Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 01:14 pm BST

PDB ID	:	7YXJ
Title	:	Drosophila melanogaster JMJD7 (dmJMJD7) in complex with Mn and 2,4-PDCA
Authors	:	Chowdhury, R.; Schofield, C.J.
Deposited on	:	2022-02-16
Resolution	:	2.45 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 following versions of software and data (see references ⓘ) were used in the production of this report:

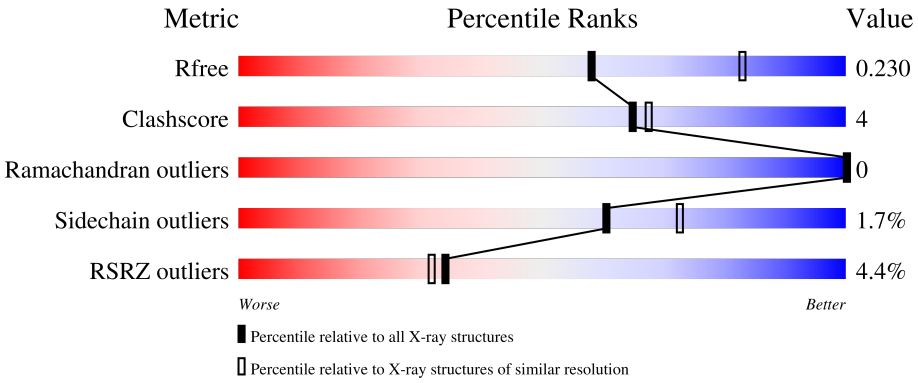
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	322	91% 6% .
1	B	322	5% 85% 11% .
1	C	322	3% 85% 11% .
1	D	322	8% 85% 10% .

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	EDO	D	502	-	-	-	X
4	EDO	D	505	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19299 atoms, of which 9211 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 GH14974p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	3	0
			4873	1603	2371	419	469	11			
1	B	309	Total	C	H	N	O	S	0	1	0
			4679	1560	2254	398	456	11			
1	C	309	Total	C	H	N	O	S	0	3	0
			4620	1548	2209	396	456	11			
1	D	308	Total	C	H	N	O	S	0	2	0
			4721	1567	2278	401	464	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9VU77
A	-4	SER	-	expression tag	UNP Q9VU77
A	-3	HIS	-	expression tag	UNP Q9VU77
A	-2	MET	-	expression tag	UNP Q9VU77
A	-1	ALA	-	expression tag	UNP Q9VU77
A	0	SER	-	expression tag	UNP Q9VU77
B	-5	GLY	-	expression tag	UNP Q9VU77
B	-4	SER	-	expression tag	UNP Q9VU77
B	-3	HIS	-	expression tag	UNP Q9VU77
B	-2	MET	-	expression tag	UNP Q9VU77
B	-1	ALA	-	expression tag	UNP Q9VU77
B	0	SER	-	expression tag	UNP Q9VU77
C	-5	GLY	-	expression tag	UNP Q9VU77
C	-4	SER	-	expression tag	UNP Q9VU77
C	-3	HIS	-	expression tag	UNP Q9VU77
C	-2	MET	-	expression tag	UNP Q9VU77
C	-1	ALA	-	expression tag	UNP Q9VU77
C	0	SER	-	expression tag	UNP Q9VU77
D	-5	GLY	-	expression tag	UNP Q9VU77
D	-4	SER	-	expression tag	UNP Q9VU77
D	-3	HIS	-	expression tag	UNP Q9VU77

Continued on next page...

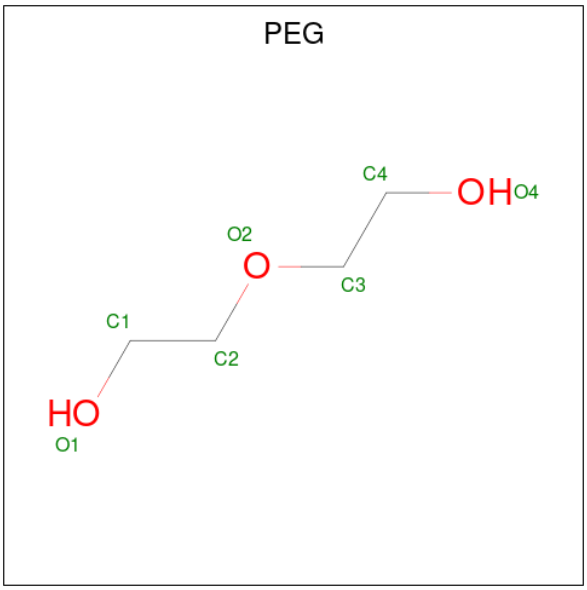
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP Q9VU77
D	-1	ALA	-	expression tag	UNP Q9VU77
D	0	SER	-	expression tag	UNP Q9VU77

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

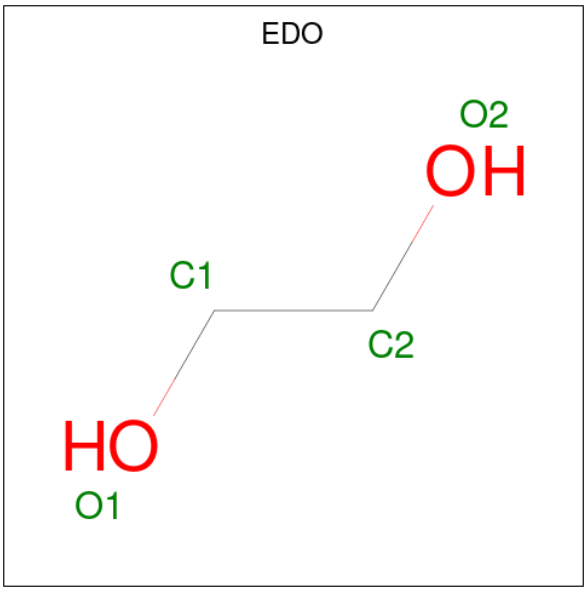
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 16 4 9 3	0	0

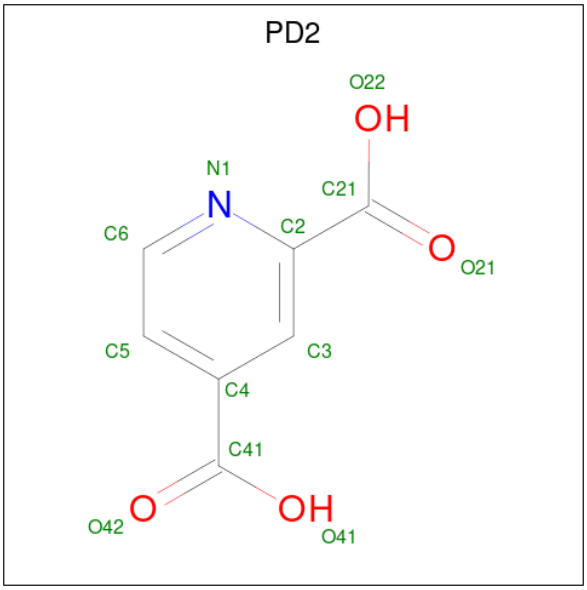
- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is PYRIDINE-2,4-DICARBOXYLIC ACID (three-letter code: PD2) (formula:

$C_7H_5NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H N O 15 7 3 1 4	0	0
5	B	1	Total C H N O 15 7 3 1 4	0	0
5	C	1	Total C H N O 15 7 3 1 4	0	0
5	D	1	Total C H N O 15 7 3 1 4	0	0

- Molecule 6 is water.

