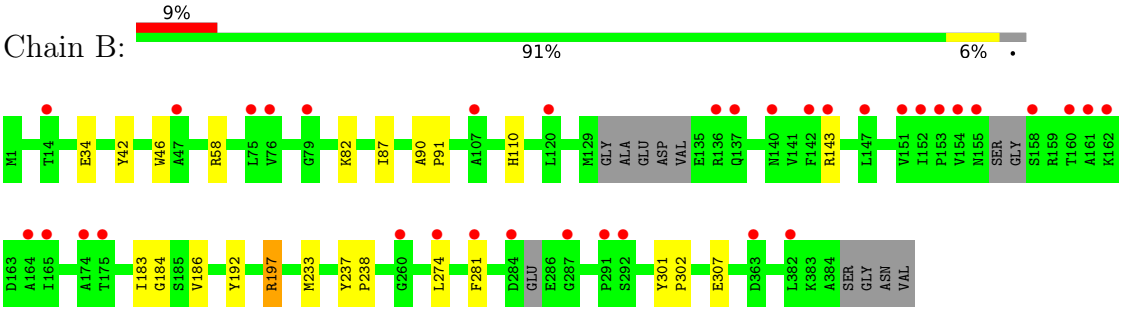
• Molecule 1: Tryptophan synthase beta chain 1



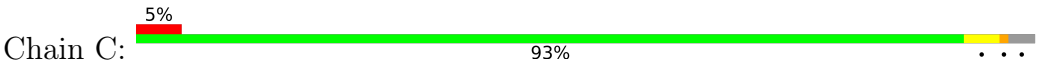
• Molecule 1: Tryptophan synthase beta chain 1

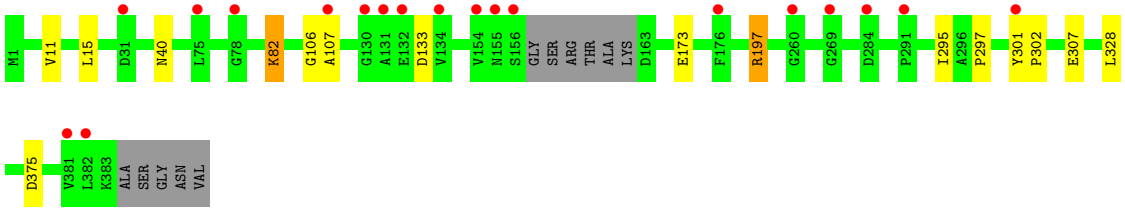


• Molecule 2: Tryptophan synthase beta chain 1



• Molecule 2: Tryptophan synthase beta chain 1




M1
V11
L15
D31
N40
L75
G78
K82
G106
A107
G130
A131
E132
D133
V134
V154
N155
S156
GLY
SER
ARG
THR
ALA
LYS
D163
E173
F176
R197
G260
G269
D284
P291
I295
A296
P297
Y301
P302
E307
L328

D375
V381
L382
K383
ALA
SER
GLY
ASN
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.22Å 109.30Å 159.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 38.16 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.75) 99.9 (38.16-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.235 , 0.261 0.242 , 0.268	Depositor DCC
R_{free} test set	7409 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11996	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FEV, LLP, PO4

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	0.32	0/2941	0.55	2/3985 (0.1%)
1	D	0.32	0/2919	0.55	1/3961 (0.0%)
2	B	0.32	0/2853	0.54	2/3867 (0.1%)
2	C	0.34	0/2867	0.56	1/3885 (0.0%)
All	All	0.33	0/11580	0.55	6/15698 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	ARG	NE-CZ-NH1	-6.23	117.19	120.30
2	B	197	ARG	NE-CZ-NH1	-6.20	117.20	120.30
2	C	197	ARG	NE-CZ-NH1	-5.76	117.42	120.30
2	B	197	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	197	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	D	197	ARG	NE-CZ-NH1	-5.08	117.76	120.30

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	2878	0	2826	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2860	0	2780	8	0
2	B	2818	0	2723	17	0
2	C	2833	0	2763	10	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	23	0	0	1	0
4	D	23	0	0	1	0
5	C	5	0	0	0	0
6	A	145	0	0	0	0
6	B	117	0	0	0	0
6	C	145	0	0	0	0
6	D	143	0	0	0	0
All	All	11996	0	11092	47	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 2.

