Full wwPDB X-ray Structure Validation Report (i)

May 14, 2024 – 08:13 PM EDT

PDB ID	:	8VRI
Title	:	E. coli peptidyl-prolyl cis-trans isomerase containing difluoro-leucines
Authors	:	Frkic, R.L.; Jackson, C.J.
Deposited on	:	2024-01-22
Resolution	:	1.65 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:

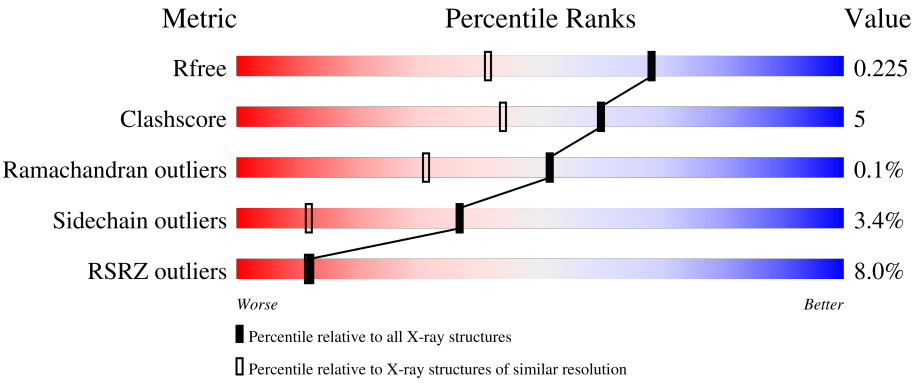
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	170	90% 9%
1	B	170	87% 12%
2	C	170	86% 9%
2	D	170	87% 9%
2	E	170	34% 84% 11%

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
2	FFL	E	115	-	-	-	X
5	EDO	B	205	-	-	-	X
5	EDO	D	207	-	-	X	-
6	PG4	B	204	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7798 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 Peptidyl-prolyl cis-trans isomerase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	170	Total	C	F	N	O	S	0	11	0
			1445	901	12	253	271	8			
1	B	170	Total	C	F	N	O	S	0	9	0
			1422	889	12	247	266	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	HIS	-	expression tag	UNP P23869
A	166	HIS	-	expression tag	UNP P23869
A	167	HIS	-	expression tag	UNP P23869
A	168	HIS	-	expression tag	UNP P23869
A	169	HIS	-	expression tag	UNP P23869
A	170	HIS	-	expression tag	UNP P23869
B	165	HIS	-	expression tag	UNP P23869
B	166	HIS	-	expression tag	UNP P23869
B	167	HIS	-	expression tag	UNP P23869
B	168	HIS	-	expression tag	UNP P23869
B	169	HIS	-	expression tag	UNP P23869
B	170	HIS	-	expression tag	UNP P23869

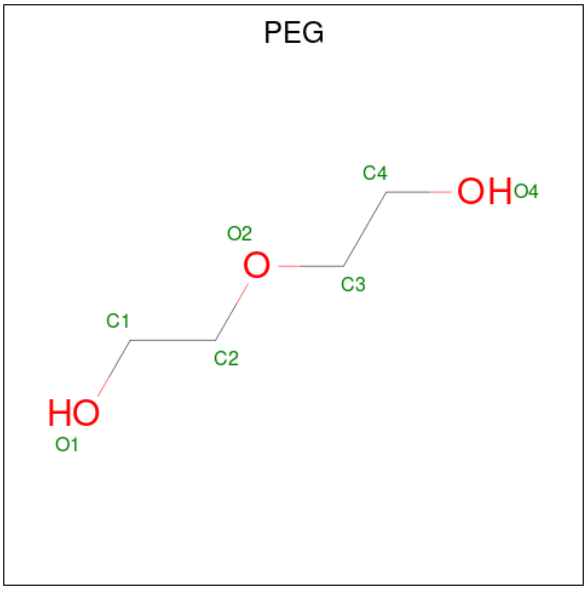
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	164	Total	C	F	N	O	S	0	4	0
			1318	823	10	226	250	9			
2	D	164	Total	C	F	N	O	S	0	3	0
			1310	819	10	222	250	9			
2	E	163	Total	C	F	N	O	S	0	0	0
			1273	796	10	218	242	7			

There are 18 discrepancies between the modelled and reference sequences:

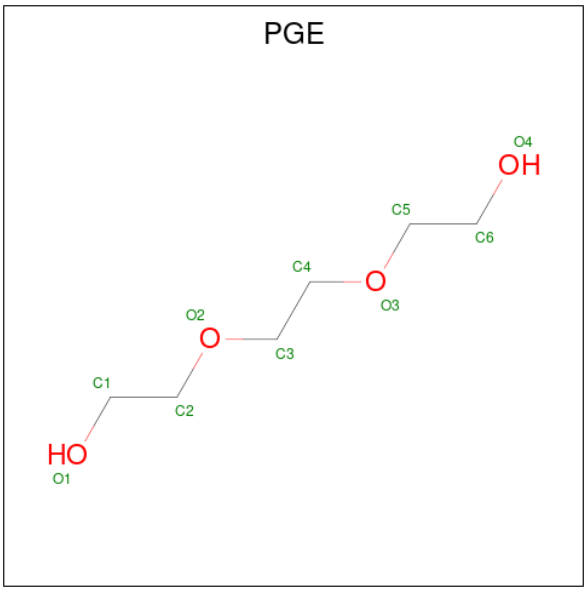
Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	expression tag	UNP P23869
C	166	HIS	-	expression tag	UNP P23869
C	167	HIS	-	expression tag	UNP P23869
C	168	HIS	-	expression tag	UNP P23869
C	169	HIS	-	expression tag	UNP P23869
C	170	HIS	-	expression tag	UNP P23869
D	165	HIS	-	expression tag	UNP P23869
D	166	HIS	-	expression tag	UNP P23869
D	167	HIS	-	expression tag	UNP P23869
D	168	HIS	-	expression tag	UNP P23869
D	169	HIS	-	expression tag	UNP P23869
D	170	HIS	-	expression tag	UNP P23869
E	165	HIS	-	expression tag	UNP P23869
E	166	HIS	-	expression tag	UNP P23869
E	167	HIS	-	expression tag	UNP P23869
E	168	HIS	-	expression tag	UNP P23869
E	169	HIS	-	expression tag	UNP P23869
E	170	HIS	-	expression tag	UNP P23869