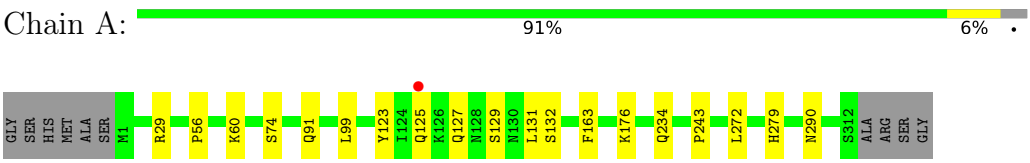
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	96	Total O 96 96	0	0
6	B	44	Total O 44 44	0	0
6	C	20	Total O 20 20	0	0
6	D	36	Total O 36 36	0	0

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.

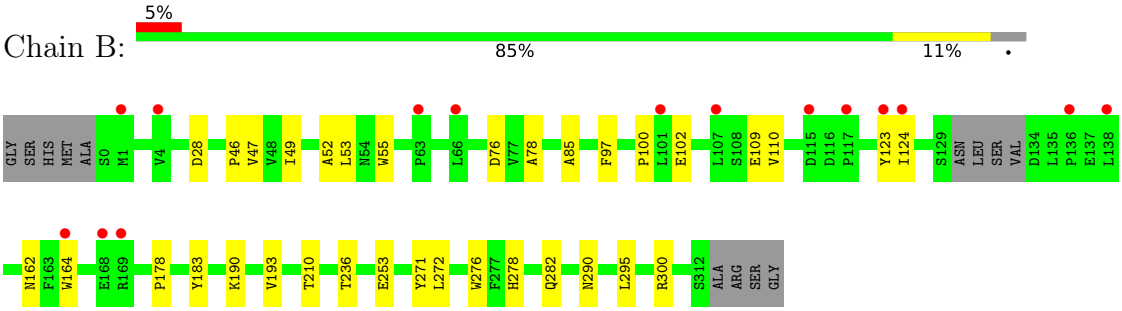
- Molecule 1: GH14974p

Chain A:



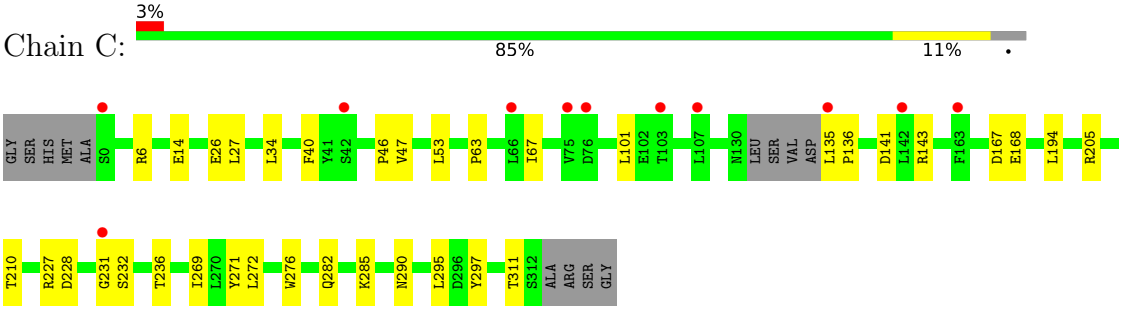
- Molecule 1: GH14974p

Chain B:



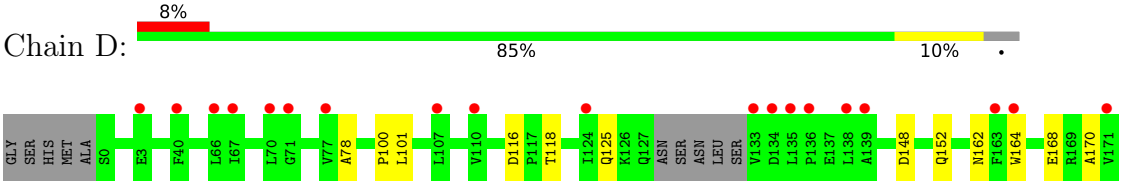
- Molecule 1: GH14974p

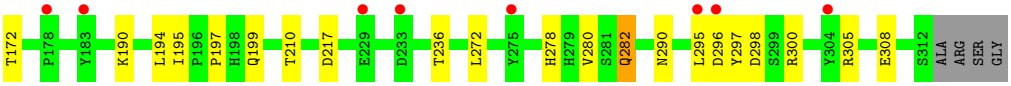
Chain C:



- Molecule 1: GH14974p

Chain D:




T172
P178
Y183
K190
L194
I195
P196
P197
H198
Q199
T210
D217
E229
D233
T236
L272
Y275
H278
H279
V280
S281
Q282
N290
L295
D296
Y297
D298
S299
R300
Y304
R305
E308
S312
ALA
ARG
SER
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.56Å 65.76Å 206.96Å 90.00° 97.78° 90.00°	Depositor
Resolution (Å)	55.35 – 2.45 55.35 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.35-2.45) 99.7 (55.35-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.206 , 0.230 0.207 , 0.230	Depositor DCC
R_{free} test set	2520 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19299	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: PD2, MN, CSO, PEG, EDO

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	0.35	0/2564	0.52	0/3500
1	B	0.35	0/2486	0.50	0/3401
1	C	0.35	0/2488	0.51	0/3410
1	D	0.34	0/2504	0.51	0/3422
All	All	0.35	0/10042	0.51	0/13733

There are no bond length outliers.

There are no bond angle outliers.