All (47) 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)
2:B:42:TYR:HB3	2:B:87:ILE:HD11	1.51	0.92
1:D:197:ARG:HD3	1:D:307:GLU:OE1	1.86	0.75
2:B:197:ARG:HD3	2:B:307:GLU:OE1	1.87	0.74
2:C:197:ARG:HD3	2:C:307:GLU:OE1	1.95	0.67
1:A:197:ARG:HD3	1:A:307:GLU:OE1	2.01	0.60
2:B:183:ILE:HD12	2:B:192:TYR:CG	2.41	0.56
2:C:106:GLY:O	2:C:133:ASP:HB3	2.07	0.55
2:B:46:TRP:CE3	2:B:87:ILE:HD12	2.42	0.54
1:A:292:SER:OG	1:A:300:ASP:O	2.25	0.52
2:C:107:ALA:HB2	2:C:297:PRO:HB2	1.92	0.50
1:D:15:LEU:HD21	1:D:173:GLU:HA	1.96	0.48
2:B:197:ARG:CD	2:B:307:GLU:OE1	2.60	0.47
1:A:18:PRO:HG3	1:A:176:PHE:CD1	2.50	0.47
2:C:82:LLP:NZ	2:C:82:LLP:O3	2.41	0.46
2:B:183:ILE:HD12	2:B:192:TYR:CD2	2.50	0.46
1:A:142:PHE:CE2	1:A:146:LEU:HD11	2.51	0.45
2:B:197:ARG:HG3	2:B:233:MET:HB3	1.98	0.45
1:D:127:ILE:HG21	1:D:144:MET:SD	2.57	0.45
1:D:295:ILE:CD1	1:D:328:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ARG:NH1	1:D:294:SER:O	2.49	0.45
2:B:110:HIS:CE1	2:B:184:GLY:HA2	2.52	0.44
2:C:15:LEU:HD21	2:C:173:GLU:HA	1.99	0.44
1:A:375:ASP:OD2	2:B:143[B]:ARG:NH2	2.51	0.44
2:C:197:ARG:CD	2:C:307:GLU:OE1	2.65	0.44
1:A:350:VAL:O	1:A:354:MET:HG3	2.17	0.44
1:A:90:ALA:HB3	1:A:91:PRO:HD3	1.99	0.44
1:D:90:ALA:HB3	1:D:91:PRO:HD3	2.00	0.44
2:B:274:LEU:HB3	2:B:281:PHE:CZ	2.53	0.43
1:A:119:ALA:O	2:B:58:ARG:NH1	2.50	0.43
2:B:274:LEU:HB3	2:B:281:PHE:CE1	2.54	0.43
2:B:42:TYR:CB	2:B:87:ILE:HD11	2.36	0.42
1:D:351:ALA:HA	1:D:354:MET:CE	2.49	0.42
2:C:295:ILE:HD13	2:C:328:LEU:HD13	2.02	0.42
1:A:289:ILE:HD11	1:A:302:PRO:HG2	2.01	0.42
4:D:403:FEV:OAG	4:D:403:FEV:NAP	2.52	0.42
1:A:351:ALA:HA	1:A:354:MET:CE	2.50	0.42
1:A:160:THR:OG1	1:A:161:ALA:N	2.52	0.41
2:B:34:GLU:OE1	2:C:40:ASN:ND2	2.53	0.41
2:B:301:TYR:CD1	2:B:302:PRO:HD2	2.55	0.41
2:B:90:ALA:HB3	2:B:91:PRO:HD3	2.03	0.41
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.56	0.41
2:C:301:TYR:CD1	2:C:302:PRO:HD2	2.56	0.41
2:C:11:VAL:HG22	2:C:15:LEU:HB2	2.02	0.40
4:A:403:FEV:NAP	4:A:403:FEV:OAG	2.53	0.40
1:D:257:LEU:HD21	1:D:321:THR:HG21	2.04	0.40
1:A:154:VAL:HG13	1:A:167:GLU:HG3	2.03	0.40
2:B:237:TYR:HB3	2:B:238:PRO:HD3	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	382/388 (98%)	376 (98%)	6 (2%)	0	100	100
1	D	383/388 (99%)	377 (98%)	5 (1%)	1 (0%)	41	22
2	B	368/388 (95%)	364 (99%)	3 (1%)	1 (0%)	41	22
2	C	372/388 (96%)	364 (98%)	8 (2%)	0	100	100
All	All	1505/1552 (97%)	1481 (98%)	22 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	VAL
2	B	186	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	284/305 (93%)	282 (99%)	2 (1%)	84	75
1	D	279/305 (92%)	275 (99%)	4 (1%)	67	52
2	B	270/304 (89%)	270 (100%)	0	100	100
2	C	276/304 (91%)	275 (100%)	1 (0%)	91	87
All	All	1109/1218 (91%)	1102 (99%)	7 (1%)	86	79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	263	SER
2	C	375	ASP
1	D	28	ARG
1	D	182	LEU
1	D	274	LEU
1	D	385	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	150	ASN
2	C	267	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)