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



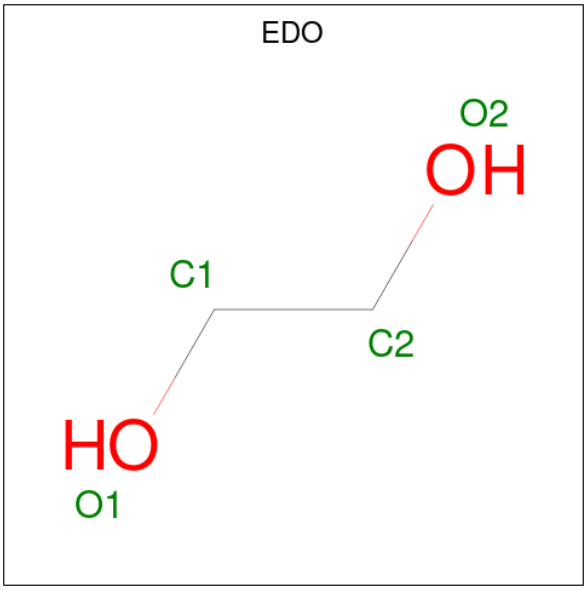
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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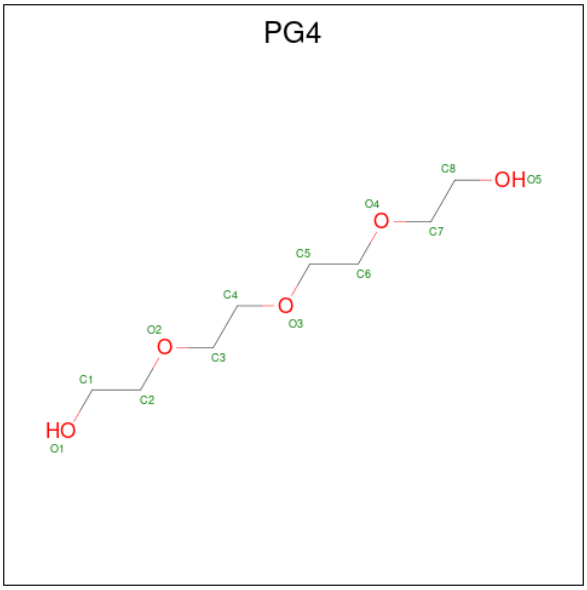
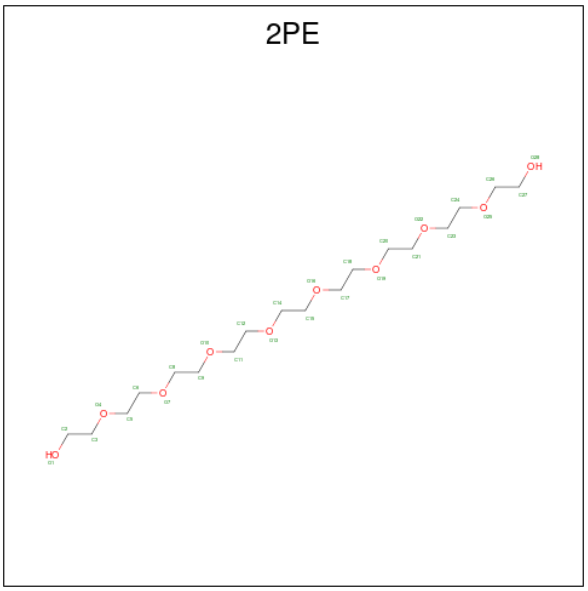
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 13 8 5	0	0

- Molecule 7 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 28 18 10	0	0
7	D	1	Total C O 28 18 10	0	0

- Molecule 8 is water.

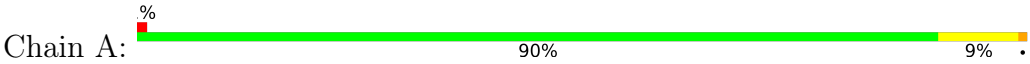
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	206	Total O 206 206	0	0
8	B	199	Total O 199 199	0	0
8	C	209	Total O 209 209	0	0
8	D	183	Total O 183 183	0	0
8	E	96	Total O 96 96	0	0

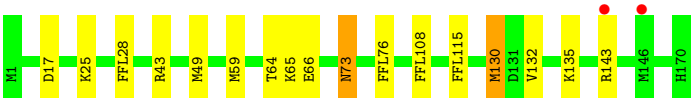
3 Residue-property plots (i)

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: Peptidyl-prolyl cis-trans isomerase B

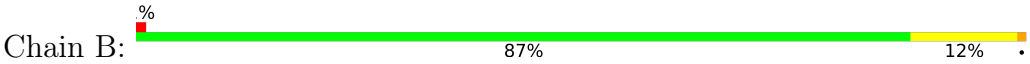
Chain A:

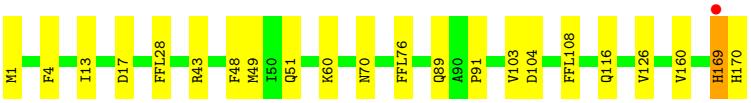




• Molecule 1: Peptidyl-prolyl cis-trans isomerase B

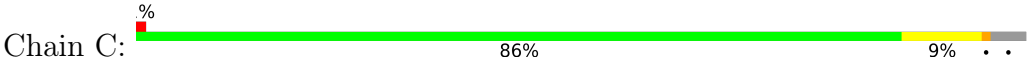
Chain B:





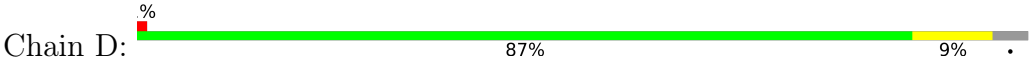
• Molecule 2: Peptidyl-prolyl cis-trans isomerase B

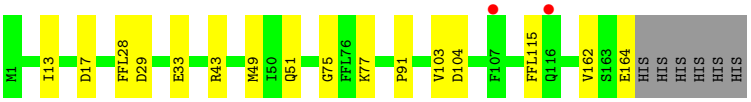
Chain C:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase B

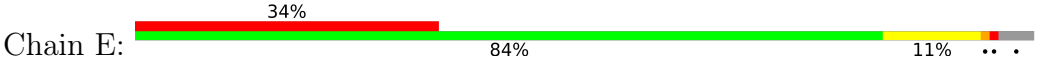
Chain D:

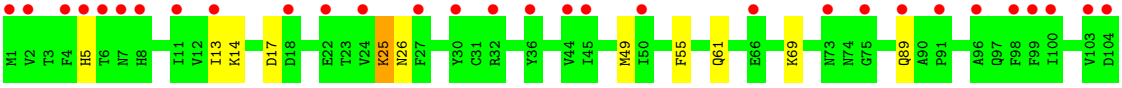


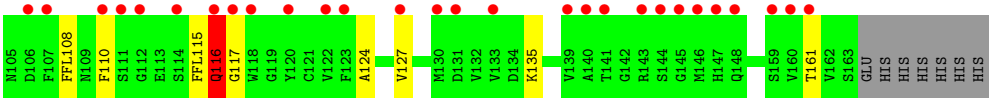


• Molecule 2: Peptidyl-prolyl cis-trans isomerase B

Chain E:






N105
D106
F107
FFL108
N109
F110
S111
G112
E113
S114
FFL115
Q116
G117
W118
G119
Y120
C121
V122
F123
A124
V127
M130
D131
V132
V133
D134
K135
V139
A140
T141
G142
R143
S144
G145
M146
H147
Q148
S159
V160
T161
V162
S163
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.66Å 83.44Å 122.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.12 – 1.65 24.12 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.12-1.65) 99.6 (24.12-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.224 0.183 , 0.225	Depositor DCC
R_{free} test set	4911 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7798	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: FME, PGE, FFL, PG4, PEG, EDO, 2PE

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	0.67	0/1404	0.75	0/1886
1	B	0.62	0/1387	0.77	0/1865
2	C	0.61	0/1289	0.76	0/1729
2	D	0.61	0/1281	0.76	0/1719
2	E	0.45	0/1244	0.61	0/1671
All	All	0.60	0/6605	0.73	0/8870

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	1445	0	1299	11	0
1	B	1422	0	1279	13	0
2	C	1318	0	1215	6	0
2	D	1310	0	1204	12	0
2	E	1273	0	1166	9	0
3	A	7	0	10	2	0
3	B	7	0	10	0	0
4	A	10	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	6	1	0
5	B	12	0	18	2	0
5	C	4	0	6	1	0
5	D	24	0	36	6	0
6	B	13	0	18	7	0
7	C	28	0	38	5	0
7	D	28	0	38	5	0
8	A	206	0	0	4	0
8	B	199	0	0	4	0
8	C	209	0	0	2	0
8	D	183	0	0	3	0
8	E	96	0	0	0	0
All	All	7798	0	6357	61	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 (61) 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:64:THR:H	3:A:201:PEG:H12	1.32	0.95
2:D:43:ARG:HH12	7:D:203:2PE:H262	1.56	0.70
1:B:103:VAL:HA	5:B:202:EDO:H21	1.75	0.69
2:E:14:LYS:HE3	2:E:127:VAL:HG11	1.74	0.69
2:C:43:ARG:HH12	7:C:201:2PE:H271	1.59	0.68
1:B:48:PHE:CZ	6:B:204:PG4:H51	2.29	0.67
2:D:91:PRO:HD2	5:D:201:EDO:H11	1.76	0.67
1:A:73[A]:ASN:ND2	8:A:303:HOH:O	2.27	0.67
1:B:48:PHE:HZ	6:B:204:PG4:H51	1.59	0.66
2:D:104:ASP:H	5:D:207:EDO:H22	1.61	0.65
1:B:51:GLN:OE1	6:B:204:PG4:H72	1.96	0.64
1:A:132:VAL:HA	1:A:135[B]:LYS:HE2	1.83	0.60
2:C:89:GLN:H	2:C:89:GLN:CD	2.04	0.60
1:A:135[B]:LYS:HE3	8:A:364:HOH:O	2.03	0.59
1:A:64:THR:N	3:A:201:PEG:H12	2.13	0.56
2:D:75:GLY:O	2:D:77:LYS:HE2	2.06	0.56
2:E:89:GLN:H	2:E:89:GLN:CD	2.10	0.55
1:B:104:ASP:OD2	5:B:205:EDO:H11	2.07	0.55
1:B:169:HIS:ND1	1:B:170:HIS:N	2.50	0.53
8:B:395:HOH:O	5:D:202:EDO:H21	2.09	0.53
1:A:25[B]:LYS:HD3	2:E:69:LYS:HZ1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ASP:H	5:D:207:EDO:C2	2.22	0.52
1:B:89:GLN:O	1:B:89:GLN:HG3	2.09	0.52
2:D:103:VAL:HB	5:D:207:EDO:H11	1.93	0.51
2:E:25:LYS:HE3	2:E:26:ASN:N	2.26	0.50
7:D:203:2PE:H201	8:D:431:HOH:O	2.12	0.50
2:C:1[A]:MET:HB3	2:C:163:SER:HB2	1.93	0.49
1:B:43:ARG:HH12	6:B:204:PG4:H52	1.77	0.49
2:E:13:ILE:HD12	2:E:124:ALA:HB1	1.94	0.49
6:B:204:PG4:O2	8:B:301:HOH:O	2.20	0.49
7:D:203:2PE:H232	8:D:431:HOH:O	2.13	0.48
2:C:13[B]:ILE:CG2	2:C:124:ALA:HB1	2.44	0.48
7:C:201:2PE:H212	7:C:201:2PE:H241	1.27	0.46
5:C:202:EDO:H12	8:C:470:HOH:O	2.15	0.46
1:B:169:HIS:HE1	8:B:308:HOH:O	1.98	0.46
1:A:43:ARG:HH22	4:A:202:PGE:H22	1.81	0.46
1:B:70:ASN:HB2	1:B:91:PRO:O	2.15	0.46
2:D:162:VAL:HG12	2:D:164:GLU:HG2	1.99	0.45
1:B:13[B]:ILE:HG22	1:B:126:VAL:HA	1.99	0.44
7:C:201:2PE:H152	8:C:488:HOH:O	2.17	0.44
2:C:146:MET:HB3	7:C:201:2PE:H122	1.98	0.43
2:D:103:VAL:CB	5:D:207:EDO:H11	2.48	0.43
1:A:65:LYS:NZ	8:A:305:HOH:O	2.36	0.43
2:D:13[B]:ILE:O	2:D:13[B]:ILE:HG13	2.17	0.43
2:E:55:PHE:CE2	2:E:61:GLN:HB2	2.53	0.43
1:A:66[A]:GLU:HG2	8:A:381:HOH:O	2.19	0.42
2:C:84:ALA:HB3	2:C:99:PHE:CZ	2.55	0.42
2:E:116:GLN:HG2	2:E:117:GLY:N	2.35	0.42
6:B:204:PG4:C5	6:B:204:PG4:H82	2.50	0.41
7:D:203:2PE:H202	8:D:465:HOH:O	2.20	0.41
2:E:5:HIS:NE2	2:E:161:THR:OG1	2.32	0.41
1:B:116:GLN:HG2	8:B:488:HOH:O	2.21	0.41
6:B:204:PG4:H52	6:B:204:PG4:H82	2.02	0.41
7:C:201:2PE:H152	7:C:201:2PE:H181	1.84	0.41
2:D:43:ARG:HH12	7:D:203:2PE:C26	2.30	0.41
2:E:110:PHE:HA	2:E:117:GLY:O	2.21	0.40
2:D:29:ASP:O	2:D:33:GLU:HG3	2.20	0.40
2:D:43:ARG:HB3	2:D:51:GLN:HB3	2.04	0.40
1:A:59:MET:HE2	1:A:59:MET:HB3	1.94	0.40
1:A:130:MET:HG2	5:A:203:EDO:H21	2.04	0.40
1:B:4:PHE:HD2	1:B:160:VAL:HG22	1.87	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	173/170 (102%)	164 (95%)	9 (5%)	0	100 100
1	B	171/170 (101%)	164 (96%)	7 (4%)	0	100 100
2	C	160/170 (94%)	152 (95%)	8 (5%)	0	100 100
2	D	159/170 (94%)	151 (95%)	8 (5%)	0	100 100
2	E	156/170 (92%)	146 (94%)	9 (6%)	1 (1%)	25 8
All	All	819/850 (96%)	777 (95%)	41 (5%)	1 (0%)	51 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	116	GLN