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	2502	2371	2368	11	0
1	B	2425	2254	2254	22	0
1	C	2411	2209	2198	22	0
1	D	2443	2278	2276	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	9	10	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	24	24	1	0
4	B	16	24	24	3	0
4	C	4	6	6	0	0
4	D	16	24	24	5	0
5	A	12	3	3	0	0
5	B	12	3	3	0	0
5	C	12	3	3	0	0
5	D	12	3	3	0	0
6	A	96	0	0	0	0
6	B	44	0	0	0	0
6	C	20	0	0	0	0
6	D	36	0	0	0	0
All	All	10088	9211	9196	79	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 (79) 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:B:49:ILE:HG22	1:B:52:ALA:HB2	1.61	0.83
1:A:176:LYS:H	3:A:502:PEG:H21	1.46	0.80
1:C:194:LEU:HD22	1:C:272:LEU:HD11	1.71	0.71
1:B:190:LYS:HD3	1:B:282:GLN:HB3	1.75	0.69
1:D:300:ARG:HD3	4:D:505:EDO:H12	1.75	0.69
1:D:295:LEU:HD11	1:D:297:TYR:CE1	2.31	0.66
1:B:164:TRP:HB3	4:B:505:EDO:H22	1.79	0.63
1:B:210:THR:HG22	1:B:236:THR:HG22	1.82	0.61
1:C:210:THR:HG22	1:C:236:THR:HG22	1.81	0.61
1:D:164:TRP:HB3	4:D:503:EDO:H11	1.84	0.59
1:D:125:GLN:HG3	1:D:164:TRP:CZ3	2.38	0.59
1:D:116:ASP:OD1	1:D:118:THR:OG1	2.20	0.58
1:B:28:ASP:OD1	4:B:504:EDO:O2	2.22	0.57
1:A:29[B]:ARG:HB3	1:A:29[B]:ARG:NH1	2.21	0.56
1:C:14:GLU:OE1	1:D:305[B]:ARG:NH2	2.38	0.56
1:D:298[B]:ASP:OD1	1:D:298[B]:ASP:N	2.39	0.55
1:A:129:SER:HG	1:A:132:SER:HG	1.55	0.55
1:B:300:ARG:HD2	4:B:502:EDO:H11	1.88	0.54
1:B:253:GLU:OE1	1:B:253:GLU:N	2.35	0.54
1:C:227:ARG:NE	1:C:231:GLY:O	2.41	0.53
1:D:295:LEU:HD11	1:D:297:TYR:CD1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:NH2	1:C:311:THR:OG1	2.42	0.52
1:D:305[A]:ARG:HD2	1:D:308:GLU:OE1	2.09	0.52
1:B:210:THR:HG22	1:B:236:THR:CG2	2.40	0.51
1:D:190:LYS:HD3	1:D:282:GLN:HB3	1.91	0.51
1:B:49:ILE:CG2	1:B:52:ALA:HB2	2.36	0.51
1:D:300:ARG:HG2	4:D:505:EDO:H11	1.93	0.50
1:D:210:THR:HG22	1:D:236:THR:CG2	2.41	0.50
1:C:63:PRO:HG2	1:C:285:LYS:HE2	1.94	0.50
1:A:176:LYS:HG2	3:A:502:PEG:H22	1.94	0.49
1:D:300:ARG:HD3	4:D:505:EDO:C1	2.42	0.49
1:B:193:VAL:O	1:B:278:HIS:HA	2.13	0.48
1:C:295:LEU:HD21	1:C:297:TYR:CZ	2.48	0.48
1:A:176:LYS:HG2	3:A:502:PEG:C2	2.44	0.48
1:B:183:TYR:OH	1:B:190:LYS:HE3	2.14	0.48
1:C:34:LEU:HD21	1:D:152:GLN:HB3	1.96	0.47
1:B:47:VAL:HG12	1:B:271:TYR:HB3	1.97	0.47
1:B:110:VAL:HG11	1:B:124:ILE:HD11	1.96	0.46
1:D:194:LEU:HD22	1:D:272:LEU:HD11	1.96	0.46
1:B:210:THR:CG2	1:B:236:THR:HG22	2.45	0.45
1:B:162:ASN:HB2	1:B:290:ASN:OD1	2.17	0.45
1:D:195:ILE:HG23	1:D:199:GLN:OE1	2.17	0.45
1:D:170:ALA:O	1:D:282:GLN:NE2	2.50	0.45
1:C:210:THR:HG22	1:C:236:THR:CG2	2.44	0.45
1:D:101:LEU:C	1:D:101:LEU:HD23	2.38	0.45
1:A:29[B]:ARG:HB3	1:A:29[B]:ARG:HH11	1.82	0.44
1:C:53:LEU:HD21	1:C:269:ILE:HD11	1.98	0.44
1:B:97:PHE:CD2	1:B:236:THR:HG21	2.52	0.44
1:C:46:PRO:HD3	1:C:276:TRP:CZ2	2.52	0.43
1:D:162:ASN:HB2	1:D:290:ASN:OD1	2.18	0.43
1:D:197:PRO:HB2	4:D:505:EDO:O1	2.19	0.43
1:D:78:ALA:HB1	1:D:100:PRO:HB2	2.00	0.43
1:B:78:ALA:HB1	1:B:100:PRO:HB2	2.01	0.43
1:C:101:LEU:C	1:C:101:LEU:HD23	2.38	0.43
1:C:227:ARG:HE	1:C:232:SER:HA	1.83	0.43
1:D:172:THR:HB	1:D:280:VAL:HB	2.01	0.43
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.83	0.43
1:B:46:PRO:HD3	1:B:276:TRP:CZ2	2.54	0.43
1:D:125:GLN:HG3	1:D:164:TRP:CE3	2.54	0.43
1:C:135:LEU:CB	1:C:136:PRO:HD3	2.49	0.42
1:C:26:GLU:O	1:C:27:LEU:HD23	2.20	0.42
1:C:40:PHE:CZ	1:C:47:VAL:HG21	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ASP:OD1	1:C:168:GLU:N	2.53	0.42
1:C:63:PRO:O	1:C:67:ILE:CG1	2.68	0.42
1:A:131:LEU:HD12	1:A:163:PHE:HB2	2.02	0.42
1:A:243:PRO:HG2	1:A:279:HIS:CD2	2.55	0.42
1:D:295:LEU:HD12	1:D:295:LEU:C	2.41	0.41
1:A:91:GLN:OE1	4:A:505:EDO:H21	2.20	0.41
1:C:47:VAL:HG12	1:C:271:TYR:HB3	2.01	0.41
1:B:109:GLU:HA	1:B:109:GLU:OE1	2.21	0.41
1:D:168:GLU:O	1:D:168:GLU:HG3	2.20	0.41
1:B:53:LEU:HD22	1:B:55:TRP:NE1	2.36	0.41
1:C:228:ASP:O	1:C:231:GLY:N	2.53	0.41
1:D:272:LEU:HD21	1:D:278:HIS:CG	2.56	0.41
1:B:85:ALA:CB	1:B:123:TYR:HE2	2.34	0.41
1:B:178:PRO:O	1:B:295:LEU:HD22	2.21	0.40
1:A:56:PRO:O	1:A:60:LYS:HG3	2.21	0.40
1:A:99:LEU:HD12	1:A:99:LEU:N	2.36	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	312/322 (97%)	306 (98%)	6 (2%)	0	100	100
1	B	305/322 (95%)	300 (98%)	5 (2%)	0	100	100
1	C	307/322 (95%)	294 (96%)	13 (4%)	0	100	100
1	D	305/322 (95%)	297 (97%)	8 (3%)	0	100	100
All	All	1229/1288 (95%)	1197 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	263/283 (93%)	256 (97%)	7 (3%)	44	57
1	B	249/283 (88%)	246 (99%)	3 (1%)	71	81
1	C	245/283 (87%)	242 (99%)	3 (1%)	71	81
1	D	254/283 (90%)	250 (98%)	4 (2%)	62	74
All	All	1011/1132 (89%)	994 (98%)	17 (2%)	60	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	123	TYR
1	A	125	GLN
1	A	127	GLN
1	A	234	GLN
1	A	272	LEU
1	A	290	ASN
1	B	76	ASP
1	B	102	GLU
1	B	272	LEU
1	C	141	ASP
1	C	282	GLN
1	C	290	ASN
1	D	148	ASP
1	D	217	ASP
1	D	282	GLN
1	D	296	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	CSO	C	19	1	3,6,7	0.61	0	0,6,8	-	-
1	CSO	B	19	1	3,6,7	0.72	0	0,6,8	-	-
1	CSO	A	19	1	3,6,7	0.63	0	0,6,8	-	-
1	CSO	D	19	1	3,6,7	0.67	0	0,6,8	-	-