2 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	$\#\|Z\| > 2$
2	LLP	B	82	2	23,24,25	2.69	5 (21%)	25,32,34	1.49	5 (20%)
2	LLP	C	82	2	23,24,25	2.60	5 (21%)	25,32,34	1.39	3 (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
2	LLP	B	82	2	-	4/16/17/19	0/1/1/1
2	LLP	C	82	2	-	3/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	82	LLP	C3-C2	7.83	1.48	1.40
2	B	82	LLP	C3-C2	7.35	1.48	1.40
2	B	82	LLP	C4'-NZ	5.92	1.47	1.27
2	B	82	LLP	C4-C5	5.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	82	LLP	C4'-NZ	5.49	1.45	1.27
2	C	82	LLP	C4-C5	5.40	1.48	1.42
2	B	82	LLP	C4-C3	5.25	1.48	1.40
2	C	82	LLP	C4-C3	4.64	1.47	1.40
2	B	82	LLP	C4-C4'	2.78	1.51	1.46
2	C	82	LLP	C4-C4'	2.29	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	82	LLP	C4-C4'-NZ	-3.48	108.35	124.31
2	B	82	LLP	C4-C4'-NZ	-3.36	108.90	124.31
2	C	82	LLP	C4-C3-C2	-3.16	118.23	120.19
2	B	82	LLP	C3-C4-C5	-2.88	116.05	118.26
2	B	82	LLP	C4-C3-C2	-2.39	118.71	120.19
2	C	82	LLP	O3-C3-C2	2.20	122.29	117.49
2	B	82	LLP	CD-CE-NZ	2.18	116.28	110.93
2	B	82	LLP	C5-C4-C4'	2.13	125.06	121.56

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	82	LLP	C4-C4'-NZ-CE
2	C	82	LLP	C4-C4'-NZ-CE
2	C	82	LLP	CG-CD-CE-NZ
2	B	82	LLP	CE-CD-CG-CB
2	B	82	LLP	CA-CB-CG-CD
2	B	82	LLP	C3-C4-C4'-NZ
2	C	82	LLP	CD-CE-NZ-C4'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	82	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	FEV	D	403	-	22,23,23	2.56	7 (31%)	26,32,32	1.59	4 (15%)
5	PO4	C	402	-	4,4,4	0.92	0	6,6,6	0.50	0
4	FEV	A	403	-	22,23,23	2.76	8 (36%)	26,32,32	1.60	4 (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	FEV	D	403	-	-	0/16/18/18	0/1/1/1
4	FEV	A	403	-	-	0/16/18/18	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	FEV	CAQ-CAR	6.10	1.54	1.48
4	A	403	FEV	CAH-CAD	-5.65	1.40	1.50
4	A	403	FEV	CAO-NAP	5.59	1.35	1.28
4	D	403	FEV	CAH-CAD	-5.58	1.40	1.50
4	D	403	FEV	CAQ-CAR	5.11	1.53	1.48
4	D	403	FEV	CAQ-NAP	-4.37	1.35	1.41
4	D	403	FEV	CAO-NAP	4.13	1.33	1.28
4	D	403	FEV	CAF-CAO	-3.55	1.39	1.46
4	A	403	FEV	CAQ-NAP	-3.50	1.36	1.41
4	A	403	FEV	PAK-OAM	3.38	1.61	1.50
4	D	403	FEV	CAB-NAC	3.36	1.41	1.34
4	A	403	FEV	CAB-NAC	3.20	1.41	1.34
4	D	403	FEV	CAI-CAA	-3.02	1.42	1.50
4	A	403	FEV	CAI-CAA	-2.99	1.42	1.50
4	A	403	FEV	CAF-CAO	-2.81	1.41	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	FEV	CAF-CAE-CAD	4.57	123.02	120.19
4	D	403	FEV	OAU-CAR-CAQ	4.30	120.50	113.42
4	A	403	FEV	OAU-CAR-CAQ	4.00	120.01	113.42
4	D	403	FEV	CAF-CAE-CAD	3.92	122.61	120.19
4	D	403	FEV	OAJ-PAK-OAM	2.89	114.57	106.47
4	D	403	FEV	CAW-CAV-CAS	-2.57	105.42	112.81
4	A	403	FEV	CAW-CAV-CAS	-2.40	105.92	112.81
4	A	403	FEV	OAN-PAK-OAJ	2.12	112.38	106.73