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	148/138 (107%)	142 (96%)	6 (4%)	30 8
1	B	146/138 (106%)	142 (97%)	4 (3%)	44 19
2	C	137/139 (99%)	129 (94%)	8 (6%)	20 3
2	D	136/139 (98%)	134 (98%)	2 (2%)	65 44
2	E	131/139 (94%)	126 (96%)	5 (4%)	33 10
All	All	698/693 (101%)	673 (96%)	25 (4%)	37 11

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	49	MET
1	A	73[A]	ASN
1	A	73[B]	ASN
1	A	130	MET
1	A	143	ARG
1	B	17	ASP
1	B	49	MET
1	B	60	LYS
1	B	169	HIS
2	C	1[A]	MET
2	C	1[B]	MET
2	C	17	ASP
2	C	49	MET
2	C	77	LYS
2	C	116	GLN
2	C	125	GLU
2	C	135	LYS
2	D	17	ASP
2	D	49	MET
2	E	17	ASP
2	E	25	LYS
2	E	49	MET
2	E	116	GLN
2	E	135	LYS

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

Mol	Chain	Res	Type
1	B	89	GLN
1	B	148	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

29 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	FFL	A	83	1	5,9,10	0.50	0	5,10,12	1.30	0
2	FFL	C	108	2	5,9,10	0.45	0	5,10,12	1.74	2 (40%)
1	FME	A	1	1	8,9,10	1.10	0	7,9,11	0.64	0
1	FFL	B	83	1	5,9,10	0.77	0	5,10,12	0.84	0
1	FFL	A	28[B]	1	5,9,10	0.34	0	5,10,12	1.79	2 (40%)
1	FFL	B	115	1	5,9,10	0.36	0	5,10,12	0.87	0
2	FFL	D	28	2	5,9,10	0.78	0	5,10,12	1.33	1 (20%)
1	FME	B	1	1	8,9,10	1.62	1 (12%)	7,9,11	1.03	0
2	FFL	C	28	2	5,9,10	0.46	0	5,10,12	1.13	1 (20%)
1	FFL	B	28[B]	-	5,9,10	0.35	0	5,10,12	1.46	1 (20%)
1	FFL	A	108	1	5,9,10	0.41	0	5,10,12	2.39	1 (20%)
1	FFL	B	108	1	5,9,10	0.30	0	5,10,12	1.88	2 (40%)
2	FFL	D	108	2	5,9,10	0.55	0	5,10,12	0.90	0
1	FFL	A	76	1	5,9,10	0.51	0	5,10,12	1.82	1 (20%)
2	FFL	D	76	2	5,9,10	0.44	0	5,10,12	0.87	0
2	FFL	E	83	2	5,9,10	0.38	0	5,10,12	0.83	0
2	FFL	C	76	2	5,9,10	0.28	0	5,10,12	0.80	0
2	FFL	E	115	2	5,9,10	0.50	0	5,10,12	2.30	3 (60%)
2	FFL	D	115	2	5,9,10	0.28	0	5,10,12	0.94	1 (20%)
2	FFL	D	83	2	5,9,10	0.44	0	5,10,12	1.05	0
1	FFL	A	28[A]	1	5,9,10	0.26	0	5,10,12	1.43	1 (20%)
1	FFL	A	115	1	5,9,10	0.37	0	5,10,12	3.81	1 (20%)
2	FFL	E	28	2	5,9,10	0.33	0	5,10,12	0.42	0
2	FFL	E	108	2	5,9,10	0.34	0	5,10,12	1.41	1 (20%)
1	FFL	B	28[A]	-	5,9,10	0.36	0	5,10,12	2.13	1 (20%)
1	FFL	B	76	1	5,9,10	0.41	0	5,10,12	2.21	1 (20%)
2	FFL	C	83	2	5,9,10	0.59	0	5,10,12	1.18	0
2	FFL	E	76	2	5,9,10	0.44	0	5,10,12	0.66	0
2	FFL	C	115	2	5,9,10	0.32	0	5,10,12	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FFL	A	83	1	-	1/9/10/12	-
2	FFL	C	108	2	-	0/9/10/12	-
1	FME	A	1	1	-	1/7/9/11	-
1	FFL	B	83	1	-	1/9/10/12	-
1	FFL	A	28[B]	1	-	0/9/10/12	-
1	FFL	B	115	1	-	5/9/10/12	-
2	FFL	D	28	2	-	3/9/10/12	-
1	FME	B	1	1	-	2/7/9/11	-
2	FFL	C	28	2	-	2/9/10/12	-
1	FFL	B	28[B]	-	-	2/9/10/12	-
1	FFL	A	108	1	-	0/9/10/12	-
1	FFL	B	108	1	-	0/9/10/12	-
2	FFL	D	108	2	-	0/9/10/12	-
1	FFL	A	76	1	-	2/9/10/12	-
2	FFL	D	76	2	-	2/9/10/12	-
2	FFL	E	83	2	-	3/9/10/12	-
2	FFL	C	76	2	-	4/9/10/12	-
2	FFL	E	115	2	-	6/9/10/12	-
2	FFL	D	115	2	-	6/9/10/12	-
2	FFL	D	83	2	-	0/9/10/12	-
1	FFL	A	28[A]	1	-	0/9/10/12	-
1	FFL	A	115	1	-	4/9/10/12	-
2	FFL	E	28	2	-	2/9/10/12	-
2	FFL	E	108	2	-	2/9/10/12	-
1	FFL	B	28[A]	-	-	1/9/10/12	-
1	FFL	B	76	1	-	1/9/10/12	-
2	FFL	C	83	2	-	2/9/10/12	-
2	FFL	E	76	2	-	1/9/10/12	-
2	FFL	C	115	2	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	FME	CA-N	-3.46	1.41	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	FFL	CG-CB-CA	-8.22	103.46	114.52
1	A	108	FFL	CD1-CG-CD2	-4.80	102.23	110.95
1	B	28[A]	FFL	CG-CB-CA	-4.37	108.64	114.52
1	B	76	FFL	CB-CG-CD1	-4.30	100.26	111.18
2	E	115	FFL	CB-CA-N	3.44	117.99	110.32
1	B	108	FFL	CD1-CG-CD2	-3.42	104.74	110.95
1	A	28[B]	FFL	CG-CB-CA	-3.22	110.19	114.52
1	A	28[A]	FFL	CG-CB-CA	-3.07	110.39	114.52
2	E	108	FFL	CG-CB-CA	2.95	118.48	114.52
2	C	108	FFL	CD1-CG-CD2	-2.87	105.74	110.95
1	B	28[B]	FFL	CG-CB-CA	-2.74	110.83	114.52
1	A	76	FFL	CG-CB-CA	-2.49	111.17	114.52
2	C	108	FFL	CB-CG-CD1	-2.40	105.09	111.18
2	E	115	FFL	CD1-CG-CD2	2.36	115.25	110.95
2	E	115	FFL	CG-CB-CA	2.23	117.52	114.52
1	B	108	FFL	CB-CG-CD1	-2.22	105.53	111.18
2	C	28	FFL	CD1-CG-CD2	-2.22	106.92	110.95
1	A	28[B]	FFL	CD1-CG-CD2	2.17	114.90	110.95
2	D	28	FFL	CG-CB-CA	-2.05	111.75	114.52
2	D	115	FFL	CG-CB-CA	-2.04	111.77	114.52