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	CSO	C	19	1	-	0/1/5/7	-
1	CSO	B	19	1	-	0/1/5/7	-
1	CSO	A	19	1	-	0/1/5/7	-
1	CSO	D	19	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	PD2	D	506	2	7,12,12	3.60	2 (28%)	8,16,16	1.53	2 (25%)
5	PD2	A	507	2	7,12,12	3.44	2 (28%)	8,16,16	1.46	1 (12%)
4	EDO	B	503	-	3,3,3	0.61	0	2,2,2	0.44	0
4	EDO	A	506	-	3,3,3	0.53	0	2,2,2	0.33	0
4	EDO	D	502	-	3,3,3	0.74	0	2,2,2	0.17	0
4	EDO	D	505	-	3,3,3	0.70	0	2,2,2	0.53	0
4	EDO	A	503	-	3,3,3	0.53	0	2,2,2	0.40	0
4	EDO	A	504	-	3,3,3	0.56	0	2,2,2	0.44	0
4	EDO	D	504	-	3,3,3	0.60	0	2,2,2	0.37	0
4	EDO	B	505	-	3,3,3	0.61	0	2,2,2	0.34	0
4	EDO	B	502	-	3,3,3	0.67	0	2,2,2	0.56	0
4	EDO	B	504	-	3,3,3	0.57	0	2,2,2	0.46	0
4	EDO	D	503	-	3,3,3	0.66	0	2,2,2	0.29	0
3	PEG	A	502	-	6,6,6	0.59	0	5,5,5	0.42	0
5	PD2	C	503	2	7,12,12	3.45	2 (28%)	8,16,16	1.76	2 (25%)
4	EDO	A	505	-	3,3,3	0.70	0	2,2,2	0.38	0
5	PD2	B	506	2	7,12,12	3.64	2 (28%)	8,16,16	1.55	1 (12%)
4	EDO	C	502	-	3,3,3	0.55	0	2,2,2	0.47	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
5	PD2	D	506	2	-	0/0/8/8	0/1/1/1
5	PD2	A	507	2	-	0/0/8/8	0/1/1/1
4	EDO	B	503	-	-	1/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	D	502	-	-	1/1/1/1	-
4	EDO	D	505	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	B	502	-	-	0/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
3	PEG	A	502	-	-	1/4/4/4	-
5	PD2	C	503	2	-	0/0/8/8	0/1/1/1
4	EDO	A	505	-	-	1/1/1/1	-
5	PD2	B	506	2	-	0/0/8/8	0/1/1/1
4	EDO	C	502	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506	PD2	C4-C41	-9.16	1.38	1.47
5	D	506	PD2	C4-C41	-9.15	1.38	1.47
5	C	503	PD2	C4-C41	-8.64	1.39	1.47
5	A	507	PD2	C4-C41	-8.62	1.39	1.47
5	B	506	PD2	C3-C4	-2.48	1.35	1.39
5	A	507	PD2	C3-C4	-2.38	1.35	1.39
5	C	503	PD2	C3-C4	-2.12	1.36	1.39
5	D	506	PD2	C3-C4	-2.01	1.36	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	503	PD2	C5-C6-N1	-3.74	119.31	123.96
5	D	506	PD2	C5-C6-N1	-3.22	119.96	123.96
5	A	507	PD2	C5-C6-N1	-3.17	120.02	123.96
5	B	506	PD2	C5-C6-N1	-3.09	120.12	123.96
5	C	503	PD2	C6-N1-C2	2.40	120.60	117.23
5	D	506	PD2	C6-N1-C2	2.06	120.12	117.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PEG	O2-C3-C4-O4
4	D	505	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	505	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
4	D	502	EDO	O1-C1-C2-O2

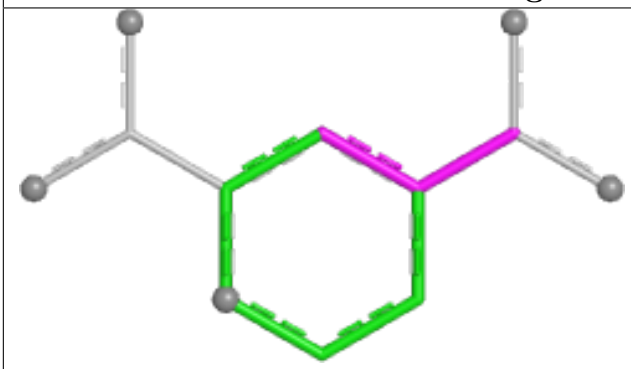
There are no ring outliers.