There are no chirality outliers.

There are no torsion outliers.

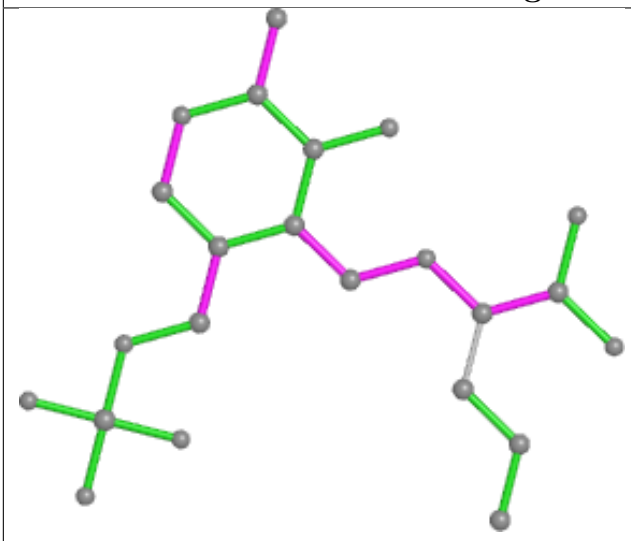
There are no ring outliers.

2 monomers are involved in 2 short contacts:

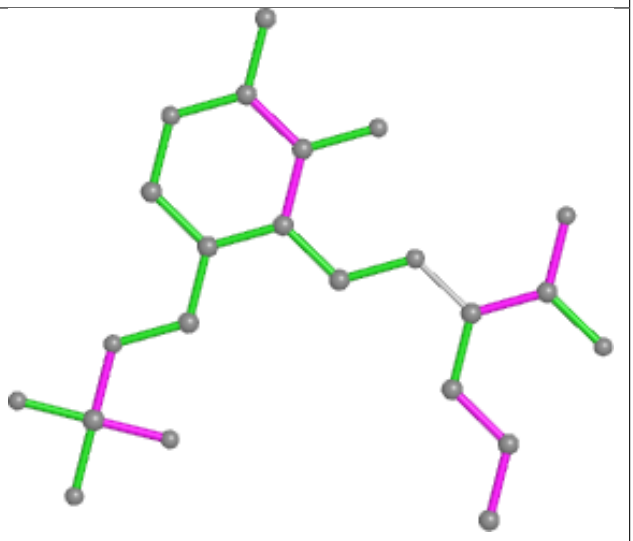
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	FEV	1	0
4	A	403	FEV	1	0

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.