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	76	FFL	F1-CD1-CG-CD2
1	A	115	FFL	CA-CB-CG-CD1
1	A	115	FFL	CA-CB-CG-CD2
1	A	115	FFL	F1-CD1-CG-CB
1	A	115	FFL	F1-CD1-CG-CD2
1	B	1	FME	C-CA-CB-CG
1	B	28[A]	FFL	F1-CD1-CG-CD2
1	B	28[B]	FFL	F1-CD1-CG-CB
1	B	28[B]	FFL	F1-CD1-CG-CD2
1	B	76	FFL	O-C-CA-CB
1	B	115	FFL	N-CA-CB-CG
1	B	115	FFL	C-CA-CB-CG
1	B	115	FFL	F2-CD2-CG-CB
1	B	115	FFL	F2-CD2-CG-CD1
2	C	28	FFL	F2-CD2-CG-CB
2	C	28	FFL	F2-CD2-CG-CD1
2	C	76	FFL	O-C-CA-CB
2	C	76	FFL	F1-CD1-CG-CB

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Mol	Chain	Res	Type	Atoms
2	C	76	FFL	F1-CD1-CG-CD2
2	C	115	FFL	C-CA-CB-CG
2	C	115	FFL	F1-CD1-CG-CB
2	C	115	FFL	F1-CD1-CG-CD2
2	D	28	FFL	F1-CD1-CG-CB
2	D	28	FFL	F1-CD1-CG-CD2
2	D	28	FFL	F2-CD2-CG-CD1
2	D	76	FFL	CA-CB-CG-CD2
2	D	76	FFL	F1-CD1-CG-CD2
2	D	115	FFL	N-CA-CB-CG
2	D	115	FFL	C-CA-CB-CG
2	D	115	FFL	CA-CB-CG-CD1
2	D	115	FFL	F1-CD1-CG-CB
2	D	115	FFL	F1-CD1-CG-CD2
2	E	28	FFL	F2-CD2-CG-CB
2	E	28	FFL	F2-CD2-CG-CD1
2	E	83	FFL	N-CA-CB-CG
2	E	83	FFL	C-CA-CB-CG
2	E	83	FFL	F1-CD1-CG-CB
2	E	108	FFL	F2-CD2-CG-CB
2	E	108	FFL	F2-CD2-CG-CD1
2	E	115	FFL	CA-CB-CG-CD1
2	E	115	FFL	F1-CD1-CG-CB
2	E	115	FFL	F1-CD1-CG-CD2
2	E	115	FFL	F2-CD2-CG-CB
2	E	115	FFL	F2-CD2-CG-CD1
1	B	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
1	A	76	FFL	CA-CB-CG-CD2
1	B	115	FFL	CA-CB-CG-CD2
2	D	115	FFL	CA-CB-CG-CD2
2	E	76	FFL	CA-CB-CG-CD2
2	E	115	FFL	CA-CB-CG-CD2
2	C	76	FFL	N-CA-CB-CG
2	C	83	FFL	C-CA-CB-CG
1	A	83	FFL	N-CA-CB-CG
1	B	83	FFL	N-CA-CB-CG
2	C	83	FFL	N-CA-CB-CG

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)

17 ligands 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	$\#\|Z\| > 2$
6	PG4	B	204	-	12,12,12	0.33	0	11,11,11	1.08	1 (9%)
5	EDO	D	202	-	3,3,3	0.57	0	2,2,2	0.16	0
5	EDO	C	202	-	3,3,3	0.41	0	2,2,2	0.88	0
5	EDO	B	201	-	3,3,3	0.46	0	2,2,2	0.62	0
5	EDO	A	203	-	3,3,3	0.52	0	2,2,2	0.63	0
7	2PE	C	201	-	27,27,27	0.23	0	26,26,26	0.25	0
3	PEG	B	203	-	6,6,6	0.20	0	5,5,5	0.04	0
5	EDO	D	205	-	3,3,3	0.48	0	2,2,2	0.38	0
5	EDO	B	202	-	3,3,3	0.41	0	2,2,2	0.18	0
5	EDO	D	204	-	3,3,3	0.61	0	2,2,2	0.06	0
5	EDO	D	206	-	3,3,3	0.52	0	2,2,2	0.19	0
5	EDO	B	205	-	3,3,3	0.53	0	2,2,2	0.57	0
7	2PE	D	203	-	27,27,27	0.18	0	26,26,26	0.43	0
5	EDO	D	201	-	3,3,3	0.52	0	2,2,2	0.32	0
3	PEG	A	201	-	6,6,6	0.27	0	5,5,5	0.14	0
5	EDO	D	207	-	3,3,3	0.47	0	2,2,2	0.34	0
4	PGE	A	202	-	9,9,9	0.36	0	8,8,8	0.62	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
6	PG4	B	204	-	-	5/10/10/10	-
5	EDO	D	202	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	202	-	-	0/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-
5	EDO	A	203	-	-	1/1/1/1	-
7	2PE	C	201	-	-	13/25/25/25	-
3	PEG	B	203	-	-	1/4/4/4	-
5	EDO	D	205	-	-	1/1/1/1	-
5	EDO	B	202	-	-	1/1/1/1	-
5	EDO	D	204	-	-	1/1/1/1	-
5	EDO	D	206	-	-	1/1/1/1	-
5	EDO	B	205	-	-	1/1/1/1	-
7	2PE	D	203	-	-	14/25/25/25	-
5	EDO	D	201	-	-	1/1/1/1	-
3	PEG	A	201	-	-	3/4/4/4	-
5	EDO	D	207	-	-	1/1/1/1	-
4	PGE	A	202	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	204	PG4	C5-O3-C4	-2.59	102.08	113.29