7 monomers are involved in 12 short contacts:

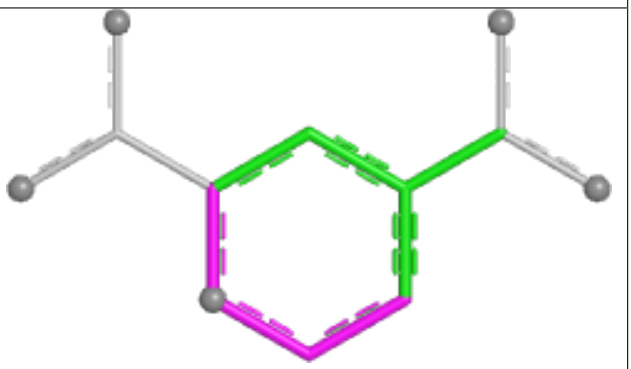
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	505	EDO	4	0
4	B	505	EDO	1	0
4	B	502	EDO	1	0
4	B	504	EDO	1	0
4	D	503	EDO	1	0
3	A	502	PEG	3	0
4	A	505	EDO	1	0

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.

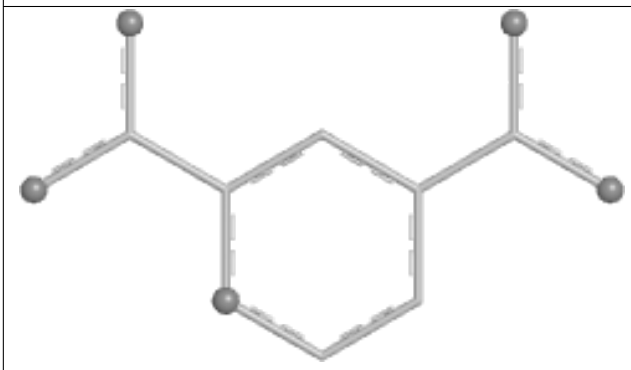
Ligand PD2 D 506



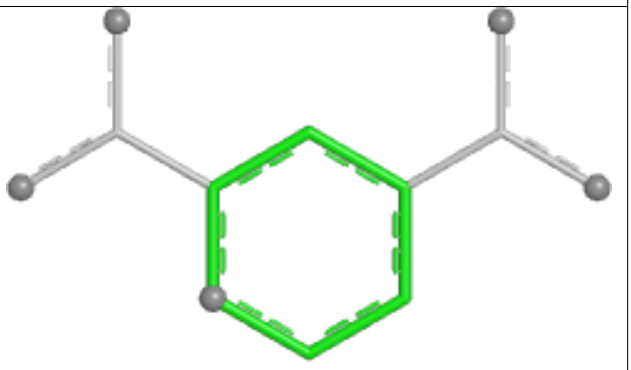
Bond lengths



Bond angles

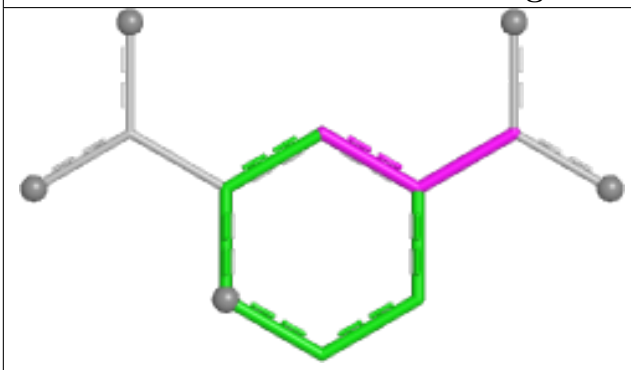


Torsions

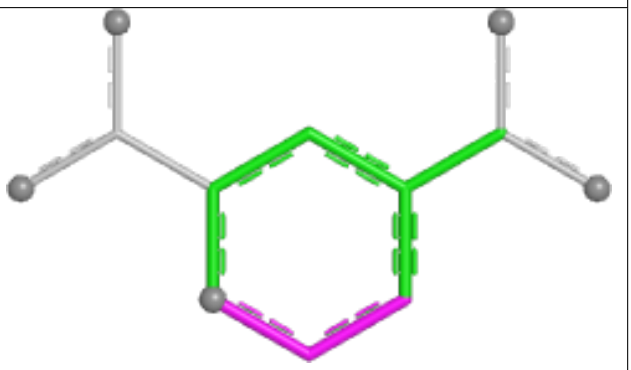


Rings

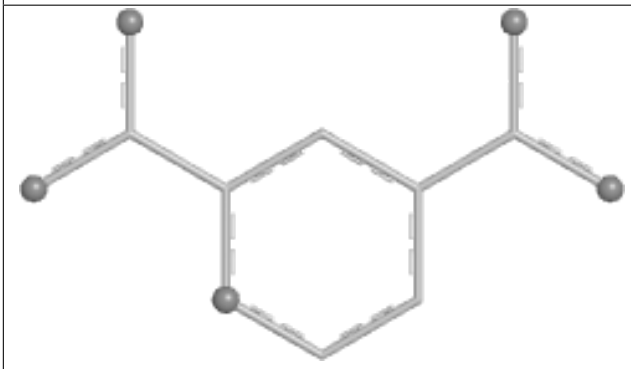
Ligand PD2 A 507



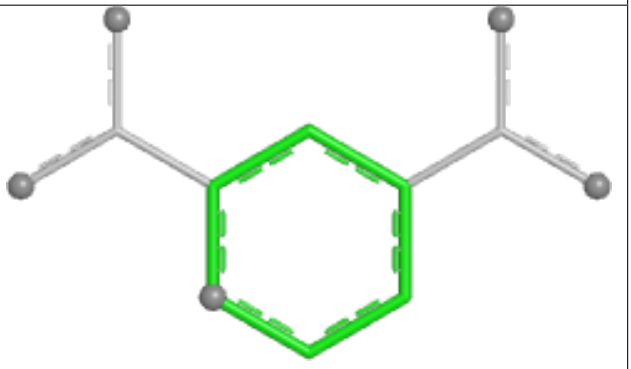
Bond lengths



Bond angles

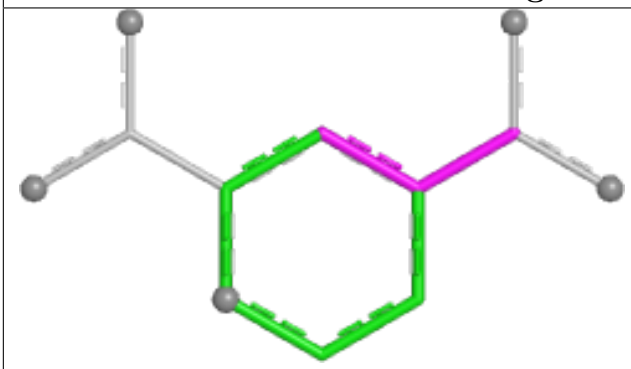


Torsions

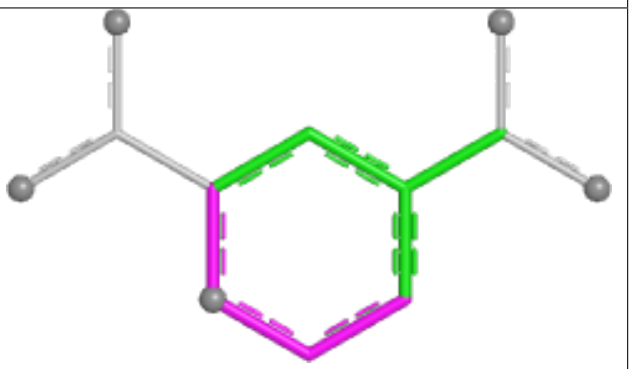


Rings

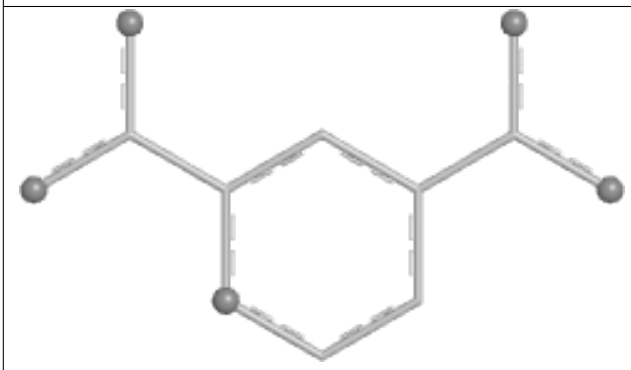
Ligand PD2 C 503



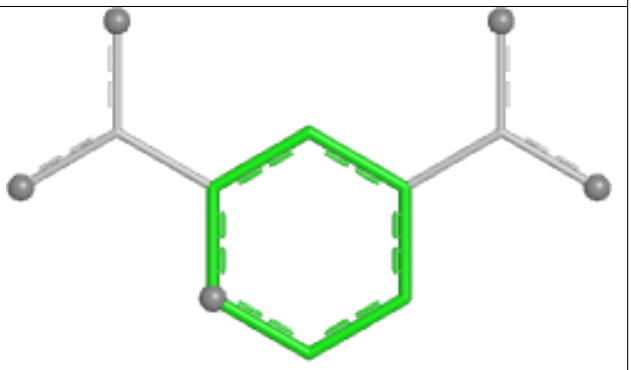
Bond lengths



Bond angles

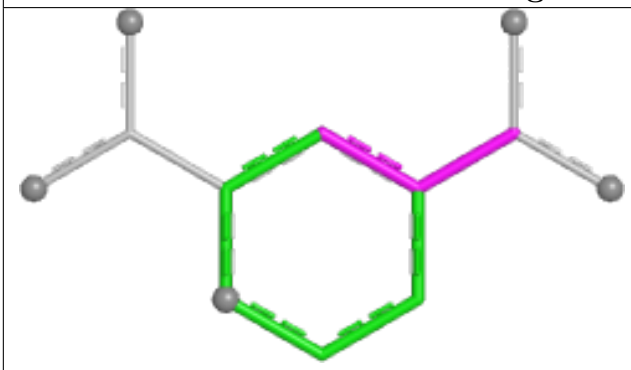


Torsions

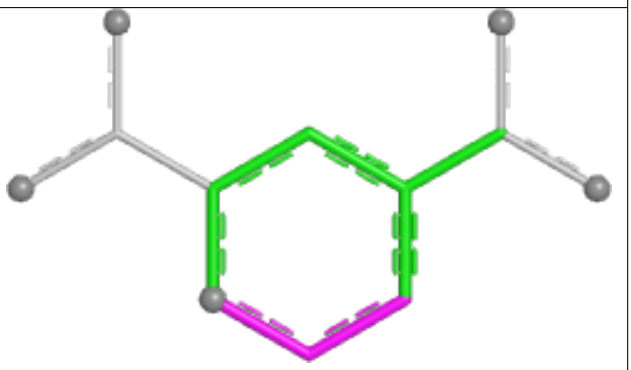


Rings

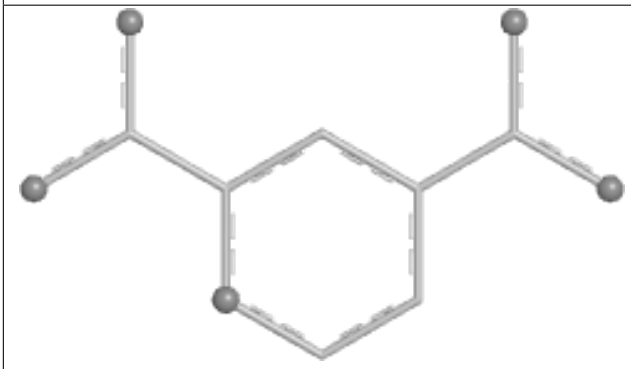
Ligand PD2 B 506



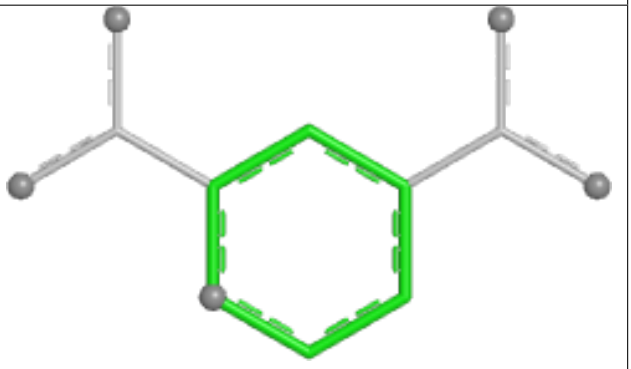
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	311/322 (96%)	0.51	1 (0%)	94	94	32, 45, 69, 103	0
1	B	308/322 (95%)	0.61	15 (4%)	29	27	36, 55, 97, 121	0
1	C	308/322 (95%)	0.45	11 (3%)	42	39	43, 64, 98, 126	0