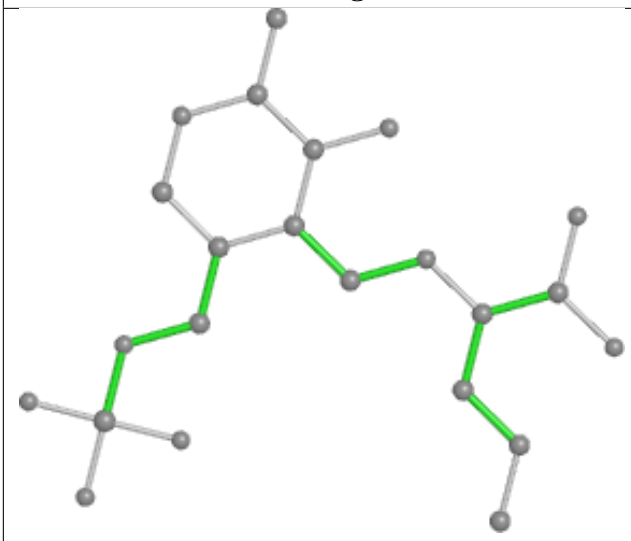
Ligand FEV D 403



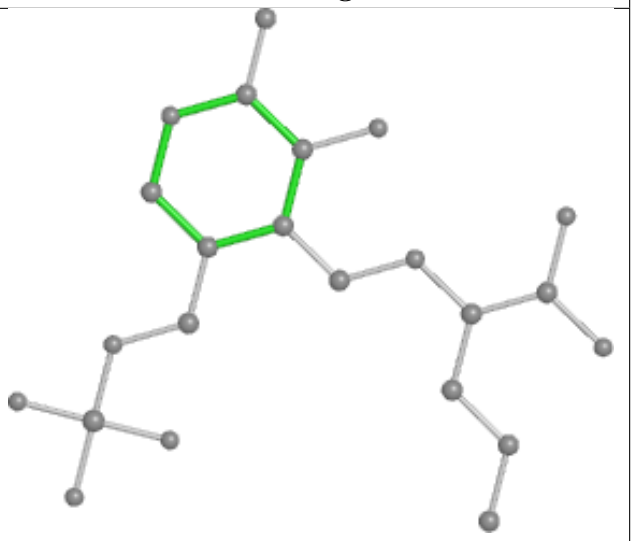
Bond lengths



Bond angles

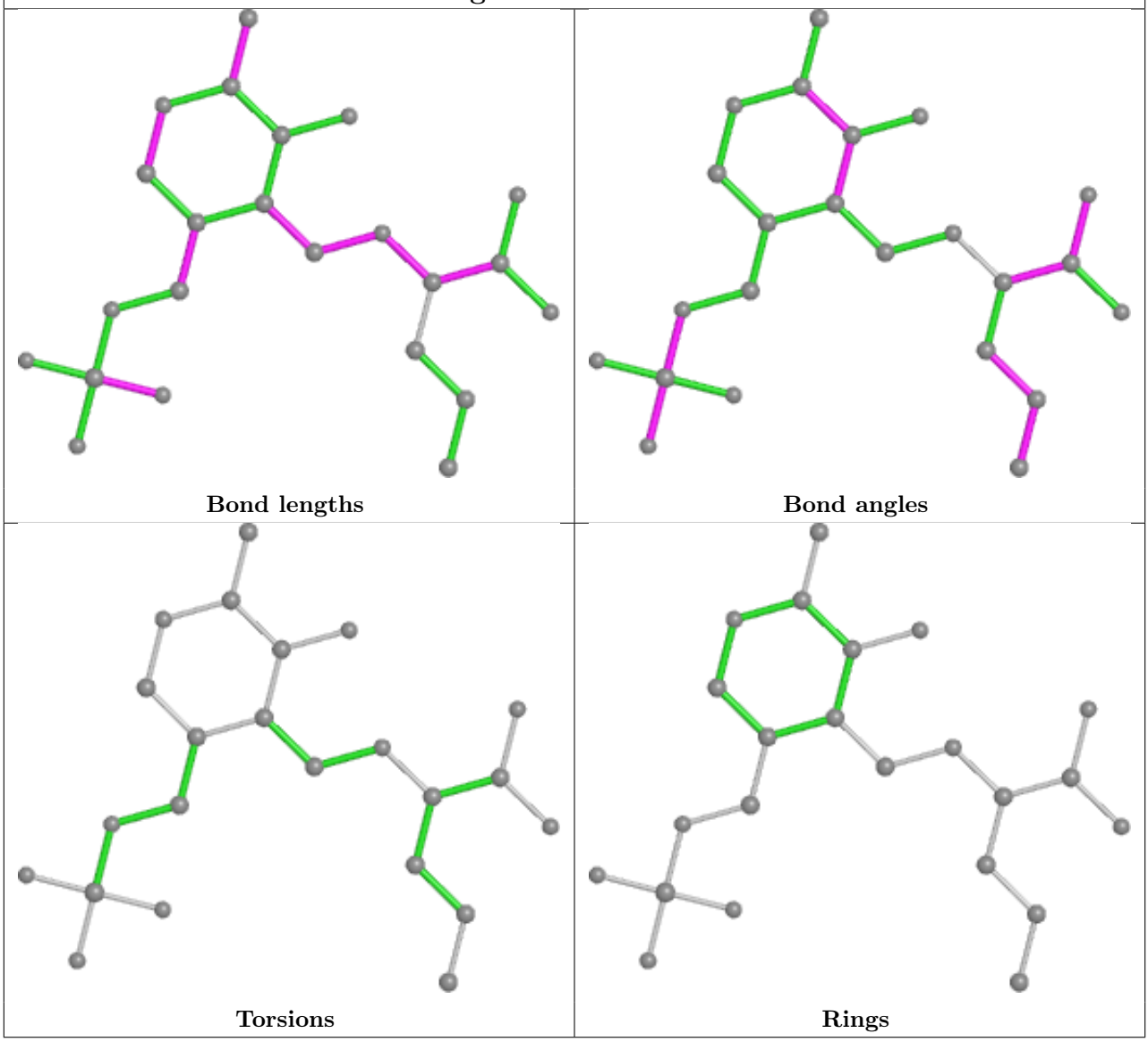


Torsions



Rings

Ligand FEV A 403



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, 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	383/388 (98%)	0.57	17 (4%)	34	40	21, 35, 57, 72	0
1	D	385/388 (99%)	0.55	32 (8%)	11	14	19, 34, 73, 101	0
2	B	375/388 (96%)	0.65	35 (9%)	8	11	23, 38, 70, 116	0
2	C	376/388 (96%)	0.46	19 (5%)	28	34	19, 32, 60, 87	0
All	All	1519/1552 (97%)	0.56	103 (6%)	17	22	19, 35, 66, 116	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	164	ALA	8.7
2	B	165	ILE	5.1
2	C	382	LEU	4.7
2	B	160	THR	4.5
2	B	174	ALA	4.2
2	B	161	ALA	4.0
1	D	178	TYR	4.0
1	A	157	GLY	3.9
2	C	155	ASN	3.9
1	D	286	GLU	3.9
2	B	162	LYS	3.8
1	D	288	GLN	3.7
2	B	136	ARG	3.7
2	B	153	PRO	3.7
1	D	75	LEU	3.6
2	B	382	LEU	3.6
2	C	154	VAL	3.5
1	D	153	PRO	3.5
2	C	156	SER	3.5
2	C	130	GLY	3.4
2	C	131	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	284	ASP	3.3
2	B	143[A]	ARG	3.3
1	D	285	GLU	3.3
2	C	107	ALA	3.3
1	D	176	PHE	3.3
2	B	14	THR	3.2
1	D	340	ILE	3.2
2	B	152	ILE	3.2
1	D	152	ILE	3.2
2	B	154	VAL	3.1
2	C	132	GLU	3.1
2	C	269	GLY	3.1
1	D	112	VAL	3.1
2	B	287	GLY	3.0
2	B	142	PHE	3.0
2	C	176	PHE	3.0