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	201	2PE	C24-C23-O22-C21
7	C	201	2PE	C27-C26-O25-C24
7	C	201	2PE	O7-C8-C9-O10
7	C	201	2PE	O10-C11-C12-O13
7	C	201	2PE	O22-C23-C24-O25
7	D	203	2PE	O22-C23-C24-O25
7	D	203	2PE	O13-C14-C15-O16
7	C	201	2PE	O4-C5-C6-O7
6	B	204	PG4	O2-C3-C4-O3
3	B	203	PEG	C4-C3-O2-C2
7	D	203	2PE	C20-C21-O22-C23
5	D	201	EDO	O1-C1-C2-O2
5	D	204	EDO	O1-C1-C2-O2
5	D	205	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	202	PGE	O1-C1-C2-O2
7	D	203	2PE	O25-C26-C27-O28
6	B	204	PG4	O3-C5-C6-O4
7	D	203	2PE	C17-C18-O19-C20
3	A	201	PEG	C4-C3-O2-C2
3	A	201	PEG	C1-C2-O2-C3
7	D	203	2PE	C11-C12-O13-C14
7	C	201	2PE	O13-C14-C15-O16
7	C	201	2PE	C17-C18-O19-C20
6	B	204	PG4	O4-C7-C8-O5
4	A	202	PGE	C4-C3-O2-C2
7	C	201	2PE	C9-C8-O7-C6
4	A	202	PGE	C3-C4-O3-C5
5	B	202	EDO	O1-C1-C2-O2
7	C	201	2PE	O19-C20-C21-O22
7	D	203	2PE	C18-C17-O16-C15
7	D	203	2PE	C6-C5-O4-C3
7	D	203	2PE	C9-C8-O7-C6
7	D	203	2PE	C14-C15-O16-C17
7	D	203	2PE	C12-C11-O10-C9
7	C	201	2PE	C18-C17-O16-C15
7	D	203	2PE	O16-C17-C18-O19
7	D	203	2PE	O19-C20-C21-O22
6	B	204	PG4	C1-C2-O2-C3
3	A	201	PEG	O1-C1-C2-O2
5	A	203	EDO	O1-C1-C2-O2
5	B	205	EDO	O1-C1-C2-O2
5	D	207	EDO	O1-C1-C2-O2
6	B	204	PG4	C5-C6-O4-C7
7	C	201	2PE	C5-C6-O7-C8
7	C	201	2PE	C23-C24-O25-C26
5	D	206	EDO	O1-C1-C2-O2
7	D	203	2PE	C2-C3-O4-C5

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	204	PG4	7	0
5	D	202	EDO	1	0
5	C	202	EDO	1	0
5	A	203	EDO	1	0

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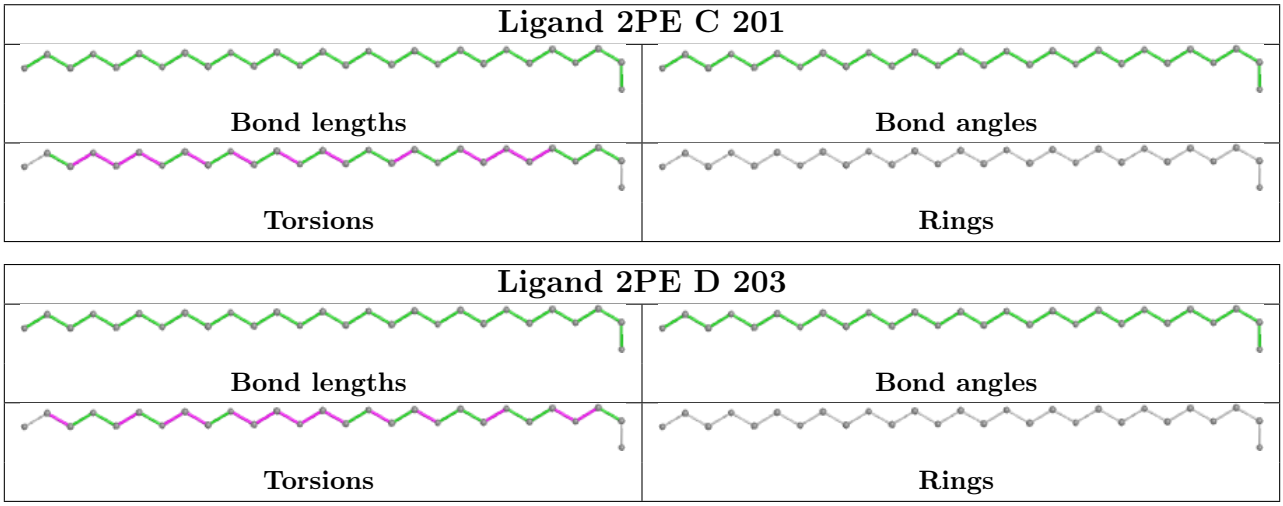
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	201	2PE	5	0
5	B	202	EDO	1	0
5	B	205	EDO	1	0
7	D	203	2PE	5	0
5	D	201	EDO	1	0
3	A	201	PEG	2	0
5	D	207	EDO	4	0
4	A	202	PGE	1	0

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.