1	D	307/322 (95%)	0.70	27 (8%)	10	7	44, 63, 101, 119	0
All	All	1234/1288 (95%)	0.57	54 (4%)	34	32	32, 58, 96, 126	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	LEU	5.7
1	D	70	LEU	4.7
1	D	138	LEU	4.3
1	D	134	ASP	4.0
1	D	163	PHE	3.8
1	D	183	TYR	3.7
1	C	107	LEU	3.7
1	D	295	LEU	3.7
1	B	107	LEU	3.4
1	B	136	PRO	3.4
1	D	71	GLY	3.3
1	B	66	LEU	3.3
1	D	66	LEU	3.3
1	C	66	LEU	3.2
1	B	123	TYR	3.1
1	D	107	LEU	3.1
1	B	138	LEU	3.1
1	D	136	PRO	3.0
1	D	139	ALA	3.0
1	C	76	ASP	3.0
1	B	4	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.0
1	C	231	GLY	2.8
1	C	103	THR	2.8
1	C	75	VAL	2.7
1	D	233	ASP	2.7
1	D	296	ASP	2.7
1	B	168	GLU	2.6
1	D	229	GLU	2.6
1	B	124	ILE	2.5
1	D	77	VAL	2.5
1	C	163	PHE	2.5
1	C	142	LEU	2.4
1	D	178	PRO	2.4
1	B	101	LEU	2.3
1	A	125	GLN	2.3
1	D	124	ILE	2.3
1	C	0	SER	2.3
1	B	115	ASP	2.3
1	C	135	LEU	2.3
1	D	110	VAL	2.2
1	B	117	PRO	2.2
1	B	164	TRP	2.2
1	D	304	TYR	2.2
1	D	171	VAL	2.2
1	B	63	PRO	2.1
1	D	3	GLU	2.1
1	B	169	ARG	2.1
1	D	164	TRP	2.1
1	D	133	VAL	2.1
1	D	275	TYR	2.1
1	C	42	SER	2.1
1	D	67	ILE	2.0
1	D	40	PHE	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
1	CSO	C	19	7/8	0.92	0.11	69,74,89,89	0
1	CSO	A	19	7/8	0.94	0.17	44,54,56,68	0
1	CSO	D	19	7/8	0.94	0.16	47,51,62,74	0
1	CSO	B	19	7/8	0.96	0.17	36,45,52,62	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.

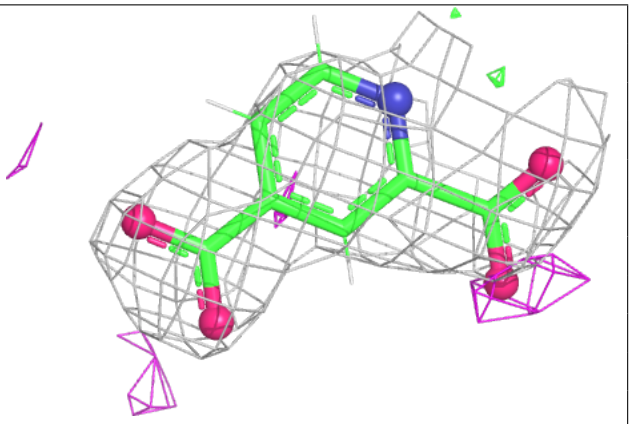