1	D	154	VAL	3.0
1	D	158	SER	3.0
2	B	155	ASN	2.9
1	D	287	GLY	2.9
1	D	147	LEU	2.9
2	B	291	PRO	2.9
2	C	291	PRO	2.8
2	C	381	VAL	2.8
2	C	260	GLY	2.8
1	D	80	ALA	2.8
1	D	289	ILE	2.7
2	B	147	LEU	2.7
2	B	151	VAL	2.7
1	D	174	ALA	2.7
1	A	295	ILE	2.7
1	A	143[A]	ARG	2.6
1	A	382	LEU	2.6
1	D	157	GLY	2.5
2	B	175	THR	2.5
1	D	164	ALA	2.5
2	C	301	TYR	2.5
1	A	155	ASN	2.5
2	B	260	GLY	2.4
1	A	142	PHE	2.4
1	D	382	LEU	2.4
1	D	28	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	156	SER	2.4
2	B	281	PHE	2.4
1	A	329	LYS	2.4
2	B	158	SER	2.4
1	A	328	LEU	2.4
2	C	31	ASP	2.4
1	A	76	VAL	2.3
1	A	256	GLY	2.3
1	D	131	ALA	2.3
2	B	107	ALA	2.3
2	C	134	VAL	2.3
2	B	274	LEU	2.3
2	C	75	LEU	2.3
2	B	120	LEU	2.2
1	A	183	ILE	2.2
2	B	292	SER	2.2
1	D	134	VAL	2.2
1	D	79	GLY	2.2
2	B	137	GLN	2.2
2	B	79	GLY	2.2
1	A	381	VAL	2.2
2	B	75	LEU	2.2
1	D	372	GLY	2.2
2	B	284	ASP	2.2
2	B	363	ASP	2.2
2	C	284	ASP	2.2
1	A	259	SER	2.1
2	B	76	VAL	2.1
1	A	158	SER	2.1
1	A	229	GLY	2.1
2	B	140	ASN	2.1
1	D	373	ARG	2.0
1	A	160	THR	2.0
1	D	281	PHE	2.0
1	D	33	GLU	2.0
1	A	80	ALA	2.0
2	B	47	ALA	2.0
1	D	259	SER	2.0
1	D	291	PRO	2.0
2	C	78	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	LLP	B	82	24/25	0.95	0.13	28,30,32,32	0
2	LLP	C	82	24/25	0.96	0.14	18,22,23,23	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