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	164/170 (96%)	-0.27	2 (1%) 79 81	9, 16, 29, 53	0
1	B	164/170 (96%)	-0.21	1 (0%) 89 90	9, 16, 34, 56	0
2	C	159/170 (93%)	-0.20	1 (0%) 89 90	10, 17, 31, 77	0
2	D	159/170 (93%)	-0.08	2 (1%) 77 80	12, 19, 39, 65	0
2	E	158/170 (92%)	1.72	58 (36%) 0 0	33, 47, 63, 83	0
All	All	804/850 (94%)	0.19	64 (7%) 12 12	9, 18, 53, 83	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	146	MET	6.6
2	E	98	PHE	5.0
2	E	116	GLN	4.8
2	E	114	SER	4.2
1	B	169	HIS	3.9
2	E	13	ILE	3.8
2	D	116	GLN	3.7
2	E	161	THR	3.7
2	E	100	ILE	3.4
2	E	160	VAL	3.3
2	E	107	PHE	3.3
2	E	11	ILE	3.2
2	E	127	VAL	3.2
2	E	106	ASP	3.1
2	E	75	GLY	3.1
2	E	117	GLY	3.0
2	E	145	GLY	3.0
2	E	143	ARG	3.0
2	E	139	VAL	3.0
2	E	148	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	144	SER	2.9
2	E	110	PHE	2.8
2	E	118	TRP	2.8
2	E	22	GLU	2.8
2	E	147	HIS	2.8
2	E	120	TYR	2.7
2	E	123	PHE	2.7
2	E	89	GLN	2.7
2	E	32	ARG	2.6
2	E	103	VAL	2.6
2	E	2	VAL	2.6
2	E	1	MET	2.5
2	E	24	VAL	2.5
2	E	133	VAL	2.5
2	E	4	PHE	2.5
2	E	130	MET	2.4
2	E	44	VAL	2.4
1	A	143	ARG	2.3
2	E	122	VAL	2.3
2	E	36	TYR	2.3
2	E	104	ASP	2.3
2	E	45	ILE	2.3
2	E	140	ALA	2.2
2	E	141	THR	2.2
2	E	50	ILE	2.2
2	E	8	HIS	2.2
2	E	73	ASN	2.2
2	E	131	ASP	2.2
2	E	96	ALA	2.2
2	E	91	PRO	2.2
2	C	73	ASN	2.2
2	E	111	SER	2.1
2	D	107	PHE	2.1
2	E	7	ASN	2.1
2	E	27	PHE	2.1
1	A	146	MET	2.1
2	E	112	GLY	2.1
2	E	99	PHE	2.1
2	E	159	SER	2.1
2	E	66	GLU	2.0
2	E	18	ASP	2.0
2	E	5	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	30	TYR	2.0
2	E	6	THR	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	FFL	E	115	10/11	0.53	0.52	98,103,118,119	0
2	FFL	E	28	10/11	0.70	0.22	45,51,65,67	0
2	FFL	D	115	10/11	0.80	0.27	52,64,79,81	0
1	FFL	B	115	10/11	0.84	0.22	50,57,64,78	0
2	FFL	E	76	10/11	0.85	0.12	46,50,59,61	0
2	FFL	E	108	10/11	0.86	0.15	36,45,48,52	0
2	FFL	C	115	10/11	0.86	0.27	37,46,72,78	0
2	FFL	E	83	10/11	0.87	0.14	35,36,38,42	0
1	FFL	A	115	10/11	0.89	0.14	21,26,42,43	0
1	FME	B	1	10/11	0.89	0.13	14,24,31,51	0
2	FFL	D	76	10/11	0.90	0.11	22,28,40,47	0
2	FFL	D	108	10/11	0.91	0.09	22,27,32,42	0
1	FFL	B	76	10/11	0.93	0.09	16,20,32,34	0
1	FFL	B	108	10/11	0.93	0.10	12,15,23,25	0
2	FFL	C	76	10/11	0.94	0.09	19,21,37,39	0
2	FFL	C	108	10/11	0.94	0.08	17,21,27,40	0
1	FFL	A	108	10/11	0.94	0.08	10,13,19,23	0
2	FFL	D	28	10/11	0.94	0.10	13,20,36,36	0
1	FFL	A	76	10/11	0.95	0.09	13,14,27,27	0
2	FFL	C	28	10/11	0.95	0.10	14,15,35,36	0
2	FFL	C	83	10/11	0.96	0.11	8,10,14,19	0
1	FFL	A	83	10/11	0.96	0.11	7,10,17,20	0
1	FFL	B	83	10/11	0.96	0.09	9,10,15,19	0
1	FME	A	1	10/11	0.96	0.07	13,16,32,32	0
1	FFL	B	28[A]	10/11	0.97	0.10	12,15,24,32	7
1	FFL	B	28[B]	10/11	0.97	0.10	12,15,21,24	7
1	FFL	A	28[B]	10/11	0.97	0.09	11,13,20,22	10
1	FFL	A	28[A]	10/11	0.97	0.09	11,13,20,21	10
2	FFL	D	83	10/11	0.98	0.12	11,13,20,21	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