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	506	4/4	0.71	0.20	64,77,84,84	0
4	EDO	D	502	4/4	0.74	0.43	51,65,72,81	0
4	EDO	D	503	4/4	0.78	0.23	65,81,86,99	0
4	EDO	D	505	4/4	0.81	0.29	53,63,72,78	0
4	EDO	B	504	4/4	0.83	0.23	54,65,75,77	0
4	EDO	A	505	4/4	0.84	0.24	45,54,59,63	0
4	EDO	D	504	4/4	0.88	0.22	53,63,74,74	0
4	EDO	B	503	4/4	0.88	0.40	52,65,79,79	0
4	EDO	A	504	4/4	0.89	0.24	46,55,59,64	0
4	EDO	B	505	4/4	0.89	0.26	62,77,80,94	0
4	EDO	B	502	4/4	0.90	0.26	46,56,60,60	0
4	EDO	C	502	4/4	0.90	0.31	58,69,72,79	0
3	PEG	A	502	7/7	0.91	0.17	46,60,72,78	0
4	EDO	A	503	4/4	0.92	0.11	61,73,80,80	0
5	PD2	D	506	12/12	0.92	0.30	56,61,74,74	0
5	PD2	C	503	12/12	0.93	0.17	54,60,75,78	0
5	PD2	A	507	12/12	0.95	0.20	37,41,48,49	0
5	PD2	B	506	12/12	0.95	0.24	47,51,63,66	0
2	MN	D	501	1/1	0.97	0.17	48,48,48,48	0
2	MN	C	501	1/1	0.99	0.16	44,44,44,44	0
2	MN	A	501	1/1	0.99	0.21	35,35,35,35	0
2	MN	B	501	1/1	1.00	0.18	43,43,43,43	0

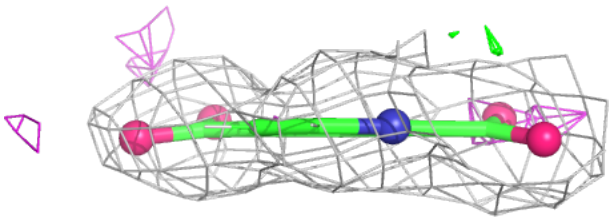
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

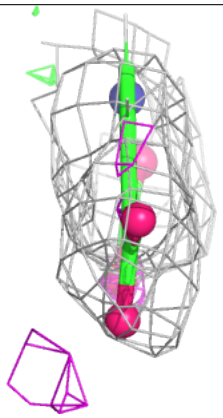
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PD2 D 506:

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

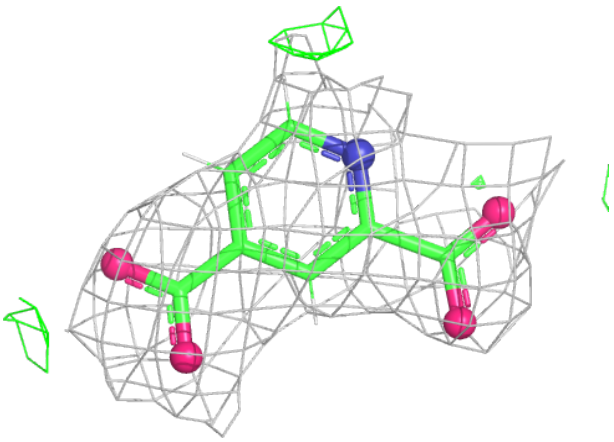


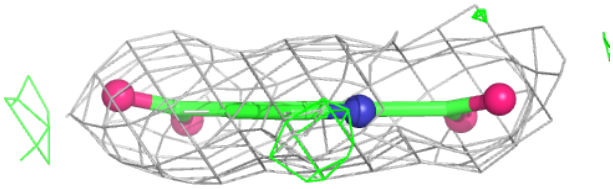


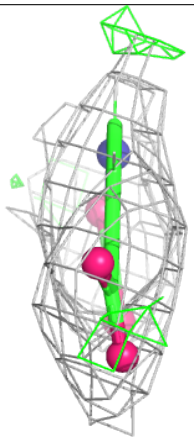


Electron density around PD2 C 503:

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

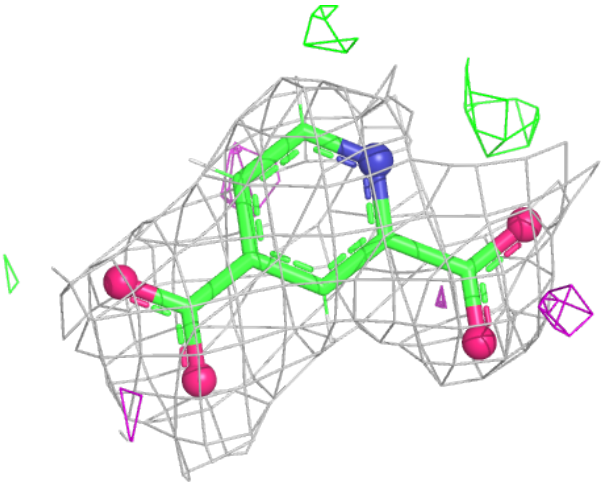


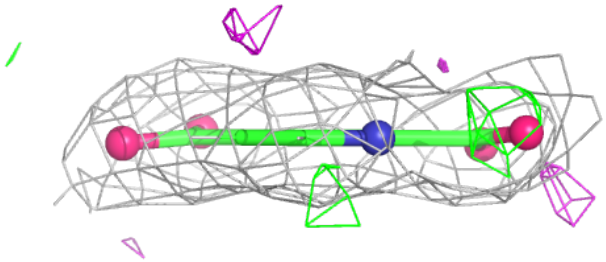


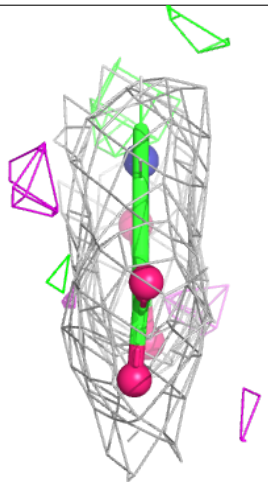


Electron density around PD2 A 507:

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

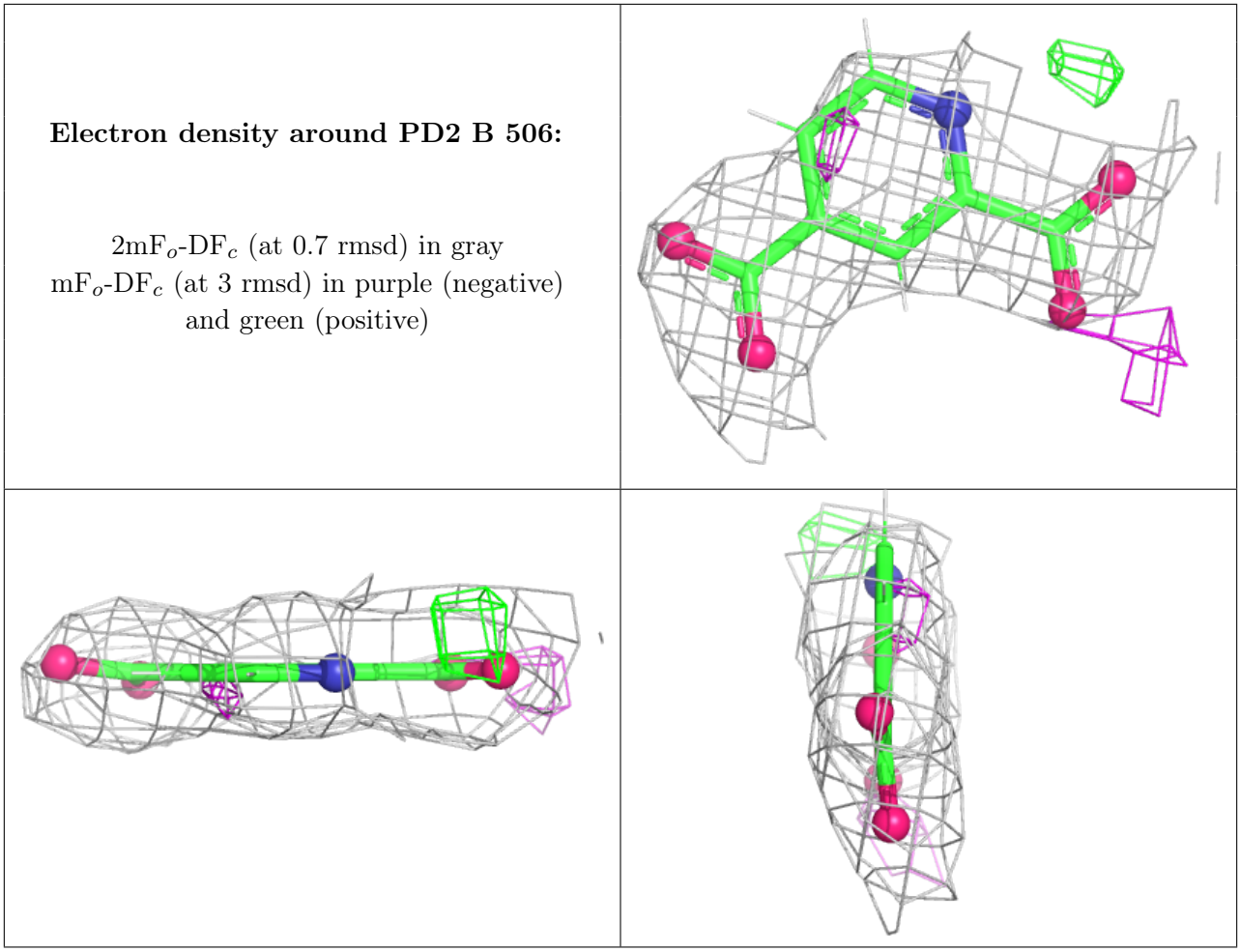






Electron density around PD2 B 506:

$2mF_o$-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.