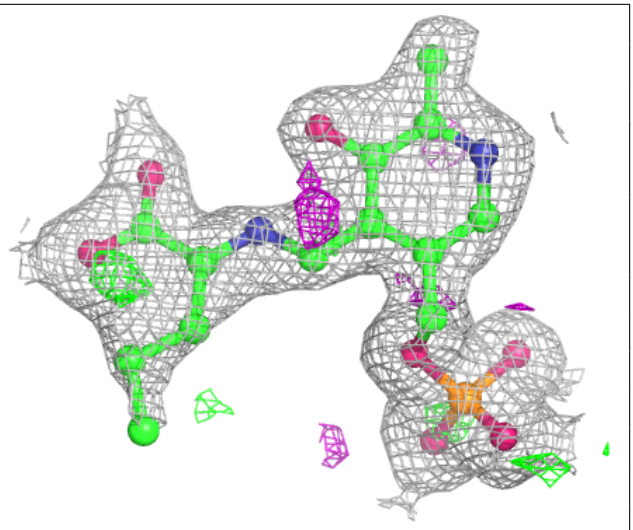
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

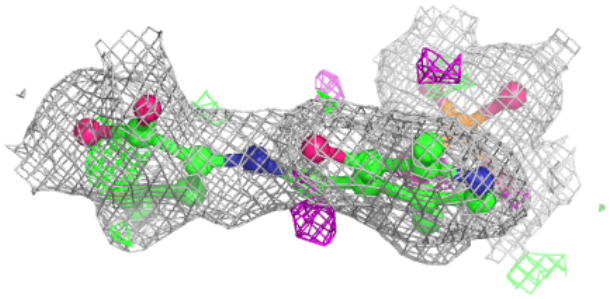
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	C	402	5/5	0.90	0.15	62,65,65,66	0
3	NA	A	402	1/1	0.93	0.33	39,39,39,39	0
4	FEV	A	403	23/23	0.94	0.17	21,30,38,39	0
4	FEV	D	403	23/23	0.95	0.14	23,27,34,35	0
3	NA	B	401	1/1	0.95	0.15	26,26,26,26	0
3	NA	A	401	1/1	0.97	0.13	24,24,24,24	0
3	NA	D	402	1/1	0.98	0.15	32,32,32,32	0
3	NA	C	401	1/1	0.98	0.12	22,22,22,22	0
3	NA	D	401	1/1	0.99	0.18	18,18,18,18	0

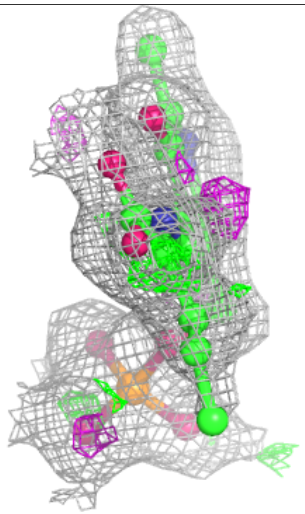
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FEV A 403:

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

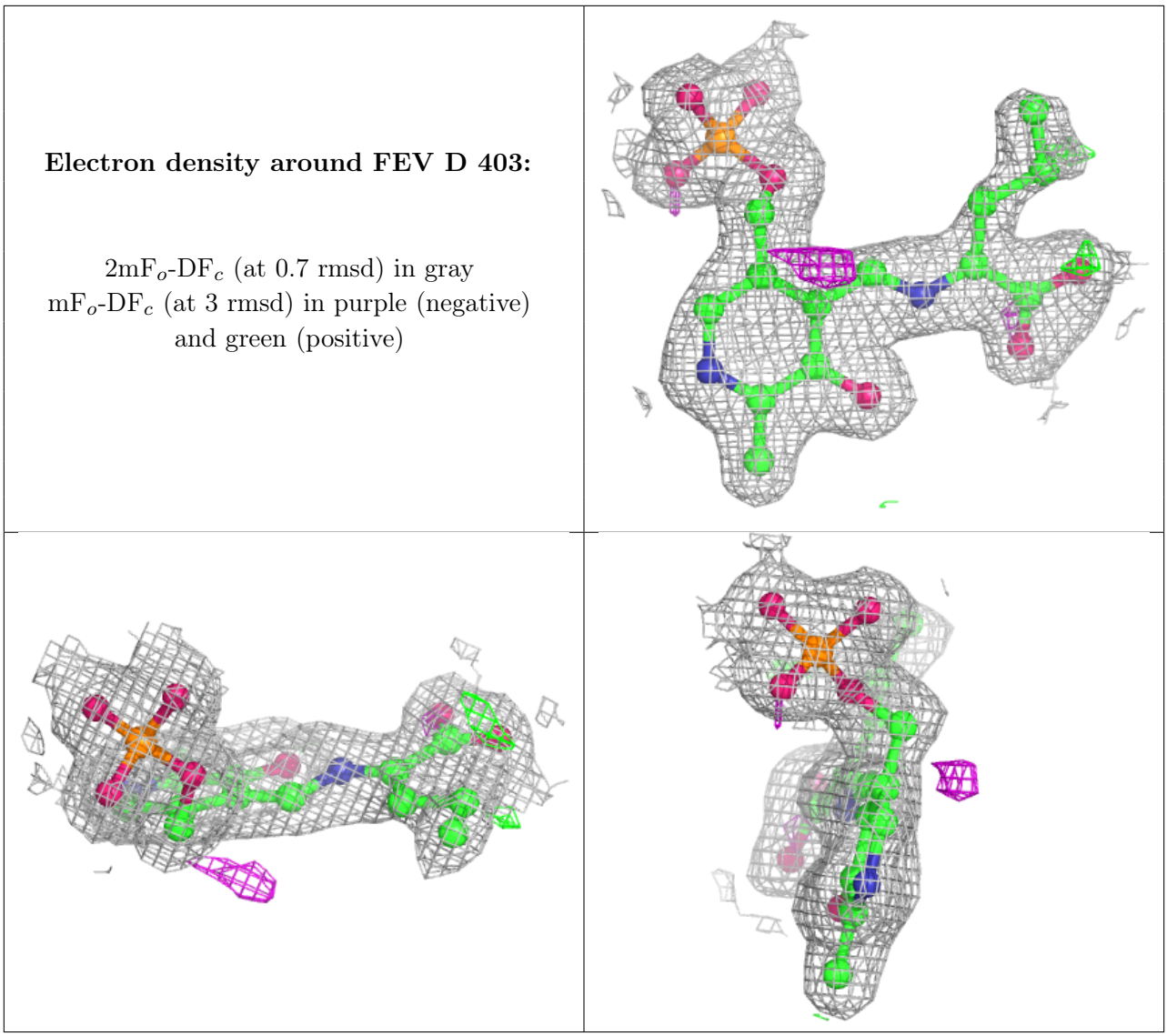






Electron density around FEV D 403:

$2mF_o$-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.