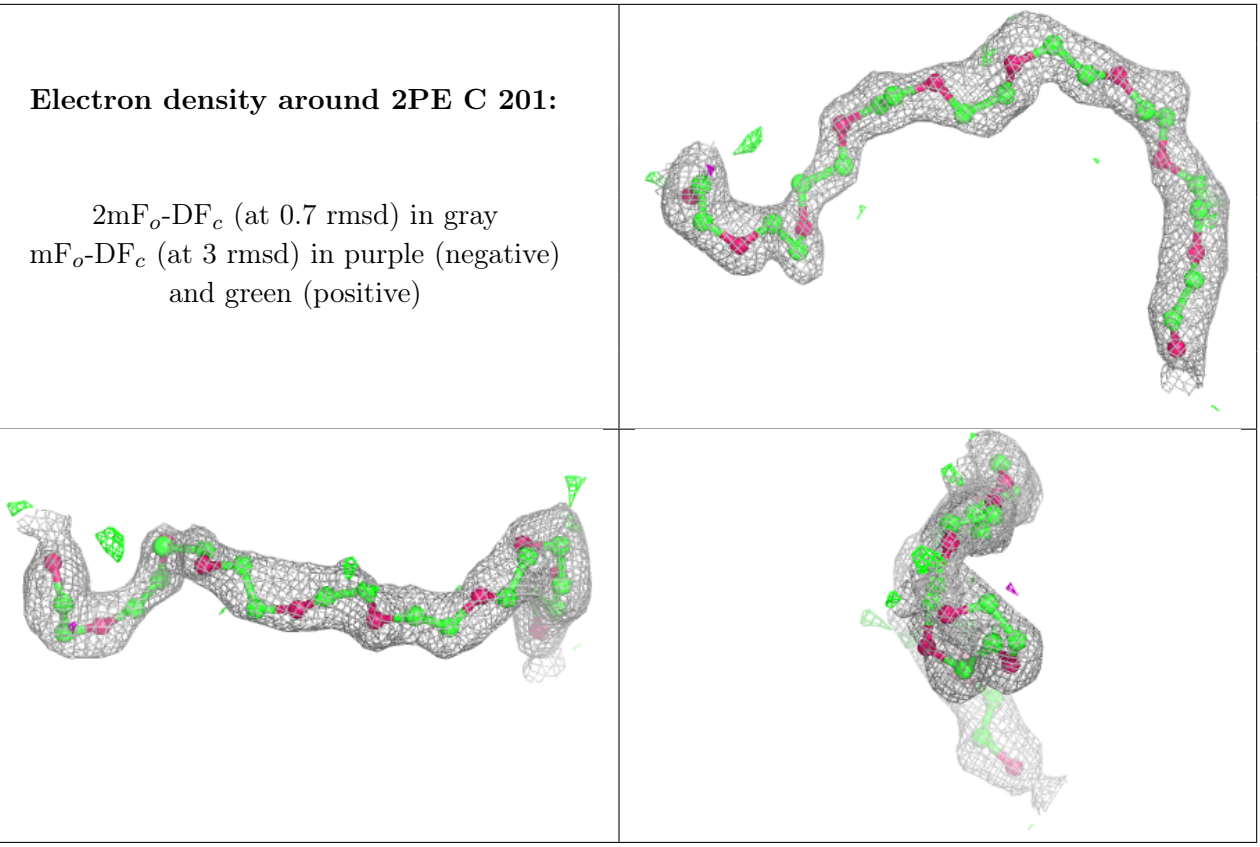
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EDO	A	203	4/4	0.72	0.17	27,27,30,43	4
5	EDO	B	205	4/4	0.74	0.41	31,35,51,73	0
3	PEG	A	201	7/7	0.75	0.22	19,31,37,39	7
5	EDO	D	206	4/4	0.75	0.27	33,38,40,49	0
3	PEG	B	203	7/7	0.76	0.29	36,41,49,52	0
7	2PE	C	201	28/28	0.76	0.17	24,36,43,47	0
6	PG4	B	204	13/13	0.84	0.17	20,31,43,45	0
5	EDO	D	205	4/4	0.84	0.25	32,36,39,45	0
5	EDO	B	202	4/4	0.85	0.15	20,27,27,31	4
5	EDO	D	207	4/4	0.85	0.34	28,33,34,38	0
7	2PE	D	203	28/28	0.85	0.12	24,35,40,44	0
5	EDO	B	201	4/4	0.87	0.27	34,35,36,38	0
4	PGE	A	202	10/10	0.88	0.12	16,27,39,44	0
5	EDO	C	202	4/4	0.89	0.36	27,32,36,50	0
5	EDO	D	201	4/4	0.89	0.29	25,27,34,38	0
5	EDO	D	202	4/4	0.92	0.15	19,20,31,45	0
5	EDO	D	204	4/4	0.93	0.21	20,32,37,43	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.

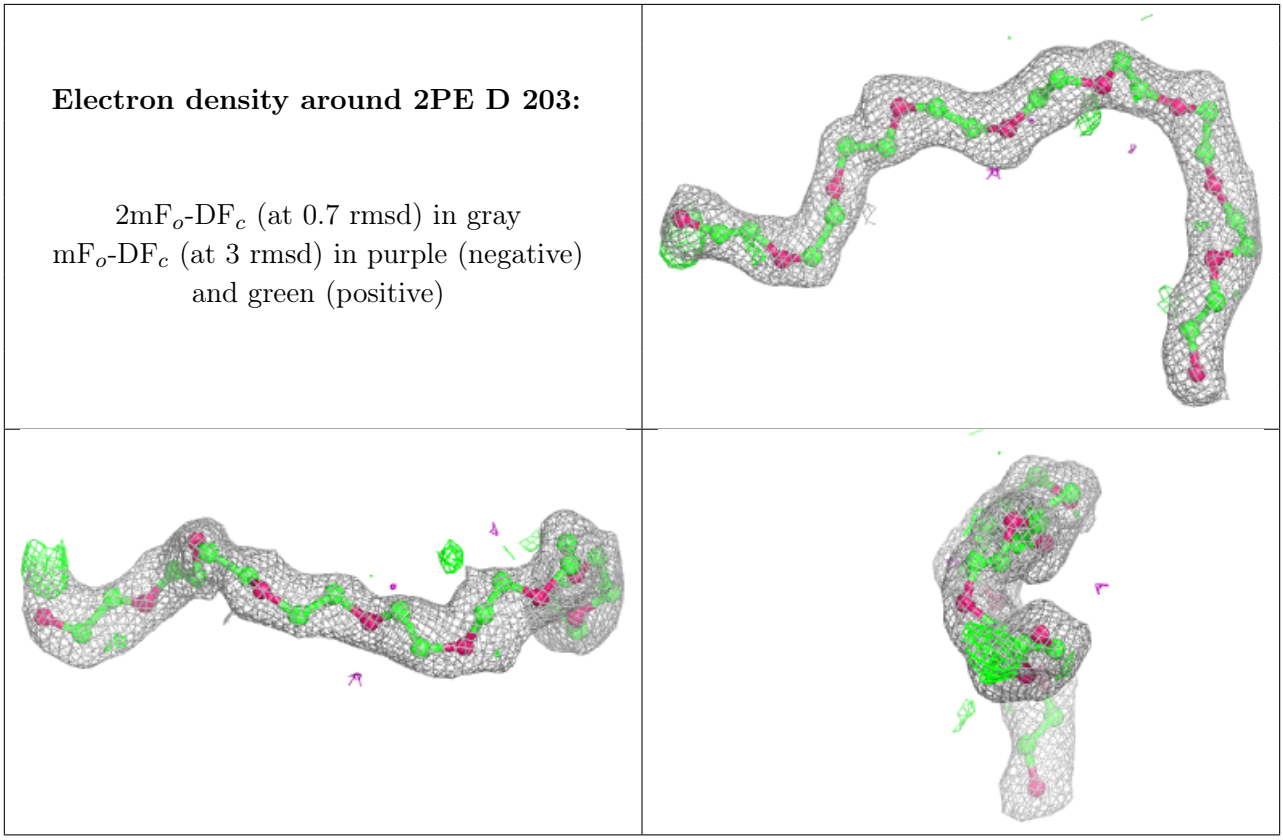
Electron density around 2PE C 201:

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



Electron density around 2PE D 203:

$2mF_o$-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.